Optimal Observation Strategies for Parameter Estimation of Distributed Systems

Faculty of Electrical Engineering, Computer Science and Telecommunications
University of Zielona Góra

Lecture Notes in Control and Computer Science Volume 5

Maciej Patan

Optimal Observation Strategies for Parameter Estimation of Distributed Systems

University of Zielona Góra Press, Poland
2004

Maciej PATAN
Institute of Control and Computation Engineering
University of Zielona Góra
ul. Podgórna 50
65-246 Zielona Góra, Poland
e-mail: M.Patan@issi.uz.zgora.pl

Referees:

- Adam KOWALEWSKI, AGH University of Science and Technology, Kraków
- Józef KORBICZ, University of Zielona Góra

The text of this book was prepared based on the author's Ph.D. dissertation

Partially supported by the State Committee for Scientific Research (KBN)
in Poland

ISBN 83-89712-03-2

Camera-ready copy prepared from the author's LaTeX2$_\varepsilon$ files.
Printed and bound by University of Zielona Góra Press, Poland.

CONTENTS

Acknowledgments

At this point, I would like to express my gratitude to the supervisor of this work, Prof. Dariusz Uciński who kindly introduced me into the field of my researches. Continuous support and supervision which I have experienced from him were an obvious stimulus. His erudition, fresh ideas and contributions have essentially improved this dissertation and cannot be overestimated.

All the friends in the Institute of Control and Computation Engineering are gratefully acknowledged for many insightful discussions, help and other activities which make the work at the institute really interesting and stimulating. Especially, I would like to thank Bartek Kuczewski for his partial contributions in the final chapter, Wojtek Paszke who helped me to improve some computer simulations and my brother Krzysztof for support within the area of diagnostics and editorial technicalities.

I also would like to address a special thanks to my mother for her continuous support which I gratefully appreciate. Finally, there exist no words to express a gratitude to my fiancee Jola who has been a medicine for my tired mind. Her endless patience and understanding have given me strength and energy to finish this work.

Notation

Symbols

$\mathbb{N}$	set of natural numbers
$\mathbb{R}$	set of real numbers
$\mathbb{R}_+$	set of positive real numbers
$\mathbb{C}$	set of complex numbers
t	time
θ, $\hat{\theta}$	unknown parameter vector and its estimate, respectively
N	number of measurements
$C(A)$	class of all continuous real-valued functions on A
$C^1(A)$	class of all continuously differentable functions on A
$\xi_N(\,\cdot\,)$	exact design of an experiment
$\xi(\,\cdot\,)$	continuous design of an experiment
I	identity matrix
$\mathbf{0}$	zero matrix
C	error covariance matrix
$K \equiv C_m(\,\cdot\,)$	observation covariance matrix
C_o	output covariance matrix

Operators and functions

$\sup \Psi(\,\cdot\,)$	least upper bound (supremum) of the functional Ψ
$\inf \Psi(\,\cdot\,)$	greatest lower bound (infimum) of the functional Ψ
E	expectation
cov	covariance
trace(A)	trace of a matrix A
det(A)	determinant of a matrix A
$\delta(\,\cdot\,)$	Dirac delta distribution
δ_k	Kronecker delta
$\operatorname{supp} \xi$	support of a measure ξ
$\otimes$	Kronecker product

Abbreviations

DPS	Distributed Parameter System
FIM	Fisher Information Matrix
LMI	Linear Matrix Inequalities
LPS	Lumped Parameter System
LSE	Least Square Estimation
MIMO	Multi-Input Multi-Output
PDE	Partial Differential Equation
SDP	Semi-Definite Programming

Chapter 1

INTRODUCTION

1.1. Introductory background

Modelling, as a method of analysing various phenomena, appears in many different areas of scientific research. A model which constitutes a mathematical representation of an examined process or object plays the major role in such an analysis. A wide range of techniques which can be used in constructing models and using them to confirm physical observations and to predict future behaviours of real systems leads to a deeper understanding of practical problems. From the mathematical point of view, models can be classified according to their form as follows (Niederliński, 1983; Sun, 1994; Karnopp *et al.*, 2000):

- Deterministic and stochastic models (w.r.t. the model dependence on random factors),
- Linear and non-linear models (w.r.t. the form of the model equations),
- Stationary and dynamic models (w.r.t. whether or not the state is time-dependent)
- Lumped parameter and distributed parameter models (w.r.t. whether or not the state depends on spatial variables).

One of the most general and important classes of systems is that of dynamic distributed parameter systems (DPS's) also called spatio-temporal dynamic systems. They are encountered in numerous practical engineering areas such as signal transmissions lines in electrical engineering (de Cogan and de Cogan, 1997) and structural mechanics in civil engineering or aircraft industry (Banks *et al.*, 1996; Flatau and Chong, 2002). From a global perspective, a rather logical consequence of the observed increase in the modern systems complexity is the fact that lumped parameter descriptions often become unsatisfactory as they may not provide a sufficient approximation of the investigated system. Thus, there exists a strongly motivated necessity for applying a more sophisticated and efficient mathematical apparatus and the development of new modelling techniques. Consequently, this leads directly to the description of the model at hand using partial differential equations (PDE's) with appropriate boundary and initial conditions. However, depending on the situation, equivalent integral or mixed integro-differential systems of equations can be considered. Despite the sophisticated formulation in the spirit of the

PDE's, such models provide a high quality and efficiency of simulations and control techniques.

Optimization and control of DPS's are active and expanding research areas (Li *et al.*, 1995; Uciński, 1999a; Lasiecka and Triggiani, 2000; Kowalewski, 2001b; Kowalewski, 2001a; Robinson, 2001). At the same time, progress in computational and applied mathematics combined with the availability of rapidly increasing computer power steadily extend the range of applications that can be simulated numerically. These developments lead to new challenges in the field of modelling. Furthermore, the classes of naturally distributed engineering systems for which estimation and control is desired has recently been enlarged. As an aftereffect, the DPS's achieve now a very important position in systems analysis and control theory and establish a separate field of research with a plenty of publications addressed to this area (Omatu and Seinfeld, 1989; Korbicz and Zgurowski, 1991; Mitkowski, 1991; Kowalewski, 1991; Sokołowski and Zolesio, 1992; Curtain and Zwart, 1995; Malanowski *et al.*, 1996; Zwart and Bontsema, 1997; Gil, 1998; Grabowski, 1999; Uciński, 1999a; Luo *et al.*, 1999; Lasiecka and Triggiani, 2000; Kowalewski, 2001a; Robinson, 2001; Sasane, 2002).

In applications, two major problems can be addressed:

- *forward problem*, which consists in determining the system state when the system parameters, spatial region, time observation interval, subsidiary conditions and control variables are known,
- *inverse problem*, which consists in recovering some of the model parameters from the collected observational data (e.g. system states and other available information) provided that the model structure is given; it is also called *parameter identification*.

The inverse problems in the context of DPS's may consist in estimation of physical parameters, forcing inputs or initial and boundary conditions. The main difficulty is that often the estimation problem is ill-conditioned (in the Hadamard sense) even if the forward problem is well-posed (Sikora, 2000; Sun, 1994; Isakov, 1998). The outstanding importance of solving inverse problems is obvious since a simulation model should be precisely calibrated based on the observations, otherwise results obtained from solving the forward problem might be unreliable. Thus, close attention should be paid to this subject, which requires more effective and robust analysis methods.

The literature related to the subject of parameter estimation in DPS's is very rich. As classical surveys systematizing the various techniques in this field, we can cite those by Kubrusly (1977) and Polis (1982), or a more recent book (Banks and Kunisch, 1989) where a broad class of estimation techniques for DPS's is presented. The interested reader can be also referred to works (Kunisch, 1988; Uciński and Korbicz, 1990; Chavent, 1991; Banks, 1992; Gibson *et al.*, 2000). However, most of contributions are focused on off-line approaches, and only few results concern on-line methods (Aihara, 1997; Demetriou, 2000).

It is well known that the efficiency of various estimation algorithms for DPS's depends significantly on the manner in which the observations are gathered from

the measurement environment. In most real situations, the measurements of the state variables in the examined processes are spatially constrained. This may be caused directly by physical restrictions of the system under consideration (e.g., actuators of the investigated plant), but more often this results from the measurement instrumentation. Although distributed measurements over the entire spatial domain are in general not available, there usually exists a possibility of taking measurement continuously in time.

A fundamental problem in parameter estimation of DPS's is to properly design the process of data acquisition from various sources. This task comprises the determination of the allocation for a limited number of sensors over the spatial domain in such a way as to maximize the estimation efficiency of the system parameters. Most often, the dependence between the sensor placement and the system performance is not intuitive and has counfounding nature. Due to the cost of obtaining data, constraints associated with measurements and requirements of increased efficiencies of identifiers, there is a dire necessity for developing some systematic methods of selecting appropriate sensor configurations and measurement strategies.

It was already indicated that the motivations to study sensor location problem stem from real-world engineering problems. One of the most interesting one is computer-assisted tomography which consist in reconstructing material parameters which characterize the inaccessible interior of an examined object based on measurements taken at the boundary without any damage of the subject of examination (Williams and Beck, 1995; Sikora, 2000). Since the observations have to be non-invasive, the problem of proper data acquisition becomes extremely difficult and the locations of the measurement electrodes are of great significance as they should provide possibly the most informative measurements.

Another inspiring application concerns optimization of air quality monitoring networks since, due to the rapid development of industry around the world, air pollution becomes a great societal problem. Protection and restitution of the natural environment requires a high accuracy of forecasts and diagnoses. To provide them, a proper calibration of models which describe the pollutant emission processes is necessary (van Loon, 1994; Sydow *et al.*, 1997; Sydow *et al.*, 1998; Berliner *et al.*, 2000). Usually, the changes in pollutant concentrations over a given area are described by PDE's of the advection-diffusion type. Since some coefficients of the equations are not measurable, accurate modelling becomes extremely difficult. In addition to this, the monitoring stations are rather costly and the problem of choosing an appropriate observation strategy is of great practical relevance indicated in many publications (Sturm *et al.*, 1994; van Loon, 1995; Andó *et al.*, 1999; Müller, 1998; Nychka *et al.*, 1998; Berliner *et al.*, 2000).

Similar problems can be found in many other engineering areas, e.g. in groundwater sources management (Sun, 1994; Kovarik, 2000), in gathering measurement data for calibration of models used in meteorology and oceanography (Daley, 1991; Bennett, 1992; Hogg, 1996; Malanotte-Rizzoli, 1996), in automated inspection of hazardous environments (Korbicz and Zgurowski, 1991; Korbicz *et al.*, 1993), in prediction of radioactive contamination (Isakov, 1998) and emerging smart mate-

rial systems (Banks *et al.*, 1996; Lasiecka, 1998).

1.2. State of the art for the sensor location problem

The sensor location problem has been attacked from various angles, but the results communicated by most authors are limited to the selection of stationary sensor positions and the context of state estimation (Kubrusly and Malebranche, 1985; El Jai and Amouroux, 1987; Amouroux and Babary, 1988; El Jai and Pritchard, 1988; El Jai, 1991; Korbicz and Uciński, 1994). An extension of state estimation methods to the parameter estimation problem is not straightforward and rather difficult, since in the latter case the current state usually depends non-linearly on unknown parameters (Korbicz and Uciński, 1994) (even if the PDE is linear in these parameters), in contrast to the dependence of the current state on the initial one, which is linear if only the system is linear. This essential difference makes the task of parameter estimation much more difficult and for that reason the number of corresponding results is much fewer (Uciński, 1999a; Uciński, 2000b).

From the perspective of the optimal sensor location problem for parameter identification in DPS's, the existing approaches can be classified into three main groups:

- methods leading to state estimation,
- methods making use of random field theory,
- methods originating in optimum experimental design.

The methods of the first group transform the original problem into a state-estimation one in such a way as to raise a possibility of applying well-developed methods of optimal sensor location for state estimation. There is rich literature concerning such problems. The interested reader can be referred to the (Kubrusly and Malebranche, 1985; Malebranche, 1988; El Jai, 1991; Azhogin *et al.*, 1988; Korbicz *et al.*, 1988; Korbicz and Zgurowski, 1991; Korbicz, 1991; Korbicz and Uciński, 1994; Uciński, 1999b). The main drawback of such an approach is that simultaneous state and parameter estimation causes the strong non-linearity of the problem. Some attempts involving sequential linearizations at the consecutive state trajectories (Malebranche, 1988) were conducted as well as suboptimal filtering (Korbicz *et al.*, 1988). Nevertheless, the approach depreciates due to the well-known difficulties encountered in non-linear state estimation analysis and it can be adopted only in simple situations.

The second group of methods are based on the application of the random field theory. However, their usefulness in the context of DPS's is rather limited, since in general transformation between system descriptions in the form of PDE's and suitable random field characteristics is not simple. Additionally, such a conversion relies only on statistics up to a given order (e.g. mean, covariance, skewness, kurtosis and higher order functions). Despite those limitations, methods of this group can be successfully applied in specific cases (Kazimierczyk, 1989; Sun, 1994).

The classical theory of optimum experimental design (Kiefer and Wolfowitz, 1959; Fedorov, 1972; Ermakov, 1983; Pázman, 1986; Atkinson and Donev, 1992; Pukelsheim, 1993; Rafajłowicz, 1996; Fedorov and Hackl, 1997; Walter and Pronzato, 1997; Uciński, 1999a) and its extensions to dynamic systems (Mehra, 1976; Goodwin and Payne, 1977; Titterington, 1980; Królikowski and Eykhoff, 1985; Walter and Pronzato, 1997) constitutes a basis of the third class of methods. Within this group of approaches the problem is cast as an optimization one, where the performance index is defined in the form of some scalar measure operating on the FIM, whose inverse, based on the Cramer-Rao inequality, plays the role of an estimate of the parameter dispersion matrix. This leads to significant simplification, because even if the precise dispersion matrix is difficult to obtain, the inverse of the FIM can be computed with relative ease.

In the context of DPS's the first formulation in this spirit was proposed by Quereshi *et al.* (1980) whose approach based on the maximization of the determinant of the FIM was used to find sensor locations and boundary perturbations in dynamic DPS's (a heat-diffusion process and a vibrating string), and Rafajłowicz (1978) for optimization of both sensor positions and a distributed control for parameter estimation of static linear DPS. A generalization of Rafajłowicz's approach to hyperbolic linear systems with known eigenvalues and eigenfunctions was delineated in (Rafajłowicz, 1981), whereas in (Rafajłowicz, 1983) an even more general framework of DPS's described in terms of Green's functions was considered.

A natural generalization which imposes itself is to apply sensors which are capable of tracking points providing at a given time moment best information about the parameters. However, communications in this field are rather limited. Rafajłowicz (1986b) considers the determinant of the Fisher Information Matrix (FIM) associated with the parameters to be estimated as a measure of the identification accuracy and looks for an optimal time-dependent measure, rather than for the trajectories themselves. The movable sensors problem was also considered in works (Rafajłowicz, 1988; 1989), however without direct reference to parameter estimation. On the other hand, Uciński, apart from generalizations of Rafajłowicz's results, developed some computational algorithms based on the FIM (Uciński, 1999a; Uciński, 2000b; Uciński and Korbicz, 2001). He reduces the problem to a state-constrained optimal-control one for which solutions are obtained via gradient techniques capable of handling various constraints imposed on sensor motions.

A quite new observational strategy, being interconnection of stationary and movable sensors techniques, is scanning. In this measurement scheme only a subset of sensors selected from among all available sensors, whose positions are fixed, take measurements during a given time interval whilst the other sensors become inactive (Demetriou, 2000) or their measurements are neglected. A reason for not using all the available sensors could be the reduction of the observation system complexity and the cost of operation and maintenance (van de Wal and de Jager, 2001). Such a scanning strategy of taking measurements can be also interpreted in terms of several sensors which are mobile. The problem has not received close attention yet (though some attempts have been made in a related context of state estimation,

see e.g. (Nakano and Sagara, 1988)). An extremely efficient approach based on directly-constrained design measures was proposed in (Uciński and Patan, 2002a), but the underlying assumptions involve its main limitation which consists in that it can be used only when the number of sensors is relatively high. One of the major difficulties in the sensor scheduling problem is its combinatorial nature. It is compounded further if sensor switchings are allowed to take place in continuous time. In (Lee *et al.*, 2001) a similar problem was considered for state estimation. In that work, the proposed solution was to make use of some recently obtained results in discrete-valued optimal control. As was already mentioned, the number of sensors is always limited. Nevertheless, the very important question, which accompanies the inverse problems in all situations is the minimization of the number of sensors which guarantees a satisfactory accuracy of parameter estimates.

Nevertheless, while applying various existing methods, some fundamental difficulties may be encountered, which make the problem extremely non-trivial. One of them is the dependence of the optimal solutions on the parameters to be identified. In order to calculate optimal sensor configurations, the true values of the estimated parameters should be known. Therefore, most of contributions in the context of DPS's are based on some *a priori* knowledge about the parameters (e.g. some nominal values can be taken). Although there exist some approaches developed to overcome those difficulties (Walter and Pronzato, 1997; Uciński, 1999a), they are not free from drawbacks. Another significant disadvantage of many results present in the literature is the so-called clusterization phenomenon, i.e. a tendency of different sensors in an optimal solution to take measurements at the same points. In addition to this, there is a lack of methods dedicated to correlated measurements, because in this situation the problem is further complicated. Finally, most of the contributions deal with the stationary sensors, but the development of new technologies leads to modern observational systems, i.e. moving and scanning sensors, which seems very attractive from the viewpoint of the degree of optimality.

In order to address those needs, there is a dire necessity for new approaches and adaptation of the existing efficient techniques. This constitutes the main motivation to write this doctoral thesis.

1.3. Contributions of the dissertation to the state-of-the-art

The primary objective of this work is to significantly extend the existing results and to develop new approaches to determining optimal observations strategies for DPS's, especially in the case of scanning sensors. Particularly, the problem is to develop new or adopt existing algorithms for different strategies and measurement error correlations. A secondary objective is to provide some efficient methods in the case when a parametric uncertainty has to be taken into account.

The following main thesis of this work is proposed:
For a broad class of distributed parameter systems a significant improvement in the parameter estimation quality is possible through the development of effective and robust methods in the sense of statistical uncertainty, using stationary, scanning and movable sensors.

In the process of testing this thesis, it was necessary both to develop a theoretical foundation for our approach and to construct several new algorithms for various types of computation. The following is a concise summary of the contributions provided by this work to the state-of-the-art in sensor location methods:

Theoretical aspects

- generalization of the classical results of optimal experiment design to MIMO systems with possible output correlation (stationary, moving and scanning sensors),
- adaptation and generalization of some algorithms of nonlinear programming and optimal experiment design to solve stationary sensor location problems,
- development of efficient methods of activating scanning sensors, in the cases of both fixed and optimal switching schedules,
- development of an approach to solve the sensor location problem in the case of correlated observations,
- introduction of optimal sensor placement methods to model-based fault diagnosis,
- adaptation of existing robust approaches to optimal sensor allocation in the presence of model parametric uncertainties (sequential designs, minimax and Bayesian criteria),
- adaptation and generalization of experimental design techniques in the presence of model structural uncertainties,

Application aspects

- application of optimal observation strategies to computer-assisted tomography and structural mechanics (static DPS),
- application of optimal observation strategies to transmission lines and advection-diffusion problems (dynamic DPS),

1.4. Dissertation outline

The organization of this dissertation follows a progression leading from basic theoretical and algorithmic foundations of sensor allocation strategies to the implementation of robust strategies for dynamic systems. This work is divided into six chapters.

Chapter 1: It contains a brief introduction to the field of optimal observation strategies for DPS's. Moreover, the main objectives to be attained are formulated.

Chapter 2: The class of the DPS's underlying the subsequent analysis is introduced and the optimal observation strategy problem is defined for specified real situations of interest in the context of this work. Main impediments met when solving the problem are delineated and illustrated with the appropriate examples. In the second part, as a connection to the next chapters, a generalization of some classical results for continuous-time MIMO lumped parameter systems is presented. The notion of continuous designs is introduced in the context of convex design theory. The applicability of some characterizations of the optimal solutions is discussed for both linear and nonlinear cases.

Chapter 3: Adaptation of continuous designs is made so as to set forth efficient algorithms for finding optimal allocation schemes of stationary sensors in the class of static DPS's. Two special situations are distinguished, i.e. the case of the measurements to be taken at a finite set of feasible locations and the case when the set of admissible sensor locations is spatially continuous. For the first situation, two subproblems are then taken into consideration, i.e. optimization of the spatial effort and avoiding sensor clusterization. For the cases so formulated efficient algorithms are proposed along with the appropriate characterization results. Some illustrative examples of applying the proposed extended techniques are presented based on the the computer-assisted tomography problem and experiments in structural mechanics.

Chapter 4: The concepts from the previous chapter are generalized and used in the context of spatio-temporal dynamic systems and continuous observations over a given time observation interval. Furthermore, a moving sensor strategy is introduced based on the so-called direct approach. From this point on, the scanning sensor strategy is investigated with attention paid to two optimization techniques, i.e. the ones with fixed and optimal switchings. In addition to that, the problem of correlated observational errors is examined and an effective algorithm is provided for such a case. As another important generalization, the introduction of sensor location techniques into the field of model-based diagnostics is considered and a suitable approach constructed based on structural hypothesis tests. The final part of the chapter contains applications concerninig various problems of practical importance, which are

- the signal propagation process in long-distance transmission lines,
- calibration of air pollution models, and
- groundwater modelling resources management.

Chapter 5: Extensions of some optimum experimental designs techniques are proposed in the presence of parametric and structural uncertainties of the model. In the first part of the chapter, sequential design techniques combined with clusterization-free designs are used to provide an efficient approach dedicated to the scanning strategy with a fixed switching schedule. Then, alternative robust

approaches are discussed. In particular, minimax and Bayesian designs are considered in this context. In the former case, the formulation in the sense of semi-infinite programming with a suitable relaxation procedure is presented. In the latter case, an approach based on statistical learning is adopted. The last part of the chapter concerns the generalization of the T-optimum design criterion to MIMO spatio-temporal dynamic systems. Moreover, a suitable iterative procedure known from the discrimination experiments for lumped systems is successfully adopted.

Chapter 6: The original contributions of this work are summarized in the context of some general context. Additionally, discussion of the possible further research directions is presented.

Chapter 2

A GENERAL FRAMEWORK FOR SENSOR LOCATION

2.1. System description

The aim here is to define the class of systems to be considered within the framework of this dissertation. Attention is especially focused on the DPS's whose mathematical models are described by the systems of n partial differential equations of the general form:

$$\mathcal{D}(x,t)\frac{\partial y(x,t)}{\partial t} = \mathcal{G}\Big(x,t,y(x,t),\nabla y(x,t),\nabla^2 y(x,t);\theta\Big), \quad (x,t)\in\Omega\times T\subset\mathbb{R}^{d+1}, \tag{2.1}$$

where

- Ω is a bounded simply-connected open domain with sufficiently regular boundary $\partial\Omega$,
- t signifies time,
- $T=(0,t_f)$ means the observation interval ($t_f<\infty$ denotes a fixed observation horizon),
- $x=(x_1,x_2,\ldots,x_d)$ stands for a spatial point belonging to the set $\bar{\Omega}=\Omega\cup\partial\Omega$,
- $y=\big(y_1(x,t),y_2(x,t),\ldots,y_n(x,t)\big)$ is the state variable with values in $\mathbb{R}^n$, and
- $\mathcal{D}$ and $\mathcal{G}$ stand for some known functions which map their arguments to $\mathbb{R}^{n\times n}$ and $\mathbb{R}^n$, respectively.

Note that this general setting includes the case when the function $\mathcal{G}$ may contain terms accounting for *a priori* known forcing inputs. The system (2.1) is supplemented with a suitable set of boundary conditions

$$\mathcal{E}\Big(x,t,y,\nabla y;\theta\Big)=0, \quad (x,t)\in\partial\Omega\times T, \tag{2.2}$$

and initial conditions

$$\mathcal{F}\Big(x,y,\nabla y;\theta\Big)=0, \quad (x,t)\in\partial\Omega\times\{0\}, \tag{2.3}$$

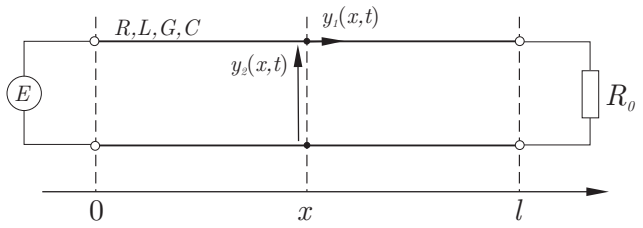


Fig. 2.1. Non-homogeneous transmission line with a load of the resistance type.

where $\mathcal{E}$ and $\mathcal{F}$ are some known functions.

The model built on (2.1)–(2.3) contains the unknown parameter vector θ whose values belong to a parameter space $\Theta_{\rm ad}$. From the practical point of view, the most significant and common situation corresponds to constant parameter values, i.e. $\theta_{\rm ad} \subset \mathbb{R}^m$, and from now on, we shall also make the assumption that the estimated parameters are constant. Note that the case of space-varying parameters can be treated in this framework through the appropriate parametrization, e.g. based on splines.

Example 2.1. As an example of the considered class of DPS's, the signal propagation process in a long-distance transmission line (e.g. a long electrical supply line or a high-frequency integrated circuit) can be examined. The large scale of such systems due to the wavelength of the propagated electromagnetic signal produces considerable spatial effects which have to be taken into account. In the case of a one-dimensional power supply line, the propagation phenomenon is described by the set of equations (Kącki, 1995; de Cogan and de Cogan, 1997)

$$\begin{aligned} -\frac{\partial y_2}{\partial t} &= L(x,t;\theta)\frac{\partial y_1}{\partial x} + R(x,t;\theta)y_1, \\ -\frac{\partial y_1}{\partial t} &= C(x,t;\theta)\frac{\partial y_2}{\partial x} + G(x,t;\theta)y_2, \quad x \in (0,l), \quad t \in (0,t_f), \end{aligned} \tag{2.4}$$

where $y_1(x,t)$ and $y_2(x,t)$ denote respectively the current intensity and voltage along the line, l is the maximal length of the line, and R, G, L, C stand for the spatial density of resistance, conductance, inductance and capacitance, respectively. In the case when the line load is only of the resistance type (cf. Fig. 2.1), the initial conditions are defined as

$$y_1(x,0) = g_1(x), \quad y_2(x,0) = g_2(x), \quad x \in (0,l) \tag{2.5}$$

while the boundary conditions at the extremities of the line are

$$\begin{aligned} & y_1(0,t) = y_{10}(t), \quad y_2(0,t) = y_{20}(t), \\ & C(x,t;\theta)R_0\left(\frac{\partial y_1}{\partial t}\right)_{x=l} + \left(\frac{\partial y_1}{\partial x}\right)_{x=l} + G(x,t;\theta)R_0\, y_1(l,t) = 0, \\ & \frac{L(x,t;\theta)}{R_0}\left(\frac{\partial y_2}{\partial t}\right)_{x=l} + \left(\frac{\partial y_2}{\partial x}\right)_{x=l} + \frac{R(x,t;\theta)}{R_0}\, y_2(l,t) = 0, \quad t \in (0,t_f) \end{aligned} \tag{2.6}$$

Although the physical interpretation of the quantities which describe the properties of the transmission channel (i.e. R, G, L, C and R_0) is well established (Kącki, 1995), their distributed nature makes grave difficulties for proper modelling. Some of these coefficients are known and available from direct measurements (e.g. R_0), yet the others contain some components which are not measurable or such a measurement could be very impractical. Therefore, a precise recovery of the model coefficients becomes a very difficult task of great importance for accurate simulation and prediction of the system behaviour.

★

Given the model structure (2.1)–(2.3) up to a finite number of constant parameters θ, the main purpose of parameter estimation is to reconstruct θ in such a way that the model response imitates the behaviour of the real state of the system $\tilde{y}$ as closely as possible. The crucial problem lies in the fact that usually not all the components of the state $\tilde{y}$ are observable, especially in real data acquisition systems. The techniques of taking measurements can be split into the following four classes (Chen and Seinfeld, 1975):

(*i*) observations at discrete spatial locations at discrete time instants,

(*ii*) observations at discrete spatial locations over a continuous time interval,

(*iii*) spatial observations at discrete time instants,

(*iv*) spatial observations continuously in a given time interval.

In general, 'ideal' spatial measurements are obviously not possible, thus the last two manners do not seem to be of serious relevance in practice. Note, however, that recent great developments in the measurement techniques and instrumentation have begun changing this situation. In many scientific areas, this type of observation techniques is successfully exploited and their outcomes cannot be overestimated (e.g. astrophysical observations of the universe in infrared or microwave ranges of the electromagnetic radiation, thermography in medical and industrial diagnostics or meteorological observations of the atmosphere from satellites). On the other hand, in the majority of engineering applications, measurements over the entire spatial domain are impossible, and methods (I) and (II) still turn out to be the most significant and applicable, and consequently they dominate in literature. This fact constitutes the main reason behind focusing our attention on these strategies of data acquisition.

2.2. Optimal measurement problem

2.2.1. Observation strategies

In general, the observation strategy can be understood as any process of taking measurements, but for the clarity for further considerations it is necessary to define such a notion more precisely. Firstly, we should provide a more formal definition of a measurement result.

Definition 2.1. (Taylor and Kuyatt, 1994) The **result of a measurement** is only an approximation or an estimate of the value of a specific quantity subjected to the measurement, that is, the **measurand** (ISO, 1996), and thus the result is complete only when accompanied by a quantitative statement of its uncertainty.

Here, it is very important to emphasize that the class of the measurements studied in this work belongs to the so-called external observations (also known as Black-Box measurements (Braake *et al.*, 1998)) made with non-inertial measuring transducers whose influence on the system performance is negligible and may be omitted. Furthermore, characteristics of real sensors often depend on both the spatial coordinates and time, and the measurement is a result of measurand averaging over some spatial domain. A common practice is, however, the assumption that this dependence can be approximated by a number of pointwise measurements. Thus, the resulting uncertainty about a measurement can be reduced to the components which are evaluated by statistical methods (i.e. an uncertainty of type A (Taylor and Kuyatt, 1994)). Otherwise, it is necessary to consider the components of uncertainty evaluated by other means than the statistical analysis of a series of observations (the so-called type B evaluation (Taylor and Kuyatt, 1994)). With such a notion of observation being a result of the measurement, it is possible to introduce the definition of the measurement space and the strategy of observations which are used within the scope of this work.

Definition 2.2. The **measurement space** is the space induced by the subset of the Cartesian product $\bar{\Omega} \times T$ in which the observations are available. A **strategy of observations** is understood as any subset of the measurement space.

In practice, the following main strategies of taking measurements can be distinguished:

Using stationary sensors. In this case observations are made at a finite number of locations continuously or discretely in time. Because the sensors positions are fixed, the resulting measurements are somewhat averaged in the time domain (of course, if the system state is time dependent). The main problem we are faced with here is the choice of the optimal sensor locations in a given admissible spatial domain.

Using moving sensors. Allowing for the mobility of the sensors, we can increase their applicability and increase the capabilities in comparison with stationary sensors. In this way observations possess an additional degree of freedom regarding potential optimality. It is a direct consequence of the possibility of taking measurements at positions which are at given time moments the most advantageous in the sense of a given performance index quantifying the information about the estimated parameters. Let us note that non-mobile sensors can be considered as movable sensors whose trajectories are reduced to fixed points. Thus the use of movable sensors constitutes a generalization including as a special case the use of stationary sensors. An observation strategy here is a set of sensor trajectories representing changes in the mea-

surement locations in time. The problem of designing optimal trajectories becomes crucial for this case.

Scanning. This strategy constitutes a combination of the previous two cases with a slight extension. In some situations, the observation system comprises multiple sensors whose positions are already specified and it is desired to activate only a subset of them during a given time interval while the other sensors remain dormant. Such a scanning strategy of taking measurements can be also interpreted in terms of several sensors which are mobile, but, since in general the number of activated sensors could vary in time, this technique is not a discrete-time version of the movable sensor method. This strategy is accompanied by the problem of determining the best spatio-temporal schedule of taking measurements.

In practical situations, Definition 2.2 may seem too abstract, especially in the case of moving observations when sensor trajectories should satisfy many constraints. However, such a formulation is convenient from the point of view of statistical analysis. Moreover, in particular situations some additional restrictions can be made providing a suitable regularization of the observation strategy.

2.2.2. Parameter estimation

Different common real situations encountered in engineering practice imply that the measurement process can be formally represented as follows:

S1. Stationary sensors, measurements discrete in time,

$$z^j(t_k) = \mathcal{H}(y(x^j, t_k; \theta), x^j, t_k) + \varepsilon(x^j, t_k), \qquad k = 1, \dots, K, \quad j = 1, \dots, N, \tag{2.7}$$

S2. Scanning sensors, measurements discrete in time,

$$z^j(t_k) = \mathcal{H}(y(x^j(t_k), t_k; \theta), x^j(t_k), t_k) + \varepsilon(x^j(t_k), t_k), \qquad k = 1, \dots, K, \quad j = 1, \dots, N, \tag{2.8}$$

S3. Stationary sensors, measurements continuous in time,

$$z^j(t) = \mathcal{H}(y(x^j, t; \theta), x^j, t) + \varepsilon(x^j, t), \quad t \in T, \quad j = 1, \dots, N, \tag{2.9}$$

S4. Movable sensors, measurements continuous in time,

$$z^j(t) = \mathcal{H}(y(x^j(t), t; \theta), x^j(t), t) + \varepsilon(x^j(t), t), \quad t \in T, \quad j = 1, \dots, N, \tag{2.10}$$

where $\mathcal{H}(\,\cdot\,)$ is a given function mapping its arguments into $\mathbb{R}^r$, $z^j(t)$ is an r-dimensional output, x^j and $x^j(t) \in X$ stand respectively for the locations of the j-th stationary and movable sensor (at time instant t), X signifies the part of Ω where the measurements can be made, and $\varepsilon^j(\,\cdot\,)$ denotes the measurement noise.

It is customary to assume that the noise is zero-mean, Gaussian, uncorrelated in both time and space (Fedorov and Hackl, 1997; Kubrusly and Malebranche, 1985), i.e. its statistics are defined as

$$\mathrm{E}[\varepsilon(x^j,t)]=0,\quad \mathrm{E}[\varepsilon(x^i,t)\varepsilon^{\mathrm{T}}(x^j,\tau)]=\delta_{ij}\delta(t-\tau)C(x^i,t), \tag{2.11}$$

$C(x^i,t)\in\mathbb{R}^{n\times n}$ is a known positive-definite matrix, δ_{ij} and $\delta(\,\cdot\,)$ stand for Kronecker's and Dirac's delta symbols, respectively. A more general situation when the measurement noise is correlated in space and time domains will be considered in more detail in Section 4.4.

The objective of the parameter estimation is to find the value of the unknown parameter vector $\hat{\theta}\in\Theta_{\mathrm{ad}}$ based on the appropriate set of process observations (2.7)–(2.10) such that the predicted response of the model (2.1)–(2.3) is close enough to the process observations (in the sense of some known quality measure). The estimation problem is customarily converted into an optimization one and then the minimization of a suitable *weighted least-squares* criterion $\mathcal{J}(\theta)$ is carried out. For situations S1–S4, we respectively have

C1. Stationary sensors, measurements discrete in time,

$$\mathcal{J}(\theta)=\frac{1}{2}\sum_{j=1}^{N}\sum_{k=1}^{K}\|z^j(t_k)-\mathcal{H}(\hat{y}(x^j,t_k;\theta),x^j,t_k)\|^2_{C(x^j,t_k)}, \tag{2.12}$$

C2. Scanning sensors, measurements discrete in time,

$$\mathcal{J}(\theta)=\frac{1}{2}\sum_{j=1}^{N}\sum_{k=1}^{K}\|z^j(t_k)-\mathcal{H}(\hat{y}(x^j(t_k),t_k;\theta),x^j(t_k),t_k)\|^2_{C(x^j(t_k),t_k)}, \tag{2.13}$$

C3. Stationary sensors, measurements continuous in time,

$$\mathcal{J}(\theta)=\frac{1}{2}\sum_{j=1}^{N}\int_T\|z^j(t)-\mathcal{H}(\hat{y}(x^j,t;\theta),x^j,t)\|^2_{C(x^j,t)}\,\mathrm{d}t, \tag{2.14}$$

C4. Movable sensors, measurements continuous in time,

$$\mathcal{J}(\theta)=\frac{1}{2}\sum_{j=1}^{N}\int_T\|z^j(t)-\mathcal{H}(\hat{y}(x^j(t),t_k;\theta),x^j(t),t)\|^2_{C(x^j(t),t)}\,\mathrm{d}t, \tag{2.15}$$

where $\hat{y}(x,t;\theta)$ is the solution to (2.1)–(2.3) for a given value of θ and

$$\|e(x,t)\|^2_A=e^{\mathrm{T}}A^{-1}e,$$

for any positive-definite symmetric matrix A. Some relevant comments concerning benefits and drawbacks of using the least-squares criterion with indications of further references can be found in the monograph by Uciński (1999a).

2.2.3. Problem formulation

It can be clearly seen that in each case the parameter estimate $\hat{\theta} = \arg\min_{\theta\in\Theta} \mathcal{J}(\theta)$ depends strongly on the coordinates of the sites where the measurements are taken. This fact allows us to consider the optimality of sensor locations leading to best estimates of θ. To achieve such a purpose, it is necessary to establish some quality measure of sensor configurations based on the accuracy of the parameter estimates obtained from the observations. Usually such a measure is related to the *Fisher Information Matrix* (FIM) commonly used in the classical theory of optimum experimental design for Lumped Parameter Systems (LPS's) (Fedorov and Hackl, 1997; Walter and Pronzato, 1997). The valuable property of the FIM is that its inverse constitutes an approximation of the covariance matrix for the estimates of the system parameters θ (Goodwin and Payne, 1977). More precisely, it is a lower bound of the above mentioned covariance matrix and it is established by the so-called Cramér-Rao inequality (Bard, 1974; Goodwin and Payne, 1977):

$$\operatorname{cov}\hat{\theta} \geqslant M^{-1}, \tag{2.16}$$

where M stands for the FIM (note that the above inequality should be interpreted in terms of the Löwner ordering of symmetric matrices, i.e. the $A \geqslant B$ means that $A - B$ must be non-negative definite). This leads to a great simplification since the inverse of the FIM, which stands for the lower bound on the right-hand side of (2.16) can often be easily computed, even in situations, when the exact dispersion matrix of the given estimator is very difficult to obtain. The assumptions regarding the noise statistics (2.11) yield the following formulae depending on the considered situation (Uciński, 1999a):

M1. Stationary sensors, measurements discrete in time,

$$M = \sum_{j=1}^{N}\sum_{k=1}^{K} G^{\mathrm{T}}(x^j, t_k)C^{-1}(x^j, t_k)G(x^j, t_k), \tag{2.17}$$

M2. Scanning sensors, measurements discrete in time,

$$M = \sum_{j=1}^{N}\sum_{k=1}^{K} G^{\mathrm{T}}(x^j(t_k), t_k)C^{-1}(x^j(t_k), t_k)G(x^j(t_k), t_k), \tag{2.18}$$

M3. Stationary sensors, measurements continuous in time,

$$M = \sum_{j=1}^{N}\int_T G^{\mathrm{T}}(x^j, t)C^{-1}(x^j, t)G(x^j, t)\,\mathrm{d}t, \tag{2.19}$$

M4. Movable sensors, measurements continuous in time,

$$M = \sum_{j=1}^{N}\int_T G^{\mathrm{T}}(x^j(t), t)C^{-1}(x^j(t), t)G(x^j(t), t)\,\mathrm{d}t, \tag{2.20}$$

where

$$G(x,t) = \left.\frac{\partial \mathcal{H}(y,t;\theta)}{\partial y}\right|_{y=y(x,t;\theta)} \frac{\partial y(x,t;\theta)}{\partial \theta}.$$

Analogously to the least-square criteria, the elements of M depend on the sensor positions. Let us introduce the collection of variables

$$\breve{\xi}_N = \{x^1, \ldots, x^N\} \tag{2.21}$$

which we call informally the simplified design of the experiment. Additionally, the design-dependent FIM $M(\breve{\xi}_N)$ will be subsequently briefly denoted by M.

Unfortunately, direct use of the FIM in optimization is inconvenient, because the above-mentioned Löwner ordering of the information matrices constitutes in general only a partial ordering over the set of all admissible components of $\breve{\xi}_N$. Thus for a complete comparison of measurement allocations, we will have to introduce a suitable scalar performance index based on the FIM, which should be minimized by a suitable selection of the sensor locations. In literature one can find various choices for such a criterion (Pázman, 1986; Walter and Pronzato, 1997; Fedorov and Hackl, 1997):

- A-optimality criterion
$$\Psi(M) = \operatorname{trace}(M^{-1}),$$
An A-optimal design supresses the variance of the estimates (but the correlation between the estimates is neglected),

- D-optimality criterion
$$\Psi(M) = -\ln\det(M),$$
A D-optimal design minimizes the volume of the uncertainty ellipsoid $E_{\hat{\theta}} = \{\theta : (\hat{\theta}-\theta)^{\mathrm{T}} M^{-1} (\hat{\theta}-\theta) \leqslant m\}$ for the parameters,

- E-optimality criterion
$$\Psi(M) = \lambda_{\max}(M^{-1}),$$
where $\lambda_{\max}(\,\cdot\,)$ stand for the maximal eigenvalue of its argument. An E-optimal design minimizes the largest width of $E_{\hat{\theta}}$ along its principal directions,

- The sensitivity criterion
$$\Psi(M) = -\operatorname{trace}(M).$$
This criterion does not possess a statistical interpretation, but it is sometimes used due to its simple form and the fact that its minimization increases the sensitivity of the outputs with respect to parameter changes.

In addition to its relative simplicity, the D-optimality has an important advantage in contrast to the E- and A-optimality criteria, namely it is invariant under linear output transformations and changes in the parameter scales (Walter and Pronzato,

1997). The simplest is the sensitivity criterion, but in many cases it leads to a singular FIM and serious problems with identifiability.

Obviously, there exist many more other performance indices, which are proposed in various publications (e.g. a class based on the variance of the system output prediction functions (Walter and Pronzato, 1997)). However, the most often used criteria are related to the eigenvalues of the FIM (e.g. minimizing the D-optimality criterion amounts to maximizing the product of all eigenvalues of M, while the use of the A-optimality criterion leads to minimizing the sum of the reciprocals of the eigenvalues). Therefore, most of the performance indices mentioned here can be treated as members of a wide class of criteria (Fedorov and Hackl, 1997; Walter and Pronzato, 1997) defined by the following functional:

$$\Psi_\gamma(M) = \begin{cases} \left[\dfrac{1}{m}\mathrm{trace}(PM^{-1}P^{\mathrm{T}})^\gamma\right]^{1/\gamma} & \text{if } \det M \neq 0, \\ \infty & \text{otherwise,} \end{cases}$$

where $P \in \mathbb{R}^{m\times m}$ is a weighting matrix. Indeed, substituting $P = I$ for $\gamma = 1$, $\gamma \to \infty$ and $\gamma \to 0$, we obtain respectively the A-, E- and D-optimum design criteria.

2.2.4. Main complications

After conversion of the original problem of choosing an optimal measurement strategy to that of minimizing the appropriate performance index, one might think that its solution is only a matter of application of some well-known nonlinear optimization algorithms. Nevertheless, the practical problems clearly shows that such an impression is extremely misleading. Severe difficulties are encountered, which make the problem highly non-trivial and explain the scarcity of publications on this subject in contrast to a similar problem for state estimation. In what follows, the main impediments in solving the prescribed problem will be indicated and discussed.

2.2.4.1. Loss of the estimator underlying properties

First of all, it should be emphasized that the approximation of the parameter dispersion matrix by the inverse of the FIM, which is based on converting the Cramer-Rao inequality into the equality, is legitimate only in situations when the measurement errors have small magnitudes and are independently distributed, the nonlinearity of the model with respect to the parameters is mild and the time horizon is comparatively large (Walter and Pronzato, 1997). Although the first assumption is rather justified in most real situations, the other two are rarely satisfied. In fact, in more precise terms, the observational time horizon should satisfy $t_f \to \infty$ (Rafajłowicz, 1986b; Walter and Pronzato, 1997). From the technical point of view, an infinite observational horizon is impossible to implement and the loss of the accuracy of the estimator should be observed. However, if the length of the observation time interval is sufficiently large, this effect is commonly neglected in applications.

The greatest difficulty, which can be often encountered in practice, is a high non-linearity of the model, and consequently the deterioration in the quality of the estimator. This situation necessitates a more detailed comment and will be discussed in further sections.

2.2.4.2. High dimensionality of the problem

In practical engineering systems, the number of allocated sensors in a given spatial region may reach from dozens to several hundreds. As examples, consider the following monitoring nets:

- Pacific Northwest Solar Radiation Network (University of Oregon) whose aim is to monitor and predict solar resources; it contains 19 stationary stations (Gueymard *et al.*, 2000);
- China Environment Monitoring Centre Network which monitors the water quality and temperature of the greatest Chinese rivers; it should contain up to 98 (by the end of 2005) stationary automatic stations;
- Southern Great Basin Digital Seismic Network for permanent observations of the seismic activity used in earthquake prediction; it has 30 stationary observational stations (Romanowicz *et al.*, 1994; Ichinose *et al.*, 1998);
- Air Quality Network of Berlin, 'BLUME' constructed for measurements of air pollution, identification of pollution sources, verification of the effect of air pollution control and prevention to detect excessive smog levels within the framework of smog alert plans; it contains 45 mobile and stationary monitoring stations with 147 measurement devices (Fedra, 1999);
- research network in the Great Lakes in the USA for spatial predictions of ozone concentration; it has approximately 160 monitoring stations (Nychka *et al.*, 1998).

Many additional examples can be provided. Since the position of each sensor is determined by at least two spatial coordinates and the optimization problem is multi-modal (when the global optimum is hidden in many local optima), severe difficulties are usually experienced when trying to solve it as a classical non-linear constrained programming task.

2.2.4.3. Phenomenon of sensor clusterization

Another acute problem is the potential sensor clusterization, i.e. the tendency of different sensors to take measurements at the same location, which is rather unacceptable in real situations. This phenomenon is a direct consequence of the assumption of spatially independent measurement errors. As an illustration of the clusterization effect, the following example can be considered.

Example 2.2. In this example we examine again the transmission line of Example 2.1 with a specified length $l = \ln(3)$, but attention will be focused only on the voltage signal y. Assume that the line is homogeneous (densities of its electrical parameters are constant along the line) without leakage conductance and inductance, i.e. $G = 0$ and $L = 0$ (this corresponds to the so-called Thomson cable (Kącki, 1995)). For notational simplicity, write down the time constant of the line as $RC = \theta_1$. Thus the signal propagation is described by the following telegraph equation of the parabolic type (de Cogan and de Cogan, 1997):

$$\theta_1 \frac{\partial y}{\partial t} = \frac{\partial^2 y}{\partial x^2}, \quad x \in \big(0, l\big), \quad t \in (0, t_f). \tag{2.22}$$

Consider the transient state of the transmission line over the observation horizon $t_f = 1$ in the case when the system at both ends is supplied by the voltage sources whose characteristics are defined by the following boundary conditions:

$$\begin{cases} y(0,t) = \theta_2 e^{\theta_1 t}, \\ y\big(\ln(3), t\big) = 2\theta_2 e^{\theta_1 t}, \quad t \in (0,1). \end{cases} \tag{2.23}$$

and initial voltage distribution

$$y(x,0) = \frac{1}{8}\theta_2\big(3\sinh(x) + 2\mathrm{e}^x\big), \quad x \in (0, \ln(3)). \tag{2.24}$$

The unknown values of the parameter vector $\theta = (\theta_1, \theta_2)$ have to be estimated with the use of two stationary sensors. To find optimal locations x^1 and x^2, the D-optimality criterion will be applied.

An exact analytical solution for this problem exists and has the form

$$y(x,t) = \frac{1}{4}\theta_2 \mathrm{e}^{\theta_1 t}\sinh(x) + \theta_2 \mathrm{e}^{\theta_1 t}\cosh(x). \tag{2.25}$$

Since the measurements are continuous in time, the FIM can be obtained from (2.19), in which $C(x,t)$ is assumed to be the identity matrix and

$$G^{\mathrm{T}}(x,t) = \left[\frac{1}{4}\theta_2 t\mathrm{e}^{\theta_1 t}\sinh(x) + \theta_2 t\mathrm{e}^{\theta_1 t}\cosh(x), \frac{1}{4}\mathrm{e}^{\theta_1 t}\sinh(x) + \mathrm{e}^{\theta_1 t}\cosh(x)\right]. \tag{2.26}$$

A computation which can be performed using a computer-algebra system shows that

$$\begin{aligned} \det\big(M(x^1, x^2)\big) = &\left(\frac{\theta_2}{16\theta_1^2}\right)^2 \big(\mathrm{e}^{4\theta_1} - 2\mathrm{e}^{2\theta_1} - 4\mathrm{e}^{2\theta_1}\theta_1^2 + 1\big) \\ &\cdot \Big(\big(\sinh(x^1) + 4\cosh(x^1)\big)^2 + \big(\sinh(x^2) + 4\cosh(x^2)\big)^2\Big)^2. \end{aligned} \tag{2.27}$$

The surface plot of $\det M(x^1, x^2)$ for $\theta = (0.05, 0.05)$ is shown in Fig. 2.2. An easy verification shows that the maximum value of the D-optimality criterion corresponds to the sensor locations

$$x^{1\star} = x^{2\star} = \ln(3). \tag{2.28}$$

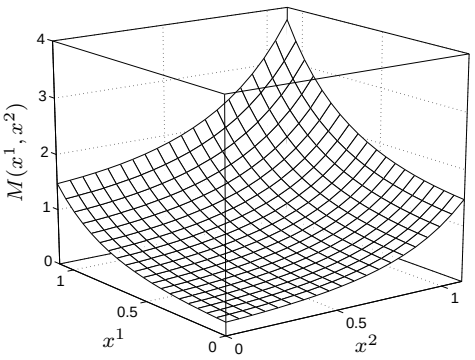


Fig. 2.2 . The surface plot of $M(x^1, x^2)$ for Example 2.2 ($\theta = (0.05, 0.05)$).

The conclusion that both the sensors must be placed at the same spatial point, which illustrates the phenomenon of clusterization, is a direct consequence of the assumptions made while constructing the simplified mathematical model of the disturbances acting on the measurements.

★

In order to avoid this tendency, the problem usually can be transformed to a combinatorial one (Uciński, 1995) when from among N_a fixed *a priori* positions the best $N < N_a$ ones are to be selected. In the case of movable sensors additional constraints imposed on sensor trajectories are required, which highly complicates the approach. Another technique dedicated especially for the scanning strategy is to apply the idea of directly constrained design measures (Fedorov and Hackl, 1997; Uciński and Patan, 2002a) which will be presented in more details in Sections 3.2 and 4.3.

2.2.4.4. Relationship between the solution and estimated parameters

Perhaps the most serious obstacle, which has to be overcome while trying to design an optimal measurement strategy is the dependence of the optimal solution on the estimated parameters. Since it is clear that these parameters are unknown prior to the experiment, in order to solve the problem, we need some preliminary estimate of their values. An illustrative example for this complication is given below.

Example 2.3. Reconsider the one-dimensional homogeneous transmission line of Example 2.1, but this time assume that the line is lossless, i.e. $G = 0$ and $R = 0$. Moreover, assume that $LC = \theta^2$, where the physical interpretation of θ is the velocity of the signal propagation along the line. The distribution of the voltage y is thus given by the hyperbolic 'wave' equation

$$\theta^2 \frac{\partial^2 y}{\partial t^2} = \frac{\partial^2 y}{\partial x^2}, \quad x \in (0, \pi), \quad t \in (0, \pi). \tag{2.29}$$

The line is supplied at each end by sinusoidal electromotive forces, which correspond to the boundary conditions

$$y(0,t) = \frac{1}{4}\cos(t), \quad y(\pi,t) = \sin(\pi\theta)\sin(t) + \frac{1}{4}\cos(\pi\theta)\cos(t), \quad t \in (0,\pi). \tag{2.30}$$

The initial voltage distribution and the rate of changes along the line are respectively given by

$$y(x,0) = \frac{1}{4}\cos(\theta x), \quad \left.\frac{\partial y(x,t)}{\partial t}\right|_{t=0} = \sin(\theta x), \quad x \in (0,\pi). \tag{2.31}$$

The analytical solution to the problem so defined is the function

$$y(x,0) = \sin(\theta x)\sin(t) + \frac{1}{4}\cos(\theta x)\cos(t). \tag{2.32}$$

Our task here is to find the location x^1 of only one sensor in such a way as to obtain the most accurate estimate of θ. Because there is only one constant parameter, the FIM is a scalar and each criterion applied leads to the same solution. The FIM can be represented as

$$\begin{aligned} M(x^1) &= \int_0^{t_f} \left(\frac{\partial u(x^1,t;\theta)}{\partial\theta}\right)^2 \mathrm{d}t \\ &= -\frac{1}{2}x^2\cos(\theta x)^2\cos(t_f)\sin(t_f) + \frac{1}{2}x^2\cos(\theta x)^2 t_f \\ &\quad + \frac{1}{4}x^2\cos(\theta x)\sin(\theta x)\cos(t_f)^2 + \frac{1}{32}x^2\sin(\theta x)^2\cos(t_f)\sin(t_f) \\ &\quad + \frac{1}{32}x^2\sin(\theta x)^2 t_f - \frac{1}{4}x^2\cos(\theta x)\sin(\theta x). \end{aligned} \tag{2.33}$$

The surface and countour plots of (2.33) corresponding to $t_f = \pi$ are shown in Fig. 2.3. The first observation is a multi-modal character of the problem as it was elucidated earlier. The second finding constitutes the essence of this example as it is clear that the optimal sensor position does depend on the value of the parameter θ. The optimal sensor position $x^{1\star}(\theta)$ is marked with a dashed line on the contour plot.

★

The dependence of the solutions on the unknown parameters is a significant drawback which implies the necessity of applying some *a priori* statistical knowledge about the parameter to be identified. Often some nominal values of physical parameters are available, otherwise there is a need for some pilot experiments conducted so as to obtain preliminary estimates of the parameters or for exploiting the so-called *sequential designs*, which comprises repeated consecutive experimentation and estimation steps. However, from the economical and technical points of view such a procedure is often impractical and difficult to implement, especially in the case of on-line algorithms. Alternatively, there are some *robust-design* techniques, which minimize the amount of statistical information necessary to find an

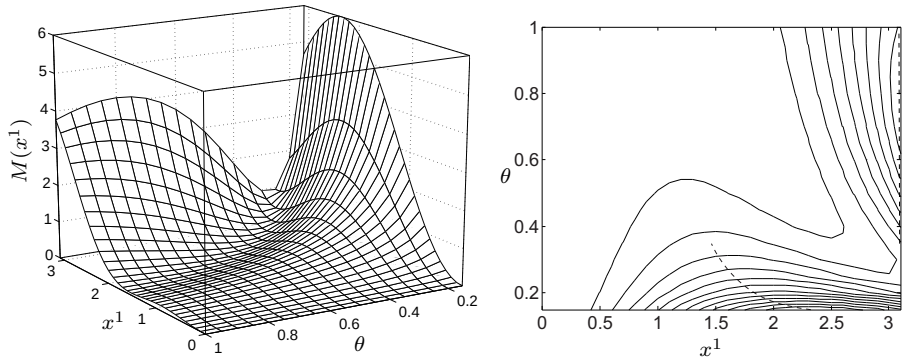


Fig. 2.3. The surface and contour plots of $M(x^1;\theta)$ in Example 2.3.

optimal solution on one hand, but on the other hand they significantly increase the complexity of the approach. This leads to the *average approach* which takes into account information about statistical distributions of unknown parameters and *minimax designs* comprising the analysis in the worst conditions possible (Walter and Pronzato, 1997).

2.3. Convex design theory for LPS's

2.3.1. Linear models

Prior to the analysis of more complex situations which are of interest in the context of the present work, it is useful to investigate first the less sophisticated case of the system linear in its parameters. If we assume that the observation conditions in the sense of the measurement locations are established arbitrarily before the experiment, such a system can be treated as an LPS with sensor positions in the role of its additional design parameters which are fixed and are not a subject of estimation. To achieve a possibly high level of generality, additionally we assume here that the system under consideration is of the MIMO type and evolves in a continuous time domain (results for the discrete case could be provided in much the same way).

Let us introduce the observation equation for the investigated system

$$z(t) = G^{\mathrm{T}}(t)\theta + \varepsilon(t), \quad t \in T = [0, t_f], \tag{2.34}$$

where t_f is a finite time horizon and $\theta \in \mathbb{R}^m$ is an unknown parameter vector. Matrix G is defined here as

$$G(t) = \begin{bmatrix} F(x^1, t) & \cdots & F(x^N, t) \end{bmatrix}, \tag{2.35}$$

where

$$F(x, t) = \begin{bmatrix} f_1(x, t) & \cdots & f_n(x, t) \end{bmatrix},$$

$x^j \in X \subset \mathbb{R}^d,\ j = 1, \ldots, N$ stand for fixed design parameters and the set of functions $f_i(\,\cdot\,,\,\cdot\,),\ i = 1, \ldots, n$ is known *a priori*. Moreover, ε is a Gaussian (zero-mean and uncorrelated in time) stochastic process playing the role of the measurement noise. Its covariance is defined by

$$\mathrm{E}\{\varepsilon(t)\varepsilon^{\mathrm{T}}(\tau)\} = C(t)\delta(t-\tau), \tag{2.36}$$

where δ means Dirac's delta distribution. The positive-definite matrix $C(\,\cdot\,) \in \mathbb{R}^{Nn\times Nn}$ is assumed here to have the following form:

$$C(t) = C_m(t) \otimes C_o(t), \tag{2.37}$$

where $C_m(t) \in \mathbb{R}^{N\times N}$ and $C_o(t) \in \mathbb{R}^{n\times n}$ are positive definite matrices defining correlations between measurements at different settings of x^j and between outputs corresponding to a fixed setting x^j, respectively (the symbol $\otimes$ denotes the Kronecker product of matrices). Furthermore, it is convenient to put the restriction that the measurements corresponding to different values of x^j are independent of each other. From a practical point of view it seems to be a rather strong constraint, but potential benefits justify this fact. Thus we make the standing assumption that

$$C_m(t) = \begin{bmatrix} \sigma^2(x^1,t) & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \sigma^2(x^N,t) \end{bmatrix} \tag{2.38}$$

where $\sigma(x^j,t),\ j = 1, \ldots, N$ can be interpreted as standard deviations of the measurement errors for different x^j's. Although the measurement covariance matrix $C_m(t)$ has diagonal form, there is no need to make additional assumptions on the matrix $C_o(t)$.

In the remainder of this chapter we shall make the following two standing assumptions:

(A1) X is compact,

(A2) $\forall i,\ f_i \in C(X \times T; \mathbb{R}^m)$.

Based on the observations $z(\,\cdot\,)$ and the known values of $G(\,\cdot\,)$, the problem of recovering θ reduces to determining the parameter vector $\hat{\theta}$ which minimizes the weighted least-squares criterion

$$\hat{\theta} = \arg\min_{\theta\in\Theta} \frac{1}{2} \int_0^{t_f} \left[z(t) - G^{\mathrm{T}}(t)\theta\right]^{\mathrm{T}} C^{-1}(t) \left[z(t) - G^{\mathrm{T}}(t)\theta\right] \mathrm{d}t \tag{2.39}$$

It is a rather simple matter to show that if only the information matrix

$$M = \int_0^{t_f} G(t)C^{-1}(t)G^{\mathrm{T}}(t)\,\mathrm{d}t \tag{2.40}$$

is non-singular, then the estimate (2.39) exists. Moreover, it is unbiased and its covariance is given by the inverse of M (Uciński, 1999a). As it is clearly seen

from (2.40), the information matrix depends on the parameters $x^j,\ j=1,\dots,N$ (through matrix G) but does not depend on the observations. The meaning of this significant fact is that it is possible to design experimental conditions by choosing $x^j,\ j=1,\dots,N$ so as to maximize the information provided by the experiment in the sense of the statistical accuracy of the estimate.

Note that the FIM can be transformed into a simpler form

$$M=\sum_{j=1}^{N}\int_0^{t_f}\sigma^{-2}(x^j,t)F(x^j,t)C_o^{-1}(t)F^{\mathrm{T}}(x^j,t)\,\mathrm{d}t=\sum_{j=1}^{N}M_j, \tag{2.41}$$

where

$$M_j=\int_0^{t_f}\sigma^{-2}(x^j,t)F(x^j,t)C_o^{-1}(t)F^{\mathrm{T}}(x^j,t)\,\mathrm{d}t. \tag{2.42}$$

The above equation expresses the additivity of the FIM with respect to the individual settings of x^j, which is the crucial property for the approach presented in what follows.

For convenience, introduce the so-called *average* (*normalized*) FIM

$$\bar{M}=\frac{1}{Nt_f}M=\frac{1}{Nt_f}\sum_{j=1}^{N}\int_0^{t_f}\sigma^{-2}(x^j,t)F(x^j,t)C_o^{-1}(t)F^{\mathrm{T}}(x^j,t)\,\mathrm{d}t, \tag{2.43}$$

which equals M up to a constant multiplier. Since most of optimality criteria used in practice satisfy the homogeneity condition

$$\Psi(\kappa M)=\gamma(\kappa)\Psi(M),\ \kappa>0$$

where $\gamma(\,\cdot\,)$ is a non-decreasing function, without loss of generality it will be used instead of M (for simplicity, the bar over M will also be omitted).

The introduction of an optimality criterion Ψ makes it possible to formulate the optimum experimental design problem as the optimization one

$$\breve{\xi}_N^{\star}=\arg\min_{\breve{\xi}_N}\Psi[M(\breve{\xi})], \tag{2.44}$$

where $\breve{\xi}=\{x^1,\dots,x^N\}$ and $x^j\in X,\ j=1,\dots,N$. A solution to the problem so formulated leads to the notion of the so-called exact designs.

Owing to the assumption (2.38), we admit of replicated measurements, i.e. some values x^j may appear several times in the optimal solution (this is an inevitable effect of the independence of measurements). Consequently, it is sensible to reformulate the problem so as to operate on the locations $x^1,\dots,x^\ell$ (relabelled different sensor locations) in lieu of $x^1,\dots,x^N$. To this end, we introduce $r_1,\dots,r_\ell$ as the numbers of replicated measurements corresponding to the points $x^1,\dots,x^\ell$. In this formulation, the x^i's are said to be the *design* or *support* points, and $p_1,\dots,p_\ell$ are called their weights. The collection of variables

$$\xi_N=\begin{Bmatrix}x^1, & x^2, & \dots, & x^\ell\\ p_1, & p_2, & \dots, & p_\ell\end{Bmatrix}, \tag{2.45}$$

where $p_i = r_i/N$, $N = \sum_{i=1}^{\ell} r_i$, is called the *exact design* of the experiment. The proportion p_i of observations performed at x^i can be considered as the percentage of experimental effort spent at that point.

On account of the above remarks, we rewrite the FIM in the form

$$M(\xi_N) = \sum_{i=1}^{\ell} p_i \frac{1}{t_f} \int_0^{t_f} \sigma^{-2}(x^i,t) F(x^i,t) C_o^{-1}(t) F^{\mathrm{T}}(x^i,t)\,\mathrm{d}t \tag{2.46}$$

Here the p_i's are rational numbers, since both r_i's and N are integers. This discrete nature of N-observation exact designs causes serious difficulties, as the resultant numerical analysis problem is not amenable to solve by standard optimization techniques, particularly when N is large. A commonly used device for this problem is to extend the definition of the design. When N is large, the p_i's can be considered as real numbers in the interval $[0,1]$, not necessarily integer multiples of $1/N$. This assumption will be also made in what follows. Obviously, we must have $\sum_{i=1}^{\ell} p_i = 1$, so we may think of the designs as probability distributions on X. This leads to the so-called *continuous* designs which constitute the basis of the modern theory of optimal experiments (Ermakov, 1983; Fedorov, 1972; Fedorov and Hackl, 1997; Atkinson and Donev, 1992; Goodwin and Payne, 1977; Pázman, 1986; Walter and Pronzato, 1997; Rafajłowicz, 1986b; Uciński, 1999a). It turns out that such an approach drastically simplifies the design. Thus, we shall operate on designs of the form

$$\xi = \begin{Bmatrix} x^1, & x^2, & \ldots, & x^{\ell}; & \displaystyle\sum_{i=1}^{\ell} p_i = 1 \\ p_1, & p_2, & \ldots, & p_{\ell} & \end{Bmatrix} \tag{2.47}$$

which concentrate Np_1 measurements at x_1, Np_2 at x_2, and so on.

At this point it is possible to further generalize the concept of the design to all probability measures ξ over X which are absolutely continuous with respect to the Lebesgue measure and satisfy by definition the condition

$$\int_X \xi(\mathrm{d}x) = 1 \tag{2.48}$$

Such a conceptual extension yields

$$M(\xi) = \int_X \left\{ \frac{1}{t_f} \int_0^{t_f} \sigma^{-2}(x,t) F(x,t) C_o^{-1}(t) F^{\mathrm{T}}(x,t)\,\mathrm{d}t \right\} \xi(\mathrm{d}x) = \int_X \Upsilon(x)\,\xi(\mathrm{d}x) \tag{2.49}$$

where

$$\Upsilon(x) = \frac{1}{t_f} \int_0^{t_f} \sigma^{-2}(x,t) F(x,t) C_o^{-1}(t) F^{\mathrm{T}}(x,t)\,\mathrm{d}t \tag{2.50}$$

and the integration in (2.48) and (2.49) is to be understood in the Lebesgue-Stieltjes sense. The function $\sigma(x,t) \in C(X \times T)$ playing the role of the standard deviation is assumed to take only positive values.

Then we may redefine the optimal design as a solution to the optimization problem

$$\xi^{\star} = \arg \min_{\xi \in \Xi(X)} \Psi[M(\xi)], \tag{2.51}$$

where $\Xi(X)$ denotes the set of all probability measures on X.

Remark 2.1. What is more, note that it is also possible and sometimes convenient to study an even more general setting by introducing a fixed measure $\xi(\mathrm{d}t)$ of observation effort in the interval T, i.e. to consider

$$\begin{aligned} M(\xi) &= \int_T \left[\int_X \sigma^{-2}(x,t) F(x,t) C_o^{-1}(t) F^{\mathrm{T}}(x,t)\, \xi(\mathrm{d}x|t) \right] \xi(\mathrm{d}t) \\ &= \iint_{X\times T} \sigma^{-2}(x,t) F(x,t) C_o^{-1}(t) F^{\mathrm{T}}(x,t)\, \xi(\mathrm{d}x, \mathrm{d}t), \end{aligned} \tag{2.52}$$

where the measure $\xi(\,\cdot\,|t)$ corresponds to a spatial measure at time t,

$$\int_X \xi(\mathrm{d}x|t) = 1 \quad \text{a.e. on } T, \tag{2.53}$$

$$\xi(\mathrm{d}t) = \int_X \xi(\mathrm{d}x, \mathrm{d}t). \tag{2.54}$$

This means that we then focus on designs ξ being non-Cartesian product measures (Rao, 1987), or in other words, we interpret sensor locations at given time moments as conditional distributions.

2.3.2. Characterization of the optimal solutions

A number of characterizations of the optimal design $\xi^\star$ can be generalized for the studied case in a rather straightforward manner based on the results reported in (Uciński, 1999a). First, let us prove some properties of the FIM given by (2.49):

Lemma 2.1. *For any $\xi \in \Xi(X)$ the matrix $M(\xi)$ is symmetric and non-negative definite.*

Proof. See Appendix A.1. ■

Let us introduce the notation $\mathfrak{M}(X)$ for the set of all admissible information matrices, i.e.

$$\mathfrak{M}(X) = \big\{ M(\xi) : \xi \in \Xi(X) \big\}. \tag{2.55}$$

Lemma 2.2. *$\mathfrak{M}(X)$ is compact and convex.*

Proof. See Appendix A.1. ■

Now we can state the following theorem which complements our knowledge of the information matrices.

Theorem 2.3. *For any matrix $M_0 \in \mathfrak{M}(X)$ there exists a design ξ that contains $\ell_0 \leqslant m(m+1)/2 + 1$ support points and $M(\xi) = M_0$. If M_0 is a boundary point of $\mathfrak{M}(X)$ then $\ell_0 \leqslant m(m+1)/2$.*

Proof. See Appendix A.1. ■

The great practical relevance of Theorem 2.3 cannot be overestimated. It allows us to dramatically reduce the dimensionality of the search space for the optimal solution. Our attention can be restricted to the designs with a limited number of support points and the concept of continuous designs, despite its abstract character, leads to a great simplification of the problem.

In order to derive necessary and sufficient conditions for the optimality of designs, some additional properties of the optimality criterion $\Psi(\,\cdot\,)$ are required:

(A3) $\forall \alpha \in [0,1], \quad \Psi[(1-\alpha)M_1 + \alpha M_2] \leqslant (1-\alpha)\Psi(M_1) + \alpha\Psi(M_2)$ (convexity),

(A4) $M_1 \leqslant M_2 \Rightarrow \Psi(M_1) \geqslant \Psi(M_2)$ (monotonicity with respect to the Löwner ordering),

(A5) $\exists q \in \mathbb{R}, \quad \Xi_q = \{\xi : \Psi[M(\xi)] \leqslant q < \infty\} \neq \emptyset$,

(A6) $\forall \xi \in \Xi_q$, $\forall \bar{\xi} \in \Xi(X)$, we have

$$\Psi[(1-\alpha)M(\xi) + \alpha M(\bar{\xi})] = \Psi[M(\xi)] + \alpha \int_X \psi(x,\xi)\bar{\xi}(\mathrm{d}x) + o(\alpha;\xi,\bar{\xi})$$

where the function $o(\,\cdot\,;\xi,\bar{\xi})$ satisfies $\lim\limits_{\alpha\downarrow 0} o(\alpha;\xi,\bar{\xi})/\alpha = 0$.

Assumptions (A3) and (A4) are rather obvious and natural as they refer to the attributes which raise a possibility of applying methods of convex optimization. (A5) guarantees the existence of designs with finite values of Ψ. The most restrictive seems Assumption (A6) as it requires the existence of a specific form of the directional derivative. But note that we have

$$\begin{aligned}
&\frac{\partial \Psi[(1-\alpha)M(\xi) + \alpha M(\bar{\xi})]}{\partial \alpha}\bigg|_{\alpha=0^+} \\
&\quad = \lim_{\alpha\to 0^+} \frac{\Psi[(1-\alpha)M(\xi) + \alpha M(\bar{\xi})] - \Psi[M(\xi)]}{\alpha} \\
&\quad = \operatorname{trace}\left[\overset{\circ}{\Psi}[M(\xi)](M(\bar{\xi}) - M(\xi))\right] \\
&\quad = \operatorname{trace}\left[\overset{\circ}{\Psi}[M(\xi)]\int_X \Upsilon(x)\,\bar{\xi}(\mathrm{d}x)\right] - \operatorname{trace}\left[\overset{\circ}{\Psi}[M(\xi)]M(\xi))\right] \\
&\quad = \int_X \left\{\operatorname{trace}\left[\overset{\circ}{\Psi}[M(\xi)]\Upsilon(x)\right] - \operatorname{trace}\left[\overset{\circ}{\Psi}[M(\xi)]M(\xi)\right]\right\} \bar{\xi}(\mathrm{d}x)
\end{aligned} \tag{2.56}$$

where

$$\overset{\circ}{\Psi}[M(\xi)] = \frac{\partial \Psi(M)}{\partial M}\bigg|_{M=M(\xi)} \tag{2.57}$$

From (2.56) it can be clearly seen that if Ψ is differentiable with respect to the elements its matrix argument, then Assumption (A6) is satisfied. Indeed, introduce the following representation of $\psi(x,\xi)$:

$$\psi(x,\xi) = \varsigma(\xi) - \phi(x,\xi), \tag{2.58}$$

where

$$\varsigma(\xi) = -\operatorname{trace}\left[\overset{\circ}{\Psi}[M(\xi)]M(\xi)\right], \tag{2.59}$$

and

$$\begin{aligned}\phi(x,\xi) &= -\operatorname{trace}\left[\overset{\circ}{\Psi}[M(\xi)]\Upsilon(x)\right] \\ &= -\operatorname{trace}\left\{\frac{1}{t_f}\int_0^{t_f}\sigma^{-2}(x,t)F^{\mathrm{T}}(x,t)\overset{\circ}{\Psi}[M(\xi)]F(x,t)C_o^{-1}(t)\,\mathrm{d}t\right\}.\end{aligned} \tag{2.60}$$

Now, we are ready to precise further characterizations of the optimal designs.

Theorem 2.4. *Suppose that Assumptions (A1)–(A6) hold. Then an optimal design $\xi^\star$ exists comprising no more than $m(m+1)/2$ support points. Moreover, the set of optimal designs is convex.*

Proof. See Appendix A.1. ■

It is purposeful to formulate the necessary and sufficient conditions for the optimality of the designs in the form of the following claim:

Theorem 2.5. *Assume that (A1)–(A6) are satisfied. Then*

(i) A design $\xi^\star$ is optimal iff

$$\min_{x\in X}\psi(x,\xi^\star) = 0, \tag{2.61}$$

(ii) The function $\psi(x,\xi^\star)$ has the zero value almost everywhere in $\operatorname{supp}\xi^\star$.

Proof. Because the explicit form of the FIM is not essential for the proof, the result can be proved in much the same way as Theorem 2.3.2 in (Fedorov and Hackl, 1997, p. 31). ■

The last theorem highlights the great decisive meaning of the function $\psi(x,\xi)$ in convex design theory, as this function completely determines the location of the support points for the optimal solution. Additionally, its local minima for any arbitrary design ξ indicate points when the measurements provide the greatest amount of information about the parameters being the subject of our interest (of course, in the sense of a chosen criterion). Using the above result, it is possible to construct a simple test for the optimality of designs. In particular,

1. If the sensitivity function $\psi(x,\xi)$ is less than or equal to 0 for all $x \in X$, then ξ is optimal.

2. If the sensitivity function $\psi(x,\xi)$ exceeds 0, then ξ is not optimal.

Applications of analytical methods for finding optimal designs are dedicated only for simple cases. In general situations, there is a need for some iterative numerical procedures. In order to state a useful theorem for checking the optimality of designs, which will be called the *equivalence theorem*, we have to prove some auxiliary results.

Lemma 2.6. *For any design $\xi \in \Xi(X)$, we have*

(i) $\displaystyle\int_X \phi(x,\xi)\,\xi(\mathrm{d}x) = \varsigma(\xi)$, *and*

(ii) $\max\limits_{x\in X} \phi(x,\xi) \geqslant \varsigma(\xi)$.

Proof. Taking into account (2.60), we obtain

$$\begin{aligned}\int_X \phi(x,\xi)\,\xi(\mathrm{d}x) &= -\int_X \operatorname{trace}\left[\overset{\circ}{\Psi}[M(\xi)]\Upsilon(x)\right]\xi(\mathrm{d}x)\\ &= -\operatorname{trace}\left[\overset{\circ}{\Psi}[M(\xi)]\int_X \Upsilon(x)\,\xi(\mathrm{d}x)\right]\\ &= -\operatorname{trace}\left[\overset{\circ}{\Psi}[M(\xi)]M(\xi)\right] = \varsigma(\xi)\end{aligned} \tag{2.62}$$

This establishes (i). Then (ii) is a direct consequence of (2.62). ■

Lemma 2.7. *If $\xi \in \Xi_q$, $\bar{\xi} \in \Xi(X)$ and $\xi_\alpha = (1-\alpha)\xi + \alpha\bar{\xi}$, then*

$$\left.\frac{\partial\Psi[M(\xi_\alpha)]}{\partial\alpha}\right|_{\alpha=0^+} = \varsigma(\xi) - \int_X \phi(x,\xi)\,\bar{\xi}(\mathrm{d}x). \tag{2.63}$$

Proof. From (2.56) we have

$$\begin{aligned}\left.\frac{\partial\Psi[M(\xi_\alpha)]}{\partial\alpha}\right|_{\alpha=0^+} &= \operatorname{trace}\left[\overset{\circ}{\Psi}[M(\xi)]\int_X \Upsilon(x)\,\bar{\xi}(\mathrm{d}x)\right] - \operatorname{trace}\left[\overset{\circ}{\Psi}[M(\xi)]M(\xi))\right]\\ &= \int_X \left\{\operatorname{trace}\left[\overset{\circ}{\Psi}[M(\xi)]\Upsilon(x)\right]\right\}\bar{\xi}(\mathrm{d}x) + \varsigma(\xi)\\ &= \varsigma(\xi) - \int_X \phi(x,\xi)\,\bar{\xi}(\mathrm{d}x).\end{aligned} \tag{2.64}$$

■

Now, we are capable of deriving our main result:

Theorem 2.8 (Generalized Equivalence Theorem). *The following conditions are equivalent:*

(i) the design $\xi^\star$ minimizes $\Psi[M(\xi)]$,

(ii) the design $\xi^\star$ minimizes $\max\limits_{x\in X} \phi(x,\xi) - \varsigma(\xi)$, and

(iii) $\max_{x\in X} \phi(x,\xi^\star) = \varsigma(\xi^\star)$

All the designs which satisfy (i)–(iii) and their convex combinations have the same information matrices equal to $M(\xi^\star)$, provided that the criterion $\Psi[\,\cdot\,]$ is strictly convex.

Proof. First, define $\xi_\alpha = (1-\alpha)\xi^\star + \alpha\xi_1$, where $\xi^\star \in \Xi_q$, and $\xi_1 \in \Xi(X)$.

$(i) \Rightarrow (ii)$ If the optimal design $\xi^\star$ minimizes $\Psi[M(\xi)]$, then $\Psi[M(\xi^\star)] \leqslant \Psi[M(\xi_\alpha)]$ for any $\xi_1 \in \Xi(X)$, therefore

$$\left.\frac{\partial \Psi[M(\xi_\alpha)]}{\partial \alpha}\right|_{\alpha=0^+} \geqslant 0, \quad \forall \xi_1 \in \Xi(X). \tag{2.65}$$

In particular substituting, $\xi = \xi^\star$ and $\bar{\xi} = \xi_x = \left\{ \begin{smallmatrix} x \\ 1 \end{smallmatrix} \right\}$ into (2.63), we get

$$\left.\frac{\partial \Psi[M(\xi_\alpha)]}{\partial \alpha}\right|_{\alpha=0^+} = \varsigma(\xi^\star) - \phi(x,\xi^\star) \geqslant 0, \quad \forall x \in X. \tag{2.66}$$

In connection with the second part of Lemma 2.6 this establishes (ii).

$(ii) \Rightarrow (iii)$ Lemma 2.6 implies that $\max_{x\in X} \phi(x,\xi) - \varsigma(\xi)$ is bounded from below by zero. From (2.66) it follows that this zero bound is achieved at any design minimizing $\Psi[M(\xi)]$ (the existence of such a design is guaranteed by Theorem 2.4). This means that if $\xi^\star$ is a design characterized in (ii), then necessarily $\max_{x\in X} \phi(x,\xi^\star) - \varsigma(\xi^\star) = 0$, which is exactly (iii).

$(iii) \Rightarrow (i)$ Let $\xi^\star \in \Xi(X)$ satisfy $\max_{x\in X} \phi(x,\xi^\star) = \varsigma(\xi^\star)$. Setting $\xi_\alpha = (1-\alpha)\xi^\star + \alpha\bar{\xi}$ for $\bar{\xi} \in \Xi(X)$, from Lemma 2.7 we obtain

$$\left.\frac{\partial \Psi[M(\xi_\alpha)]}{\partial \alpha}\right|_{\alpha=0^+} = \varsigma(\xi^\star) - \int_X \phi(x,\xi^\star)\,\bar{\xi}(\mathrm{d}x) \geqslant \varsigma(\xi^\star) - \max_{x\in X} \phi(x,\xi^\star) = 0, \tag{2.67}$$

which implies the optimality of $\xi^\star$.

The unicity of the information matrix for each optimal design follows from the convexity of the set $\mathfrak{M}(X)$ and the strict convexity of the function $\Psi : M \mapsto \Psi[M]$ (from classical optimization theory it is known that there exists at most one global minimum of a strictly convex function over a convex set). ■

Substituting a particular design criterion to Theorem 2.8, we obtain a specialized version of the equivalence theorem. There is no doubt that the most famous classical result is the equivalence theorem defined for the case of the D-optimality, formulated first in (Kiefer and Wolfowitz, 1959) for a static regression model. The form of the appropriate sensitivity functions for most popular criteria are listed in Table 2.1.

Table 2.1. Components of the sensitivity function for the most common optimality criteria.

$\Psi[M(\xi)]$	$\phi(x,\xi)$	$\varsigma(x,\xi)$
$-\ln\det M(\xi)$	$\operatorname{trace}\left\{\frac{1}{t_f}\int_0^{t_f}\sigma^{-2}(x,t)F^{\mathrm{T}}(x,t)M^{-1}(\xi)F(x,t)C_o^{-1}(t)\,\mathrm{d}t\right\}$	m
$\operatorname{trace}M^{-1}(\xi)$	$\operatorname{trace}\left\{\frac{1}{t_f}\int_0^{t_f}\sigma^{-2}(x,t)F^{\mathrm{T}}(x,t)M^{-2}(\xi)F(x,t)C_o^{-1}(t)\,\mathrm{d}t\right\}$	$\operatorname{trace}M^{-1}(\xi)$
$-\operatorname{trace}M(\xi)$	$\operatorname{trace}\left\{\frac{1}{t_f}\int_0^{t_f}\sigma^{-2}(x,t)F^{\mathrm{T}}(x,t)F(x,t)C_o^{-1}(t)\,\mathrm{d}t\right\}$	$\operatorname{trace}M(\xi)$

2.3.3. Nonlinear models

From now on, we shall discuss a more complicated situation when the considered system is not linear with respect to the parameters. This is a straightforward consequence of the attempt of adopting results from preceding section in parameter estimation of DPS's, because even if a system of PDE's constituting the model is linear, the state depends on the parameters in a highly non-linear manner. This creates grave difficulties and makes the closed-form solutions almost unavailable in most practical situations.

The sought generalization in (2.34) can be achieved by replacing the term $G^{\mathrm{T}}(t)\theta$ by the nonlinear multi-output system response

$$y(t;\theta)=\begin{bmatrix}y(x^1,t;\theta)\\ \vdots\\ y(x^N,t;\theta)\end{bmatrix}, \tag{2.68}$$

where

$$y(x,t;\theta)=\begin{bmatrix}y_1(x,t;\theta) & \cdots & y_n(x,t;\theta)\end{bmatrix}^{\mathrm{T}}. \tag{2.69}$$

Analogously to (2.39), the least-squares estimator is then defined by

$$\hat{\theta}=\arg\min_{\theta\in\Theta}\frac{1}{2}\int_0^{t_f}\left[z(t)-y(t,\theta)\right]^{\mathrm{T}}C^{-1}(t)\left[z(t)-y(t,\theta)\right]\,\mathrm{d}t. \tag{2.70}$$

In contrast to the linear case, this estimator is generally biased and the analytical form of the parameter covariance matrix, due to its dependence on θ, is extremely difficult. Most of the results for this case have only asymptotic character (Banks and Fitzpatrick, 1990; Fitzpatrick, 1991; Yin and Fitzpatrick, 1992; Fitzpatrick, 1995; Fitzpatrick and Yin, 1995).

To derive an expression for the dispersion matrix, it is customary to linearize the system response in the vicinity of a prior estimate θ^0 of the unknown parameter vector θ. This estimate is assumed to be close enough to the true value of θ. Then,

the system state can be approximated by expanding the function $y(t;\theta)$ in the Taylor series and retaining only the linear terms:

$$y(t;\theta) \cong y(t;\theta^0) + \left.\frac{\partial y(t;\theta)}{\partial \theta}\right|_{\theta=\theta^0} (\theta - \theta^0) \tag{2.71}$$

where

$$\frac{\partial y(t;\theta)}{\partial \theta} = \begin{bmatrix} \dfrac{\partial y(x^1,t;\theta)}{\partial \theta} \\ \vdots \\ \dfrac{\partial y(x^N,t;\theta)}{\partial \theta} \end{bmatrix} \tag{2.72}$$

and

$$\frac{\partial y(x,t;\theta)}{\partial \theta} = \begin{bmatrix} \dfrac{\partial y_1(x,t;\theta)}{\partial \theta_1} & \cdots & \dfrac{\partial y_1(x,t;\theta)}{\partial \theta_m} \\ \vdots & \ddots & \vdots \\ \dfrac{\partial y_n(x,t;\theta)}{\partial \theta_1} & \cdots & \dfrac{\partial y_n(x,t;\theta)}{\partial \theta_m} \end{bmatrix} \tag{2.73}$$

is the Jacobian of the system response y with respect to the vector θ. Substituting (2.71) into (2.34), we obtain the following observation equation

$$z(t) \approx y(t;\theta^0) + \left.\frac{\partial y(t;\theta)}{\partial \theta}\right|_{\theta=\theta^0} (\theta - \theta^0) + \varepsilon(t), \tag{2.74}$$

or equivalently, after some rearrangement,

$$z'(t) = z(t) - y(t;\theta^0) + \left.\frac{\partial y(t;\theta)}{\partial \theta}\right|_{\theta=\theta^0} \theta^0 \approx \left.\frac{\partial y(t;\theta)}{\partial \theta}\right|_{\theta=\theta^0} \theta + \varepsilon(t). \tag{2.75}$$

In this way, we get an analogue of the (2.34) for the nonlinear case. The respective form form of the average FIM (approximation of the inverse of $\operatorname{cov}\hat{\theta}$ up to a constant multiplier) is then

$$M(\xi_N) = \sum_{i=1}^{\ell} p_i \frac{1}{t_f} \int_0^{t_f} \sigma^{-2}(x^i,t) F(x^i,t) C_o^{-1}(t) F^{\mathrm{T}}(x^i,t)\,\mathrm{d}t, \tag{2.76}$$

where

$$F(x^i,t) = \left(\frac{\partial y(x^i,t;\theta)}{\partial \theta}\right)^{\mathrm{T}}_{\theta=\theta^0}. \tag{2.77}$$

It is clearly seen that information matrix (2.76) depends on the prior estimate around which the model is linearized and it is valid only when the approximation (2.71) is accurate. In this sense the results obtained from such an approach have only a local character. However, it can be shown that under rather mild assumptions the estimator (2.70) is strongly consistent, i.e.

$$a.s. \lim_{N\to\infty} \hat{\theta} = \theta,$$

where $a.s.\lim$ denotes the *almost sure* limit (convergence with probability one). For detailed consistency results, the reader can be referred to (Fitzpatrick, 1991; Fitzpatrick, 1995; Banks and Fitzpatrick, 1990; Fitzpatrick and Yin, 1995).

If both $y(x,t)$ and $F(x,t)$ are continuous in $\bar{\Omega} \times T$, then all the results from Sections 2.3.1 and 2.3.2, are directly applicable without any changes. In particular, the analogue of the FIM (2.78) can be written as

$$M(\xi) = \int_X \Upsilon(x)\, \xi(\mathrm{d}x), \tag{2.78}$$

where $X \in \bar{\Omega}$ is the region of admissible sensor locations, and

$$\Upsilon(x) = \frac{1}{t_f} \int_0^{t_f} \sigma^{-2}(x,t) \left(\frac{\partial y(x^i,t;\theta)}{\partial \theta} \right)^{\mathrm{T}}_{\theta=\theta^0} C_o^{-1}(t) \left(\frac{\partial y(x^i,t;\theta)}{\partial \theta} \right)_{\theta=\theta^0} \mathrm{d}t. \tag{2.79}$$

2.4. Concluding remarks

There is no doubt that the preparation of experimental conditions in the sense of choosing a suitable observational strategy has a great influence on the expected accuracy of parameter estimates, especially in the context of DPS's. In this chapter, the class of spatio-temporal dynamic systems, on which attention of this work is focused, was described along with the problem of choosing an optimal observation strategy for parameter estimation within this class. The problem once formulated and transformed to an optimization one is far form being trivial. In spite of the elegant formulation based on the use of a performance index defined on the Fisher information matrix, severe impediments exist such as the loss of some underlying properties of the estimator being a consequence of the dependence of the optimal solution on the estimated parameters, the sensor clusterization phenomenon or a high dimensionality of the problem. Thus, the well-known non-linear programming algorithms are neither directly applicable, nor provide effective solutions for practical engineering applications. Bearing this in mind, the remainder of this dissertation is dedicated to overcoming these difficulties to some extent.

In the second part of this chapter, the notion of continuous designs was introduced, which dramatically reduces the problem dimensionality. Furthermore, the generalization of some classical results from experimental design theory to multi-response systems with possibly correlated outputs was presented for the purpose of providing fundamental results which characterize the solutions and thus indicate possible numerical procedures. The inherent nonlinearity of DPS's with respect to the estimated parameters is certainly a problem of paramount importance and one of main complications in the delineated approach. However, under some assumptions, the results derived for linear-in-parameter systems can be extended to the class of nonlinear models based on suitable approximations of the FIM.

Such a generalized classical theory paves the way to numerous applications of DPS's and, being crucial for specific problems, constitutes close connection with the chapters which follow.

Chapter 3

OPTIMAL MEASUREMENT STRATEGIES FOR STATIC DPS'S

This chapter is devoted to tailoring the optimum experimental design theory delineated in the previous chapter to the subclass of DPS's, which are independent of time, i.e. to static DPS's. Such systems appear in many engineering applications and it is worth of paying them close attention since some solutions can be derived and then extended to more general cases.

In the context of general DPS's, determination of optimal designs in closed form is rather limited to simplest problems. The most frequent situation is then exploitation of iterative numerical routines, which offer a greater flexibility and an ability for providing a sufficient approximation to the optimal solution.

The main idea here is to reformulate the problem in the spirit of optimization of a scalar measure defined on the FIM related to the estimated parameters. Then well-known methods of optimum experimental design for non-linear models can be adopted to the setting of the sensor location problem at hand, or alternatively, standard non-linear programming procedures could be employed. One of the main objectives of this chapter is to elucidate how some extremely fast and efficient numerical algorithms of optimum experimental design can be altered to the framework of sensor location for static multiresponse DPS's with an appropriate theoretical substantiation.

3.1. Problem reformulation and notation

The appropriate mathematical description of the considered DPS subclass can be obtained from (2.1) by assuming that $D(x,t) = \mathbf{0}$, i.e. it is a zero matrix. What is more, as it has been mentioned above the system state does not depend on time, even if there are some time-dependent components of the PDE (e.g. such components could compensate one another and have no influence on the state). Taking this into account, without loss of generality we can describe the models under consideration in a simpler form given by the system of n (possibly non-linear) partial differential equations

$$\mathcal{G}\Big(x, y, \nabla y, \nabla^2 y; \theta\Big) = 0, \quad x \in \Omega \subset \mathbb{R}^d, \tag{3.1}$$

subject to the boundary conditions

$$\mathcal{E}\Big(x, y, \nabla y; \theta\Big) = 0, \quad x \in \partial\Omega, \tag{3.2}$$

where all the symbols have the same meaning as defined in Section 2.1.

Fortunately, the connection between the optimal observation strategy problem for the class of static distributed systems and the general optimum experimental design theory is in those circumstances rather straightforward. In particular, the vector of unknown parameters $\theta \in \mathbb{R}^m$ has to be estimated based on the data described by the simplified form of the observation equation (2.7):

$$z_j^i = y(x^i; \theta) + \varepsilon_{ij}, \quad i = 1, \ldots, \ell, \quad j = 1, \ldots, r_i. \tag{3.3}$$

The measurements are taken at different locations x^i, while ε_{ij} denotes the spatially uncorrelated Gaussian measurements noise satisfying

$$\mathrm{E}\{\varepsilon_{ij}\} = 0, \quad \mathrm{E}\{\varepsilon_{ij}\varepsilon_{qs}^{\mathrm{T}}\} = \sigma_i \delta_{iq} \delta_{js} C_o, \tag{3.4}$$

δ_{ij} being the Kronecker delta, $C_o \in \mathbb{R}^{n\times n}$ a known positive-definite matrix responsible for correlation between system outputs, and the σ_i's the standard deviations of the measurement errors. Note that replications are admitted, i.e. $r_i \geqslant 1$ measurements may be taken at a point x^i.

If we assume that some, albeit rough, *a priori* estimate of the parameter vector θ^0 is available e.g. from preliminary experiments, and parameter estimation is carried out with use of the least-squares method, the goal here can be defined analogously to the one from Section 2.3.1. For the exact design of the experiment ξ_N defined by (2.45) the specific form of the average-per-observation FIM is

$$M(\xi_N) = \sum_{i=1}^{\ell} \frac{p_i}{\sigma_i^2} G(x^i) C_o^{-1} G^{\mathrm{T}}(x^i), \tag{3.5}$$

where $p_i = r_i/N$, $N = \sum_{i=1}^{\ell} r_i$ and

$$G(x^i) = \left(\frac{\partial y(x^i;\theta)}{\partial \theta}\right)_{\theta=\theta^0}$$

is the Jacobi matrix consisting of the sensitivity coefficients (Uciński, 1999a). Applying the concept of continuous designs we have also the appropriate counterpart of (2.49):

$$M(\xi) = \int_X \Upsilon(x)\, \xi(\mathrm{d}x), \tag{3.6}$$

where

$$\Upsilon(x) = \int_X \sigma^{-2}(x) G(x) C_o^{-1} G^{\mathrm{T}}(x)\, \xi(\mathrm{d}x). \tag{3.7}$$

The problem is to find a design

$$\xi^\star = \arg \min_{\xi \in \Xi(X)} \Psi[M(\xi)], \tag{3.8}$$

where $\Xi(X)$ is the set of all admissible designs (i.e. all probability distributions on X, the spatial domain where measurements are allowed). In such a way direct applicability of all theorems and concepts of Section 2.3.2 can be established with minor changes.

Within the scope of the data acquisition methods which are of interest in the context of this dissertation, two important situations have to be individually characterized since the underlying theory and numerical techniques which can be applied need some separate description and comments. To be more precise, the next sections will be devoted to the case of a discrete finite set of admissible support points X and as the second topic the support set of non-zero measure will be considered.

3.2. Finite set of allowable measurement points

Our basic assumption in this section, is that the set of admissible support points X, where the observations of the measurands are possible, is finite. Because the number of locations from X is limited, then any design $\xi \in \Xi(X)$ is uniquely determined by the collection of the corresponding weights. Such a description is is very convenient as the problem is reduced to the optimization of weights.

3.2.1. Optimization of the experimental effort

It was already mentioned, the weight assigned to a measurement point can be interpreted as the proportion of observations performed at this point, or the percentage of experimental effort spent at it. The potential solutions are of considerable interest while assessing which sensors are more informative than the others and allow for complexity reduction of the measurement system.

In the case under consideration, i.e. the design for fixed sensor locations, the problem (3.8) can be rewritten as

$$p^\star = \arg\min_p \Psi[M(\xi)] \tag{3.9}$$

subject to

$$p \in \mathbb{S} = \left\{ p = (p_1, \ldots, p_\ell) : \; p_i \geqslant 0, \; i = 1, \ldots, \ell; \quad \sum_{i=1}^{\ell} p_i = 1 \right\} \tag{3.10}$$

for the FIM $M(\xi)$ given by (3.5) and with variable $p \in \mathbb{R}^\ell$. This is a finite-dimensional optimization problem over the canonical simplex $\mathbb{S}$.

Obviously, it is always possible to exploit some general constrained optimization routines in order to solve the problem formulated above. However, due to a relatively simple form of the constraints, a more straightforward procedure can be proposed, which reduces to using a gradient projection method (Walter and Pronzato, 1997). The first step is to find a feasible direction, i.e. the one which guarantees a decrease in the value of the criterion Ψ and then a step is taken along

this line. The result is projected on $\mathbb{S}$, thereby obtaining a new feasible weight vector. Generation of a new candidate point can be formalized as follows:

$$p_+^{(k)} = \Pi_{\mathbb{S}}[p^{(k)} + \eta\delta(p^{(k)})], \tag{3.11}$$

where $\delta(p^{(k)}) \in \mathbb{R}^\ell$ is the vector representing a feasible direction of weight modification and η is some coefficient which controls the correction process, and $\Pi_{\mathbb{S}}[\,\cdot\,]$ stands for orthogonal projection onto the convex set of admissible weights $\mathbb{S}$.

The derivatives

$$\frac{\partial\Psi[M(\xi)]}{\partial p_i} = \phi(x^i,\xi), \quad i = 1,\ldots,\ell \tag{3.12}$$

are easy to calculate, so the very first idea is to choose the direction $\delta(p^{(k)})$ determined by the negative gradient $-\nabla_p\Psi$ as in steepest descent. Also note that there exist many possible choices of determining the step coefficient η. It can be taken as a suitable constant or may be adapted in some manner, e.g. according to the rules

$$\eta_{k+1} = \begin{cases} \gamma_1\eta_k & \text{if } \Psi[M(\xi^{(k)})] \leqslant \Psi[M(\xi^{(k-1)})], \\ \eta_k/\gamma_2 & \text{otherwise,} \end{cases} \tag{3.13}$$

where $\gamma_1 > 1$ and $\gamma_2 > 1$ are appropriate fixed parameters, or optimally, i.e.

$$\eta_{k+1} = \arg\min_{\eta} \Psi\big[M(\xi_+^{(k)})\big], \tag{3.14}$$

where $\xi_+^{(k)}$ denotes the 'trial' design with weights defined by (3.11).

Now, it is possible to formulate the following steepest-descent type algorithm:

Algorithm 3.1. *Gradient projection weight optimization algorithm for a fixed finite set of measurement points*

Step 1. Guess a starting set of weights $p_1^{(0)} \in \mathbb{S}$. Choose some positive tolerance $\epsilon \ll 1$. Set $k = 0$.

Step 2. Compute

$$p^{(k+1)} = \Pi_{\mathbb{S}}\Big[p^{(k)} - \eta_k\nabla_p\ \Psi\big[M(\xi)\big]\big|_{p=p^{(k)}}\Big]$$

where

$$\eta_{k+1} = \arg\min_{\eta} \Psi\big[M(\xi_+^{(k)})\big]$$

Step 3. If the condition

$$\|p^{(k+1)} - p^{(k)}\| < \epsilon$$

is satisfied then *STOP*, otherwise increment k by one and go to Step 2.

♦

At first sight, the gradient projection procedure above is rather easy in implementation due to its simplicity, but unfortunately it inherits all the drawbacks of stepeest-descent-like algorithms. For example, the convergence rate dramatically decreases in the vicinity of the minimum. This can be avoided to some extent with a suitable choice of the correction step η. As for projection onto the canonical simplex $\mathbb{S}$, an algorithm can be developed which is almost as simple as a closed-form solution. Indeed, the point $p = \Pi_{\mathbb{S}}[p_+]$ is defined as the solution to the problem: Minimize

$$\sum_{i=1}^{\ell}(p_i - p_{i+})^2 \tag{3.15}$$

subject to

$$p_i \geqslant 0, \quad i = 1, \ldots, \ell, \quad \sum_{i=1}^{\ell} p_i = 1. \tag{3.16}$$

A very elegant and simple algorithm for solving this task was proposed by Tuenter (2001). Without loss of generality, assume that $p_{1+} \geqslant p_{2+} \geqslant \cdots \geqslant p_{\ell+}$, since this is only a matter of reordering the elements of p_+. It can be shown that problem (3.15)–(3.16) can be then reduced to a univariate one of the form: Minimize

$$f_{\mathrm{obj}}(q) = \frac{1}{q}\Big(1 - \sum_{i=1}^{q} p_{i+}\Big)^2 + \sum_{i=q+1}^{\ell} p_{i+}^2 \tag{3.17}$$

subject to

$$\sum_{i=1}^{q}(p_{i+} - p_{q+}) \leqslant 1, \quad q \in \{1, \ldots, \ell\}. \tag{3.18}$$

It is a simple matter to check that the sequence

$$S_q = \sum_{i=1}^{q}(p_{i+} - p_{q+}) \tag{3.19}$$

satisfies the recursion formula

$$S_q = S_{q-1} + (q-1)(p_{(q-1)+} - p_{q+}), \quad S_1 = 0. \tag{3.20}$$

Then the objective function from (3.17) satisfies

$$f_{\mathrm{obj}}(q) = f_{\mathrm{obj}}(q-1) - \frac{1}{q(q-1)}(1 - S_q)^2, \quad f_{\mathrm{obj}}(1) = 1 - 2p_{1+} + \sum_{i=1}^{\ell} p_{i+}^2. \tag{3.21}$$

It is easily seen that the sequence $\{f_{\mathrm{obj}}(q)\}_{q=1}^{\ell}$ is non-increasing. Then the solution can be determined by finding $q^\star$ as the largest index q which fulfils $S_q \leqslant 1$. Such

an index exists, since $S_1 = 0$, and it can be extremely easily determined from the recursion formula (3.20). This defines the components of the sought projection

$$p_i^\star = \begin{cases} p_{i+} + \dfrac{1}{q^\star}\Bigl(1 - \displaystyle\sum_{i=1}^{q^\star} p_{i+}\Bigr) & \text{for } \ 1 \leqslant i \leqslant q^\star, \\ 0 & \text{for } \ i > q^\star. \end{cases} \tag{3.22}$$

A detailed proof can be found in (Tuenter, 2001). In spite of the simplicity of this briefly delineated algorithm, it still involves some additional numerical effort. Moreover, the projection operator is not differentiable, so that the line search with respect to η in (3.14) requires a non-derivative algorithm (e.g. a golden-search one). Consequently, the effective usage of the proposed weight optimization algorithm requires practical experience from the user to overcome several impediments.

All these considerations imply that it could be expedient to take into account some other possible directions of weight modification, different from the gradient projection one in order to derive simpler procedures with comparable efficiency. One of such alternatives is the approach based on the mapping $\mathcal{T} : \Xi(X) \to \Xi(X)$ defined by

$$\mathcal{T}\xi = \begin{Bmatrix} x^1, & \dots, & x^\ell \\ p_1\phi(x^1,\xi)/\varsigma(\xi), & \dots, & p_\ell\phi(x^\ell,\xi)/\varsigma(\xi) \end{Bmatrix}. \tag{3.23}$$

From Theorem 2.8 it follows that a design $\xi^\star$ is optimal if it is a fixed point of the mapping $\mathcal{T}$, i.e.

$$\mathcal{T}\xi^\star = \xi^\star. \tag{3.24}$$

Certainly, from Lemma 2.6 it follows that the sum of weights is invariant with respect to $\mathcal{T}$. Thus the projection problem no longer exist. As for the interpretation of this function, consider the situation when a design ξ is not optimal. Then the mapping $\mathcal{T}$ increases the weights of those support points of ξ at which the sensitivity function takes a high values, i.e. $\phi(x,\xi) > \varsigma(\xi)$ in such a way decreasing its maximal values. This is attained at the cost of decreasing the weights for support points with small values of $\phi(x,\xi)$ (where $\phi(x,\xi) < \varsigma(\xi)$).

Therefore, the following algorithm can be used as an implementation of the above idea:

Algorithm 3.2. *Feasible-direction weight optimization algorithm*

Step 1. Guess a discrete starting design $\xi^{(0)}$ such that $p_i^{(0)} > 0$ for $i = 1, \dots, \ell$. Choose some positive tolerance $\epsilon \ll 1$. Set $k = 0$.

Step 2. If the condition

$$\frac{\phi(x^i,\xi^{(k)})}{\varsigma(\xi)} < 1 + \epsilon, \quad i = 1, \dots, \ell.$$

is satisfied, then *STOP*.

Step 3. Construct the next design $\xi_+^{(k)}$ by determining its weights according to the rule

$$p_{i+}^{(k)} = p_i^{(k)} \frac{\phi(x^i, \xi^{(k)})}{\varsigma(\xi^{(k)})}, \quad i = 1, \ldots, \ell,$$

Step 4. For an appropriate value of $0 < \alpha_k < 1$, set

$$\xi^{(k+1)} = (1 - \alpha_k)\xi^{(k)} + \alpha_k \xi_+^{(k)}$$

increment k by one and go to Step 2.

♦

Note that the algorithm above is nothing but a feasible direction method, cf. (Bertsekas, 1999). The convergence of the proposed iterative routine to the optimal design depend on a suitable choice of the sequence $\{\alpha_k\}$. The possible selections are as follows:

(a) the sequence α_k satisfies the conditions

$$\lim_{k\to\infty} \alpha_k = 0, \quad \sum_{k=0}^{\infty} \alpha_k = \infty, \tag{3.25}$$

(b) α_k is the solution of the problem

$$\alpha_k = \arg \min_{\alpha\in[0,1]} \Psi\big[(1-\alpha)M(\xi^{(k)}) + \alpha M(\xi_+^{(k)})\big], \tag{3.26}$$

(c) α_k is taken as the value of α_{k-1} divided repeatedly by $\gamma < 1$ until it satisfies

$$\Psi[M(\xi_{k-1})] > \Psi[M(\xi_k)]. \tag{3.27}$$

The following convergence result is valid.

Theorem 3.1. *Assume that the optimality criterion $\Psi[\,\cdot\,]$ is strictly monotonous in the sense that $\Psi[M_1] < \Psi[M_2]$ provided that $M_1 \geqslant M_2$ for $M_1 \neq M_2$. If $\{\xi^{(k)}\}$ is a sequence of designs obtained according to **Algorithm 3.2** and the rule* (3.26)*, then the sequence $\{\Psi[M(\xi^{(k)})]\}$ is non-increasing, and it converges to* $\min\{\Psi[M(\xi)] : \xi \in \Xi(X)\}$.

Proof. See Appendix A.2. ■

Generalization of the proof for the remaining cases is possible, although it is not trivial.

Analysing Step 3 of this fixed-point based algorithm, after some rearrangement we have

$$p_{i+}^{(k)} = p_i^{(k)} + \underbrace{p_i^{(k)} \left(\frac{1}{\varsigma(\xi^{(k)})} - \frac{1}{\phi(x^i, \xi^{(k)})} \right)}_{\eta} \phi(x^i, \xi^{(k)}), \quad i = 1, \ldots, \ell. \tag{3.28}$$

It is thus clear that the descent direction in this case is not certainly the negative gradient one. Notwithstanding this fact, such a direction automatically keeps the design in the simplex $\mathbb{S}$ and in such a way the effort of mapping $\mathcal{T}$ is not disturbed by any additional activity. Moreover, Step 4 can be omitted or at least simplified for many particular criteria, which will be discussed later in this section. Practical experiments show that the expected convergence rate can be in some situations comparable or even better than in the case of Algorithm 3.1 and with a great stability of performance. Besides the high efficiency coming from the numerical simplicity, the ease of implementation should be noticed as a great benefit of the procedure.

A decided advantage of both the delineated algorithms is simultaneous correction of all the weights, which leads to a significant increase in the convergence rate. Moreover, their applicability can be extended to a wide class of experimental design problems, in accordance with the following guidelines (Rafajłowicz, 1996):

1. The set of admissible support points X is finite. In this case the proposed routine converges to the optimal design as described above.

2. The set X is a bounded subset of $\mathbb{R}^d$. In such a framework the following alternatives can be distinguished:

   (a) If we know a small finite set $X_d \subset X$, which contains the optimal locations of the support points, the proposed routine can be used to find the optimal weights. The optimal design obtained for the set X_d constitutes simultaneously the optimal one for the set X. The main impediment is selection of a suitable subset X_d. For this purpose, other algorithms can be successfully applied and such possibilities will be discussed in Section 3.3.

   (b) We can choose a finite set $X_d \subset X$ with sufficiently distributed elements over the set X. For this set the algorithm can be applied, in the same manner as in Case 1. It guarantees that the resultant design is close enough to the optimal one (for the set X_d, of course), but for the quality assessment of the obtained solution an additional analysis is necessary.

From this point, some special cases require a more serious discussion as they are very important in the framework of this dissertation. Algorithm 3.2, being a generalization of the approach to the D-optimal criterion delineated in (Rafajłowicz, 1986b; Pázman, 1986; Torsney, 1988), can be further improved when applied to particular situations.

D-optimum experimental effort. For the D-optimum criterion and the case of only one response (i.e. $n = 1$) it can be shown that the line search in Algorithm 3.2 is not necessary. Therefore, it can be omitted in order to simplify the procedure. This leads to the following scheme, whose convergence was proved in (Pázman, 1986; Torsney, 1983; Torsney, 1988; Pukelsheim and Torsney, 1991) in the framework of the classical optimum experimental design problem:

Algorithm 3.3. *Optimization algorithm for finding a D-optimum experimental effort*

Step 1. Guess a discrete starting design $\xi^{(0)}$ such that $p_i^{(0)} > 0$ for $i = 1, \ldots, \ell$. Choose some positive tolerance $\epsilon \ll 1$. Set $k = 0$.

Step 2. If the condition

$$\frac{\phi(x^i, \xi^{(k)})}{m} < 1 + \epsilon, \quad i = 1, \ldots, \ell.$$

is satisfied, then *STOP*.

Step 3. Construct the next design $\xi^{(k+1)}$ by determining its weights according to the rule

$$p_i^{(k+1)} = p_i^{(k)} \frac{\phi(x^i, \xi^{(k)})}{m}, \quad i = 1, \ldots, \ell.$$

Increment k by one and go to Step 2.

♦

In such a way, the efficient and extremely simple procedure known in optimum experimental design for static systems can be used within the framework of the sensor location for static DPS's.

Nevertheless, the convex combination of designs which appears in Step 4 of Algorithm 3.2 can still be exploited to significantly improve the convergence rate since the transformation $\mathcal{T}$ does not guarantee the best correction of the weights. To illustrate the performance of the foregoing iterative routines, we give the following example.

Example 3.1. Consider the finite set of possible support locations $X = \{-2, -1, 0, 1, 2\}$ and the following vector of basis functions:

$$f^{\mathrm{T}}(x) = [1, x^2, e^{-x}].$$

The task is to found an optimal experimental effort for the D-optimality criterion using iterative procedures given by Algorithm 3.3 and its generalized version with selection of the convex combination of designs according to formula (3.26). The initial design was chosen in the form

$$\xi^{(0)} = \begin{Bmatrix} -2 & -1 & 0 & 1 & 2 \\ 0.3 & 0.3 & 0.2 & 0.1 & 0.1 \end{Bmatrix},$$

for which $\det M(\xi^{(0)}) = 12.209$. Using the equivalence theorem it is easy to check that the D-optimal design is

$$\xi^{\star} = \begin{Bmatrix} -2 & -1 & 0 & 1 & 2 \\ \frac{1}{3} & 0 & \frac{1}{3} & 0 & \frac{1}{3} \end{Bmatrix}$$

and $\det M(\xi^{\star}) = \frac{16}{27}(e^4 + e^{-4}) - \frac{32}{27} \simeq 31.180$. After four iterations, the algorithms generated the following approximations of the D-optimal design:

$$\xi_1^{(4)} = \begin{Bmatrix} -2 & -1 & 0 & 1 & 2 \\ 0.33 & 0.05 & 0.26 & 0.03 & 0.32 \end{Bmatrix}, \; \xi_2^{(4)} = \begin{Bmatrix} -2 & -1 & 0 & 1 & 2 \\ 0.34 & 0.00 & 0.35 & 0.00 & 0.31 \end{Bmatrix}$$

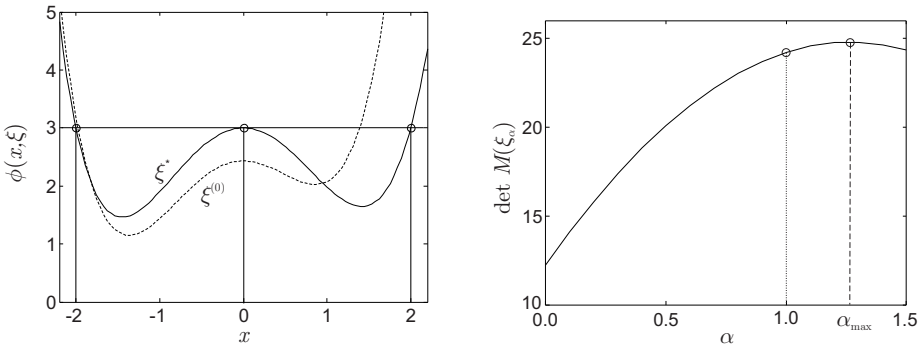


Fig. 3.1. Illustration of Example 3.1: (a) sensitivity functions for the initial and D-optimal designs (dashed and solid lines, respectively), (b) the choice of the best correction coefficient in the line search (at the first iteration)

Table 3.1. Consecutive steps of procedures from Example 3.1.

Iteration	Algorithm 3.3	Algorithm 3.3 with α-correction	
k	$\det M(\xi^{(k)})$	α_k	$\det M(\xi^{(k)})$
0	12.209	–	12.209
1	24.210	1.264	24.780
2	25.933	1.265	26.927
3	27.365	2.764	30.381
4	28.510	2.956	31.013
$\det M(\xi^\star) \simeq 31.180$			

with determinants $\det M(\xi_1^{(4)}) = 28.510$ and $\det M(\xi_2^{(4)}) = 31.013$, respectively. The detailed results are gathered in Table 3.1 and illustrated in Fig. 3.1(a), where the sensitivity functions are presented for the initial and optimal solutions. It can be seen that the sensitivity function attains its maximal value $m = 3$ at the points X which have non-zero weights. For the non-optimal design, at some support points the sensitivity function exceeds the number of parameters. Algorithm 3.3 with improvements has a high convergence rate at the expense of a lower numerical efficiency connected with the finding of the optimal value for the coefficient α. An analysis of Fig. 3.1(b) clarifies that if implementation of Step 4 of Algorithm 3.2 is justified from the computational point of view, then a significant increase in the convergence rate can be achieved, otherwise it can be neglected and convergence is still maintained although at the cost of its slowing down. The monotonicity of the function $\det M_\alpha(\xi)$ on the unit interval suggests that it may be worthwile to slightly extend the admissible interval in which the optimal coefficient α is sought. But this should be done carefully as this interval has to provide nonnegative design

weights. Another important observation is that the weights of the D-optimal design are all equal to $1/m$ over the set of m support points, which is in the excellent agreement with theory (cf. Silvey, 1980, p. 42).

★

Other criteria. Simplification of Algorithm 3.2 regarding criteria other than the D-optimal one still demands a more careful analysis (Torsney, 1983; Torsney, 1988; Pukelsheim and Torsney, 1991). In general, Assumptions (A1)–(A6) do not guarantee a generalization of the conclusions from the previous subsection to the whole class of interesting criteria.

Namely, it can be proven that for various criteria satisfying (A1)–(A6) without Step 4 of Algorithm 3.2 the convergence to an optimal solution cannot be guaranteed. To demonstrate it, consider the following counter-example based on the mapping $\mathcal{T}$ for the A-optimum criterion.

Example 3.2. Assume that the finite set of possible support locations is $X = \{0, 1\}$ and the vector of basis functions has the form

$$f^{\mathrm{T}}(x) = [1, x].$$

Consider the design

$$\xi^{(0)} = \begin{Bmatrix} 0 & 1 \\ p & 1-p \end{Bmatrix}, \quad p \in (0, 1)$$

with the information matrix

$$M(\xi^{(0)}) = \begin{bmatrix} 1 & 1-p \\ 1-p & 1-p \end{bmatrix}.$$

Applying the mapping $\mathcal{T}$ (defined for the A-optimality) to the design $\xi^{(0)}$, we have

$$\xi^{(1)} = \left\{ \begin{matrix} 0 \\ \left(p \dfrac{\operatorname{trace}[f^{\mathrm{T}}(0) M^{-2}(\xi^{(0)}) f(0)]}{\operatorname{trace} M^{-1}(\xi^{(0)})} \right) \end{matrix} \quad \begin{matrix} 1 \\ \left((1-p) \dfrac{\operatorname{trace}[f^{\mathrm{T}}(1) M^{-2}(\xi^{(0)}) f(1)]}{\operatorname{trace} M^{-1}(\xi^{(0)})} \right) \end{matrix} \right\}$$

After some algebra, we get

$$\xi^{(1)} = \left\{ \begin{matrix} 0 \\ \left(\dfrac{2-2p}{2-p} \right) \end{matrix} \quad \begin{matrix} 1 \\ \left(\dfrac{p}{2-p} \right) \end{matrix} \right\}$$

and the corresponding FIM takes the form

$$M(\xi^{(1)}) = \begin{bmatrix} 1 & \dfrac{p}{2-p} \\ \dfrac{p}{2-p} & \dfrac{p}{2-p} \end{bmatrix}.$$

If only p lies inside the interval $(0, 1)$, then matrices $M(\xi^{(0)})$ and $M(\xi^{(1)})$ are nonsingular. Now it is easy to check that

$$\operatorname{trace} M^{-1}(\xi^{(0)}) = \frac{2-p}{p-p^2} = \operatorname{trace} M^{-1}(\xi^{(1)})$$

so mapping $\mathcal{T}$ gives no decrease in the value of $\Psi[M(\xi)] = \operatorname{trace} M^{-1}(\xi)$. Moreover, further computations show, that

$$\xi^{(2)} = \mathcal{T}(\mathcal{T}\xi^{(0)}) = \mathcal{T}\xi^{(1)} = \xi^{(0)}.$$

If $p \neq 2 - \sqrt{2}$ then oscillations between two non-optimal designs are observed and consequently the mapping $\mathcal{T}$ does not lead to convergence. However, it can be shown that the function $\operatorname{trace} M^{-1}(\alpha\xi^{(k)} + (1-\alpha)\xi^{(k+1)})$ whose explicit form is

$$\Psi(\alpha; p) = \frac{(p-2)(2\alpha - 4\alpha p + \alpha p^2 + 2)}{(2\alpha - 4\alpha p + \alpha p^2 + p)(-2 + 2p + 2\alpha - 4\alpha p + \alpha p^2)}$$

has a local minimum at the point

$$\alpha^\star = \frac{\sqrt{2}(2-p) - 2}{2 - 4p + p^2}$$

which lies inside the interval $(0, 1)$.

★

The meaning of the above conclusion is that not for every criterion it is possible to extremely simplify the iterative procedure which determines the optimal experimental effort. If this is not the case, then we can come back to Algorithm 3.2 in its general form.

Reduction of the measurement space. It is clear that the numerical complexity of the considered class of algorithms depends linearly on the number of admissible support points belonging to the set X, i.e. on the power of this set. Note that the choice of the initial weights for Algorithm 3.3 is not crucial for the convergence, but no weights can be equal to zero, because it would be then impossible to change them. This simple observation may lead to a significant improvement, since if during the run of the procedure a weight achieves a value close to zero, it is rather impossible that it will be increased in next iterations. Deletion of such points significantly decreases the number of admissible locations in consecutive steps of the algorithm and thus it increases the efficiency. To assure that the weight values sum up to unity, we modify them e.g. according to the formula

$$p_{i\ \text{new}} = p_{i\ \text{old}} + \frac{\sigma}{|N_m|}, \quad i \in N_m \tag{3.29}$$

where σ is the sum of the weights of deleted points, N_m is the set containing the indices of the points which remain in the design and $|N_m|$ is the cardinality of N_m. Since this is connected with a very low numerical cost, the general effect is very beneficial.

There exist other possibilities for a further reduction of the computational burden while determining optimal sensor locations, but they are not that obvious and easy to interpret. For example, based on some matrix algebra dependencies it can be shown that for the D-optimality the following result can be helpful (Pronzato, 2003):

Proposition 3.2. *Let X be some finite design space, $X = \{x^i \in \mathbb{R}^d,\ i = 1, \ldots, \ell\}$, and $\xi^{(k)}$ be any design measure on X, with*

$$\epsilon_k = \max_{x^i \in X} \phi(x^i, \xi^{(k)}) - m. \tag{3.30}$$

Then any point x^i such that

$$\phi(x^i, \xi^{(k)}) < mr(\epsilon_k) \tag{3.31}$$

with

$$r(\epsilon) = 1 + \frac{\epsilon}{2} - \frac{\sqrt{\epsilon(4+\epsilon)}}{2} \tag{3.32}$$

cannot be a support point of a D-optimum design measure on X.

Proof. The generalization of the proof given by Pronzato (2003) for the multi-output case is straightforward and since the proof has a rather technical character, it is omitted. ■

When using any algorithm of D-optimum design, one can thus remove all the points satisfying (3.31) from the design space X in each iteration. Clearly, the acceleration that can be expected depends on the employed algorithm and the cardinality of X. Removing support points based on Proposition 3.2 implies some additional computations. Consequently, the best results can be obtained for the high power of the set X, otherwise the gain might not compensate the additional computational effort and a deceleration of the procedure may occur.

Approach based on Semi-Definite Programming (SDP). One more approach is proposed here since it makes it possible to employ very powerful algorithms for convex optimization based on Linear Matrix Inequalities (LMI's) or, more generally, on Semi-Definite Programming (SDP) which has recently become a dynamically expanding research area. The SDP problem can be regarded as an extension of linear programming where the component-wise inequalities between vectors are replaced by matrix inequalities, or equivalently, the first orthant is replaced by the cone of positive semidefinite matrices. Most interior-point methods for linear-programming have been generalized to semidefinite programs (Sturm, 1997). As in linear programming, these methods have polynomial worst-case complexity, and perform very well in practice. SDP has been successfully applied in engineering (from control theory to structural design) and combinatorial optimization (Boyd *et al.*, 1994; Sturm, 1997; Dullerud and Paganini, 2000; Du and Xie, 2002; Boukas and Liu, 2003; Boyd and Vandenberghe, 2004).

Although potential applications of SDP in optimum experimental design were indicated in (Vandenberghe and Boyd, 1998), the idea has not been pursued in the optimum experimental design community. In what follows, we present how to implement Vandenberge and Boyd's concept in the context of sensor location on finite support sets. Its decided advantage contrary to the standard experiment design techniques is a possibility of solving problems for a wide class of design

criteria, even for those which are non-differentiable (e.g. the E-optimality criterion). In such a way this novel formulation creates a very attractive alternative for classical approaches to the optimization of the experimental effort.

Particularly, the problem (3.9)–(3.10) can be formulated in terms of the SDP (Boyd and Vandenberghe, 2004) as follows:

D-optimal design. For the determinant criterion, the considered convex weight optimization problem can be formulated as follows: Minimize

$$\Psi_p(p_1, \ldots, p_\ell) = \ln\det M^{-1}(\xi) \tag{3.33}$$

subject to

$$p_i \geqslant 0, \quad i = 1, \ldots, \ell, \quad \sum_{i=1}^{\ell} p_i = 1, \tag{3.34}$$

and

$$M(\xi) = \sum_{i=1}^{\ell} p_i G(x^i) G^{\mathrm{T}}(x^i). \tag{3.35}$$

With no loss of generality, all covariance matrices were set to identity. In some situations it is convenient and just simpler to solve the problem operating on the convex space of admissible information matrices $\mathfrak{M}$, rather than on the design space $\Xi(X)$ itself (e.g. if the number of parameters is low compared with the cardinality of $\Xi(X)$, i.e. $m \ll \ell$).

It can be shown (Vandenberghe and Boyd, 1996a) that by introducing the Lagrange dual function

$$g(\lambda, \nu) = \min_{p_i,\, i=1,\ldots,\ell} \left\{ \ln\det M^{-1}(\xi) + \sum_{i=1}^{\ell} \lambda_i p_i + \nu \left(\sum_{i=1}^{\ell} p_i - 1 \right) \right\}, \tag{3.36}$$

where $\lambda = (\lambda_1, \ldots, \lambda_\ell)$ and ν are the Lagrange multipliers associated with the inequality and equality constraints in (3.34), respectively, the problem can be converted to the following dual problem (Vandenberghe and Boyd, 1996a; Boyd and Vandenberghe, 2004): Maximize

$$\Psi(M) = \ln\det M \tag{3.37}$$

subject to

$$\operatorname{trace} G(x^i) M G^{\mathrm{T}}(x^i) \leqslant 1, \; i = 1, \ldots, \ell, \tag{3.38}$$

which is a convex problem with the variable $M = M(\xi)$ defined on the cone of positive definite matrices $\mathbb{S}_+^m$. The interpretation of the dual problem in the case of single output systems is very clear, namely the optimal solution $M^\star$ determines the minimum volume ellipsoid, centred at the origin, given

by $\Theta_D = \{\theta : \theta^{\mathrm{T}} M^\star \theta \leqslant 1\}$, that contains the points $G(x^1), \ldots, G(x^\ell)$. The return to the primal problem can be done by the complementary slackness,

$$p_i^\star \big(1 - \operatorname{trace} G^{\mathrm{T}}(x^i) M^\star G(x^i)\big) = 0, \quad i = 1, \ldots, \ell, \tag{3.39}$$

that is, the optimal experiment strategy contains only those locations which lie on the surface of the minimum volume ellipsoid Θ_D.

A-optimal design. By analogy, for other criteria the suitable problem reformulation can also be performed. Thus, the A-optimal experimental design problem can be cast as that of minimizing

$$\Psi_p(p_1, \ldots, p_\ell) = \operatorname{trace} M^{-1}(\xi) \tag{3.40}$$

subject to

$$p_i \geqslant 0, \ i = 1, \ldots, \ell, \quad \sum_{i=1}^{\ell} p_i = 1, \tag{3.41}$$

where $M(\xi)$ is defined by (3.35). This problem can be converted into the following equivalent SDP one (Vandenberghe and Boyd, 1996b): Minimize

$$\Psi_u(u) = \sum_{i=1}^{\ell} u_i \tag{3.42}$$

subject to

$$\begin{bmatrix} M(\xi) & I \\ I & \operatorname{diag}(u) \end{bmatrix} \geqslant 0, \quad p_i \geqslant 0, \ i = 1, \ldots, \ell, \quad \sum_{i=1}^{\ell} p_i = 1. \tag{3.43}$$

with variables $u \in \mathbb{R}^m$ and $p \in \mathbb{R}^\ell$.

The dual problem in this case has the following form (Vandenberghe and Boyd, 1996b; Boyd and Vandenberghe, 2004): Maximize

$$\Psi(M) = (\operatorname{trace} M^{1/2})^2 \tag{3.44}$$

subject to

$$\operatorname{trace} G(x^i) M G^{\mathrm{T}}(x^i) \leqslant 1, \ i = 1, \ldots, \ell, \quad M \geqslant 0, \tag{3.45}$$

where $M = M(\xi) \in \mathbb{S}_+^m$. As for the D-optimal design, for single response systems the optimal solution $M^\star$ determines a minimal ellipsoid (in the sense of its average widths along the principal directions) consisting points $G(x^1), \ldots, G(x^\ell)$. The quantities $p^\star$ and $M^\star$ also satisfy the condition (3.39), so the dual problem can be easily reverted to the primal one.

E-optimal design. For E-optimal designs, the norm of the parameter covariance matrix estimate is minimized, i.e. the maximum eigenvalue of the FIM inverse. Since the diameter of the parameter confidence ellipsoid is proportional to $\|M^{-1}(\xi)\|_2^{1/2}$, the primal problem can be cast as follows: Minimize

$$\Psi_p(p_1,\ldots,p_\ell) = \|M^{-1}(\xi)\|_2 \tag{3.46}$$

subject to

$$p_i \geqslant 0,\ i=1,\ldots,\ell, \quad \sum_{i=1}^{\ell} p_i = 1. \tag{3.47}$$

It can be reformulated as an SDP problem by considering minimization of (Boyd and Vandenberghe, 2004)

$$\Psi_v(v) = v \tag{3.48}$$

subject to

$$M(\xi) \geqslant vI, \quad p_i \geqslant 0,\ i=1,\ldots,\ell, \quad \sum_{i=1}^{\ell} p_i = 1. \tag{3.49}$$

Then, the dual problem takes the form (Boyd and Vandenberghe, 2004): Maximize

$$\Psi(M) = \operatorname{trace} M \tag{3.50}$$

subject to

$$\operatorname{trace} G(x^i) M G^{\mathrm{T}}(x^i) \leqslant 1,\ i=1,\ldots,\ell, \quad M \geqslant 0, \tag{3.51}$$

where $M = M(\xi)$. This formulation of the E-optimum experimental design enables us to employ efficient numerical algorithms for solving convex optimization problems over LMI's. This is extremely important because of the fact that due to the non-differientiability of the criterion, no such algorithms have been proposed in the optimum experimental design community.

Sensitivity criterion. For this very simple case the original problem constitutes the SDP formulation per se (this is because it is a linear programming task): Maximize

$$\Psi_p(p_1,\ldots,p_\ell) = \operatorname{trace} M(\xi) \tag{3.52}$$

subject to

$$p_i \geqslant 0,\ i=1,\ldots,\ell, \quad \sum_{i=1}^{\ell} p_i = 1, \tag{3.53}$$

and the corresponding dual problem is as follows: Minimize

$$\Psi_v(v) = v \tag{3.54}$$

subject to

$$\sum_{j=1}^{m} G_j(x^i) G_j^{\mathrm{T}}(x^i) \leqslant v - z_i, \quad i = 1, \ldots, \ell, \quad z_i \geqslant 0, \tag{3.55}$$

where G_j denotes the j-th row of the matrix $G(x^i)$.

At this juncture it could be expedient to present a suitable example to illustrate the benefits of the SDP formulation of the problem. However, since the advantages of such an approach lie in the powerful numerical algorithms dedicated to more complex tasks, an appropriate example will be given in Section 3.4 devoted to practical applications.

3.2.2. Clusterization-free designs

The assumption of independent observations is advantageous from a theoretical point of view, but it can hardly be justified when in an optimal solution several sensors are to take measurements near one another (this phenomenon was indicated earlier as a *sensor clusterization* effect (Fedorov, 1996; Müller, 1998; Uciński, 1999a)). Indeed, in the spatial data collection schemes there is usually no possibility of replicated measurements, i.e. different sensors cannot take measurements at one point without influencing one another. In addition to this, classical optimum experimental design techniques do not take into account local correlations which determine the spatial locations of measurements. Anyway, several sensors situated in the close vicinity of one another usually do not give more information than a single sensor.

In order to avoid such clustered sensor configurations, we can adopt the idea of operating on the density of sensors (Fedorov, 1989; Cook and Fedorov, 1995; Fedorov and Hackl, 1997) (i.e. the number of sensors per unit area), rather than on the sensor locations, which is justified when the total number of sensors N is sufficiently large. In contrast to the designs discussed in the previous section, however, the crucial restriction is imposed that the density of sensor allocation must not exceed some prescribed level. This corresponds to the condition

$$\xi(\mathrm{d}x) \leqslant \omega(\mathrm{d}x), \tag{3.56}$$

where $\omega(\mathrm{d}x)$ signifies the maximal possible 'number' of sensors per $\mathrm{d}x$ (Fedorov and Hackl, 1997) such that

$$\int_X \omega(\mathrm{d}x) \geqslant 1. \tag{3.57}$$

Introducing a performance measure Ψ, the following optimization problem can be formulated:

$$\xi^\star = \arg\min_{\xi \in \Xi} \Psi[M(\xi)] \tag{3.58}$$

subject to

$$\xi(\mathrm{d}x) \leqslant \omega(\mathrm{d}x). \tag{3.59}$$

Definition 3.1. The design $\xi^\star$ corresponding to the solution of the problem (3.58)–(3.59) formulated above is said to be a (Ψ, ω)**-optimal design** (Fedorov and Hackl, 1997).

To precise some valuable properties of the designs so defined, in addition to Assumptions (A1)–(A6) it is necessary to impose the following restriction:

(A7) $\omega(\mathrm{d}x)$ is atomless, i.e. for any $\Delta X \subset X$ there exists a $\Delta X' \subset \Delta X$ such that

$$\int_{\Delta X'} \omega(\mathrm{d}x) < \int_{\Delta X} \omega(\mathrm{d}x). \tag{3.60}$$

In what follows, we write $\bar{\Xi}(X) \subset \Xi(X)$ for the collection of all the design measures which satisfy the requirement

$$\xi(\Delta X) = \begin{cases} \omega(\Delta X) & \text{for } \Delta X \subset \operatorname{supp} \xi, \\ 0 & \text{otherwise.} \end{cases} \tag{3.61}$$

Definition 3.2. For any given design ξ, we will say that the function $\psi(\,\cdot\,, \xi)$ defined by (2.58) **separates** sets X_1 and X_2 with respect to $\omega(\mathrm{d}x)$ if for any two sets $\Delta X_1 \subset X_1$ and $\Delta X_2 \subset X_2$ with equal non-zero measures we have

$$\int_{\Delta X_1} \psi(x, \xi)\, \omega(\,\mathrm{d}x) \leqslant \int_{\Delta X_2} \psi(x, \xi)\, \omega(\,\mathrm{d}x). \tag{3.62}$$

It is then possible to formulate the main result which provides a characterization of (Ψ, ω)-optimal designs.

Theorem 3.3. *Let Assumptions (A1)–(A7) hold. Then:*

(i) There exists an optimal design $\xi^\star \in \bar{\Xi}(X)$, and

(ii) A necessary and sufficient condition for $\xi^\star \in \bar{\Xi}$ to be (Ψ, ω)-optimal is that $\psi(\,\cdot\,, \xi^\star)$ separates $X^\star = \operatorname{supp} \xi^\star$ and its complement $X \setminus X^\star$ with respect to the measure $\omega(\mathrm{d}x)$.

Proof. The results of the theorem are strongly related to the theory of moment spaces and since for the case of static MIMO DPS's investigated here the result constitutes a direct adaptation of Theorem 4.3.1 of (Fedorov and Hackl, 1997, p. 63), it is omitted. Comprehensive ideas of the proof can also be found in (Cook and Fedorov, 1995, p.64). ■

From a practical point of view, Theorem 3.3 means that at all the support points of an optimal design $\xi^\star$ the mapping $\psi(\,\cdot\,, \xi^\star)$ should be less than anywhere else, i.e. preferably $\operatorname{supp} \xi^\star$ should coincide with minimum points of $\psi(\,\cdot\,, \xi^\star)$, which

amounts to allocating observations to the points at which we know least of all about the system response.

If we were able to construct a design with this property, then it would be qualified as an optimal design. This conclusion forms a basis for numerical algorithms of constructing solutions to the problem under consideration.

As regards the interpretation of the resultant optimal designs (provided that we are in a position to calculate at least their approximations), one possibility is to partition X into subdomains ΔX_i of relatively small areas and then to allocate to each of them the number

$$N^\star(\Delta X_i) = \left\lceil N \int_{\Delta X_i} \xi^\star(\mathrm{d}x) \right\rceil \tag{3.63}$$

of sensors whose positions may coincide with nodes of some uniform grid (here $\lceil \zeta \rceil$ denotes the least integer greater than or equal to ζ). This grid can consist e.g. of points at which sensors may be located, which will be exploited in what follows.

Clearly, unless the considered design problem is quite simple, we must employ a numerical algorithm to make the outlined concept useful. Theorem 3.3 allows us to develop a simple iterative procedure for constructing optimal designs. Since $\xi^\star(\mathrm{d}x)$ should be non-zero in the areas where $\psi(\,\cdot\,, \xi^\star)$ takes on a smaller value, the central idea is to move some measure from areas with higher values of $\psi(\,\cdot\,, \xi^{(k)})$ to those with smaller values, as we expect that such a procedure will improve $\xi^{(k)}$. This idea is implemented in the following iterative algorithm (Fedorov and Hackl, 1997; Uciński, 1999a):

Algorithm 3.4. *Clusterization-free sensing algorithm*

Step 1. Guess an initial design $\xi^{(0)} \in \bar{\Xi}(X)$. Set $k = 0$.

Step 2. Set $X_1^k = \operatorname{supp} \xi^{(k)}$ and $X_2^k = X \setminus X_1^k$. Determine

$$x_1^k = \arg \max_{x \in X_1^k} \psi(x, \xi^{(k)}), \qquad x_2^k = \arg \min_{x \in X_2^k} \psi(x, \xi^{(k)}).$$

If $\psi(x_1^k, \xi^{(k)}) > \psi(x_2^k, \xi^{(k)}) + \epsilon$, where $\epsilon \ll 1$, then find two sets $S_1^k \subset X_1^k$ and $S_2^k \subset X_2^k$ such that $x_1^k \in S_1^k$, $x_2^k \in S_2^k$ and

$$\int_{S_1^k} \omega(\mathrm{d}x) = \int_{S_2^k} \omega(\mathrm{d}x) = \alpha_k$$

(i.e. the measures of S_1^k and S_2^k must be identical) for some $\alpha_k > 0$. Otherwise *STOP*.

Step 3. Construct $\xi^{(k+1)}$ such that

$$\operatorname{supp} \xi^{k+1} = X_1^{k+1} = (X_1^k \setminus S_1^k) \cup S_2^k.$$

Increment k and go to Step 2.

♦

Convergence is guaranteed if the sequence $\{\alpha_n\}_{n=0}^{\infty}$ satisfies the conditions

$$\lim_{k\to\infty} \alpha_k = 0, \quad \sum_{k=0}^{\infty} \alpha_k = \infty, \tag{3.64}$$

which is established in much the same way as in (Fedorov, 1989).

Within the framework of sensor placement, we usually have $\omega(\mathrm{d}x) = \varrho(x)\mathrm{d}x$, where ϱ is a density function. But in this situation we may restrict our attention to constant ϱ's (in fact, there always exist a possibility of proposing an appropriate transformation of coordinates). Moreover, while implementing the algorithm on a computer, all integrals are replaced by sums over some regular grid elements. Analogously, the sets X, X_1^k, X_2^k, S_1^k and S_2^k then simply consist of grid elements (or potential sensor locations). Consequently, the above iterative procedure may be considered as an exchange-type algorithm with the additional constraint that every grid element must not contain more than one supporting point and the weights of all supporting points are equal to $1/N$. In practice, α_n is usually fixed and, what is more, one-point exchanges are most often adopted, i.e. $S_1^k = \{x_1^k\}$ and $S_2^k = \{x_2^k\}$, which substantially simplifies implementation. Let us note, however, that convergence to an optimal design is assured only for decreasing α_n's and hence some oscillations in $\Psi[M(\xi^{(k)}]$ may sometimes be observed. A denser spatial grid usually constitutes a remedy for this predicament (Müller, 1998).

As a verification and practical illustration of the the proposed approach, an appropriate example should be considered to bring some overview of ideas and performance of the algorithm.

Example 3.3. Consider the problem of determining the electrostatic potential y on a disc centred at the origin with unit radius $\Omega = \{(x_1, x_2) : x_1^2 + x_2^2 < 1\}$ (cf. Fig. 3.2) with homogeneous coefficient of dielectricity equal to θ_1. The boundary of the disc is grounded, i.e the potential is equal to zero. The density of the charge in the domain can be modelled via a function $q(x) = 1 - 7x_1^2 - x_2^2 - 2\theta_2^2$. This leads to the problem of solving Poisson's equation

$$\nabla \cdot (\theta_1 \nabla y(x)) = q(x), \quad x \in \Omega, \tag{3.65}$$

subject to the Dirichlet boundary conditions

$$y(x) = 0, \quad x \in \partial\Omega. \tag{3.66}$$

We wish to find the best D-optimal design to identify the coefficient of dielectricity and the free term of the force function or, more precisely, the vector of coefficients $\theta = (\theta_1, \theta_2)$, based on the clusterization-free strategy. Our aim is to select the best 51 sensor locations from among 149 admissible points which constitute the (15×15)-point uniform grid lying inside the domain Ω (see Fig. 3.2, where the dots represents the possible locations and the open circles actual sensor positions). The clusterization-free sensing algorithm, once implemented using the Lahey/Fujitsu Fortran 95 v.5.6 compiler and then applied to this problem, found a solution in only 53 iterations for the accuracy $\epsilon < 10^{-5}$ in a negligible time (below 1 sec. on a

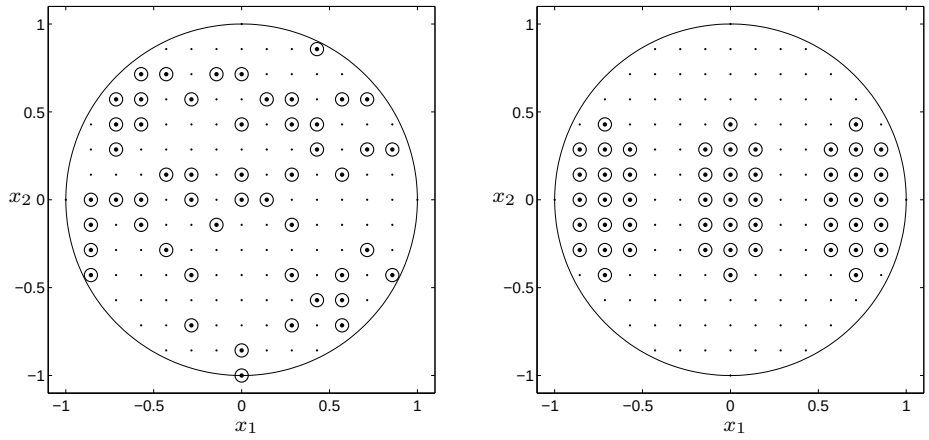


Fig. 3.2. D-optimal clusterization-free strategy for Example 3.3: (a) initial design, (b) optimal solution.

PC equipped with Duron 900 MHz processor and running under Windows 2000). The randomly generated initial design and the obtained best sensor placement are shown in Figs. 3.2(a) and (b), respectively.

To compare the performance of routines, the weight optimization algorithm has been also applied to the problem so defined. Starting from randomly generated weights, after only 95 iterations for an accuracy of $\epsilon \leqslant 10^{-5}$ and the same simulation environment, Algorithm 3.3 reached the approximated optimum design

$$\xi^\star \approx \left\{ \begin{matrix} (-0.714, 0.000) & (0.000, 0.000) & (0.714, 0.000) \\ 0.250 & 0.500 & 0.250 \end{matrix} \right\} \tag{3.67}$$

in a blink of an eye, cf. Fig. 3.3. It is now clear that the sensors located in accordance with the clusterization-free strategy tend to assemble in the vicinity of the points calculated based on the replication design approach. In both the cases the symmetry of the problem with respect to the coordinate axes is perfectly retained.

On the other hand, the problem defined by (3.65) and (3.66) possesses the closed-form solution

$$y(x_1, x_2) = -\frac{1}{2\theta_1}(x_1^2 + \theta_2^2)(1 - x_1^2 - x_2^2). \tag{3.68}$$

Now, it can be easily shown that the design

$$\xi^\star = \left\{ \begin{matrix} (-\frac{\sqrt{2}}{2}, 0) & (0, 0) & (\frac{\sqrt{2}}{2}, 0) \\ \frac{1}{4} & \frac{1}{2} & \frac{1}{4} \end{matrix} \right\} \tag{3.69}$$

is D-optimal. Its comparison with (3.67) clearly proves the quality of the numerical results and the efficiency of the proposed algorithms. Investigating further, we

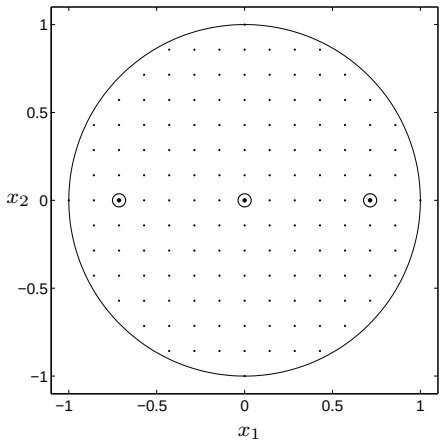


Fig. 3.3. D-optimal experimental design with replications allowed.

deduce that due to the symmetry of the problem, any design of the form

$$\left\{ \begin{array}{ccc} (-\frac{\sqrt{2}}{2}, 0) & (0,0) & (\frac{\sqrt{2}}{2}, 0) \\ \alpha & \frac{1}{2} & \frac{1}{2} - \alpha \end{array} \right\}, \quad 0 \leqslant \alpha \leqslant \frac{1}{2} \tag{3.70}$$

is also D-optimal! This is an immediate consequence of the fact that the solution is not unique and the set of optimal designs is not necessarily finite. In addition to that, there exists a D-optimal design with $m = 2$ support points and equal weights, which is compatible with theory.

★

3.3. Continuous case

Although the algorithms proposed so far are quite efficient and simple, they operate only on a finite set of available support points, and for some problems this approach may be too restrictive, especially for the case when the measurement domain is continuous. To increase the quality of the approximated solutions, some systematic algorithms are necessary, which operate on the continuous set of points where the measurements may be taken. Fortunately, the characterization constituting the general equivalence theorem from Section 2.3.2 indicates some ideas useful in construction of sequential numerical algorithms. The underlying reasoning relies on a correction of a non-optimal design $\xi^{(k)}$ obtained after k iterations by convex combination with another design $\xi_+^{(k)}$, which hopefully improves the current solution, i.e.

$$\xi^{(k+1)} = (1 - \alpha_k)\xi^{(k)} + \alpha_k \xi_+^{(k)} \tag{3.71}$$

for some convenient α_k.

In this manner the experimental effort related to the design $\xi^{(k)}$ is reduced, and instead, the measurements at some locations corresponding to the design $\xi_+^{(k)}$ are taken. The question is: How to find a suitable design $\xi_+^{(k)}$ which would guarantee a better value of the optimality criterion? The answer is indicated by Theorem 2.8. First, recall the fact that the points of the optimum design $\xi^\star$ coincide with the maxima of the function $\psi(x,\xi^\star)$. In such a way, by addition of an appropriate design measure to the maxima of $\psi(x,\xi)$, an improvement in the current design can be expected. Indeed, if we take into account one-point designs $\xi_+^{(k)} = \{{x \atop 1}\}$, then combining Lemmas 2.7 and 2.6, we have that the directional derivative is negative, i.e.

$$\left.\frac{\partial \Psi[M(\xi^{(k+1)})]}{\partial \alpha_k}\right|_{\alpha_k=0+} = \varsigma(\xi_k) - \phi(x,\xi_k) < 0 \tag{3.72}$$

which yields a decrease in the value of $\Psi[M(\xi^{(k+1)})]$ for a sufficiently small α_k.

First-order algorithm for a general case. The sequential numerical design algorithms based on the ideas indicated above, which have been continually refined since the early 1960s, can be employed with some modifications to the sensor locations problem for parameter estimation. The general form of the one-point correction version of the delineated procedure can be embodied in the following scheme (Ermakov, 1983; Rafajłowicz, 1996; Fedorov and Hackl, 1997; Walter and Pronzato, 1997; Uciński, 1999a):

Algorithm 3.5. *General first-order algorithm*

Step 1. Let $\xi^{(0)}$ be any non-degenerate design measure. Set $k = 0$. Choose some positive tolerance $\epsilon \ll 1$.

Step 2. Find $x^k = \arg\max_{x\in X} \phi(x,\xi^{(k)})$.

Step 3. If $\phi(x^k,\xi^{(k)}) \leqslant \varsigma(\xi^{(k)}) + \epsilon$ then STOP.

Step 4. For an appropriate value of $0 < \alpha_k < 1$, set

$$\xi^{(k+1)} = (1-\alpha_k)\xi^{(k)} + \alpha_k \xi(x^k)$$

where $\xi(x^k)$ is the design with only one support point x^k and weight equal to 1. Increment k by one and go to Step 2.

♦

On the analogy of Algorithm 3.2 dedicated to finite measurement spaces, it can be shown that the suitable choice of the sequence $\{\alpha_k\}$ guarantees the convergence of Algorithm 3.5. Common versions of the algorithm depending on the choice of $\{\alpha_k\}$ are (Fedorov and Hackl, 1997; Uciński, 1999a):

(a) Wynn's formula

$$\lim_{k\to\infty} \alpha_k = 0, \quad \sum_{k=0}^{\infty} \alpha_k = \infty, \tag{3.73}$$

(b) Fedorov's formula

$$\alpha_k = \arg\min_{\alpha} \Psi\big[(1-\alpha)M(\xi^{(k)}) + \alpha M(\xi(x^k))\big], \tag{3.74}$$

(c) adaptation formula

$$\alpha_k = \begin{cases} \alpha_{k-1} & \text{if } \Psi[(1-\alpha_{k-1})M(\xi^{(k)}) + \alpha_{k-1}M(\xi(x^k))], \\ \gamma\alpha_{k-1} & \text{otherwise,} \end{cases} \tag{3.75}$$

where $\gamma < 1$ is suitably chosen.

Note that Algorithm 3.5 makes use of only information about the gradient of the performance index and the rule (3.74) results in the steepest-descent algorithm. The conclusion is that the convergence rate of the presented numerical technique is comparable with its gradient counterparts from mathematical programming. That is, typically, a significant decrease in the performance index measure in the first few iterations is observed and then serious moderation of the convergence rate occurs as the minimum is approached. Some second-order generalizations of Algorithm 3.5 are possible for specific criteria (Ermakov and Zhigljavsky, 1987), but they involve a high complexity of implementation and are connected with an improvement in the design weights, rather than the support points and in this context the characteristics of the first-order algorithm are satisfactory as the most significant support points are usually found in just few iterations.

From the point of view of this dissertation the decided advantage of Algorithm 3.5 is a possiblity of its extension to the field of optimum experimental design for the wide class of DPS's mentioned above. However, such an adaptation and further efficiency improvements require a little more comprehensive disscusion about the implementation details.

Implementation details. Despite the fact that the above procedure offers a higher level of freedom regarding optimality in comparison with the algorithms dedicated to the discrete case, it still suffers from disadvantageous effects such as high numerical complexity and clusterization of support points. Therefore the general first-order algorithm does not solve all the theoretical and technical problems which can be encountered in the area of DPS's and its applicability is far from being trivial. While implementing the algorithm, various problems should be addressed. The main of them are listed below:

1. In literature some improvements of the first-order algorithm can be found, whose intention is to increase the convergence rate.

   (a) One of them is the idea of adding in each iteration all points which coincide with the maxima of $\phi(x, \xi^{(k)})$. Such an approach in the context of DPS's demands global maximization in multi-dimensional spaces. Such an adaptation is connected with a dramatically increased numerical complexity. Because of this, the multi-point correction is rather unavailable and not suggested.

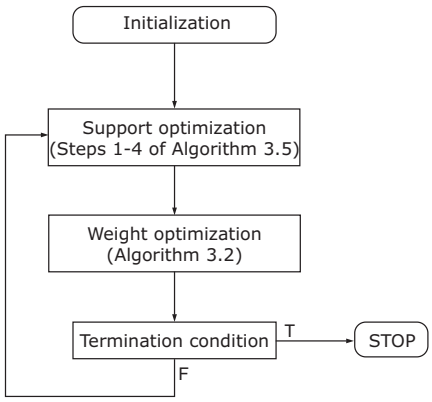


Fig. 3.4. Scheme of the two-phase design optimization algorithm.

(b) Inverting the underlying idea of Algorithm 3.5, it is possible to achieve an additional decrease in the performance index by removing some design measure from noninformative support points of the design $\xi^{(k)}$ and distributing this measure among the other design points. This leads to an accelerated version of the algorithm consisting in the simultaneous addition of potentially significant support points and elimination of worthless ones from the design.

(c) In order to increase the efficiency of deleting redundant support points and to improve the quality of Step 4, the weight optimization algorithm for the discrete case can be exploited as a complement for one of the rules (3.73)–(3.75) since in Step 4 the design measure for a newly selected point is uniformly subtracted from the current support points. This leads to the procedure being a direct generalization of the two-phase design optimization algorithm proposed by Rafajłowicz (1996) for the D-optimum criterion in the case of the one-dimensional regression. The general scheme of such a routine is illustrated in Fig. 3.4.

2. While implementing various versions of Algorithm 3.5, one may encounter numerous technical problems. The main of them are the following:

(a) The added support points tend to cluster in the vicinity of the optimal ones. One of the possible simple solutions is to represent all sites in a given cluster as one support point placed in the centre of the cluster with the weight equal to the sum of the weights for all clustered sites.

(b) Step 4 requires some comment concerning the choice of an optimal factor α in the variant of the stepeest descent rule. In a general case, when multi-output systems are taken into account (or dynamic systems), the situation is slightly different from the static case of linear regression for which it is possible to determine a closed-form solution. Here an optimal α has to be found numerically and, because the searching range is

fixed, golden-section or Fibbonacci methods will cope quite fine with this task.

(c) The removal of points with negligible weights is suggested in order to obtain designs with relatively small numbers of support points (Rafajłowicz, 1996).

3. The crucial bottleneck of Algorithm 3.5 is Step 2, both from computational and implementation point of view. First of all, complications are related to the necessity of calculating a global maximum of $\phi(x, \xi)$ over all points $x \in X$. Since this function has multimodal nature and convergence can be guaranteed only if the added support point lies close to the global optimum, realization of this task becomes very difficult. Therefore, an effective global optimization procedure is required, which is crucial for efficient implementation. A major impediment while using PDE systems as DPS descriptions is that this involves a high cost of gradient evaluation, or approximations of the gradient may fail to be satisfactory (e.g. there may occur some scaling problems or insufficient smoothness of the underlying functions). Based on numerous computer experiments it was found that in order to overcome those difficulties, some procedures of the stochastic type are especially suited for many practical problems. One of the examples which was successfully exploited is the extremely simple Adaptive Random Search (ARS) strategy proposed in (Walter and Pronzato, 1997). It is dedicated to situations where the set of admissible measurement points X is a hypercube, i.e.

$$X = \{x = (x_1, \ldots, x_d) : x_{i\,\min} \leqslant x_i \leqslant x_{i\,\max}\}. \tag{3.76}$$

The adaptive strategy can be split into two stages, which are repeatedly alternated. The first is the variance selection phase which consist in selecting an element from the sequence

$$\{\sigma^{(i)}\}, \quad i = 1, \ldots, i_{\max}, \tag{3.77}$$

where

$$\sigma^{(1)} = x_{\max} - x_{\min} \tag{3.78}$$

and

$$\sigma^{(i)} = 10^{-i+1}\sigma^{(1)}. \tag{3.79}$$

In such a manner the range of σ ensures both proper exploration properties over X and a sufficient accuracy of optimum localization. Because larger values of σ decrease the possibility of getting stuck in local minima, they are used more often (see Step 2.5) than the smaller ones.

The second phase (variance exploration) is dedicated to exploring the search space with use of the most suitable value of $\sigma^{(i)}$ (in the sense of the best evaluated

point from the first phase) and consists in repetitive random perturbation of the best point obtained so far. After that the algorithm can be stopped or the first phase is resumed.

In iteration j a perturbation of the point $x^{(j)}$ is made according to the rule

$$x_+^{(j)} = \Pi_X(x^{(j)} + r^{(j)}), \tag{3.80}$$

where Π_X is the orthogonal projection operator onto X. The quantity $r^{(j)}$ is a displacement vector randomly generated according to a multinormal distribution $\mathcal{N}(0, \operatorname{cov} r^{(j)})$, where

$$\operatorname{cov} r^{(j)} = \begin{bmatrix} \sigma_1^{(i)} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \sigma_d^{(i)} \end{bmatrix}. \tag{3.81}$$

where i is selected arbitrarily.

A detailed scheme of the ARS algorithm is as follows (J stands for the optimization criterion):

Algorithm 3.6. *ARS algorithm*

Step 1. (Initialization) Choose $x^{(0)}$, $k_{\max}$, $i_{\max}$, $j_{\max}$, $\sigma^{(1)}$, and set $x_{\text{best}} = x^{(0)}$, $k = 1$, $i = 1$.

Step 2. (Variance-selection phase)

2.1. Set $j = 1$, $x^{(j)} = x^{(0)}$ and $\sigma^{(i)} = 10^{-i+1}\sigma^{(1)}$.

2.2. Perturb $x^{(j)}$ according to (3.80) to get a new trial point $x_+^{(j)}$.

2.3. If $J(x_+^{(j)}) \leqslant J(x^{(j)})$ then $x^{(j+1)} = x_+^{(j)}$ else $x^{(j+1)} = x^{(j)}$.

2.4. If $J(x_+^{(j)}) \leqslant J(x_{\text{best}})$ then $x_{\text{best}} = x_+^{(j)}$, $i_{\text{best}} = i$.

2.5. If $j \leqslant j_{\max}/i$ then increment j and go to Step 2.2.

2.6. If $i < i_{\max}$ then set $i = i + 1$ and go to Step 2.1.

Step 3. (Variance-exploitation phase)

3.1. Set $j = 1$, $x^{(j)} = x_{\text{best}}$, $i = i_{\text{best}}$ and $\sigma^{(i)} = 10^{-i+1}\sigma^{(1)}$.

3.2. Perturb $x^{(j)}$ according to (3.80) to get a new trial point $x_+^{(j)}$.

3.3. If $J(x_+^{(j)}) \leqslant J(x^{(j)})$ then $x^{(j+1)} = x_+^{(j)}$ else $x^{(j+1)} = x^{(j)}$.

3.4. If $J(x_+^{(j)}) \leqslant J(x_{\text{best}})$ then $x_{\text{best}} = x_+^{(j)}$.

3.5. If $j \leqslant j_{\max}$ then increment j and go to Step 3.2.

3.6. If $n = n_{\max}$ then STOP.

3.7. Set $n = n + 1$, $x^{(0)} = x_{\text{best}}$ and resume from Step 2.1.

♦

Since the ARS does not take into account the information about the gradient of the performance index, a significant numerical efficiency could hardly be expected. However, because of its valuable properties regarding global convergence and simplicity (even for a high-dimensional search space) it seems to be more flexible and suitable in the case of DPS's than many classical nonlinear programming approaches. Numerous practical applications show that for static DPS's such a non-gradient optimizer is very efficient. Otherwise, if the operational characteristics are not satisfactory, the performance of the ARS can be improved by combination with various other techniques, or we can employ other optimization methods, which will be indicated in the next chapter where spatio-temporal dynamic systems will be considered.

One more technical adaptation is very important and requires some comment. Usually, in practical engineering problems the continuous design space X is not a hypercube, so it may seem that the application of the ARS algorithm is rather restricted. But one valuable property of the function $\phi(x,\xi)$ comes in handy. From Lemma 2.6 we have

$$\max_{x\in X}\phi(x,\xi)\geqslant\varsigma(\xi).$$

Taking this into account, it is easy to propose a suitable procedure. For example, X can be embedded in some set H being a hypercube, i.e. $X\subseteq H$. Then some suitable penalty function can be constructed, e.g. the modified criterion

$$J(x)=\begin{cases}\phi(x,\xi) & \text{if } x\in X,\\ \varsigma(\xi) & \text{if } x\in H\setminus X\end{cases}\tag{3.82}$$

can be maximized. Since in the proposed stochastic approach the gradient is not used, the possible non-continuity of the minimized function has no influence on the performance.

It is difficult to even indicate all the existing improvements of the first-order algorithms and their implementation problems in the limited area of this section. Therefore, for a more detailed discussion the reader is referred to the relevant literature (Ermakov, 1983; Torsney, 1988; Rafajłowicz, 1996; Rafajłowicz, 1998; Fedorov and Hackl, 1997; Walter and Pronzato, 1997).

Rounding procedures. Note that except for the clusterization-free strategy, the discussed types of algorithms are oriented to calculating only approximate (continuous) designs. Namely, in the concept of approximated design measures we neglected the fact that in real experiments the number of measurements r_i to be taken at each support point x^i is integer-valued and the value of the weight $p_i=r_i/N$ is rational. Nevertheless, the number of potential support points in the spatial setting is usually quite large and the set of candidate points is continuous (in the case of Algorithm 3.5) so that we can expect that some rounding procedure (Pukelsheim and Rieder, 1992; Rafajłowicz, 1996) of the approximate designs calculated by the proposed algorithms will yield sufficiently good exact designs. In such circumstances satisfactory results can be achieved using the simple numerical

rounding

$$r_i^\star = \begin{cases} \lceil p_i N \rceil & \text{if } \lceil p_i N \rceil - p_i N \leqslant 0.5, \\ \lfloor p_i N \rfloor & \text{otherwise,} \end{cases} \tag{3.83}$$

where $\lceil a \rceil$ denotes the least integer greater than or equal to a and $\lfloor a \rfloor$ stands for the greatest integer less than or equal to a. If $\sum_{i=1}^{\ell} r_i^\star = N_r \neq N$ then the correction $(N - N_r)/N$ can be made to the weight of an arbitrary chosen support point, or alternatively, $|N - N_r|$ points can be randomly selected and their weights suitably updated.

3.4. Applications

3.4.1. Computer-assisted tomography

3.4.1.1. Background and problem description

The main aim of Computer-Assisted Tomography (CAT) is data acquisition from an inaccessible interior of an object which is examined based on exterior measurements (Black Box measurements) without any damage of the examined subject (Williams and Beck, 1995; Sikora, 2000). In general, CAT exploits various physical phenomena and data media such as photons, magnetic fields, gamma rays, X-rays, ultrasounds and finally electric currents or electron beams. Depending on the phenomenon used, the data are processed with a computer system in such a way as to obtain the appropriate map of the corresponding material parameters (Sikora, 2000; West *et al.*, 2000). For example, for X-rays it can be the coefficient of their suppression, for gamma rays the concentration of the radioactive contrast injected into the object, and finally resistance or impedance in electrical tomography.

Recently, due to its advantageous properties, Electrical Impedance Tompography (EIT) has became a major trend in many process engineering applications and scientific research. The EIT can be divided (Sikora, 2000) into resistive tomography when the examined objects are conducting (biomedicine and electronic industry), capacitive tomography when they are insulators or dielectric materials (energetic and refinery industry) and eddy-current tomography. The most significant examples can be taken from chemical and pharmaceutical industries to examine the homogeneity of a product, analysis and diagnostics in material engineering (Sikora, 2000), fluid-dynamic modelling (laminar and turbulent flows) (Lemonnier and Peytraud, 1998; West *et al.*, 2000; Kim *et al.*, 2002) or groundwater contamination control and monitoring of water reservoirs. Finally, medical applications such as the clinical problem of left venticular failure (Noble *et al.*, 1999) or diagnostics of brain aneurism (Sikora, 2000) can be citied. The main benefits from using EIT are as follows:

- non-invasiveness of the low-density currents,
- high sensitivity,

- maintenance security,
- small costs of instrumentation and its exploitation, and
- portability of devices.

However, the nonlinear trajectories of data carrier movements (e.g. electrons) in EIT result in complex algorithms of image reconstruction.

The impedance tomography is a two-step process (Lemonnier and Peytraud, 1998; Sikora, 2000). The experiment provides the data which characterize the electrical response of a two-phase medium and in the second step the distribution of the electrical properties is reconstructed from these data. Consequently, two problems can be distinguished. The first is the so-called *forward* (or direct) problem, which comprises the determination of the field potential distribution over a given domain Ω with suitable boundary conditions and full knowledge about the considered domain. Since both the resistive and the capacitive tomography have similar formulations, resistive EIT can be addressed here with no loss of generality. Therefore, the forward problem is described in the simplest case by the Laplace equation (Lemonnier and Peytraud, 1998; Kim *et al.*, 2002)

$$\nabla \cdot (\sigma(x) \nabla y(x)) = 0, \quad x \in \Omega, \tag{3.84}$$

where y is the electrical potential and σ is the conductivity coefficient. Equation (3.84) is supplemented by Dirichlet boundary conditions at those point of the boundary $\partial\Omega$ which are contiguous with the electrodes and von Neumann boundary conditions on the rest of $\partial\Omega$.

EIT inversion consist in solving the second problem, the so-called *inverse* problem, defined for material parameters, (in this case the conductivity coefficient of distributed type). For a given potential distribution over the boundary, a suitable form of $\sigma(x)$ is constructed based on some lack-of-fit criterion defining the discrepancy between the modelled and measured responses. The reconstruction techniques can be split into three main groups (West *et al.*, 2000):

- *Pixel-based tomography*, in which the picture is represented by an array of pixel values. This technique has enjoyed much success in medical applications. However, it is well known that such an approach is ill-conditioned and regularization is required. In the presence of significant measurement noise such regularization may be very complicated and solutions cannot be reliable. Additionally, it is difficult to obtain a large amount of linearly independent measurements, which results in a relatively low picture resolution. This substantially reduces the range of possible applications.
- The *parametric-model approach*. The object image can be modelled here to produce a parameterization of the tomogram, thereby providing a suitable regularization. The general philosophy is to incorporate those features of the object for which the tomogram is elucidated. Thus, the parameters identified during reconstruction are exactly those necessary for image interpretation. In such a way, the computational effort is efficiently spent. Nevertheless, it

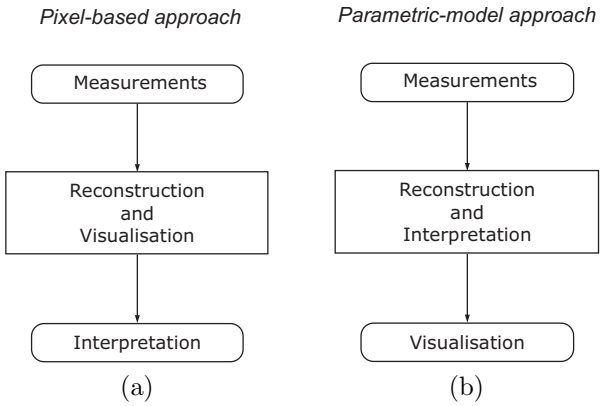


Fig. 3.5 . Schemes illustrating differences between the reconstruction approaches: (a) pixel-based and (b) parametric-model methods.

should be emphasized that the assumed model of the object is crucial for this technique. Hence, it is necessary to properly analyse the industrial process or the object properties.

- The *general basis-function approach* being an intermediate solution connecting the two techniques mentioned above. The tomogram could be built upon basis functions (Vauhkonen *et al.*, 1997), which suit the geometry of the problem or the geometry of boundaries and additionally provide some regularization of the reconstruction problem. The weights of the basis functions (e.g. wavelets) stand for the unknown parameters which have to be estimated, but have no particular interpretation in terms of the investigated object characterizations.

Figure 3.5 illustrates the differences between the techniques listed above. The pixel-based approach is directly linked to image reconstruction and visualisation. The interpretation is often based on the displayed tomogram (e.g. in medical applications), however it is impractical in some applications such as automated process control, especially where the tomograms have to be interpreted on-line. In the parametric-model approach there is a direct connection between the interpretation and reconstruction which makes this approach interesting in industrial applications. Nevertheless, it is clear that the quality of parameter estimators has a crucial significance for the reconstruction accuracy.

At this point it should be stressed that real applications involve most often fully three-dimensional models. This leads to the requirement of significant computational power in the process of numerically solving the problems involved. Notwithstanding those facts, such sophisticated situations do not possess the asset of illustrative presentation. On the other hand, the methodology used within the framework of this thesis does not demand any changes when increasing the problem dimensionality. This accounts for the fact that for a full presentation of

properties characterizing both the problem of computer-assisted tomography and approaches to solve it, 2D problems will be investigated below. The extension to the third dimension thus becomes only a matter of computation power.

Boundary parameterization. Since the measurements cannot be taken inside the object being the subject of examination, the measurement space is restricted at least to its surface. Usually, the most significant observations can be expected in the closest vicinity of the object, that is the measurement electrodes are placed on the boundary of the examined system, which then automatically becomes the set of admissible sensor locations. To avoid additional constraints of the design space arising from the restrictions above and to simplify the numerical implementation, a suitable parameterization of the boundary should be introduced. Generally, the dimension of the measurement space X can be thus decreased (at least by one) and additionally it is sometimes possible to provide several valuable properties such as the compactness or convexity of X, which cannot be overestimated from the point of view of implementation. As particular situations entirely determine the form and properties of such mappings, they will be discussed in more detail within the framework of specific examples.

3.4.1.2. Numerical experiments

Electrolysis process. The first example regarding the application of the proposed methodology regards the optimal sensor location for parameter estimation in reconstruction of an electrolysis process. Consider two circular metallic conductors which are placed on a plane of thin conductive medium with a spatially-varying conductivity coefficient like a blotting paper with varying thickness wetted by a weak electrolyte. The domain of interest Ω is shown in Fig. 3.6(a) and its boundary $\Gamma = \bigcup_{i=1}^{3} \Gamma_i$ is split into three disjoint subsets:

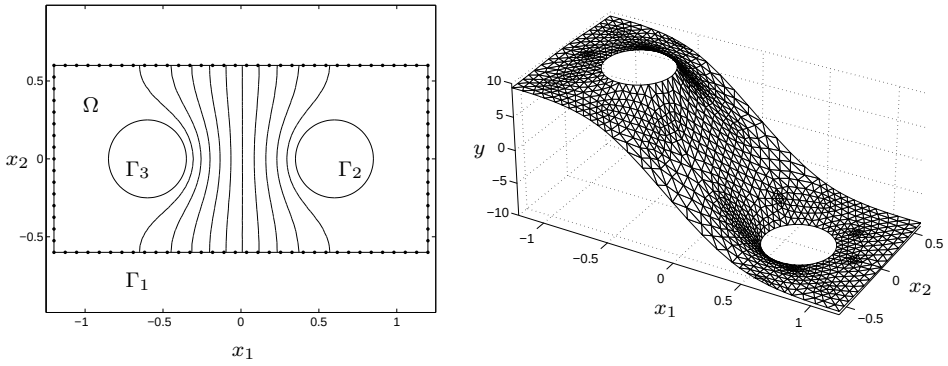
$$\begin{aligned} \Gamma_1 = {} & \big\{(-1.2, x_2) : -0.6 \leqslant x_2 \leqslant 0.6\big\} \cup \big\{(1.2, x_2) : -0.6 \leqslant x_2 \leqslant 0.6\big\} \\ & \cup \big\{(x_1, -0.6) : -1.2 \leqslant x_1 \leqslant 1.2\big\} \cup \big\{(x_1, 0.6) : -1.2 \leqslant x_1 \leqslant 1.2\big\}, \\ \Gamma_2 = {} & \big\{(x_1, x_2) : (x_1 + 0.6)^2 + x_2^2 = (0.25)^2\big\}, \\ \Gamma_3 = {} & \big\{(x_1, x_2) : (x_1 - 0.6)^2 + x_2^2 = (0.25)^2\big\}. \end{aligned} \tag{3.85}$$

A steady current flow through the plates in connection with the absence of external current sources results in the physical model for this problem expressed in the form of the Laplace equation

$$\nabla \cdot \big(\sigma(x) \nabla y(x)\big) = 0, \quad x \in \Omega \subset \mathbb{R}^2, \tag{3.86}$$

where y is the potential of the electric field in the conductive medium. The respective boundary conditions are

$$\begin{cases} \dfrac{\partial y(x)}{\partial n} = 0 & \text{if } x \in \Gamma_1 \text{ (on the outer boundaries)}, \\ y(x) = 10 & \text{if } x \in \Gamma_2 \text{ (for the left metallic plate)}, \\ y(x) = -10 & \text{if } x \in \Gamma_3 \text{ (for the right metallic plate)}. \end{cases} \tag{3.87}$$



(a) (b)

Fig. 3.6. Domain Ω with admissible discrete sensor locations with the contour plot of an electric potential function ($\theta = (0.4, -0.5, 0.6)$) (a) and the surface plot of the potential (b)

where $\partial y/\partial n$ denotes the derivative in the direction of the unit outward normal to Γ.

Our task is to find a D-optimum design to reconstruct the spatial distribution of the conductivity coefficient modelled in the form

$$\sigma(x) = \theta_1 + x_2^2 \exp\left(\theta_2 (x_1 - \theta_3)^2\right) \tag{3.88}$$

or, more precisely, to optimally estimate the vector of constant parameters $\theta = (\theta_1, \theta_2, \theta_3)$. In order to obtain an approximation of the D-optimal design, Algorithms 3.1, 3.3 and 3.4 for the discrete case and 3.5 for the continuous domain were implemented in a computer program with the Lahey/Fujitsu Fortran 95 compiler v.5.6 using a PC running Windows 2000.

The system equation accompanied by the sensitivity equations form a system of elliptic PDE's which has to be solved and the solution is to be stored in memory. For this purpose, the procedures from the Matlab PDE Toolbox (Littlefield, 1997) based on a Finite Element Method (FEM) solver (function `assempde`) were adopted with the initial estimate of $\theta^0 = (0.4, -0.5, 0.6)$ taken as a nominal one. The distribution of the electric potential is illustrated in Fig. 3.6. All covariance matrices $C(x)$ were then set to unity (a scalar system).

The measurement electrodes may be placed only on the outer boundary Γ_1, which automatically becomes the design space X. For this reason it is convenient to derive its suitable parameterization. The simplest way to do so is to use the

length $\lambda \in [0, 7.2]$ of Γ_1, i.e.

$$x_1(\lambda) = \begin{cases} \lambda - 1.2 & \text{if } 0 \leqslant \lambda < 2.4, \\ 1.2 & \text{if } 2.4 \leqslant \lambda < 3.6, \\ 4.8 - \lambda & \text{if } 3.6 \leqslant \lambda < 6.0, \\ -1.2 & \text{if } 6.0 \leqslant \lambda \leqslant 7.2, \end{cases}, \quad x_2(\lambda) = \begin{cases} -0.6 & \text{if } 0 \leqslant \lambda < 2.4, \\ \lambda - 3.0 & \text{if } 2.4 \leqslant \lambda < 3.6, \\ 0.6 & \text{if } 3.6 \leqslant \lambda < 6.0, \\ 6.6 - \lambda & \text{if } 6.0 \leqslant \lambda \leqslant 7.2. \end{cases} \tag{3.89}$$

Optimization of experimental effort. For the discrete case the set X of possible locations for measurement electrodes was proposed as a uniform grid along the length of the outer boundary Γ_1 (cf. Fig. 3.6(a))

$$X = \left\{ x(\lambda_i) : \lambda_i = \frac{7.2}{98}(i-1), \quad i = 1, \ldots, 98 \right\}.$$

This set will be used for all the routines dedicated for the discrete case in the considered example. Those support points with uniform distribution of weights $p_i^{(0)} = 1/98,\ i = 1, \ldots, 98$ formed the starting design for weight optimization procedures. Besides the implemented approaches, for the sake of comparison, the problem was also treated as a nonlinear constrained optimization one and solved numerically using the procedure `DLCONF` from IMSL Fortran 90 MP Library v.4.0 based on the sequential quadratic programming with linear constraints (Visual Numerics, 1997). For this nontrivial experimental design problem, all procedures operating on the finite measurement space lead to striking consistence of results. For any applied algorithm the support points of approximated designs with weights over the threshold value 0.01 were the same and slight differences concern only the weight values. For example, the steepest descent weight optimization routine (Algorithm 3.1) with the rule (3.14) (implemented using the golden-search routine) converged with the accuracy of $\epsilon \leqslant 10^{-4}$ after 134 iterations to the following approximation of the D-optimal design:

$$\xi^* = \left\{ \begin{array}{rl} \text{support} & \text{weight} \\ (-1.2, -0.6), & 0.166292 \\ (-1.2, 0.6), & 0.166292 \\ (-0.2545, -0.6), & 0.100013 \\ (-0.2545, 0.6), & 0.100013 \\ (-0.1818, -0.6), & 0.067811 \\ (-0.1818, 0.6), & 0.067811 \\ (0.3272, -0.6), & 0.165885 \\ (0.3272, 0.6), & 0.165885 \end{array} \right\}. \tag{3.90}$$

Figure 3.7 shows the corresponding results from which it can be easily seen that the optimal design is concentrated at those points at which the so-called sensitivity function $\phi(x, \xi^*)$ takes its maximal value in the discrete domain, which is equal to the number of estimated parameters, i.e. $m = 3$. Our intuition suggests that we could expect the symmetry of the problem along the axis $x_2 = 0$ in the obtained approximation to the optimal design and, in fact, (3.90) seems to satisfy such a

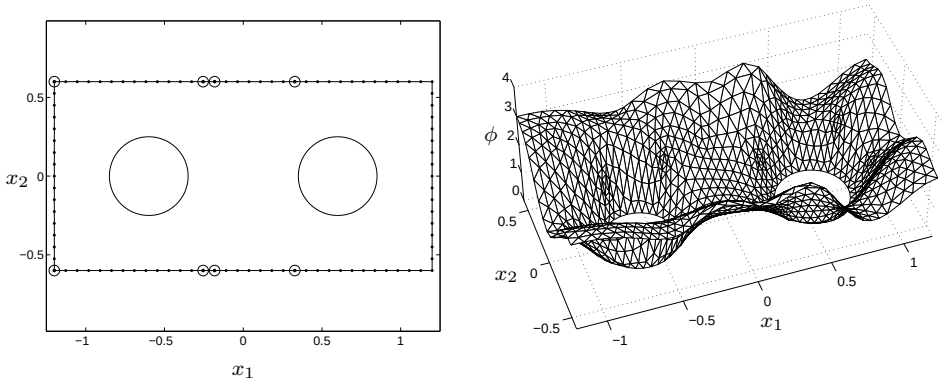


Fig. 3.7. D-optimal discrete measurement strategy (open circles indicate the D-optimum sensor locations) (a), and the surface plot of the sensitivity function (b).

conjecture since the points can be connected into pairs with approximately equal weights and the same x_1 spatial coordinates while the values of x_2 are opposite (see Fig. 3.7(a)). It is pointless to present here solutions from all algorithms as they are very similar. More detailed results and the values of the D-optimum design criterion are presented in Table 3.2. To increase the efficiency of the solution, the steepest descent algorithm for the continuous measurement space was used along with the ARS strategy of determining the significant design support and the possibility of removing noninformative points. Starting from the design

$$\xi^{(0)} = \begin{Bmatrix} (0.1, 0.6), & (0.3, 0.6), & (0.5, 0.6), & (0.8, 0.6) \\ 0.25, & 0.25, & 0.25, & 0.25 \end{Bmatrix}, \tag{3.91}$$

Table 3.2. Results in EIT for the electrolysis example.

Algorithm	Accuracy	Iterations	Time	$\det M(\xi^\star)$
Steepest descent weight optimization with golden search	10^{-4}	74	~ 5 s	6.6124
Feasible-direction weight optimization	10^{-4}	301	~ 3 s	6.6180
Linearly constrained sequential quadratic programming	10^{-4}	–	~ 10 s	6.6072
Two-phase support & weight optimization with ARS	10^{-6}	3	~ 20 s	6.6459
Clusterization-free method with one-point correction	10^{-5}	18	< 1 s	5.8706

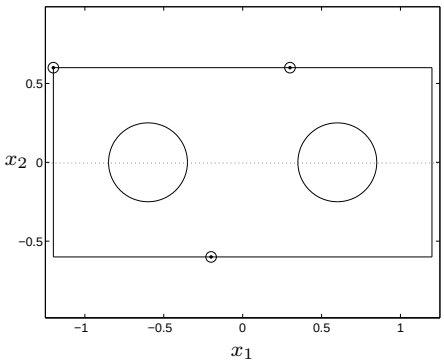


Fig. 3.8. D-optimal continuous measurements allocation.

the algorithm attained the optimal solution in only three repetitions of the main loop. The weight optimization phase was performed using Algorithm 3.3. The approximated design was

$$\xi^\star = \begin{Bmatrix} (-1.1999, 0.6), & (-0.2, -0.6), & (0.3, 0.6) \\ 0.3333, & 0.3333, & 0.3333 \end{Bmatrix} \tag{3.92}$$

which is shown in Fig. 3.8. In this case the improvement is almost unnoticeable (by means of the criterion value), which proves that the discretization of the boundary was adequate to obtain a reasonably high quality of the solution. However, from Fig. 3.8 a very important property of Algorithm 3.5 is seen, namely a tendency to minimize the redundancy of the design support. Indeed, the three support points constitute the minimal number for this problem and since the corresponding weights of the final approximation of an optimal design are practically equal, one third of the sensors should be assigned to each support point.

At first sight, the symmetry of the problem (the axis of the symmetry is shown as a dotted line in Fig. 3.8) is not retained. But if a new design is created by symmetrically mirroring any support point with respect to the symmetry axis, an equivalent approximation of the optimal design can be obtained. As an example, consider the following design, which is symmetric in the sense of both the support and weights:

$$\xi_2^\star = \left\{ \begin{array}{rl} (-1.1999, 0.6), & 0.1667 \\ (-1.1999, -0.6), & 0.1667 \\ (-0.2, 0.6), & 0.1667 \\ (-0.2, -0.6), & 0.1667 \\ (0.3, 0.6), & 0.1667 \\ (0.3, -0.6), & 0.1667 \end{array} \right\}. \tag{3.93}$$

It is obtained from (3.92) by mirroring (the weight of each site was divided by 2).

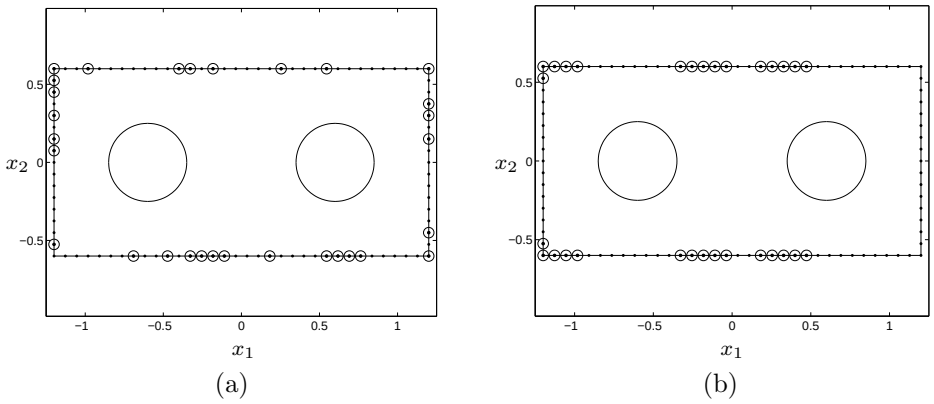


Fig. 3.9 . Initial (a) and D-optimal (b) designs for the clusterization-free algorithm.

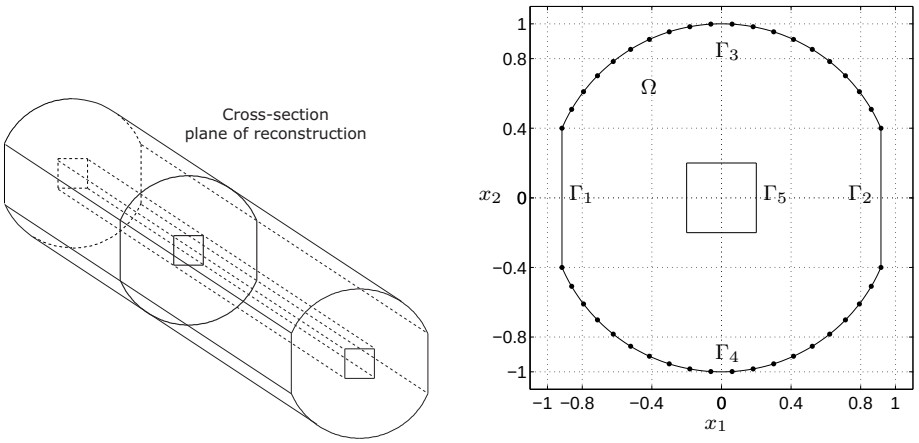
The FIM for both the designs has exactly the same form:

$$M(\xi^*) = \begin{bmatrix} 0.32690 & 0.09555 & -0.03299 \\ 0.09555 & 0.09798 & -0.07867 \\ -0.03299 & -0.07867 & 0.07423 \end{bmatrix}.$$

From a statistical point of view, such pairs of symmetrical support points are rather disadvantageous since they provide identical information about the system. Another observation is the possibility of the existence of more than one equivalent approximation to the optimal design. The performance of the algorithm can be reviewed in Table 3.2, from which it becomes clear that the possible improvement in the solution, if any, is obtained at the cost of an increased complexity of the algorithm. On the other hand, for 3D problems such a situation is very often strongly justified.

Replication free optimization. As a last approach applied in our experiment, the clusterization-free algorithm was used in the simplest form of a sequential one-point exchange procedure. In this case, the aim was to choose 30 locations of measurement electrodes from the set X defined at the beginning of the example. An initial design was created by randomly selecting support points. The algorithm calculated the solution very quickly (18 iterations for $\varepsilon \leqslant 10^{-5}$). The initial and final distributions of the optimal support points are shown in Fig. 3.9. The quality of the solution is evidently worse in the sense of the D-optimality criterion. It is a direct consequence of the constraints imposed on the design measure. However, the clusterization effect is avoided and the D-optimal observational strategy tends to take the measurements in the vicinity of the best support points of the replicated designs obtained earlier.

Material flaw detection. The next example concerns the EIT used for inspection of objects regarding possible defects of their structures. This problem is widely



(a) (b)

Fig. 3.10. The metallic core (a) and its cross-section plane with discrete available sensor locations pointed out (b).

encountered in many practical problems (e.g. chemical, nuclear and building industries or medicine applications). The aim of the tomography here is to detect possible inhomogeneities of a material, which suggest possible flaws.

Consider a metallic core with rectangular crack inside which is shown with its cross-section in Fig. 3.10. During the experiment only one cross-section plane for each reconstruction process is considered. The left and right boundaries Γ_1 and Γ_2 (cf. Fig. 3.10(b)) are supplied with constant voltage to force the flow of a low density steady current. Hence, the planar reconstruction forward problem can be simplified to the form of the two-dimensional Laplace equation (3.86), subject to the following boundary conditions:

$$\begin{cases} \dfrac{\partial y(x)}{\partial n} = 0 & \text{if } x \in \Gamma_i,\ i \in \{3,4,5\}, \\ y(x) = 5 & \text{if } x \in \Gamma_1, \\ y(x) = 0 & \text{if } x \in \Gamma_2, \end{cases} \tag{3.94}$$

where y stands for the electric potential.

The material homogeneity aberrations are assumed to be modelled with the use of the exponential functions involved into conductivity parameter mapping (Lemonnier and Peytraud, 1998):

$$\sigma(x) = \sigma_0 + \sum_{j=1}^{N_f} \sigma_j(x), \tag{3.95}$$

where

$$\sigma_j(x) = \sigma_{j,\max} \exp\big(- \|(x - a_j)\|_B^2\big), \quad j = 1, \ldots, N_f. \tag{3.96}$$

Here σ_0 is the value of the conductivity for normal conditions, $N_f \in \mathbb{N}$ signifies the number of possible structural flaws, $\sigma_{j,\max}$ is the maximal amplitude of the conductivity deviation caused by a particular defect, $a_j \in \mathbb{R}^2$ can be interpreted as the centre of such a defect and $B \in \mathbb{R}^{2\times 2}$ denotes the parameter vector describing its spatial spread.

It is assumed that from previous experiments a rather rough location of only one structural imperfection of the object is available with parametric characterization of its distribution over the domain. Hence, the corresponding reconstructed conductivity coefficient can be expressed as

$$\sigma(x_1, x_2) = \sigma_0 + \sigma_{\max} \exp\big(-\theta_1(x_1 - \theta_2)^2 - \theta_3(x_2 - \theta_4)^2\big) \tag{3.97}$$

where $\sigma_0 = 0.1$, $\sigma_{\max} = 0.2$ and $\theta = (30.0, 0.3, 80.0, 0.7)$.

Our task here is to find the most informative strategy of data acquisition for estimation of parameter vector θ applying this time different optimality criteria.

The measurements can be taken on the boundaries denoted by Γ_3, Γ_4 and Γ_5, but since the interior boundary Γ_5 is virtually inaccessible, only $\Gamma_3 \cup \Gamma_4$ constitutes the set of admissible sensor locations. Hence, it is easy to propose the following boundary parameterization:

$$x_1(\lambda) = \cos\lambda, \quad x_2 = \sin\lambda, \tag{3.98}$$

with λ satisfying

$$\arcsin 0.4 \leqslant \lambda \leqslant \pi - \arcsin 0.4, \quad \text{or} \quad \pi + \arcsin 0.4 \leqslant \lambda \leqslant 2\pi - \arcsin 0.4 \tag{3.99}$$

In this experiment, the set X of possible sensor locations was chosen as a uniform grid of 20 sites along each boundary Γ_3 and Γ_4 (cf. Fig. 3.10(b)) which results in the set of 40 points

$$X = \Big\{ x(\lambda_i) : \lambda_i = \arcsin 0.4 + \frac{\pi - 2\arcsin 0.4}{19}(i-1), \\ \lambda_{i+20} = \pi + \lambda_i, \quad i = 1, \ldots, 20 \Big\}.$$

The relatively small cardinality of the admissible location set means that the formulation of the problem in terms of the SDP approach is quite easy and convenient. In order to account for different criteria (E, A, sensitivity) these problems were reformulated as convex optimization tasks with LMI constraints. Then the Matlab compatible SeDuMi v.1.02 SDP solver written by Sturm (1997) based on the interior-point primal-dual approach was used in connection with additionally implemented Matlab routines.

As a complement, also the weight optimization algorithm of Section 3.2.1 was applied (in the case of D-optimality) with the initial design formed by a uniform weight distribution over the finite set X. The PDE system was solved with the Matlab PDE Toolbox and simulations were conducted in the hardware-software computational environment established by a PC with Pentium IV 1.7GHz processor and 768MB RAM running Windows 2000. The results (after removing locations

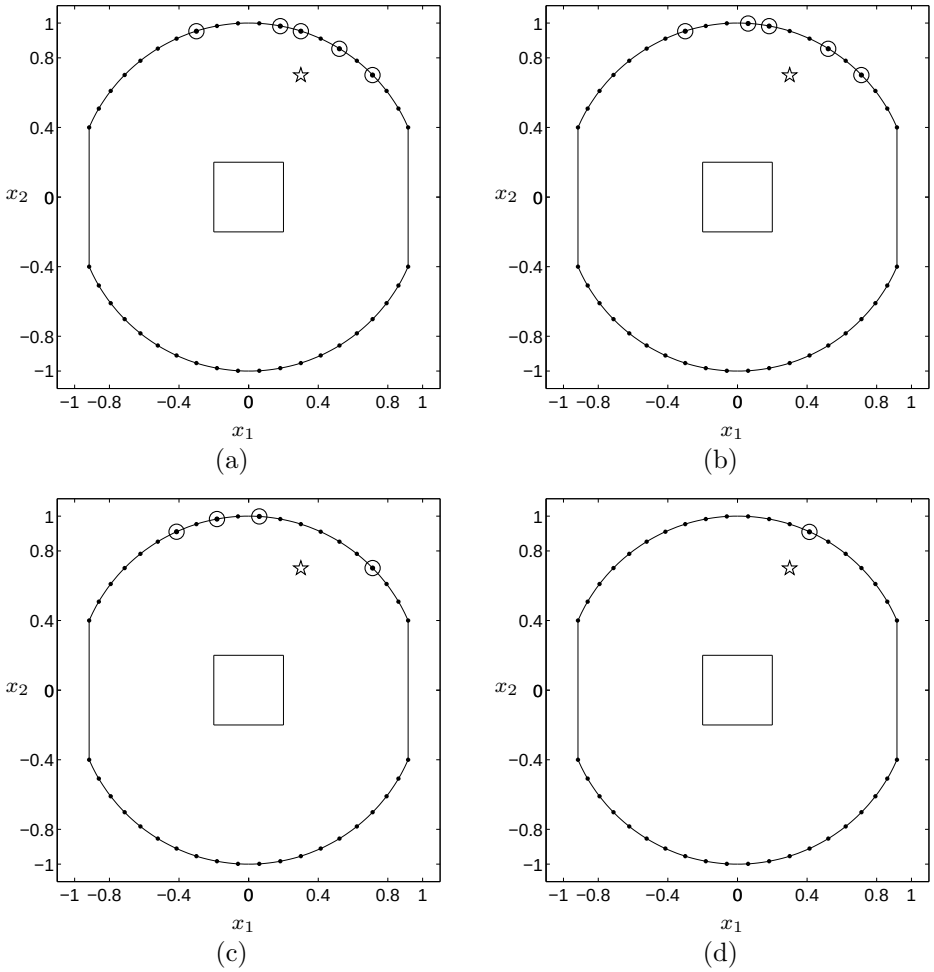


Fig. 3.11. Optimal designs for various criteria: (a) D-optimum, (b) A-optimum, (c) E-optimum and (d) sensitivity criterion.

with weight less than 0.01) are illustrated in Fig. 3.11. The points denote the possible sensor locations while open circles stand for the optimal ones. Additionally, the star stands for the position of the material non-homogeneity centre. In spite of the fact that a detailed interpretation of the sensor locations is not trivial, an intuitively clear observation of the tendency of taking measurements in a close vicinity of the structural defect of the object can be made, where the measurements are expected to be the most informative. Unfortunately, in the case of the sensitivity criterion a common drawback of this quality measure occurs as the optimal design is degenerated and concentrated in only one point. The A- and D-optimal locations look very similar, but there exist a significant difference regarding design weights.

Approximations of the optimal designs obtained from the exploited approaches were:

- D-optimality (steepest descent weight optimization),

$$\xi_D^\star = \left\{ \begin{array}{cc} (0.711, 0.700), & 0.249892 \\ (0.521, 0.852), & 0.244113 \\ (0.300, 0.952), & 0.225804 \\ (0.181, 0.982), & 0.033782 \\ (-0.300, 0.952), & 0.246409 \end{array} \right\},$$

- A-optimality (SDP approach)

$$\xi_A^\star = \left\{ \begin{array}{cc} (0.711, 0.700), & 0.366007 \\ (0.521, 0.852), & 0.116856 \\ (0.061, 0.997), & 0.239722 \\ (0.181, 0.982), & 0.228461 \\ (-0.300, 0.952), & 0.047558 \end{array} \right\},$$

- E-optimality (SDP approach)

$$\xi_E^\star = \left\{ \begin{array}{cc} (0.711, 0.700), & 0.438980 \\ (0.061, 0.997), & 0.444876 \\ (-0.181, 0.982), & 0.063655 \\ (-0.414, 0.909), & 0.052488 \end{array} \right\},$$

- sensitivity criterion (SDP approach)

$$\xi_{\text{sens}}^\star = \left\{ \begin{array}{cc} (0.414, 0.909), & 1 \end{array} \right\}.$$

The efficiency of the algorithms combined with a small-medium scale of the problem leads to a very short computation time (below 5 seconds in the worst case).

Table 3.3. Results and performance measures in EIT for the material flaw detection example.

Criterion/Solver	Accuracy	Iterations	Time
A-optimum (SeDuMi)	10^{-4}	24	~ 5 s
D-optimum (steepest descent weight optimization)	10^{-4}	86	~ 1 s
E-optimum (SeDuMi)	10^{-4}	16	~ 5 s
sensitivity criterion (SeDuMi)	10^{-4}	9	~ 1 s

The results are compared in Table 3.3. Notice that the problem is extremely difficult in this case, since the most informative measurements can be taken inside the object (this is a common situation), which may lead to the ill-conditioning of the FIM (it can be very close to singularity).

3.4.2. Elasticity in the structural mechanics of smart materials

3.4.2.1. Background

As an auxiliary application, multi-output systems encountered in structural mechanics are considered for the purpose of a proper illustration of the proposed approaches. A variety of engineering applications for this class of problems establish a motivation to pay close attention to such systems. Especially the field of *smart material* systems (also referred to as intelligent, adaptive or controllable systems) occupy now a prominent position in structural mechanics. This is a direct consequence of the technological advances in material science in combination with the increasing requirements on controller design, which have led to the development of many structural systems employing advanced sensors and actuators (Flatau and Chong, 2002). By utilizing the physical properties of smart materials, significant improvements in the system behaviour control can be achieved regarding traditional servomechanisms. The smart material structures being the combination of advanced sensors, actuators and microprocessors have already revolutionized the design of many control systems and still promise an ongoing progression in the future. They are generally created through a synthesis, but also through their integration with conventional structural materials such as steel, concrete or composites (Flatau and Chong, 2002). Smart materials can be divided into few major groups according to their physical properties (Banks *et al.*, 1996; Dorfman *et al.*, 2001; Flatau and Chong, 2002):

- piezoelectric and ferroelectric elements and magnetostrictive transducers, which possess an ability to convert the electric charge, field and current (via the induced magnetism), respectively, to mechanical forces and vice versa,
- electrorheological and magnetorheorogical fluids, which can change their state of aggregation (between liquid and solid) in the presence of electric and magnetic fields, dramatically altering basic material properties,
- electroactive polymers, which change their shape in response to applied fields,
- shape memory alloys being a class of metal compounds which possess the capability to sustain and recover relatively large strains without undergoing a plastic deformation and can generate force through temperature changing across the transition state,
- fiber optic sensors using the refractive properties of light to measure mechanical strains.

The development of intelligent structures that can monitor their own conditions, detect impeding failures, control or heal damages, and adapt to changing environments can be observed in numerous research areas and the range of important practical applications for smart materials is extremely wide. Some significant examples are listed below (Gandhi and Thompson, 1992; Banks *et al.*, 1996; Boresi and Chong, 2000; Flatau and Chong, 2002):

- the design of smart spacecraft and aircraft skins embedded with fiber optic sensors to detect structural flaws,
- semi-active vibration absorbers in civil constructions (bridges, buildings, etc.) with both the actuating and sensor elements to counter violent vibrations,
- flying microelectromechanical systems with remote control for surveying and rescue missions,
- stealth submarine vehicles with swimming muscles made of special polymers,
- design, modelling and development of active aperture antennas,
- ultra-precison shape-controlled positioners,
- remote sensing of damage in large civil structures, and
- design of robust helicopter rotors.

Such multidisciplinary mechanical and civil infrastructure systems encountered in mechanical, electrical, civil, control, computer, aeronautical and aircraft engineering have collectively created a new entity at the interface of these research areas.

The different physical phenomena determining the advantageous features of intelligent materials usually have distributed form by definition. Thus, a proper analysis automatically requires suitable modelling with the use of the finesse mathematical apparatus. The PDE or integro-differential equation systems thus became a natural way to provide the relevant accuracy. For instance, a model of structural elasticity can be derived in the form of Lamé's PDE's (Kącki, 1995; Banks *et al.*, 1996). Another example is a stress-strain relation described by the Donell-Mushtari equations in weak (integral) or strong (differential) forms (Banks *et al.*, 1996). Due to the limited space, it is impossible to outline even rough fundamentals of the corresponding mathematical theory as it exceeds the scope of this thesis. The literature on the problem is very extensive, and a detailed description of smart materials and structures can be found e.g. in the pertinent monographs (Banks *et al.*, 1996; Boresi and Chong, 2000).

3.4.2.2. Numerical experiments

Transverse loads applied to a thin plate. Consider a thin sheet of material being an extremely simple model of the aircraft lifting surface. This surface has a displacement in the out-of-plane direction as a result of external and internal forces

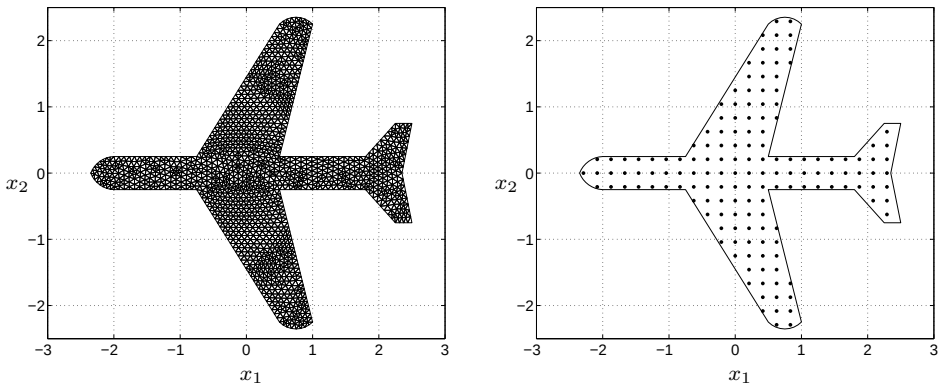


Fig. 3.12. Domain Ω with a triangular finite element mesh (a), and the admissible sensor locations for discrete approaches (b).

being a result of an applied load or the air resistance. The control of those possibly dangerous effects and a damage detection constitute the main application area of smart materials in the aircraft industry and space technology (Boresi and Chong, 2000).

In order to simplify such an extremely sophisticated problem and to expose its illustrative properties as an example, think of a plate resting or clamped in a frame, with various weights placed on the plate. Under these conditions, the transverse displacement y_1 satisfies the biharmonic equation (Kącki, 1995)

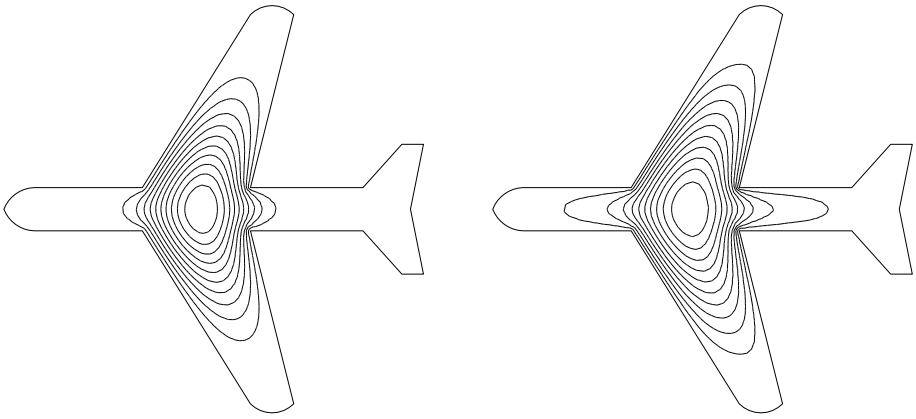
$$\nabla^4 y_1(x) = f(x, y_1(x)), \quad x \in \Omega \tag{3.100}$$

which is equivalent to the pair of the second-order elliptic equations

$$\begin{aligned} &\nabla^2 y_1(x) = y_2(x), \\ &\nabla^2 y_2(x) = f(x, y_1(x)), \quad x \in \Omega, \end{aligned} \tag{3.101}$$

where y_2 is the surface curvature and f plays the role of an applied force distributed over the domain Ω (note that in general it also depends on y_1). The first of these equations is a Poisson one involving the Laplacian of the original unknown y_1. The second gives the right-hand side of the biharmonic equation. Taken together, they define two coupled second-order elliptic equations for the biharmonic system. The simplest set of boundary conditions is that for a simply supported sheet of material, with the displacement and the sheet curvature both equal to zero on the boundary. That is equivalent to the boundary conditions

$$\begin{aligned} &\nabla^2 y_1(x) = 0, \quad x \in \partial\Omega, \\ &\nabla^2 y_2(x) = 0, \quad x \in \partial\Omega. \end{aligned} \tag{3.102}$$



(a) (b)

Fig. 3.13. Contour plots of the transverse displacements (a) and the curvature (b) for the aircraft example ($\theta = (-2.5, 0.7, 0.9, -0.8)$).

Another set of conditions that is commonly applied is that for a clamped sheet with zero Dirichlet conditions for the displacement and von Neumann natural conditions for the curvature on the boundary. The domain Ω in the form of a plane-shaped figure is shown in Fig. 3.12(a) with an unstructured triangular mesh.

The main purpose is the determination of the optimal sensor locations which provide the best accuracy of the parameter estimates playing the major role in external force control. The function f is assumed to be in the form

$$f(x, y_1) = \gamma y_1(x) + \theta_1 + \theta_2 x_1^2 + \theta_3 x_2^2 + \theta_4 x_1^2 x_2^2, \tag{3.103}$$

where $\theta = (\theta_1, \theta_2, \theta_3, \theta_4)$ is an unknown vector of constant parameters and γ stands for some known coefficient which represents the dependence between the surface curvature and the displacement. The function f is expected to describe in a reasonably simple form the downward displacements in the fuselage and upwards displacements on the wings. The value of $\gamma = 0.1$ was assumed as a nominal one, and the rough estimate $\theta^0 = (-2.5, 0.6, 0.9, -0.8)$ was assumed to be derived from a prior process analysis.

In this experiment the solution to the forward problem (3.101)–(3.102) was generated by the Fastflo v.3.0 environment based on the FEM approach with several procedures written for this purpose in *Fasttalk* language (a built-in feature of Fastflo) especially dedicated to PDE's. The simulations were performed with the use of a low-cost PC (Pentium IV 1.7GHz processor, 768MB RAM) running Windows 2000. The solution illustrated in the contour plots in Fig. 3.13 was then transferred into the Fortran environment where the design optimization procedures mentioned in the preceding sections were used, namely the weight optimization routines, the clusterization-free strategy and the support-weight optimization algorithm.

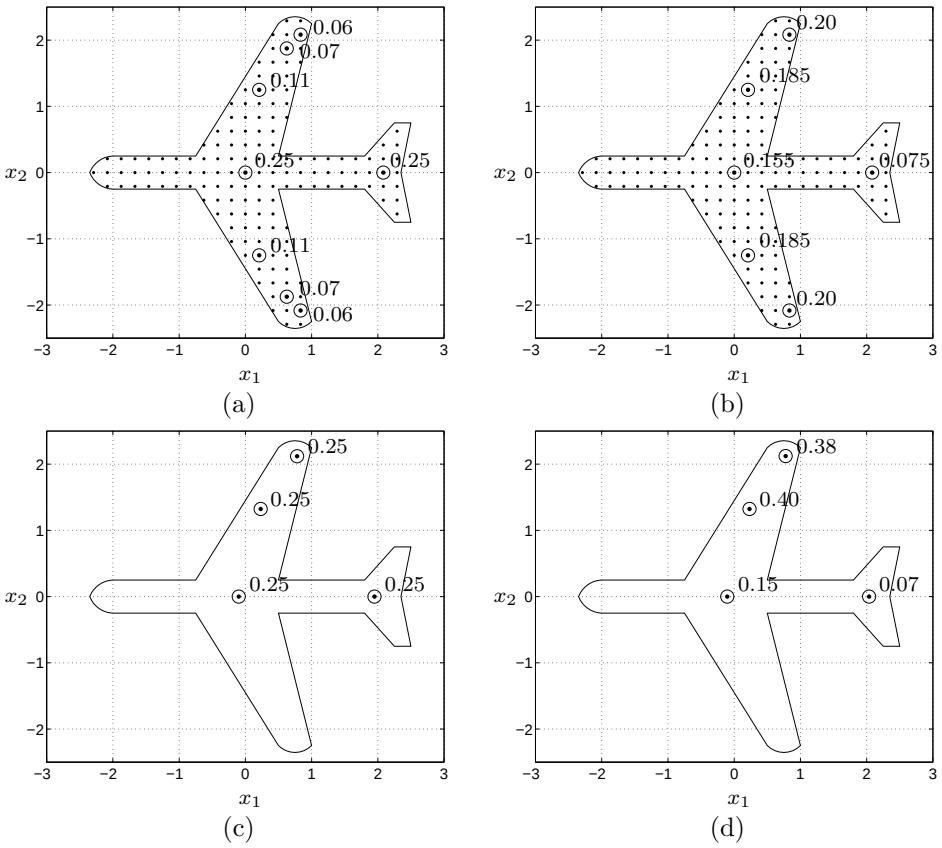


Fig. 3.14. Optimal designs: (a) D-optimum design in the discrete case, (b) A-optimum design in the discrete case, (c) D-optimum design in the continuous case, and (d) A-optimum design in the continuous case.

In order to apply the algorithms dedicated to a finite measurement space, a suitable discretization of the domain Ω was provided, i.e. a set of admissible sensor locations was constructed using those points of the uniform rectangular (25×25) grid which lie inside Ω (cf. Fig. 3.12(b)). The feasible-direction weight optimization procedure produced the solution after 137 and 272 iterations (for the D- and A-optimum criteria, respectively) with accuracy $\epsilon \leqslant 10^{-5}$ starting from randomly generated weights. The 153-point discretized domain appears very adequate as the results are almost identical to the continuous domain case taking account of the problem symmetry with respect to the axis $x_2 = 0$ (cf. remarks regarding the electrolysis example). The approximations of optimal locations with the corresponding experimental effort for both the discrete and continuous cases are illustrated in Fig. 3.14.

The generalized first-order algorithm proved again its ability to minimize the

redundancy of the resulting designs which were achieved in 6 (D-optimum) and 4 (A-optimum) repetitions of the main loop. Once more, the locations for those criteria are very similar, but the experimental effort makes these approaches distinct. The sensor locations reflect the fact that the most informative measurements can be obtained at the centre of the fuselage with greatest downward displacements and wings with greatest upward ones.

The cardinality of X is large enough to apply the clusterization-free strategy for the sake of comparison. The forty-point designs obtained after only 32 (D-optimal) and 34 (A-optimal) iterations in almost non-measurable operational time are shown in Fig. 3.15. This time the difference between D- and A-optimal strategies became clearer, nevertheless the resemblance to the replicated designs is rather obvious.

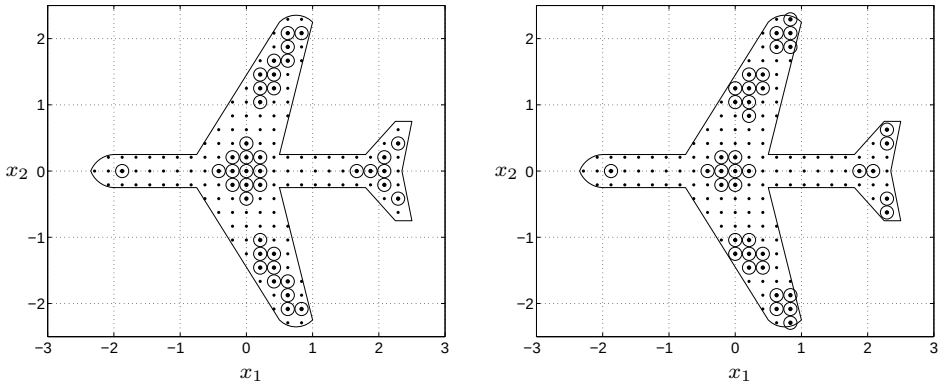


Fig. 3.15. (a) D-optimum and (b) A-optimum clusterization-free designs for the aircraft example.

3.5. Concluding remarks

The results contained in this chapter show that some well-known methods of optimum experimental design for linear regression models can be easily extended to the setting of the sensor location problem for multidimensional static DPS's. The advantage of introducing continuous designs lies in the fact that the problem dimensionality is dramatically reduced. Moreover, with some minor changes, sequential numerical design algorithms, which have been continually refined since the early 1960s, can be employed here. Unfortunately, this approach does not prevent sensors from clustering which is a rather undesirable phenomenon in potential applications if the measurements are to be taken simultaneously. Clusterization is a consequence of the assumption that the measurement noise is spatially uncorrelated. This means that in an optimal solution different sensors often tend to

take measurements at the same point, which is most often unacceptable from the technical point of view.

Alternatively, we may seek to find an optimal design not within the class of all designs, but rather in a restricted subset of competing replication-free designs. To implement this idea, some recent advances in spatial statistics are employed, and in particular Fedorov's idea of directly constrained design measures is adapted to our framework. As a consequence, this leads to a very efficient and particularly simple exchange-type algorithm. Bear in mind, however, that this approach should in principle be used if the number of sensors is relatively high in comparison with the number of admissible support points. If this is not the case, we can resort to standard optimization routines. To the best of author's knowledge, the presented algorithms have not been applied yet to systems described by partial differential equations, in spite of their decided advantages. The only exception is the monograph (Uciński, 1999a) where an attempt was made to implement the continuous first-order algorithm in the case of a parabolic equation and the seminal works (Patan and Uciński, 2002; Uciński and Patan, 2002a; Uciński and Patan, 2002c; Uciński and Patan, 2002b) which concern the different theoretical and practical aspects of the delineated algorithms. Especially, the SDP (or even LMI) based approach has received no attention yet with respect to its tailoring to the area of static and dynamic DPS's, especially for some classes of non-differentiable criteria such as the E-optimality one.

The efficiency and usefulness of the proposed approaches was verified via computer simulations for vital engineering problems of tomography (MISO systems) and structural elasticity of smart materials (MIMO systems) proving their flexibility and ability for providing accurate approximations of optimal solutions in non-trivial practical situations. However, the very important problem of correlated measurements which appear in practical applications (especially in computer-assisted tomography) was silently omitted as some approaches will be proposed in a more general context.

Recapitulating, the following is a concise summary of contributions developed in this chapter to the state-of-the-art in optimal sensor location for parameter estimation in static DPS's:

- A characterization of continuous designs in the problem of stationary sensor allocation for static DPS's is provided, which leads to a great reduction in the problem dimensionality and complexity.

- It is clarified how to adapt some existing algorithms of nonlinear programming and optimum experimental design for finding numerical approximations to the optimum experimental effort for single and multi-output static DPS's. Particularly, the gradient projection and feasible-direction methods were tailored to the optimization on a finite set of admissible locations. Additionally, the SDP approach was presented here, which is a completely new technique in the context of DPS's. For the case of experimental effort optimization on sets with non-zero measures the two-phase first-order algorithm with an ARS global optimization strategy was adapted.

- A characterization of the replication-free approach is provided, which allows us to avoid the sensor clusterization effect. This technique with the corresponding exchange-type algorithm is adopted to the framework of static DPS's.
- The delineated algorithms were tested via computer simulations on engineering problems such as computer-assisted electrical impedance tomography and the structural mechanics of smart materials.

Chapter 4

OPTIMAL MEASUREMENT STRATEGIES FOR SYSTEMS WITH SPATIO-TEMPORAL DYNAMICS

In the field of spatio-temporal systems being a substantial generalization of the systems considered up to now, the variety of possible observation strategies is naturally much richer. On account of the explicit time presence in the studied processes, besides stationary observations, scanning and movable observation strategies can be applied. Such a possibility is very interesting due to the greater flexibility of the methods, because the appropriate strategy can be chosen as a result of a compromise between practical conditions and the required accuracy. However, most of the contributions to the measurement optimization problem concern the choice of stationary sensor positions and there have been relatively few contributions to the experimental design for those systems (for surveys, see (Kubrusly and Malebranche, 1985; Rafajłowicz, 1986a; Uciński, 1992; Korbicz and Uciński, 1994; Uciński, 2000c; Uciński, 2000b; Uciński and Korbicz, 2001)). Of course, one may argue that there exist a few works dealing with the problem of determining sensor positions for optimal state estimation (Kubrusly and Malebranche, 1985; Azhogin *et al.*, 1988). At this point, however, it should be noted again that the state estimation problem is essentially different from the optimal measurement problem for parameter identification since in the latter case the current state depends strongly non-linearly on unknown parameters, while its dependence on the initial state is linear. The sensor location problem was considered in various aspects (for reviews, we refer the reader to (Uciński, 1999a; Uciński, 2000a; Uciński, 2000c; Kubrusly and Malebranche, 1985; Sun, 1994)).

For dynamic DPS's the very first idea is to extend the approaches developed for stationary sensors in previous chapter in the spirit of the classical optimum experimental design theory for lumped systems (Fedorov and Hackl, 1997; Müller, 1998; Pázman, 1986; Walter and Pronzato, 1990). In spite of a great convenience of such an approach, the main drawback of stationary sensors in the context of spatio-temporal systems is the lack of flexibility regarding the system dynamics. The measurements are taken during the whole observation horizon at the same locations. Consequently, in many situations the observations may be inadequate and the measurement data do not provide suitable information about the system dynamics. This is the main reason why it is worth to pay closer attention to the other strategies mentioned above, which are more flexible and have more capabilities than non-mobile observations, since they exploit the time-measurement

domain in a more effective manner, thereby offering additional degrees of freedom regarding optimality. Hence, the sensors positions do not have to be assigned to the most informative points in the average sense, but they can track the ones which give at a particular time instant the most significant knowledge about the estimated parameters of interest.

Potential vital applications where such strategies can be employed were introduced in Section 2.2, e.g. the design of monitoring networks for air and water pollution, the scanning strategies in the measurement of strain and stress (smart structures) or various types of transmission lines. These are only some examples, which can be found in an extremely wide family of real engineering problems connected with dynamic DPS's.

Allowing the sensors to change their positions lead directly to the moving sensors strategy. But contributions to this field are rather limited and here the interesting results from (Uciński, 1999a; Uciński, 2000b; Uciński and Korbicz, 2001) based on the optimal control techniques can be distinguished. However, the problem and its solutions are far from being trivial. Thus, a slightly less sophisticated strategy of scanning sensors appears to be very attractive as it leads to less complex solutions and also offers an increased degree of optimality.

In such a way, the main objective here becomes a generalization of techniques proposed in the preceding chapter and dedicated to stationary sensors towards the class of dynamic DPS's and showing how to adapt modified versions of the corresponding algorithms. Moreover, complementary systematic approaches for movable and scanning sensors will be introduced with special emphasis on the latter technique.

Another problem arises when mutual relations not only between system outputs, but also between measurements made by different sensors cannot be neglected. In practical applications this is very often the case, especially in the field of DPS's, since spatio-temporal observations are commonly determined by local correlations, which are unaccounted for by standard optimal experimental design techniques delineated in Section 2.3. This is a consequence of the fact that in this case the problem formulation based on the FIM does not allow us to exploit the convexity of the relevant optimality criteria, which precludes the construction of simple sequential algorithms based on convex optimization theory. The problem is extremely difficult, since the information from different locations cannot be separated. A large majority of publications dedicated to optimal observation strategies for parameter estimation in DPS's simply neglect and omit such impediments, or treat them in a simplified form (e.g. either time or spatial correlations are taken into account). An additional objective here is to propose a suitable approach to overcome those difficulties (at least to a certain degree).

4.1. Observations from stationary sensors

Dynamic DPS's constitute a non-trivial generalization of the systems considered in the previous chapter, as their states depend not only on the space variable, but also on time t. If there are no particular assumptions on this time variable which

would make it substantially different from the space variable, then the systems with spatio-temporal dynamics can be considered exactly in the same manner as static DPS's. Consequently, the methodology developed in the previous chapter is directly applicable with no changes at all and the observations can be treated as pointwise measurements in the space-time continuum. Unfortunately, such an assumption is very inadequate and impractical since in the measurement process the time is beyond of the experimenter's control in contrast to the spatial sensor allocations $x^1, \ldots, x^N$. This feature is crucial from the point of view of a further analysis, because it entirely determines the properties of the possible observational strategies. At this point, it should be noted that the variable t can be associated with other variables such as temperature, gas pressure, radiation or any uncontrolled quantity. Depending on the situation, the results can be easily adopted to a particular case since no more specific features related to physical quantities such as time are assumed. Nevertheless, within the framework of this dissertation attention is focused on time-dependent systems owing to their great practical relevance.

In real-world problems, the data acquisition process often has to satisfy multiple criteria. Usually the measurements should provide not only information about system parameters, but also the character of the statistical trend in the system behaviour or its dynamics should be sufficiently represented. In the light of the dynamic character of the state dependence on time, it becomes clear that this can be exploited in the observation process and sensors may take the measurements according to the suitable strategy built on the system dynamics and the fact that the measurements can be taken in continuous time (in contrast to the spatial domain). From this point of view, the following two possibilities of increasing the quality of solutions (regarding their degree of optimality) can be distinguished:

- appropriately selecting spatial sensor locations, which are assumed to vary in time,
- properly choosing the time schedule of taking measurements for each sensor.

Both the cases directly lead to more complex strategies of observations, namely the use of mobile sensors in the former and scanning ones in the latter. Since a more detailed analysis of those techniques is contained in the next part of the chapter, at this point let us consider the simplest situation in which stationary sensors are used to take measurements at specified time moments or continuously in time. Such a situation is most frequently encountered in practice, as it is simple to implement. Monitoring networks used in real engineering problems (e.g. atmospheric observations) are most commonly based on stationary sensors. For this reason such an approach is worth of paying attention to.

4.1.1. Adaptation of the notion of continuous designs

For the class of dynamic DPS's, their mathematical model follows from (2.1)–(2.3) by assuming that matrix $\mathcal{D}(x,t)$ is non-zero. If the measurements are taken by N stationary sensors and, for simplicity, the n-th dimensional system state $y(x,t)$ is

assumed to be directly measurable, then the measurements are governed by the following observation equation derived from (2.9):

$$z^j(t) = y(x^j, t; \theta) + \varepsilon(x^j, t), \quad t \in T, \quad j = 1, \ldots, N, \tag{4.1}$$

where $z^j(t)$ is an r-dimensional output (in this case $r = n$), $y(x, t; \theta) \in \mathbb{R}^n$ denotes the system state at time t and a spatial point $x \in X \in \Omega \cup \partial\Omega$, $T = \{t_k,\ k = 1, \ldots, t_K : t_1 \leqslant t_1 \leqslant \cdots \leqslant t_K\}$ for the discrete case and $T = [0, t_f]$ for the continuous case. In general, the random measurements errors represented by the random field $\varepsilon^j(\,\cdot\,)$ may be correlated, but since this subject will be discussed in a broaden context in Section 4.4, at this point let us assume, by analogy to (2.37), that the errors are zero-mean and correlated only in output space, i.e. their statistics are given by the relations

$$\mathrm{E}[\varepsilon(x^j, t)] = 0, \quad \mathrm{E}[\varepsilon(x^q, t)\varepsilon^{\mathrm{T}}(x^s, \tau)] = \delta_{qs}\delta(t - \tau)C(x^q, t). \tag{4.2}$$

where $0 \leqslant C(x^j, t) \in \mathbb{R}^{n \times n}$, $\delta(\,\cdot\,)$ and δ_{qs} being Dirac's and Kronecker's delta functions, respectively.

If an observation strategy implies that the measurements are taken at any time instant $t \in T$, then this fact will directly influence the form of the criterion of parameter estimation. The generalized LS criterion takes the form

$$J(\theta) = \frac{1}{2}\sum_{j=1}^{N} \mathcal{A}_T \left\{[z^j(\,\cdot\,) - \hat{y}(x^j, \,\cdot\,; \theta)]^{\mathrm{T}} C^{-1}(x, \,\cdot\,)[z^j(\,\cdot\,) - \hat{y}(x^j, \,\cdot\,; \theta)]\right\} \tag{4.3}$$

where $\mathcal{A}_T$ is some known operator responsible for the suitable weighting of the measurements over the set of the time instants at which the observations are made and $\hat{y}(\,\cdot\,; \theta)$ is the solution to (2.1)–(2.3) corresponding to the parameter vector θ. The form of (4.3) explicitly shows that the measurements are averaged in some sense established by the weighting operator. Moreover, it is clear that they depend upon the entire time schedule, rather than on the time itself. Such an observation is of crucial importance here, since if there is no particular information concerning the significance of measurements at specified time instants (they are uniformly weighted), then the operator $\mathcal{A}_T$ is equivalent to the mean over the set T and in this context the observations have to be understood as averaged over time.

However, the arbitrary time schedule implies that the notion of exact and continuous designs can be adopted in a virtually unchanged form from static DPS's. In such a way, we shall operate only on sensor locations. Formally, after a suitable relabelling of different sensor allocations, a design can be denoted exactly in the same form as for static DPS's (2.45), i.e.

$$\xi_N(T) = \begin{Bmatrix} x^1, & x^2, & \ldots, & x^\ell \\ p_1, & p_2, & \ldots, & p_\ell \end{Bmatrix}, \tag{4.4}$$

where $p_i = r_i/N$, $N = \sum_{i=1}^{\ell} r_i$, $i = 1, \ldots, \ell$. By analogy to (2.45), the proportion p_i of the observations performed at x^i can be considered as the percentage of the

experimental effort spent at that point. In further considerations, the more concise notation ξ_N will be used to denote the exact design. Similarly, ξ will stand for the corresponding continuous design.

The above definition of the design is extremely convenient. It enables the adaptation of the entire methodology developed for static DPS's in Chapter 3 with relative ease. This results from the fact that the approaches presented for static DPS's are invariant with respect to the explicit form of the FIM. As a result, the only adaptation needed is an appropriately defined form of the FIM. The average-per-observation FIM can be written down as (Uciński, 1999a)

$$M(\xi_N) = \sum_{i=1}^{\ell} p_i \frac{1}{K} \sum_{k=1}^{K} G^{\mathrm{T}}(x^j, t_k) C^{-1}(x^j, t_k) G(x^j, t_k), \tag{4.5}$$

for the discrete case, and

$$M(\xi_N) = \sum_{i=1}^{\ell} p_i \frac{1}{t_f} \int_0^{t_f} G^{\mathrm{T}}(x^j, t) C^{-1}(x^j, t) G(x^j, t)\, \mathrm{d}t, \tag{4.6}$$

in the continuous case, where

$$G(x,t) = \left(\frac{\partial \mathcal{H}(y,t;\theta)}{\partial y} \right)_{y=y(x,t;\theta)} \left(\frac{\partial y(x,t;\theta)}{\partial \theta} \right)_{\theta=\theta^0} \tag{4.7}$$

is the matrix of the sensitivity coefficients corresponding to a prior estimate of parameters θ^0.

With the information matrices so defined the characterizations of the optimal solutions presented in Section 2.3 are almost directly applicable to the considered case, including all properties and theorems, and in particular the Equivalence Theorem. What is more, the approaches and algorithms developed in Sections 3.2.1, 3.3 (effort optimization with first-order, feasible-direction and SDP routines) and 3.2.2 (clusterization-free approach) can be easily adopted to the case of the measurements which are averaged over the time horizon, without major modifications. The only complication becomes the increased numerical effort related to the calculation of the informational matrices.

Bearing in mind that the use of stationary sensors taking measurements which are averaged over time is one of the simplest solutions and this is because it is most commonly encountered in real problems, it should be emphasized that there exist some substantial drawbacks of such an approach. The main disadvantage is that its flexibility is often insufficient to assure that the observational process will fit enough to the system dynamics. In addition to this, for systems with spatio-temporal dynamics the clusterization effect has a much more complex nature. Generally, in the estimation of m unknown parameters, a one-point design might result in a non-singular FIM in contrast to static MIMO DPS's where the minimal number of measurements which give a chance for estimation of m parameters is equal to $\lceil m/r \rceil$ ($\lceil \zeta \rceil$ stands for the minimal integer number greater than or equal to ζ). It is a direct consequence of the fact that averaging over time implies

that the rank of the information matrix for a given spatial point x^j can be equal to the number of parameters, regardless of the choice of x^j. This clarifies why sensors tend to cluster more frequently in this situation. On the other hand, we should remember that the minimal number of measurements so defined does not guarantee a high quality of estimation. Finally, because of those impediments, the applicability of the proposed algorithms needs a more careful analysis and more flexible approaches are necessary, such as mobile or scanning sensors. This constitutes the further part of the chapter where a suitable comparison of the discussed strategies will be presented.

4.2. Spatially movable sensors

When adapting the idea of continuous designs to the field of movable observations, it has to be emphasized that the connection between the classical experimental design theory and the problem of determining optimal sensor movements is beyond doubt rather complex. The main obstacle is the representation of the sensor motion trajectories in the form of generalized conditional distributions, or more precisely, Radon probability measures on the Borel sets of a given compact set of admissible locations (Rafajłowicz, 1986b; Uciński, 1999a). Despite this impediment, however, some relevant approaches can still be established and successfully applied.

4.2.1. Direct approach

The direct approach proposed by Rafajłowicz (1986b) for the scalar case has become one of the very scare classical references on moving sensors. It was then complemented by Uciński (1999a). In what follows, another generalization will be presented. Denote by X the compact set, in which the state $y \in \mathbb{R}^n$ of a DPS can be measured.

Definition 4.1. The mapping $T \ni t \mapsto x(t) \in X$, where $x(\,\cdot\,)$ is measurable in the Lebesgue sense, stands for the **trajectory** of the sensor motion.

The term 'trajectory' is used to emphasize the dependence of $x(t)$ on time. Such trajectories are elements of the corresponding design space. For discrete-time observations, i.e. $T = \{t_k,\ k = 1, \ldots, K : t_1 \leqslant t_1 \leqslant \cdots \leqslant t_K\}$ the trajectory of the j-th sensor may be interpreted as a vector containing a series of observations that are taken at consecutive time moments t_k, i.e.

$$x^j = [x^j(t_1), \ldots, x^j(t_K)]^{\mathrm{T}}. \tag{4.8}$$

For the continuous observation interval $T = [0, t_f]$, each trajectory is determined by an observation curve for the j-th sensor

$$x^j(t) \in X, \quad \text{a.e. on } T. \tag{4.9}$$

Now we can formulate our main objective, which is the design of an optimal measurement strategy for estimation of the unknown system parameter vector

$\theta \in \mathbb{R}^m$, while the observations are made by N pointwise sensors. Reasoning will be provided for the continuous time domain, as it is a more general situation and a suitable discretization a finite set T can be proposed with no difficulties. Thus, the observation equation is then given by (2.10), which can be rewritten in the following simplified form:

$$z^j(t) = y(x^j(t), t; \theta) + \varepsilon(x^j(t), t), \quad t \in T, \quad j = 1, \ldots, N, \tag{4.10}$$

where $z^j(t)$ is the r-dimensional output, $y(x, t; \theta) \in \mathbb{R}^n$ denotes the system state at time t and a spatial point $x \in \Omega \cup \partial\Omega$, and $\varepsilon^j(\,\cdot\,)$ denotes the measurement noise, which is assumed to be a realization of a white Gaussian random field with statistics defined by

$$\mathrm{E}[\varepsilon(x,t)] = 0, \quad \mathrm{E}[\varepsilon(x,t)\varepsilon^{\mathrm{T}}(\chi,\tau)] = \delta(x-\chi)\delta(t-\tau)C(x,t), \tag{4.11}$$

where $0 \leqslant C(x,t) \in \mathbb{R}^{n\times n}$ and $\delta(\,\cdot\,)$ stands for Dirac's delta function. According to (4.11), correlations between observations on the same trajectory may occur, but observations from different trajectories are not correlated. This fact is crucial for the approach as the additivity of the information matrices for measurements from different trajectories is assured.

Another important assumption is that there exists a neighbourhood of some known preliminary estimate θ^0 of the unknown parameter θ where the state $y(x, t; \,\cdot\,)$ is continuously differentiable with respect to θ. In such a way, the average Fisher information matrix is given by (Uciński, 1999a)

$$M = \frac{1}{Nt_f} \int_0^{t_f} \left\{ \sum_{j=1}^{N} G^{\mathrm{T}}(x^j(t),t) C^{-1}(x^j(t),t) G(x^j(t),t) \right\} \mathrm{d}t, \tag{4.12}$$

where $G(x,t)$ defined by (4.7) is required to be continuous in $\bar{\Omega} \times T$.

On the other hand, the assumption of independent measurements leads directly to the clusterization effect for some time moments, i.e. at a given time moment more than one sensor may take measurements at a point $x^j(t)$. Taking this into account, by suitably relabelling the sensors (i.e. such that $i_1 \neq i_2 \Rightarrow x^{i_1}(t) \neq x^{i_2}(t)$, $1 \leqslant i_1, i_2 \leqslant \ell(t)$ where $\ell(t)$ is the number of different sensor locations at time t) the following collection of variables may be introduced by analogy to exact design for a specified time moment t:

$$\xi_N(t) = \begin{Bmatrix} x^1(t) & \ldots & x^{\ell}(t) \\ p_1(t) & \ldots & p_{\ell}(t) \end{Bmatrix}, \tag{4.13}$$

where $p_i(t) = r_i(t)/N$, $\sum_{i=1}^{\ell(t)} r_i(t) = 1$ and $r_i(t)$ denotes the number of sensors occupying the position $x^i(t)$. Hence the FIM may be rewritten as

$$M(\xi_N) = \frac{1}{t_f} \int_0^{t_f} \left\{ \sum_{i=1}^{\ell(t)} p_i(t) G^{\mathrm{T}}(x^i(t),t) C^{-1}(x^i(t),t) G(x^i(t),t) \right\} \mathrm{d}t. \tag{4.14}$$

Analogously to the case of stationary sensors, the notion of the exact design can be extended to the more general form of a probability measure ξ over X, which can be considered as a function

$$\xi : T \ni t \mapsto \xi(\mathrm{d}x|t) \in \Xi_t(X) \tag{4.15}$$

where $\Xi_t(X)$ is the set of all probability measures on X. In our further considerations, $\Xi(X)$ will be understood as the family of all such mappings ξ.

This yields the following form of the FIM:

$$M(\xi) = \frac{1}{t_f} \int_0^{t_f} \left\{ \int_X G^{\mathrm{T}}(x,t) C^{-1}(x,t) G(x,t)\, \xi(\mathrm{d}x|t) \right\} \mathrm{d}t \tag{4.16}$$

Introducing a fixed measure $\xi(\mathrm{d}t)$ of the observation effort in the interval T, we arrive at a further generalization, i.e.

$$\begin{aligned} M(\xi) &= \int_T \left\{ \int_X G(x,t)^{\mathrm{T}} C^{-1}(x,t) G(x,t)\, \xi(\mathrm{d}x|t) \right\} \xi(\mathrm{d}t) \\ &= \iint_{X\times T} G^{\mathrm{T}}(x,t) C^{-1}(x,t) G(x,t)\, \xi(\mathrm{d}x, \mathrm{d}t), \end{aligned} \tag{4.17}$$

with the marginal distribution defined as

$$\xi(\mathrm{d}t) = \int_X \xi(\mathrm{d}x, \mathrm{d}t). \tag{4.18}$$

Notice that the identity $\xi(\mathrm{d}t) \equiv \mathrm{d}t/t_f$ corresponds to the uniform distribution of the experimental effort. In other words, $\xi(\mathrm{d}t)$ defines a 'density' of replications.

The problem of finding an optimal observation strategy problem can be reformulated as follows:

$$\xi^\star = \arg \min_{\xi \in \Xi(X)} \Psi[M(\xi)], \tag{4.19}$$

where $\xi(\mathrm{d}t)$ is assumed to be fixed *a priori*. Obviously, introduction of the measure

$$\xi(\mathrm{d}t) = \frac{1}{t_f}\, \mathrm{d}t \tag{4.20}$$

brings us back to (4.16). The time dependent measure $\xi^\star(\mathrm{d}x|t)$ can be considered as the optimal generalized trajectory.

To transfer the results from the standard case (stationary sensors), conditions (A3)–(A5) from page 38 are assumed to be satisfied and instead of (A6) the following assumption is necessary:

(A8) $\forall \xi \in \Xi_q = \{\xi : \Psi[M(\xi)] \leqslant q < \infty\}, \forall \bar{\xi} \in \Xi(X)$,

$$\Psi[(1-\alpha)M(\xi) + \alpha M(\bar{\xi})] = \Psi[M(\xi)] + \alpha \iint_{X\times T} \psi(x,t,\xi) \bar{\xi}\,(\mathrm{d}x, \mathrm{d}t) + o(\alpha; \xi, \bar{\xi})$$

where the scalar q is chosen so that $\Xi_q \neq \emptyset$.

For differentiable criteria Ψ, we have

$$\begin{aligned}\Delta\Psi\big(M(\xi),M(\bar{\xi})\big) &= \left.\frac{\partial\Psi[(1-\alpha)M(\xi)+\alpha M(\bar{\xi})]}{\partial\alpha}\right|_{\alpha=0^+}\\ &= \operatorname{trace}\Big[\overset{\circ}{\Psi}[M(\xi)]\big(M(\bar{\xi})-M(\xi)\big)\Big]\\ &= \iint_{X\times T}\Big\{\operatorname{trace}\Big[\overset{\circ}{\Psi}[M(\xi)]G^{\mathrm{T}}(x,t)C^{-1}(x,t)G(x,t)\Big]\\ &\quad-\operatorname{trace}\Big[\overset{\circ}{\Psi}[M(\xi)]M(\xi)\Big]\Big\}\,\bar{\xi}(\mathrm{d}x,\mathrm{d}t),\end{aligned} \tag{4.21}$$

where

$$\overset{\circ}{\Psi}[M(\xi)] = \left.\frac{\partial\Psi(M)}{\partial M}\right|_{M=M(\xi)}$$

Hence, the function $\psi(x,t,\xi)$ takes the form

$$\psi(x,t,\xi) = \varsigma(\xi) - \phi(x,t,\xi), \tag{4.22}$$

where

$$\varsigma(\xi) = -\operatorname{trace}\Big[\overset{\circ}{\Psi}[M(\xi)]M(\xi)\Big] \tag{4.23}$$

and

$$\phi(x,t,\xi) = -\operatorname{trace}\Big[G^{\mathrm{T}}(x,t)\overset{\circ}{\Psi}[M(\xi)]G(x,t)C^{-1}(x,t)\Big]. \tag{4.24}$$

At this point, the following necessary and sufficient condition for optimality can be formulated:

Theorem 4.1. *A design $\xi^\star$ is optimal iff*

$$\int_T \min_{x\in X}\psi(x,t,\xi^\star)\,\xi(\mathrm{d}t) = 0. \tag{4.25}$$

***Proof*.** See Appendix A.3. ■

In such a way, it is possible to formulate the following version of the general equivalence theorem:

Corollary 4.2. *The following statements are equivalent*

(i) the design $\xi^\star$ minimizes $\Psi[M(\xi)]$,

(ii) the design $\xi^\star$ minimizes $\displaystyle\int_T \max_{x\in X}\phi(x,t,\xi)\,\bar{\xi}(\mathrm{d}t) - \varsigma(\xi)$, and

(iii) $\displaystyle\int_T \max_{x\in X}\phi(x,t,\xi^\star)\bar{\xi}(\mathrm{d}t) = \varsigma(\xi^\star)$

Corollary 4.2 constitutes a generalization of Rafajłowicz's result for D-optimum designs (Rafajłowicz, 1986b, Th. 1). Moreover, in (Rafajłowicz, 1986b) some further sufficient optimality conditions are given, whose use allows us to reduce the problem to a series of optimization problems for each time moment separately.

4.2.2. Parameterization of the trajectories

The main drawback of the approach delineated in the previous section is that the resulting trajectories are only guaranteed to be measurable in the Lebesgue sense, which may be insufficient in real applications. Such a complication can be avoided by an appropriate parameterization of the trajectories. In such a way, some conditions can be imposed on the regularity of the solutions and, additionally, the dimension of the optimization problem can sometimes can be reduced.

To focus our attention, assume that the sensor trajectories can be approximated by the parametric curves of the form

$$x^j(t) = \kappa(t, \zeta^j), \quad t \in T, \tag{4.26}$$

where ζ^j is a constant parameter vector belonging to a compact set $A \subset \mathbb{R}^s$. Here κ denotes a known function which is assumed to be sufficiently flexible to approximate the trajectory of the j-th sensor. Moreover, it is required that for any values of ζ^j and t, functions $\kappa(\,\cdot\,, \zeta^j)$ and $\kappa(t, \,\cdot\,)$ be continuous. Restricting our attention to the trajectories lying completely inside the set of admissible locations X (i.e. each point of the trajectory belongs to X), we assume the existence of a non-empty set

$$Z = \{\zeta \in A : \kappa(t, \zeta) \in X, \forall t \in T), \} \tag{4.27}$$

which is rather natural and not particularly restrictive in practice. It can be easily verified that Z is also compact.

From now on it is easy to derive the following form of the average FIM for N moving sensors:

$$M = \frac{1}{N t_f} \int_0^{t_f} \left\{ \sum_{j=1}^{N} G^{\mathrm{T}}\big(\kappa(t, \zeta^j), t\big) C^{-1}\big(\kappa(t, \zeta^j), t\big) G\big(\kappa(t, \zeta^j), t\big) \right\} \mathrm{d}t. \tag{4.28}$$

Obviously, from (4.28) it can be seen that the independent measurements taken by different sensors is exploited here, thereby leading to the allowance of replicated trajectories. By suitably relabelling and thus distinguishing ℓ different paths of sensors, we get

$$M(\xi_N) = \frac{1}{t_f} \int_0^{t_f} \left\{ \sum_{i=1}^{\ell} p_i(t) G^{\mathrm{T}}\big(\kappa(t, \zeta^i), t\big) C^{-1}\big(\kappa(t, \zeta^i), t\big) G\big(\kappa(t, \zeta^i), t\big) \right\} \mathrm{d}t, \tag{4.29}$$

with a new formulation of the design

$$\xi_N = \begin{Bmatrix} \zeta^1 & \zeta^2 & \dots & \zeta^\ell \\ p_1 & p_2 & \dots & p_\ell \end{Bmatrix} \tag{4.30}$$

$p_i = r_i/N$, r_i being the number of sensors moving along the i-th curve.

In terms of the designs interpreted as generalized probability measures ξ for all Borel sets of Z including single points, the counterpart of (4.29) can be defined as

$$M(\xi) = \int_Z \Upsilon(\zeta)\, \xi(\mathrm{d}\zeta), \tag{4.31}$$

where

$$\Upsilon(\zeta) = \frac{1}{t_f} \int_0^{t_f} G^{\mathrm{T}}\big(\kappa(t,\zeta),t\big) C^{-1}\big(\kappa(t,\zeta),t\big) G\big(\kappa(t,\zeta),t\big)\, \mathrm{d}t. \tag{4.32}$$

If the optimal design $\xi^\star$ is understood as the one which minimizes the scalar measure $\Psi[M(\xi)]$, it is clear that the form of the reformulated problem is exactly the same as that from Section 2.3.1 (p. 36) with ζ, Z and $G^{\mathrm{T}}\big(\kappa(t,\zeta),t\big)$ substituted for x, X and $F(x,t)$, respectively. As a result, the corresponding theory, characterizations of solutions and other results remain valid in this context. Furthermore, note that the dimension of this optimization problem is s, the dimension of vector ζ.

In addition to the dimensionality reduction, the approximation (4.26) offers a possibility of imposing various constraints on the trajectories. For instance, a limited velocity of the motion of the i-th sensor can be expressed in the form of the constraint

$$\|\partial\kappa(t,\zeta^i)/\partial t\|^{1/2} \leqslant V_i, \quad t \in T \tag{4.33}$$

whereas the bounded length of the same trajectory can be introduced as

$$\int_0^{t_f} \|\partial\kappa(t,\zeta^i)/\partial t\|\, \mathrm{d}t \leqslant L_i. \tag{4.34}$$

In spite of the relative simplicity of the ideas presented above, the main drawback of the outlined approach still remains a high computational cost. To provide a sufficient approximation of the trajectories and to ensure their appropriate flexibility (the family of admissible movement curves should be rich enough), the size of the parameter vector ζ has to be much larger than in the case of stationary sensors, where the size of the design variable was simply equal to the number of spatial coordinates. Furthermore, the most cumbersome phase of the algorithm presented in Section 3.3 is solving the global non-linear constrained programming problem in each iteration. The problem becomes extremely hard in the context of systems with spatio-temporal dynamics, since we are faced with the necessity of solving both systems of PDE's, and optimization problems of high complexity, which demands multidisciplinary approaches.

Obviously, an efficient global optimizer should be employed and one of the possible solutions is a combination of stochastic global optimizers with classical methods of hard selection. In computer simulations performed in this work the ARS strategy (cf. Section 3.3) was exploited in conjunction with the sequential quadratic programming algorithm employed during the local search. The scheme of such a hybrid algorithm is presented in Fig. 4.1. The aim of the ARS strategy is to establish a rough estimate of the optimal trajectory lying in the convergence

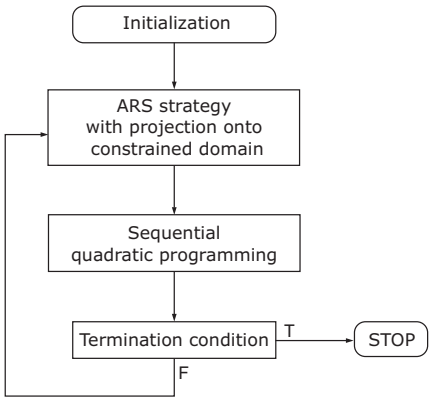


Fig. 4.1 . Hybrid ARS strategy enhanced with sequential quadratic programming.

region of the method used for local optimization. In such a way, emphasis should be put on the exploratory performance of the algorithm, and not on the accuracy. Then the sequential quadratic programming is applied to the solution produced by the ARS with the goal of determining an accurate approximation of the optimal solution. Nevertheless, having in mind that the ARS strategy is not dedicated to constrained optimization tasks the problem of the projection onto the set of admissible trajectories appears, which may lead to an additional optimization subproblem for some non-linear constraints.

Consequently, the computational burden connected with the proposed approach usually remains quite heavy. However, such a cost is unavoidable when trying to increase the degree of freedom regarding optimality. It is then necessary to search and to develop alternative approaches which would minimize the numerical effort spent on finding a solution. In this context, some techniques of optimizing measurement schedules based on optimal-control theory are indicated in (Uciński, 2000c; Uciński, 2000b; Uciński, 2001; Uciński and Korbicz, 2001; Uciński, 1999a).

In order to illustrate the potential benefits of applying mobile sensors in implementation of the observational strategies, let us consider the following example.

Example 4.1. For the sake of comparison with the case of stationary sensors, it is worth to consider a less sophisticated problem which possesses a closed-form solution. For this reason, we study signal propagation over an infinite one-dimensional transmission line over the time interval $T = [0, 1]$ governed by the homogeneous wave equation of the form

$$\frac{\partial^2 y(x,t)}{\partial t^2} = \theta^2 \nabla^2 y(x,t), \quad -\infty \leqslant x \leqslant \infty, \quad 0 < t \leqslant 1, \tag{4.35}$$

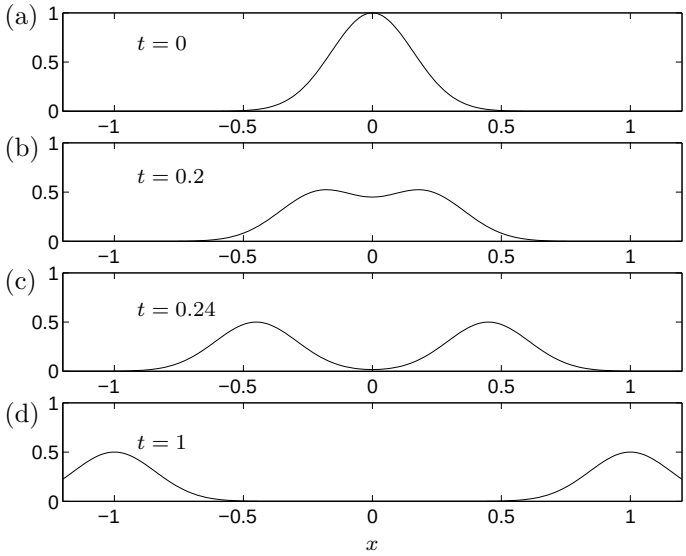


Fig. 4.2. Propagation of a voltage impulse in the infinite transmission line from Example 4.1.

subject to the initial conditions

$$\begin{cases} y(x,0) = \exp(-20x^2) & -\infty \leqslant, x \leqslant \infty, \\ \left.\dfrac{\partial y(x,t)}{\partial t}\right|_{t=0} = 0, & -\infty \leqslant x \leqslant \infty. \end{cases} \tag{4.36}$$

The initial Cauchy problem above describes the propagation of a voltage impulse with amplitude y and velocity θ along the line. From a practical point of view, the assumption of an infinite length of the line is not too abstract as the distributed nature of such a system appears when its dimensions are much greater than the wavelength of the signal.

The considered problem posseses a closed-form solution of the fundamental form

$$y(x,t) = \frac{1}{2}\exp\big(-20(x-\theta t)^2\big) + \frac{1}{2}\exp\big(-20(x+\theta t)^2\big). \tag{4.37}$$

Moreover, the process is symmetric with respect to the central point $x = 0$. The propagation of the signal is shown in Fig. 4.2.

Our task consists in finding a best allocation for stationary sensors and then trajectories of mobile sensors which assure the best estimate of the velocity θ, whose nominal value is assumed to be equal to $\theta^0 = 1.0$. As this velocity is finite, the measurement space X can be arbitrarily bounded by the appropriate fixed values $x_{\min}$ and $x_{\max}$, such that $X = \{x : x_{\min} \leqslant x \leqslant x_{\max}\}$. The identification of one unknown system parameter in this case can be performed with the use of only one sensor, i.e. $\ell = 1$. The form of the FIM in such a situation can be represented

as

$$\begin{aligned} M(\chi(\,\cdot\,)) &= \int_0^{t_f} \left(\frac{\partial y(\chi(t), t; \theta)}{\partial \theta} \right)^2_{\theta=\theta^0} \mathrm{d}t \\ &= \int_0^1 \Big(20(\chi(t) - t) t \exp\big(-20(\chi(t) - t)^2 \big) \\ &\quad - 20(\chi(t) + t) t \exp(-20\big(\chi(t) + t\big)^2) \Big)^2 \mathrm{d}t. \end{aligned} \tag{4.38}$$

Since we have only one parameter to be estimated, the FIM reduces to a scalar. Thus, the minimum of any optimality criterion defined on the FIM corresponds to the maximum value of the FIM. To determine an optimal trajectory $\chi(\,\cdot\,)$, we have to solve the variational problem of maximizing of the functional (4.38) with respect to the motion curve $\chi(\,\cdot\,)$. Unfortunately, the exact solution does not posses a closed form, however it can be easily found numerically, since for any time moment t the optimal sensor location corresponds to the maximum of the integrand in (4.38). Moreover, from Fig. 4.2 it is clear that the signal is the superposition of two interfering exponential impulses which start at the point $x = 0$ and then propagate in opposite directions. If these symmetrical pulses are relatively 'narrow', then after some short transient period the mutual interference can be neglected, which dramatically simplifies this problem. In such a case the optimal trajectories can be approximated by the functions which describe the motion of the extrema of the sensitivity $\partial y/\partial\theta$ for each single impulse separately. It is easy to verify that these extrema of the signal (4.37) move according to

$$\chi^\star(t) \approx \pm t \pm \frac{\sqrt{2}}{2\sqrt{20}}, \tag{4.39}$$

which constitutes the desired approximation of the optimal solution. Furthermore, due to the symmetry of the problem, any design with support points being a combination of the trajectories above is also optimal. The value of the optimality criterion is in this case equal to $M(\chi^\star(t)) \approx 2.7065$.

A solution for the case of a stationary sensor can be obtained by reduction of the trajectory to a constant function independent of time, i.e. $\chi(t) = \chi$. Then we obtain the one-dimensional optimization problem of maximizing the FIM in the form

$$\begin{aligned} M(\chi) &= \int_0^{t_f} \left(\frac{\partial y(\chi, t; \theta)}{\partial \theta} \right)^2_{\theta=\theta^0} \mathrm{d}t \\ &= \frac{1}{640} \Big(\sqrt{10\pi}(3+80\chi^2)\big(\operatorname{erf}(2\sqrt{10} - 2\chi\sqrt{10}) + \operatorname{erf}(2\sqrt{10} + 2\chi\sqrt{10}) \big) \\ &\quad + (6 - 160\chi^2)\sqrt{10\pi} \operatorname{erf}(2\sqrt{10}) \exp\left(-40\chi^2\right) + \big(6400\chi^2 - 6640 \\ &\quad + 6320 \sinh\left(80\chi\right) - 6640 \cosh\left(80\chi\right)\big) \exp\left(-40\chi^2 - 40\right) \Big) \end{aligned} \tag{4.40}$$

where

$$\operatorname{erf}(\alpha) = \frac{2}{\sqrt{\pi}} \int_0^\alpha \exp\left(-\zeta^2\right) \mathrm{d}\zeta$$

stands for a so-called error function (Redfern, 1996).

It could hardly be expected that a solution in a simple closed form exists, but a numerical solution to this problem can be achieved rather easily. Due to the problem symmetry, any of the locations

$$\chi^\star \approx \pm 0.7371$$

is an approximate solution with the criterion value $M(\chi^\star) \approx 1.3763$ which is almost half of the corresponding value for the movable sensor strategy. It thus becomes clear why it is worth of paying attention to an optimal exploitation of the sensor motion dynamics through more flexible observation strategies.

In order to solve this problem numerically, the hybrid ARS strategy with sequential quadratic programming was implemented in Fortran/Fujitsu Fortran 95 v.5.6 to establish the approximations of optimal sensors trajectories which assure as accurate estimation of the parameter θ as possible. The time interval was partitioned into 20 subintervals determined by the grid $t_k = k/2$, $k = 0, \ldots, 20$. According to this partitioning, the trajectories were parameterized with the use of linear splines, i.e. any trajectory was uniquely established with a vector of 21 spatial positions corresponding to discrete time instants. From a randomly generated two-point initial design, the algorithm achieved an approximation of the optimal trajectory after only 3 iterations (about 10 on Pentium IV 1.7GHz, 768MB RAM under Windows 2000) with accuracy $\epsilon \leqslant 10^{-4}$. The results are shown in Fig. 4.3(a) with one of possible analytical solutions. Open circles indicate consecutive sensor positions at evenly distributed time intervals. The starting positions and weights assigned to the trajectories are additionally indicated.

For comparison, the same problem was solved for the case of stationary sensors with the use of a two-phase first-order algorithm with the ARS global optimizer from Section 3.3 and the same accuracy of the solution. The resulting optimal design obtained in two iterations was

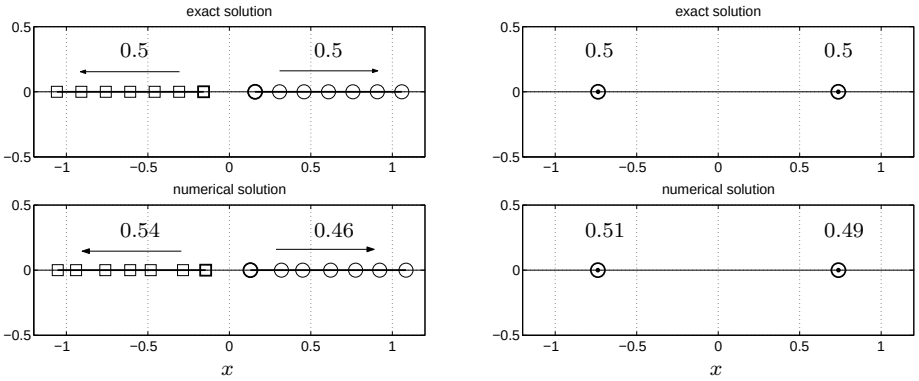
$$\xi^\star = \begin{Bmatrix} -0.7382 & 0.738 \\ 0.4942 & 0.5058 \end{Bmatrix} \tag{4.41}$$

and is shown in Fig. 4.3(b) together with the 'exact' solution.

In the problem above both the algorithms proved their advantages, but we have to realize that the considered example is not too sophisticated. In more complex situations, experiments reveal that the numerical effectiveness dramatically decreases due to obvious reasons, especially in the case of mobile sensors owing to the necessity of solving global optimization problems in high-dimensional search spaces which result from trajectory discretizations.

★

Remark 4.1. There is another very important interpretation of the sensors weights which has not been mentioned yet, although it has significance for movable observations and could be exploited here. Based on the generalized weighted least-squares



(a) (b)

Fig. 4.3. Optimal solutions and their approximations: (a) mobile sensors, (b) stationary sensors.

method where the performance index

$$J(\theta) = \frac{1}{2}\sum_{j=1}^{N}\int_{T} w_j[z^j(t) - \hat{y}(x^j(t),t;\theta)]^{\mathrm{T}} C^{-1}(x^j(t),t)[z^j(t) - \hat{y}(x^j(t),t;\theta)]\,\mathrm{d}t \tag{4.42}$$

is minimized, each weight can be interpreted as the reciprocal of the variance of the observation error along a given trajectory

$$w_j = \sigma^{-2}(x^j(t),t), \quad j = 1,\ldots,N. \tag{4.43}$$

Thus we may think of the weights as the sensitivities of the measurement devices. Such an interpretation is not only very reasonable, but also very practical from an engineering point of view, as it allows us to include such considerations into the analysis of the experiment without essential changes.

4.3. Scanning sensors

Notwithstanding the fact that the optimal measurement problem for spatially movable sensors seems to be very attractive from the viewpoint of the degree of optimality, it is inherently connected to high computational costs and complex implementations. Such circumstances bring about the necessity of searching for alternative strategies of taking measurements which would offer an increased degree of optimality and minimize the numerical effort. It has to be pointed out that, in general, mobile observations can be proposed for a limited set of problems and then they become the best strategy.

In some situations, however, the observation system comprises multiple sensors whose positions are already specified and it is desired to activate only a subset of them during a given time interval while the other sensors remain dormant (Demetriou, 2000). A reason for not using all the available sensors could be

the reduction of the observation system complexity and the cost of operation and maintenance (van de Wal and de Jager, 2001). Such a scanning strategy of taking measurements can be also interpreted in terms of several sensors which are mobile. To the best the of author's knowledge, the problem has received no attention yet (though some attempts have been made in a related area of state estimation, see e.g. (Nakano and Sagara, 1988; Korbicz, 1991)), except for the approaches proposed in (Uciński and Patan, 2002a; Patan and Uciński, 2003). Therefore the aim of the present section is to outline some constructive methodology to fill this gap.

4.3.1. Fixed switching schedule

4.3.1.1. Problem decomposition and notation

When the number of sensors is relatively high and the sensor switchings are arbitrarily fixed (i.e. the discretization of the time interval is known *a priori*), a first idea is to decompose the problem into a series of subproblems defined for given time instants and suitable adaptation of the clusterization-free strategy set forth in Section 3.2.2.

The DPS under consideration is defined by (2.1)–(2.3) in a simply-connected open spatial domain $\Omega \subset \mathbb{R}^d$, and its state at spatial point $x \in \Omega$ and time instant $t \in T = [0, t_f]$, $t_f < \infty$, is an n-dimensional vector $y(x, t; \theta)$. As usual, θ represents an unknown constant parameter vector which must be estimated using observations of the system.

In what follows, we form an arbitrary partition of the time interval T by choosing points $0 < t_1 < t_2 < \cdots < t_K = t_f$ defining subintervals $T_k = [t_{k-1}, t_k]$, $k = 1, \ldots, K$. We then consider N moving sensors which possibly change their locations at the beginning of each time subinterval but then remain stationary till the end of this subinterval. In other words, the measurement process can be formally represented in the form of the output equation (2.8), or assuming that the state is directly measured, by its simpler version

$$z^j(t) = y(x_k^j, t; \theta) + \varepsilon(x_k^j, t), \quad t \in T_k \tag{4.44}$$

for $j = 1, \ldots, N$ and $k = 1, \ldots, K$, where $z^j(t)$ is an r-dimensional output, $x_k^j \in X$ stands for the location of the j-th sensor on the subinterval T_k, X signifies the part of Ω where the measurements can be made, and $\varepsilon(\,\cdot\,, \cdot\,)$ denotes the zero-mean, Gaussian and white measurement noise defined with exactly the same characteristics as for the case of mobile sensors (4.11).

Sensor positions which guarantee the best accuracy of the least-squares estimates of θ are then found by choosing x_k^j for $j = 1, \ldots, N$ and $k = 1, \ldots, K$ so as to minimize a scalar measure of performance Ψ defined on the average FIM, which takes here the form (Rafajłowicz, 1986b)

$$M = \frac{1}{N} \sum_{k=1}^{K} \sum_{j=1}^{N} \Upsilon_k(x_k^j), \tag{4.45}$$

where

$$\Upsilon_k(x)=\frac{1}{t_f}\int_{T_k} G^{\mathrm{T}}(x,t)C^{-1}(x,t)G(x,t)\,\mathrm{d}t,\quad G(x,t)=\left(\frac{\partial y(x,t;\theta)}{\partial\theta}\right)_{\theta=\theta^0}, \tag{4.46}$$

θ^0 stands for a prior estimate to the unknown parameter vector θ, G means the Jacobi matrix of the sensitivity coefficients defined on the analogy of (4.7) and C denotes the positive definite matrix responsible for the correlations between the outputs, which is constructed in the same manner as in (4.11).

Owing to the assumption of independent measurements made by different sensors (i.e. replicated observations), we may distinguish only different sensor locations in each time interval and define the exact design of the experiment for subinterval T_k so that it consists of the following collection of variables:

$$\xi_k^N=\begin{Bmatrix} x_k^1, & x_k^2, & \dots, & x_k^{\ell(k)} \\ p_k^1, & p_k^2, & \dots, & p_k^{\ell(k)} \end{Bmatrix}, \tag{4.47}$$

where $\ell(k)$ and $r_k^1,\dots,r_k^{\ell(k)}$ denote the number of different locations and the numbers of replications corresponding to the k-th time subinterval, respectively. Obviously, for all k we have $p_k^i=r_k^i/N$, $N=\sum_{i=1}^{\ell(k)} r_k^i$, $i=1,\dots,\ell(k)$.

On account of the above remarks, the FIM can be rewritten in the form

$$M(\xi_N)=\sum_{k=1}^{K}\sum_{i=1}^{\ell(k)} p_k^i\,\Upsilon_k(x_k^i). \tag{4.48}$$

Relaxing the notion of the design, we obtain the equivalent notation in terms of the probability measures ξ_k:

$$M(\xi)=\sum_{k=1}^{K}\int_X \Upsilon_k(x)\,\xi_k(\mathrm{d}x), \tag{4.49}$$

where

$$\xi=(\xi_1,\dots,\xi_K) \tag{4.50}$$

and, by definition, we have

$$\int_X \xi_k(\mathrm{d}x)=1,\quad k=1,\dots,K. \tag{4.51}$$

The integration in (4.51) and (4.49) is to be understood in the Lebesgue-Stieltjes sense.

Then we redefine the optimal design as a solution to the optimization problem

$$\xi^\star=\arg\min_{\xi\in\Xi(X)}\Psi[M(\xi)], \tag{4.52}$$

where $\Xi(X)$ denotes the set of all designs of the form (4.50).

To provide a suitable reasoning for the scanning approach, the validity of the conditions (A1)–(A5) from pages 34 and 38 is assumed and in place of (A6) the following counterpart is taken, which will be used in the remainder of this section:

(A9) $\forall \xi \in \Xi_q = \{\xi : \Psi[M(\xi)] \leqslant q < \infty\} \neq \emptyset$, $\forall \bar{\xi} \in \Xi(X)$:

$$\Psi[(1-\alpha)M(\xi) + \alpha M(\bar{\xi})] = \Psi[M(\xi)] + \alpha \sum_{k=1}^{K} \int_X \psi_k(x,\xi)\, \bar{\xi}_k(\mathrm{d}x) + o(\alpha;\xi,\bar{\xi}). \tag{4.53}$$

Just as in the previous considerations regarding stationary and mobile sensors, Assumption (A9) simply amounts to the existence of the directional derivative whose form must be on one hand specific, but on the other hand, for most practical criteria such a condition is not particularly restrictive.

In fact, requiring Ψ to be differentiable with respect to the individual elements of its matrix argument, we obtain

$$\psi_k(x,\xi) = \underbrace{\operatorname{trace}\Big[\mathring{\Psi}[M(\xi)]\Upsilon_k(x)\Big]}_{-\phi_k(x,\xi)} - \underbrace{\operatorname{trace}\Big[\mathring{\Psi}[M(\xi)]M_k(\xi_k)\Big]}_{-\varsigma_k(\xi)}, \tag{4.54}$$

where

$$\mathring{\Psi}[M(\xi)] = \left.\frac{\partial \Psi(M)}{\partial M}\right|_{M=M(\xi)}.$$

In order to establish the main result, which is only the matter of a suitable formulation of the conclusions resulting from the considerations above, we first give some auxiliary assertions being counterparts of Lemmas 2.6 (p. 40) and 2.7 (p. 40).

Lemma 4.3. *For any design $\xi = (\xi_1, \ldots, \xi_K) \in \Xi(X)$ and all $k = 1, \ldots, K$ we have*

(i) $\displaystyle\int_X \phi_k(x,\xi)\, \xi_k(\mathrm{d}x) = \varsigma_k(\xi)$, *and*

(ii) $\displaystyle\max_{x\in X} \phi_k(x,\xi) \geqslant \varsigma_k(\xi)$.

Proof. From (4.54), we obtain

$$\begin{aligned}\int_X \phi_k(x,\xi)\, \xi_k(\mathrm{d}x) &= -\int_X \operatorname{trace}\Big[\mathring{\Psi}[M(\xi)]\Upsilon_k(x)\Big]\, \xi_k(\mathrm{d}x) \\ &= -\operatorname{trace}\left[\mathring{\Psi}[M(\xi)] \int_X \Upsilon_k(x)\, \xi_k(\mathrm{d}x)\right] \\ &= -\operatorname{trace}\Big[\mathring{\Psi}[M(\xi)]M_k(\xi_k)\Big] = \varsigma_k(\xi).\end{aligned} \tag{4.55}$$

This establishes (i). Then

$$\varsigma_k(\xi) = \int_X \phi_k(x,\xi)\, \xi_k(\mathrm{d}x) \leqslant \int_X \max_{x\in X} \phi_k(x,\xi)\, \xi_k(\mathrm{d}x) = \max_{x\in X} \phi_k(x,\xi), \tag{4.56}$$

which proves the second claim of the lemma. ■

Lemma 4.4. *If* $\xi = (\xi_1, \ldots, \xi_K) \in \Xi_q$, $\bar{\xi} = (\bar{\xi}_1, \ldots, \bar{\xi}_K) \in \Xi(X)$ *and* $\xi_\alpha = (1-\alpha)\xi + \alpha\bar{\xi}$, *then*

$$\left.\frac{\partial \Psi[M(\xi_\alpha)]}{\partial \alpha}\right|_{\alpha=0^+} = \varsigma(\xi) - \sum_{k=1}^{K} \int_X \phi_k(x,\xi)\, \bar{\xi}_k(\mathrm{d}x),$$

where

$$\varsigma(\xi) = \sum_{k=1}^{K} \varsigma_k(\xi).$$

Proof. Taking into account (4.53) and (4.54), we have

$$\begin{aligned}
&\left.\frac{\partial \Psi[M(\xi_\alpha)]}{\partial \alpha}\right|_{\alpha=0^+} \\
&\quad = \sum_{k=1}^{K} \int_X \left\{ \mathrm{trace}\left[\overset{\circ}{\Psi}[M(\xi)] \Upsilon_k(x) \right] - \mathrm{trace}\left[\overset{\circ}{\Psi}[M(\xi)] M(\xi_k) \right] \right\} \bar{\xi}(\mathrm{d}x) \qquad (4.57) \\
&\quad = -\sum_{k=1}^{K} \int_X \phi_k(x,\xi)\, \bar{\xi}_k(\mathrm{d}x) + \sum_{k=1}^{K} \varsigma_k(\xi).
\end{aligned}$$

■

Now, it is possible to formulate the Equivalence Theorem for the scanning strategy

Theorem 4.5. *The following statements are equivalent:*

(i) the design $\xi^\star = (\xi_1^\star, \xi_2^\star, \ldots, \xi_K^\star)$ *minimizes* $\Psi[M(\xi)]$,

(ii) $\max_{x \in X} \phi_k(x, \xi^\star) = \varsigma_k(\xi^\star), \quad k = 1, \ldots, K.$

Proof. See Appendix A.3. ■

Remark 4.2. The result above establishes the direct applicability of the theory and algorithms developed for stationary sensors, since the problem can be decomposed to a finite set of 'virtually independent' problems, where continuous-time observations are taken by stationary sensors over subintervals T_k. Indeed, it is not difficult to construct simple sequential algorithms which exploit in each iteration procedures from Chapter 3 separately for each consecutive time step (the only element joining the subproblems is the common global FIM), determining a new design ξ used in the next iteration. This raises attractive possibilities for parallel implementations of the algorithm. Nevertheless, the assumption of a known arbitrary switching schedule may be too restrictive in some situations.

4.3.1.2. Problem reformulation and optimality conditions

In real engineering problems the scanning observation strategy is usually realized with the use of dedicated scanning networks or sometimes even with mobile monitoring stations. The assumption of independent observations, which is beneficial from a theoretical point of view, cannot be justified when the clusterization of measurements should be avoided, as usually the spatial data acquisition techniques do not raise a possibility of replicated observations at a single site. Consequently, a natural way to alleviate those impediments seems application of the extremely efficient approach connected to the clusterization-free designs delineated in Section 3.2.2, where the idea of operating on the density of sensors (i.e. the number of sensors per unit area), rather than on the sensor locations has been exploited. However, it has to be underlined once more that such an approach can be justified only for a sufficiently large total number of sensors N.

Similarly to the designs discussed in Section 3.2.2, we impose the crucial restriction that the density of sensor allocation must not exceed some prescribed level, which in general can be defined separately for each observation subinterval T_k. This can be expressed with the condition

$$\xi_k(\mathrm{d}x) \leqslant \omega_k(\mathrm{d}x), \quad k = 1, \ldots, K, \tag{4.58}$$

where $\omega_k(\mathrm{d}x)$ signifies the maximal possible 'number' of sensors per $\mathrm{d}x$ (Fedorov and Hackl, 1997) such that

$$\int_X \omega_k(\mathrm{d}x) \geqslant 1. \tag{4.59}$$

Note that in the spirit of such a general formulation, the number of activated sensors may vary in time, which is not a common situation in practice. However, since a constant number of active sensors can be achieved by imposing the trivial condition that for any two intervals T_{k_1} and T_{k_2}, $k_1, k_2 \in 1, \ldots, K$ the corresponding maximal densities are equal, i.e. $\omega_{k_1}(dx) = \omega_{k_2}(dx)$, this presents no particular difficulty. Moreover, the increased flexibility of the scanning strategy becomes in such a way more exposed.

We are thus faced with the following optimization problem being the appropriate form of (3.58) and (3.59): Find

$$\xi^\star = \arg\min_{\xi \in \Xi} \Psi[M(\xi)], \tag{4.60}$$

subject to

$$\xi_k(\mathrm{d}x) \leqslant \omega_k(\mathrm{d}x), \quad k = 1, \ldots, K. \tag{4.61}$$

The design $\xi^\star$ above is then said to be a (Ψ, ω)-*optimal design* (Fedorov and Hackl, 1997; Uciński and Patan, 2002a) on the analogy of Definition 3.1 (p. 62), introduced in the context of directly constrained design measures.

Apart from Assumptions (A1)–(A5) and (A9), a proper mathematical formulation calls for the following proviso:

(A10) $\omega_k(\mathrm{d}x)$ is atomless, i.e. for any $\Delta X \subset X$ there exists a $\Delta X' \subset \Delta X$ such that

$$\int_{\Delta X'} \omega_k(\mathrm{d}x) < \int_{\Delta X} \omega_k(\mathrm{d}x), \quad k = 1, \ldots, K. \tag{4.62}$$

In what follows, we write $\bar{\Xi}(X) \subset \Xi(X)$ for the collection of all the design measures (4.50) which satisfy the requirement

$$\xi_k(\Delta X) = \begin{cases} \omega_k(\Delta X) & \text{for } \Delta X \subset \operatorname{supp} \xi_k, \\ 0 & \text{for } \Delta X \subset X \setminus \operatorname{supp} \xi_k, \end{cases} \tag{4.63}$$

$k = 1, \ldots, K$.

Definition 4.2. For any given design ξ, the function $\psi_k(\,\cdot\,, \xi)$ defined by (4.54) **separates** sets X_1 and X_2 with respect to $\omega_k(\mathrm{d}x)$ if for any two sets $\Delta X_1 \subset X_1$ and $\Delta X_2 \subset X_2$ with equal non-zero measures we have

$$\int_{\Delta X_1} \psi_k(x, \xi)\, \omega_k(\mathrm{d}x) \leqslant \int_{\Delta X_2} \psi_k(x, \xi)\, \omega_k(\mathrm{d}x). \tag{4.64}$$

Then a suitable reformulation of the main result which characterizes the (Ψ, ω)-optimal designs takes the following form:

Theorem 4.6. *Let Assumptions (A1)–(A5),(A9) and (A10) hold. Then:*

(i) There exists an optimal design $\xi^\star \in \bar{\Xi}(X)$, and

(ii) A necessary and sufficient condition for $\xi^\star \in \bar{\Xi}$ to be (Ψ, ω)-optimal is that $\psi_k(\,\cdot\,, \xi^\star)$ separates $X_k^\star = \operatorname{supp} \xi_k^\star$ and its complement $X \setminus X_k^\star$ with respect to the measure $\omega_k(\mathrm{d}x)$ for $k = 1, \ldots, K$.

This constitutes a direct generalization of Theorem 3.3 from page 62 and the main ideas with suitable references for the proof are the same.

4.3.1.3. Scanning policy

A practical interpretation of Theorem 4.6 is that at all support points of an optimal design component $\xi_k^\star$ the function $\psi_k(\,\cdot\,, \xi^\star)$ should take lower values than at other points. This amounts to allocating observations in the vicinity of the points where the least is known about the system response (automatically, measurements at such locations will be the most informative).

One of the interpretations of the resultant optimal designs is obtained after partitioning the domain X into subdomains ΔX_i (with relatively small areas). Then, on the subinterval T_k, we allocate to each of them the number

$$N_k^\star(\Delta X_i) = \left\lceil N \int_{\Delta X_i} \xi_k^\star(\mathrm{d}x) \right\rceil \tag{4.65}$$

of sensors whose positions may coincide with nodes of some grid which further could represent the possible locations of the scanning sensors.

Making use of the above properties, there is a possibility to develop some numerical algorithms of constructing approximated solutions to the analysed problem. Since $\xi_k^\star(\mathrm{d}x)$ should be non-zero in the areas where $\psi_k(\,\cdot\,,\xi^\star)$ takes on smaller values, the main idea is to move some measure from the areas with higher values of $\psi_k(\,\cdot\,,\xi^n)$ to those with smaller values, as we expect that such a procedure will improve ξ^n. This is embodied by the iterative algorithm presented below, being the natural extension of the clusterization-free strategy algorithm presented in Section 3.2.2 to scanning observations (Uciński and Patan, 2002a):

Algorithm 4.1. *Clusterization-free scanning strategy algorithm*

Step 1. Guess an initial design $\xi^{(0)} \in \bar{\Xi}$. Set $n = 0$.

Step 2. For $k = 1,\ldots,K$ separately set $X_1^n(k) = \operatorname{supp}\xi_k^{(n)}$ and $X_2^n(k) = X \setminus X_1^n(k)$. Determine

$$x_1^n(k) = \arg\max_{x\in X_1^n(k)} \psi_k(x,\xi^{(n)}), \qquad x_2^n(k) = \arg\min_{x\in X_2^n(k)} \psi_k(x,\xi^{(n)}).$$

If $\psi_k(x_1^n(k),\xi^{(n)}) > \psi_k(x_2^n(k),\xi^{(n)}) + \epsilon$, where $\epsilon \ll 1$, then find two sets $S_1^n(k) \subset X_1^n(k)$ and $S_2^n(k) \subset X_2^n(k)$ such that $x_1^n(k) \in S_1^n(k)$, $x_2^n(k) \in S_2^n(k)$ and

$$\int_{S_1^n(k)} \omega_k(\mathrm{d}x) = \int_{S_2^n(k)} \omega_k(\mathrm{d}x) = \alpha_n$$

(i.e. the measures of $S_1^n(k)$ and $S_2^n(k)$ must be identical) for some $\alpha_n > 0$. Otherwise, set $S_1^n(k) = S_2^n(k) = \emptyset$. If $\psi_k(x_1^n(k),\xi^n) < \psi_k(x_2^n(k),\xi^n) + \epsilon$ for all $k = 1,\ldots,K$, then STOP.

Step 3. Construct $\xi^{(n+1)}$ such that

$$\operatorname{supp}\xi_k^{(n+1)} = X_1^{n+1}(k) = (X_1^n(k) \setminus S_1^n(k)) \cup S_2^n(k).$$

for $k = 1,\ldots,K$. Increment n and to go Step 2.

♦

The convergence of the algorithm is guaranteed if the sequence $\{\alpha_n\}_{n=0}^\infty$ satisfies the conditions

$$\lim_{n\to\infty} \alpha_n = 0, \quad \sum_{n=0}^{\infty} \alpha_n = \infty. \tag{4.66}$$

The maximal numbers of sensors allocated to the spatial element $\mathrm{d}x$ can be usually expressed as $\omega_k(\mathrm{d}x) = \varrho_k(x)\mathrm{d}x$, $k = 1,\ldots,K$, where the ϱ_k's play the roles of density functions. But then it is always possible to propose an appropriate change of coordinates which allows us to restrict attention to constant ϱ_k's.

The proposed approach inherits all of more and less valuable characteristics of the adopted clusterization-free strategy. For instance, a computer implementation forces the replacement of all integration operators by summing over some suitable regular grid elements. Furthermore, the sets X, $X_1^n(k)$, $X_2^n(k)$, $S_1^n(k)$ and $S_2^n(k)$

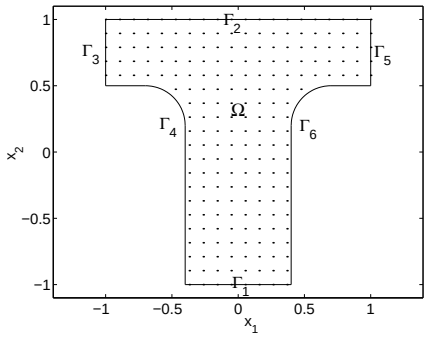


Fig. 4.4. Membrane and potential sites where the sensors can be placed in the Example 4.2.

then simply consist of grid elements (in this case these are the potential sensor locations). As a result, a rather abstract form of the above iterative procedure is reduced to an exchange-type algorithm with the additional constraint that every grid element must not contain more than one support point in each time subinterval and the weights of all supporting points are equal. An additional assumption is that the α_n's are fixed and one-point exchanges are most often adopted, i.e. $S_1^n(k) = \{x_1^n(k)\}$ and $S_2^n(k) = \{x_2^n(k)\}$, which leads directly to an extremely simple and efficient implementation. On the other hand, the convergence to an optimal design is assured only for a properly decreasing sequence $\{\alpha_n\}_{n=0}^{\infty}$ and since it is not generally true for fixed α_n's, some minor oscillations in $\Psi[M(\xi^{(n)})]$ may occur when the density of the spatial grid is not sufficient.

Example 4.2. As an example, consider a vibrating T-shaped membrane shown in Fig. 4.4. The membrane is fixed on the top and bottom boundaries, and is free elsewhere. The amplitude $y(x,t)$ of the transverse vibrations over a given time interval $T = [0, 10]$ is described by the hyperbolic equation

$$\frac{\partial^2 y(x,t)}{\partial t^2} = \nabla \cdot \big(\gamma(x)\nabla y(x,t)\big) + 20\exp\big(-50[x_2 - (0.2t-1)]^2\big) \quad \text{in } \Omega, \quad (4.67)$$

subject to the boundary and initial conditions

$$\begin{cases} y(x,t) = 0 & \text{on } \{\Gamma_1 \cup \Gamma_2\} \times T, \\ \dfrac{\partial y(x,t)}{\partial n} = 0 & \text{on } \{\Gamma_3 \cup \Gamma_4 \cup \Gamma_5 \cup \Gamma_6\} \times T, \\ y(x,0) = 0 & \text{in } \Omega, \\ \dfrac{\partial y(x,0)}{\partial t} = 0 & \text{in } \Omega. \end{cases} \quad (4.68)$$

The coefficient of the transverse elasticity has the distributed form

$$\gamma(x) = \theta_1 + \theta_2 x_1^2 + \theta_3 x_2, \quad (4.69)$$

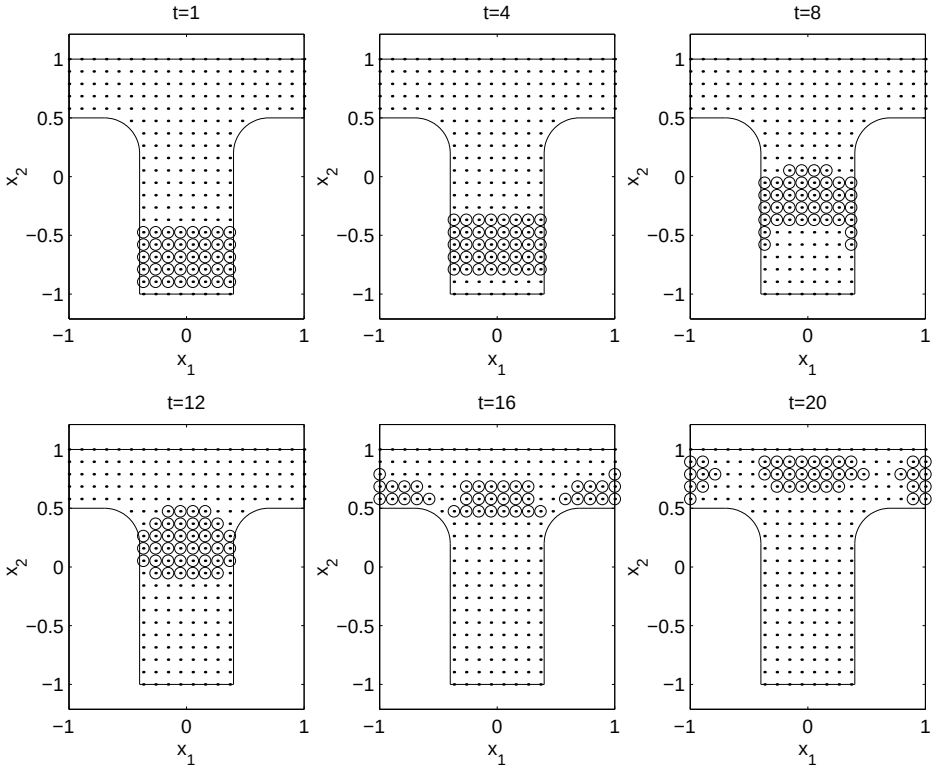


Fig. 4.5. Consecutive sensor configurations for the D-optimality criterion in the T-shaped membrane example.

where parameter values $\theta_1 = 100.0$, $\theta_2 = 5.0$ and $\theta_3 = 25.5$ were assumed to be nominal and known prior to the experiment. Our purpose is to construct a D-optimal scanning strategy for determining most accurate estimates of the true parameters θ_1, θ_2 and θ_3 when applying $N = 40$ scanning sensors and the partition of T defined by the switching points $t_k = k/2$, $k = 0, \ldots, 20$. The resulting optimal solution is shown in Fig. 4.5, where open circles indicate the actual sensor positions.

The initial design was generated by randomly selecting its support points. A simple one-point correction algorithm was employed ($\epsilon = 10^{-2}$) which produced the solution after only 53 iterations, practically within 10 s on a low-cost PC (Pentium II, 300 Mhz, using the Lahey/Fujitsu Fortran 95 compiler).

As regards the forcing term in our model, it approximates the action of a line source whose support is constantly oriented along the x_1-axis and moves with constant speed from the bottom to the top boundary of Ω. This is reflected by the consecutive configurations of the scanning sensors which also advance upwards.

★

4.3.2. Optimal switching schedule

Although the approach based on directly-constrained design measures proposed in the preceding section turns out to be extremely efficient in practice, its main limitation is that it can be used only when the number of sensors is relatively high (Uciński and Patan, 2002a). One of the major difficulties in the sensor scheduling problem is its combinatorial nature. It is compounded further if the sensor switchings are allowed to take place in continuous time, i.e. they are not established arbitrarily. In (Lee *et al.*, 2001) a similar problem was considered for state estimation. In that work, the proposed solution was to make use of some recently obtained results on discrete-valued optimal control problems. By introducing the transformation described in (Lee *et al.*, 2001), it was shown that the original discrete-valued control problem with variable switching times can be transformed into an equivalent continuous-valued optimal control problem which can then be solved using readily available optimal-control techniques. The aim of the considerations presented in what follows and originally developed in (Patan and Uciński, 2003) for the scalar case is to outline how this approach can be adopted to calculating optimal switching schedules for parameter estimation. This does not constitute a trivial task, as the natures of the sensor location problems for state and parameter estimation are of different character.

4.3.2.1. Optimal sensor scheduling problem

The considered class of MIMO spatio-temporal systems is described just like in the previous section, i.e. it is defined by (2.1)–(2.3) with the same notation and assumptions regarding spatial and temporal domains.

In what follows, we suppose that there are N stationary sensors located at given points $x^1, \ldots, x^N$ of $\Omega \cup \partial\Omega$. The additional assumption that at a given time moment only one sensor may be active while the others remain dormant simplifies considerations and provides the clarity of analysis and discussion. A sensor activation schedule can be represented by a function (Lee *et al.*, 2001)

$$u : T \to \Lambda = \{1, \ldots, N\}. \tag{4.70}$$

In particular, $u(t) = j$ means that the j-th sensor is used at time t. Hence the set of admissible sensor schedules is given by the set

$$\mathcal{U} = \{u : T \to \Lambda \mid u(\,\cdot\,) \text{ is measurable}\}. \tag{4.71}$$

Each sensor makes noisy observations of the state continuously in time, which can be formally represented as

$$z(t) = \sum_{j=1}^{N} \chi_{\{u(t)=j\}}(t)\big[y(x^j, t; \theta) + \varepsilon^j(t)\big] \tag{4.72}$$

for $t \in T$, where

$$\chi_{\{u(t)=j\}}(t) = \begin{cases} 1 & \text{if } u(t) = j, \\ 0 & \text{otherwise,} \end{cases} \tag{4.73}$$

and $\varepsilon^j(\,\cdot\,)$ denotes the measurement noise assumed to be zero-mean, Gaussian, and uncorrelated in both time and space.

Sensor positions which guarantee the best accuracy of the least-squares estimates of θ are then found by choosing $u(\,\cdot\,) \in \mathcal{U}$ so as to minimize some scalar measure of performance Ψ defined on the average FIM given in this situation by (Quereshi *et al.*, 1980)

$$M = \sum_{j=1}^{N} \int_0^{t_f} \chi_{\{u(t)=j\}}(t) G^{\mathrm{T}}(x^j,t) C^{-1}(x^j,t) G(x^j,t)\,\mathrm{d}t, \tag{4.74}$$

where G stands for the matrix of sensitivity coefficients defined by (4.7) and C is some known positive definite matrix of the same structure as in (4.11).

Thus we formulate the sensor location problem as the optimization one

$$\Psi\big[M(u(\,\cdot\,))\big] \longrightarrow \min \tag{4.75}$$

with respect to $u(\,\cdot\,) \in \mathcal{U}$.

4.3.2.2. Equivalent Mayer problem

Note that the sensor selection problem (4.75) can be cast as an optimal-control problem in Mayer form. Indeed, defining the quantity

$$\Pi(t) = \sum_{j=1}^{N} \int_0^{t} \chi_{\{u(\tau)=j\}}(\tau) G^{t}(x^j,\tau) C^{-1}(x^j,\tau) G(x^j,\tau)\,\mathrm{d}\tau, \tag{4.76}$$

we get

$$M = \Pi(t_f). \tag{4.77}$$

Thus the finding of $u(\,\cdot\,) \in \mathcal{U}$ minimizing $\Psi\big[M(u(\,\cdot\,))\big]$ amounts to the following problem:

Problem 1. Choose $u^\star(\,\cdot\,) \in \mathcal{U}$ to minimize the performance index

$$J(u(\,\cdot\,)) = \Psi[\Pi(t_f)], \tag{4.78}$$

subject to the constraint in the form of the nonlinear differential equation

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\Pi(t) &= \sum_{j=1}^{N} \chi_{\{u(t)=j\}}(t) G^{\mathrm{T}}(x^j,t) C^{-1}(x^j,t) G(x^j,t), \\ \Pi(0) &= 0. \end{aligned} \tag{4.79}$$

Problem 1 is an optimal control one in which the main difficulty is that the range set of the control is discrete and hence not convex. Furthermore, choosing the appropriate elements from the control set in an appropriate order is, in fact, a nonlinear combinatorial optimization problem.

4.3.2.3. A computational procedure based on the CPET

A first approach to handle Problem 1 is to view this optimal discrete-valued control problem as that of determining the switching points of the optimal discrete-valued control directly, but this may lead to serious numerical difficulties since the switchings (i.e. possible discontinuities) may occur at any time in the interval $[0, t_f]$. A novel problem transformation called the Control parameterization Enhancing Technique (CPET) was proposed in (Lee *et al.*, 1999) to address these difficulties. Under the CPET, the switching points are mapped onto the integers, and the transformed problem is just an ordinary optimal control problem with known and fixed switching points. It can then be readily solved numerically by numerous existing techniques.

As in (Lee *et al.*, 2001), where the CPET was employed to construct an optimal sensor schedule for finding optimal mean-square estimates of the system state, we set $Q = rN^2$, where r is an assumed maximum number of times any sensor $i \in \Lambda$ is being selected. We introduce a new time scale variable s which varies from 0 to Q. Let $\mathcal{V}$ denote the class of non-negative piecewise constant scalar functions defined on $[0, Q)$ with fixed interior knot points located at $\{1, 2, \ldots, Q-1\}$. The CPET transformation from $t \in [0, t_f]$ to $s \in [0, Q]$ is defined by the differential equation

$$\frac{\mathrm{d}t}{\mathrm{d}s} = v(s), \quad t(0) = 0, \tag{4.80}$$

where the scalar function $v(\,\cdot\,) \in \mathcal{V}$ is called the enhancing control which satisfies

$$\int_0^Q v(s)\,\mathrm{d}s = t_f. \tag{4.81}$$

Furthermore, we introduce a fixed function $\mu : [0, Q] \to \Lambda$,

$$\mu(s) = (i \bmod N) + 1, \quad s \in [i, i+1), \tag{4.82}$$

for $i = 0, 1, \ldots, Q-1$. The idea of this CPET transformation is to let any $u(t) \in \mathcal{U}$ be naturally represented by a $v(s) \in \mathcal{V}$ whenever this fixed $\mu(s)$ is defined.

Substituting (4.80) into (4.78)–(4.79) and setting $P(s) = \Pi(t(s))$, we obtain the following equivalent problem:

Problem 2. Find a $v \in \mathcal{V}$ such that the cost functional

$$\mathcal{J}(v(\,\cdot\,)) = \Psi[P(Q)] \tag{4.83}$$

is minimized, subject to the constraints

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}s}P(s) &= v(s)\left[\sum_{j=1}^{N} \chi_{\{\mu(s)=j\}}(t) G^{\mathrm{T}}(x^j, t(s)) C^{-1}(x^j, t(s)) G(x^j, t(s))\right], \\ P(0) &= 0. \end{aligned} \tag{4.84}$$

and (4.81).

Problem 2 can be solved with relative ease, as the switching points of the original control are mapped onto the set of integers in chronological order. Piecewise integration can now be easily performed since discontinuity points in the s-domain are known and fixed.

Theorem 4.7. *Assume that the maximum number of selections (or activations) of any sensor $j \in \Lambda$ is finite and equal to r. Then Problems 1 and 2 are equivalent if $Q \geqslant rN^2$.*

Proof. This result may be proved in much the same way as the corresponding theorem in (Lee *et al.*, 2001) and thus the proof is omitted. ■

Remark 4.3. Note that the delineated method can be extended to the case of several scanning sensors with no major difficulties. The only change we need to make is the definition of Λ. In particular, if n sensors are to be used, there are altogether $N' = \binom{N}{n}$ ways of activating n sensors from a total of N sensors. Then, we can define $\Lambda = \{1, \ldots, N'\}$ and the meaning of each $j \in \Lambda$ is to be understood as one of the sensor combinations.

Remark 4.4. Another question is the determination of an optimal number of switchings, as in the above algorithm a fixed maximal number of switchings is assumed. A heuristic approach proposed in (Lee *et al.*, 1999) to circumvent this problem is the following: Starting with a fixed r, we solve Problem 1. We then increment the number of switchings and solve Problem 1 again. If there is no decrease in the optimal cost, we adopt the previous value of r to be the optimal number of switchings, otherwise we increase r further.

Example 4.3. As an illustrative example to verify the performance of the proposed approach, consider the air pollutant transport process over a given area. At the initial time instant, a pollutant is emitted to the atmosphere from the left side of a spatial domain Ω shown in Fig. 4.3 together with the velocity field of the transport medium, which was assumed to be a solid rotation field. The problem considered here is similar to the Molenkamp-Crowley advection test combined with a diffusion process (Berkvens *et al.*, 1999).

The concentration $y(x,t)$ of substances over a given unit time interval $T = [0,1]$ is described by the following advection-diffusion equation:

$$\frac{\partial y(x,t)}{\partial t} + \nabla \cdot \big(v(x)y(x,t)\big) = \nabla \cdot \big(d(x)\nabla y(x,t)\big), \quad x \in \Omega$$

subject to the boundary and initial conditions:

$$\begin{aligned} \frac{\partial y(x,t)}{\partial n} &= 0, && (x,t) \in \partial\Omega \times T, \\ y(x,0) &= 20e^{-50[(x_1-0.3)^2+x_2^2]}, && x \in \Omega, \end{aligned}$$

The distributed diffusion coefficient was modelled in the following form:

$$d(x) = \theta_1 + \theta_2 x_1^2 + \theta_3 x_2^2 + \theta_4 x_1 x_2, \tag{4.85}$$

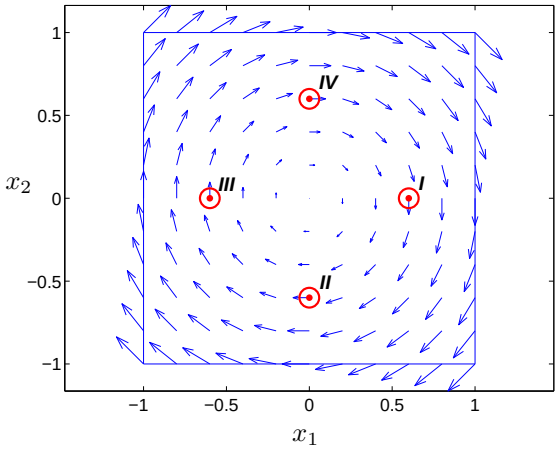


Fig. 4.6 . Domain with available sensors positions and the wind velocity field.

where the parameters $\theta = (0.08, 0.03, 0.02, 0.05)$ were assumed to be nominal. The aim of the experiment was to find an optimal sensor activation policy for determining the most accurate estimate of the true parameter vector θ. At one time instant only two sensors from among four possible data sources (see Fig. 4.3) could be activated. The consecutive combinations of activated sensors are coded as successive integers (see Table 4.1) which also stand for the levels of the input control signal u_c. A computer program was implemented in the Matlab 6.1 environment using

Table 4.1. Combinations of activated sensors

u_c	Active sensors
1	I, II
2	II, III
3	III, IV
4	I, IV
5	I, III
6	II, IV

a standard PC (Pentium IV processor, 1.7GHz, 768MB RAM) running Windows 2000. The system of state and sensitivity PDE's was first solved with the use of another program written in Matlab with the aid of PDE Toolbox routines (using a triangular grid with 1500 nodes and 21 divisions of the time interval). The sensitivity coefficients were then linearly interpolated and stored. Finally, to solve the constrained optimization problem (4.83)–(4.84) the `fmincon` routine from the Matlab Optimization Toolbox was employed. The constraints in the form of the ODE

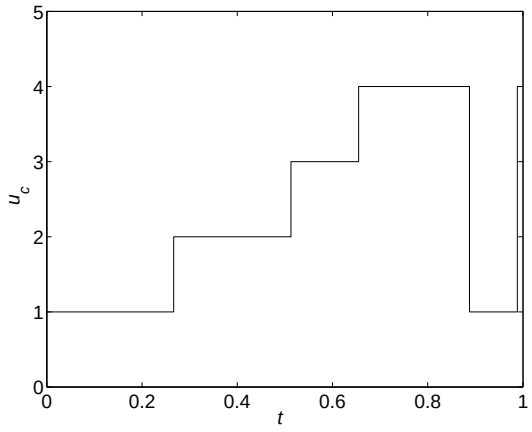


Fig. 4.7. D-optimal sensor switching policy of Example 4.3.

system (4.84) were implemented using the `ode45` routine from the Matlab ODE suite (piecewise integration over each interval of the s-domain where the solution is continuous). Let us note here that the integral equation (4.81) was transformed to its differential form and added to the constraints. The maximal number of switchings used in our simulations was assumed to be equal to 2 (this means that any sensor combination could be activated maximum twice). The CPET approach produced the following control signal within approximately 3 minutes:

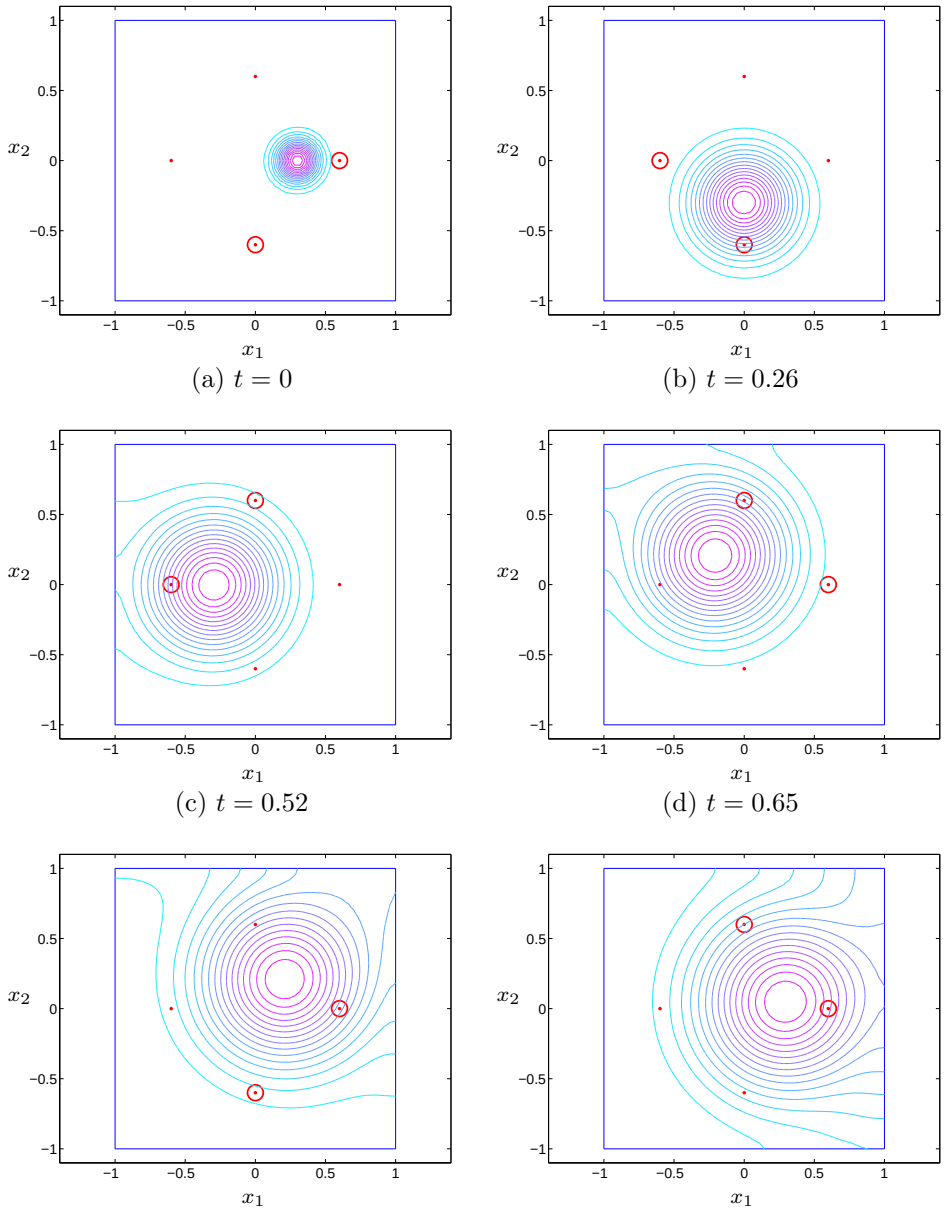
$$u_c(t) = \begin{cases} 1, & 0.00 \leqslant t < 0.26, \\ 2, & 0.26 \leqslant t < 0.52, \\ 3, & 0.52 \leqslant t < 0.65, \\ 4, & 0.65 \leqslant t < 0.88, \\ 1, & 0.88 \leqslant t < 0.98, \\ 4, & 0.98 \leqslant t < 1.00. \end{cases}$$

This solution is plotted in Fig. 4.7. Figure 4.8 illustrates the optimal sensor activation policy versus contour plots of pollutant concentration, where open circles indicate the active sensor locations and points indicate the available sensor positions.

★

4.4. Optimal measurement strategies for correlated observations

Until now, one of the most characteristic properties of spatial data acquisition techniques, namely the fact that observations made at different sites are often determined by local correlations, was consequently omitted, which is on one hand very convenient and leads to elegant solutions, but on the other hand, it is not



(a) $t = 0$ (b) $t = 0.26$

(c) $t = 0.52$ (d) $t = 0.65$

(e) $t = 0.88$ (f) $t = 0.98$

Fig. 4.8. Contour plots of pollutant concentrations and consecutive sensor switchings in Example 4.3.

justified in a high number of applications. In addition to this, usually there is no possibility of using replicated measurements. In fact, most often in practice the experimental conditions are extremely difficult to reconstruct or such a procedure is unacceptable (a good example here is the process of pollutant emission to the natural environment). This fact is of crucial importance as the classical concept of design measures is not applicable to this case.

The situation for dynamic DPS's is even more complicated since the measurements are usually taken according to some regular schedule or they are continuously recorded. Thus, random errors can be correlated both in time and space. Obviously, such simultaneous correlation dependencies involve an extremely difficult nature of the problem. For this reason, to the best of the author's knowledge, most contributions are focused only on the spatially or time correlated measurements separately with no attention paid to the correlated outputs.

To deal with the problem, two main approaches can be distinguished. The first idea is to exploit some well-known numerical techniques of constrained optimization where suitably defined additional constraints representing admissible distances between observations in time and space are imposed. Direct application of optimization techniques by no means excludes the clusterization effect, but when the number of sensors is quite high, the problem complexity considerably increases. In terms of the interpretation and applicability, such an approach is very attractive in the context of mobile sensors (Uciński, 1999a). The second approach consists in taking into account the mutual correlations between all measurements by appropriately modifying the information matrix. This alternative approach constitutes the subject of the next section.

4.4.1. Correlated measurement errors

For simplicity, the considerations are limited to stationary sensors with the observations taken in accordance with some discrete time schedule. Generalizations to more general models and observation strategies (i.e. scanning and movable sensors) can be made with minor difficulties of technical nature. Let us assume that the random errors in the model (2.7) are correlated and the covariance structure is known (either the covariance matrix C or the covariance kernel is given). If the system state y is directly measurable, this is equivalent to the output equation

$$z^j(t_k) = y(x^j, t_k; \theta) + \varepsilon(x^j, t_k), \quad j = 1, \ldots, N, \quad k = 1, \ldots, q, \tag{4.86}$$

where $z^j(\,\cdot\,)$ is an r-dimensional output, $t_k \in T = [0, t_f]$ and the zero-mean random field $\varepsilon(\,\cdot\,)$ representing measurement errors is described by the known continuous covariance kernel

$$\mathrm{E}[\varepsilon(x, \chi)\varepsilon^{\mathrm{T}}(t, \tau)] = K(x, \chi, t, \tau). \tag{4.87}$$

The generalized least-squares estimate of the unknown parameter vector θ from the set of experimental observations (4.86) is given by

$$\hat{\theta} = \arg\min_{\theta\in\Theta} \sum_{i_1=1}^{r}\sum_{i_2=1}^{r}\sum_{j_1=1}^{N}\sum_{j_2=1}^{N}\sum_{k_1=1}^{q}\sum_{k_2=1}^{q} w_{\ell_1\ell_2}\big[z_{i_1}^{j_1}(t_{k_1}) - y_{i_1}(x^{j_1}, t_{k_1};\theta)\big] \times\big[z_{i_2}^{j_2}(t_{k_2}) - y_{i_2}(x^{j_2}, t_{k_2};\theta)\big] \tag{4.88}$$

where $\ell_1 = rq(j_1-1)+r(k_1-1)+i_1,\ \ell_2 = rq(j_2-1)+r(k_2-1)+i_1,\ 1\leqslant \ell_1,\ell_2 \leqslant L = rNq$.

The weights $w_{\ell_1\ell_2}$ constitute the elements of the inverse of the covariance matrix

$$C^{-1} = W = \begin{bmatrix} w_{11} & \cdots & w_{1L} \\ \vdots & \ddots & \vdots \\ w_{L1} & \cdots & w_{LL} \end{bmatrix} = \begin{bmatrix} K(x^1,x^1) & \cdots & K(x^1,x^N) \\ \vdots & \ddots & \vdots \\ K(x^N,x^1) & \cdots & K(x^N,x^N) \end{bmatrix}^{-1} \tag{4.89}$$

where

$$K(x,\chi) = \begin{bmatrix} K(x,\chi,t_1,t_1) & \cdots & K(x,\chi,t_1,t_K) \\ \vdots & \ddots & \vdots \\ K(x,\chi,t_K,t_1) & \cdots & K(x,\chi,t_K,t_K) \end{bmatrix}, \quad K(x,\chi,t,\tau)\in\mathbb{R}^{r\times r}.$$

Notice that if any two sensors are placed at the same location, then the corresponding columns (and rows) of C are identical, which leads to the singularity of the covariance matrix. Since the replications of the measurements are no longer justified, the following compact notation for the design of experiment will be subsequently used in the further analysis

$$\xi = \{x^1,\ldots,x^N\}. \tag{4.90}$$

In the case considered, the Fisher Information Matrix (FIM) takes the form

$$M(\xi) = F^{\mathrm{T}}C^{-1}F, \tag{4.91}$$

where

$$F=\begin{bmatrix} F(x^1) \\ \vdots \\ F(x^N) \end{bmatrix},\ F(x)=\begin{bmatrix} \nabla_\theta^{\mathrm{T}} y(x,t_1,\theta^0) \\ \vdots \\ \nabla_\theta^{\mathrm{T}} y(x,t_K,\theta^0) \end{bmatrix},\ \nabla_\theta y(x,t,\theta^0)=\begin{bmatrix} \partial y(x,t,\theta^0)/\partial\theta_1 \\ \vdots \\ \partial y(x,t,\theta^0)/\partial\theta_m \end{bmatrix} \tag{4.92}$$

and θ^0 stands for a prior estimate of the unknown parameter vector θ.

Unfortunately, the information matrix (4.91) does not inherit the advantages of its predecesor (2.17). The valuable property of the additivity of information matrices corresponding to single observations is no longer valid. Thus, the information pieces from individual observations cannot be separated and therefore direct application of the results from convex optimization is rather impossible. Furthermore,

as was already mentioned, the classical definition of the design measures as the proportion of the experimental effort is generally impractical. From among all designs, the one which minimizes the performance index Ψ has to be selected. This can be formulated as the optimization problem

$$\xi^\star = \arg \min_{\xi \in \Xi(X)} \Psi[M(\xi)] \tag{4.93}$$

which, besides a similar notation, does not have much in common with (2.51). For example, it is not convex any more and direct application of the numerical algorithms known from convex optimization is impossible.

4.4.1.1. An exchange-type procedure for computation of optimal designs

Practical determination of optimal designs in the context of correlated measurements creates significant problems of numerical nature. For that reason, there are few available results on this subject, in which the contributors try to imitate some iterative methods of optimal design construction for the uncorrelated case. Usually the authors assume the correlation-free framework with many well-developed techniques of finding acceptable designs. Since correlations between observations in real spatio-temporal dynamic systems are rather natural, such an assumption can often hardly be accepted.

For calculation of exact designs, it is possible to adapt the exchange-type numerical scheme proposed by Brimkulov *et al.* (1986) which originally was used for the determination of the D-optimum sampling points for parameter estimation in linear models of random fields.

A generalized version of this algorithm is outlined below. Starting from an arbitrary initial N-point design $\xi^{(0)}$, in each iteration this procedure generates a new support point which is included into the current design instead of an existing point which will be deleted, in such a way as to maximize the resulting decrease in the performance index Ψ of the FIM. For iteration ℓ the following notation is used: $F^{(\ell)}$ is the current matrix of sensitivity coefficients in (4.92), $W^{(\ell)}$ stands for the current weighting matrix (4.89), $M^{(\ell)}$ means the resulting FIM and $D^{(\ell)}$ stands for its inverse. In addition to that, $\Lambda = \{1, \ldots, N\}$ and $\xi^{(\ell)}_{x^j \leftarrow x}$ denotes the design in which the support point x^j is replaced by x.

Algorithm 4.2. *Exchange-type algorithm for correlated measurements*

Step 1. Select an initial design $\xi^{(0)} = \{x^{1(0)}, \ldots, x^{N(0)}\}$ such that $t_i^{(0)} \neq t_j^{(0)}$ for $i, j \in \Lambda$ and $i \neq j$. Calculate the matrices $F^{(0)}$, $W^{(0)}$ and $M^{(0)}$. If $M^{(0)}$ is singular (i.e. $\det M^{(0)} = 0$), then select a new initial design and repeat this step.

Step 2. Calculate $D^{(0)}$. Set $\ell = 0$.

Step 3. Determine

$$(j^*, x^*) = \arg \min_{(j,x) \in \Lambda \times X} \Delta(x^j, x),$$

where $\Delta(x^j, x) = \left\{\Psi[M(\xi^{(\ell)}_{x^j \leftrightarrows x})] - \Psi[M(\xi^{(\ell)})]\right\}/\Psi[M(\xi^{(\ell)})]$.

Step 4. If $|\Delta(x^{j^*}, x^*)| \leqslant \delta$, where δ is some given positive tolerance, then STOP. Otherwise, set $\xi^{(\ell+1)} = \xi^{(\ell)}_{x^{i^*} \leftrightarrows x^*}$ and determine $F^{(\ell+1)}$, $W^{(\ell+1)}$, $M^{(\ell+1)}$ and $D^{(\ell+1)}$ corresponding to $\xi^{(\ell+1)}$. Set $\ell \leftarrow \ell + 1$ and go to Step 3.

♦

From the point of view of nonlinear programming, treating the design problem as an optimization one with a collection of decision variables $\xi = \{x^1, \ldots, x^N\}$ and the performance index $\Psi[M(\xi)]$, the algorithm outlined above is very similar to the Gauss-Seidel algorithm (Findeisen *et al.*, 1980). The only difference lies in the update which takes place only for the coordinate x^j for which the resulting decrease in $\Psi[M(\xi)]$ is the largest. In the classical Gauss-Seidel relaxation scheme (also known as the block coordinate ascent method, cf. Bertsekas, 1999), each iteration consists of N one-dimensional search steps with respect to variables $x^1, \ldots, x^N$ taken in cyclic order. If an increase in $\Psi[M(\xi)]$ is attained for some j after performing the search, then the corresponding variable x^j is immediately updated. Consequently, the presented simple exchange routine has similar properties regarding convergence to the Gauss-Seidel algorithm and in particular only convergence to a local minimum is assured. From a practical point of view, in order to obtain an approximation to a global minimum, several restarts of the algorithm from different initial designs are necessary.

In spite of the great simplicity of Algorithm 4.2, its main inconvenience results from the fact that the form of the FIM is much more cumbersome that in the case of independent measurements and automatically the computational effort of updating matrices in Steps 3 and 4 is not acceptable in most practical situations. Fortunately, for particular criteria (e.g. D-optimality) there exist possibilities of optimizing those updates through elimination of matrix inversions, which leads to a dramatic reduction in the computational cost.

4.4.1.2. Implementation details for the D-optimum criterion

When the goal is to determine a D-optimum design using Algorithm 4.2, the speed can be substantially improved by suitable optimization of the computations. This may be achieved through elimination of time-consuming matrix inversions and calculation of the determinants following the ideas from (Brimkulov *et al.*, 1986).

Implementation of the optimization appearing in Step 3 of Algorithm 4.2 requires multiple repetition of the passage from design $\xi^{(\ell)}$ to $\xi^{(\ell)}_{x^j \leftrightarrows x}$. Such a task can be split into two stages: the removal of location x^j from $\xi^{(\ell)}$ and then the inclusion of a new point x in place of the deleted one. Obviously, both the stages imply suitable updates in all the matrices corresponding to the current design. But before we will give the appropriate update formulae, it is necessary to prove some valuable results which lead to the extreme efficiency of the considered stage of the algorithm.

First, consider the inclusion of a new point x into the actual design. In order to determine the updated version of the FIM (for $N+1$ spatial locations) define

$$V(x) = \big[K(x,x^1),\ldots,K(x,x^N)\big]^{\mathrm{T}}, \qquad B(x) = -C_N^{-1}V(x), \tag{4.94}$$

$$\Gamma(x) = [K(x,x) - V^{\mathrm{T}}(x)C_N^{-1}V(x)]^{-1}, \quad G(x) = \big[F^{\mathrm{T}}(x) + F_N^{\mathrm{T}}B(x)\big], \tag{4.95}$$

where C_N and F_N play the roles of the covariance and sensitivity matrices defined for the design $\xi = \{x^1,\ldots,x^N\}$, respectively. Now we are able to formulate the following result

Proposition 4.8. *Let M_N be the information matrix for the design $\xi_N = \{x^1, x^2,\ldots,x^N\}$. Then the information matrix for the design $\xi_{N+1} = \xi_N \cup \{x\}$ is given by the formula*

$$M_{N+1} = M_N + G(x)\Gamma(x)G^{\mathrm{T}}(x).$$

Proof. See Appendix A.3. ■

Remark 4.5. Note that C_{N+1}^{-1} decomposes into

$$C_{N+1}^{-1} = \left[\begin{array}{c:c} V_N & L(x) \\ \hdashline L^{\mathrm{T}}(x) & \Gamma(x) \end{array}\right]. \tag{4.96}$$

Making use of (A.22), we can express C_N and M_N by the elements of C_{N+1} and M_{N+1}, respectively:

$$C_N = V_N - B(x)\Gamma(x)B^{\mathrm{T}}(x) = V_N - L(x)\Gamma^{-1}(x)L^{\mathrm{T}}(x) \tag{4.97}$$

$$M_N = M_{N+1} - G(x)\Gamma(x)G^{\mathrm{T}}(x), \quad G(x) = F^{\mathrm{T}}(x) + F_N^{\mathrm{T}}L(x)\Gamma^{-1}(x) \tag{4.98}$$

In order to construct a numerical procedure for determining optimal experiment designs, it is necessary to establish relationships between the information matrices after removing a support point and adding a new one to the design. Assume that a point $x_r \in \xi_N = \{x^1,\ldots,x^N\}$ is to be replaced by a new point x_a. Then, without loss of generality, we can assume that $x_r = x^N$. In fact, it is always possible to rearrange the points in the design and all matrices (by swapping appropriate rows and columns) in such a way as to obtain the location x_r in the N-th position. Such an interchange makes the resulting formulae clearer and more elegant, while simplifying the implementation. Denote by $\tilde{\xi}_N = \big\{\xi_N \setminus \xi(x^N)\big\} \cup \xi(x_a)$ the resulting design. Then Proposition 4.8 yields the following relation between the information matrices $\tilde{M}_N$ and M_N corresponding to the designs $\tilde{\xi}_N$ and ξ_N:

$$\tilde{M}_N = M_N - G(x^N)\Gamma(x^N)G^{\mathrm{T}}(x^N) + G(x_a)\Gamma(x_a)G^{\mathrm{T}}(x_a). \tag{4.99}$$

Based on this result, it is possible to formulate a more precise relation in terms of the performance index Ψ, in particular for the determinants of both the designs.

Proposition 4.9. *Let $\tilde{M}_N$ be the FIM for the design $\tilde{\xi}_N = \{x^1, \dots, x^{N-1}, x_a\}$ and M_N be the FIM for $\xi_N = \{x^1, \dots, x^N\}$. Then*

$$\det(\tilde{M}_N) = \det(M_N)\det(I + \Upsilon),$$

where

$$\Upsilon = \left[\begin{array}{c:c} D_a\Gamma(x_a) & \imath D_{ar}\Gamma(x^N) \\ \hdashline \imath D_{ar}^{\mathrm{T}}\Gamma(x_a) & -D_r\Gamma(x^N) \end{array}\right], \quad \imath = \sqrt{-1}$$

and

$$\begin{aligned} D_a &= G^{\mathrm{T}}(x_a)D_{N+1}G^{\mathrm{T}}(x_a), \quad D_r \ = G^{\mathrm{T}}(x^N)D_N G^{\mathrm{T}}(x^N), \\ D_{ar} &= G^{\mathrm{T}}(x_a)D_{N+1}G^{\mathrm{T}}(x^N), \quad D_N = M_N^{-1}. \end{aligned}$$

Proof. See Appendix A.3. ■

Remark 4.6. From (A.29) it follows immediately that

$$\big(\det(\tilde{M}_N) - \det(M_N)\big)/\det(M_N) = \det(I + \Upsilon) - 1. \tag{4.100}$$

Moreover, the inverse of $\tilde{M}_N$ can be expressed as

$$\tilde{D}_N = \tilde{M}_N^{-1} = \big[M_N + G\Gamma G^{\mathrm{T}}\big]^{-1} = D_N - D_N G(\Gamma^{-1} + G^{\mathrm{T}}D_N G)^{-1}G^{\mathrm{T}}D_N. \tag{4.101}$$

So it is clear that in order to compute the performance ratio $\Delta(x^j, x)$ and suitable updates of the matrices in Step 3 which are time-consuming operations, we may operate on matrices whose size is $N/2$ times smaller in the case of calculating determinants and N times smaller while inverting them as a whole.

Based on the above results, we are capable of precisely establishing the necessary calculations during the passage from the design $\xi^{(\ell)}$ to $\xi^{(\ell)}_{x^N \leftrightarrows x}$, which guarantees the extreme reduction in the computational burden.

The detailed scheme of the computations is as follows:

Stage 1: Deletion of x^N from $\xi^{(\ell)}$. Write $F^{(\ell)}$ as

$$F^{(\ell)} = \left[\begin{array}{c} F_r \\ \hdashline F(x^N) \end{array}\right], \tag{4.102}$$

where $F_r \in \mathbb{R}^{rK(N-1)\times m}$ and $F(x^N) \in \mathbb{R}^{rK\times m}$. Deletion of x_N from design $\xi^{(\ell)}$ implies removing $F(x^N)$ from $F^{(\ell)}$, so that we then have F_r instead of $F^{(\ell)}$. Consequently, some updates of matrices $W^{(\ell)}$ and $M^{(\ell)}$ are also necessary. Namely, decomposing the symmetric matrix $W^{(\ell)}$ according to Remark 4.5 as

$$W^{(\ell)} = C^{-1\,(\ell)} = \left[\begin{array}{c:c} V_r & L(x^N) \\ \hdashline L^{\mathrm{T}}(x^N) & \Gamma_r(x^N) \end{array}\right], \tag{4.103}$$

where $V_r \in \mathbb{R}^{rK(N-1)\times rK(N-1)}$, $L(x^N) \in \mathbb{R}^{rK(N-1)\times rK}$, $\Gamma_r(x^N) \in \mathbb{R}^{rK\times rK}$, and setting

$$G_r(x^N) = F^{\mathrm{T}}(x^N) + F_r^{\mathrm{T}} L(x^N)\Gamma_r^{-1}(x^N), \tag{4.104}$$

we are able to calculate the following counterparts of $W^{(\ell)}$ and $M^{(\ell)}$:

$$W_r = V_r - L(x^N)\Gamma_r^{-1}(x^N)L^{\mathrm{T}}(x^N), \quad M_r = M^{(\ell)} - G_r(x^N)\Gamma_r(x^N)G_r^{\mathrm{T}}(x^N). \tag{4.105}$$

Stage 2: Inclusion of x into the design resulting from Stage 1. At this stage a new sensitivity matrix $F_a(x)$ is constructed

$$F_a(x) = \left[\begin{array}{c} F_r \\ \hdashline F(x) \end{array}\right], \tag{4.106}$$

where $F(x)$ is defined according to (4.92). Such an augmentation influences the form of the matrices W_r and M_r obtained at Stage 1. Analyzing the proof of Proposition 4.8, it is easy to deduce the respective updated versions $W_a(x)$ and $M_a(x)$. Rewritting (4.94) and (4.95) as follows:

$$V(x) = \left[K(x,x^1),\ldots,K(x,x^{N-1})\right]^{\mathrm{T}}, \quad B(x) = -W_r V(x), \tag{4.107}$$

$$\Gamma_a(x) = [K(x,x) - V^{\mathrm{T}}(x)W_r V(x)]^{-1}, \quad G_a(x) = \left[F^{\mathrm{T}}(x) + F_r^{\mathrm{T}} B(x)\right], \tag{4.108}$$

we obtain

$$W_a(x) = \left[\begin{array}{c:c} W_r + B(x)\Gamma_a(x)B^{\mathrm{T}}(x) & B(x)\Gamma_a(x) \\ \hdashline \Gamma_a(x)B^{\mathrm{T}}(x) & \Gamma_a(x) \end{array}\right], \tag{4.109}$$

$$M_a(x) = M_r + G_a(x)\Gamma_a(x)G_a^{\mathrm{T}}(x). \tag{4.110}$$

Remark 4.7. It is not clearly seen, but it can be easily verified that $G_a(x^j) = \mathbf{0}$ for $j = 1,\ldots,N-1$. In combination with (4.109), this confirms the fact that an additional observation at the same point does not provide more information about the estimated parameters and inclusion of such a point into the design does not alter the information matrix. Consequently, the resulting optimal design should be automatically replication-free.

Once the point x^N has been replaced by x, the ratio $\Delta(x^N, x)$ in Step 3 of Algorithm 4.2 can be calculated based on Proposition 4.9 as

$$\Delta(x^N,x) = \det\left(I + \left[\begin{array}{c:c} D_a(x)\Gamma_a(x) & \imath D_{ar}(x)\Gamma_r(x^N) \\ \hdashline \imath D_{ar}^{\mathrm{T}}(x)\Gamma_a(x) & -D_r\Gamma_r(x^N) \end{array}\right]\right) - 1, \tag{4.111}$$

where $\imath = \sqrt{-1}$ and

$$\begin{gathered} D_a(x) = G_a^{\mathrm{T}}(x)D^{(\ell)}G_a^{\mathrm{T}}(x), \quad D_r = G_r^{\mathrm{T}}(x^N)D^{(\ell)}G_r^{\mathrm{T}}(x^N), \\ D_{ar}(x) = G_a^{\mathrm{T}}(x)D^{(\ell)}G_r^{\mathrm{T}}(x^N). \end{gathered} \tag{4.112}$$

A result of performing Step 3 is the pair of points $x^{j^*} \in \xi^{(\ell)}$ and $x^* \in X$ which ensure the largest increase in the performance ratio (this amounts to minimization of the D-optimality criterion) in the current iteration. In such a way, the update of the matrices in Step 4 looks as follows:

$$F^{(\ell+1)} = F_a(x^*), \quad W^{(\ell+1)} = W_a(x^*), \quad M^{(\ell+1)} = M_a(x^*), \tag{4.113}$$

$$D^{(\ell+1)} = D^{(\ell)} - D^{(\ell)}G(\Gamma^{-1} + G^{\mathrm{T}}D^{(\ell)}G)^{-1}G^{\mathrm{T}}D^{\ell}, \tag{4.114}$$

where

$$G = \left[\, G_a(x) \,\vdots\, \imath G_r(x^N) \,\right], \quad \Gamma = \left[\begin{array}{c:c} \Gamma(x) & \mathbf{0} \\ \hdashline \mathbf{0} & \Gamma(x^N) \end{array}\right], \quad \imath = \sqrt{-1}. \tag{4.115}$$

Finally, the new value for the criterion (D-optimality) is equal to

$$\det(M^{(\ell+1)}) = \det(M^{(\ell)}) \det(I + \Delta(x^N, x^*)). \tag{4.116}$$

Thus, applying the above formulae the efficiency of the algorithm can be significantly improved and its performance imitates Fedorov's exchange algorithm for determining exact designs for the uncorrelated case (Fedorov, 1972).

4.4.2. A final comment on the correlation structure

The results discussed in the previous section are essentially based on *a priori* knowledge of the covariance structure for measurement errors. Such a situation is possible, but rather uncommon in practice, and thus the form of the correlations has to be estimated. Nevertheless, there are several classes of processes for which it is possible to construct the covariance kernel in closed form or the corresponding eigenvalues and eigenfunctions are known, which allows us to expand the kernel into a series. For example, the spatial kernel for the Brownian motion is described by (Butkovskiy, 1982)

$$k(x, \chi) = \min(x, \chi), \quad 0 \leqslant x, \chi \leqslant 1,$$

and its eigenvalues and eigenfunctions are

$$\lambda_i = (i - 1/2)^{-2}\pi^{-2}, \quad f_i(x) = \sqrt{2}\sin\big((i - 1/2)\pi x\big), \quad i = 1, 2, \ldots,$$

respectively. Another example is the Poisson kernel, whose shape can be controlled by a parameter β (Butkovskiy, 1982)

$$k(x, \chi) = \frac{1 - \beta^2}{1 - 2\beta\cos 2\pi(x - \chi) + \beta^2}, \quad 0 \leqslant x, \chi \leqslant 1, \quad 0 \leqslant \beta \leqslant 1$$

and

$$\lambda_0 = 1,\ \lambda_{2i-1} = \lambda_{2i} = \beta^i,$$
$$f_0(x) = 1,\ f_{2i-1} = \sqrt{2}\cos(2i\pi x),\ f_{2i}(x) = \sqrt{2}\sin(2i\pi x),\ i = 1, 2, \ldots$$

However, for most real-world problems it is impossible to represent the covariance kernels in a simple closed form. Then a standard approach is to use some approximations based on the series expansion. It can be shown that under very mild conditions the series

$$k_n(x,\chi) = \sum_{i=1}^{n} \lambda_i f_i(x) f_i(\chi), \quad x,\chi \in X,$$

where λ_i and $f_i(x)$ are respectively the eigenvalues and eigenfunctions of the covariance kernel $k(x,\chi)$, is uniformly and absolutely convergent (Kanwal, 1971). Therefore for a sufficiently large n the kernel $k_n(x,\chi)$ can be a sufficient approximation of $k(x,\chi)$. For instance, the covariance kernel for two dimensional transport problems including heat convection or diffusion over a finite domain can be expressed as (Butkovskiy, 1982)

$$k(x,\chi) = 4\sum_{i=1}^{\infty}\sum_{j=1}^{\infty} \lambda_{ij} \sin(i\pi x_1)\sin(j\pi x_2)\sin(i\pi\chi_1)\sin(j\pi\chi_2), \tag{4.117}$$

where $X = \{x : 0 \leqslant x_1, x_2 \leqslant 1\}$. The corresponding eigenvalues and eigenfunctions are

$$\lambda_{ij} = \exp\left[-\sigma^2\pi^2(i^2+j^2)\right], \quad f_{ij}(x) = 2\sin(i\pi x_1)\sin(j\pi x_2), \quad i,j = 1,2,\ldots$$

and σ is some constant. When X becomes infinite with respect to any coordinate, the above-mentioned physical processes lead to Gaussian-type kernels, which are in particular of the isotropic form (Nychka and Saltzman, 1998)

$$k(x,\chi) = \sigma^2 \exp\left(-\|x-\chi\|/\beta\right)$$

or its extension allowing for the use of different marginal variances

$$k(x,\chi) = \sigma(x)\sigma(\chi)\exp\left(-\|x-\chi\|/\beta\right).$$

This type of kernels will be subsequently exploited within the framework of some applications considered in this work.

Allowing for correlations between the measurement errors in time domain further complicates the situation, but qualitatively it does not change much from a methodological point of view. Nevertheless, the practical engineering problems often rule out any possibilities of obtaining closed forms of covariance kernels and more complex approaches are necessary. To resolve those difficulties, suitable techniques of the direct estimation of the covariance matrix can be proposed (Fedorov, 1996) which complement the delineated methodology. Of course, we have to remember that if the expected measurement error is only of instrumental nature, the 'white noise' becomes automatically the most reasonable model with a known covariance kernel which is still of interest for many practical applications.

Example 4.4. At this juncture, trying to give some representative and illustrative example, consider an atmospheric pollutant transport-chemistry process over

a unit circle. In contrast to Example 4.3, however, assume that the velocity of the transport medium is zero everywhere. Instead, we take into account an active source of pollution and reaction, which leads to the decay of pollutant concentration $y(x,t)$. The entire process over the observation interval $T=[0,10]$ is modelled with the following diffusion-reaction equation:

$$\frac{\partial y(x,t)}{\partial t}=\theta_1\Big[\nabla^2 y(x,t)+4y(x,t)-4\theta_2 e^{-4\theta_1 t}\Big],\quad x\in\Omega=\{x: x_1^2+x_2^2<1\}, \tag{4.118}$$

where the second term on the right-hand side is responsible for the reaction and the last term represents some exponential source of contamination over Ω. Equation (4.118) is supplemented by suitable boundary and initial conditions

$$y(x,t)=0, \qquad (x,t)\in\partial\Omega\times T, \tag{4.119}$$

$$y(x,0)=\theta_2(1-x_1^2-x_2^2), \qquad x\in\Omega. \tag{4.120}$$

This time the task consists in determining the locations of an arbitrary number of stationary sensors for estimation of the diffusion coefficient θ_1 and the relative amplitude of the source θ_2. The measurements are assumed to be corrupted by the noise which is zero-mean and correlated in time and space with covariance kernel $k(x,\chi,t,\tau)=\exp(-\rho_t|t-\tau|)\exp(-\rho_x\|x-\chi\|)$.

The problem (4.118)–(4.120) has the closed-form solution, i.e.

$$y(x,t)=\theta_2(1-x_1^2-x_2^2)e^{-4\theta_1 t}. \tag{4.121}$$

The nominal parameter values $\theta_1=0.05$ and $\theta_2=0.02$ were used. The central symmetry of the problem and the fact that the sensitivities $\partial y/\partial\theta_1$ and $\partial y/\partial\theta_2$ take their maximal values at point $(x_1,x_2)=(0,0)$ suggest that a one-point design

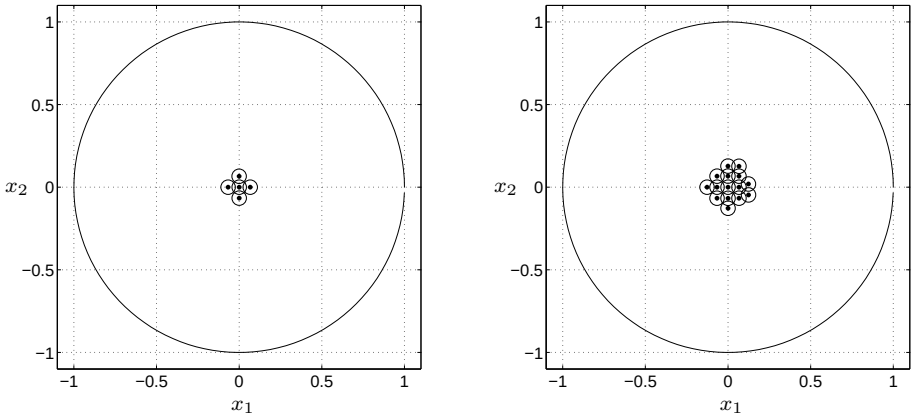
$$\xi^\star=\{(0,0)\} \tag{4.122}$$

is D-optimal for the stationary sensor strategy on the assumption of independent measurements. Indeed, passing the polar coordinates it can be verified that the determinant of the FIM in the case of a one-point design takes the form

$$\begin{aligned}\det(M(\xi))=&\frac{1}{4}e^{-8}-\frac{9}{2}e^{-4}+\frac{1}{4}-r^2+18e^{-4}r^2-27e^{-4}r^4+\frac{3}{2}r^4-r^6+\frac{1}{4}r^8\\&-e^{-8}r^2+\frac{3}{2}e^{-8}r^4-e^{-8}r^6+18e^{-4}r^6+\frac{1}{4}e^{-8}r^8-\frac{9}{2}e^{-4}r^8,\end{aligned} \tag{4.123}$$

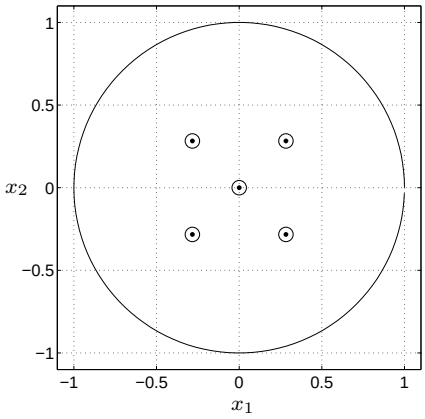
where $r=\sqrt{x_1^2+x_2^2}$ and $0\leqslant r\leqslant 1$. Function (4.123) takes its maximal value at $r=0$, which corresponds to the centre of the circular domain which is the most informative point for observations, and it can be easily checked that (4.122) is optimal.

In order to find optimal locations for taking measurements, a program based on the developed algorithm was written in Matlab v. 6.5. R12.1 and run on a

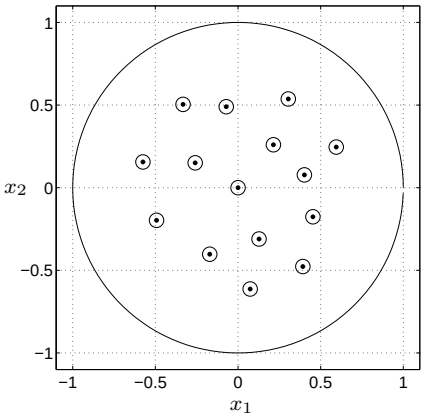


(a) $N = 5,\ \rho_x = 100$

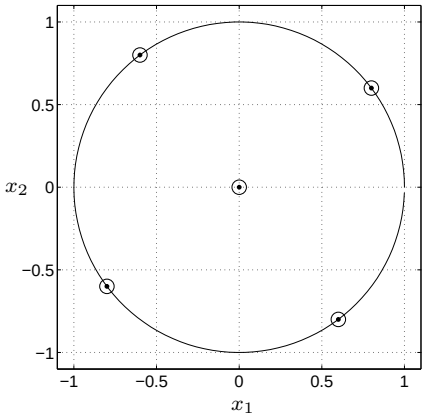
(d) $N = 15,\ \rho_x = 100$



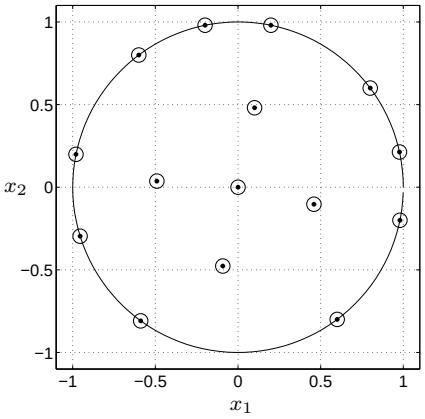
(b) $N = 5,\ \rho_x = 5$



(e) $N = 15,\ \rho_x = 5$



(c) $N = 5,\ \rho_x = 1$



(f) $N = 15,\ \rho_x = 1$

Fig. 4.9 . D-optimum sensor allocation for $N = 5$ and 15 measurements for small ($\rho_x = 100$), medium ($\rho_x = 5$) and considerable ($\rho_x = 1$) spatial correlations, respectively.

PC equipped with Duron 900MHz CPU and running Windows 2000. The two-dimensional search for a candidate to include into the current design was implemented using the routine `fmincon` from the Optimization Toolbox.

The influence of the mutual correlations of observations on the sensor allocation was tested by varying the coefficient ρ_x. For clarity, the correlation in time was assumed to be negligible (i.e. $\rho_t = 100$). The results obtained for relative small and medium numbers of measurements are presented in Fig. 4.9.

An analysis of the obtained results leads to the conclusion that the level of correlation directly affects the distances between the sensors which are increasing when the correlation is more intense. If the correlation is small, then the measurements tend to cluster in the vicinity of the optimal design support for the case of independent measurements. Another important remark is that the higher the correlation, the lower the criterion value. This effect results from a more global character of the mutual influence between random error realizations in the case of higher correlation values. Due to the interference with the estimation of the unknown parameters, the valuable information in observations is reduced. Note that due to the problem symmetry every solution constructed by rotation of those presented in Fig. 4.9 by any angle is an equivalent approximation of the optimal sensors allocation. This phenomenon also affects the performance of the algorithm and for numerical reasons in the case of $N = 15$ measurements the solutions are not as regular as in the simplest case when $N = 5$.

★

4.5. Optimal experiment design in model-based diagnostics

Nowadays, we can observe an extremely fast development of methods of fault detection and isolation (FDI) for dynamical systems. There exist a wide variety of different techniques with many potential applications and rich literature. For surveys, the interested reader is referred to (Isermann, 1997; Frank and Köppen-Seliger, 1997; Chen and Patton, 1999; Patton and Korbicz, 1999; Duch *et al.*, 2000; Patton *et al.*, 2000; Chiang *et al.*, 2001; Korbicz *et al.*, 2001; Korbicz *et al.*, 2004). Nevertheless, there is a lack of effective methods specialized in dynamic DPS's. Furthermore, within the framework of FDI systems, the optimization of the data acquisition process which increases the reliability of the diagnosis is most often neglected and the contributions are very scarce. Some approaches to fill this gap are indicated in the works (Patan and Patan, 2001; 2003) related to LPS's and in (Uciński, 2003; Kuczewski *et al.*, 2003; Kuczewski *et al.*, 2004; Demetriou, 2000) in the context of fault diagnosis in DPS's.

A proper recognition of an abnormal behaviour of the examined object leads to the necessity of the very precise fitting of a nominal model corresponding to the conditions of normal work of real physical phenomena associated with it, as well as the need for the appropriate models of abnormal work. In the context of analytical models, the diagnosis is a practical realization of a proper selection of the appropriate model structure in accordance with the current system performance mode. On the other hand, in any possible working conditions the calibration of a

model is strongly dependent on the strategy of taking measurements. In such a way, the problem of sensor location becomes one of the most important ones for fault detection in DPS's. This task comprises minimization of the diagnosis uncertainty through selection of the appropriate strategy of taking measurements for a limited number of transducers located in a given spatial area. In the background of diagnostic problems, the main difficulty is a definition of suitable relations between the quality of the system diagnosis and the observational strategy. In this section, we shall indicate how classical hypothesis testing can be used in the model-based diagnosis and especially fault detection with the use of the approach set forth by Uciński (2003) in order to construct a qualitative criterion of sensor allocation based on the notion of D_s-optimum designs.

4.5.1. A parameter estimation approach to fault detection in DPS's

Parameter estimation is one of the fundamental methods from among all analytical techniques of fault detection (Korbicz *et al.*, 2004). Its role is of significance in situations, when the abnormal system state appears not only in the form of output changes but also as fluctuations of model parameters. This is a very common situation in practice if only the parameters have a physical interpretation built upon a proper analysis of various quantities which are crucial for the considered process. Unfortunately, they are usually directly non-measurable and application of effective parameter estimation algorithms is required in order to obtain their estimates. The very basic idea is a comparison of such estimates with some known nominal values of parameters treating possible differences as residuals which contain information about potential faults. Then based on some thresholding techniques the appropriate decision making system can be constructed (Korbicz *et al.*, 2004).

Consider the process, whose nominal mode $y(x,t)$ of work is described by the mathematical model (2.1)–(2.3) with $\theta = \theta_{\rm nom}$, where $\theta_{\rm nom}$ is some vector of constant parameters which are characteristic for this state. Assuming for simplicity that the process states are observed directly over some finite time horizon using N stationary sensors, the observations can be presented in the form

$$z^j(t) = y(x^j, t; \theta_{\rm nom}) + \varepsilon(x^j, t), \quad t \in T = [0, t_f], \quad j = 1, \ldots, N, \tag{4.124}$$

$\varepsilon(\,\cdot\,,\,\cdot\,)$ being the measurement noise uncorrelated in space and time such that

$$\mathrm{E}[\varepsilon(x^i, t)\varepsilon^{\mathrm{T}}(x^j, t)] = \sigma^2 \delta_{ij} \delta(t - \tau).$$

A further assumption is that the estimation of the unknown parameter vector $\theta_{\rm nom}$ is performed via minimization of the least-squares criterion

$$J(\theta) = \sum_{j=1}^{N} \int_0^{t_f} \|z^j(t) - \hat{y}(x^j, t; \theta)\|^2 \,\mathrm{d}t, \quad \theta \in \Theta_{\rm ad} \tag{4.125}$$

where $\Theta_{\rm ad}$ is the set of admissible parameters and $\hat{y}(\,\cdot\,,\,\cdot\,;\theta)$ denotes the solution to (2.1)–(2.3) corresponding to a given parameter θ. A vector $\hat{\theta}$ minimizing $J(\theta)$

stands for the estimate of the true value of θ_{nom}. Generally, in practical situations only a subset of all parameters can be used for diagnosis. If such a situation takes place, then without loss of generality the parameters of interest can be distinguished by partitioning the parameter vector into

$$\theta^{\mathrm{T}} = \left[\, \theta_1 \ \ldots \ \theta_s \,\vdots\, \theta_{s+1} \ \ldots \ \theta_m \,\right] = \left[\, \alpha^{\mathrm{T}} \,\vdots\, \beta^{\mathrm{T}} \,\right] \tag{4.126}$$

where α is a vector of s parameters which are essential for a proper detection and β is the vector of some parameters which are a part of the model but are not significant for detection (although they can be used for fault isolation or are some representation of the model uncertainty). Based on the observations, it is possible to test the simple hypothesis

$$H^0 : \alpha = \alpha_{\text{nom}}, \tag{4.127}$$

where α_{nom} is the nominal value for the vector α corresponding to the normal system performance.

The 'continuous' generalization of the likelihood function for the considered experiment takes the following form (Goodwin and Payne, 1977):

$$L(z;\theta) = \left(\frac{1}{2\pi\sigma^2}\right)^{N/2} \exp\left\{ -\frac{1}{2\sigma^2} \sum_{j=1}^{N} \int_0^{t_f} \|z^j(t) - \hat{y}(x^j, t; \theta)\|^2 \,\mathrm{d}t \right\}. \tag{4.128}$$

Setting $\Theta_0 = \{\theta \in \Theta : \alpha = \alpha_{\text{nom}}\}$, we can define the following generalized likelihood ratio:

$$\lambda(z) = \frac{\sup\limits_{\theta\in\Theta} L(z;\theta)}{\sup\limits_{\theta\in\Theta_0} L(z;\theta)} = \exp\left\{ -\frac{1}{2\sigma^2}(J(\hat{\theta}) - J(\tilde{\theta}) \right\} \tag{4.129}$$

where

$$\hat{\theta} = \arg\min_{\theta\in\Theta} J(\theta), \qquad \tilde{\theta} = \arg\min_{\theta\in\Theta_0} J(\theta). \tag{4.130}$$

It should be pointed out that a number of different variations in the maximum likelihood ratio exist. One variation is to swap the numerator and the denominator. Another is to calculate the supremum over ${\Theta_0}^C$ (A^C denotes a complement of the set A) in the denominator of (4.129) instead of Θ (Lehmann, 1986).

The likelihood ratio test is widely used in statistics. The reason is partly that it is the optimal test in the case when both the null and alternative hypotheses are simple, i.e. Θ_0 and Θ_0^C reduce to one-element sets (cf. the Neyman-Pearson lemma (Garthwaite and Jolliffe, 1995)). The proofs for optimality also exist for many other cases where H^0 is simple (Garthwaite and Jolliffe, 1995). In many cases where a theoretical justification is missing, the likelihood ratio can still be shown to be very good in practice (Lehmann, 1986). Nevertheless, there also exist few situations for which the likelihood ratio is not adequate. Commonly the generalized log-likelihood ratio is used, because it can be shown that assuming the validity of the null hypothesis H^0 the sequence $\{2\ln\lambda(y)\}$ for $N \to \infty$ is weakly convergent to a χ^2 random variable on s degrees of freedom (Goodwin and Payne, 1977). The

meaning of this fact is that we can compare the observed value of $2\ln\lambda(y)$ with some threshold k_γ obtained from the cumulative χ^2 distribution on s degrees of freedom where k_γ is such that $100(1-\gamma)\%$ of the distribution lies to the left of k_γ. The decision rule for a given significance level γ, which represents a fixed range of model uncertainty, takes the following form:

$$S = \begin{cases} S^1 & \text{if } 2\ln\lambda(y) \geqslant k_\gamma \quad (\text{reject } H^0) \\ S^0 & \text{if } 2\ln\lambda(y) < k_\gamma \quad (\text{accept } H^0) \end{cases} \tag{4.131}$$

The potential rejection of H^0 indicates an essential deviation of the vector α from the nominal value of this parameter and is a base for detection of abnormal states in the system.

4.5.2. D_s-optimum detectability problem

The basic concepts presented in the previous section are probably well known to statisticians and decision theorists. However, because of their usefulness for fault diagnosis problems, they deserve some attention. When the null hypothesis H^0 is true, we do not want to reject H^0. The mistake in rejecting H^0 when H^0 is true is called the Type I error. Similarly, accepting H^0 when the alternative hypothesis of the form $H^1 : \alpha = \alpha^1 \neq \alpha_{\text{nom}}$ is true is called the Type II error (Domański, 1990). In fault diagnosis, there is a connection between these errors and the probability of a false alarm, missed detection, and missed isolation. We will not go into the details here but this connection will be discussed in the following. At this point, it is at least clear that to achieve low probabilities of false alarms, missed detection, and missed isolation, we have to keep the probabilities of Type I and II errors low. Thus the probabilities of Types I and II are a kind of performance measure for a single hypothesis test. It is not possible to minimize both the errors simultaneously (Domański, 1990). Therefore, a classical approach is to minimize the Type II error with a prescribed level of the Type I error.

If only a subset of s parameters is of interest, with the parameter vector partitioning given by (4.126), the power of the presented hypothesis test can be increased by maximization of the D_s-optimality criterion (Goodwin and Payne, 1977) of the following form:

$$\Psi_s[M] = \det[M_{\alpha\alpha} - M_{\alpha\beta}M_{\beta\beta}^{-1}M_{\alpha\beta}^{\mathrm{T}}], \tag{4.132}$$

where $M \in \mathbb{R}^{m\times m}$ is the FIM corresponding to the vector θ, which can be partitioned into blocks

$$M = \left[\begin{array}{c:c} M_{\alpha\alpha} & M_{\alpha\beta} \\ \hdashline M_{\alpha\beta}^{\mathrm{T}} & M_{\beta\beta} \end{array}\right] \tag{4.133}$$

and

$$M_{\alpha\alpha} \in \mathbb{R}^{s\times s}, \quad M_{\alpha\beta} \in \mathbb{R}^{s\times(m-s)}, \quad M_{\beta\beta}^{-1} \in \mathbb{R}^{(m-s)\times(m-s)}.$$

In the case considered the information matrix is defined as a simpler analogue of (2.19)

$$M = \frac{1}{N}\sum_{j=1}^{N} \Upsilon(x^j), \tag{4.134}$$

where

$$\Upsilon(x) = \frac{1}{t_f}\int_0^{t_f} G^{\mathrm{T}}(x,t)G(x,t)\,\mathrm{d}t, \tag{4.135}$$

and

$$G(x,t) = \left(\frac{\partial y(x,t;\theta)}{\partial \theta}\right)_{\theta=\theta_{\mathrm{nom}}}. \tag{4.136}$$

Maximization of the criterion (4.132) can be achieved by a suitable sensor allocation. The process is equivalent to minimizing the determinant of the estimate of the covariance matrix for vector α. Furthermore,

$$\Psi_s[M] = \frac{\det M}{\det M_{\beta\beta}}. \tag{4.137}$$

At this point, the problem of increasing the reliability of the diagnosis can be formulated as the problem of maximizing $\Psi_s[M]$ with respect to the sensor locations $x^j,\ j = 1,\ldots,N$ belonging to an admissible set of locations X.

Remark 4.8. Denoting by ξ some arbitrarily chosen design measure and introducing the decomposition

$$M^{-1} = \left[\begin{array}{c:c} D_{\alpha\alpha} & D_{\alpha\beta} \\ \hdashline D_{\alpha\beta}^{\mathrm{T}} & D_{\beta\beta} \end{array}\right] \tag{4.138}$$

where $D_{\alpha\alpha} \in \mathbb{R}^{s\times s},\ D_{\alpha\beta} \in \mathbb{R}^{s\times(m-s)},\ D_{\beta\beta}^{-1} \in \mathbb{R}^{(m-s)\times(m-s)}$, from the Equivalence Theorem for D_s-optimum designs (Fedorov, 1972) an analogue of the variance of the prediction can be established from the system response. In particular, we have the following form of the sensitivity function and its components:

$$\psi(x,\xi) = \varsigma(\xi) - \phi(x,\xi), \tag{4.139}$$

$$\varsigma(\xi) = \mathrm{trace}\left[\overset{\circ}{\Psi}[M(\xi)]M(\xi)\right] = s, \tag{4.140}$$

$$\phi(x,\xi) = \mathrm{trace}\left[\overset{\circ}{\Psi}[M(\xi)]\Upsilon(x)\right], \tag{4.141}$$

where

$$\overset{\circ}{\Psi}[M(\xi)] = \frac{\partial\Psi(M)}{\partial M} = \left[\begin{array}{c:c} D_{\alpha\alpha} & D_{\alpha\beta} \\ \hdashline D_{\alpha\beta}^{\mathrm{T}} & D_{\beta\beta} - M_{\beta\beta}^{-1} \end{array}\right]. \tag{4.142}$$

At this point it is clear that those simple modifications of the sensitivity function pave the way for the applicability of a wide range of methods. For example, all approaches dedicated to the stationary sensors case developed in Chapter 3 can be used directly without further improvements.

4.5.3. Fault isolation using structured hypothesis testing

In order to propose an extension of the delineated approach for providing the fault isolation stage of the diagnosis, we propose to use the principle of structured hypothesis tests which assume that all of the individual tests ρ_i are hypothesis tests (Nyberg, 1999). Then the diagnosis system consists of a finite set of hypothesis tests and a decision logic. The classical, statistical or decision theoretic definition of the hypothesis test is adopted, e.g. see (Berger, 1985; Lehmann, 1986). This means that a hypothesis test is a procedure to select between exactly two hypotheses characterized by $\theta \in \Theta_0$ and $\theta \in \Theta_0^C$ based on sample data. This is in contrast to 'multiple hypothesis testing' that is often found in literature (Basseville and Nikiforov, 1993).

Denote by $F_i,\ i = 0, \ldots, Q$ all available system work modes, where F_0 is the mode of the normal work. Introducing the collection of sets

$$M_0 = \{F_0\}, \quad M_i = \{F_0, F_i\}, \quad i = 1, \ldots, Q, \tag{4.143}$$

the null hypothesis for the i-th test, i.e. H_i^0, can be defined as the belonging of the fault mode, present in the process, to a specific set M_i. Then the alternative hypothesis H_i^1 is that the present fault mode does not belong to M_i, and thus it must belong to the complement M_i^C. In this way, each individual hypothesis test contributes with a piece of information about which fault modes can be present. The task of the decision logic module is a suitable combination of any piece of partial information in order to make a diagnosis decision.

If F_q is an actual system-fault mode, then the i-th hypothesis test comprises the null and alternative hypotheses which can be written down as

$$\begin{cases} H_i^0 : F_q \in M_i & \text{if some fault mode in } M_i \text{ can explain the observations,} \\ H_i^1 : F_q \in M_i^C & \text{otherwise.} \end{cases}$$

An alternative is to use the definition of the sets Θ_i which are the sets of admissible parameters describing each mode of system work separately. The hypotheses can now be expressed as

$$\begin{cases} H_i^0 : \theta \in \Theta_i & \text{if some value of } \theta \in \Theta_i \text{ can explain the observations,} \\ H_i^1 : \theta \notin \Theta_i & \text{otherwise.} \end{cases}$$

The commonly used convention in the hypothesis testing literature is that when H_i^0 is rejected, we assume that H_i^1 is true. But when H_i^0 is not rejected, then in particular nothing special is assumed for the present.

For each hypothesis test ρ_i, it is necessary to find a test quantity and a rejection region. Test quantity is a function which maps the observations of system outputs y and eventually measurable inputs u into some scalar measure of model uncertainty. Based on such a performance index the decision system is able to formulate a partial diagnosis through some thresholding techniques. The typical scheme of hypothesis testing is illustrated in Fig. 4.10. In many textbooks the

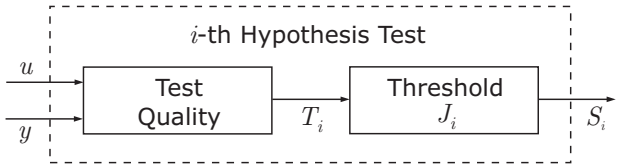


Fig. 4.10. Block structure of the hypothesis test.

test quantity $T_i(u, y)$ is also called the test statistic (Domański, 1990; Basseville and Nikiforov, 1993; Nyberg, 1999). It can be interpreted as a random variable, which is often identified with a residual generator or the sum of squared prediction errors of a parameter estimator. In many applications, a deterministic view is taken and $T_i(u, y)$ is not seen as a random variable but just as a function of the data (Nyberg, 1999; Patan and Patan, 2003). In the considered case it was shown that the likelihood ratio analogous to (4.129) can be used, i.e.

$$T_i(u, y) \sim \frac{\sup\limits_{\theta \in \Theta} L(z; \theta)}{\sup\limits_{\theta \in \Theta_i} L(z; \theta)}, \quad i = 1, \ldots, Q. \tag{4.144}$$

Formally, the general decision rule for hypothesis test ρ_i is defined as

$$S_i = \begin{cases} S_i^1 & \text{if } T(u, y) \geqslant J_i \quad (\text{reject } H_i^0) \\ S_i^0 & \text{if } T(u, y) < J_i \quad (\text{accept } H_i^0) \end{cases} \tag{4.145}$$

The rejection region of each test is thereby implicitly defined by a threshold J_i which can be arbitrarily established according to some significance level (i.e. the error of Type I) by analogy to (4.131). The meaning of such a decision rule is that we have to design a test quantity $T_i(u, y)$ which is at least below the threshold if the observations fit to the hypothesis H_i^0, i.e. a fault mode in M_i can explain the data. On the other hand, if the data arising from the observations match a fault mode which is not in M_i, $T_i(u, y)$ should be large or at least above the threshold. In terms of the traditional terminology, the fault modes in M_i are said to be decoupled (Nyberg, 1999).

Remark 4.9. Due to non-trivial problems with restoration of initial and boundary conditions in the case of abnormal system work, it is not difficult to see that for proper detection and isolation of faults, the observation system should perform the data acquisition in a complex manner. This means that it is necessary to construct solutions separately for each mode of work and then combine them into one complex system. For this reason the clusterization-free approach seems to be more adequate, as in practice a part of sensors might be used simultaneously to isolate different faults of the system.

The proposed approach can be considered as a first attempt to establish an interconnection between parameter-estimation based FDI for DPS's and the sensor location problem. It should be emphasized that still some open problems remain

which need close attention. One of the most important questions is the lack of on-line identification methods for spatio-temporal systems. The existing approaches rely on a set of linearizations which often hide the complex nature of the considered problem and consequently lead to excessive modelling errors and unacceptable false alarms. Another essential impediment is application of fixed thresholds which represent arbitrarily chosen ranges of model uncertainty (or measurement noise). A low level of such a threshold would lead to a greater number of false alarms, while a too high one would decrease the sensitivity of the detection system. Problems of this kind still require further developments of effective and qualitative FDI techniques, but this subject lies beyond the scope of this dissertation.

4.6. Applications

4.6.1. Transmission lines

4.6.1.1. Background

Transmission lines appear in many different contexts arising from the examples in previous chapters where practical engineering applications were indicated. A classical instance of physical realization for transmission lines are long-distance electrical supply lines, but nowadays, due to a dramatic increase in the timing frequencies in the modern technologies of integrated circuits like processors, they become another strong demonstrative example of transmission lines with distributed nature. In general, a transmission line is an entity which is characterized by its inseparable electrical properties, namely inductance, capacitance and resistance, which are distributed along its dimensions. Strictly speaking, in any real electrical component there will always occur some time delays. Those quantities will depend on the system dimensions, so it is useful to use distributed densities (linear, surface or spatial depending on the system dimensionality).

The time taken for an electrical signal to traverse the line is determined by the local velocity of light, which strongly depends on the permittivity of the material of which the line is made. An analysis of transient states in the line is equivalent to investigating propagation of the electrical signal $y(x,t)$ (a voltage or a current intensity) and determination of those signals leads directly to solving systems of partial differential equations. These, in turn, can be defined in the form similar to (2.4), but usually it is more convenient to study only one signal separately.

Apart from physical interpretations of line properties, an electrical impulse travelling on a network of lossy transmission lines obeys the telegraph equation stemming from fundamental laws of electromagnetics. The most general form of the equation describing the underlying signal propagation in a given domain Ω is (Polyanin, 2002)

$$\frac{\partial^2 y(x,t)}{\partial t^2} + \vartheta_1(x,t)\frac{\partial y(x,t)}{\partial t} = \vartheta_2(x,t)\nabla^2 y(x,t) - \vartheta_3(x,t)y(x,t) + f(x,t),\ x \in \Omega. \tag{4.146}$$

The first term on the left-hand side of this equation represents lossless propagation of a wave or an impulse. The second terms on both the sides account for the

effects of power dissipation in the distributed resistance. The last term on the right-hand side is responsible for possible force inputs. Introducing the notions of spatio-temporal densities of resistance $R(x,t)$, inductance $L(x,t)$, capacitance $C(x,t)$ and leakage conductivity $G(x,t)$, the distributed parameters in (4.146) can be rewritten as

$$\vartheta_1 = \frac{GL + RC}{LC}, \quad \vartheta_2 = (LC)^{-1}, \quad \vartheta_3 = \frac{RG}{LC}.$$

Additionally the quantity $\sqrt{\vartheta_1(x,t)}$ can be interpreted as the directional velocity of the wave propagation which, in general, can be anisotropic.

The telegraph equation is not easy to treat in a general way and modellers usually tend to consider special situations when some terms in (4.146) become insignificant. The instances commonly encountered in practice are as follows (Kącki, 1995):

- *Thomson's cable*, i.e. inductionless line ($L = 0$) without leakage conductivities ($G = 0$); in such circumstances the telegraph equation reduces to the equation of the parabolic type

$$R(x,t)C(x,t)\frac{\partial y(x,t)}{\partial t} = \nabla^2 y(x,t) + f(x,t), \tag{4.147}$$

- *Lossless line*, i.e. $R = 0$ and $G = 0$; then the considered process is governed by the hyperbolic 'wave' equation

$$L(x,t)C(x,t)\frac{\partial^2 y(x,t)}{\partial t^2} = \nabla^2 y(x,t) + f(x,t), \tag{4.148}$$

- *Homogeneous line*, where the parameters $R, L, G, C = const$, i.e. they are independent of time and space.

It becomes now clear that the initial conditions most often formulated in problems related to transmission lines can be of two types (Kącki, 1995), namely only the distribution of $y(x,t)$ along the line at the initial time instant is given, which can be written as

$$y(x,0) = \varphi(x), \quad x \in \Omega, \tag{4.149}$$

or additionally the rate of signal changes along the line is given, that is

$$\left(\frac{\partial y(x,t)}{\partial t}\right)_{t=0} = \psi(x), \quad x \in \Omega. \tag{4.150}$$

A definition of boundary conditions requires more attention, because they strongly depend on supply sources and the type of load which is used on the boundaries. Furthermore, their strict form is also forced by the physical interpretation of the quantity y. For example, if a line is an open circuit (insulated) at some point belonging to the boundary, the suitable boundary condition will be

$$\left(\frac{\partial y(x,t)}{\partial n}\right)_{x=x_b} = 0, \quad x_b \in \partial\Omega, \quad t \geqslant 0,$$

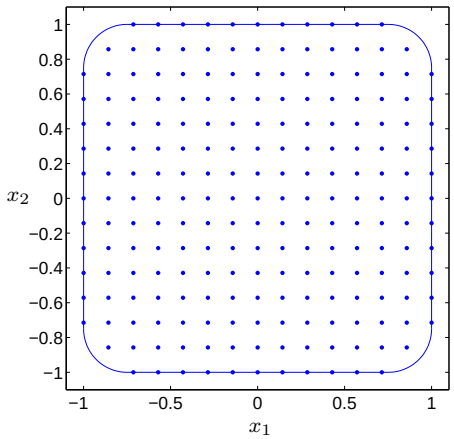


Fig. 4.11 . The conductor and a grid of detectors.

if y is interpreted in terms of a voltage signal, and

$$y(x_b, t) = 0, \quad x_b \in \partial\Omega, \quad t \geqslant 0$$

for y being the current intensity. In the case of a short-circuit at the point x_b, the two equations above should be exchanged according to the voltage and current signals, respectively.

If a transmission line is loaded at boundaries, then the boundary condition is determined by the system of internal connections between the elements R_0, L_0 and C_0 of the receiver. In such a way, there exist an infinite number of possible formulations of boundary conditions as there are an infinite number of electrical circuits characterized by the lumped parameters R_0, L_0 and C_0 which can be connected to the line as loads. The situation will be even more complicated if a receiver belongs to the class of DPS's. A suitable instance was presented in Example 2.1.

4.6.1.2. Numerical experiments

Signal propagation. As the first application example of the methodology developed within the scope of this chapter, we study the propagation of a disturbance in a thin square-shaped conducting plate with rounded corners. On its surface a collection of measurement sensors were placed forming a uniform grid of size 15×15 shown in Fig. 4.11. The material of the plate is non-isotropic and is assumed to be a lossless environment (a signal leakage and power supression are assumed to be negligible) because of a relatively small scale of object. Thus, the transmission of the voltage signal $y(x, t)$ over the conductor in time interval $T = [0, 1]$ can be described by the wave equation of the form

$$\frac{\partial^2 y(x,t)}{\partial t^2} = v(x)^2 \nabla^2 y(x,t), \quad x \in \Omega, \ t \in T, \tag{4.151}$$

where $v(x)$ is the velocity of signal propagation inside the medium being the reciprocal of the product of the surface densities of inductance $L(x)$ and capacitance $C(x)$, which have distributed character and should be appropriately modelled. To this end, the following parametrization for the velocity is assumed:

$$v(x) = \theta_1 + \theta_2 x_1^2 + \theta_3 x_2^2, \tag{4.152}$$

where $\theta = (\theta_1, \theta_2, \theta_3)$ is the vector of unknown parameters which are of interest as they define a parametric map of suitable material properties. As a preliminary estimate of θ, the vector $(1.0, 0.5, 3.0)$ was assumed.

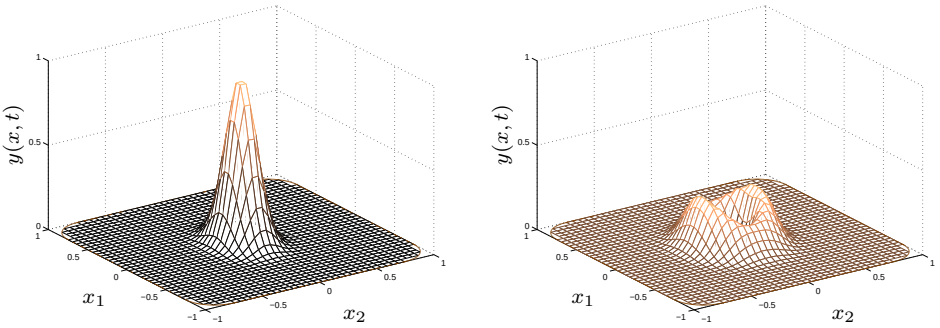
The boundaries of the conductor are insulated and at the initial time instant at the centre of Ω a disturbance is generated which is further transmitted to the rest of the area. This is reflected by the following boundary and initial conditions:

$$\begin{aligned} \frac{\partial y(x,t)}{\partial n} &= 0, && (x,t) \in \partial\Omega \times T, \\ y(x,0) &= e^{-50(x_1^2 + 0.5x_2^2)}, && x \in \Omega, \\ \left(\frac{\partial y(x,t)}{\partial t}\right)_{t=0} &= 0, && x \in \Omega. \end{aligned}$$

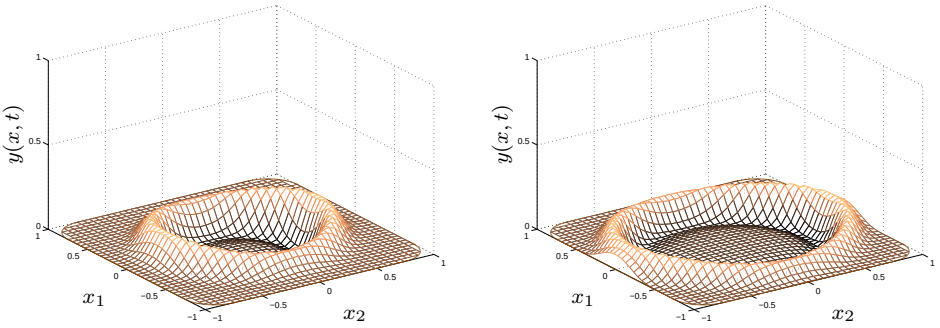
First, the wave equation (4.151) and the respective sensitivity equations were solved with the use of the Matlab PDE Toolbox for the time domain divided into 20 subintervals and a spatial mesh composed of about 2500 triangles and 1300 nodes. The solution is presented in Fig. 4.12 where the process dynamics can be easily observed. It can be seen that the disturbance propagates with slightly different velocities and amplitudes with respect to the direction.

To determine an optimal scanning strategy in order to maximize the estimation accuracy of θ, the clusterization-free scanning strategy with fixed switching schedule (Algorithm 4.1) was adopted as the most adequate and implemented as a Fortran routine (compiler Lahey/Fujitsu v.5.7). The switching table was determined arbitrarily as the sequence of points synchronized with the solution of the PDE's system, i.e. $t_k = k/20$, $k = 0, \ldots, 20$. The task was to choose $N = 50$ measurements sites in each consecutive time step from among all 213 available sensor positions. The starting design was randomly generated and the desired accuracy was set at the level of $\epsilon \leqslant 10^{-4}$. The algorithm found the approximated D-optimal design in only 72 iterations which took less than 10 s on a PC equipped with a Duron 900Mhz processor and running Windows 2000. The results are shown in Fig. 4.13. The activated sensors tend to take measurements at the wave front of the spreading disturbance.

For comparison with other possible observation strategies, two more algorithms were used, namely the a two-phase procedure (Algorithm 3.5) for determining the allocation of stationary sensors in the continuous domain and an enhanced two-phase procedure with a combined ARS–SQP approach for finding sensor motion trajectories. In both the cases the assumed accuracy of the solution was equal to $\epsilon \leqslant 10^{-4}$ and the starting designs contained 3 randomly generated support



(a) $t = 0.05$ (b) $t = 0.35$



(c) $t = 0.75$ (c) $t = 1.00$

Fig. 4.12 . Impulse propagation in a lossless transmission line.

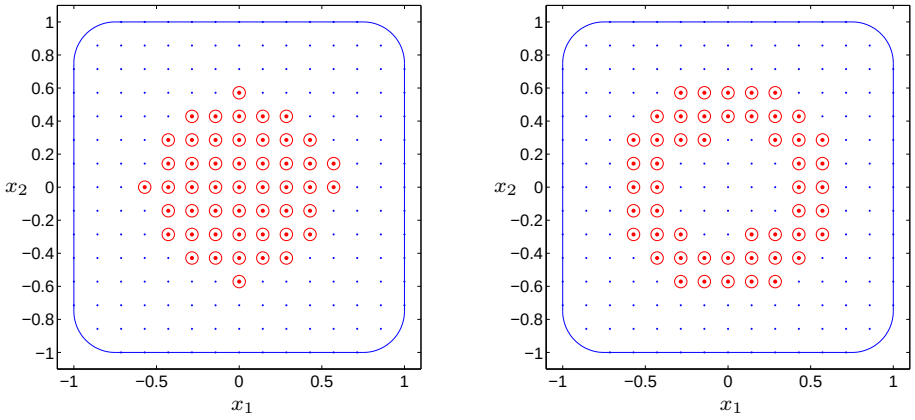
elements with equal weights. For the case of stationary sensors, a solution was obtained after 4 iterations which took 20 s. It has the following form:

$$\xi^\star = \begin{Bmatrix} (0.00, 0.00) & (0.15, 0.02) & (1.00, 0.00) \\ 0.31 & 0.14 & 0.55 \end{Bmatrix} \tag{4.153}$$

For mobile sensors additional constraints were imposed on the maximal length of trajectories which must not exceed a value of 1.1 (this slightly is more than the radius of the circle inscribed into the domain). The starting points of the trajectories were also optimized and each trajectory was parametrized with linear splines according to the division of the time domain. No particular constraints were imposed on the motion dynamics of the sensors. The algorithm for determining D-optimal sensors motion curves converged in 5 iterations of the main loop (35 s). The solution consists of two symmetrical trajectories

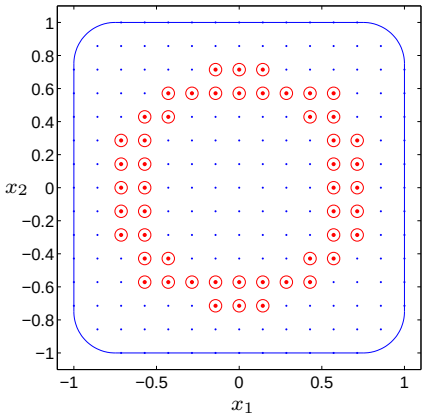
$$\xi^\star = \begin{Bmatrix} x^1(\,\cdot\,) & x^2(\,\cdot\,) \\ 0.46 & 0.54 \end{Bmatrix} \tag{4.154}$$

Both results are compared in Fig. 4.14 where circles and triangles on the right panel

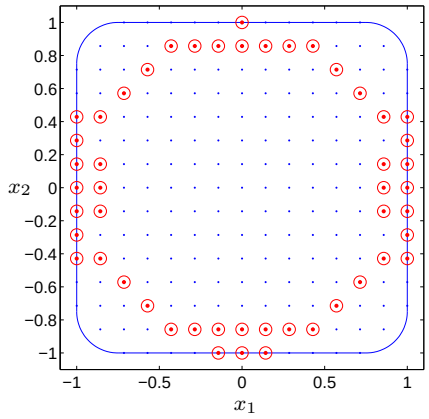


(a) $t = 0.05$

(b) $t = 0.35$



(c) t=0.75



(d) t=1.00

Fig. 4.13. Selected D-optimal switchings for the scanning strategy in the signal propagation example.

denote selected consecutive locations of movable sensors at evenly distributed time instants. The locations of stationary sensors are indicated with open circles on the left panel.

As the velocity of the signal propagation and its magnitude is the greatest in direction of the x_1 axis, the behaviour of movable sensors can be easily explained, because they move to the areas where the changes of the wavefront are the greatest. However, the location of the stationary sensors is not that easy to interpret. The intuition completely fails in this case and this strategy seems to be the least adequate as the process dynamics can hardly be retrieved from the observations.

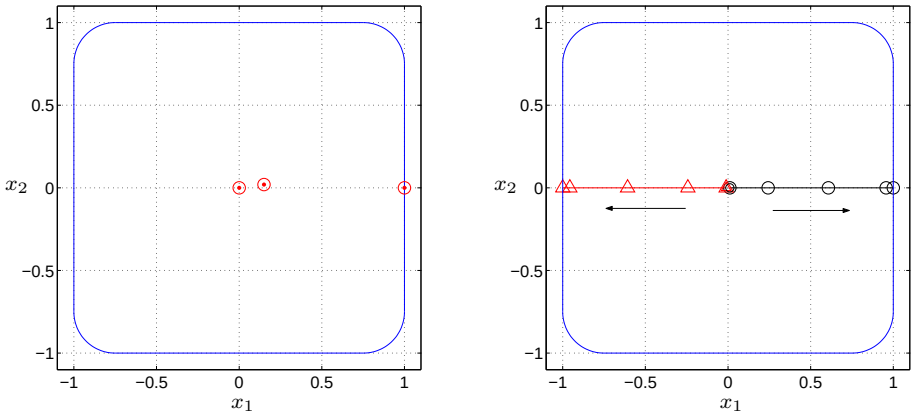


Fig. 4.14. D-optimal strategies for the transmission line example: (a) stationary sensors, (b) movable sensors.

4.6.2. Calibration of air-pollution models

The air quality has become an important societal issue. As air pollutants, we can enumerate gases, liquids, or solid substances suspended in the atmosphere in concentrations which may affect the natural environment including human, animal or vegetation health. Most commonly encountered air-pollution problems are urban smog, acid deposisions, global ozone reduction and a global climate change. The urban smog has recently become one of the most important questions of atmospheric modelling as both an environmental and a social problem. It is characterized by the local buildup of high concentrations of gases and particles caused by industry or traffic emissions, smokestacks, other human-made sources, or formed by secondary processes in the atmosphere.

Atmospheric problems belong to extremely difficult modelling tasks. There exist numerous causes of such a situation. One of them is a high number of different processes which constitute the complicated dynamics of changes in the air environment including (Jacobson, 1999):

- dynamical and thermodynamical processes (changes in the wind speed and direction, air pressure, temperature and density; turbulences),
- transport processes (emissions; transport, dry deposition and sedimentation of gases, aeorosols and cloud drops; energy transport),
- gas processes (gas photochemistry, gas-to-particle conversion),
- radiative processes (infrared and solar radiative transfer),
- aerosol/cloud processes (nucleation; coagulation; condensation/evaporation; deposition/ sublimation; reversible and irreversible kinetic chemistry),

Table 4.2. Scales of atmospheric problems (Jacobson, 1999).

Scale	Dimension [m]	Exemplary processes
Molecular	$\ll 2 \times 10^{-3}$	Molecular diffusion, molecular viscosity
Micro	2×10^{-3}–$2 \cdot 10^{3}$	Eddies, car exhaust, cumulus clouds
Meso	2×10^{3}–$2 \cdot 10^{6}$	Gravity waves, thunderstorms and tornados, urban air pollution and local winds
Synoptic	5×10^{2}–10^{7}	Weather fronts, tropical storms, hurricanes, high- and low-pressure systems
Planetary	$> 10^{7}$	Global wind systems, global warming, stratospheric ozone reduction

and many more. Additionally, all of the above-mentioned processes are coupled through various interactions among them, which further complicate the analysis.

Another considerable cause is the variety of spatial scales of atmospheric problems, from the molecular to the planetary scales. The particular processes are summarized in Table 4.2 adopted from Jacobson (1999). This gives only a very rough overview of problems which may be encountered, but just enough to understand the complexity of the subject.

Due to the rapid development of industry around the world, the problem of protection and restitution of the natural environment becomes of crucial importance. In this context, optimization of air quality monitoring networks is one of the most interesting questions (Munn, 1981). In general two main streams of the considered tasks may be distinguished (Jacobson, 1999):

(a) Forecast problems, where the main aim is to provide the expected levels of pollutant concentrations which allow us to prevent or minimize the further release of dangerous substances. The time derivative should be found based on the so-called *prognostic equation*. Examples of such equations are the species continuity equations or the thermodynamic energy equation.

(b) Diagnostic problems, where emphasis is laid on the detection of some existing abnormal situations. This involves the analysis of the so-called *diagnostic equation* in which the time derivative does not have to be solved. The state and hydrostatic equations are examples of such diagnostic equations.

Apart from the type of problems motivating a forecast, or a suitable diagnosis, the appropriate air-pollutant model over a given urban area is necessary. The propagation process of air-pollutants emitted to the atmosphere is caused by the advection transport of those substances in air masses and, as a result, of the diffusion being the effect of air turbulent pulsations. All processes take place

in mesoscale (see Tab. 4.2). Besides diffusion in a small scale, fluctuations of the velocity and the direction of winds in short- and long-time scales are of importance. The averaged streams of the substances spreading in air masses usually have convection and advection components, and their averaged fluctuation motions may be interpreted as diffusion in the background of the basic average movement. Taking into account the kinetic chemistry of pollutants, this leads directly to air-pollution models in the form of systems of advection-diffusion-reaction equations (Marchuk, 1985; Zlatev, 1995; Hundsdorfer, 1996; Sydow *et al.*, 1997; Sydow *et al.*, 1998; Jacobson, 1999) describing the concentrations $y(x,t)$ of the interacting substances

$$\begin{aligned}\frac{\partial y_k(x,t)}{\partial t} + \nabla\cdot\big(v(x,t)y_k(x,t)\big) &= \nabla\cdot\big(d(x,t)\nabla y_k(x,t)\big)\\ &+ f_k(x,t,y_1,\ldots,y_r),\quad k=1,\ldots,r,\quad x\in\Omega,\quad t\in T\end{aligned} \tag{4.155}$$

subject to the set of boundary and initial conditions

$$\begin{aligned}\frac{\partial y_k(x,t)}{\partial n} &= 0 && \text{for } (x,t)\in\partial\Omega\times T \quad \text{if } v\cdot n \geqslant 0\\ y_k(x,t) &= 0 && \text{for } (x,t)\in\partial\Omega\times T \quad \text{if } v\cdot n < 0\\ y_k(x,0) &= y_0^k(x) && \text{for } x\in\Omega.\end{aligned}$$

The quantity $v(x,t)$ represent the velocity field vector of the transport medium such as water or air. Usually it is directly measurable, or can be computed based on meteorological or hydrodynamical data. From this point of view, a suitable modelling of the velocity over a given domain Ω in time interval T does not present essential difficulties. But the diffusion coefficient $d(x,t)$ which may contain parameterizations of the turbulences being the result of small spontaneous fluctuations which dissipate and create conditions for other disturbances, is generally non-measurable. Thus the appropriate modelling becomes a very difficult problem. Finally, the terms $f_k(\,\cdot\,)$ describe the nonlinear chemistry coupling the different species together with emmissions (sources) and depositions (sinks).

In most air pollution models the transport is dominated by the advection term, and there can be strong local sources. Moreover, the reaction terms are usually very stiff, i.e. some reactions take place on very small scales in comparison with the the overall time scale. In such a way the calibration of the diffusivity tensor in (4.155) is extremely difficult and requires parameter estimation based on observations from a monitoring network. Since the cost of instrumentation (monitoring stations) is rather high, the problem of working out a proper strategy for the measurement process becomes very important. The necessity of optimal control of observational systems is often indicated in works concerned with air-quality monitoring networks (Sturm *et al.*, 1994; Nychka *et al.*, 1998; Müller, 1998).

4.6.2.1. Numerical experiments

Calibration of smog prediction models. One of the most interesting instances of air-pollutant monitoring is prediction of smog, being a mixture of many gases,

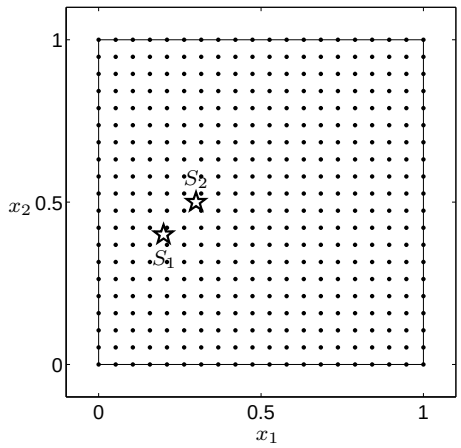


Fig. 4.15. Considered urban area with two emission sources and the available scanning grid.

aerosols and water vapour. In order to construct a proper prognosis of pollutant concentrations, we need a suitable prediction model, and in this case it may be established in the form of a PDE system describing the transport-chemistry of many components. Such a model should be accurately calibrated as it will directly influence the efficiency of the forecast. To slightly simplify the situation, consider the transport-chemistry of only two air pollutants over a given urban area, which are mutually interconnected with a consecutive reaction of the reversible type (Atkins, 1998)

$$P_1 \underset{k_2}{\overset{k_1}{\rightleftharpoons}} P_2, \tag{4.156}$$

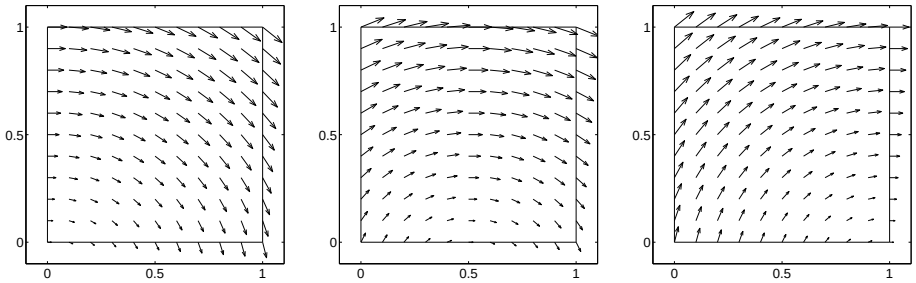
where P_1 and P_2 denote chemical compounds, and k_1 and k_2 are the rates of the forward and reverse reactions, respectively.

The entire process can be described by the system of advection-diffusion-reaction equations

$$\begin{aligned}
&\frac{\partial y_1(x,t)}{\partial t} + \nabla \cdot \big(v(x,t) y_1(x,t)\big) = \nabla \cdot \big(d_1(x) \nabla y_1(x,t)\big) - k_1 y_1(x,t) + k_2 y_2(x,t),\\
&\frac{\partial y_2(x,t)}{\partial t} + \nabla \cdot \big(v(x,t) y_2(x,t)\big) = \nabla \cdot \big(d_2(x) \nabla y_2(x,t)\big) + k_1 y_1(x,t) - k_2 y_2(x,t),
\end{aligned} \tag{4.157}$$

where $y = (y_1, y_2)$ is the vector of concentrations observed in the normalized time interval $T = [0, 1]$. The spatial variable x belongs to the urban area rescaled to the domain Ω with the boundary Γ shown in Fig. 4.15. The last terms on the right-hand side with coefficients k_1 and k_2 are responsible for the changes in the concentrations due to the reaction (4.156).

At the initial time instant, two sources of pollutants (indicated with stars in Fig. 4.15) located at points $S_1 = (0.2, 0.4)$ and $S_2 = (0.3, 0.5)$ emit different substances to the atmosphere, which spread all over the domain Ω due to the



(a) $t = 0$ (b) $t = 0.5$ (c) $t = 1$

Fig. 4.16 . Temporal changes in the wind velocity field.

combination of diffusion and advection processes. The velocity vector v varies in space and time, and changes according to the following model of the velocity field:

$$v(x,t) = (y + 1/4, -x + t), \tag{4.158}$$

which is illustrated in Fig. 4.16.

The contamination mentioned above can be expressed by the following boundary and initial conditions:

$$\begin{aligned}
\frac{\partial y_1(x,t)}{\partial n} &= 0 && \text{if } (x,t) \in \Gamma \times T,\\
\frac{\partial y_2(x,t)}{\partial n} &= 0 && \text{if } (x,t) \in \Gamma \times T,\\
y_1(x,0) &= 20e^{-50[(x_1-0.2)^2+(x_2-0.4)^2]} && \text{if } x \in \Omega,\\
y_2(x,0) &= 10e^{-40[(x_1-0.3)^2+(x_2-0.5)^2]} && \text{if } x \in \Omega.
\end{aligned} \tag{4.159}$$

In our simulation study the following form of the distributed diffusion coefficients was assumed:

$$\begin{aligned}
d_1(x) &= \theta_1 + \theta_2 x_1 x_2,\\
d_2(x) &= \theta_3 + \theta_4 x_1 x_2,
\end{aligned} \tag{4.160}$$

where the nominal vector of parameter values $\theta = (0.04, 0.015, 0.03, 0.025)$ was assumed to be taken from preceding experiments and the reaction rates were predetermined as $k = (k_1, k_2) = (0.1, 0.05)$. The purpose was to find a D-optimal sensor allocation strategy for determining the most accurate estimates of the true parameters $\theta_i,\ i = 1, \ldots, 4$. The experiment consisted in comparison of the strategies employing stationary, movable, and scanning sensors. To this end, the hardware/software simulation environment was established by a PC equipped with Pentium IV 1.7GHz processor, 768MB RAM and running Windows 2000. The solutions of the PDE's were obtained with a Matlab Toolkit written by the author especially for this purpose with the aid of the PDE Toolbox (we employed 30 divisions of the time interval and a triangular spatial mesh consisting of about 400

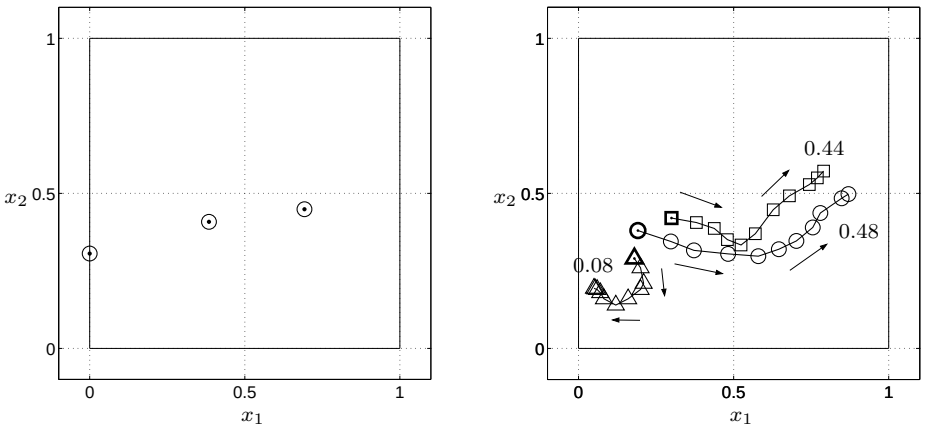


Fig. 4.17. D-optimal locations of stationary sensors (a) versus movable sensors trajectories (b).

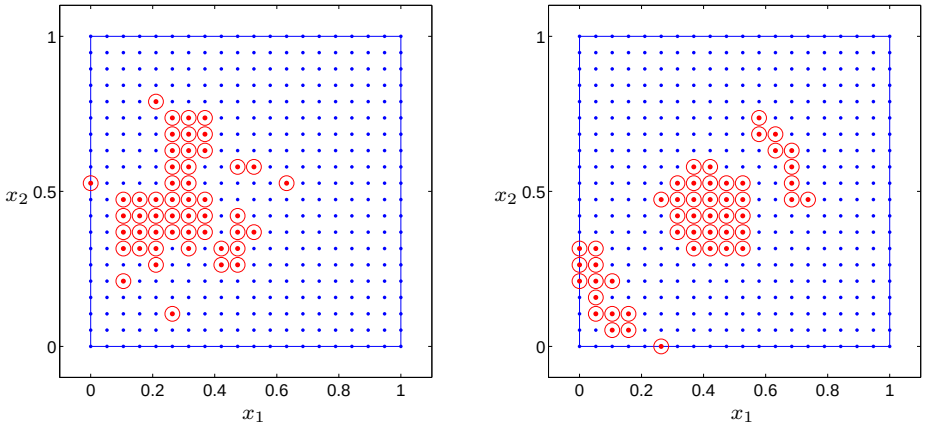
nodes and 800 triangles). All design optimization algorithms were implemented using the Fortran 95 Lahey/Fujitsu v.5.7 compiler.

In the first examined case (i.e. the stationary sensors), Algorithm 3.5 was used for a continuous support set and, starting from a randomly generated four-point initial design, after 7 iterations for accuracy $\epsilon \leqslant 10^{-6}$, the ultimate design

$$\xi^\star = \begin{Bmatrix} (0.000, 0.306) & (0.385, 0.408) & (0.692, 0.449) \\ 0.31 & 0.30 & 0.39 \end{Bmatrix}$$

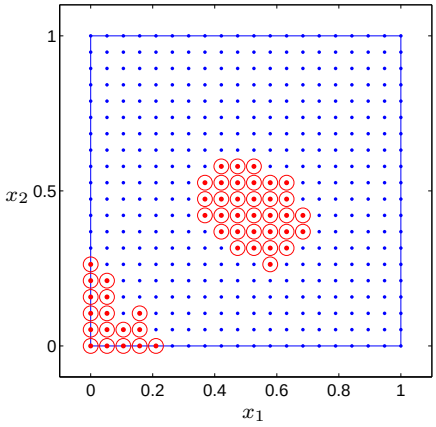
was obtained. It corresponds to the criterion value $\det(M(\xi^\star)) = 7.4139\,\mathrm{E}\,22$. The solution is shown in Fig. 4.17(a).

As the second simulated strategy, application of movable sensors was studied. In order to simplify the calculations, the trajectories were discretized by introducing 10 divisions of the observation interval and then interpolating them with linear splines. Although such an approach produces non-smooth curves, it reduces the number of components for individual support elements (for each spatial location at a given time instant we need only two spatial coordinates) and is the simplest in implementation. The starting positions of motion curves also were optimized and the only constraint imposed on the trajectories was that their maximal length should not exceed unity. The algorithm started from a four-trajectory initial design and after 10 iterations (which took about 8 min) was terminated with the design presented in Fig. 4.17(b) for the same accuracy as for stationary sensors. It is clear that the sensors move to the areas where the greatest changes in pollutant concentrations occur, which approximately follow the wind direction. In contrast to the stationary sensors, the results are much more intuitive, which also affects the value of the criterion ($\det(M(\xi^\star)) = 3.6475\,\mathrm{E}\,23$). The accuracy is significantly greater, which confirms our earlier theoretical hypotheses.

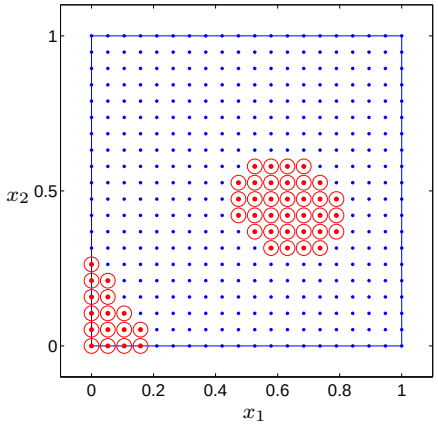


(a) $t = 0.064$

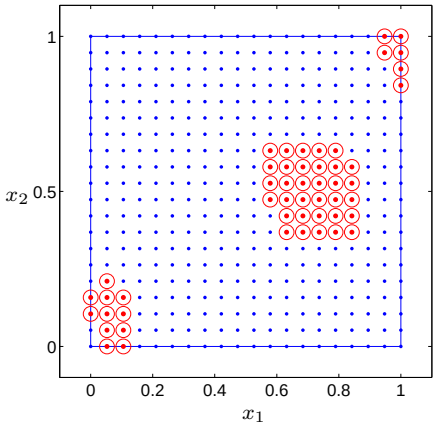
(b) $t = 0.258$



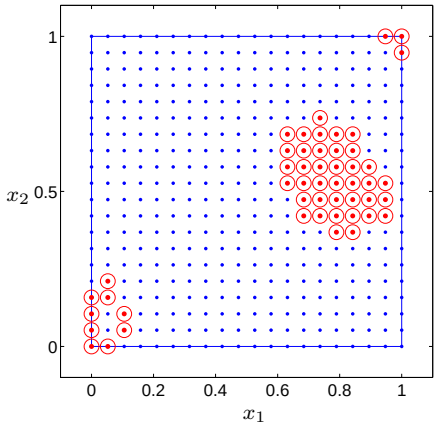
(c) $t = 0.451$



(d) $t = 0.645$



(e) $t = 0.839$



(f) $t = 1.000$

Fig. 4.18. D-optimal sensor allocations for selected time moments in the air-quality monitoring example from Section 4.6.2.1.

Finally, for the same task the scanning strategy was investigated with the assumption that the sensors may be placed on the uniform grid of size 20×20 (see Fig. 4.15) and for the partition of T defined by the switching points $t_k = k/30$, $k = 0, \ldots, 30$. From among 400 admissible sites the task was to choose the best 60 points over any resulting time subinterval. After 304 iterations ($\epsilon \leqslant 10^{-5}$), in less than 10 seconds the one-point correction algorithm produced a solution. The results are shown in Fig. 4.18, where open circles indicate the actual active sensor locations and points stand for the available locations. The corresponding value of the criterion in this case was equal to $\det(M(\xi^\star)) = 9.2249\,\mathrm{E}\,22$. The accuracy of solving a relatively large system of 10 PDE's (2 system responses and 8 sensitivities of the observed states) is slightly affected by a reasonably low density of the finite element approximation mesh which was used (258 nodes and 412 triangles). Consequently, the sensor configurations in the first iterations are also a little perturbed, which can be observed in Fig. 4.18(a).

4.6.3. Managing groundwater resources

Groundwater modelling is another interesting and motivating application which can be considered in the context of the practical usefulness of the developed methodology. Groundwater is one of the natural resources which sustained extensive damage in the past decade due to the man's industrial activities (Sun, 1996; Kovarik, 2000). The significance of this problem cannot be overestimated since even ordinary events of day-to-day human life (e.g. solid and liquid waste dumps, storing and processing the chemicals) may cause pollution of soil or surface water. The pollutants spread through a covering layer and after some time they reach and pollute the groundwater (Sun, 1994; Sun, 1996; Rijtema and Elias, 1996; Kovarik, 2000). In recent years the problem is not only to find a well with a given amount of water discharge, but also to fulfil some quality requirements (Sun, 1996).

A high cost and long period of time for remediation of pollution (compared with that for surface water) results in the fact that groundwater contamination is one of the most serious environmental problems that may damage the human health and cause the water shortage. In the protection and improvement of groundwater quality, two challenging problems may be encountered (Sun, 1996):

- for uncontaminated resources, it is required to predict and control the potential sources of pollution,
- for contaminated resources, it is required to provide suitable remediation processes.

Both the cases imply directly the necessity of predicting the pollutant distribution in groundwater. Since field experiments cannot be exploited for this purpose, the only tool which remains is mathematical modelling. But the main impediment which appears is the high complexity of the analysis, since there are many processes involved in the transport and dynamics of resources, such as hydrodynamic flow and dispersion, mass transport in porous media, sorption and decay of substances and many more. The whole field of the groundwater modelling theory and

Table 4.3. Applications of groundwater modelling

Model	Example
Groundwater flow	Water supply, connection between ground and surface water, regional aquifier analysis, artificial recharge, drainage and dewatering
Heat/Energy transport	Geothermal utilization, heat and cold storage under the ground, heat pollution in groundwater
Mass transport	Groundwater contamination, sea water intrusion, soil reformation, radionuclide waste repositories, impact of river pollution on groundwater,
Media deformation	Weather fronts, tropical storms, hurricanes, high- and low-pressure systems

its potential applications extensively enlarges (the most significant examples are contained in Tab. 4.3) but the detailed analysis of the subject is beyond the scope of this dissertation, so the interested reader can be referred to the relevant comprehensive literature (Dagan, 1989; Bear *et al.*, 1993; Sun, 1994; Sun, 1996; Rijtema and Elias, 1996; Kovarik, 2000).

In general, there exist several classes of models which are exploited in various contributions, but one of the most commonly used ones is the model based on the hydrodynamic dispersion (Dagan, 1989; Bear *et al.*, 1993; Sun, 1996; Kovarik, 2000). This is based on the description with the use of the set of *hydrodynamic* PDE's of advection-diffusion type similar to (4.155):

$$\begin{aligned}\frac{\partial y_k(x,t)}{\partial t} + \nabla \cdot \big(v(x,t) y_k(x,t)\big) &= \nabla \cdot \big(d(x,t)\rho \nabla (y_k(x,t)/\rho)\big) \\ &+ f_k(x,t,y), \quad k = 1,\dots,r, \quad x \in \Omega, \quad t \in T,\end{aligned} \tag{4.161}$$

with exactly the same notation as in the case of (4.155), with additional variable ρ which denotes the density of the fluid. Generally, the variation in the concentration may affect the density and viscosity of the fluid. Further, changes in those variables may cause the state of the flow field to change. In other words, all the above-mentioned variables are interconnected and therefore a single equation of hydrodynamic dispersion is not enough to describe the process in the general case. To solve the problem of groundwater quality in a saturated domain Ω in a given observation interval T, additional differential equations are required, namely the *continuity equation*

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho v(x,t)) = 0, \tag{4.162}$$

the *kinetic equations*

$$v_i(x,t) = -\frac{k_{ij}}{\mu\nu}\left(\frac{\partial p}{\partial x_j} + \rho g \frac{\partial z}{\partial x_i}\right), \quad i,j = 1,\ldots,d \tag{4.163}$$

and the *hydrodynamic state equations*

$$\rho = \rho(y,p), \quad \mu = \mu(y,p), \tag{4.164}$$

where p is the pressure, ρ and μ denote respectively the density and viscosity of the fluid, the k_{ij}'s are the components of the hydraulic conductivity tensor, ν stands for the effective porosity and d is the spatial dimensionality of the problem. From a hydraulic point of view, the boundaries can be split into three groups (Kovarik, 2000):

- *Impermeable* boundaries, where there is neither groundwater inflow, nor outflow. This part is characterized by Neumann conditions, with zero derivative of the concentration in the directions of the unit outward normal of $\partial\Omega$.
- *Permeable* boundaries, where the groundwater flows in and out, and this makes the choice of boundary conditions difficult. This choice depends on the experience of the hydrologists. If the boundary is the river or a lake bank, Dirichlet conditions are often used, but such a condition is very strong because it presumes an ideal interaction between the water level in the river and the groundwater surface. Thus, alternatively, mixed boundary conditions are sometimes used.
- *A boundary with phreatic surface*, where the pressure on a free surface equals the atmospheric pressure (which can be neglected). This leads to the constant boundary condition in the Dirichlet form.

Since the groundwater is a limited resource, it should be exploited with a maximum economic benefit while maintaining a minimum environmental damage. This can be obtained only through an intelligent management and utilization. The cost of the experiment is usually very high and causes the necessity to consider additional problems related to the optimal strategy of the measurement process. For example, the optimization of the number and locations of observational wells should be taken into account, as well as the observational frequency (Sun, 1994) and decisions on the variables which have to be directly measured.

Finally, we have to emphasize that although most often a full 3D model is advisable, it is obvious that some problems can be solved succesfully in two dimensions reducing to a great extent the computational effort. There exist suitable transformations of three-dimensional groundwater flows to two dimensions, which are possible to apply in many cases (Kovarik, 2000).

4.6.3.1. Numerical experiments

Control of observation well exploitation. Consider a confined aquifer lying on a river bank. The other boundaries are assumed to be of impermeable type or the flow

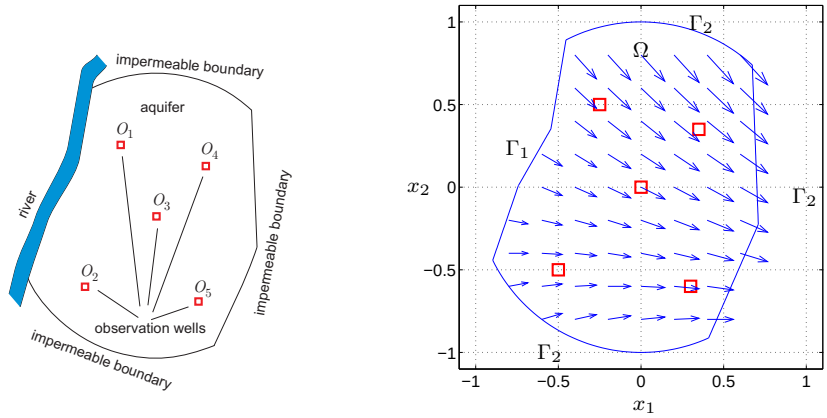


Fig. 4.19. The general overview of a confined aquifer (a) and the velocity field with locations of observation wells from Section 4.6.3.1.

throughout them is negligible. There are five possible locations for the observation wells, O_1 to O_5. The situation is shown in Fig. 4.19. The river is a source of pollution, which spreads over the aquifer due to the hydrodynamic transport and dispersion. For illustrative convenience, a two-dimensional model will be considered as the description of the contamination process. Similar problems can be found in (Sun, 1994; Kovarik, 2000) together with more sophisticated practical applications. In contrast to the atmospheric pollution, the transport of substances in porous media takes place in a much larger scale of time. The duration of such processes may be equal to months and even years, so the pollution effects are also more permanent. In such a way, from a numerical point of view, it is convenient to suitably normalize the time scale.

This leads to the model for changes in the pollutant concentration $y(x,t)$ over the domain Ω in a unit time interval T given by

$$\frac{\partial y(x,t)}{\partial t} + \nabla \cdot \big(v(x)y(x,t)\big) = \nabla \cdot \big(d(x)\nabla y(x,t)\big), \quad x \in \Omega, \;\; t \in T = [0,1]. \quad (4.165)$$

From the equation above it can be seen that the pollutant is assumed not to affect the density of groundwater, i.e. it is approximately constant in time. An additional assumption is that the bank of the river is contaminated all along its length adjacent to the domain Ω with the same constant rate. Moreover, an initial contamination of the aquifer with the considered substance can be neglected. Thus

(4.165) can be supplemented with the following boundary and initial conditions:

$$\begin{aligned} y(x,t) &= 10, \quad (x,t) \in \Gamma_1 \times T, \quad \text{(river bank)} \\ \frac{\partial y(x,t)}{\partial n} &= 0, \quad (x,t) \in \Gamma_2 \times T, \quad \text{(impermeable boundary)} \\ y(x,0) &= 0, \quad x \in \Omega. \end{aligned} \tag{4.166}$$

Since exploratory wells of observation and pumping types are very expensive, the monitoring of water quality should be optimized in order to reduce the number of data sources and to properly use the available data. Because in our case the possible number of observation wells is rather small, the application of the scanning strategy with an optimal switching schedule seems to be the most appropriate approach.

The parametric form of the distributed hydrodynamic dispersion was assumed as

$$d(x) = \theta_1 + \theta_2 \tanh(\theta_3 x_2), \tag{4.167}$$

where the elements of the vector $\theta^0 = (0.15, -0.02, 2.00)$ were taken as the nominal values of the parameters. The velocity of the transport medium was taken in the simple closed form

$$v = (v_{x_1}, v_{x_2}) = (0.1x_1 + 0.4,\ -0.3x_2 - 0.1x_1 - 0.2), \tag{4.168}$$

which is illustrated in Fig. 4.19(b).

Table 4.4. Combinations of the activated observation wells

Active wells	Control u_c
O_1, O_2	1
O_1, O_3	2
O_1, O_4	3
O_1, O_5	4
O_2, O_3	5
O_2, O_4	6
O_2, O_5	7
O_3, O_4	8
O_3, O_5	9
O_4, O_5	0

The main aim of the experiment was to find an optimal sensor activation policy for determining the most accurate estimates of the true parameters θ_1 to θ_3. As the number of the exploited wells should be minimal, a reasonable choice it to use at every time instant only two from among the five available locations (cf. Fig. 4.19). The set of ten combinations of active wells, which were coded as

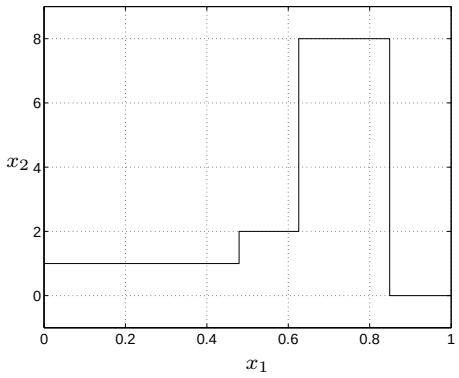


Fig. 4.20. D-optimal control signal for activation of observation wells.

successive integers being the levels of the input control signal u_c, is gathered in Table 4.4.

In this example the implementation was performed entirely in the Matlab 6.5 environment. The PDE's were solved using exactly the same routines as in the previous application example with a finite-element approximation of the domain (483 nodes, 893 triangles) and 40 divisions of the time interval. Finally, the procedure based on the CPET approach with the `fmincon` Matlab function in the role of the optimizer produced the following control signal (cf. Fig. 4.20) describing the changes in the active well locations:

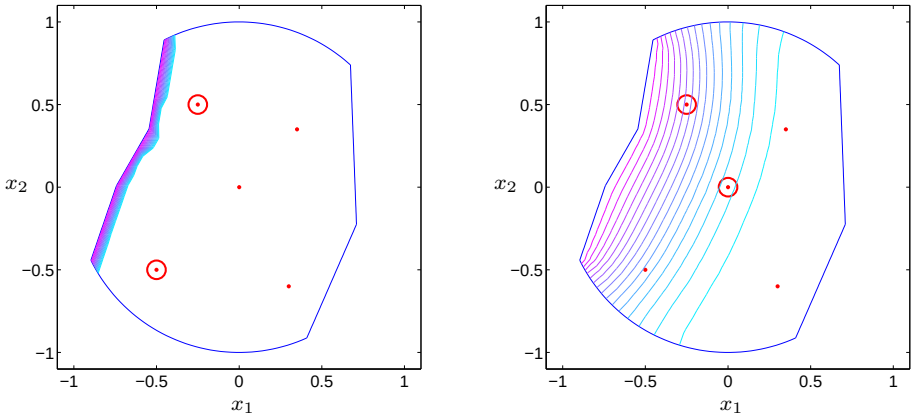
$$u_c(t) = \begin{cases} 1 & \text{if } 0.000 \leqslant t < 0.479, \\ 2 & \text{if } 0.479 \leqslant t < 0.626, \\ 8 & \text{if } 0.626 \leqslant t < 0.849, \\ 0 & \text{if } 0.849 \leqslant t \leqslant 1.000. \end{cases}$$

The maximal number of switchings was assumed to be equal to 2 and the time of calculations was about 12 minutes.

Figure 4.21 illustrates the optimal sensor activation policy versus contour plots of the pollutant concentration, where open circles indicate the actually exploited observation wells. The sensor activation strategy can be interpreted based on the observation that the measurements are taken possibly close to the forehead of the 'pollutant wave' moving from the river bank to the right boundary of the aquifer. This fact is reflected by the sensor activation schedule as the greatest changes in the concentration occur there.

4.7. Concluding remarks

Observation strategies for DPS's involving stationary sensors with time-continuous or time-discrete measurements are commonly exploited techniques in engineering



(a) $t = 0$ (b) $t = 0.479$

(c) $t = 0.626$ (d) $t = 0.849$

Fig. 4.21. Consecutive switchings of the activated observational wells versus contour plots of the pollutant concentration.

applications due to their attractive properties such as the low complexity of the observational system and a wide variety of methods. In this chapter it was shown that construction of appropriate information matrices leads to a generalization of the methodology and algorithms developed for multi-output static DPS's in Chapter 3, including optimization of the experimental effort (well-known nonlinear programming procedures and the novel SDP approach) as well as clusterization-free designs. Nevertheless, such strategies are not always adequate to dynamic DPS's because of their low flexibility to fit into the system dynamics, which results in a significant decrease in the estimation quality.

A remedy is to employ more sophisticated measurement strategies, which may influence the experiment conditions operating directly on the time variable or indirectly through the dynamics of sensor motions. Both the approaches may

significantly increase the possibilities to efficiently exploit the dynamics of the considered system. In first part of the chapter, the advantages of applying mobile sensors were delineated based on the direct approach (Rafajłowicz, 1986b; Uciński, 1999a) whose origin is in the classical methods of optimum experiment design. The key idea is to convert the problem to operating on design measures, rather than on the trajectories themselves. Such an approach seems to be attractive as some well-known classical design algorithms can be adopted. Consequently, the appropriate procedure based on Fedorov's first-order algorithm is proposed in this work. However, it should be emphasized that the applicability of the direct approach for more complicated tasks is limited since difficult numerical problems can be encountered, which is connected to discretizations of the trajectories and the necessity of solving global optimization problems. On the other hand, only a few alternatives exist in this field (Uciński, 1999a).

The second possibility is the scanning strategy, which can be split into two subcases, namely the situation when the time schedule of sensor switchings is fixed *a priori* and when it also constitutes a design variable. Within the framework of this chapter, a computationally attractive approach was proposed for the optimal placement of scanning sensors in both the situations. In the former case, our solution extends some ideas employed for constructing replication-free designs proposed by Fedorov (Fedorov and Hackl, 1997; Cook and Fedorov, 1995; Fedorov, 1989) who restricted his attention solely to static systems. Accordingly, much more efficient scanning measurement policies can be determined compared with the stationary sensor strategies which have been considered in the literature so far. In spite of its somewhat abstract assumptions, the resulting algorithm of exchange type is very easy to implement, which leads to extremely good performances.

Bear in mind, however, that the clusterization-free approach should in principle be used if the number of sensors is relatively high. If this is not the case, we can resort to standard discrete optimization routines which ensure that the constraints on the design measure are satisfied.

In order to select an optimal switching table, a computational scheme based on the control parameterization enhancing technique was proposed in order to determine optimal schedules of scanning sensors which measure the state of a given DPS. The aim of this monitoring network is to accurately determine estimates of the unknown system parameters. Consequently, the highly combinatorial nature of the original problem is alleviated in a sense. The point is not in the computational effort, but in the possibility of applying widely available non-linear programming algorithms to the resulting transformed optimal control problem.

Furthermore, the question of correlated observations, being one of the most serious problems which may appear in applications, was discussed. The local and global mutual correlations between measurements are usually neglected and there are very few contributions devoted to this subject. One possible approach is to directly introduce additional constraints into the problem which concern the acceptable minimal distances between sensors. Although this technique seems to be very attractive due to its simple formulation, it is practically impossible to consider global correlation relations. Instead, we set forth an alternative approach which

is based on including mutual correlations between the measurements directly into the information matrix. Then an efficient exchange-type procedure dedicated to the multi-response DPS's was developed. It constitutes a broad generalization of the algorithm proposed by Brimkulov *et al.* (1986). However, we still should bear in mind that numerical problems may occur due to the singularity of the covariance matrix and the notion of the pseudoinverse must then be used (Pukelsheim, 1993). This problem can be accounted for with relative ease by some minor changes in the implementation. Nevertheless, the ultimate algorithm is very simple to implement and additional improvements discussed in the chapter extremely increase its efficiency.

In the last part of the chapter, sensor location techniques were proposed for the model-based diagnostics of DPS's based on the structural hypothesis testing. To the best of the author's knowledge, such an approach is one of the first attempts addressed to this area. In spite of the initial state of the investigations in the field, the results could hardly be overestimated in numerous applications, e.g. in air pollution systems or in hazardous environments.

The following stands for a concise summary of contributions developed in this chapter to the state-of-the-art in optimal sensor location for parameter estimation in spatio-temporal systems:

- Generalization of the results and algorithms from previous chapter to dynamic DPS's in the case of stationary sensors.
- Derivation of optimality conditions for non-parameterized and parameterized trajectories, and application of the two-phase first-order algorithm with adaptive random search (Walter and Pronzato, 1997) and sequential quadratic programming to construct optimal trajectories of mobile sensors,
- Development of expeditious methods of activating scanning sensors, and specifically:
  - introduction of an approach based on clusterization-free designs for an arbitrarily fixed switching schedule,
  - transformation of the problem to an equivalent Mayer formulation of optimal control in the case of an optimized switching schedule, which can then be solved using the CPET approach.
- Development of an approach to solve the sensor location problem in the case of correlated observations. Specifically, a method which includes mutual correlations between measurements directly into the measurement covariance matrix is proposed and a relaxation algorithm is developed for solving the resulting computational problem.
- Introduction of optimal sensor placement methods to model-based fault detection. Adaptation of the parametric approach to describe system modes of work and the development of methods for the reliability maximization of fault detection and isolation based on structured hypothesis testing.

Chapter 5

SENSOR LOCATION IN THE PRESENCE OF PARAMETRIC AND STRUCTURAL MODEL UNCERTAINTIES

In Section 2.2.4 we indicated that, in general, for a nonlinear parameterization of the system responses optimum experimental conditions strongly depend on the unknown parameter values which only have to be estimated. This causes one of the main complications related to the determination of the optimal experimental conditions. A common approach is then to design the experiment for some reasonable nominal parameter values whose knowledge is a prerequisite for applying the locally optimal sensor location methods described in the previous chapters. Since the uncertainty of those nominal values is not taken into account, the practical application of such procedures is limited to situations when the system responses change slowly in the set of admissible parameters.

Often, the parameter estimates at hand are far from their true values, and in addition to this, properties of locally optimal sensor locations can be very sensitive to changes in these parameters (Ford *et al.*, 1989). Neglecting the problem of the parametric uncertainty may make the solution far from the optimal one. Consequently, this may lead to the question about the practical usefulness of the non-linear experimental design (Walter and Pronzato, 1990).

To overcome those difficulties, several attempts have been made in the literature regarding general optimum experimental design theory either by application of the sequential approach (Fedorov, 1972; Ford *et al.*, 1989; Walter and Pronzato, 1990; Walter and Pronzato, 1997), modification of the obtained locally optimal designs (Landaw, 1980), introduction of designs in the average sense (Pronzato and Walter, 1985; Walter and Pronzato, 1997; Uciński, 1999a; Uciński, 1999b) or so-called minimax designs (Pronzato and Walter, 1988; Walter and Pronzato, 1997; Uciński, 1999a; Uciński, 1999b). However, none of the listed techniques is without drawbacks and the problem still remains open.

Another and even more difficult situation which can be encountered in practice is that the form of the model is far from being known with such a certainty as it was assumed in the previous chapters. Sometimes several alternative models are proposed for the same physical situation but it is unknown which is the most adequate one. For example, such a situation is typical in fault diagnosis where different modes of the system work are described by different models, but the actual one is unknown and has to be detected (Korbicz *et al.*, 2004). We have

to conduct experiments that will allow us to select the model which best fits the data. This leads directly to model discrimination designs (Fedorov, 1972; Bard, 1974; Atkinson and Fedorov, 1975; Atkinson and Donev, 1992; Burke *et al.*, 1994; Fedorov and Hackl, 1997; Uciński and Bogacka, 2002; Kuczewski and Uciński, 2003; Kuczewski *et al.*, 2004) which make it possible to find solutions in the presence of structural model uncertainties.

The main goal of this chapter is to briefly present the existing methods which take into account model uncertainties and to show how to adapt them in the framework of the sensor location problem. To the best of our knowledge, in the context of the scanning measurement strategies such robust approaches have received no attention yet, whereas for stationary and movable sensors the only attempts were made by Uciński (1999a; 1999b). In addition to this, the introduction of the discrimination experiments into the field of DPS's is provided where very few contributions exist (Kuczewski and Uciński, 2003; Kuczewski *et al.*, 2003; Kuczewski *et al.*, 2004) contrary to the corresponding theory for LPS's.

5.1. Sequential design techniques

Since it is clear that for any design ξ the FIM elements depend on the true vector of parameters θ_{true} which is obviously unknown, determination of an optimal design requires finding some compact domain Θ_{ad} containing θ_{true} and where $M(\xi, \theta)$ varies insignificantly for $\theta \in \Theta_{\text{ad}}$. In the case when initial information about the parameters is missing, the only solution is to conduct an additional analysis for predetermination of the region Θ_{ad}. Nevertheless, it is impossible to construct an optimal design for such an experiment without sufficient knowledge about parameters, because most often optimal sensor locations depend on θ. This leads directly to the very reasonable idea of repetition of the experimental and estimation steps several times. This is equivalent to the division of the resources (e.g. the time horizon) into small parts which are related to the corresponding consecutive stages of the experiment. A general scheme is shown in Fig. 5.1. Each stage consists of

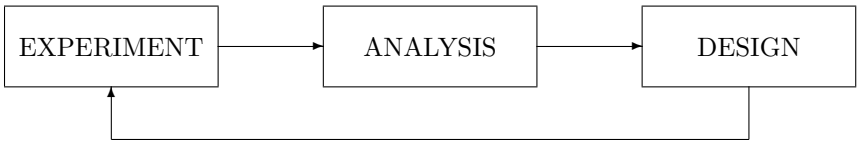


Fig. 5.1 . A general scheme of sequential design.

three sequential tasks: first a measurement process is conducted (some preliminary nondegenerate design can be used in the first stage), then the obtained data are used for parameter estimation or an additional analysis and, at last a locally optimal sensor placement is determined based on the updated calculated parameter estimates. The sequential experiment finishes as a prescribed level of accuracy regarding parameter estimates is achieved or, alternatively, the maximum number

of stages is exceeded.

Owing to its simplicity, the idea of sequential designs is relatively easy to implement and could be used in conjunction with a wide class of design optimization algorithms without substantial difficulties. Because the analytical determination of optimal designs is possible only in simple cases, this property is of great practical relevance. Nevertheless, some non-trivial problems sometimes appear which have to be taken into account, cf. (Ford *et al.*, 1989):

- How many stages of the experiment should be chosen to guarantee the prescribed accuracy?
- What is the character of the dependence of the final design upon initial parameter estimates?
- Is the sequential procedure convergent, and if so, does the convergence can be understood in the approximation sense (i.e. does the generated design asymptotically tend to the locally optimal one for the true parameter values θ_{true})?

Some existing results being partial answers to the questions mentioned above and which justify sequential techniques can be found in (Fedorov, 1972; Ford *et al.*, 1989; Walter and Pronzato, 1990; Walter and Pronzato, 1997). However, it should be noted that this approach often becomes impractical, due to a possibly too long experimental time and a too high experimental cost which are required. But the main disadvantage seems to be the fact that sequential designs necessitate the experimentation stage to be renewable. Since for some classes of systems this is rarely possible (e.g. biological systems) it is clear that such an approach cannot be treated as a universal remedy for the discussed shortcomings of local designs.

5.1.1. Sequential designs for the scanning strategy

Some of the approaches considered within the framework of this dissertation are especially suited for adaptation when implementing sequential designs strategies. The most important of them is scanning which provides by definition the division of the experimental resources (time interval) into separate parts. This fact can often be exploited to extend the approach using sequential techniques in such a way as to obtain a higher level of robustness to parametric uncertainty.

Theorem 4.5 for a fixed time switching schedule in the scanning strategy makes it possible to decompose the problem into a set of subproblems concerning determination of particular components of the design $\xi = (\xi_1, \ldots, \xi_K)$, cf. (4.50), corresponding to the consecutive time subintervals $T_k,\ k = 1, \ldots, K$. On one hand this offers a possibility of parallelization of numerical procedures (see Remark 4.2), but on the other hand, a sequential version of the algorithm can be proposed which is very convenient in this case. Providing for each design step an additional estimation phase which is supposed to improve our knowledge about the system parameters, we obtain the general scheme of such a procedure shown in Fig. 5.2 (Patan and Uciński, 2004). In such a way, typical conditions in the scanning measurement

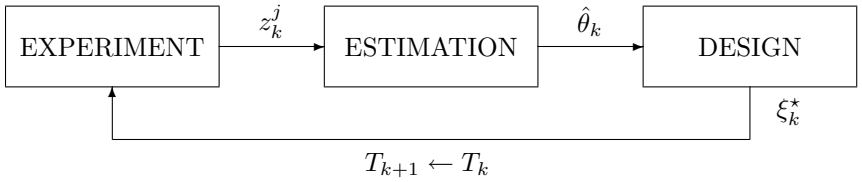


Fig. 5.2. Sequential design for scanning strategy.

strategy make it possible to apply the sequential design technique to implement alternate experimental and estimation stages in a very natural manner. Then our basic idea is to extend the results to the so-called clusterization-free designs set forth in Section 4.3.1 taken in conjunction with some techniques taken from the sequential design theory. The resulting extended multi-point correction algorithm of exchange type is described in the following.

5.1.1.1. Robust scanning algorithm

The activation policy of scanning sensors implies that no replications of measurements are allowed during each phase of the experiment and at most one observation may be made at each available sensor position. In this situation, as a particular implementation of the multi-correction version of Algorithm 4.1, we can use the approach which consists in selecting in every time step the best N-element subset S^* of a given P-element set X of all potential points where measurements may be taken, provided that $N < P$. This idea is realized with the following iterative routine (Patan and Uciński, 2004):

Algorithm 5.1. *Sequential multi-point correction algorithm*

Step 1. Select the number K of sequential design stages. Introduce the partition $t_0 = 0 < t_1 < \cdots < t_K = t_f$ of the time interval $T = [0, t_f]$. Construct the subintervals $T_k = [t_{k-1}, t_k]$, $k = 1, \ldots, K$. Guess an initial N-element set $S_1^0 \subset X = \{x^1, \ldots, x^P\}$. Set $R_1^0 = X \setminus S_1^0$, $k = 1$. Choose some positive tolerance $\varepsilon \ll 1$.

Step 2. If $k > K$ then STOP, otherwise set $s = 0$, construct the design ξ_k^s by setting

$$w_{s,j}^{(k)} = \begin{cases} 1/N & \text{if } x^j \in S_k^s, \\ 0 & \text{if } x^j \in R_k^s, \end{cases}$$

and conduct the corresponding experiment. Solve the problem

$$\hat{\theta}_k = \arg \min_{\theta \in \Theta_{\mathrm{ad}}} \sum_{j=1}^{P} w_{s,j}^{(k)} \int_{T_k} \|z^j(t) - y(x^j, t; \theta)\|^2 \, \mathrm{d}t.$$

Step 3. Set $R_k^s = X \setminus S_k^s$.

Step 4. Determine $M(\xi_k^s;\hat{\theta}_k)$ and for $j=1,\ldots,P$ calculate

$$\psi(x^j,\xi_k^s)=\operatorname{trace}\Big[\overset{\circ}{\Psi}(\xi_k^s)\Upsilon(x^j)\Big]-\frac{1}{K}\operatorname{trace}\Big[\overset{\circ}{\Psi}(\xi_k^s)M(\xi_k^s;\hat{\theta}_k)\Big],$$

where

$$\overset{\circ}{\Psi}(\xi_k^s)=\left.\frac{\partial\Psi(M)}{\partial M}\right|_{M=M(\xi_k^s;\hat{\theta}_k)},$$

and

$$\Upsilon(x)=\frac{1}{t_f}\int_{T_k}G^{\mathrm{T}}(x,t)C^{-1}(x,t)G(x,t)\,\mathrm{d}t,\quad G(x,t)=\left(\frac{\partial y(x,t;\theta)}{\partial\theta}\right)_{\theta=\hat{\theta}_k}.$$

Step 5. If $\max\limits_{x^j\in R_k^s}\psi(x^j,\xi_k^s)<\min\limits_{x^j\in S_k^s}\psi(x^j,\xi_k^s)+\varepsilon$, then set $S_{k+1}^0=S_k^s$, increment k by one and go to Step 2.

Step 6. Sort the values of the function ψ obtained in Step 4 in non-increasing order and relabel points x^j as v^r in order to have

$$\psi(v^1,\xi_k^s)\geqslant\psi(v^2,\xi_k^s)\geqslant\ldots\geqslant\psi(v^P,\xi_k^s).$$

Step 7. Construct $S_k^{j+1}=\{v^1,\ldots,v^N\}$. Increment s by one and go to Step 3.

♦

Based on the notion of clusterization-free designs in the k-th stage of the experiment, this exchange-type algorithm constructs a sequence of sets S^s converging to a set S_k^* which is optimal in the sense of the criterion Ψ (Section 4.3.1). As was already mentioned, the procedure described above constitutes an extension of the practical realization of Algorithm 4.1 originally proposed in (Uciński and Patan, 2002a).

In spite of a reasonably simple scheme, the efficiency of this iterative routine depends strictly on the effectiveness of the solution to the estimation problem from Step 2, which constitutes the major drawback of the proposed approach. It is a direct consequence of the lack of on-line identification methods for DPS's, which was already indicated in Section 4.6. But it should be pointed out that in spite of this inconvenience, in order to construct an appropriate design in each consecutive time step only a rough estimate of the unknown parameters is necessary, and the solution of the estimation problem does not have to possess a high accuracy, which raises possibilities of accelerating this phase in any experimental stage. On the other hand, the high accuracy of parameter estimation is the main goal of the approach, and therefore apart from design phase, the high accuracy of estimation must simultaneously be provided. Moreover, for some problems the duration of the studied process is sufficiently long (e.g. for groundwater modelling the pollution transport takes months or even years) to apply an efficient off-line estimation algorithms.

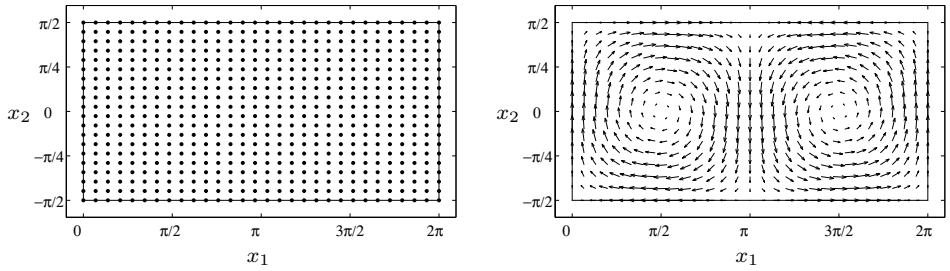


Fig. 5.3 . Domain with admissible sensor locations (a) and a wind velocity field (b).

Example 5.1. In order to test the proposed algorithm, consider the transport-chemistry problem of air pollutants over a given area similar to Example 4.3. The wind power and direction are assumed to be described by the symmetric solid rotational velocity field of the form

$$v(x) = \Big(2\pi \cos\big(x_1 - \frac{\pi}{2}\big) \sin(x_2), -2\pi \sin\big(x_1 - \frac{\pi}{2}\big) \cos(x_2)\Big), \tag{5.1}$$

which is illustrated in Fig. 5.3 along with the possible sensor locations over the area $\Omega = [0, 2\pi] \times [-\pi/2, \pi/2]$. At the initial time instant, a contamination substance is emitted to the atmosphere near the centre of the top boundary of Ω. The changes in the pollutant concentration $y(x, t)$ over a normalized unit time interval $T = [0, 1]$ are in such a situation described by the following advection-diffusion process equation:

$$\frac{\partial y(x,t)}{\partial t} + \nabla \cdot \big(v(x) y(x,t)\big) = \nabla \cdot \big(d(x) \nabla y(x,t)\big), \quad (x,t) \in \Omega \times T, \tag{5.2}$$

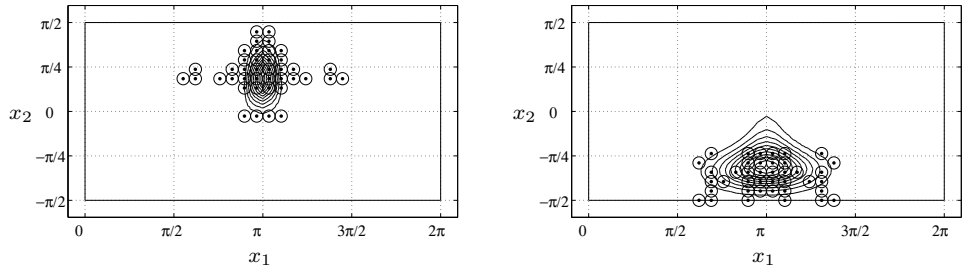
supplemented with the boundary and initial conditions:

$$\begin{array}{rll} \dfrac{\partial y(x,t)}{\partial n} & = 0, & (x,t) \in \partial\Omega \times T, \\ y(x,0) & = 10 e^{-50[(x_1-\pi)^2 + (x_2-1)^2]}, & x \in \Omega. \end{array} \tag{5.3}$$

Our aim is to determine optimal experimental conditions in the sense of a D-optimum activation policy for scanning sensors in order to estimate the unknown parameters of the spatially-varying diffusion coefficient

$$d(x) = \theta_1 + \theta_2 (x_1 - \pi)^2 + \theta_3 x_2. \tag{5.4}$$

Sensors may be placed on the uniform grid of size 30×20 (cf. Fig. 5.3(a)) and the partition of T is defined *a priori* by the switching points $t_k = k/20$, $k = 0, \ldots, 20$. The initial design was formed from randomly generated $N = 40$ points. The algorithm was implemented with the use of the Lahey/Fujitsu Fortran 95 compiler



(a) $t = 0.1;\ \hat{\theta}_0 = (0.072, 0.012, 0.091)$ (b) $t = 0.4;\ \hat{\theta}_0 = (0.118, 0.032, 0.049)$

(c) $t = 0.65;\ \hat{\theta}_0 = (0.112, 0.039, 0.046)$ (d) $t = 0.95;\ \hat{\theta}_0 = (0.106, 0.056, 0.049)$

Fig. 5.4. Selected consecutive stages of the sequential scanning configurations with the contour plots of pollutant concentrations.

and a PC (Pentium IV, 1.7 GHz). All covariance matrices were set to identity and the estimation phase was performed using simulated output data with the noise of normal distribution and the variance equal to 2% of the simulated output). The true value of the parameter vector was assumed to equal $\theta_{\text{true}} = (0.1, 0.05, 0.05)$. The ultimate consecutive sensor configurations are shown in Fig. 5.4, where open circles indicate the activated sensor locations. As can be easily seen from Fig. 5.4, the symmetry of the problem along the x_1 axis is retained and the sensors are activated near the region where the greatest changes in the concentrations take place. Moreover, the updates of the parameters lie in the vicinity of the postulated true values. For the estimation phase the sequential quadratic programming procedure `DNCONF` from the IMSL library (v.4.0) was used. Despite the time consuming estimation of system parameters, the computational time for the finite-element grid consisting of 1600 nodes was approximately 1 minute.

★

5.2. Optimal designs in the minimax sense

5.2.1. Problem formulation

When trying to develop more systematic approaches to tackle the parametric uncertainty of the model than sequential designs, one of the possible solutions is to

optimize the performance of the experiment for the worst possible case in the set of admissible parameters $\Theta_{\rm ad}$. The most attractive property of this idea is that any further hypothesis about the distribution of the parameters is not needed. Focusing all attention and effort on providing possibly maximum information to a parameter vector θ which is the most difficult to identify in $\Theta_{\rm ad}$, the problem can be brought down to the minimization of the criterion

$$J_{\rm MM}(\xi) = \max_{\theta\in\Theta_{\rm ad}} J(\xi,\theta) = \max_{\theta\in\Theta_{\rm ad}} \Psi[M(\xi,\theta)]. \tag{5.5}$$

The most popular choice in the literature seems minimization of the MMD-optimality criterion (Walter and Pronzato, 1997; Uciński, 1999d; Uciński, 1999a)

$$J_{\rm MMD}(\xi) = \max_{\theta\in\Theta_{\rm ad}} \big[-\ln\det M(\xi,\theta)\big]. \tag{5.6}$$

The minimax criterion (5.5) defines the optimal design as

$$\xi^\star_{\rm MM} = \arg\min_{\xi\in\Xi(X)} \big\{ \max_{\theta\in\Theta_{\rm ad}} \Psi[M(\xi),\theta]\big\}, \tag{5.7}$$

where $\Theta_{\rm ad}$ is assumed to be compact. To characterize the minimax designs, assume that both $\Psi(\,\cdot\,,\,\cdot\,)$ and $\partial\Psi(\,\cdot\,,\,\cdot\,)/\partial M$ are continuous. Moreover, conditions (A3)–(A5) from page 38 are assumed to be satisfied together with the following assertion:

(A11) $\forall\xi\in\Xi_q(\theta)=\{\xi:\Psi[M(\xi,\theta)]\leqslant q<\infty\}$, $\forall\bar\xi\in\Xi(X)$:

$$\Psi[(1-\alpha)M(\xi,\theta)+\alpha M(\bar\xi,\theta)] = \Psi[M(\xi,\theta)]+\alpha\int_X \psi(x,\xi,\theta)\bar\xi(\mathrm{d}x)+o(\alpha;\xi,\bar\xi)$$

where the scalar q is chosen to assure that $\Xi_q(\theta)\neq\emptyset$ and $\lim\limits_{\alpha\to0} o(\alpha;\xi,\bar\xi)/\alpha=0$ uniformly in $\Theta_{\rm ad}$.

This allows us to formulate the following result, being the necessary and sufficient condition for the optimality of a minimax design:

Theorem 5.1. *A design $\xi^\star_{MM}$ is optimal iff there exist a probability measure $\omega^\star$ defined on $\Theta_{\rm ad}(\xi)=\big\{\hat\theta:\Psi[M(\xi,\hat\theta)]=\max\limits_{\theta\in\Theta_{\rm ad}}\Psi[M(\xi,\theta)]\big\}$ such that*

$$\min_{x\in X}\int_{\Theta_{\rm ad}(\xi)}\psi(x,\xi^\star_M,\theta)\,\omega^\star(\mathrm{d}\theta)\geqslant 0.$$

Proof. The proof is based on the results of game theory in conjunction with some properties of the max functions. Nevertheless, since the explicit form of the function ψ is not essential here, the proof for the MIMO systems proceeds in the same way as in Theorem 2.6.1 from (Fedorov and Hackl, 1997, p. 42). ■

Clearly, the practical application of Theorem 5.1 is by no means more difficult than the corresponding conditions for locally optimal designs. The optimization of the minimax criteria provides reasonably good results for the worst possible

values of parameters, which potentially may occur more than once, but for the other parameter vectors the quality of the optimal design might be questionable. As a final comment, let us indicate one more drawback of the minimax designs, namely that invariant criteria with respect to transformations of θ for calculation of locally optimal designs may not maintain this valuable property with respect to the minimax approach (Ford *et al.*, 1989).

5.2.2. Minimax optimization via relaxation

There exist very few efficient numerical algorithms devoted to solving general minimax problems, and in addition to this, most of them are limited to the situations where the optimization is performed over finite sets. Since both ξ and θ belong to infinite sets, the solution of the problem (5.5) becomes a rather hard task except for rare situations where for some regression models the $MM\Psi$-optimal design can transformed into a conventional Ψ-optimal one (Pronzato and Walter, 1988). However, in (Uciński, 1999a) the considered optimization problem (5.5) is proposed to be exchanged with minimization of a scalar α, with respect to

$$\max_{\theta\in\Theta_{\rm ad}} \Psi[M(\xi,\theta)] \leqslant \alpha. \tag{5.8}$$

This is equivalent to the set of constraints

$$\{\Psi[M(\xi,\theta)] \leqslant \alpha, \;\; \theta \in \Theta_{\rm ad}\} \tag{5.9}$$

which is obviously infinite.

The so redefined problem can be solved with the use of some numerical procedures for inequality constrained Semi-Infinite Programming (SIP) (Polak, 1997; Reemtsen, 2001). In this vein, an intuitive approach can be proposed for construction of a finite set containing representative values of θ, which is equivalent to relaxing the problem by taking into account only a finite number of constraints (5.9). This is embodied in the simple relaxation algorithm proposed by Shimizu and Aiyoshi (1980) and its well performance was proven in non-linear experimental design problems for LPS's (Pronzato and Walter, 1988; Walter and Pronzato, 1997) and DPS's (Uciński, 1999c). The general form of this procedure can be represented by the following scheme (Uciński, 1999a):

Algorithm 5.2. *Minimax optimization algorithm via relaxation*

Step 1. Set $k = 1$. Choose an initial parameter vector $\theta^1 \in \Theta_{\rm ad}$ and define the first set of representative values $\Theta^k_{\rm rep} = \{\theta^1\}$.

Step 2. Solve the current relaxed problem

$$\xi^{(k)} = \arg \min_{\xi\in\Xi(X)} \left\{ \max_{\theta\in\Theta^k_{\rm rep}} \Psi[M(\xi,\theta)] \right\}.$$

Step 3. Solve the maximization problem

$$\theta^{k+1} = \arg \max_{\theta\in\Theta_{\rm ad}} \Psi[M(\xi^{(k+1)},\theta)].$$

Step 4. If

$$\Psi[M(\xi^{(k)}, \theta^{k+1})] \leqslant \max_{\theta \in \Theta^k_{\rm rep}} \Psi[M(\xi^{(k)}, \theta)] + \epsilon,$$

where ϵ is a predefined small positive constant, then STOP, otherwise $\Theta^{k+1}_{\rm rep} = \Theta^k_{\rm rep} \cup \{\theta^{k+1}\}$, increment k, and go to Step 2.

♦

Shimizu and Aiyoshi (1980) showed that the above routine terminates in a finite number of iterations for any ϵ. As was mentioned earlier, the usefulness of the algorithm was confirmed for the case of stationary sensors (Uciński, 1999c). To the best of the author's knowledge, however, the procedure has not been verified yet in the case of scanning sensors. Its applicability to mobile sensors is rather limited due to problems with solving the minimax optimization problem in Step 2. Some indications of possible alternatives can be found in (Uciński, 1999a; Uciński, 1999b; Uciński, 1999d). At this juncture, it would be beneficial to present some illustrative example. But in order to compare different approaches, the results of the corresponding experiments will be postponed to the end of the next section.

5.3. Optimal designs in the average sense

5.3.1. Problem statement

A common opinion is that methods based on the minimax interpretation of the parametric robustness of design lead to overly conservative solutions (Vidyasagar, 2001). This flaw stems from the worst-case nature of the associated performance index. Indeed, it is possible that a design $\xi_1(\theta)$ will be preferred to a design $\xi_2(\theta)$, even though the former seems to be worse than the latter for 'most' realizations of θ. Therefore, if a minimax performance index is used, then all the efforts will be spent on determining the worst-case situation, which might be a non-representative case.

Sometimes, it is more reasonable to waive such strong requirements and consider designs which are satisfactory for 'most' realizations of $\theta \in \Theta_{\rm ad}$. This leads directly to designs in the average sense. When the set $\Theta_{\rm ad}$ of possible values of θ is compact, then a very logical way to capture this idea is to employ an approach based on a probabilistic description of the prior uncertainty of the unknown system parameters. This uncertainty is assumed to be characterized by the distribution μ which is deduced from the *a priori* knowledge about the considered system (e.g. it results from previously made observations collected on similar systems). This distribution represents additional experimenters' knowledge which is accessible *a priori* and regards the confidence level about representative values of the unknown parameters. For such an interpretation of the statistical relations between the parameters and the system behaviour, it is possible to define the criterion to be minimized as the expectation of the corresponding 'local' performance index, i.e.

$$J_E(\xi) = \mathop{\rm E}_{\theta} \big\{ \Psi_{\rm E}[M(\xi, \theta)] \big\} = \int_{\Theta_{\rm ad}} \Psi_{\rm E}[M(\xi, \theta)] \, \mu({\rm d}\theta). \tag{5.10}$$

A common assumption is to choose the measure μ as

$$\mu(\mathrm{d}\theta) = p(\theta)\,\mathrm{d}\theta, \tag{5.11}$$

where p denotes the probability density function for θ. In real-world problems the direct transformation of the *a priori* knowledge about parameters into a statistical distribution in closed form is rather difficult, or such knowledge is far from being complementary. Then, commonly encountered examples of p can be applied (Sun, 1994; Uciński, 1999a):

- In the case when the parameter vector θ_{true} is known with probability very close to unity, the prior distribution

  $$p(\theta) = \delta(\theta - \theta^0),$$

  can be used, where $\delta(\,\cdot\,)$ is the Dirac delta function.

- In the case when θ is limited to the region Θ_{ad}, but no further information is provided, the uniform distribution on Θ_{ad} may be assumed, i.e.

  $$p(\theta) = \begin{cases} 1/V(\Theta_{\mathrm{ad}}) & \text{for } \theta \in \Theta_{\mathrm{ad}}, \\ 0 & \text{otherwise,} \end{cases}$$

  where $V(\Theta_{\mathrm{ad}})$ denotes the volume of Θ_{ad} in the Lebesgue sense.

- In the case when the θ distribution can be estimated with the accuracy up to characteristics of second order (e.g. the expected value $\mathrm{E}(\theta)$ and the covariance matrix $\mathrm{cov}(\theta)$ are available), but there is no other information, the following multidimensional normal distribution can be assumed:

  $$p(\theta) = (2\pi)^{-m/2}\big(\det(\mathrm{cov}\,\theta)\big)^{-1/2} \exp\left(-\frac{1}{2}\big(\theta - \mathrm{E}(\theta)\big)^{\mathrm{T}}(\mathrm{cov}\,\theta)^{-1}\big(\theta - \mathrm{E}(\theta)\big)\right).$$

  The appropriate regularization and normalization should be imposed if values of $p(\theta)$ in the vicinity of the Θ_{ad} limits are not negligible.

According to (5.10), a design that is optimal in the average sense can be defined as

$$\xi_E^\star = \arg \min_{\xi \in \Xi(X)} \int_{\Theta_{\mathrm{ad}}} \Psi_{\mathrm{E}}[M(\xi,\theta)]\,\mu(\mathrm{d}\theta), \tag{5.12}$$

and is often called a Bayesian design. As the integral in (5.12) plays the role of a linear operator, Theorems 2.5 (p. 39) and 2.8 (p. 40) can be relatively easily reformulated by introducing the following functions:

$$\psi(x,\xi) = \int_{\Theta_{\mathrm{ad}}} \hat{\psi}(x,\xi,\theta)\,\mu(\mathrm{d}\theta), \tag{5.13}$$

$$\phi(x,\xi) = \int_{\Theta_{\mathrm{ad}}} \hat{\phi}(x,\xi,\theta)\,\mu(\mathrm{d}\theta), \tag{5.14}$$

$$\varsigma(\xi) = \int_{\Theta_{\mathrm{ad}}} \hat{\varsigma}(\xi,\theta)\,\mu(\mathrm{d}\theta), \tag{5.15}$$

where $\hat{\psi}(x,\xi,\theta)$, $\hat{\phi}(x,\xi,\theta)$ and $\hat{\varsigma}(\xi,\theta)$ are the equivalents of (2.58)–(2.60), respectively, calculated for a particular realization of the parameter vector θ. In such a way, the optimality conditions and equivalence results can be generalized to the case of Bayesian designs. As regards the existence of optimal solutions, Theorem 2.4 can also be adopted, but with the essential difference that the maximal number of support points cannot be guaranteed to be less than or equal to the value of $m(m+1)/2$. This is a consequence of the fact that Caratheodory's theorem cannot be directly applied since Ψ_E depends on different matrices $M(\xi,\theta)$ for different vectors θ (Uciński, 1999a).

Since analytical solutions can be obtained only for very simple cases, efficient numerical techniques are required. Unfortunately, Theorem 2.8 rewritten in this new framework yields efficient solutions only in the case when the distribution μ is discrete with a reasonably moderated number of support points. The main complication in applying any numerical approach from the previous chapters arises from the fact that in order to solve the problem (5.12), respective expectations have to be evaluated, which leads to time-consuming calculations of the multidimensional integrals (cf. (5.13)–(5.15)). However, to overcome those difficulties, some stochastic algorithms can be applied to avoid direct numerical evaluation of the statistical expectations, which will be briefly presented in the next section.

At this point, it should be emphasized that the class of Bayesian criteria is much wider than the corresponding class of their local counterparts. For example, only for D-optimality there exist various choices of suitable functions (Walter and Pronzato, 1997), e.g.

- ED-optimality criterion

$$J_{\mathrm{ED}}(\xi) = \mathop{\mathrm{E}}_{\theta}\big\{ -\det M(\xi,\theta)\big\},$$

- EID-optimality criterion

$$J_{\mathrm{EID}}(\xi) = \mathop{\mathrm{E}}_{\theta}\big\{[\det M(\xi,\theta)]^{-1}\big\},$$

- ELD-optimality criterion

$$J_{\mathrm{ELD}}(\xi) = \mathop{\mathrm{E}}_{\theta}\big\{ -\ln\det M(\xi,\theta)\big\}.$$

The above criteria usually lead to different optimal solutions, and therefore their practical usefulness depends on some prior experience of the experimenter. The advantages and disadvantages of particular variants are presented in (Walter and Pronzato, 1997).

5.3.2. Bayesian optimization via statistical learning

5.3.2.1. Background

As was indicated earlier, a direct application of numerical algorithms developed in the previous chapters to solving (5.12) is highly complicated by the necessity of tremendous calculations related to the evaluation of the expectations of a

local optimality criterion. However, the situation when a criterion is not given explicitly or its evaluation requires great computational efforts is standard for stochastic-approximation techniques. For that reason, those methods seem attractive as they iteratively yield approximated solution without determination of the functional to be optimized. Such an approach was introduced and successfully applied to the finite-dimensional case by Walter and Pronzato (1987; 1997) and extended to the sensor location problem for DPS's by Uciński (1999a), where a simple classical Robbins-Monro algorithm (Pflug, 1996; Spall, 2003), also known as the stochastic-gradient algorithm, was used. For instance, in the case when $s = \operatorname{supp}\xi$ is optimized, we obtain the following iterative scheme (Uciński, 1999a):

$$s^{k+1} = \Pi_{S_{\rm ad}}\left(s^k - \gamma^k \left(\frac{\partial \Psi[M(s,\theta^k)]}{\partial s}\right)^{\rm T}_{s=s^k}\right), \quad k = 0, 1, \ldots \tag{5.16}$$

where θ^k is randomly generated according to the prior distribution μ and $\Pi_{S_{\rm ad}}$ stands for the orthogonal projection onto the set $S_{\rm ad}$. The decreasing sequence $\{\gamma_k\}$ has to satisfy the following conditions:

$$\gamma_k \geqslant 0, \quad \sum_{k=0}^{\infty} \gamma_k = \infty, \quad \sum_{k=0}^{\infty} \gamma_k^2 < \infty. \tag{5.17}$$

It can be shown that the validity of some classical assumptions (Ermakov and Zhigljavsky, 1987; Kushner and Yin, 1997; Spall, 2003), where the system state y is sufficiently smooth, ensures the almost sure convergence of the above algorithm.

However, within the framework of this work, another alternative approach will be proposed, which is based on the statistical learning theory. It was originally developed in the context of the robust controller design (Vidyasagar, 1997; 1998; 2001). This constitutes the subject of the next subsections.

5.3.2.2. Relations between various types of minima

First, assume that the criterion $\Psi[M(\xi,\theta)]$ can take only non-positive values (this assumption is not too restrictive, as e.g. the D-optimality criterion satisfies it). Then, consider a measure of the system performance for vector θ and design ξ which takes values from the unit interval. This can be achieved by the following transformation of Ψ:

$$\Psi_{\rm E}[M(\xi,\theta)] = \frac{1}{1 - \Psi[M(\xi,\theta)]}. \tag{5.18}$$

Once a probability measure μ is chosen, the objective function to be minimized can be defined as

$$J_E(\xi) = {\rm E}\{\Psi[M(\xi,\theta)]\}, \tag{5.19}$$

which implies that a design ξ is occasionally permitted to be inadequate for conditions which are not likely to occur, i.e. which are associated with low probability values. In such a way the problem of determining a Bayesian design is reduced to finding the minimum of a function $J(\xi) : \Xi(X) \to [0,1]$. As was already mentioned,

finding the exact value of this minimum $J^\star$ belongs to extremely cumbersome problems. This leads to the idea of 'nearly' minimizing $J(\,\cdot\,)$, and consequently to the necessity of introducing the concept of a 'near minimum' which would increase its applicability. Let us start with the most simple definition of such a quantity (Vidyasagar, 2001):

Definition 5.1. Let $J : \Xi(X) \to \mathbb{R}$ and suppose that $\epsilon > 0$ is a given number. A number $J_0 \in \mathbb{R}$ is said to be a *Type 1 near minimum of* $J(\,\cdot\,)$ *to accuracy* ϵ, or an approximate near minimum of $J(\,\cdot\,)$ to accuracy ϵ if

$$\inf_{\xi\in\Xi(X)} J(\xi) - \epsilon \leqslant J_0 \leqslant \inf_{\xi\in\Xi(X)} J(\xi) + \epsilon \tag{5.20}$$

An approximate near minimum is probably most commonly identified with the notion of a 'near' minimum. Nevertheless, for the robust approach considered in the average sense, the determination of even an approximation to $J^\star$ is related to a high computational cost, which makes its practical application almost impossible. Therefore, it is necessary to look for other notions of near minima, which will be more useful. One of possibilities is provided with the following definition (Vidyasagar, 2001):

Definition 5.2. Let $J : \Xi(X) \to \mathbb{R}$, and assume that ν is a given probability measure on $\Xi(X)$, and that $\alpha > 0$ is a given number. A number $J_0 \in \mathbb{R}$ is said to be a *Type 2 near minimum of* $J(\,\cdot\,)$ *to level* α, or a probable near minimum of $J(\,\cdot\,)$ to level α, if $J_0 \geqslant J^\star$, and in addition

$$\nu\{\xi \in \Xi(X) : J(\theta) < J_0\} \leqslant \alpha.$$

In other words, J_0 is a probable near minimum of $J(\,\cdot\,)$ to level α if there exists a set S with probability $\nu(S) \leqslant \alpha$, such that

$$\inf_{\xi\in\Xi(X)} J(\xi) \leqslant J_0 \leqslant \inf_{\xi\in\Xi(X)\setminus S} J(\xi). \tag{5.21}$$

Examples of some algorithms for finding Type 2 near minima can be found in (Tempo *et al.*, 1997), for the case where the probability distribution is continuous and in (Vidyasagar, 1997) where this assumption is removed. However, the main impediment becomes the fact that those algorithms require the performance index $J(\theta)$ to be computable for any given $\xi \in \Xi(X)$. To relax this requirement, the following ultimate notion of near minimum can be proposed (Vidyasagar, 2001):

Definition 5.3. Let $J : \Xi(X) \to \mathbb{R}$, and suppose that ν is a given probability measure on $\Xi(X)$, and that $\epsilon, \alpha > 0$ are given numbers. A number $J_0 \in \mathbb{R}$ is said to be a *Type 3 near minimum of* $J(\,\cdot\,)$ *to accuracy* ϵ *and level* α, or a probably approximate near minimum of $J(\,\cdot\,)$ to accuracy ϵ and level α, if $J_0 \geqslant J^\star - \epsilon$, and in addition

$$\nu\{\xi \in \Xi(X) : J(\xi) < J_0 - \epsilon\} \leqslant \alpha.$$

This can be interpreted as the existence of an 'exceptional' set $S \subseteq \Xi(X)$ with probability $\nu(S) \leqslant \alpha$ such that

$$\inf_{\xi\in\Xi(X)} J(\xi) - \epsilon \leqslant J_0 \leqslant \inf_{\xi\in\Xi(X)\setminus S} J(\xi) + \epsilon \tag{5.22}$$

It becomes clear that a probably approximate near minimum (Type 3) is a combination of Type 1 and 2 near minima according to the relationships between them established by formulae (5.20)–(5.22).

5.3.2.3. A general approach to finding approximate near minima

Although evaluation of the expectations (5.19) is an excessively costly task, it is possible to approximate them to an arbitrarily chosen accuracy. This is achieved by approximating the expectations by sample means based on a series of randomly generated parameters. More precisely, assume that $\theta_{\mathrm{ms}} = [\theta^1, \ldots, \theta^m]^{\mathrm{T}} \in \Theta_{\mathrm{ad}}^m$ is a collection of *independent identically distributed* (i.i.d.) samples from Θ_{ad}, generated according to the probability measure μ. With such a multisample θ_{ms}, for any design ξ it is possible to define the empirical mean of the criterion $J(\,\cdot\,)$ as

$$\hat{J}(\xi) = \hat{\mathrm{E}}\{\Psi[M(\xi;\theta)];\theta_{\mathrm{ms}}\} = \frac{1}{m}\sum_{j=1}^{m} \Psi[M(\xi;\theta^j)], \quad \xi \in \Xi(X). \tag{5.23}$$

Defining the quantity

$$q(m,\epsilon) = \mu^m\left\{\theta_{\mathrm{ms}} \in \Theta_{\mathrm{ad}}^m : \sup_{\xi\in\Xi(X)} |\hat{\mathrm{E}}\{\Psi[M(\xi;\theta)];\theta_{\mathrm{ms}}\} - J(\xi)| > \epsilon\right\}, \tag{5.24}$$

it can be said with the confidence $1 - q(m,\epsilon)$ that every single empirical mean approximates the corresponding true value $J(\xi)$ with accuracy ϵ. Choosing m large enough such that $q(m,\epsilon) < \delta$, where the parameter δ is given *a priori*, it can be said with confidence $1 - \delta$ that the function $\hat{J}(\xi)$ is a sufficiently close approximation to the original criterion $J(\xi)$. This implies that the exact minimizer of the former function is an approximate near minimizer of the latter to accuracy ϵ, cf. (Vidyasagar, 2001) for a detailed discussion.

Note that there always exists a nonzero probability, i.e. $q(\,\cdot\,)$, that the algorithm may fail to produce an approximate near minimum of $J(\,\cdot\,)$. By increasing the number m of generated samples θ, this probability can be established on an arbitrarily small level, although, it always is positive.

Going further, another problem can be considered, namely how to determine a probable near minimum of $\hat{J}(\,\cdot\,)$, which is equivalent to the question about adequate estimates of the number of samples for θ and ξ, i.e. m and n, respectively. From the discussion presented in (Vidyasagar, 1997; 2001), it is clear that such a probable near minimum of the approximated function $\hat{J}(\,\cdot\,)$ would simultaneously be a probably approximate near minimum of the original objective function $J(\,\cdot\,)$.

It turns out that there exist a couple of approaches for this purpose which can be found e.g. in (Tempo *et al.*, 1997; Vidyasagar, 1997; 1998). Especially, one

particular algorithm developed by Vidyasagar (2001) for determining probably approximate near minima is in the focus of our interest. Suppose that $\epsilon, \alpha, \delta > 0$ are given. The objective is to construct a probably approximate (Type 3) near minimum of $J(\xi) = \mathrm{E}_\theta\{\Psi[M(\xi;\theta)]\}$ to accuracy ϵ and level α, with confidence $1-\delta$.

Algorithm 5.3. *Statistical learning algorithm for determination of Type 3 near minima*

Step 1. Select integers m, n such that

$$n \geqslant \frac{\ln(2/\delta)}{\ln[1/(1-\alpha)]} \quad \text{and} \quad m \geqslant \frac{1}{2\epsilon^2} \ln\left(\frac{4n}{\delta}\right)$$

Step 2. Generate i.i.d. samples $\xi_1, \xi_2, \ldots, \xi_n$ according to ν and $\theta^1, \ldots, \theta^m$ according to μ. Define

$$\hat{J}_i = \frac{1}{m} \sum_{j=1}^{m} \Psi[M(\xi_i;\theta^j)], \quad i = 1, \ldots, n$$

and

$$\hat{J}_0 = \min_{1 \leqslant i \leqslant n} \hat{J}_i.$$

Then with confidence $1-\delta$, it can be said that $\hat{J}_0$ is a probably approximate near minimum of $J(\,\cdot\,)$ to accuracy ϵ and level α.

♦

A full proof of the claim in Algorithm 5.3 can be found in (Vidyasagar, 1997; 2001). Algorithm 5.3 is extremely easy to implement and in addition to that, it does not require any assumptions about the character of the criterion J apart from the requirement that its range is a subset of the interval $[0, 1]$. However, the disadvantage of the considered procedure is the dependence of the number m of θ-samples on the number of ξ-samples, i.e. n. Another drawback is the necessity of the normalization (5.18) (this is because we must have $0 \leqslant J(\xi) \leqslant 1$ for any $\xi \in \Xi(X)$), which results in a very flat surface of the criterion in the vicinity of the minimum. In such a way, a practical realization of the routine requires small values of parameters ϵ, δ, α which leads to very high values of repetition numbers m and n. Consequently, the resulting computational effort may be comparable with standard methods.

At this point it would be advantageous to present some appropriate example in order to clarify differences between the delineated approaches. Bearing in mind that robust designs imply serious difficulties from the viewpoint of numerical complexity, we shall study a less cumbersome instance with only one spatial dimension.

Example 5.2. Consider a one-dimensional homogeneous and inductance-free transmission line of length π. The propagation of the voltage signal y over the time horizon $T = [0, 1]$ is described by the parabolic equation

$$\frac{\partial y(x,t)}{\partial t} = \theta_1 \nabla^2 y(x,t) + \theta_2 y(x,t), \quad (x,t) \in \Omega \times T = [0,\pi] \times [0,1]. \tag{5.25}$$

The ends of the line are short-circuited and the initial signal distribution along the line is known, which is reflected by the following boundary and initial conditions:

$$\begin{cases} y(0,t) = y(\pi,t) = 0, & 0 \leqslant t \leqslant 1, \\ y(x,0) = \sin(x) + \sin(2x), & 0 \leqslant x \leqslant \pi. \end{cases} \tag{5.26}$$

The solution of the considered problem can be found in closed form as

$$y(x,t) = e^{(\theta_2 - \theta_1)t} \sin(x) + e^{(\theta_2 - 4\theta_1)t} \sin(2x). \tag{5.27}$$

In our example the unknown parameter vector $\theta = (\theta_1, \theta_2)$ was assumed to belong to the compact set $\Theta_{\text{ad}} = [0, 1]^2$ with the uniform distribution of θ. To simplify our problem, the set of admissible support points was restricted to the uniform grid resulting from 29 divisions of Ω (i.e. evenly distributed 30 nodes). In such a way, the potential measurement sites were the elements of the set

$$X = \{x^j : x^j = j\pi/29, \quad j = 0, \ldots, 29\}. \tag{5.28}$$

The main objective was to estimate θ as accurately as possible, based on measurements taken at points from X. To this end, ED- and MMD-optimum design procedures were implemented in the Lahey/Fujitsu Fortran 95 programming environment and run on a PC (Pentium IV, 1.7GHz, 768 MB RAM). More precisely, Algorithm 3.3 for optimizing experimental effort was adopted with direct numerical evaluation of the expectations (integration of the criterion was performed with use of the procedure `DTWODQ` from the IMSL Fortran 90 ver. 4.0 Library which embodies the adaptive integration based on the Gauss-Kronrod rule). Such an approach was compared with Algorithm 5.3 based on the estimation of mathematical expectations. Furthermore, to provide a more comprehensive context, the minimax relaxation (Algorithm 5.2) was used to obtain an approximation to the robust design in the minimax sense. For all procedures, the initial design was randomly generated and in the final solutions the points with weights below 0.01 were removed and their experimental effort uniformly distributed among the other supports. In the case of the relaxation procedure proposed by Shimizu and Aiyoshi, the starting set of representative values of θ was chosen as $\Theta^1_{\text{rep}} = \{(0.5, 0.5)\}$ and the final design was obtained for the worst case corresponding to $\theta = (0.3, 1.0)$. All results are presented in Table 5.1.

To fully understand the obtained results, note that the similarity of the designs in the minimax and average senses is not just a coincidence. The set Θ_{ad} was specially prepared so as to provide such results. In fact, extremely cumbersome calculations made with the help of any reasonable computer-algebra system (e.g.

Table 5.1. Comparison of robust approaches

Algorithm	Iterations	Time	Approx. solution
Weight optimization with numerical integration ($\epsilon = 10^{-2}$)	273	~ 2 h	$\begin{Bmatrix} 0.975 & 2.167 \\ 0.50 & 0.50 \end{Bmatrix}$
Statistical learning ($\delta = 0.02, \alpha = 0.02, \epsilon = 10^{-2}$)	$n = 228$ $m = 107275$	~ 50 min	$\begin{Bmatrix} 0.975 & 2.167 \\ 0.49 & 0.51 \end{Bmatrix}$
Minimax relaxation ($\epsilon = 10^{-2}$)	3	~ 5 min	$\begin{Bmatrix} 0.975 & 2.167 \\ 0.50 & 0.50 \end{Bmatrix}$

Maple Rel. 9 was used here) show that for both average and minimax designs it is possible to obtain closed-form solutions which have the same form, i.e.

$$\xi_E^\star = \xi_M^\star = \begin{Bmatrix} \arctan(\sqrt{2}) & \pi - \arctan(\sqrt{2}) \\ \frac{1}{2} & \frac{1}{2} \end{Bmatrix} \tag{5.29}$$

Unfortunately, due to the limited space here, it is not possible to present the detailed calculations (e.g. the closed form of the ED-optimality criterion possesses several hundreds of components). However, this fact proves the quality of the obtained approximations as the support of any design represents the discrete locations from X which are the closest to the optimal values. It becomes clear that from a practical point of view the integration is a critical operation which extends the time of computations. The approach via statistical learning might be some kind of remedy, but it requires broad experience regarding selection of suitable values for the algorithm parameters. Sometimes a too restrictive demand of high accuracy and confidence levels leads to very large sizes of the samples and the advantages of such an approach are not obvious. On the other hand, the minimax optimization algorithm leads to global optimization problems with respect to the design space and the parameter space, which are very difficult to analyse. For searching the parameter space and seeking an approximate global optimum, once more the ARS approach proved its usefulness. In such a way, for this demonstrative problem the minimax approach appears as the one with the lowest operational time.

★

5.4. Discrimination between rival model structures

5.4.1. Introduction

The process of proper model calibration should contain two components: the selection of a model structure and estimation of the relevant parameters. Until now, we have limited our considerations to the latter problem, and have focused attention on the accuracy of the identifiers, while simultaneously neglecting the model structure error. Nevertheless, in real-world engineering problems, the error arising from

an improper model structure often dominates the measurement and computation errors.

Being the initial part of modelling and simulation of many physical phenomena, the structure identification of complex process models constitutes an essential part of that methodology. Usually the choice of a particular model structure is ambiguous, since the mechanisms of many complex processes are not fully known. A detailed analysis of the considered phenomenon often leads to a simplified model of the investigated system, but occasionally several plausible models can be used. A specially designed experiment to discriminate between those rival models constitutes a good source of information about the model fit. Moreover, the very important aspects of the model level of complexity and cost of the experiment can be included into the criterion of the best model choice.

Motivations to develop some discrimination techniques come from practical problems. A representative example is the prediction of the pollution level in groundwater resources (Sun, 1994; 1996) where facing the extremely complicated structures of real aquifers the problem of proper selection of the complexity level for the conceptual model cannot be omitted. As it was mentioned earlier, the phenomena of that kind are modelled with the aid of partial differential equations of advection-diffusion-reaction type, where the main difficulty is that only a part of model parameters (e.g. wind velocities) belong to the set of measurable quantities. In contrast, the diffusion coefficients or parameters occurring in chemical reactions cannot be directly measured. This inconvenience, which results from the fact that we deal with a conjunction of a few complicated phenomena (transport, diffusion and chemical reactions in the considered case), significantly complicates the appropriate modelling of such systems and requires various simplifying assumptions when constructing an applicable model. Other pertinent examples can be found in the modelling of atmospheric pollutant transport problems (Kuczewski *et al.*, 2004) or fault diagnosis in dynamical systems (Patan and Patan, 2003).

The main and most important aspect of structure discrimination is the introduction of an appropriate quantitative criterion used to compare the quality of different designs. However, the high level of complexity in the case of the experimental design for discrimination between models has limited its application to relatively simple models of static systems. Various criteria were considered in (Atkinson and Fedorov, 1975; Burke *et al.*, 1994; Stewart *et al.*, 1988). Recently the criterion, called the T-optimality criterion, introduced by Atkinson and Fedorov (1975) was generalized to discrimination between two rival multiresponse dynamic models given in the form of ordinary differential equations with observations corrupted by white noise (Uciński and Bogacka, 2002; Kuczewski and Uciński, 2002).

Within the scope of this work, the approach based on T-optimum designs is generalized to find optimal stationary sensor locations, which allows us to perform the most reliable discrimination between two models of a process with spatiotemporal dynamics (Kuczewski *et al.*, 2003; 2004). The proposed iterative numerical procedure for computing optimum designs consists in solving a maximin problem where global optimization techniques have to be employed. The generalization to the case of several plausible models can be made without major difficulties.

5.4.2. Design problem in context

The class of systems considered here is, in general, the same as that established in Section 2.1, i.e. it is described by (2.1)–(2.3) in a simply-connected bounded open domain $\Omega \subset \mathbb{R}^d$ with sufficiently smooth boundary $\partial\Omega$.

For simplicity, only stationary sensors will be studied and the measurements are assumed to be independent of one another. This leads to the observational process described by the following equation:

$$z_i^j(t) = y(x^j, t) + \varepsilon_i(x^j, t), \quad t \in T = [0, t_f], \quad j = 1, \ldots, \ell; \;\; i = 1, \ldots, r_j, \;\; (5.30)$$

where ℓ denotes the number of measurement sensors, $x^j \in \Omega$ stands for sensor locations ($x^j \neq x^i$ for $j \neq i$) and $\varepsilon_i(x^j, t)$ represents the statistical uncertainty resulting from possible measurement errors. We make the assumption that the errors $\varepsilon_i(x^j, t)$ can be described by a spatially uncorrelated Gaussian stochastic process. Moreover, the measurements can be taken repeatedly at a particular location, which is taken into account in (5.30) by introducing the replication term r_j, $\sum_{j=1}^{\ell} r_j = N$.

According to (2.1)–(2.3), since the uncertainty of the boundary and initial conditions (i.e. functions $\mathcal{E}$ and $\mathcal{F}$) does not differ from the uncertainty of the system equation structure, it is very convenient to restrict our attention to the main assumption of the proposed approach, which is the conformity of the examined model structure $\mathcal{G}$ with $\mathcal{G}_1(\,\cdot\,, \tilde{\theta}_1)$ or $\mathcal{G}_2(\,\cdot\,, \tilde{\theta}_2)$, where functions $\mathcal{G}_1$ and $\mathcal{G}_2$ are given *a priori*, and $\tilde{\theta}_1 \in \Theta_1 \subset \mathbb{R}^{m_1}$ and $\tilde{\theta}_2 \in \Theta_2 \subset \mathbb{R}^{m_2}$ stand for vectors of unknown but *constant* parameter values (Θ_1 and Θ_2 are some compact sets). The aim of the experiment is to determine which of the models $\mathcal{G}_1$ and $\mathcal{G}_2$ is compatible with the investigated phenomenon.

The proposed solution can be delineated as follows (Kuczewski *et al.*, 2004; Fedorov and Hackl, 1997): The least-squares estimate of parameters $\tilde{\theta}^k$ in the considered case can be expressed by the equation:

$$\hat{\theta}_k = \arg \min_{\theta_k \in \Theta_k} \sum_{j=1}^{\ell} \sum_{i=1}^{r_j} w_j \int_T \|z_i^j(t) - \eta_k(x^j, t; \theta_k)\|^2 \mathrm{d}t, \quad (5.31)$$

for $k = 1, 2$, where $w_j = r_j/N$, $\eta_k(x^j, t; \theta_k)$ is the solution of (2.1)–(2.3) with $\mathcal{G}(\,\cdot\,) = \mathcal{G}_k(\,\cdot\,, p_k)$, and $\|\cdot\|$ stands for the Euclidean norm.

Without loss of generality, we can assume that the first of the considered models $\mathcal{G}_1$ is 'true', i.e. it is compatible with the investigated phenomenon. This assumption entails the condition of the knowledge of the parameter vector $\tilde{\theta}^1$ (this value can be obtained as a result of a pilot experiment or some nominal values can be used if accessible). Then the problem of the best model selection reduces to maximization of the following criterion subject to weights w_j and spatial locations x^j (Fedorov and Hackl, 1997):

$$T_{12}^0(\xi_N) = \min_{\theta_2 \in \Theta_2} \sum_{j=1}^{\ell} \sum_{i=1}^{r_j} w_j \int_T \|\eta(x^j, t) - \eta_2(x^j, t; \theta_2)\|^2 \, \mathrm{d}t, \quad (5.32)$$

where $\eta(x,t) = \eta_1(x,t;\tilde{\theta}^1)$, and the set of variables

$$\xi_N = \begin{Bmatrix} x^1, & \ldots, & x^\ell \\ w_1, & \ldots, & w_\ell \end{Bmatrix} \tag{5.33}$$

is called the *N-observation normalized exact experimental design*. The quantities x^j and w_j are called the support and weights, respectively.

The criterion (5.32) defines some measure of the discrepancy between the responses of both the models. Then the resultant optimum design has an effect on the maximum lack of fit of model $\mathcal{G}_2$ in the sense of the sum of the squared errors calculated for optimum estimates of the θ_2 parameter vector. It is intuitively clear that the solution strongly depends on which model is assumed to be 'true', as well as on the true values of the parameters in this model ($\tilde{\theta}_1$ in the considered case). We wish to choose a design which is optimal for some particular value of $\tilde{\theta}_1$ in the hope that it is not too bad whatever the true $\tilde{\theta}_1$ happens to be. The dependence of the optimal solution on the model parameters is an unappealing characteristic of nonlinear experimental designs. In such a way we are faced again with the parametric uncertainty of the model and methods presented in preceding sections could be used in order to surmount this difficulty.

Allowing for replicated observations at the support points x^j entails serious difficulties, as the resultant numerical analysis problem is not amenable to be solved by standard optimization techniques, particularly when N is large. This is caused by the discrete nature of the N-observation exact designs, since the weights w_j are rational numbers. To alleviate this inconvenience, once again the notion of the design can be relaxed to all probability measures ξ over X which are absolutely continuous with respect to the Lebesgue measure and satisfy by definition the normalization condition $\int_X \xi(\mathrm{d}x) = 1$, which leads to continuous designs which dramatically simplify the problem. The 'continuous' equivalent of the criterion (5.32) can be then expressed for the considered case as follows:

$$T_{12}(\xi) = \min_{\theta_2 \in \Theta_2} \int_X \left\{ \int_T \|\eta(x,t) - \eta_2(x,t;\theta_2)\|^2 \, \mathrm{d}t \right\} \xi(\mathrm{d}x) \tag{5.34}$$

and the design

$$\xi^\star = \arg \max_{\xi \in \Xi(X)} T_{12}(\xi) \tag{5.35}$$

is called locally T_{12}-optimum.

5.4.3. Optimality conditions and numerical construction of T_{12}-optimum designs

In order to derive necessary and sufficient conditions for the optimality of designs, the following assumptions are required:

(B1) Sets X i Θ_2 are compact,

(B2) η is a continuous function on $X \times T$,

(B3) η_2 is a continuous function on $X \times T \times \Theta_2$.

Then, the results presented in (Atkinson and Fedorov, 1975) can be easily generalized to prove the following claim (Uciński and Bogacka, 2002):

Theorem 5.2. *If the optimization problem* (5.34) *possesses a unique solution* $\theta_2^\star \in \Theta_2$ *for a design* $\xi^\star$*, then the necessary and sufficient condition for the* T_{12}*-optimality of* $\xi^\star$ *is*

$$\int_T \|\eta(x,t) - \eta_2(x,t;\theta_2^\star)\|^2 \,\mathrm{d}t \leqslant T_{12}(\xi^\star), \qquad \forall\ x \in X. \tag{5.36}$$

For each support point in $\xi^\star$ *the inequality is replaced by equality in* (5.36)*. Moreover, the set of all possible optimum designs* $\xi^\star$ *is convex.*

Below we present a numerical scheme of computing locally T-optimum continuous designs, which constitutes a generalization of the iterative procedure set forth by Atkinson and Fedorov (1975) in the case of static systems. However, its usefulness was also shown in the case of discrimination between multiresponse dynamic system models described by ordinary differential equations (Kuczewski and Uciński, 2002) and for DPS's (Kuczewski *et al.*, 2004). The procedure can be schematically depicted as the sequence of the following steps:

Algorithm 5.4. *Two-model discrimination algorithm*

Step 1. Choose an initial nonsingular design $\xi^{(0)}$. Set $s = 1$.

Step 2. In the s-th iteration, find

$$\hat{\theta}_2^{(s)} = \arg\min_{\theta_2 \in \theta_2} \sum_{j=1}^{\ell} w_j \int_T \|\eta(x^j,t) - \eta_2(x^j,t;\theta_2)\|^2 \mathrm{d}t$$

$$x^{(s)} = \arg\max_{x \in X} \int_T \|\eta(x,t) - \eta_2(x,t;\hat{\theta}_2^{(s)})\|^2 \mathrm{d}t$$

Step 3. If $\phi(x^{(s)}) - \Delta(\xi^{(s)}) \leqslant \epsilon$, where

$$\phi(x) = \int_T \|\eta(x,t) - \eta_2(x,t;\hat{\theta}_2^{(s)})\|^2 \mathrm{d}t, \qquad \Delta(\xi) = \sum_{j=1}^{\ell} w_j \phi(x^j),$$

then $\xi^\star = \xi^{(s)}$ and STOP, otherwise go to Step 4

Step 4. Choose α_s from $0 \leqslant \alpha_s \leqslant 1$ and determine the convex combination of designs:

$$\xi^{(s+1)} = (1 - \alpha_s)\xi^{(s)} + \alpha_s \xi(x^{(s)}),$$

where $\xi(x^{(s)})$ stands for the design concentrated only at one point $x^{(s)}$ with unit weight. Set $s = s + 1$ and return to Step 2.

♦

The choice of the sequence $\{\alpha_s\}$ is ambiguous (Atkinson and Fedorov, 1975) and should be detailed. The simulation presented in what follows was performed with $\alpha_s = 1/(1+\ell)$, where ℓ denotes the size of the design, but the optimal value of coefficient α_s can be easily found in each iteration, e.g. with the golden search method. Although the number of support points in the optimum design is not set *a priori*, the algorithm possesses the property of finding designs which are optimal. To achieve this, techniques of avoiding the clusterization phenomenon have to be used.

The simplest possibility is the periodical exchange of clusters for single points with the averaged position and summed weights within cluster components. Another solution consists in retaining in the design only those members of clusters, which came up at the latest, since they represent the most valuable information — the longer the process runs, the better solutions the iterative procedure produces (of course if the whole iterative process converges). Finally, the points with relatively small weights should be removed from the resultant design. Thresholds steering the maximum cluster diameter, the minimum weight of the support points and the accuracy ϵ should be selected experimentally.

The most important part of the algorithm, which directly affects the convergence of the proposed procedure, is the solution of the global optimization problem which appears in Step 2 of the scheme. It is the most time-consuming part of the algorithm as well, since the system state is given implicitly as the solution of a particular PDE and each evaluation of the cost function for different model parameters is related to the necessity of solving the underlying PDE. Getting stuck in a local minimum usually leads to premature convergence or the lack of convergence at all. Therefore, an effective implementation of some global optimization method is of crucial significance in the implementation of the presented approach.

Example 5.3. In order to illustrate the properties of the proposed algorithm, a computer experiment was performed. For this purpose, the process of pollutant transport-diffusion over a given area Ω was considered. Assume that the pollutant concentration y over the time interval $T = [0, 1]$ is described by the model in the form of the advection-diffusion equation

$$\frac{\partial y(x,t)}{\partial t} + \nabla \cdot (v(x)u(x,t)) = \nabla \cdot (d_1(x)\nabla y(x,t)), \quad (x,t) \in \Omega \times T, \tag{5.37}$$

subject to initial and boundary conditions

$$\begin{aligned} y(x,0) &= 100e^{-100(x_1^2+x_2^2)}, && x \in \Omega, \\ \frac{\partial y(x,t)}{\partial n} &= 0, && (x,t) \in \partial\Omega \times T. \end{aligned} \tag{5.38}$$

The diffusion coefficient was assumed in the form:

$$d_1(x) = 0.1 + 0.1x_1^4 + 0.1x_2^4.$$

The velocity of the transport medium was modelled as a radial field directed

outwards with a source situated at point $P = (0, 0)$:

$$v(x) = \left(\frac{x_1^3}{\sqrt{(x_1^2 + x_2^2)}}, \frac{x_2^3}{\sqrt{(x_1^2 + x_2^2)}} \right). \tag{5.39}$$

The domain Ω, boundary $\partial\Omega$, contour of the initial concentration of the substance $y(x, 0)$ and the gradient of the transport medium velocity are shown in Fig. 5.5. The

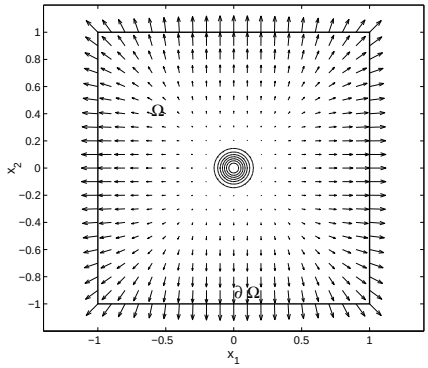


Fig. 5.5. Setting of Example 5.3: the considered domain, its boundary, initial concentration of a pollutant (contour plot) and velocity field.

alternative model has no advection component, so only diffusion of the pollutant is considered. The model is expressed by the equation

$$\frac{\partial y(x,t)}{\partial t} = \nabla \cdot (d_2(x) \nabla y(x,t)) \qquad \text{in } x \in \Omega \tag{5.40}$$

with boundary and initial conditions (5.38) in the same domain and the same observation horizon as in the previous model (5.37). The diffusion coefficient of the alternative model has the form preserving symmetry:

$$d_2(x) = \theta_1 + \theta_2 (x_1^4 + x_2^4). \tag{5.41}$$

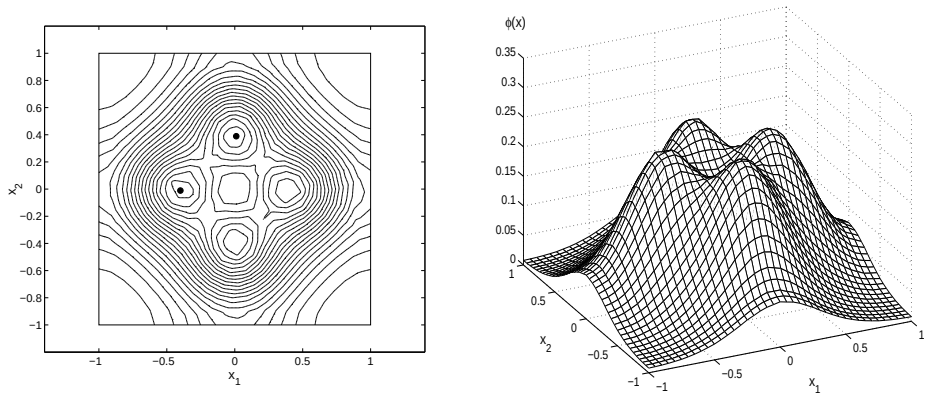
The values of the alternative model parameters were assumed to satisfy $\theta_1, \theta_2 \in [0.01, 0.2]$. A program for computing the optimum design was written completely in the Matlab 6.5 environment. Solutions of the advection-diffusion-reaction PDE's were obtained using the finite-element method with a separate program based on the Matlab PDE Toolbox.

The resulting optimum design includes two points and has the form

$$\xi^\star = \left\{ \begin{array}{cc} (-0.4002, -0.0110), & (0.0120, 0.3890) \\ 0.2097, & 0.7903 \end{array} \right\}$$

and the parameters of the alternative model with respect to $\xi^\star$ have the values: $\theta_2^\star = (\theta_{2,1}^\star, \theta_{2,2}^\star) = (0.1004, 0.1048)$. The obtained sensitivity function

$$\phi(x) = \int_T \|\eta(x,t) - \eta_2(x,t;\hat{\theta}_2)\|^2 \mathrm{d}t \tag{5.42}$$



(a) (b)

Fig. 5.6. Contour plot of the sensitivity function $\phi(x)$ with optimum sensor locations (a) and a 3D plot of the sensitivity function $\phi(x)$ (b).

defining the discrepancy between the responses of the models for the optimum sensor location is shown in Fig. 5.6. It is worth of noticing that the support points are located at the maxima of the $\phi(x)$ function which is consistent with the outlined theory. As can be seen in Fig. 5.6, the sensitivity function is symmetric, which results from the problem symmetry. The function has four maxima, where the values of the T_{12} criterion equal one another, but the sensors are located only at two of them. This situation is caused by unavoidable numerical inaccuracies of computations (even the smallest possible float difference between the values of the appropriate criterion decides which of the points will be included into design during the present iteration of the algorithm).

★

5.5. Concluding remarks

Within the scope of this chapter it was expressed than the parametric and structural model uncertainties are major impediments encountered in the problem of optimal sensor location for DPS's, which makes it extremely nontrivial. However, in the former case it was shown that difficulties arising from the dependence of the optimal solutions on the parameters to be identified can be circumvented to some extent by the introduction of the so-called sequential and robust designs.

In the first part of the chapter, an approach was proposed based on a combination of two concepts: sequential designs and the scanning strategy with a fixed time switching schedule. Although sequential designs constitute a well-known technique, the resulting time and cost of the experiment may be too long or too large. Moreover, it is often difficult to obtain strong results in a mathematical sense. However, from a practical point of view the approach is very simple for imple-

mentation and very easy to combine with other approaches. Furthermore, in some processes, the partitioning of resources (e.g. time discretization), being the most characteristic property of sequential designs, is given by definition. This is used to provide a characterization of a simple and effective computational scheme based on the concepts of clusterization-free and sequential designs. However, such an approach inherits some drawbacks which have to taken into account, i.e. the necessity of consecutive parameter estimation in each stage of the experiment, which is a main difficulty in the light of the lack of on-line identification methods for DPS's.

Alternatively, as more systematic approaches, designs in minimax and average senses can be introduced on the analogy of the standard procedure in optimum experimental design for nonlinear regression models. Despite the critical importance of the problem, to the best of the author's knowledge the only contributions to this issue in the context of DPS's are works of Uciński (1999a; 1999d; 1999b). Suitable characterizations of the optimality conditions for continuous designs, as well as some known numerical algorithms for obtaining approximate solutions are discussed. A proper choice between these two approaches is equivalent to the selection of the most adequate practical conditions which have to be satisfied during the experiment. If there is no arbitrary knowledge about the distribution of the unknown parameters and the worst possible performance of the experiment should be optimized, then minimax designs can be a right choice. Another situation when the prior distribution of the parameters to be estimated is available and we are interested in a design whose performance is good enough for the great majority of parameter realizations, the best suited will be a design in the averaged sense. The algorithms described in the middle part of this chapter make it possible to apply both the approaches mentioned above, with a reasonable numerical effort. Especially, the use of the statistical learning approaches leads to essential improvements in the determination of the designs in the average sense.

The problem of structural uncertainty is even more meaningful, and at the same time, more difficult. However, in a situation when some finite set of models describing the examined phenomenon is known and the goal is to choose the best fitted one, it was shown that this problem can be addressed using the concept of designs dedicated to model discrimination. In the final part of this chapter, a generalization of the T-optimality criterion fitting to the considered case of discrimination between two DPS's models was presented. The proposed iterative procedure for computing optimum designs consists in solving a maximin problem where global optimization techniques have to be employed. This requires an efficient global optimizer, or alternatively, a parallel realization of the algorithm. Furthermore, note that generalizations to the case of several plausible models can be made without major difficulties.

Summarizing, the following is a short list of contributions of this work to the state-of-the-art in robust optimum experimental design:

- A new technique was developed, being the conjunction of the clusterization-free designs for the scanning strategy and sequential design techniques. This is embodied in a very simple and efficient exchange-type numerical procedure. In addition to that, it is clarified how to adapt some existing algorithms

delineated in the previous chapters, which establishes a promising attempt to optimally locate scanning sensors in parameter estimation of distributed systems with respect to parametric uncertainties.

- A characterization of the robust designs in the minimax and average senses with appropriate discussion was provided. As a novelty proposed to extend the issue of determination of robust designs in the average sense, the procedure based on statistical learning theory was adopted, which is an alternative to the standard methods aimed at the local case since it allows for avoiding the multi-dimensional integration.

- The T-optimum design criterion and optimum design characterizations were generalized to the MIMO spatio-temporal dynamic systems. Moreover, a suitable iterative procedure known from the discrimination experiments for lumped systems was successfully adopted.

At this moment, despite a critical character of the problem, no technique exists which is free form drawbacks and there is no doubt that the subject of robust experimental design is still open for research. However, with some approaches proposed in this chapter, the gap in the methodology of preparing the data acquisition process for parameter estimation in DPS's is filled at least to some extent.

Chapter 6

CONCLUSIONS AND FUTURE RESEARCH DIRECTIONS

There is no doubt that optimization and control of DPS's are intensively expanding research areas with a high number of potential applications. The process of data acquisition, being an integral part of control design, is fundamental as in distributed systems it exerts a strong influence on the accuracy of estimation, the quality of control and prediction of system behaviour. But the problem of sensor location for parameter estimation in DPS's is very difficult since its intrinsic non-linearity rather excludes simple methods. Furthermore, most often, the dependence between the observations and the system performance is not intuitive and has counfounding nature. Despite these facts, the problem has been considered by many authors and a number of relevant contributions have already been reported in the literature. In addition to this, some new approaches to determining optimal sensor locations are still proposed in order to provide a more general context, a wider range of potential criteria and better understanding of interconnection between the optimal locations and the quality of the identifiers. On the other hand, engineers expect efficient techniques which are easy to implement and provide benefits overcoming the cost of application.

In such a way, although various results for the sensor location problem exist, they are rarely applied in practice by engineers. This seems to be a direct consequence of the complexity of most sensor location approaches which lead to sophisticated and inefficient algorithms. Moreover, the existing methods are often intricate and difficult in implementation. However, taking into account that the progress in computational mathematics combined with the rapidly increasing computer power steadily extend the range of potential applications, there is a strong necessity to develop more effective systematic approaches which pave the way to the algorithms of great efficiency and reasonable complexity.

In the light of the conclusions above, the original objective of the research reported in this dissertation was to develop effective and reliable methods to solve the sensor location problems encountered in practical applications for a wide class of DPS's. In order to accomplish this task the appropriate theoretical substantiation for the adopted approach was developed. Furthermore, some known methods have been generalized and several new algorithms have been constructed. The following is a final concise summary of the contributions provided by this work to the state-of-the-art in optimal sensor location for parameter estimation in DPS's:

- Systematizes and generalizes the classical results of optimal experiment design for stationary sensors to MIMO systems with possible output correlation.

- Adapts some algorithms of nonlinear programming and optimal experiment design to solve the stationary sensor location problems. In particular, it provides:

  - adaptation of gradient projection and feasible-direction methods,
  - transformation to a semi-definite programming task and application of some well-developed SDP algorithms and LMI techniques, which are, to the best of the autor's knowledge, a completely new technique in the context of the sensor location problem for parameter estimation.

  The delineated algorithms were tested via computer simulations on engineering problems such as computer-assisted electrical impedance tomography and structural mechanics.

- Derives optimality conditions for non-parameterized and parameterized trajectories, and applies the two-phase first-order algorithm with adaptive random search (Walter and Pronzato, 1997) to construct optimal trajectories of mobile sensors,

- Develops expeditious methods of activating scanning sensors, and in particular:

  - introduces an approach based on clusterization-free designs for an arbitrarily fixed switching schedule,
  - transforms the problem to the equivalent Mayer problem of optimal control in the case of an optimized switching schedule; it is then solved using the CPET approach.

  These scanning techniques, as well as the approaches employing mobile and stationary sensors, were validated and compared on simulations of dynamic processes of signal propagation in transmission lines and atmospheric and groundwater pollution.

- Develops an approach to solve the sensor location problem in the case of correlated observations. Specifically, a method which includes mutual correlations between measurements directly into the measurement covariance matrix is proposed and a relaxation algorithm is developed for solving the resulting computational problem.

- Introduces methods of optimal sensor placement to the model-based fault diagnosis. It adapts the parametric based approach to describe system modes of work and develops methods of the reliability maximization of fault detection and isolation based on structured hypothesis testing.

- Develops some approaches to optimal sensor allocation in the presence of model parametric and structural uncertainties:
  - Develops a new technique, which is a conjunction of the clusterization-free designs for the scanning strategy and sequential design techniques. In addition to this, it provides an extremely efficient exchange-type numerical procedure.
  - Provides a characterization of robust designs in the minimax and average senses with the appropriate discussion. As a novelty here, an original application of statistical learning theory should be stressed, which is an alternative to standard methods from the local case multi-dimensional integration is avoided.
  - Generalizes the T-optimum design criterion and optimum design characterizations to MIMO spatio-temporal dynamic systems. Moreover, a suitable iterative procedure known from the discrimination experiments for lumped systems was successfully adopted.

As was pointed out in (Uciński, 1999a), the decided advantage of the approach suggested in this work is its independence of a particular form of the PDE's system which is used as a model of the considered spatio-temporal process. The only requirement then becomes the existence of sufficiently regular solutions to the state and sensitivity equations.

From an engineering point of view, the proposed approach leads to more transparent solutions and many efficient and easy-to-implement numerical procedures. The author strongly believes that these advantages establish a firm position of such a methodology regarding applications in engineering. In addition to this, note that few alternatives exist in the literature. Nevertheless, there still remain open problems which require closer attention and indicate possible applications. In what follows, a brief discussion of possible areas for further investigation is presented.

Application for time-delayed systems. As the specific form of partial differential equations is not crucial for the approach, it seems natural to extend the proposed methodology to the case of systems with possible time delays. A comprehensive treatment of such DPS's from an optimal control perspective is given in (Kowalewski, 2001a). However, the main problem which has to be addressed while trying to derive such a generalization is to answer the question whether or not the approach based on FIM is still applicable. The works of Fitzpatrick (1990; 1995; 1995) indicate some conditions of the estimator consistency which can be used to establish the desired applicability for particular cases.

Further development of the approaches robust to the structural model uncertainty. In the model-based systems analysis, a proper calibration of the model involves two stages, namely an appropriate selection of the model structure and then the estimation of its parameters. Although the former stage is of great practical relevance,

the problem of the model quality assessment is usually omitted due to its difficulty. However, for some problems regarding DPS's, where the model responses are of considerable importance, some systematic approaches are required as the model structure plays a major role in the process of building the prediction of system outputs.

Further development of approaches for correlated measurements. It is clear that in real-world problems the independence of the observations often cannot be sufficiently justified and mutual correlations between measurements should be taken into account. Since the classical concept of the design measures is not applicable in this case, this fact is of crucial importance as it significantly increases the problem complexity. In Section 4.4, an exchange-type relaxation algorithm was adopted and its efficiency for the D-optimality criterion was dramatically improved. Attempts to extend those concepts to other criteria would be quite natural. The close connection of correlated measurements with practical problems makes such results very desirable.

Simultaneous estimation and experimental design. Most of the approaches considered within the scope of this dissertation concern implementation of the sensor allocation strategies before conducting the experiment, i.e. they work off-line. The only exception are the sequential design techniques discussed within the framework of parameter uncertainties. From a practical point of view, it would be interesting to investigate the problem of simultaneously taking measurements, estimating the parameters and updating the locations of scanning or movable sensors. But, as was indicated earlier, the main obstacle is the lack of on-line estimation methods for DPS's and the relevant literature is very limited (Demetriou and Rosen, 1993; Demetriou, 2000; Aihara, 1997). Nevertheless, potential applications make this research direction extremely important.

Model based fault diagnosis. Recently, the modern diagnostics is a dynamically developing and, at the same time, very important research field with numerous engineering applications. In Section 4.5, a first attempt to the model based diagnosis in distributed systems was delineated. In spite of the very rich literature for LPS's, the number of contributions for DPS's is very limited. Moreover, the above-mentioned lack of on-line estimation methods appears again as a crucial difficulty here. Nevertheless, due to the importance of this subject, there is a need for further developments and increasing the reliability of the diagnosis through the appropriate sensor location is a very challenging area for investigations.

Streszczenie

Temat rozprawy dotyczy ważnego problemu optymalizacji czasoprzestrzennego rozmieszczania czujników pomiarowych w układach o parametrach rozłożonych, które sformułowano już u schyłku lat sześćdziesiątych, jednak do dziś brak jest uniwersalnych i łatwych do zastosowania rozwiązań. Istotna trudność wynika z konieczności stosowania metod analizy nieliniowej, bowiem nawet w sytuacji gdy równanie różniczkowe cząstkowe jest liniowe ze względu na identyfikowane parametry, jego rozwiązanie jest na ogół nieliniową funkcją tych parametrów. Stosunkowo dużo miejsca w literaturze poświęcono rozmieszczaniu zadanej liczby czujników stacjonarnych, w pewnych sytuacjach możliwe jest jednak stosowanie czujników mogących wykonywać pomiary również w trakcie ruchu lub przy zastosowaniu tzw. „skanowania" czyli odpowiedniej aktywacji czujników pomiarowych. Taki sposób obserwacji wydaje się dość atrakcyjny zarówno z praktycznego punktu widzenia, gdyż czujniki nie są związane z ustalonymi punktami pomiarowymi i mogą przemieszczać się do obszarów, które dostarczają w danej chwili więcej informacji o obserwowanym obiekcie, jak również z punktu widzenia teorii sterowania, gdyż prowadzi do wielu interesujących problemów wymagających nieklasycznych rozwiązań.

Do podstawowych celów pracy należało istotne rozszerzenie istniejących rezultatów oraz opracowanie nowych podejść do określania optymalnych strategii obserwacji w estymacji dla układów o parametrach rozłożonych. W tym kontekście poruszane są m.in. problemy generalizacji istniejącej metodologii na rzecz wielowyjściowych układów z dynamiką czasoprzestrzenną oraz rozwinięcie efektywnych algorytmów określania optymalnych strategii obserwacji w oparciu o bezpośrednio ograniczone miary planów. Ponadto opracowano niezwykle skuteczne podejścia do określania optymalnych harmonogramów aktywacji czujników skanujących w przypadku ustalonych i optymalnych momentów przełączeń.

Drugoplanowe cele dotyczyły dostarczenia odpowiedniej metodyki postępowania w przypadku występowania niepewności parametrycznej modelu. Rozważane są tutaj nowatorskie techniki adaptujące kryteria bayesowskie i minimaksowe oraz zastosowanie planowania sekwencyjnego do realizacji strategii on-line z użyciem czujników skanujących. Inne istotne uogólnienia zawarte w pracy dotyczą technik planowania eksperymentu w przypadku skorelowanych szumów pomiarowych oraz ich zastosowanie w diagnostyce uszkodzeń.

Wszystkie wymienione podejścia zostały przetestowane i porównane na bazie symulacji numerycznych dotyczących ważkich i potencjalnych problemów praktycznych tj. impedancyjnej tomografii komputerowej i mechaniki strukturalnej oraz w problemach estymacji parametrów w liniach transmisyjnych i do kalibracji modeli rozprzestrzeniania się zanieczyszczeń w powietrzu i wodach gruntowych.

Appendix A

PROOFS OF SOME THEORETICAL RESULTS

A.1. Proofs of Theorems from Chapter 2

Proof of Lemma 2.1

The symmetry of the matrix is a direct consequence of the definition (2.49) since the matrix $C_o^{-1}(t)$ is symmetric. The proof of the non-negative definiteness starts with the observation that $C_o^{-1}(t)$ is positive definite for any t, therefore it can be represented in the form $C_o^{-1}(t) = A(t)A^{\mathrm{T}}(t)$, where $A(t)$ is a lower-triangular square matrix. From this it follows that

$$\begin{aligned}\forall b \in \mathbb{R}^m, \;\; b^{\mathrm{T}} M(\xi) b &= \int_X \left\{ \frac{1}{t_f} \int_0^{t_f} \sigma^{-2}(x,t) b^{\mathrm{T}} F(x,t) A(t) A^{\mathrm{T}}(t) F^{\mathrm{T}}(x,t) b \, \mathrm{d}t \right\} \xi(\mathrm{d}x) \\ &= \int_X \left\{ \frac{1}{t_f} \int_0^{t_f} \sigma^{-2}(x,t) \|\alpha(x,t)\|^2 \, \mathrm{d}t \right\} \xi(\mathrm{d}x)\end{aligned} \tag{A.1}$$

where $\alpha(x,t) = A^{\mathrm{T}}(t) F^{\mathrm{T}}(x,t) b$. Since the integrand is non-negative, the integral itself must be non-negative, which completes the proof. ■

Proof of Lemma 2.2

According to the assumptions concerning $\sigma(x,t)$ it is clear that $\sigma^{-2}(x,t) \in C(X \times T)$. In combination with (A2) this means that the function $\Upsilon(x)$ in (2.49) is continuous in X. The compactness of $\mathfrak{M}(X)$ is thus a direct consequence of assumption (A1) as shown in (Uciński, 1999a, Lem. 3.2, p. 42).

To prove the convexity, let us introduce the design

$$\xi = (1-\alpha)\xi_1 + \alpha\xi_2, \tag{A.2}$$

where $\xi_1, \xi_2 \in \Xi(X)$ and $\alpha \in [0,1]$. Now, constructing the convex combination of the matrices corresponding to ξ_1, ξ_2 we have

$$\begin{aligned}(1-\alpha)M(\xi_1) + \alpha M(\xi_2) &= (1-\alpha) \int_X \Upsilon(x) \xi_1(\mathrm{d}x) + \alpha \int_X \Upsilon(x) \xi_2(\mathrm{d}x) \\ &= \int_X \Upsilon(x) [(1-\alpha)\xi_1(\mathrm{d}x) + \alpha\xi_2(\mathrm{d}x)] = M(\xi)\end{aligned} \tag{A.3}$$

According to (2.55), $M(\xi) \in \mathfrak{M}(X)$ which proves the second part of the lemma. ■

Proof of Theorem 2.3

To derive the discussed property of the information matrices, we need the following classical result (Fedorov, 1972; Pukelsheim, 1993).

Theorem A.1 (Carathéodory's theorem). *Let S be the the set of all possible $s_\mu = \int_{S_0} s\mu(\mathrm{d}s)$, where μ is any probability measure defined on S_0 and $s \in S_0 \subset \mathbb{R}^d$ (S is the convex hull of the S_0). Then each point of S can be represented in the form*

$$s_\mu = \sum_{i=1}^{d_0} \mu_i s_i, \tag{A.4}$$

where $s_i \in S_0$ and $d_0 \leqslant d+1$. If s_μ is the boundary point of S, then $d_0 \leqslant d$.

The main idea of the proof can be found in (Fedorov and Hackl, 1997, Th. 2.3.1, p. 30), however it is expedient to present it here as this result is essential in our considerations.

The set $\mathfrak{M}(X)$ is the convex hull of the set $S_0 = \{\Upsilon(x) : x \in X\}$. The dimension of this set is $d = m(m+1)/2$ due to the symmetry of the matrix $\Upsilon(x)$ (it is sufficient to use only elements lying over and on the main diagonal). Applying the Carathedéodory theorem, we may represent M_0 as a convex combination of no more than d_0 points from S_0:

$$M_0 = \sum_{i=1}^{d_0} p_i \Upsilon(x_i), \quad \sum_{i=1}^{d_0} p_i = 1 \tag{A.5}$$

where $d_0 \leqslant d+1$ in a general case and $d_0 \leqslant d$ for boundary points. Choosing

$$\xi = \begin{Bmatrix} x^1 & \cdots & x^{d_0} \\ p_1 & \cdots & p_{d_0} \end{Bmatrix},$$

we have $M_0 = M(\xi)$ (2.46) and this is precisely the assertion of the theorem. ■

Proof of Theorem 2.4

The existence of an optimal design $\xi^\star$ follows from the compactness of $\mathfrak{M}(X)$ (see Lem. 2.2) and the existence of designs with finite measure Ψ, cf. (A5). From the monotonicity of the criterion Ψ in (A4) it follows that $M(\xi^\star)$ has to be a boundary point of $\mathfrak{M}(X)$. Indeed, if we assume that $M(\xi^\star)$ is an interior point of $\mathfrak{M}(X)$ then there exists $\alpha > 1$ such that $\alpha M(\xi^\star) \in \mathfrak{M}(X)$. Consequently, there exist some design ξ, whose information matrix is given by $\alpha M(\xi^\star)$ (cf. Th. 2.3). But then we have

$$\Psi[M(\xi^\star)] > \Psi[M(\alpha\xi^\star)] = \Psi[M(\xi)]$$

and this contradicts the optimality of the design $\xi^\star$. Thus, if $M(\xi^\star)$ is a boundary point of $\mathfrak{M}(X)$, from the second part of Theorem 2.3 we obtain the existence of a design with no more than $m(m+1)/2$ support points.

For the second part of the assertion, assume that $\xi_1^\star$ and $\xi_2^\star$ are optimal and $\xi^\star = \alpha\xi_1^\star + (1-\alpha)\xi_2^\star$. From the convexity of $\Psi(\,\cdot\,)$ (A3) and the set $\mathfrak{M}(X)$, we have

$$\begin{aligned}\Psi[M(\xi^\star)] &= \Psi[\alpha M(\xi_1^\star) + (1-\alpha)M(\xi_2^\star)] \leqslant \alpha\Psi[M(\xi_1^\star)] + (1-\alpha)\Psi[M(\xi_2^\star)] \\ &= \alpha \min_{\xi\in\Xi(X)} \Psi[M(\xi)] + (1-\alpha) \min_{\xi\in\Xi(X)} \Psi[M(\xi)] = \min_{\xi\in\Xi(X)} \Psi[M(\xi)],\end{aligned}$$

that is to say, $\xi^\star$ is an optimal design. ■

A.2. Proofs of Theorems from Chapter 3

Proof of Theorem 3.1

Since we deal with a feasible-direction method, the convergence analysis proceeds in much the same way as in the clasical framework of this category of methods, cf. (Bertsekas, 1999, p. 213). We must only show that the direction, i.e. $M(\xi_+^{(k)}) - M(\xi^{(k)})$ is also a descent direction, i.e.

$$\frac{\partial}{\partial\alpha}\Psi\left\{M(\xi^{(k)}) + \alpha\big[M(\xi_+^{(k)}) - M(\xi^{(k)})\big]\right\}\Big|_{\alpha=0^+} < 0. \tag{A.6}$$

To this end, let us notice that for any design $\xi \in \Xi(X)$ such that $M(\xi) > 0$, we have

$$\varsigma(\xi) > 0.$$

Indeed, the function $\Psi[\,\cdot\,]$ is convex if and only if (Bertsekas, 1999, Prop. 3.3, p. 675)

$$\Psi[M(\xi) + A] \geqslant \Psi[M(\xi)] + \operatorname{trace}\left\{\overset{\circ}{\Psi}[M(\xi)]A\right\}, \quad \forall A \geqslant 0. \tag{A.7}$$

This gives

$$-\operatorname{trace}\left\{\overset{\circ}{\Psi}[M(\xi)]A\right\} \geqslant \Psi[M(\xi)] - \Psi[M(\xi) + A] > 0, \tag{A.8}$$

for all non-zero $A \geqslant 0$, which is valid due to the assumed monotonicity of $\Psi[\,\cdot\,]$. According to Lemma in (Pukelsheim, 1993, p. 9), this is equivalent to the condition

$$-\overset{\circ}{\Psi}[M(\xi)] > 0. \tag{A.9}$$

This clearly forces

$$\varsigma(\xi) = -\operatorname{trace}\left\{\overset{\circ}{\Psi}[M(\xi)]M(\xi)\right\} > 0. \tag{A.10}$$

We are now in a position to show our claim. It follows that

$$\begin{aligned}
&\frac{\partial}{\partial\alpha}\,\Psi[(1-\alpha)M(\xi^{(k)})+\alpha M(\xi_+^{(k)})]\Big|_{\alpha=0^+}\\
&\quad=\operatorname{trace}\left\{\overset{\circ}{\Psi}[M(\xi^{(k)})][M(\xi_+^{(k)})-M(\xi^{(k)})]\right\}\\
&\quad=\operatorname{trace}\left\{\overset{\circ}{\Psi}[M(\xi^{(k)})]\sum_{i=1}^{\ell}p_i^{(k)}\,\frac{\phi(x^i,\xi^{(k)})-\varsigma(\xi^{(k)})}{\varsigma(\xi^{(k)})}M(\xi^{(k)})\right\}\\
&\quad=-\sum_{i=1}^{\ell}p_i^{(k)}\,\frac{\phi(x^i,\xi^{(k)})-\varsigma(\xi^{(k)})}{\varsigma(\xi^{(k)})}\phi(x^i,\xi^{(k)})=-\operatorname{E}\left[\frac{\phi(x,\xi^{(k)})-\varsigma(\xi^{(k)})}{\varsigma(\xi^{(k)})}\phi(x,\xi^{(k)})\right]\\
&\quad=-\frac{\operatorname{E}\left[\phi^2(x,\xi^{(k)})\right]-\varsigma(\xi^{(k)})\operatorname{E}\left[\phi(x,\xi^{(k)})\right]}{\varsigma(\xi^{(k)})}=-\frac{\operatorname{E}\left[\phi^2(x,\xi^{(k)})\right]-\operatorname{E}^2\left[\phi(x,\xi^{(k)})\right]}{\varsigma(\xi^{(k)})}\\
&\quad=-\frac{\operatorname{var}\left(\phi(x,\xi^{(k)})\right)}{\varsigma(\xi^{(k)})}<0
\end{aligned}\tag{A.11}$$

provided that not all $M\big(\xi(x^i)\big),\ i=1,\ldots,\ell$ are equal. Here we have treated the weights $p_i^{(k)},\ i=1,\ldots,\ell$ as a probability distribution on the set of support points $x^i,\ i=1,\ldots,\ell$. ■

A.3. Proofs of Theorems from Chapter 4

Proof of Theorem 4.1

Since the explicit form of the FIM is not crucial for the proof, the considered generalization to the multi-response systems can be obtained by following the reasoning of the relevant result from (Uciński, 1999a, Thm. 4.1, p. 79). First, the convexity of Ψ yields a necessary and sufficient condition for optimality of $\xi^\star$:

$$\begin{aligned}
\inf_{\bar\xi\in\Xi(X)}\Delta\Psi\big(M(\xi^\star),M(\bar\xi)\big)&=\inf_{\bar\xi\in\Xi(X)}\operatorname{trace}\left[\overset{\circ}{\Psi}[M(\xi^\star)]\big(M(\bar\xi)-M(\xi^\star)\big)\right]\\
&=\operatorname{trace}\left[\overset{\circ}{\Psi}[M(\xi^\star)]\big(M(\xi^\star)-M(\xi^\star)\big)\right]=0.
\end{aligned}\tag{A.12}$$

Setting $x^\star(t) = \arg\min_{x\in X} \psi(x,t,\xi^\star)$, we get

$$\begin{aligned}\int_T \psi(x^\star(t),t,\xi^\star)\,\xi(\mathrm{d}t) &= \int_T \left\{\int_X \psi(x,t,\xi^\star)\delta\big(x-x^\star(t)\big)\,\mathrm{d}x\right\}\xi(\mathrm{d}t)\\ &\geqslant \inf_{\bar\xi}\int_T \left\{\int_X \psi(x,t,\xi^\star)\,\bar\xi(\mathrm{d}x|t)\right\}\xi(\mathrm{d}t)\\ &\geqslant \inf_{\bar\xi}\int_T \left\{\int_X \min_{x\in X}\psi(x,t,\xi^\star)\,\bar\xi(\mathrm{d}x|t)\right\}\xi(\mathrm{d}t)\\ &= \inf_{\bar\xi}\int_T \psi(x^\star(t),t,\xi^\star)\left\{\int_X \bar\xi(\mathrm{d}x|t)\right\}\xi(\mathrm{d}t)\\ &= \int_T \psi(x^\star(t),t,\xi^\star)\,\xi(\mathrm{d}t)\end{aligned} \tag{A.13}$$

Hence

$$\inf_{\bar\xi}\int_T \left\{\int_X \psi(x,t,\xi^\star)\,\bar\xi(\mathrm{d}x|t)\right\}\xi(\mathrm{d}t) = \int_T \psi(x^\star(t),t,\xi^\star)\,\xi(\mathrm{d}t). \tag{A.14}$$

Combining the last equation with (A.12) and (4.21) gives (4.25), which completes the proof. ■

Proof of Theorem 4.5

At the beginning, introduce the design $\xi_\alpha = (1-\alpha)\xi^\star + \alpha\bar\xi$, where $\xi^\star = (\xi_1^\star,\ldots,\xi_K^\star) \in \Xi_q$, and $\bar\xi = (\bar\xi_1,\ldots,\bar\xi_K) \in \Xi(X)$.

$(i) \Rightarrow (ii)$ If $\xi^\star = \arg\min_{\xi\in\Xi(X)} \Psi[M(\xi)]$, then

$$\left.\frac{\partial\Psi[M(\xi_\alpha)]}{\partial\alpha}\right|_{\alpha=0^+} \geqslant 0, \quad \forall\bar\xi \in \Xi(X). \tag{A.15}$$

From Lemma 4.4, setting $\xi = \xi^\star$ and $\bar\xi$ such that

$$\bar\xi_k = \begin{cases} \xi_k^\star & \text{if } k \neq i,\\ \left\{\begin{smallmatrix} x \\ 1 \end{smallmatrix}\right\} & \text{if } k = i,\end{cases} \tag{A.16}$$

we get

$$\begin{aligned}\left.\frac{\partial\Psi[M(\xi_\alpha)]}{\partial\alpha}\right|_{\alpha=0^+} &= \sum_{k=1}^K \varsigma_k(\xi^\star) - \sum_{\substack{k=1\\k\neq i}}^K \int_X \phi_k(x,\xi^\star)\xi_k^\star(\mathrm{d}x) - \phi_i(x,\xi^\star)\\ &= \sum_{k=1}^K \varsigma_k(\xi^\star) - \sum_{k=1}^K \int_X \phi_k(x,\xi^\star)\xi_k^\star(\mathrm{d}x) - \phi_i(x,\xi^\star)\\ &\quad + \int_X \phi_i(x,\xi^\star)\xi_i^\star(\mathrm{d}x) = \varsigma_i(\xi^\star) - \phi_i(x,\xi^\star) \geqslant 0\end{aligned} \tag{A.17}$$

The result is

$$\phi_i(x, \xi^\star) \leqslant \varsigma_i(\xi^\star), \tag{A.18}$$

which clearly forces

$$\max_{x \in X} \phi_i(x, \xi^\star) \leqslant \varsigma_i(\xi^\star). \tag{A.19}$$

Part (ii) of Lemma 4.3 now yields the desired conclusion

$(ii) \Rightarrow (i)$ Let $\xi^\star \in \Xi(X)$ satisfy (ii). We have

$$\begin{aligned} \left.\frac{\partial \Psi[M(\xi_\alpha)]}{\partial \alpha}\right|_{\alpha=0^+} &= \sum_{k=1}^{K} \Big[\varsigma_k(\xi^\star) - \int_X \phi_k(x, \xi^\star) \bar{\xi}_k(\mathrm{d}x)\Big] \\ &\geqslant \sum_{k=1}^{K} \big[\varsigma_k(\xi^\star) - \max_{x \in X} \phi_k(x, \xi^\star)\big] = 0, \end{aligned} \tag{A.20}$$

which completes the proof. ■

Proof of Proposition 4.8

We write C_N for the measurement covariance matrix corresponding to the design ξ_N. The respective covariance matrix C_{N+1} for the design $\xi_{N+1} = \xi_N \cup \{x\}$ takes the following form:

$$C_{N+1} = \left[\begin{array}{c:c} C_N & V(x) \\ \hdashline V^{\mathrm{T}}(x) & K(x,x) \end{array}\right]. \tag{A.21}$$

Applying the Frobenius formula (Ermakov and Zhigljavsky, 1987, Thm. 1.16,p. 301) for inverting the block matrix C_{N+1}, we obtain

$$C_{N+1}^{-1} = \left[\begin{array}{c:c} C_N^{-1} + B(x)\Gamma(x)B^{\mathrm{T}}(x) & B(x)\Gamma(x) \\ \hdashline \Gamma(x)B^{\mathrm{T}}(x) & \Gamma(x) \end{array}\right]. \tag{A.22}$$

Since $F_{N+1}^{\mathrm{T}} = \left[\begin{array}{c:c} F_N^{\mathrm{T}} & F^{\mathrm{T}}(x) \end{array}\right]$, from (A.22) we get

$$\begin{aligned} M_{N+1} =& F_{N+1}^{\mathrm{T}} C_{N+1}^{-1} F_{N+1} = \overbrace{F_N^{\mathrm{T}} C_N^{-1} F_N}^{M_N} + \Big[F_N^{\mathrm{T}} B(x)\Gamma(x)B^{\mathrm{T}}(x)F_N \\ &+ F^{\mathrm{T}}(x)\Gamma(x)B^{\mathrm{T}}(x)F_N + F_N^{\mathrm{T}} B(x)\Gamma(x)F(x) + F^{\mathrm{T}}(x)\Gamma(x)F(x)\Big] \\ =& M_N + \big[F^{\mathrm{T}}(x) + F_N^{\mathrm{T}} B(x)\big]\Gamma(x)\big[F(x) + B^{\mathrm{T}}(x)F_N\big] \\ =& M_N + G(x)\Gamma(x)G^{\mathrm{T}}(x), \end{aligned} \tag{A.23}$$

what is the desired conclusion. ■

Proof of Proposition 4.9

Formula (4.99) can be rewritten as

$$\tilde{M}_N = M_N + G\Gamma G^{\mathrm{T}}, \tag{A.24}$$

where

$$G = \left[\, G(x_a) \,\vdots\, \imath G(x^N) \,\right], \quad \Gamma = \left[\begin{array}{c:c} \Gamma(x_a) & \mathbf{0} \\ \hdashline \mathbf{0} & \Gamma(x^N) \end{array}\right], \quad \imath = \sqrt{-1}. \tag{A.25}$$

The determinant of the block matrix (cf. Fedorov, 1972, Thm. 1.1.13, p. 16) can be calculated as

$$\det\left(\left[\begin{array}{c:c} M_N & G \\ \hdashline G^{\mathrm{T}} & \Gamma^{-1} \end{array}\right]\right) = \det(M_N)\det(\Gamma^{-1} + G^{\mathrm{T}}M_N^{-1}G). \tag{A.26}$$

But the same determinant can be rewritten as

$$\det\left(\left[\begin{array}{c:c} M_N & G \\ \hdashline G^{\mathrm{T}} & \Gamma^{-1} \end{array}\right]\right) = \det(\Gamma^{-1})\det(M_N + G\Gamma G^{\mathrm{T}}). \tag{A.27}$$

Combination of (A.26) and (A.27) yields

$$\begin{aligned} \det(\tilde{M}_N) &= \det(M_N + G\Gamma G^{\mathrm{T}}) = \det(M_N)\det(\Gamma^{-1} + G^{\mathrm{T}}M_N^{-1}G)/\det(\Gamma^{-1}) \\ &= \det(M_N)\det(\Gamma^{-1}\Gamma + G^{\mathrm{T}}M_N^{-1}G\Gamma) \\ &= \det(M_N)\det(I + G^{\mathrm{T}}M_N^{-1}G\Gamma). \end{aligned} \tag{A.28}$$

Finally, taking into account (A.25), we get

$$\begin{aligned} &\det(\tilde{M}_N) \\ &= \det(M_N)\det\left(I + \left[\begin{array}{c} G^{\mathrm{T}}(x_a) \\ \hdashline \imath G^{\mathrm{T}}(x^N) \end{array}\right] M_N^{-1} \left[\, G(x_a) \,\vdots\, \imath G(x^N) \,\right] \left[\begin{array}{c:c} \Gamma(x_a) & \mathbf{0} \\ \hdashline \mathbf{0} & \Gamma(x^N) \end{array}\right]\right) \\ &= \det(M_N)\left(I + \left[\begin{array}{c:c} G^{\mathrm{T}}(x_a)D_N G(x_a)\Gamma(x_a) & \imath G^{\mathrm{T}}(x_a)D_N G(x^N)\Gamma(x^N) \\ \hdashline \imath G^{\mathrm{T}}(x^N)D_N G(x_a)\Gamma(x_a) & -G^{\mathrm{T}}(x^N)D_N G(x_a)\Gamma(x^N) \end{array}\right]\right) \end{aligned} \tag{A.29}$$

which completes the proof. ■

BIBLIOGRAPHY

Aihara S. I. (1997): *Consistency of Extended Least Square Parameter Estimate for Stochastic Distributed Parameter Systems.* — in G. Bastin and M. Gevers (eds), Proc. 4-th European Control Conf., Brussels, Belgium, 1–4 July, 1997, EUCA. (published on CD-ROM)

Amouroux M. and Babary J. P. (1988): *Sensor and Control Location Problems.* — in M. G. Singh (ed.), Systems & Control Encyclopedia. Theory, Technology, Applications, Oxford: Pergamon Press, pp. 4238–4245.

Andó B., Cammarata G., Fichera A., Graziani S. and Pitrone N. (1999): *A Procedure for the Optimization of Air Quality Monitoring Networks.* — IEEE Transactions on Systems, Man, and Cybernetics – Part C: Applications and Reviews, Vol. 29, No. 1, pp. 157–163.

Atkins P. W. (1998): *Physical Chemistry.* — Oxford: Oxford University Press.

Atkinson A. C. and Donev A. N. (1992): *Optimum Experimental Design.* — Oxford: Oxford University Press.

Atkinson A. C. and Fedorov V. V. (1975): *The design of experiments for discriminating between two rival models.* — Biometrica, Vol. 62, pp. 57–70.

Azhogin V. V., Zgurovski M. Z. and Korbicz J. (1988): *Filtration and Control Methods for Stochastic Distributed-Parameter Processes.* — Kiev: Vysha Shkola. (in Russian)

Banks H. T. (1992): *Computational Issues in Parameter Estimation and Feedback Control Problems for Partial Differential Equation Systems.* — Physica D, Vol. 60, pp. 226–238.

Banks H. T. and Fitzpatrick B. G. (1990): *Statistical Methods for Model Comparison in Parameter Estimation Problems for Distributed Systems.* — Journal of Mathematical Biology, Vol. 28, pp. 501–527.

Banks H. T. and Kunisch K. (1989): *Estimation Techniques for Distributed Parameter Systems.* — Systems & Control: Foundations & Applications, Boston: Birkhäuser.

Banks H. T., Smith R. C. and Wang Y. (1996): *Smart Material Structures: Modeling, Estimation and Control.* — Research in Applied Mathematics, Paris: Masson.

Bard Y. (1974): *Nonlinear Parameter Estimation.* — New York, San Francisco, London: Academic Press.

Basseville M. and Nikiforov I. (1993): *Detection of Abrupt Changes.* — New York: Prentice-Hall.

Bear J., Tsang C.-F. and de Marsily G. (1993): *Flow and Contaminant Transport in Fractured Rock.* — New York: Academic Press.

Bennett A. F. (1992): *Inverse Methods in Physical Oceanography.* — Cambridge Monographs on Mechanics and Applied Mathematics, Cambridge: Cambridge University Press.

Berger J. O. (1985): *Statistical Decision Theory and Bayesian Analysis.* — Springer-Verlag.

Berkvens P. J. F., Botchev M. A., Lioen W. M. and Verwer J. (1999): *A Zooming Technique for Wind Transport of Air Pollution.* — Technical Report MAS-R9921, Centrum voor Wiskunde en Informatica, Amsterdam.

Berliner M. L., Nychka D. and Hoar T. (eds) (2000): *Studies in the Atmospheric Sciences.* — Vol. 144 of Lecture Notes in Statistics, Berlin: Springer-Verlag.

Bertsekas D. P. (1999): *Nonlinear Programming.* — Optimization and Computation Series, 2-nd edn, Belmont: Athena Scientific.

Boresi A. P. and Chong K. P. (2000): *Elasticity in engineering mechanics.* — New York: John Wiley & Sons.

Boukas E. and Liu Z. (2003): *Deterministic and Stochastic Time Delay Systems.* — Control Engineering, Birkhäuser.

Boyd S., Ghaoui L. E., Feron E. and Balakrishnan V. (1994): *Linear Matrix Inequalities in System and Control Theory.* — Vol. 15 of SIAM Studies in Applied Mathematics, Philadelphia: SIAM.

Boyd S. and Vandenberghe L. (2004): *Convex Optimization.* — Cambridge: Cambridge University Press.

Braake H. A. B., van Can H. J. L. and Verbruggen H. B. (1998): *Semi-mechanistic modeling of chemical processes with neural networks.* — Engineering Applications of Artificial Intelligence, Vol. 11, No. 4, pp. 507–515.

Brimkulov U. N., Krug G. K. and Savanov V. L. (1986): *Design of Experiments in Investigating Random Fields and Processes.* — Moscow: Nauka. (in Russian)

Burke A. L., Duever T. A. and Pendilis A. (1994): *Model discrimination via designed experiments; Discriminating between the terminal and penultimate models on the basis of composition data.* — Macromolecules, Vol. 27, pp. 386–399.

Butkovskiy A. G. (1982): *Green's Functions and Transfer Functions Handbook.* — New York: Wiley.

Chavent G. (1991): *On the Theory and Practice of Non-Linear Least-Squares.* — Adv. Water Resources, Vol. 14, No. 2, pp. 55–63.

Chen J. and Patton R. J. (1999): *Robust Model-Based Fault Diagnosis for Dynamic Systems.* — Berlin: Kluwer Academic Publishers.

Chen W. H. and Seinfeld J. H. (1975): *Optimal Location of Process Measurements.* — International Journal of Control, Vol. 21, No. 6, pp. 1003–1014.

Chiang L. H., Russel E. L. and Braatz R. D. (2001): *Fault Detection and Diagnosis in Industrial Systems.* — London: Springer.

Cook D. and Fedorov V. (1995): *Constrained Optimization of Experimental Design.* — Statistics, Vol. 26, pp. 129–178.

Curtain R. F. and Zwart H. (1995): *An Introduction to Infinite-Dimensional Linear Systems Theory.* — Texts in Applied Mathematics, New York: Springer-Verlag.

Dagan G. (1989): *Flow and Transport in Porous Formations.* — Berlin: Springer-Verlag.

Daley R. (1991): *Atmospheric Data Analysis.* — Cambridge: Cambridge University Press.

de Cogan D. and de Cogan A. (1997): *Applied Numerical Modelling for Engineers.* — New York: Oxford University Press.

Demetriou M. A. (2000): *Activation Policy of Smart Controllers for Flexible Structures with Multiple Actuator/Sensor Pairs.* — in A. El Jai and M. Fliess (eds), Proc. 14-th Int. Symp. Mathematical Theory of Networks and Systems, Perpignan, France, 19–23 June, 2000, . (published on CD-ROM)

Demetriou M. A. and Rosen I. G. (1993): *On the Persistence of Excitation in the Adaptive Estimation of Distributed Parameter Systems.* — Technical Report 93–4, Center for Applied Mathematical Sciences, University of Southern California, Los Angeles.

Domański C. (1990): *Statistical Tests.* — Warsaw: Polish Scientific Publishers. (in Polish)

Dorfman S., Fuks D., Gordon A., Kotomin E. and Wyder P. (2001): *Some nonlinear properties of ferroelectric smart materials.* — Physica B, Vol. 304, pp. 339–347.

Du C. and Xie L. (2002): H_∞ *Control and Filtering of Two-dimensional Systems.* — Vol. 278 of Lecture Notes in Control and Information Sciences, Springer-Verlag.

Duch W., Korbicz J., Rutkowski L. and Tadeusiewicz R. (eds) (2000): *Biocybernetics and Biomedical Engineering 2000. Neural Networks*. — Warszawa: Akademicka Oficyna Wydawnicza, PLJ. (in Polish)

Dullerud G. E. and Paganini F. (2000): *A Course in Robust Control Theory. A convex approach*. — Vol. 36 of Texts in Applied Mathematics, Springer-Verlag, New York.

El Jai A. (1991): *Distributed Systems Analysis via Sensors and Actuators*. — Sensors and Actuators A, Vol. 29, pp. 1–11.

El Jai A. and Amouroux M. (eds) (1987): *Proceedings of the First International Workshop on Sensors and Actuators in Distributed Parameter Systems, Perpignan, France, 16–18 December, 1987*. — IFAC, Perpignan.

El Jai A. and Pritchard A. J. (1988): *Sensors and Controls in the Analysis of Distributed Systems*. — New York: John Wiley & Sons.

Ermakov S. M. (ed.) (1983): *Mathematical Theory of Experimental Design*. — Moscow: Nauka. (in Russian)

Ermakov S. M. and Zhigljavsky A. A. (1987): *Mathematical Theory of Optimal Experiments*. — Moscow: Nauka. (in Russian)

Fedorov V. V. (1972): *Theory of Optimal Experiments*. — New York: Academic Press.

Fedorov V. V. (1989): *Optimal Design with Bounded Density: Optimization Algorithms of the Exchange Type*. — Journal of Statistical Planning and Inference, Vol. 22, pp. 1–13.

Fedorov V. V. (1996): *Design of Spatial Experiments: Model Fitting and Prediction*. — Technical Report TM-13152, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

Fedorov V. V. and Hackl P. (1997): *Model-Oriented Design of Experiments*. — Lecture Notes in Statistics, New York: Springer-Verlag.

Fedra K. (1999): *Urban Environmental Management: Monitoring, GIS, and Modeling*. — Computer, Environment and Urban Systems, Vol. 23, pp. 443–457.

Findeisen W., Szymanowski J. and Wierzbicki A. (1980): *Optimization theory and numerical methods*. — Warsaw: Polish Scientific Publishers. (in Polish)

Fitzpatrick B. G. (1991): *Bayesian Analysis in Inverse Problems*. — Inverse Problems, Vol. 7, pp. 675–702.

Fitzpatrick B. G. (1995): *Large Sample Behavior in Bayesian Analysis of Nonlinear Regression Models*. — Journal of Mathematical Analysis and Applications, Vol. 192, pp. 607–626.

Fitzpatrick B. G. and Yin G. (1995): *Empirical Distributions in Least Squares Estimation for Distributed Parameter Systems.* — Journal of Mathematical Systems, Estimation, and Control, Vol. 5, No. 1, pp. 37–57.

Flatau A. B. and Chong K. P. (2002): *Dynamic smart material and structural systems.* — Engineering Structures, Vol. 24, pp. 261–270.

Ford I., Titterington D. M. and Kitsos C. P. (1989): *Recent Advances in Nonlinear Experimental Design.* — Technometrics, Vol. 31, No. 1, pp. 49–60.

Frank P. M. and Köppen-Seliger B. (1997): *New developments using AI in fault diagnosis.* — Artificial Intelligence, Vol. 10, No. 1, pp. 3–14.

Gandhi M. V. and Thompson B. S. (1992): *Smart Materials and Structures.* — New York: Chapman and Hall.

Garthwaite I. T. and Jolliffe B. J. (1995): *Statistical Interference.* — Prentice Hall.

Gibson J. S., George H. and Wu C.-F. (2000): *Least-squares estimation of input/output models for distributed linear systems in the presence of noise.* — Automatica, Vol. 36, pp. 1427–1442.

Gil M. I. (1998): *Stability of Finite and Infinite Dimensional Systems.* — Boston: Kluwer Academic Publishers.

Goodwin G. C. and Payne R. L. (1977): *Dynamic System Identification. Experiment Design and Data Analysis.* — Mathematics in Science and Engineering, New York: Academic Press.

Grabowski P. (1999): *Lecture Notes on Optimal Control Systems.* — Cracow: University of Mining and Metallurgy Publishers.

Gueymard C. A., Laulainen N. S., Vaughan J. K. and Vignola F. E. (2000): *China's Dust Affects Solar Resource in U.S.: A Case Study.* — Proceedings of the 2000 Annual Conference American Solar Energy Society, Heidelberg, pp. 383–389.

Hogg N. G. (1996): *Oceanographic Data for Parameter Estimation.* — in P. Malanotte-Rizzoli (ed.), Modern Approaches to Data Assimilation in Ocean Modeling, Elsevier Oceanography, Amsterdam: Elsevier, pp. 57–76.

Hundsdorfer W. H. (1996): *Numerical Solution of Advection-Diffusion-Reaction Equations.* — Technical Report NM-N9603, Centrum voor Wiskunde en Informatica, Amsterdam.

Ichinose G. A., Smith K. D. and Anderson J. G. (1998): *Moment Tensor solutions of the 1994 to 1996 Double Spring Flat, Nevada, Earthquake Sequence and Implications for Local Tectonic Models.* — Bull. Seism. Soc. Am., Vol. 88, pp. 1363–1378.

Isakov V. (1998): *Inverse Problems for Partial Differential Equations.* — Applied Mathematical Sciences, New York: Springer-Verlag.

Isermann R. (ed.) (1997): *Supervision, Fault Detection and Diagnosis of Technical Systems.* — Special Section Control Engineering Practice, Vol. 5, No. 5.

ISO (1996): *International Vocabulary of Basic and General Terms in Metrology.* — Warsaw: International Organisation of Standarization. (Polish edition)

Jacobson M. Z. (1999): *Fundamentals of atmospheric modelling.* — Cambridge: Cambridge University Press.

Kanwal R. P. (1971): *Linear Integral Equations, Theory and Technique.* — New York: Academic Press.

Karnopp D. C., Margolis D. L. and Rosenberg R. C. (2000): *System Dynamics: Modeling and Simulation of Mechatronic Systems.* — New Yersey: Interscience.

Kazimierczyk P. (1989): *Optimal Experiment Design; Vibrating Beam under Random Loading.* — Technical Report 7/1989, Institute of Fundamental Technological Research, Polish Academy of Sciences, Warsaw.

Kącki E. (1995): *Partial Differential Equations in Problems of Physics and Technics.* — 4-th edn, Warsaw: Wydawnictwa Naukowo-Techniczne. (in Polish)

Kiefer J. and Wolfowitz J. (1959): *Optimum Designs in Regression Problems.* — The Annals of Mathematical Statistics, Vol. 30, pp. 271–294.

Kim M. H., Kim S., Lee H. J., Lee Y. J. and Kim K. Y. (2002): *An experimental study of electrical impedance tomography for the two-phase flow visualization.* — International Comm. Heat Mass Transfer, Vol. 29, No. 2, pp. 193–202.

Korbicz J. (1991): *Discrete-scanning observation problem for stochastic non-linear disrete-time distributed parameter systems.* — International Journal of Systems Science, Vol. 22, No. 9, pp. 1647–1662.

Korbicz J., Kościelny J., Kowalczuk Z. and Cholewa W. (2004): *Fault Diagnosis. Models, Artificial Intelligence, Applications.* — Berlin, Heidelberg: Springer-Verlag.

Korbicz J., Patan K. and Obuchowicz A. (2001): *Neural network fault detection system for dynamic processes.* — Bulletin of the Polish Academy of Sciences. Technical Sciences., Vol. 49, No. 2, pp. 301–321.

Korbicz J. and Uciński D. (1994): *Sensors Allocation for State and Parameter Estimation of Distributed Systems.* — in W. Gutkowski and J. Bauer (eds), Proc. IUTAM Symposium, Zakopane, Poland, 31 August–3 September, 1993, Berlin: Springer-Verlag, pp. 178–189.

Korbicz J., Uciński D., Pieczyński A. and Marczewska G. (1993): *Knowledge-Based Fault Detection and Isolation System for Power Plant.* — Applied Mathematics and Computer Science, Vol. 3, No. 3, pp. 613–630.

Korbicz J., Zgurovsky M. Z. and Novikov A. N. (1988): *Suboptimal Sensors Location in the State Estimation Problem for Stochastic Non-Linear Distributed Parameter Systems.* — International Journal of Systems Science, Vol. 19, No. 9, pp. 1871–1882.

Korbicz J. and Zgurowski M. Z. (1991): *Estimation and Control of Stochastic Distributed-Parameter Systems.* — Warsaw: Polish Scientific Publishers. (in Polish)

Kovarik K. (2000): *Numerical Models in Grounwater Pollution.* — Berlin, Heidelberg, New York: Springer-Verlag.

Kowalewski A. (1991): *Optimal Control Problems of Distributed Parameter Systems with Boundary Conditions Involving Time Delays.* — Scientific Bulletins of the University of Mining and Metallurgy, Series Automatics, Cracow: University of Mining and Metallurgy Publishers. (in Polish)

Kowalewski A. (2001a): *Optimal Control of Infinite Dimensional Distributed Parameter Systems with Delays.* — Cracow: University of Mining and Metallurgy Press.

Kowalewski A. (2001b): *Optimal control of time delay parabolic systems.* — Optimization, Vol. 50, No. 1–2, pp. 205–232.

Królikowski A. and Eykhoff P. (1985): *Input Signals Design for System Identification: A Comparative Analysis.* — Prep. 7-th IFAC/IFORS Symp. Identification and System Parameter Estimation, York, pp. 915–920.

Kubrusly C. S. (1977): *Distributed Parameter System Identification: A Survey.* — International Journal of Control, Vol. 26, No. 4, pp. 509–535.

Kubrusly C. S. and Malebranche H. (1985): *Sensors and Controllers Location in Distributed Systems—A Survey.* — Automatica, Vol. 21, No. 2, pp. 117–128.

Kuczewski B., Patan M. and Uciński D. (2003): *Optimal sensor location in fault detection of distributed parameter systems.* — in Z. Kowalczuk (ed.), 6-th National Conference on Diagnostics of Industrial Processes, 15-17 September, Władysławowo, Poland, 2003, Gdańsk: Technical University Press, pp. 213–218. (in Polish)

Kuczewski B., Patan M. and Uciński D. (2004): *Discrimination between Models of Distributed Parameter Systems Using T-optimum Experimental Design.* — in R. Wyrzykowski (ed.), Lecture Notes in Computer Science, Berlin Heidelberg: Springer-Verlag, Vol. 3019.

Kuczewski B. and Uciński D. (2002): *Optimal design of measurement strategies for discrimination between multiresponse dynamic models.* — in S. Domek and R. Kaszyński (eds), Proc. 8-th IEEE Int. Conf. Methods and Models in Automation and Robotics, Międzyzdroje, Poland, 2–5 September, Szczecin: Technical University Press, Vol. 1, pp. 593–598.

Kuczewski B. and Uciński D. (2003): *Optimal Measurement Policies for Discrimination between Models of Dynamic Systems*. — in R. Kaszyński (ed.), Proc. 9-th IEEE Int. Conf. Methods and Models in Automation and Robotics, Międzyzdroje, Poland, 25–28 August, Szczecin: Technical University Press, Vol. 2, pp. 1239–1244.

Kunisch K. (1988): *A Review of Some Recent Results on the Output Least Squares Formulation of Parameter Estimation Problems*. — Automatica, Vol. 24, No. 4, pp. 531–539.

Kushner H. J. and Yin G. G. (1997): *Stochastic Approximation Algorithms and Applications*. — Applications of Mathematics, New York: Springer-Verlag.

Landaw E. M. (1980): *Optimal experiment design for biologic compartmental systems with applications to pharmacokinetics*. — PhD thesis, University of California, Los Angeles, USA.

Lasiecka I. (1998): *Active Noise Control in an Acoustic Chamber: Mathematical Theory*. — in S. Domek, R. Kaszyński and L. Tarasiejski (eds), Proc. 5-th Int. Symp. Methods and Models in Automation and Robotics, Międzyzdroje, Poland, 25–29 August 1998, Szczecin: Technical University Press, Vol. 1, pp. 13–22.

Lasiecka I. and Triggiani R. (2000): *Control Theory for Partial Differential Equations: Continuous and Approximation Theories*. — Vol. I and II of Encyclopedia of Mathematics and Its Applications, Cambridge: Cambridge University Press.

Lee H. W. J., Teo K. L. and Lim A. E. B. (2001): *Sensor scheduling in continuous time*. — Automatica, Vol. 37, pp. 2017–2023.

Lee H. W. J., Teo K. L., Rehbock V. and Jennings L. S. (1999): *Control parametrization enhancing technique for optimal discrete-valued control problems*. — Automatica, Vol. 35, pp. 1401–1407.

Lehmann E. L. (1986): *Testing Statistical Hypotheses*. — 2-nd edn, Springer-Verlag.

Lemonnier H. and Peytraud J. F. (1998): *Is 2D impedance tomography a rielable technique for two-phase flow*. — Nuclear Engineering and Design, Vol. 184, pp. 253–268.

Li X., Yong J. and Li H.-C. (1995): *Optimal Control Theory for Infinite Dimensional Systems (Systems and Control)*. — Berlin: Springer-Verlag.

Littlefield B. (1997): *MATLAB User's Guide*. — Prentice Hall Professional Technical Reference.

Luo Z.-H., Guo B.-Z. and Morgul O. (1999): *Stability and Stabilization of Infinite Dimensional Systems with Applications*. — Heidelberg: Springer-Verlag.

Malanotte-Rizzoli P. (ed.) (1996): *Modern Approaches to Data Assimilation in Ocean Modeling*. — Elsevier Oceanography, Amsterdam: Elsevier.

Malanowski K., Nahorski Z. and Peszyńska M. (eds) (1996): *Modelling and Optimization of Distributed Parameter Systems*. — International Federation for Information Processing, Boston: Kluwer Academic Publishers.

Malebranche H. (1988): *Simultaneous State and Parameter Estimation and Location of Sensors for Distributed Systems*. — International Journal of Systems Science, Vol. 19, No. 8, pp. 1387–1405.

Marchuk G. I. (1985): *Mathematical modelling in problems of natural environment*. — Warsaw: Polish Scientific Publishers. (in Polish)

Mehra R. K. (1976): *Optimization of Measurement Schedules and Sensor Designs for Linear Dynamic Systems*. — IEEE Transactions on Automatic Control, Vol. 21, No. 1, pp. 55–64.

Mitkowski W. (1991): *Stabilization of Dynamic Systems*. — Warsaw: Wydawnictwa Naukowo-Techniczne. (in Polish)

Müller W. G. (1998): *Collecting Spatial Data. Optimum Design of Experiments for Random Fields*. — Contributions to Statistics, Heidelberg: Physica-Verlag.

Munn R. E. (1981): *The Design of Air Quality Monitoring Networks*. — London: MacMillan.

Nakano K. and Sagara S. (1988): *Optimal Scanning Measurement Problem for a Stochastic Distributed-Parameter System*. — International Journal of Systems Science, Vol. 19, No. 7, pp. 1069–1083.

Niederliński A. (1983): *Systems and control: introduction to automation and cybernetics*. — Warsaw: Polish Scientific Publishers. (in Polish)

Noble T. J., Morice A. H., Channer K. S., Milnes P., Harris N. D. and Brown B. H. (1999): *Monitoring patients with left ventricular failure by electrical impedance tomography*. — The European Journal of Heart Failure, Vol. 1, pp. 379–384.

Nyberg M. (1999): *Model Based Fault Diagnosis: Methods, Theory, and Automotive Engine Applications*. — PhD thesis, Linköping University, Linköping, Sweden.

Nychka D., Piegorsch W. W. and Cox L. H. (eds) (1998): *Case Studies in Environmental Statistics*. — Lecture Notes in Statistics, Vol. 132, New York: Springer-Verlag.

Nychka D. and Saltzman N. (1998): *Design of Air-Quality Monitoring Networks*. — in D. Nychka, W. W. Piegorsch and L. H. Cox (eds), Case Studies in Environmental Statistics, Lecture Notes in Statistics, Vol. 132, New York: Springer-Verlag, pp. 51–76.

Omatu S. and Seinfeld J. H. (1989): *Distributed Parameter Systems: Theory and Applications*. — Oxford Mathematical Monographs, New York: Oxford University Press.

Patan M. and Patan K. (2001): *Parametric identification of the continuous time systems using experimental design optimization*. — in J. Korbicz (ed.), Proc. 5-th National Conference on Diagnostics of Industrial Processes, 17-19 September, Łagów, Poland, 2001, Zielona Góra: Technical University Press, pp. 95–101. (in Polish)

Patan M. and Patan K. (2003): *Calibration of diagnostic models for two tank system using optimal experiment design*. — in Z. Kowalczuk (ed.), 6-th National Conference on Diagnostics of Industrial Processes, 15-17 September, Władysławowo, Poland, 2003, Gdańsk: Technical University Press, pp. 189–194. (in Polish)

Patan M. and Uciński D. (2002): *Optimal location of sensors for parameter estimation of static distributed systems*. — in R. Wyrzykowski, J. Dongarra, M. Paprzycki and J.Waśniewski (eds), Lecture Notes in Computer Science, Berlin Heidelberg: Springer-Verlag, Vol. 2328, pp. 729–738.

Patan M. and Uciński D. (2003): *Optimal Strategies of Scanning Sensors for Parameter Estimation of Distributed Systems*. — in R. Kaszyński (ed.), Proc. 9-th IEEE Int. Conf. Methods and Models in Automation and Robotics, Międzyzdroje, Poland, 25–28 August, Szczecin: Technical University Press, Vol. 1, pp. 115–120.

Patan M. and Uciński D. (2004): *Robust activation strategy of scanning sensors via sequential design in parameter estimation of distributed systems*. — in R. Wyrzykowski (ed.), Lecture Notes in Computer Science, Berlin Heidelberg: Springer-Verlag, Vol. 3019.

Patton R. J., Frank P. M. and Clark R. (2000): *Issues of Fault Diagnosis for Dynamic Systems*. — Berlin: Springer-Verlag.

Patton R. J. and Korbicz J. (eds) (1999): *Advances in Computational Intelligence*. — Special Issue International Journal of Applied Mathematics and Computer Science, Vol. 9, No. 3.

Pázman A. (1986): *Foundations of Optimum Experimental Design*. — Mathematics and Its Applications, Dordrecht: D. Reidel Publishing Company.

Pflug G. C. (1996): *Optimization of Stochastic Models. The Interface Between Simulation and Optimization*. — Engineering and Computer Science: Discrete Event Dynamic Systems, Boston: Kluwer Academic Publishers.

Polak E. (1997): *Optimization. Algorithms and Consistent Approximations*. — Applied Mathematical Sciences, New York: Springer-Verlag.

Polis M. P. (1982): *The Distributed System Parameter Identification Problem: A Survey of Recent Results*. — Proc. 3-rd IFAC Symp. Control of Distributed Parameter Systems, Toulouse, France, pp. 45–58.

Polyanin A. D. (2002): *Linear Partial Differential Equations for Engineers and Scientists*. — New York: Chapman and Hall/CRC.

Pronzato L. (2003): *Removing non-optimal support points in D-optimum designs algorithms*. — Statistics and Probability Letters, Vol. 63, pp. 223–228.

Pronzato L. and Walter É. (1985): *Robust Experiment Design via Stochastic Approximation*. — Mathematical Biosciences, Vol. 75, pp. 103–120.

Pronzato L. and Walter É. (1988): *Robust Experiment Design via Maximin Optimization*. — Mathematical Biosciences, Vol. 89, pp. 161–176.

Pukelsheim F. (1993): *Optimal Design of Experiments*. — Probability and Mathematical Statistics, New York: John Wiley & Sons.

Pukelsheim F. and Rieder S. (1992): *Efficient Rounding of Approximate Designs*. — Biometrica, Vol. 79, No. 4, pp. 763–770.

Pukelsheim F. and Torsney B. (1991): *Optimal Weights for Experimental Design on Linearly Independent Support Points*. — Annals of Statistics, Vol. 19, No. 3, pp. 1614–1625.

Quereshi Z. H., Ng T. S. and Goodwin G. C. (1980): *Optimum Experimental Design for Identification of Distributed Parameter Systems*. — International Journal of Control, Vol. 31, No. 1, pp. 21–29.

Rafajłowicz E. (1978): *Design of Experiments for Parameter Identification of the Static Distributed Systems*. — Systems Science, Vol. 4, No. 4, pp. 349–361.

Rafajłowicz E. (1981): *Design of Experiments for Eigenvalue Identification in Distributed-Parameter Systems*. — International Journal of Control, Vol. 34, No. 6, pp. 1079–1094.

Rafajłowicz E. (1983): *Optimal Experiment Design for Identification of Linear Distributed-Parameter Systems: Frequency Domain Approach*. — IEEE Transactions on Automatic Control, Vol. 28, No. 7, pp. 806–808.

Rafajłowicz E. (1986a): *Choice of Optimum Input Signals in Linear Distributed-Parameter Systems Identification*. — Monographs, Wrocław: Technical University Press. (in Polish)

Rafajłowicz E. (1986b): *Optimum Choice of Moving Sensor Trajectories for Distributed Parameter System Identification*. — International Journal of Control, Vol. 43, No. 5, pp. 1441–1451.

Rafajłowicz E. (1988): *Distributed Parameter Systems Analysis by Tracking Stationary Points of Their States*. — International Journal of Systems Science, Vol. 19, No. 4, pp. 613–620.

Rafajłowicz E. (1989): *Reduction of Distributed System Identification Complexity Using Intelligent Sensors*. — International Journal of Control, Vol. 50, No. 5, pp. 1571–1576.

Rafajłowicz E. (1996): *Algorithms of Experimental Design with Implementations in MATHEMATICA*. — Warsaw: Academic Publishers PLJ. (in Polish)

Rafajłowicz E. (1998): *Selective Random Search for Optimal Experiment Designs*. — in A. C. Atkinson, L. Pronzato and H. P. Wynn (eds), MODA 5 – Advances in Model-Oriented Data Analysis and Experimental Design: Proceedings of the 5-th International Workshop in Marseilles, France, June 22–26, 1998, Contributions to Statistics, Heidelberg: Physica-Verlag, chapter 9, pp. 75–83.

Rao M. M. (1987): *Measure Theory and Integration*. — New York: Wiley & Sons.

Redfern D. (1996): *The Maple Handbook*. — New York: Springer-Verlag.

Reemtsen R. (2001): *Semi-infinite programming: Discretization methods*. — in C. A. Floudas and P. M. Pardalos (eds), Encyclopedia of Optimization, Dordrecht: Kluwer Academic Publishers, pp. 100–107.

Rijtema P. E. and Elias V. (eds) (1996): *Regional approaches to water pollution in the environment*. — Dordrecht: Kluwer Academic Publishers.

Robinson J. C. (2001): *Infinite-Dimensional Dynamical Systems : An Introduction to Dissipative Parabolic PDEs and the Theory of Global Attractors*. — Cambridge: Cambridge University Press.

Romanowicz B., Neuhauser D., Gogaert B. and Oppenheimer D. (1994): *Accessing Northern California Earthquake Data via Internet*. — EOS, Vol. 75, pp. 258–261.

Sasane A. (2002): *Hankel Norm Approximation for Infinite-Dimensional Systems*. — Vol. 277 of Lecture Notes in Control and Information Sciences, Heidelberg: Springer-Verlag.

Shimizu K. and Aiyoshi E. (1980): *Necessary Conditions for Min-Max Problems and Algorithms by a Relaxation Procedure*. — IEEE Transactions on Automatic Control, Vol. AC-25, No. 1, pp. 62–66.

Sikora J. (2000): *Numerical approaches to the impedance and eddy-currental tomography*. — Warsaw: Technical University Press. (in Polish)

Silvey S. D. (1980): *Optimal Design*. — London: Chapman and Hall.

Sokołowski J. and Zolesio J.-P. (1992): *Introduction to Shape Optimization: Shape Sensitivity Analysis*. — Computational Mathematics, Berlin: Springer-Verlag.

Spall J. C. (2003): *Introduction to stochastic search and optimization; Estimation, Simulation, and Control.* — New Jersey: Wiley-Interscience.

Stewart W. E., Shon Y. and Box G. E. P. (1988): *Discrimination and goodness of fit of multiresponse mechanistic models.* — AIChE Journal, Vol. 44, No. 6, pp. 1404–1412.

Sturm J. F. (1997): *Primal-Dual Interior Point Approach to Semidefinite Programming.* — PhD thesis, Erasmus Universiteit Rotterdam, Rotterdam, the Netherlands.

Sturm P. J., Almbauer R. A. and Kunz R. (1994): *Air Quality Study for the City of Graz, Austria.* — in H. Power, N. Moussiopoulos and C. A. Brebbia (eds), Urban Air Pollution, Vol. 1, Southampton: Computational Mechanics Publications, chapter 2, pp. 43–100.

Sun N.-Z. (1994): *Inverse Problems in Groundwater Modeling.* — Theory and Applications of Transport in Porous Media, Dordrecht: Kluwer Academic Publishers.

Sun N.-Z. (1996): *Mathematical Modeling of Groundwater Pollution.* — New York: Springer-Verlag.

Sydow A., Lux T., Mieth P., Schmidt M. and Unger S. (1997): *The DYMOS Model System for the Analysis and Simulation of Regional Air Pollution.* — in R. Grützner (ed.), Modellierung und Simulation im Umweltbereich, Wiesbaden: Vieweg-Verlag, pp. 209–219.

Sydow A., Lux T., Rosé H., Rufeger W. and Walter B. (1998): *Conceptual Design of the Branch-Oriented Simulation System DYMOS (Dynamic Models for Smog Analysis).* — Transactions of the Society for Computer Simulation International, Vol. 15, No. 3, pp. 95–100.

Taylor B. N. and Kuyatt C. E. (1994): *Guidelines for Evaluating and Expressing the Uncertainty of NIST Measurement Results.* — Technical Note 1297, National Institute of Standards and Technology, Washington.

Tempo R., Bai E. W. and Dabbene F. (1997): *Probabilistic robustness analysis: Explicit bounds for the minimum number of sampling points.* — Systems & Control Letters, Vol. 30, pp. 237–242.

Titterington D. M. (1980): *Aspects of Optimal Design in Dynamic Systems.* — Technometrics, Vol. 22, No. 3, pp. 287–299.

Torsney B. (1983): *A moment inequality and monotonicity of an algorithm.* — in K. O. Kortanek and A. V. Fiacco (eds), Proc. of the Int. Symp. on Semi-infinite Programming and Applications, University Texas at Austin, Vol. 215 of Lecture Notes in Econom. and Math. Systems, New York: Springer-Verlag, pp. 249–260.

Torsney B. (1988): *Computing Optimising Distributions with Applications in Design, Estimation and Image Processing.* — in Y. Dodge, V. V. Fedorov and H. P. Wynn (eds), Optimal Design and Analysis of Experiments, Amsterdam: Elsevier, pp. 316–370.

Tuenter H. J. H. (2001): *The Minimum L_2-Distance Projection onto the Canonical Simplex: A Simple Algorithm.* — Algo Research Quarterly, Vol. Dec 2001, pp. 53–55.

Uciński D. (1992): *Optimal Sensor Location for Parameter Identification of Distributed Systems.* — Applied Mathematics and Computer Science, Vol. 2, No. 1, pp. 119–134.

Uciński D. (1995): *Optimal Selection of Measurement Locations for Identification of Parameters in Distributed Systems.* — in S. Bańka, S. Domek and Z. Emirsajłow (eds), Proc. 2-nd Int. Symp. Methods and Models in Automation and Robotics, Międzyzdroje, Poland, 30 August–2 September 1995, Szczecin: Technical University Press, Vol. 1, pp. 175–180.

Uciński D. (1999a): *Measurement Optimization for Parameter Estimation in Distributed Systems.* — Zielona Góra: Technical University Press.

Uciński D. (1999b): *Optimum Design of Sensor Locations in Parameter Estimation of Distributed Systems.* — Studia z Automatyki i Informatyki, Vol. 24, pp. 151–167. (in Polish)

Uciński D. (1999c): *Robust Design of Sensor Locations in Parameter Estimation of Distributed Systems.* — in Z. Bubnicki and J. Józefczyk (eds), Proc. 13-th Nat. Conf. Automatics, Opole, 21–24 September, Wrocław, Vol. 1, pp. 289–292. (in Polish)

Uciński D. (1999d): *A Technique of Robust Sensor Allocation for Parameter Estimation in Distributed Systems.* — in P. M. Frank (ed.), Proc. 5-th European Control Conf., Karlsruhe, Germany, 31 August–3 September, 1999, EUCA.

Uciński D. (2000a): *Optimal Selection of Measurement Locations for Parameter Estimation in Distributed Processes.* — International Journal of Applied Mathematics and Computer Science, Vol. 10, No. 2, pp. 357–379.

Uciński D. (2000b): *Optimal Sensor Location for Parameter Estimation of Distributed Processes.* — International Journal of Control, Vol. 73, No. 13, pp. 1235–1248.

Uciński D. (2000c): *Optimization of Sensors' Allocation Strategies for Parameter Estimation in Distributed Systems.* — Systems Analysis–Modelling–Simulation, Vol. 37, pp. 243–260.

Uciński D. (2001): *Sensor Motion Planning with Design Criteria in Output Space.* — in A. C. Atkinson, P. Hackl and W. Müller (eds), *mODa 6*, Proc. 6-th Int.

Workshop on Model-Oriented Data Analysis, Puchberg//Schneeberg, Austria, 2001, Heidelberg: Physica-Verlag, pp. 235–242.

Uciński D. (2003): *On optimum experimental design for technical diagnostics of processes*. — in Z. Kowalczuk (ed.), 6-th National Conference on Diagnostics of Industrial Processes, 15-17 September, Władysławowo, Poland, 2003, Gdańsk: Technical University Press, pp. 207–212. (in Polish)

Uciński D. and Bogacka B. (2002): *Construction of T-Optimum Designs for Multiresponse Dynamic Models*. — Proceedings in Computational Statistics : 15th Symposium Held in Berlin, Germany, Berlin, pp. 267–272.

Uciński D. and Korbicz J. (1990): *Parameter Identification of Two-Dimensional Distributed Systems*. — International Journal of Systems Science, Vol. 21, No. 2, pp. 2441–2456.

Uciński D. and Korbicz J. (2001): *Optimal Sensor Allocation for Parameter Estimation in Distributed Systems*. — Journal of Inverse and Ill-Posed Problems, Vol. 9, No. 3, pp. 301–317.

Uciński D. and Patan M. (2002a): *Optimal location of discrete scanning sensors for parameter estimation of distributed systems*. — Proc. 15th Trennial World Congress of the International Federation of Automatic Control, Barcelona, Spain, Oxford: Pergamon Press. (published on CD-ROM)

Uciński D. and Patan M. (2002b): *Optimal observation strategies in parameter estimation of distributed systems*. — Proc. 14-th Nat. Conf. of Automatic Control, KKA'02, Zielona Góra, Poland, 24–27 June, Zielona Góra: Zielona Góra University Press, Vol. 1, pp. 331–336. (in Polish)

Uciński D. and Patan M. (2002c): *Optimization of the measurement effort in parameter estimation of distributed systems*. — in S. Domek and R. Kaszyński (eds), Proc. 8-th IEEE Int. Conf. Methods and Models in Automation and Robotics, Szczecin, Poland, 2–5 September, Szczecin: Technical University Press, Vol. 1, pp. 195–200.

van de Wal M. and de Jager B. (2001): *A Review of Methods for Input/Output Selection*. — Automatica, Vol. 37, pp. 487–510.

van Loon M. (1994): *Numerical Smog Prediction, I: The Physical and Chemical Model*. — Technical Report NM-R9411, Centrum voor Wiskunde en Informatica, Amsterdam.

van Loon M. (1995): *Numerical Smog Prediction, II: Grid Refinement and Its Application to the Dutch Smog Prediction Model*. — Technical Report NM-R9523, Centrum voor Wiskunde en Informatica, Amsterdam.

Vandenberghe L. and Boyd S. (1996a): *Determinant maximization with linear matrix inequality constraints*. — Siam Review, Vol. 40, pp. 49–95.

Vandenberghe L. and Boyd S. (1996b): *Semidefinite programming.* — Siam Review, Vol. 38, pp. 49–95.

Vandenberghe L. and Boyd S. (1998): *Connections between semi-infinite and semidefinite programming.* — in R. Reemtsen and J.-J. Rückmann (eds), Semi-Infinite Programming, Boston: Kluwer Academic Publishers, pp. 277–294.

Vauhkonen M., Kaipio J. P., Somersalo E. and Karjalainen P. A. (1997): *Electrical impedance tomography with basis constraints.* — Inverse Problems, Vol. 13, pp. 523–530.

Vidyasagar M. (1997): *A Theory of Learning and Generalization with Applications to Neural Networks and Control Systems.* — London: Springer-Verlag.

Vidyasagar M. (1998): *Statistical Learning Theory and Randomized Algorithms for Control.* — IEEE Control Systems, Vol. 18, No. 6, pp. 69–85.

Vidyasagar M. (2001): *Randomized algorithms for robust controller synthesis using statistical learning theory.* — Automatica, Vol. 37, pp. 1515–1528.

Visual Numerics (1997): *IMSL: Fortran Subroutines for Mathematical Applications.* — Visual Numerics. (printed on CD-ROM)

Walter É. and Pronzato L. (1987): *Robust Experiment Design: Between Qualitative and Quantitative Identifiabilities.* — in É. Walter (ed.), Identifiability of Parametric Models, Oxford: Pergamon Press, pp. 104–113.

Walter É. and Pronzato L. (1990): *Qualitative and Quantitative Experiment Design for Phenomenological Models—A Survey.* — Automatica, Vol. 26, No. 2, pp. 195–213.

Walter É. and Pronzato L. (1997): *Identification of Parametric Models from Experimental Data.* — Communications and Control Engineering, Berlin: Springer-Verlag.

West R. M., Jia X. and Williams R. A. (2000): *Parametric modelling in industrial process tomography.* — Chemical Engineering Journal, Vol. 77, pp. 31–36.

Williams R. A. and Beck M. S. (1995): *Process Tomography: Principles, Techniques, and Applications.* — Oxford: Butterworth-Heinemann.

Yin G. and Fitzpatrick B. G. (1992): *On Invariance Principles for Distributed Parameter Identification Algorithms.* — Informatica, Vol. 3, No. 1, pp. 98–118.

Zlatev Z. (1995): *Computer Treatment of Large Air Pollution Models.* — Dordrecht: Kluwer Academic Publishers.

Zwart H. and Bontsema J. (1997): *An Application-Driven Guide through Infinite-Dimensional Systems Theory.* — in G. Bastin and M. Gevers (eds), European Control Conference 1997: Plenaries and Mini-Courses, Ottignies/Louvain-la-Neuve: CIACO, pp. 289–328.