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Measurement Optimization for Parameter Estimation in Distributed Systems

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Contents

List of symbols

$\mathbb{N}$	set of natural numbers
A^n	given a set A, it is the Cartesian product $\underbrace{A \times \cdots \times A}_{n \text{ times}}$
$\mathbb{R}^n$	finite-dimensional Euclidean space
t_f	total time of the observation process
t	time
Ω	simply-connected, open and bounded subset of $\mathbb{R}^n$
$x = (x_1, \ldots, x_n)$	point of Ω
$\Gamma \equiv \partial\Omega$	boundary of Ω
$\bar{\Omega}$	$\Omega \cup \partial\Omega$
Q	space-time domain $\Omega \times]0, t_f[$
$F \circ G$	composition of mappings F and G
$F \mid A$	restriction of a mapping $F : X \to Y$ to a subset $A \subset X$, i.e. the mapping $F \circ j$, where $j : A \ni x \mapsto x \in X$ is the canonical injection of A into X
ℓ_n^p	$\mathbb{R}^n$ endowed with the norm $\|x\|_{\ell_n^p} = \left(\sum_{i=1}^{n} \|x_i\|^p \right)^{1/p}$

ℓ_n^∞ — $\mathbb{R}^n$ endowed with the norm $\|x\|_{\ell_n^\infty} = \max\limits_{1\le i\le n} |x_i|$

$C(\bar\Omega)$ — class of all continuous real-valued functions on $\bar\Omega$

$C^1(\bar\Omega)$ — class of all continuously differentiable functions on $\bar\Omega$

$C^{2,1}(\bar Q)$ — class of all the functions f continuous on $\bar Q$ together with the derivatives $\partial f/\partial t$, $\partial f/\partial x_i$, $\partial^2 f/\partial x_i \partial x_j$, $1 \le i, j \le n$

$L^p(\Omega)$ — space of classes of measurable functions f on Ω such that $\int_\Omega |f(x)|^p \,\mathrm{d}x < \infty$; this is a Banach space for the norm

$$\|f\|_{L^p(\Omega)} = \left\{ \int_\Omega |f(x)|^p \,\mathrm{d}x \right\}^{1/p}$$

$L^\infty(\Omega)$ — space of classes of measurable functions f on Ω such that $x \mapsto |f(x)|$ is essentially bounded, i.e. $\exists\, C < \infty$, $|f(x)| \le C$ a.e. in Ω; this is a Banach space for the norm

$$\begin{aligned} \|f\|_{L^\infty(\Omega)} &= \operatorname*{ess\,sup}_{x\in\Omega} |f(x)| \\ &= \inf\big\{ C : |f(x)| \le C \text{ a.e. in } \Omega \big\} \end{aligned}$$

$\mathcal{L}(X, Y)$ — set of all bounded linear operators from X to Y; if X and Y are both Banach spaces, then so is $\mathcal{L}(X, Y)$, endowed with norm

$$\|A\|_{\mathcal{L}(X,Y)} = \sup_{x\neq 0} \frac{\|Ax\|_Y}{\|x\|_X}$$

$\mathcal{L}(X)$ — $\mathcal{L}(X, X)$

X' — dual space of X, i.e. $\mathcal{L}(X, \mathbb{R})$

$\operatorname{supp} f$ — support of f

$\partial^\alpha f$ — for a multi-index $\alpha = (\alpha_1, \dots, \alpha_n) \in \mathbb{N}^n$ it is equal to $\partial^{|\alpha|} f / \partial x_1^{\alpha_1} \dots \partial x_n^{\alpha_n}$, where $|\alpha| = \alpha_1 + \cdots + \alpha_n$

$\mathcal{D}(\Omega)$ space of smooth (i.e. infinitely differentiable) functions which have compact support in Ω; a sequence $\{\varphi_m\}$ of $\mathcal{D}(\Omega)$ tends to φ in $\mathcal{D}(\Omega)$ if

(i) $\bigcup_m \operatorname{supp}\varphi_m \subset K \subset \Omega$, where K is compact

(ii) for each $\alpha \in \mathbb{N}^n$, $\partial^\alpha \varphi_m$ tends uniformly to $\partial^\alpha \varphi$

$\mathcal{D}'(\Omega)$ space of distributions on Ω, i.e. the set of 'continuous' linear forms on $\mathcal{D}(\Omega)$: if T is a distribution on Ω and if $\langle T, \varphi\rangle$ stands for the pairing between $\mathcal{D}'(\Omega)$ and $\mathcal{D}(\Omega)$, then for every sequence $\{\varphi_m\}_{m=1}^{\infty}$ converging to φ in $\mathcal{D}(\Omega)$, $\langle T, \varphi_m\rangle$ tends to $\langle T, \varphi\rangle$

$H^1(\Omega)$ first-order Sobolev space, i.e. the set $\{f \in L^2(\Omega) : \partial f/\partial x_i \in L^2(\Omega),\ 1 \le i \le n\}$; this is a Hilbert space with scalar product

$$(f,g)_{H^1(\Omega)} = \int_\Omega \left(fg + \sum_{i=1}^{n} \frac{\partial f}{\partial x_i}\frac{\partial g}{\partial x_i} \right) \mathrm{d}x$$

$H^2(\Omega)$ second-order Sobolev space, i.e. the set $\{f \in L^2(\Omega) : \partial f/\partial x_i,\ \partial^2 f/\partial x_i \partial x_j \in L^2(\Omega),\ 1 \le i, j \le n\}$; this is a Hilbert space with scalar product

$$(f,g)_{H^2(\Omega)} = \int_\Omega \Big\{ \sum_{|\alpha|\le 2} \partial^\alpha f\, \partial^\alpha g \Big\} \mathrm{d}x$$

$H_0^1(\Omega)$ closure of $\mathcal{D}(\Omega)$ in the space $H^1(\Omega)$; for domains with Lipschitz boundaries it may be concluded that $H_0^1(\Omega) = \{v \in H^1(\Omega) : v\big|_\Gamma = 0\}$

$H^{-1}(\Omega)$ dual space of $H_0^1(\Omega)$, i.e. $H^{-1}(\Omega) = \mathcal{L}(H_0^1(\Omega), \mathbb{R})$; this is a Hilbert space with norm

$$\|F\|_{H^{-1}(\Omega)} = \sup_{0 \ne f \in H_0^1(\Omega)} \frac{|\langle F, f\rangle|}{\|f\|}$$

$L^2(0, t_f; X)$ space of classes of functions f from $]0, t_f[$ to a Banach space X such that f is measurable with respect to the Lebesgue measure and

$$\|f\|_{L^2(0,t_f;X)} = \left(\int_0^{t_f} \|f(t)\|_X^2 \, \mathrm{d}t \right)^{1/2} < \infty$$

$C([0, t_f]; X)$ space of all those functions which are continuous from $[0, t_f]$ to a Banach space X; this is a Banach space endowed with norm

$$\|f\|_{C([0,t_f];X)} = \sup_{t \in [0,t_f]} \|f(t)\|_X$$

A note on abbreviations

LPS	lumped parameter system
DPS	distributed parameter system
ODE	ordinary differential equation
PDE	partial differential equation
FIM	Fisher information matrix
OSL	optimal sensor location
SLI	OSL for system identification
SLE	OSL for state estimation

Preface

It is well-understood that the choice of experimental conditions for distributed systems has a significant bearing upon the accuracy achievable in parameter-estimation experiments. Since for such systems it is impossible to observe their states over the entire spatial domain, close attention has been paid to the problem of optimally locating discrete sensors to estimate the unknown parameters as accurately as possible. Such an optimal sensor location problem has been widely investigated by many authors since the beginning of the 1970s (for surveys, see Kubrusly and Malebranche, 1985; Rafajłowicz, 1986b; Uciński, 1992; Korbicz and Uciński, 1994; Uciński, 1999a), but the existing methods are either restricted to one-dimensional spatial domains for which some theoretical results can be obtained for idealized linear models, or onerous, not only discouraging interactive use but also requiring a large investment in software development. The potential systematic approaches could be of significance, e.g. for environmental monitoring, meteorology, surveillance, hydrology and some industrial experiments, which are typical exemplary areas where we are faced with the sensor location problem, especially owing to serious limitations on the number of costly sensors.

This was originally the main motivation to pursue the laborious research detailed in this monograph. My efforts on optimum experimental design for distributed-parameter systems began some ten years ago at a time when rapid advances in computing capabilities and availability held promise for significant progress in the development of a practically useful as well as theoretically sound methodology for such problems. At present, even low-cost personal computers allow us to solve rather routinely certain computational problems which would have been out of the question several years ago.

The aim of this monograph is to give an account of both classical and recent work on sensor placement for parameter estimation in dynamic distributed systems modelled by partial differential equations. We focus our

attention on using real-valued functions of the Fisher information matrix of parameters as the performance index to be minimized with respect to the positions of pointwise sensors. Particular emphasis is placed on determining the 'best' way to guide moving sensors and making the solutions independent of the parameters to be identified. The bulk of the material in the corresponding chapters is taken from a collection of my original research papers. My main objective has been to produce useful results which can be easily translated into computer programmes.

The study of this subject is at the interface of the following fields:

- optimum experimental design,
- partial differential equations,
- non-linear programming,
- optimal control,
- stochastic processes, and
- numerical methods.

Consequently, in order to give the reader a clear image of the proposed approach, the adopted strategy is to indicate direct arguments in relevant cases which preserve the essential features of the general situation, but avoid many technicalities.

This book is organized as follows. In Chapter 1, a brief summary of concrete applications involving the sensor location problem is given. Some of these examples are used throughout the monograph to motivate and illustrate the demonstrated developments. A concise general review of the existing literature and a classification of methods for optimal sensor location are presented. Chapter 2 provides a detailed exposition of the measurement problem to be discussed in the remainder of the book and expounds the main complications which make this problem difficult. In Chapter 3 our main results for stationary sensors are stated and proved. Their extensions to the case of moving internal observations are reported in Chapter 4. A more realistic situation with non-negligible dynamics of the vehicles conveying the sensors and various restrictions imposed on their motions is also studied therein and the whole problem is then formulated as a state-constrained optimal-control problem. Chapter 5 establishes some methods to overcome the difficulties related to the dependence of the optimal solutions on the

parameters to be identified. Finally, some concluding remarks are made in Chapter 6.

It is a pleasure to express my sincere thanks to a number of people:

- Professor Józef Korbicz for suggesting the problem and for his continuous support and advice,
- Professor Ewaryst Rafajłowicz, whose works introduced me to the field of experimental design for distributed-parameter systems, for many valuable suggestions, and
- Professor Abdelhaq El Jai for his active interest in the publication of this monograph.

In addition, I wish to express my gratitude to all my colleagues and friends who have helped me in many, many ways over the years.

D. Uciński

Chapter 1

Introduction

1.1 The optimum experimental design problem in context

Distributed-parameter systems (DPS's) are dynamical systems whose state depends not only on time but also on spatial coordinates. They are frequently encountered in practical engineering problems. Examples of a thermal nature are furnaces for heating metal slabs or heat exchangers, examples of a mechanical nature are large flexible antennas, aircrafts and robot arms, examples of an electrical nature are energy transmission lines.

Appropriate mathematical modelling of DPS's yields most often partial differential equations (PDE's), but descriptions by integral equations or integro-differential equations can sometimes be considered. Clearly, such models involve using very sophisticated mathematical methods, but in recompense for this effort we are in a position to describe the process more accurately and to implement more effective control strategies. Early lumping, which means approximation of a PDE by ordinary differential equations of possibly high order, may completely mask the distributed nature of the system and therefore is not always satisfactory.

For the past thirty years DPS's have occupied an important place in control and systems theory. This position has grown in relevance due to the ever-expanding classes of engineering systems which are distributed in nature, and for which estimation and control are desired. DPS's, or more generally, infinite-dimensional systems are now an established area of research with a long list of journal articles, conference proceedings and several textbooks to its credit (Curtain and Zwart, 1995; Klamka, 1991; Mitkowski, 1991; Lasiecka and Triggiani, 2000; Grabowski, 1999; Kowalewski, 1991;

Sokołowski and Zolesio, 1992; Emirsajłow, 1991; Malanowski *et al.*, 1996; El Jai and Amouroux, 1990; Zwart and Bontsema, 1997; Omatu and Seinfeld, 1989; Korbicz and Zgurowski, 1991). What is more, the field of potential applications could hardly be considered come to an end (Banks *et al.*, 1996; Lasiecka, 1998; Uciński and El Jai, 1997; Uciński and El Yacoubi, 1998; Uciński and El Yacoubi, 1999).

One of the basic and most important questions in DPS's is parameter estimation which refers to the determination from observed data of unknown parameters in the system model such that the predicted response of the model is close, in some well-defined sense, to the process observations (Omatu and Seinfeld, 1989). The parameter estimation problem is also referred to as the parameter identification or simply the inverse problem (Isakov, 1998). There are many areas of technological importance in which identification problems are of crucial significance. The importance of inverse problems in the petroleum industry, for example, is well-documented (Ewing and George, 1984; Korbicz and Zgurowski, 1991). One class of such problems involves determination of the porosity (the ratio of pore volume to total volume) and permeability (a parameter measuring the ease with which the fluids flow through the porous medium) of a petroleum reservoir based on field production data. Another class of inverse problems of interest in a variety of areas is to determine the elastic properties of an inhomogeneous medium from observations of reflections of waves travelling through the medium. The literature on the subject of DPS identification is considerable. Kubrusly (1977) and Polis (1982) have surveyed the field by systematically classifying the various techniques. A more recent book by Banks and Kunisch (1989) is an attempt to present a thorough and unifying account of a broad class of identification techniques for DPS models, also see (Banks, 1992; Uciński and Korbicz, 1990).

In order to identify the unknown parameters (in other words, to calibrate the considered model), the system's behaviour or response is observed with the aid of some suitable collection of sensors termed the measurement or observation system. In many industrial processes the nature of state variables does not allow much flexibility as to which they can be measured. For variables which can be measured on-line, it is usually possible to make the measurements continuously in time. However, it is generally impossible to measure process states over the entire spatial domain. For example (Phillipson, 1971), the temperature of molten glass flowing slowly in a forehearth is described by a linear parabolic PDE, whereas the displacements occasioned by dynamic loading on a slender airframe can be described

by linear second-order hyperbolic PDE's. In the former example, temperature measurements are available at selected points along the spatial domain (obtained by a pyrometer or some other device), whereas, in the latter case, strain gauge measurements at selected points on the airframe are reduced to yield the deflection data. In both the cases the measurements are incomplete in the sense that the entire spatial profile is not available. Moreover, the measurements are inexact by virtue of inherent errors of measurement associated with transducing elements and also because of the measurement environment.

The inability to take distributed measurements of process states leads to the question where to locate sensors so that the information content of the resulting signals with respect to the distributed state and PDE model be as high as possible. This is an appealing problem since in most applications these locations are not pre-specified and therefore provide design parameters. The location of sensors is not necessarily dictated by physical considerations or by intuition and, therefore, some systematic approaches should still be developed in order to reduce the cost of instrumentation and to increase the efficiency of identifiers.

As was already mentioned, the motivations to study the sensor location problem stem from practical engineering issues. Optimization of air quality monitoring networks is among the most interesting ones. As is well-known, due to traffic emissions, residential combustion and industry emissions, air pollution has become a big social problem. One of the tasks of environmental protection systems is to provide expected levels of pollutant concentrations. In case smog is expected, a local community can be warned and some measures can be taken to prevent or minimize the release of prescribed substances and to render such substances harmless. But to produce such a forecast, a smog prediction model is necessary (Sydow *et al.*, 1997; Sydow *et al.*, 1998; van Loon, 1994; Holnicki *et al.*, 1986), which is usually chosen in the form of an advection-diffusion PDE. Its calibration requires parameter estimation (e.g. the unknown spatially-varying turbulent diffusivity tensor should be identfied based on the measurements from monitoring stations (Omatu and Matumoto, 1991b; Omatu and Matumoto, 1991a)). Since measurement transducers are usually rather costly and their number is limited, we are inevitably faced with the problem of how to optimize their locations in order to obtain the most precise model. A need for the appropriate strategies of optimally allocating monitoring stations is constantly indicated in the works which report the implementations of systems to perform air quality management (Andó *et al.*, 1999; van Loon, 1995; Sturm

et al., 1994; Nychka *et al.*, 1998; Müller, 1998). Of course, some approaches have already been advanced (Müller, 1998; Fedorov, 1996). Due to both the complexity of urban and industrial areas and the influence of meteorological quantities, the suggested techniques are not easy to apply and further research effort is required.

Another stimulating application concerns groundwater modelling employed in the study of groundwater resources management, seawater intrusion, aquifer remediation, etc. To build a model for a real groundwater system, some observations of state variables such as the head and concentration are needed. But the cost of experiments is usually very high, which results in many efforts regarding e.g. optimizing the decisions on the state variables to be observed, the number and location of observation wells, and the observation frequency (see (Sun, 1994) and references given therein). Besides, it is easy to imagine that similar problems appear e.g. in the recovery of valuable minerals and hydrocarbon from underground permeable reservoirs (Ewing and George, 1984), in gathering measurement data for calibration of mathematical models used in meteorology and oceanography (Navon, n.d.; Malanotte-Rizzoli, 1996; Bennett, 1992; Daley, 1991; Hogg, 1996), in automated inspection in static and active environments, or in hazardous environments where trial-and-error sensor planning cannot be used (e.g. in nuclear power plants (Korbicz and Zgurowski, 1991; Korbicz *et al.*, 1993)), or, in recent years, in emerging smart material systems (Banks *et al.*, 1996; Lasiecka, 1998).

1.2 A general review of literature

In general, the following main strategies of taking measurements can be distunguished:

- locating a given number of stationary sensors,
- using moving sensors, and
- scanning, i.e. only a part of a given total number of stationary sensors take measurements at a given time moment.

As a matter of fact, every real measuring transducer averages the measured quantity over some portion of the spatial domain. In most applicatons, however, this averaging is approximated by assuming that pointwise measurements are available at a number of spatial locations. Otherwise, the

problem of finding an optimal geometry of the sensor support can be formulated (El Jai, 1991).

Trying to implement the above-mentioned techniques, we are faced with the corresponding problems:

- How to determine an optimal sensor placement in a given admissible spatial domain?
- How to design optimal sensor trajectories?
- How to select the best subset of all available sensors to take measurements at given time moments?

Additionally, in all cases we should also address the question of a minimal number of sensors which will guarantee sufficient accuracy of the estimates.

The literature on optimal sensor location in DPS's is plentiful, but the bulk of works deal with state estimation, see (Kubrusly and Malebranche, 1985; El Jai and Pritchard, 1988; Amouroux and Babary, 1988; El Jai and Amouroux, 1987) for surveys of the state-of-the-art in the mid 1980s or more recent overviews (El Jai, 1991; Korbicz and Uciński, 1994; Uciński, 1999a). There have been considerably fewer works on this subject related to parameter identification. This is mainly because a direct extension of the appropriate results from state estimation is not straightforward and has not been pursued. That problem is essentially different from the optimal measurement problem for parameter identification, since in the latter case the current state usually depends strongly non-linearly on unknown parameters (Korbicz and Uciński, 1994), even though the PDE is linear in these parameters, while the dependence of the current state on the initial one is linear for linear systems, which makes state estimation easier.

The existing methods of sensor location for parameter identification can be gathered in three major groups:

1. Methods leading to state estimation,
2. Methods employing random fields analysis, and
3. Methods using optimum experimental design theory.

Group 1 brings together some attempts to transform the problem into a state-estimation one (by augmenting the state vector) and then to use well-developed methods of optimal sensor location for state estimation. However, since the state and parameter estimation are to be carried out simultaneously, the whole problem becomes strongly non-linear. To overcome

this difficulty, a sequence of linearizations at consecutive state trajectories was performed by Malebranche (1988) and a special suboptimal filtering algorithm was used by Korbicz *et al.* (1988). Nevertheless, the viability of this approach is rather questionable owing to the well-known severe difficulties inherent in non-linear state estimation.

The methods of Group 2 are based on random fields theory. Since DPS's are described by PDE's, direct application of that theory is impossible, and therefore this description should be replaced by characteristics of a random field, e.g. mean and covariance functions. Such a method for a beam vibrating due to the action of a stochastic loading was considered by Kazimierczyk (1989) who made extensive use of optimum experimental design for random fields (Brimkulov *et al.*, 1986). Although the flexibility of this approach seems rather limited, it can be useful in some case studies (see e.g. Sun, 1994).

The methods belonging to major Group 3 originate from the classical theory of optimum experimental design (Kiefer and Wolfowitz, 1959; Fedorov, 1972; Fedorov and Hackl, 1997; Pázman, 1986; Pukelsheim, 1993; Ermakov, 1983; Rafajłowicz, 1996; Walter and Pronzato, 1997) and its extensions to models for dynamic systems, especially in the context of the optimal choice of sampling instants and input signals (Mehra, 1974; Mehra, 1976; Goodwin and Payne, 1977; Titterington, 1980; Kalaba and Spingarn, 1982; Królikowski and Eykhoff, 1985; Walter and Pronzato, 1997). Consequently, the adopted optimization criteria are essentially the same, i.e. various scalar measures of performance based on the Fisher information matrix (FIM) associated with the parameters to be identified are minimized. The underlying idea is to express the goodness of parameter estimates in terms of the covariance matrix of the estimates. For sensor location purposes, one assumes that an unbiased and efficient (or minimum-variance) estimator is employed so that the optimal sensor placement can be determined independently of the estimator used. This leads to a great simplification since the Cramér-Rao lower bound for the afore-mentioned covariance matrix is merely the inverse of the FIM, which can be computed with relative ease, even though the exact covariance matrix of a particular estimator is very difficult to obtain.

There is a fundamental complication in the application of the resulting optimal location strategies and that is the dependence of the optimal solutions on the parameters to be identified. It seems that we have to know their true values in order to calculate an optimal sensor configuration for estimating them. As a result, practically all the works in context are based

on the assumption of *a-priori* estimates for the true parameters.

As regards dynamic DPS's, the first treatment in this spirit for the sensor location problem was proposed by Quereshi *et al.* (1980). Their approach was based on maximization of the determinant of the FIM and examples regarding a damped vibrating string and a heat-diffusion process were used to illustrate the advantages and peculiarities of the method. Besides sensor location, the determination of boundary perturbations was also considered. In order to avoid computational difficulties, sinusoidal excitations were assumed and the position of a single sensor was optimized.

The same optimality criterion was used by Rafajłowicz (1978) in order to optimize both sensor positions and a distributed control for parameter estimation of a static linear DPS. Reduction of the problem to a form, where results of the classical theory of optimum experimental design can be applied, was accomplished after eigenfunction expansion of the solution to the PDE considered and subsequent truncation of the resulting infinite series. Consequently, the FIM was associated with system eigenvalues, rather than with the system parameters. A separation principle was proved which allows the possibility of finding an optimal control and an optimal sensor configuration independently of each other. The delineated approach was generalized in (Rafajłowicz, 1981) to a class of DPS's described by linear hyperbolic equations with known eigenfunctions and unknown eigenvalues. The aim was to find conditions for optimality of measurement design and of optimal spectral density of the stochastic input. It was indicated that common numerical procedures from classical experimental design for linear regression models could be adopted to find optimal sensor location. Moreover, the demonstrated optimality conditions imply that the optimal input comprises a finite number of sinusoidal signals and that optimal sensor positions are not difficult to find in some cases. A similar problem was studied in (Rafajłowicz, 1983) in a more general framework of DPS's which can be described in terms of Green's functions.

The idea of generalizing methods of optimum experimental design for parameter identification of lumped systems was also applied to solve the optimal measurement problem for moving sensors (Rafajłowicz, 1986c). The approach was based on looking for a time-dependent measure, rather than for the trajectories themselves. Various sufficient optimality conditions were presented, among others the so-called *quasi-maximum principle*. In spite of their somewhat abstract forms, they made it possible to solve relatively easily a number of non-trivial examples. The problem of moving sensors in DPS's was also revisited in (Rafajłowicz, 1988; Rafajłowicz, 1989a), but

without direct reference to parameter estimation.

As regards other works by the same author which pertain to the optimal measurement problem for DPS's, let us also mention (Rafajłowicz, 1987) where the notion of equi-informative sensor-actuator configurations in the sense of the coincidence of the corresponding FIM's was introduced and studied for a class of static DPS's, and (Rafajłowicz, 1995) where a sensor allocation was sought so as to maximize the identification accuracy for the mean values of random pointwise inputs to a static DPS described by Green's function. In turn, optimization of input signals for a fixed sensor configuration was exhaustively treated by Rafajłowicz (1984; 1986a; 1986b; 1989b; 1990) and Rafajłowicz and Myszka (1986).

The approach based on maximization of the determinant of the appropriate FIM is not restricted to theoretical considerations and there are examples which do confirm its effectiveness in practical applications. Thus, in (Munack, 1984) a given number of stationary sensors were optimally located using non-linear programming techniques for a biotechnological system consisting of a bubble column loop fermenter. On the other hand, Sun (1994) advocates using optimum experimental design techniques to solve inverse problems in groundwater modelling. How to monitor the water quality around a landfill place is an example of such a network design. Sun's monograph constitutes an excellent introductory text to applied experimental design for DPS's, as it covers a broad range of issues motivated by engineering problems. Non-linear programming techniques are also used there to find numerical approximations to the respective exact solutions.

A similar approach was used by Kammer (1990; 1992) for on-orbit modal identification of large space structures. Although the respective models are not PDE's, but their discretized versions obtained through the finite-element method, the proposed solutions can still be of interest owing to the striking similitude of both the formulations. A fast and efficient approach was delineated for reducing a relatively large initial candidate sensor location set to a much smaller optimum set which retains the linear independence of the target modes and maintains the determinant of the FIM resulting in improved modal response estimates.

A related optimality criterion was given in (Point *et al.*, 1996) by the maximization of the Gram determinant which is a measure of the independence of the sensitivity functions evaluated at sensor locations. The authors argue that such a procedure guarantees that the parameters are identifiable and the correlation between the sensor outputs is minimized. The form of the criterion itself resembles the D-optimality criterion pro-

posed by Quereshi *et al.* and Rafajłowicz, but the counterpart of the FIM takes on much larger dimensions, which suggests that the approach involves more cumbersome calculations. The delineated technique was successfully applied to a laboratory-scale catalytic fixed-bed reactor (Vande Wouwer *et al.*, 1999).

In summary, this brief review of the state-of-the-art in the sensor location problem indicates that, as was already emphasized by Kubrusly and Malebranche (1985), more attention should be paid to the problem of sensor allocation for parameter identification of DPS's, as from an engineering point of view the use of the existing scarce methods is restricted owing to computational and/or realizing difficulties. Few works have appeared about the results regarding two- or three-dimensional spatial domains and spatially-varying parameters. Thus, some generalizations are still expected in this connection. Furthermore, most of the contributions deal with stationary sensors. On the other hand, the optimal measurement problem for spatially movable sensors seems to be very attractive from the viewpoint of the degree of optimality and should receive more attention. Similarly, the dependence of the solutions on the values assumed for the unknown parameters to be identified should be addressed with greater care, as this limitation of the existing methods seems to be one of the main impediments to persuade engineers to apply these methods in practice.

This monograph constitutes an attempt to systematize the existing approaches to the sensor location problem and to meet the above-mentioned needs created by practical applications through the development of new techniques and algorithms or adopting methods which have been successful in akin fields of optimum experimental design. It is an outgrowth of original research papers and some results which have not been published yet. We believe that the approach outlined here has significant practical and theoretical advantages which will make it, with sufficient development, a versatile tool in numerous sensor location problems encountered in engineering practice.

Chapter 2

Parameter identification and sensor location: Basic concepts

2.1 System description

In this section, we introduce the class of systems to be considered. Let Ω be a bounded simply-connected open domain of a d-dimensional Euclidean space $\mathbb{R}^d$ with sufficiently smooth boundary $\partial\Omega$. Since the results outlined in this monograph are strongly motivated by two-dimensional situations, the explicit formulae will be written down for $d = 2$, but bear in mind that they can easily be generalized to $d = 3$ or limited to $d = 1$. Accordingly, the spatial coordinate vector will be denoted by $x = (x_1, x_2) \in \bar{\Omega} = \Omega \cup \partial\Omega$. As our fundamental state system we consider the scalar (possibly non-linear) distributed-parameter system described by a partial differential equation of the form

$$\frac{\partial y}{\partial t} = \mathcal{F}\left(x, t, y, \frac{\partial y}{\partial x_1}, \frac{\partial y}{\partial x_2}, \frac{\partial^2 y}{\partial x_1^2}, \frac{\partial^2 y}{\partial x_2^2}, \theta\right), \quad x \in \Omega, \quad t \in T \tag{2.1}$$

where t stands for time, $T = (0, t_f)$, $y = y(x, t)$ denotes the state variable with values in $\mathbb{R}$ and $\mathcal{F}$ is some known function which may include terms accounting for given *a-priori* forcing inputs. The system evolves from $t = 0$ to $t = t_f < \infty$, the period over which observations are available.

Equation (2.1) is accompanied by the boundary condition of the general form

$$\mathcal{E}\left(x, t, y, \frac{\partial y}{\partial x_1}, \frac{\partial y}{\partial x_2}, \theta\right) = 0, \quad x \in \partial\Omega, \quad t \in T \tag{2.2}$$

and the initial condition

$$y(x,0) = y_0(x), \quad x \in \Omega \tag{2.3}$$

where $\mathcal{E}$ and y_0 denote some known functions.

We assume the existence of a unique solution to (2.1)–(2.3), which is sufficiently regular. The system model above contains an unknown parameter vector denoted by θ (note that it may also appear in the boundary conditions), which is assumed to belong to a parameter space Θ. The possible forms of Θ are (Omatu and Seinfeld, 1989):

1. Constant parameters

$$\Theta_1 = \left\{\theta = (\theta_1, \theta_2, \ldots, \theta_m) \in \mathbb{R}^m\right\}$$

2. Assumed functional form, i.e. some or all components of θ are assumed to have known functional forms which themselves contain unknown parameters. Thus,

$$\theta = \theta(x,t,y) = g(x,t,y,\theta_1,\theta_2,\ldots,\theta_m)$$

where θ_i, $i = 1,\ldots,m$ are unknown constants and the functional form of each component of g is assumed to be known:

$$\Theta_2 = \left\{\theta = (\theta_1, \theta_2, \ldots, \theta_m) \in \mathbb{R}^m\right\}$$

3. General functions of space x, and/or time t, and/or the state y, i.e.

$$\Theta_3 = \{\theta = (\theta_1(x,t,y), \ldots, \theta_m(x,t,y))\}$$

where the parameter space in this case is infinite-dimensional.

From a practical point of view, Case 2 does not differ in anything from Case 1, and Case 3 must be approximated eventually by a finite-dimensional space to obtain numerical results (within certain limitations discussed on p. 16), so in what follows we will focus our attention on Case 1, which is also a common procedure in the literature.

Example 2.1. A chief aim of the intensive studies on the atmospheric aspects of air pollution is to be able to describe mathematically the spatio-temporal distribution of contaminants released into the atmosphere. The phenomenon of pollutant advection and diffusion over a spatial domain Ω

containing an urban region is governed by the equation (Holnicki *et al.*, 1986)

$$\frac{\partial y}{\partial t} = -v_1 \frac{\partial y}{\partial x_1} - v_2 \frac{\partial y}{\partial x_2} + \kappa \left(\frac{\partial^2 y}{\partial x_1^2} + \frac{\partial^2 y}{\partial x_2^2} \right) - \gamma y + \frac{1}{H}(E - \sigma y) + Q \quad \text{in } \Omega \times T$$

subject to the boundary condition

$$\begin{aligned} \frac{\partial y}{\partial n}(x,t) &= 0 \quad \text{on } \partial\Omega \times T \text{ for } \langle v, n \rangle \geq 0 \\ y(x,t) &= 0 \quad \text{on } \partial\Omega \times T \text{ for } \langle v, n \rangle < 0 \end{aligned}$$

and the initial condition

$$y(x,0) = y_0 \quad \text{in } \Omega$$

where $y = y(x,t)$ denotes the pollutant concentration, $v_i = v_i(x,t)$, $i = 1,2$ stand respectively for the x_1 and x_2 directional wind velocities, $v = (v_1, v_2)$, $Q = Q(x,t)$ signifies the intensity of the pointwise emission sources, all these quantities being averaged in the vertical direction over the mixing layer whose height is H. The term $E - \sigma y$ represents the ground-level stream of the pollutant, where $E = E(x,t)$ is the intensity of the area emission and σ denotes the dry deposition coefficient. Furthermore, κ is the horizontal diffusion coefficient and γ is the wet deposition factor which usually depends on the precipitation intensity. Here the notation $\partial y/\partial n$ means the partial derivative of y with respect to the outward normal of $\partial\Omega$, n, and $\langle \cdot, \cdot \rangle$ is used to denote the scalar product of ordinary vectors.

Some parameters which appear as coefficients in this model are known or can be obtained from direct observations (e.g. the wind field v is usually available from weather forecasting centres), but the others cannot be measured (e.g. the diffusivity κ, cf. Omatu and Matumoto, 1991b; Omatu and Matumoto, 1991a) and consequently they constitute components of the vector θ introduced above. Due to spatial changes in environmental conditions, it is highly likely that the unknown parameters will also be spatially varying. Their precise determination is essential to the process of accurately simulating and predicting the spatial distribution of air pollutant concentrations. ♢

The objective of parameter estimation is to choose a parameter $\theta^\star$ in Θ so that the solution y to (2.1)–(2.3) corresponding to $\theta = \theta^\star$ agrees with

the 'true' observed state $\tilde{y}$. In general, however, measurements of the state may not be possible, rather only measurements for some observable part of the actual state $\tilde{y}$ may be available (Banks and Kunisch, 1989). This is related to the fact that there are several possible manners in which the measurements themselves are made. For example, measurements may be carried out (Chen and Seinfeld, 1975)

(M1) over the entire spatial domain continuously in time,

(M2) over the entire spatial domain at discrete points in time,

(M3) at discrete spatial locations continuously in time, or

(M4) at discrete spatial locations at discrete points in time.

Manners (M1) and (M2) are considered to be of little significance, since it is generally not possible to carry out measurements over the entire domain of the system. Some authors adopt them notwithstanding and obtain 'distributed' measurements by an appropriate interpolation of the pointwise data (Kunisch, 1988; Lamm, 1987). Note, however, that recent technological advances in measuring instrumentation are very promising for this type of observation (e.g. thermography cameras used to continuously monitor manufacturing processes, scanning tunnelling microscopes for imaging solid surfaces, or scanning thermal conductivity microscopes capable of producing thermal conductivity maps of specimen surfaces with sub-micron resolution).

In contrast, measurements at discrete spatial locations are commonly encountered in engineering applications and, as a consequence, they dominate in the literature on parameter identification. Manner (M3) causes the problem of choosing the spatial locations and Manner (M4) involves a choice of both spatial locations and measurement timing. If measurements can only be made intermittently, the time interval between measurements is usually determined by the time requirements of the analytical procedure. If the meaurements are not costly, then one will take data as frequently as possible. As long as the timing of measurements is not a decision variable, Manners (M3) and (M4) are basically equivalent. Thus we focus here on Manner (M3) only. Based on the developed ideas, it is a simple matter to procure the corresponding results for Manner (M4).

Consequently, it is further assumed that the observation process is described by the equation of the form

$$z(t) = y_{\mathrm{m}}(t) + \varepsilon_{\mathrm{m}}(t), \quad t \in T \tag{2.4}$$

where

$$y_{\mathrm{m}}(t) = \mathrm{col}[y(x^1,t),\dots,y(x^N,t)]$$
$$\varepsilon_{\mathrm{m}}(t) = \mathrm{col}[\varepsilon(x^1,t),\dots,\varepsilon(x^N,t)]$$

$z(t)$ is the N-dimensional observation vector, $x^j \in \bar{\Omega}$, $j = 1,\dots,N$ denote the pointwise and stationary sensor locations, and $\varepsilon = \varepsilon(x,t)$ is a white Gaussian noise process (a formal time derivative of a Wiener process) whose statistics are

$$\mathrm{E}\{\varepsilon(x,t)\} = 0, \quad \mathrm{E}\{\varepsilon(x,t)\varepsilon(x',t')\} = q(x,x',t)\delta(t-t') \tag{2.5}$$

δ being the Dirac delta function concentrated at the origin.

Note that pointwise sensors require a corresponding smoothness of solutions to (2.1)–(2.3). In fact, each solution y may be thought of as a collection of functions of space parametrized by time, $\{y(\cdot,t)\}_{t\in T}$. But a 'snapshot' $y(\cdot,t) \in L^2(\Omega)$ need not be continuous and it is therefore not meaningful to talk about its values at particular points. On the other hand, explicitly requiring $y(\cdot,t)$ to be continuous is not convenient, since $C(\bar{\Omega})$ is not a Hilbert space. Consequently, we must be careful in specifying the functional framework for our problem. For the rest of this book, we shall consider pointwise observations generally assuming that $\mathcal{F}$, $\mathcal{E}$ and the boundary $\partial\Omega$ are sufficiently regular to ensure the enclosure of outputs into $L^2(T;\mathbb{R}^N)$. Let us observe that this condition is met e.g. if $y \in L^2(T;H^2(\Omega))$, where $H^2(\Omega)$ is the second-order Sobolev space. In fact, from the Sobolev embedding theorem (Curtain and Pritchard, 1977, Th. 8.5, p. 141) it follows that $H^2(\Omega) \subset C(\bar{\Omega})$ with continuous injection provided that the dimension of Ω (i.e. d) is less than or equal to three. This means that there exists a constant $K \in (0,\infty)$ such that

$$\|v\|_{C(\bar{\Omega})} \le K\|v\|_{H^2(\Omega)}, \quad \forall v \in H^2(\Omega) \tag{2.6}$$

The result is

$$\begin{aligned}\|y_{\mathrm{m}}\|^2_{L^2(T;\mathbb{R}^N)} &= \int_T \|y_{\mathrm{m}}(t)\|^2_{\mathbb{R}^N}\,\mathrm{d}t \le N\int_T \|y(\cdot,t)\|^2_{C(\bar{\Omega})}\,\mathrm{d}t \\ &\le NK^2\int_T \|y(\cdot,t)\|^2_{H^2(\Omega)}\,\mathrm{d}t = NK^2\|y\|^2_{L^2(T;H^2(\Omega))}\end{aligned} \tag{2.7}$$

2.2 Parameter identification

Based on a collection of data $\{z(t)\}_{t\in T}$ which has been observed from our physical process, we wish to calibrate the model (2.1)–(2.3), i.e. to determine

a parameter vector $\hat{\theta}$ such that the predicted response of the model is close, in some well-defined sense, to the process observations. Such calibration is generally performed for one of the following objectives: 1) accurate determination of parameter values which may have some physical significance, such as specific heat and thermal conductivity of materials; 2) response prediction and forecasting; and 3) control system design. Mathematically, the problem is usually cast as an optimization one, which leads to the so-called *weighted least-squares* approach to parameter estimation in which we seek to minimize the output-error criterion (also called the fit-to-data criterion)

$$\mathcal{J}(\theta) = \frac{1}{2}\int_T \|z(t) - \hat{y}_{\mathrm{m}}(t;\theta)\|^2_{Q^{-1}(t)}\,\mathrm{d}t \tag{2.8}$$

where $Q(t) = \big[q(x^i, x^j, t)\big]_{i,j=1}^N \in \mathbb{R}^{N\times N}$ is assumed to be positive definite,

$$\|a\|^2_{Q^{-1}(t)} = a^{\mathrm{T}}Q^{-1}(t)a, \quad \forall\, a \in \mathbb{R}^N$$
$$\hat{y}_{\mathrm{m}}(t;\theta) = \mathrm{col}[\hat{y}(x^1, t;\theta), \ldots, \hat{y}(x^N, t;\theta)]$$

and $\hat{y}(\,\cdot\,,\,\cdot\,;\theta)$ stands for the solution to (2.1)–(2.3) corresponding to a given parameter θ.

A decided advantage of using (2.8) stems from the fact that the system model within which the unknown parameters are imbedded is a DPS is largely irrelevant and hence techniques for the estimation of parameters in lumped-parameter systems can be readily extended to the distributed-parameter case. Moreover, it can often be used effectively even if only a minimal data set is available. In turn, a disadvantage is that this criterion is almost never quadratic in the parameters and therefore the addressed optimization problem may be poorly conditioned (e.g. the surface plot of the criterion may be very flat). Another drawback to this approach manifests itself when the infinite-dimensional parameter space is replaced by a space of finite dimension. If the number of parameters is kept small, a well-behaved solution results. However, the modelling error introduced is significant, since the corresponding subspace of θ's is too restricted to provide a good approximation of an arbitrary θ. As the number of parameters is increased, on the other hand, numerical instabilities appear, manifested by spatial oscillations in the estimated θ, the frequency and amplitude of which are inconsistent with the expected smoothness of the true θ. Restoring a type of problem stability necessitates employing some regularization approaches (Lamm, 1987; Kunisch, 1988; Banks and Kunisch, 1989; Banks,

1992; Chavent, 1991; Kravaris and Seinfeld, 1985), which leads to an increased technical complexity. But in spite of these inconveniences, in actual fact (2.8) is commonly adopted as the first choice in parameter estimation problems. For some alternatives, the interested reader is referred to the comprehensive monographs (Banks and Kunisch, 1989; Banks *et al.*, 1996).

2.3 Measurement location problem

Clearly, the parameter estimate $\hat{\theta}$ resulting from minimization of the fit-to-data criterion depends on the sensor positions since one can observe the quantity z in the integrand on the right-hand side of (2.8). This fact suggests that we may attempt to select sensor locations which lead to best estimates of the system parameters. To form a basis for the comparison of different locations, a quantitative measure of the 'goodness' of particular locations is required. A logical approach is to choose a measure related to the expected accuracy of the parameter estimates to be obtained from the data collected. Such a measure is usually based on the concept of the *Fisher Information Matrix* (FIM) (Sun, 1994; Rafajłowicz, 1986c) which is widely used in optimum experimental design theory for lumped systems (Walter and Pronzato, 1997; Fedorov and Hackl, 1997). When the time horizon is large, the nonlinearity of the model with respect to its parameters is mild and the measurement errors are independently distributed and have small magnitudes, the inverse of the FIM constitutes an approximation of the covariance matrix for the estimate of θ (Walter and Pronzato, 1997; Fedorov and Hackl, 1997). Derivation of this fundamental property is centred on the use of the Cramér-Rao inequality[†] (Goodwin and Payne, 1977)

$$\operatorname{cov} \hat{\theta} \geq M^{-1} \tag{2.9}$$

as the starting point (here M is just the FIM), which requires the additional qualification that the estimator $\hat{\theta}$ is unbiased. Accordingly, it is sensible to assume that the estimator is *efficient* (minimum-variance) in the sense that the parameter covariance matrix achieves the lower bound, i.e. (2.9) becomes an equality, which is justified in many situations (Rafajłowicz, 1986b). This leads to a great simplification since the minimum variance given by the Cramér-Rao lower bound can be easily computed in a number of estimation problems, even though the exact covariance matrix of a particular estimator is very difficult to obtain.

[†] Recall that (2.9) should be interpreted in terms of the Loewner ordering of symmetric matrices, i.e. the matrix $\operatorname{cov} \hat{\theta} - M^{-1}$ is required to be non-negative definite.

It is customary to restrict investigations to spatial uncorrelated observations, i.e.

$$\mathrm{E}\{\varepsilon(x^i,t)\varepsilon(x^j,t')\} = \sigma^2\delta_{ij}\delta(t-t') \tag{2.10}$$

where δ_{ij} denotes the Kronecker delta function and $\sigma > 0$ is the standard deviation of the measurement noise. The reason obviously lies in the simplicity of a subsequent analysis. Such an assumption yields the following explicit form of the FIM (Quereshi *et al.*, 1980):

$$M = \frac{1}{\sigma^2}\sum_{j=1}^{N}\int_0^{t_f}\left(\frac{\partial y(x^j,t)}{\partial\theta}\right)^{\mathrm{T}}\left(\frac{\partial y(x^j,t)}{\partial\theta}\right)\mathrm{d}t \tag{2.11}$$

which is encountered in the bulk of the literature on sensor location. We shall also adopt this approach in the remainder of this chapter.

Clearly, the elements of M depend on the corresponding sensor positions. We shall emphasize this dependence setting

$$s = (x^1,\ldots,x^N) \in \mathbb{R}^{2N} \tag{2.12}$$

and writing here and subsequently $M = M(s)$.

Optimal sensor positions for system identification can be found by choosing the components of s so as to minimize some scalar measure of performance Ψ based on the FIM. Various choices exist for such a function (Walter and Pronzato, 1997; Fedorov and Hackl, 1997; Pukelsheim, 1993; Pázman, 1986), including e.g. the following:

- The D-optimality (determinant) criterion

$$\Psi(M) = -\log\det M \tag{2.13}$$

- The E-optimality criterion (smallest-eigenvalue; $\lambda_{\max}(\,\cdot\,)$ denotes the maximum eigenvalue of its argument)

$$\Psi(M) = \lambda_{\max}(M^{-1}) \tag{2.14}$$

- The A-optimality (trace) criterion

$$\Psi(M) = \operatorname{trace} M^{-1} \tag{2.15}$$

- The sensitivity criterion

$$\Psi(M) = -\operatorname{trace} M \tag{2.16}$$

A D-optimum design minimizes the volume of the uncertainty ellipsoid for the estimates. An E-optimum design minimizes the length of the largest axis of the same ellipsoid. An A-optimum design suppresses the average variance of the estimates. An important advantage of D-optimality is that it is invariant under scale changes in the parameters and linear transformations of the output, whereas A-optimality and E-optimality are affected by these transformations. The sensitivity criterion is often used due to its simplicity, but it sometimes leads to serious problems with identifiability as it may result in a singular FIM (Zarrop and Goodwin, 1975), so in principle it should be used only to obtain startup locations for one of the above criteria. The introduction of an optimality criterion renders it possible to formulate the sensor location problem as an optimization problem.

The above criteria are no doubt the most popular ones in modern experimental design theory, but they are by no means the only options. In fact, there is a plethora of other criteria which are labelled by other letters (some authors even speak of 'alphabetic' criteria (Fedorov and Hackl, 1997)). A rather general class of optimality criteria employs the following family of costs functions (Fedorov and Hackl, 1997; Walter and Pronzato, 1997):

$$\Psi_\gamma(M) = \begin{cases} \left[\dfrac{1}{m}\operatorname{trace}(PM^{-1}P^{\mathrm{T}})^\gamma\right]^{1/\gamma} & \text{if } \det M \neq 0 \\ \infty & \text{if } \det M = 0 \end{cases} \tag{2.17}$$

where $P \in \mathbb{R}^{m\times m}$ is a weighting matrix. For example, setting $P = I_m$ (the identity matrix), we obtain $\gamma = 1$, $\gamma \to \infty$ and $\gamma \to 0$ for the A-, E- and D-optimum design criteria, respectively.

Example 2.2. On order to illustrate the introduced ideas, consider a thin rod or wire whose lateral surface is impervious to heat (i.e. insulated). For modelling purposes, we assume the rod coincides with the x-axis from $x = 0$ to $x = 1$, is made of uniform material, and has a uniform cross-section. We know that the initial temperature of the rod is specified as $\sin(\pi x)$. The temperature distribution $y = y(x,t)$ at some later time in the absence of any heat source is then a solution to the one-dimensional heat equation

$$\frac{\partial y}{\partial t}(x,t) = \theta\frac{\partial^2 y}{\partial x^2}(x,t), \quad x \in (0,1),\ t \in (0,t_f) \tag{2.18}$$

and the prescribed initial condition

$$y(x,0) = \sin(\pi x), \quad x \in (0,1) \tag{2.19}$$

where θ stands for the diffusivity of the material forming the rod. The temperature inside the rod will also be affected by how the ends of the rod exchange heat energy with the surrounding medium. Suppose the two ends of the rod are at time $t = 0$ suddenly placed in contact with ice packs at $0°$ and that the temperature at the ends is maintained at all later times. This corresponds to the boundary conditions

$$y(0,t) = y(1,t) = 0, \quad t \in (0, t_f) \tag{2.20}$$

The model is specified up to the value of the diffusivity coefficient θ which is not known exactly. Assume that the temperature $y(x,t)$ can be measured continuously by one thermocouple and the measurements are described by

$$z(t) = y(x^1, t) + \varepsilon(t) \tag{2.21}$$

where the measurement noise ε is Gaussian and white with variance σ^2, and x^1 signifies the measurement location. It is desired to select an optimal sensor location x^1 so as to obtain a best estimate of θ. This is to be accomplished prior to the experiment itself and the subsequent identification process.

In order to settle our problem, at first let us note that (2.18)–(2.20) has the solution

$$y(x,t) = \exp(-\theta\pi^2 t)\sin(\pi x) \tag{2.22}$$

Hence the FIM (which reduces to a scalar, since there is only one parameter to be identified) is of the form

$$\begin{aligned} M(x^1) &= \frac{1}{\sigma^2}\int_0^{t_f}\left(\frac{\partial y(x^1,t)}{\partial\theta}\right)^2 \mathrm{d}t \\ &= \frac{1}{\sigma^2}\int_0^{t_f}\left\{-\pi^2 t\exp(-\theta\pi^2 t)\sin(\pi x)\right\}^2 \mathrm{d}t \\ &= \underbrace{\frac{1}{\sigma^2}\pi^4\int_0^{t_f} t^2\exp(-2\theta\pi^2 t)\,\mathrm{d}t}_{\text{a positive constant}}\sin^2(\pi x) \end{aligned} \tag{2.23}$$

and it is evident that it attains a maximum at $x^1 = 1/2$. Since practically all the design criteria in common use meet the condition of monotonicity (cf. (A4) on p. 44), the centre of the rod corresponds to a point of minimum

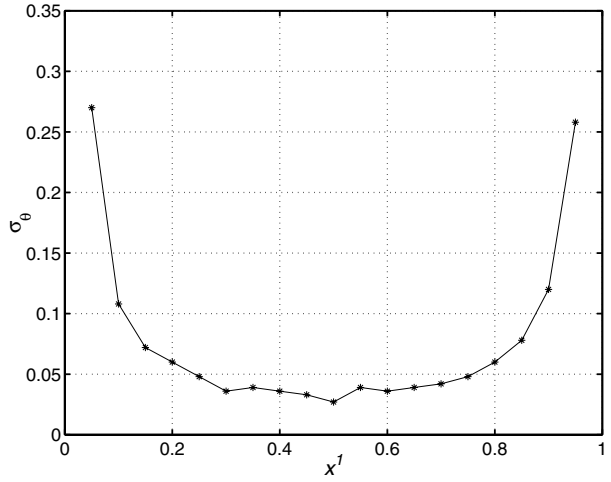


Figure 2.1: Empirical mean-squared estimation error for θ of (2.18)–(2.20) versus different sensor locations.

of $\Psi[M(x^1)]$ for any Ψ as well. That is where the sensitivity of the output with respect to changes in θ is maximal. Consequently, measurements at the centre convey more information about the dynamics of our heat transfer process.

The benefits of the optimum sensor location can be evaluated via simulations. For that purpose, a computer code was written to simulate the system behaviour for $\theta_{\text{true}} = 1$ and $t_f = 0.2$. An $\mathcal{N}(0, 0.05)$ normal distribution was assumed for the noise and uniform sampling with time period $\Delta t = 0.01$ simulated time-continuous measurements. As potential sensor locations, the points $x_i^1 = 0.05i$, $i = 1, \ldots, 19$ were tested by performing $L = 150$ identification experiments at each of them (to this end, the routine `dbrent` from (Press *et al.*, 1996) was used as the minimizer). Figure 2.1 shows the empirical mean-squared estimation error

$$\hat{\sigma}_\theta(x^1) = \sqrt{\frac{1}{L-1}\sum_{j=1}^{L}\left(\hat{\theta}_j(x^1) - \frac{1}{L}\sum_{\ell=1}^{L}\hat{\theta}_\ell(x^1)\right)^2}$$

as a function of the sensor location. As predicted, the best point for taking measurements is just the centre of the rod, since at that point the dispersion of the estimates is the least of all. Also note that the accuracy of the estimates is almost ten times as great for the optimal point as for the outermost

allowable locations, which indicates that even sophisticated techniques of sensor placement can be worthwile if we wish to identify the parameters with great precision. ♢

2.4 Main impediments to solving the sensor placement problem

Transformation of the initial sensor location problem to minimization of a criterion defined on the FIM may lead to the conclusion that the remainder is only the question of selecting an appropriate solver from a library of numerical optimization routines. Unfortunately, the reality turns out to be harsher than the previous perfunctory analysis suggests. This is mainly because of the four problems outlined in what follows, which explain to a certain extent why so few works have been published on this subject so far when compared e.g. with the sensor location problem for state estimation.

2.4.1 High dimensionality of the multi-modal optimization problem

In practice, the number of sensors to be placed in a given region may be quite large. For example, in the research carried out to find spatial predictions for ozone in the Great Lakes of the United States, measurements made by approximately 160 monitoring stations were used (Nychka and Saltzman, 1998). When trying to treat the task as a constrained non-linear programming problem, the actual number of variables is even doubled, since the position of each sensor is determined by its two spatial coordinates, so that the resulting problem is rather of large scale. What is more, a desired global extremum is usually hidden among many, poorer, local extrema. Consequently, to directly find a numerical solution may be extremely difficult. Some approach which makes this problem dimensionality substantially lower is delineated on p. 39.

2.4.2 Loss of the underlying properties of the estimator for finite horizons of observation

As a matter of fact, the approximation of the covariance matrix for the parameter estimates by the inverse of the FIM is justified when $t_f \to \infty$ (Rafajłowicz, 1986c; Walter and Pronzato, 1997). In practice, this is a rare case, as the observation horizon is usually limited by imposed technical

requirements. But the resulting loss in accuracy is commonly neglected in practical applications.

2.4.3 Sensor clusterization

One of the most serious problems, which complicate the selection of measurement points, is sensors' clusterization being 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 one point, which is obviously unacceptable from the technical point of view. This phenomenon is illustrated with the following example.

Example 2.3. Let us consider the following one-dimensional heat equation:

$$\frac{\partial y(x,t)}{\partial t} = \theta_1 \frac{\partial^2 y(x,t)}{\partial x^2}, \quad x \in (0,\pi), \quad t \in (0,1)$$

supplemented by the conditions

$$\begin{cases} y(0,t) = y(\pi,t) = 0, & t \in (0,1) \\ y(x,0) = \theta_2 \sin(x), & x \in (0,\pi) \end{cases}$$

We assume that constant coefficients θ_1 and θ_2 are unknown and to be estimated based on the data gathered by two stationary sensors. Let us try to determine the sensors' locations x^1 and x^2 so as to maximize the determinant of the FIM.

Of course, in this elementary case the solution can be obtained in closed form as

$$y(x,t) = \theta_2 \exp(-\theta_1 t) \sin(x)$$

There is no loss of generality in assuming $\sigma = 1$ as this value has no influence on the sensor positions. After some easy calculations, we get

$$\begin{aligned} &\det(M(x^1,x^2)) \\ &\quad = \underbrace{\frac{\theta_2^2}{16\theta_1^4}\left(-4\theta_1^2\exp(-2\theta_1) - 2\exp(-2\theta_1) + \exp(-4\theta_1) + 1\right)}_{\text{constant term}} \\ &\qquad \cdot \underbrace{\left(2 - \cos^2(x^1) - \cos^2(x^2)\right)^2}_{\text{term dependent on } x^1 \text{ and } x^2} \end{aligned}$$

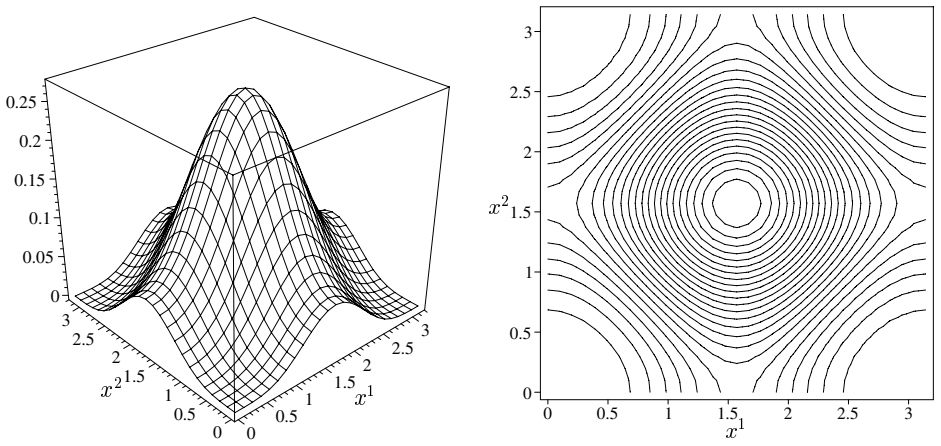


Figure 2.2: Surface and contour plots of $\det M$ of Example 2.3 versus the sensors' locations ($\theta_1 = 0.1$, $\theta_2 = 1$).

Figure 2.2 shows the corresponding surface and contour plots. Clearly, the maximum of the above criterion is attained for

$$x^{1\star} = x^{2\star} = \frac{\pi}{2}$$

but this means that both the sensors should be placed at the same point being the centre of the interval $(0, \pi)$. ♢

In the literature on stationary sensors, a common remedy for such a predicament is to guess *a priori* a set of N' possible locations, where $N' > N$, and then to seek the best set of N locations from among the N' possible, so that the problem is then reduced to a combinatorial one (Uciński, 1995). (If the system is solved numerically, the maximum value of N' is the number of grid points in the domain $\bar{\Omega}$.)

2.4.4 Dependence of the solution on the parameters to be identified

Another great difficulty encountered while trying to design the sensors' locations is the dependence of the optimal solution on the parameters to be identified, which are yet unknown before the experiment. In other words, one cannot determine an optimal design setting for estimating θ without having to specify an initial estimate θ^0 of θ. This peculiarity is illustrated with the following example.

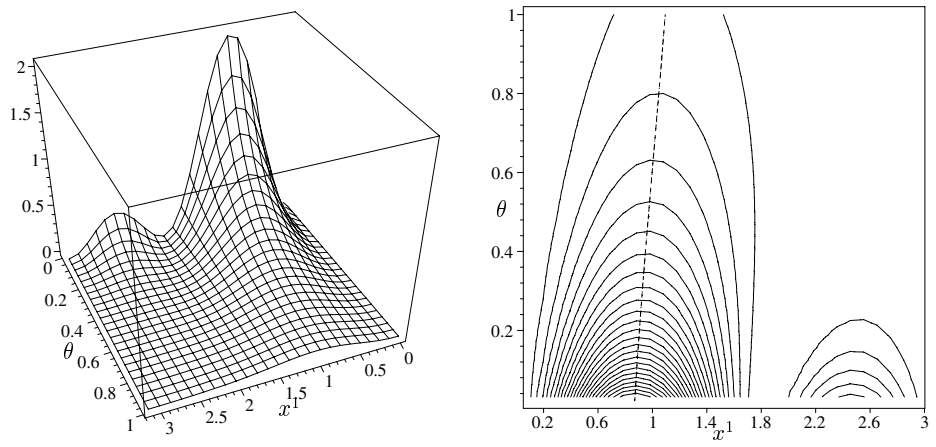


Figure 2.3: Surface and contour plots for $M(x^1)$ of Example 2.4 as a function of the parameter θ (the dashed line represents the best measurement points).

Example 2.4. Let us reconsider the heat process of Example 2.3

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

with the same homogeneous boundary conditions and a slightly changed initial condition:

$$\begin{cases} y(0,t) = y(\pi,t) = 0, & t \in (0,t_f) \\ y(x,0) = \sin(x) + \frac{1}{2}\sin(2x), & x \in (0,\pi) \end{cases}$$

Its solution can be easily found in explicit form as

$$y(x,t) = \exp(-\theta t)\sin(x) + \frac{1}{2}\exp(-4\theta t)\sin(2x)$$

This time we assume that we have at our disposal only one stationary sensor and we would like it to be placed at a best position x^1 in order to estimate the constant parameter θ as precisely as possible.

Based on the previous considerations and using any reasonable computer-algebra system, we can write down the following expression for the FIM

(here again we assume $\sigma = 1$):

$$\begin{aligned} M(x^1) &= \int_0^{t_f} \left(\frac{\partial y(x^1, t; \theta)}{\partial \theta} \right)^2 \mathrm{d}t \\ &= \frac{1}{4\theta^3} \Big\{ -\sin^2(x^1) \left(2\theta^2 t_f^2 + 2t_f\theta + 1 \right) \exp(-2t_f\theta) \\ &\quad - \frac{32}{125} \cos(x^1) \sin^2(x^1) \left(10t_f\theta + 2 + 25\theta^2 t_f^2 \right) \exp(-5t_f\theta) \\ &\quad - \frac{1}{4} \cos^2(x^1) \sin^2(x^1) \left(1 + 32\theta^2 t_f^2 + 8t_f\theta \right) \exp(-8t_f\theta) \\ &\quad + \frac{1}{500} \sin^2(x^1) \left(500 + 256 \cos(x^1) + 125 \cos^2(x^1) \right) \Big\} \end{aligned}$$

Since there is only one parameter to be identified, the FIM is actually a scalar value and hence finding a minimum of any design criterion Ψ defined on it leads to the same solution due to the monotonicity of Ψ. Figure 2.3 shows the corresponding graphs after setting $t_f = 1$, from which two important features can be deduced. First of all, there may exist local minima of Ψ which interfere with numerical minimization of the adopted performance criterion. Apart from that, the optimal sensor position which corresponds to the global minimum of $\Psi(M(x^1))$ depends on the true value of θ (cf. the dashed line joining points $(0.87, 0)$ and $(1.1, 1)$ on the contour plot). $\diamondsuit$

This dependence on θ is an unappealing characteristic of nonlinear optimum-experimental design and was most appropriately depicted by Cochran (Khuri and Cornell, 1996): 'You tell me the value of θ and I promise to design the best experiment for estimating θ.' This predicament can be partially circumvented by relying on a nominal value of θ, the results of a preliminary experiment or a *sequential design* which consists in multiple alternation of experimentation and estimation steps. Unfortunately, such strategies are often impractical, because the required experimental time may be too long and the experimental cost may be too high. An altervative is to exploit the so-called *robust-design* strategies (Walter and Pronzato, 1997; Sun, 1994) which allow us to make optimal solutions independent of the parameters to be identified. The approach (called the *average-optimality* approach) relies on a probabilistic description of the prior uncertainty in θ, characterized by a prior distribution $\pi_{\mathrm{p}}(\theta)$ (this distribution may have been inferred, e.g. from previous observations collected on similar processes). In the same spirit, the *minimax optimality* produces the best sensor positions in the worst circumstances. Both the approaches are treated in detail in Chapter 5.

2.5 Deterministic interpretation of the FIM

It is worth pointing out that Fisher's information matrix may also be given a deterministic interpretation. To this end, set up a somewhat more abstract conceptual framework for the identification problem under consideration. First, we define three function spaces (Chung and Kravaris, 1988; Kravaris and Seinfeld, 1985): the parameter space Θ, the state space Y and the observation space Z, to which belong θ, y and z, respectively. The set of physically admissible parameters is denoted by $\Theta_{\text{ad}} \subset \Theta$. Then solving the PDE for a given value of θ is represented by a solution operator $\mathcal{S} : \Theta_{\text{ad}} \to Y$ defined by

$$y = \mathcal{S}(\theta) \tag{2.24}$$

The type of measurement available is characterized by an observation operator $O : Y \to Z$ defined by

$$y_{\text{m}} = \mathcal{O}(y) \tag{2.25}$$

Combining (2.24) and (2.25), y_{m} is given by

$$y_{\text{m}} = \Phi(\theta) \tag{2.26}$$

where $\Phi = \mathcal{O} \circ \mathcal{S}$ signifies the composite mapping of $\mathcal{S}$ and $\mathcal{O}$. The situation is depicted in Fig. 2.4 (Chavent, 1987).

Given an observation $z \in Z$, the inverse problem under consideration consists in finding a model parameter $\hat{\theta}$ which solves the operator equation

$$\Phi(\hat{\theta}) = z \tag{2.27}$$

Because of the measurement and model errors, this equation usually has no solution, so we attempt to solve it approximately by minimizing on Θ_{ad} the least-squares functional

$$\mathcal{J}(\theta) = \frac{1}{2}\|\Phi(\theta) - z\|_Z^2 \tag{2.28}$$

which quantifies the discrepancy between experimentally measured and analytically predicted response data.

Our task now is to study the differentiability of $\mathcal{J}$ at a given point $\bar{\theta} \in \Theta_{\text{ad}}$. Let us orient Φ by the requirement that it be continuously Fréchet differentiable in a neighbourhood of $\bar{\theta}$ and, additionally, that it

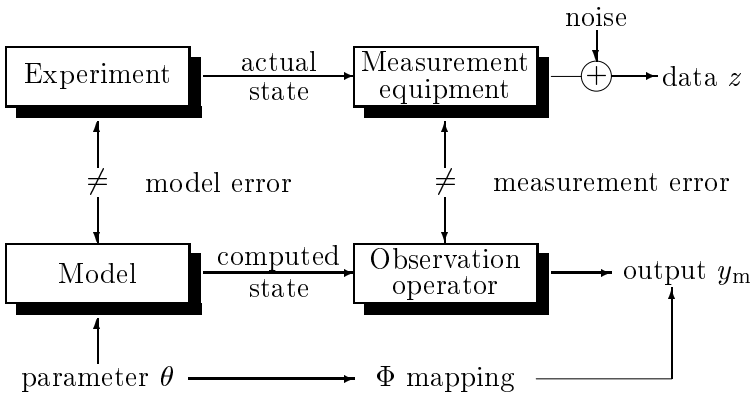


Figure 2.4: An interpretation of the identification problem.

have the second-order Gâteaux derivative at $\bar{\theta}$. Making use of the chain rule of differentation, we see at once that $\mathcal{J}$ itself is continuously Fréchet differentiable and

$$\mathcal{J}'(\bar{\theta})\delta\theta = \langle \Phi(\bar{\theta}) - z, \Phi'(\bar{\theta})\delta\theta \rangle_Z = \langle \Phi'^*(\bar{\theta}) \left[\Phi(\bar{\theta}) - z \right], \delta\theta \rangle_\Theta \tag{2.29}$$

or, equivalently,

$$\nabla \mathcal{J}(\bar{\theta}) = \Phi'^*(\bar{\theta}) \left[\Phi(\bar{\theta}) - z \right] \tag{2.30}$$

where $\nabla \mathcal{J}(\bar{\theta})$ stands for the gradient of $\mathcal{J}$ at $\bar{\theta}$ and $\Phi'^*(\bar{\theta})$ is the adjoint operator of $\Phi'(\bar{\theta})$.

Furthermore, we deduce that

$$\begin{aligned}
&\frac{1}{\lambda}\{\mathcal{J}'(\bar{\theta} + \lambda\delta\theta')\delta\theta - \mathcal{J}'(\bar{\theta})\delta\theta\} \\
&\qquad = \frac{1}{\lambda}\{\langle \Phi(\bar{\theta} + \lambda\delta\theta') - z, \Phi'(\bar{\theta} + \lambda\delta\theta')\delta\theta \rangle_Z \\
&\qquad\quad - \langle \Phi(\bar{\theta}) - z, \Phi'(\bar{\theta})\delta\theta \rangle_Z \} \\
&\qquad = \langle \frac{1}{\lambda}\{\Phi(\bar{\theta} + \lambda\delta\theta') - \Phi(\bar{\theta})\}, \Phi'(\bar{\theta} + \lambda\delta\theta')\delta\theta \rangle_Z \\
&\qquad\quad + \langle \Phi(\bar{\theta}) - z, \frac{1}{\lambda}\{\Phi'(\bar{\theta} + \lambda\delta\theta')\delta\theta - \Phi'(\bar{\theta})\delta\theta\} \rangle_Z
\end{aligned} \tag{2.31}$$

From this, letting $\lambda \to 0$ and using the continuity of Φ', we get

$$\begin{aligned}\lim_{\lambda\to 0}\frac{1}{\lambda}\big\{\mathcal{J}'(\bar\theta+\lambda\delta\theta')\delta\theta-\mathcal{J}'(\bar\theta)\delta\theta\big\}\\ =\langle\Phi'(\bar\theta)\delta\theta',\Phi'(\bar\theta)\delta\theta\rangle_Z+\langle\Phi(\bar\theta)-z,\Phi''(\bar\theta)(\delta\theta,\delta\theta')\rangle_Z\end{aligned}\tag{2.32}$$

the limit being uniform with respect to all $\delta\theta$ such that $\|\delta\theta\|_\Theta = 1$. Consequently, the second-order Gâteaux derivative of $\mathcal{J}$ exists and is given by

$$\begin{aligned}\mathcal{J}''(\bar\theta)(\delta\theta,\delta\theta')=\langle\delta\theta',\Phi'^*(\bar\theta)\Phi'(\bar\theta)\delta\theta\rangle_\Theta\\ +\langle\Phi(\bar\theta)-z,\Phi''(\bar\theta)(\delta\theta,\delta\theta')\rangle_Z\end{aligned}\tag{2.33}$$

If the measurements and model errors are small and $\bar\theta$ is in the proximity of a global minimum of $\mathcal{J}$, then the second term on the right-hand side may be neglected using the fact that $\Phi(\bar\theta)-z\approx 0$. Hence

$$\mathcal{J}''(\bar\theta)(\delta\theta,\delta\theta')\approx\langle\delta\theta',\Phi'^*(\bar\theta)\Phi'(\bar\theta)\delta\theta\rangle_\Theta\tag{2.34}$$

which forces

$$H(\bar\theta)\approx\Phi'^*(\bar\theta)\Phi'(\bar\theta)\tag{2.35}$$

where $H(\bar\theta)$ denotes the Hessian of $\mathcal{J}$ at $\bar\theta$.

Let us unravel now what (2.35) means in case $\Theta=\mathbb{R}^m$ and $Z=L^2(T;\mathbb{R}^N)$, where $T=(0,t_f)$. As was already noted, this setting corresponds to an N-sensor parameter-output mapping

$$y_{\mathrm{m}}(\,\cdot\,)=\Phi(\theta)=\mathrm{col}[y(x^1,\,\cdot\,;\theta),\dots,y(x^N,\,\cdot\,;\theta)]\tag{2.36}$$

Clearly, there exist partial Fréchet derivatives Φ'_{θ_i} of Φ with respect to individual parameters $\theta_i\in\mathbb{R}$ and each of them may be identified with an element $g_i(\bar\theta)\in Z$ (see Appendix A.4), so that we have

$$\delta y_{\mathrm{m}}=\Phi'(\bar\theta)\delta\theta=\sum_{i=1}^m\delta\theta_i g_i(\bar\theta)\tag{2.37}$$

An easy computation shows that

$$\begin{aligned}\langle h,\Phi'(\bar\theta)\delta\theta\rangle_Z&=\langle h,\sum_{i=1}^m\delta\theta_i g_i(\bar\theta)\rangle_Z\\ &=\sum_{i=1}^m\langle h,g_i(\bar\theta)\rangle_Z\delta\theta_i=\langle A(\bar\theta)h,\delta\theta\rangle_{\mathbb{R}^m},\quad\forall\,h\in Z\end{aligned}\tag{2.38}$$

where $A(\bar{\theta})h = \mathrm{col}[\langle h, g_1(\bar{\theta})\rangle_Z, \ldots, \langle h, g_m(\bar{\theta})\rangle_Z]$, which yields $\Phi'^*(\bar{\theta}) \equiv A(\bar{\theta})$. For the composite mapping in (2.35) we thus get

$$\begin{aligned} H(\bar{\theta}) &= \begin{bmatrix} \langle g_1(\bar{\theta}), g_1(\bar{\theta})\rangle_Z & \cdots & \langle g_m(\bar{\theta}), g_1(\bar{\theta})\rangle_Z \\ \vdots & & \vdots \\ \langle g_1(\bar{\theta}), g_m(\bar{\theta})\rangle_Z & \cdots & \langle g_m(\bar{\theta}), g_m(\bar{\theta})\rangle_Z \end{bmatrix} \\ &= \sum_{j=1}^{N} \int_0^{t_f} \gamma_j(t;\bar{\theta})\gamma_j^{\mathrm{T}}(t;\bar{\theta})\,\mathrm{d}t \end{aligned} \tag{2.39}$$

where $\gamma_j(\,\cdot\,;\bar{\theta}) = \mathrm{col}[g_{1j}(\bar{\theta})(\,\cdot\,), \ldots, g_{mj}(\bar{\theta})(\,\cdot\,)]$, g_{ij} being the j-th component of g_i (viz. the component of the derivative which corresponds to the i-th parameter and the j-th sensor), $i = 1, \ldots, m$, $j = 1, \ldots, N$. But if the solution to (2.1)–(2.3) is sufficiently regular and $\bar{\theta}$ is merely the actual parameter vector, then (2.39) is nothing but the FIM calculated for $\sigma = 1$. The interpretation of the FIM as the Hessian of the least-squares criterion will be exploited in Section 3.5, p. 70.

2.6 Calculation of sensitivity coefficients

A basic step in the design of optimal sensor positions is to devise an effective numerical procedure for the computation of the so-called sensitivity coefficients, i.e. the derivatives of the states with respect to system parameters, which is necessary to form the elements of the appropriate FIM. The problem is closely related to design sensitivity analysis which plays a critical role in inverse and identification studies, as well as numerical optimization and reliability analyses (Haug *et al.*, 1986; Eslami, 1994; Banichuk, 1990; Tortorelli and Michaleris, 1994) for which there exist many comprehensive monographs and surveys. In the context of parameter estimation of DPS's the problem of calculating sensitivities dates back to early works of Chavent (1974). As for more recent developments, let us cite the monograph by Sun (1994) where the issue was addressed from an engineering point of view with application to groundwater resources management. At the other extreme, Brewer (1982) studied the differentiability with respect to a parameter of the solution to a linear inhomogeneous abstract Cauchy problem by employing the theory of strongly continuous semigroups. Some of his ideas were then used to identify spatially-varying unknown coefficients in parabolic PDE's via quasilinearization (Hammer, 1996).

In what follows, three classical methods of calculating sensitivities are briefly delineated and compared. The reader interested in technical formalities regarding the method widely exploited throughout this monograph is referred to Appendices B.2 and C.2. In order to maintain the discussion at a reasonable level of clarity and to avoid tedious calculations, we will consider the system (2.1) with initial conditions (2.3) and Dirichlet boundary conditions

$$y(x,t) = b(x,t) \quad \text{on } \partial\Omega \times T \tag{2.40}$$

where b is some prescribed function.

2.6.1 Finite-difference method

The finite-difference method is undoubtedly the easiest method to implement as it does not require any analytical or programming effort by the user, but suffers from computational inefficiency and possible errors. We employ the Taylor series expansion to approximate the derivative, which gives

$$y(x,t;\theta + \Delta\theta_i e_i) = y(x,t;\theta) + \frac{\partial y(x,t;\theta)}{\partial \theta_i}\Delta\theta_i + o(\Delta\theta_i) \tag{2.41}$$

where

$$e_i = (0,0,\ldots,0,\overbrace{1}^{i\text{-th component}},0,\ldots,0) \tag{2.42}$$

and $\Delta\theta_i$ represents the parameter perturbation. The above is solved for $\partial y/\partial\theta_i$ to obtain the forward-difference approximation

$$\frac{\partial y(x,t;\theta)}{\partial \theta_i} = \frac{y(x,t;\theta + \Delta\theta_i e_i) - y(x,t;\theta)}{\Delta\theta_i} + O(\Delta\theta_i) \tag{2.43}$$

where we see that the truncation error of the approximation is of order $O(\Delta\theta_i)$. Thus, a smaller $\Delta\theta_i$ yields a more accurate approximation. However, if $\Delta\theta_i$ is too small, then numerical round-off error will erode the accuracy of the computations. The simultaneous choice of the perturbation $\Delta\theta_i$ and of a numerical tolerance used for the numerical simulation of the model equation is critical and may be delicate in some applications (Point *et al.*, 1996). To obtain a second-order accurate approximation, the central-difference approximation

$$\frac{\partial y(x,t;\theta)}{\partial \theta_i} = \frac{y(x,t;\theta + \Delta\theta_i e_i) - y(x,t;\theta - \Delta\theta_i e_i)}{2\Delta\theta_i} + o(\Delta\theta_i) \tag{2.44}$$

is commonly employed.

Forward and central differences require respectively $m+1$ and $2m+1$ simulation runs of the model (2.1), (2.3), (2.40) to get all the sensitivity coefficients for a given $\theta \in \mathbb{R}^m$, i.e. this number is proportional to the number of unknown parameters.

2.6.2 Direct-differentation method

In the direct-differentation method we differentiate the system equations (2.1), (2.3), (2.40) with respect to the individual parameters, which gives, after some rearrangement, the so-called *sensitivity equations*

$$\begin{aligned}\frac{\partial}{\partial t}\left[\frac{\partial y}{\partial \theta_i}\right] = {} & \frac{\partial \mathcal{F}}{\partial y}\frac{\partial y}{\partial \theta_i} + \frac{\partial \mathcal{F}}{\partial y_{x_1}}\frac{\partial}{\partial x_1}\left[\frac{\partial y}{\partial \theta_i}\right] + \frac{\partial \mathcal{F}}{\partial y_{x_2}}\frac{\partial}{\partial x_2}\left[\frac{\partial y}{\partial \theta_i}\right] \\ & + \frac{\partial \mathcal{F}}{\partial y_{x_1 x_1}}\frac{\partial^2}{\partial x_1^2}\left[\frac{\partial y}{\partial \theta_i}\right] + \frac{\partial \mathcal{F}}{\partial y_{x_2 x_2}}\frac{\partial^2}{\partial x_2^2}\left[\frac{\partial y}{\partial \theta_i}\right] \\ & + \frac{\partial \mathcal{F}}{\partial \theta_i} \qquad \text{in } Q = \Omega \times T\end{aligned} \tag{2.45}$$

subject to

$$\frac{\partial y}{\partial \theta_i}(x,0) = 0 \quad \text{in } \Omega \tag{2.46}$$

$$\frac{\partial y}{\partial \theta_i}(x,t) = 0 \quad \text{on } \Sigma = \partial\Omega \times T \tag{2.47}$$

for $i = 1, \ldots, m$, where y_{x_j} and $y_{x_j x_j}$ denote

$$\frac{\partial y}{\partial x_j} \quad \text{and} \quad \frac{\partial^2 y}{\partial x_j^2}$$

respectively, $j = 1, 2$.

Let us note that these equations are linear even if the system equation is non-linear. All the derivatives of $\mathcal{F}$ are calculated for a solution to (2.1), (2.3), (2.40) corresponding to a given value of θ and therefore this solution must be obtained prior to solving sensitivity equations and then stored, or computed simultaneously with these.

If the system equation is linear, then the form of the sensitivity problem is exactly the same as that of simulating the original system. Consequently, we can use the same computer code to solve both of them. The total computational effort is the same as that of using the finite-difference method

($m+1$ simulation runs), but this time the results obtained are exact (for the numerical solution) and the difficulty of determining the size of perturbation increments can thus be avoided.

2.6.3 Adjoint method

Suppose that the values of all the sensitivity coefficients are required at a point $x^0 \in \Omega$ for a given time moment $t^0 \in T$. It turns out that this can be accomplished without the necessity of solving sensitivity equations, as this step can be eliminated via the calculus of variations. Indeed, the variation in y due to variations in the parameter vector θ is given by the solution of

$$\begin{aligned}\delta y_t = &\frac{\partial \mathcal{F}}{\partial y}\delta y + \frac{\partial \mathcal{F}}{\partial y_{x_1}}\delta y_{x_1} + \frac{\partial \mathcal{F}}{\partial y_{x_2}}\delta y_{x_2} \\ &+ \frac{\partial \mathcal{F}}{\partial y_{x_1x_1}}\delta y_{x_1x_1} + \frac{\partial \mathcal{F}}{\partial y_{x_2x_2}}\delta y_{x_2x_2} + \frac{\partial \mathcal{F}}{\partial \theta}\delta\theta \quad \text{in } Q = \Omega \times T\end{aligned} \tag{2.48}$$

subject to

$$\delta y(x,0) = 0 \quad \text{in } \Omega \tag{2.49}$$

$$\delta y(x,t) = 0 \quad \text{on } \Sigma = \partial\Omega \times T \tag{2.50}$$

We introduce the adjoint state $\psi = \psi(x,t)$, multiplying (2.48) by it and integrating the result over Q while making use of the Green formulae (cf. Appendix B.1), to give

$$\begin{aligned}&\int_\Omega \psi\delta y\big|_{t=t_f}\,\mathrm{d}x \\ &\quad= \int_Q \left\{\frac{\partial\psi}{\partial t} + \psi\frac{\partial \mathcal{F}}{\partial y} - \frac{\partial}{\partial x_1}\left(\psi\frac{\partial \mathcal{F}}{\partial y_{x_1}}\right) - \frac{\partial}{\partial x_2}\left(\psi\frac{\partial \mathcal{F}}{\partial y_{x_2}}\right)\right. \\ &\qquad\left. + \frac{\partial^2}{\partial x_1^2}\left(\psi\frac{\partial \mathcal{F}}{\partial y_{x_1x_1}}\right) + \frac{\partial^2}{\partial x_2^2}\left(\psi\frac{\partial \mathcal{F}}{\partial y_{x_2x_2}}\right)\right\}\delta y\,\mathrm{d}x\,\mathrm{d}t \\ &\qquad+ \int_\Sigma \psi\left\{\frac{\partial \mathcal{F}}{\partial y_{x_1x_1}}\delta y_{x_1}\nu_1 + \frac{\partial \mathcal{F}}{\partial y_{x_2x_2}}\delta y_{x_2}\nu_2\right\}\mathrm{d}\sigma\,\mathrm{d}t \\ &\qquad+ \int_Q \psi\frac{\partial \mathcal{F}}{\partial\theta}\delta\theta\,\mathrm{d}x\,\mathrm{d}t\end{aligned} \tag{2.51}$$

where ν_i's signify the direction cosines of the unit outward normal to $\partial\Omega$. The quantity ψ acts as the Lagrange multiplier and for now it is arbitrary.

Writing the value of y at (x^0, t^0) in the form

$$y(x^0,t^0) = \int_Q y(x,t)\delta(x_1 - x_1^0)\delta(x_2 - x_2^0)\delta(t - t^0)\,\mathrm{d}x\,\mathrm{d}t \tag{2.52}$$

where δ is the Dirac delta function, we see that

$$\delta y(x^0,t^0) = \int_Q \delta y(x,t)\delta(x_1 - x_1^0)\delta(x_2 - x_2^0)\delta(t - t^0)\,\mathrm{d}x\,\mathrm{d}t \tag{2.53}$$

The summation of (2.51) and (2.53) gives

$$\begin{aligned}
&\delta y(x^0,t^0)\\
&\quad = -\int_\Omega \psi\delta y\big|_{t=t_f}\,\mathrm{d}x + \int_Q \Bigg\{ \frac{\partial\psi}{\partial t} + \psi\frac{\partial\mathcal{F}}{\partial y} - \frac{\partial}{\partial x_1}\left(\psi\frac{\partial\mathcal{F}}{\partial y_{x_1}}\right)\\
&\qquad - \frac{\partial}{\partial x_2}\left(\psi\frac{\partial\mathcal{F}}{\partial y_{x_2}}\right) + \frac{\partial^2}{\partial x_1^2}\left(\psi\frac{\partial\mathcal{F}}{\partial y_{x_1x_1}}\right) + \frac{\partial^2}{\partial x_2^2}\left(\psi\frac{\partial\mathcal{F}}{\partial y_{x_2x_2}}\right)\\
&\qquad + \delta(x_1 - x_1^0)\delta(x_2 - x_2^0)\delta(t - t^0)\Bigg\}\delta y\,\mathrm{d}x\,\mathrm{d}t\\
&\quad + \int_\Sigma \psi\left\{\frac{\partial\mathcal{F}}{\partial y_{x_1x_1}}\delta y_{x_1}\nu_1 + \frac{\partial\mathcal{F}}{\partial y_{x_2x_2}}\delta y_{x_2}\nu_2\right\}\mathrm{d}\sigma\,\mathrm{d}t\\
&\quad + \int_Q \psi\frac{\partial\mathcal{F}}{\partial\theta}\delta\theta\,\mathrm{d}x\,\mathrm{d}t
\end{aligned} \tag{2.54}$$

Since ψ is arbitrary, we may select it to annihilate the terms related to δy. We therefore specify that ψ be governed by

$$\begin{aligned}
\frac{\partial\psi}{\partial t} = &-\psi\frac{\partial\mathcal{F}}{\partial y} + \frac{\partial}{\partial x_1}\left(\psi\frac{\partial\mathcal{F}}{\partial y_{x_1}}\right) + \frac{\partial}{\partial x_2}\left(\psi\frac{\partial\mathcal{F}}{\partial y_{x_2}}\right) - \frac{\partial^2}{\partial x_1^2}\left(\psi\frac{\partial\mathcal{F}}{\partial y_{x_1x_1}}\right)\\
&- \frac{\partial^2}{\partial x_2^2}\left(\psi\frac{\partial\mathcal{F}}{\partial y_{x_2x_2}}\right) - \delta(x_1 - x_1^0)\delta(x_2 - x_2^0)\delta(t - t^0) \quad \text{in } Q
\end{aligned} \tag{2.55}$$

subject to the final condition

$$\psi(x,t_f) = 0 \quad \text{in } \Omega \tag{2.56}$$

and the boundary condition

$$\psi(x,t) = 0 \quad \text{on } \Sigma \tag{2.57}$$

Substituting (2.55)–(2.57) into (2.54), we obtain

$$\delta y(x^0, t^0) = \int_Q \psi \frac{\partial \mathcal{F}}{\partial \theta} \delta\theta \, \mathrm{d}x \, \mathrm{d}t \tag{2.58}$$

and hence

$$\frac{\partial y}{\partial \theta}(x^0, t^0) = \int_Q \psi \frac{\partial \mathcal{F}}{\partial \theta} \, \mathrm{d}x \, \mathrm{d}t \tag{2.59}$$

which is due to the fact that $\theta \in \mathbb{R}^m$.

From what has just been outlined, it follows that the adjoint method is implemented as follows:

1. Solve the state equation (2.1) from $t = 0$ to $t = t_f$ subject to (2.3), (2.40) and store the resulting values of the state y obtained on a spatial grid at selected time instants.

2. Solve the adjoint problem (2.55) backwards in time, i.e. from $t = t_f$ to $t = 0$, subject to (2.56) and (2.57) using interpolated values of y.

3. Compute $\partial y(x^0, t^0)/\partial\theta$ from the reduced equation (2.59).

A decided advantage of the method lies in the fact that the amount of computations is not proportional to the number of unknown parameters, as only solution of one adjoint equation is required in addition to the solution of the state equation (compare this with the necessity of solving $m+1$ equations in the finite-difference and direct-differentiation methods). Moreover, the adjoint method also yields exact (for the numerical solution) results.

However, the solution of the adjoint problem may be computationally more delicate than that of the original problem. In particular, the adjoint PDE contains point sources, which makes the spatial discretization more complicated (Point *et al.*, 1996; Holtz and Arora, 1997) and eventually the resulting increase in computation time may outweigh the benefits from the reduction in the number of equations. Moreover, the adjoint equation frequently proves to be numerically unstable, especially for long terminal times. This means that any round-off error which becomes 'mixed into' the calculation at an early stage is successively magnified until it comes to swamp the true answer. But the main drawback to the method is that it is primarily intended to calculate the sensitivity vector at a number of points in the space-time domain Q which is less than the number of parameters. This makes its usefuleness questionable in optimally locating sensors, but it can be valuable in some studies related to identifiability (Sun, 1994).

2.7 A final introductory note

The undeniable relationship between the sensor location and the achievable accuracy in parameter identification for distributed systems motivates the development of systematic methods for finding points which are best suited for taking measurements. This chapter has dealt with the characterization of the optimal sensor location problem from formulation to discussion of some specific technical issues, such as calculation of the sensitivity coefficients. The problem has been ultimately formalized as minimization of some scalar measure of performance based on the Fisher information matrix whose inverse constitutes the Cramér-Rao bound on the covariance matrix for the estimates. Unfortunately, some severe difficulties encountered while naïvely trying to treat this problem as an ordinary non-linear programming problem exclude straightforward approaches to find the corresponding solutions. Owing to the same reasons, the existing techniques are limited to some particular situations and are far from being flexible enough to tackle a broad class of problems facing engineers who deal with applications. Accordingly, the remainder of this monograph is intended as an attempt to fill this gap (at least to a certain extent), to overcome some of the shortcomings of the earlier approaches, and to provide a unified methodology for optimally locating measurement transducers along a given spatial domain.

Chapter 3

Locally optimal location of stationary sensors

3.1 Optimum experimental design for continuous-time linear-in-parameters lumped models

As an introduction to the measurement system design for DPS's, we shall first investigate a slightly simpler linear case of a lumped system. The presented results are in principle rather easy alterations of their counterparts from the classical theory of optimum experimental design, the main difference being the assumption of continuous-time observations in lieu of a finite collection of measurements at selected time instants.

Consider the dynamic system

$$z(t) = F^{\mathrm{T}}(t)\theta + \varepsilon(t), \quad t \in T = [0, t_f] \tag{3.1}$$

where t denotes time and t_f is a fixed finite time horizon. Here $\theta \in \mathbb{R}^m$ signifies a vector of constant parameters and F is given by

$$F(\,\cdot\,) = \Big[f(x^1, \,\cdot\,) \quad \ldots \quad f(x^N, \,\cdot\,) \Big] \tag{3.2}$$

where the quantities $x^1, \ldots, x^N$ are treated as variables whose values belong to a compact set $X \subset \mathbb{R}^n$ (for now, we freeze their values) and $f \in C(X \times T; \mathbb{R}^m)$ is known *a priori*. Furthermore, ε is a zero-mean white (in time) Gaussian process which plays the role of a disturbance. Its covariance meets the condition

$$\mathrm{E}\big\{\varepsilon(t)\varepsilon^{\mathrm{T}}(\tau)\big\} = C(t)\delta(t-\tau) \tag{3.3}$$

where δ denotes the Dirac delta function and $C(t) \in \mathbb{R}^{N\times N}$ is symmetric and positive-definite for any $t \in T$.

In this setting, the parameter estimation problem is as follows: Given the history of F, i.e. the set $\{F(t)\}_{t\in T}$, and the outcomes of the measurements $\{z(t)\}_{t\in T}$ find, among all possible values of the parameter vector θ, a parameter which minimizes the weighted least-squares criterion

$$\mathcal{J}(\theta) = \frac{1}{2}\int_0^{t_f} \left[z(t) - F^{\mathrm{T}}(t)\theta\right]^{\mathrm{T}} C^{-1}(t)\left[z(t) - F^{\mathrm{T}}(t)\theta\right] \mathrm{d}t \tag{3.4}$$

Differentiating (3.4) with respect to θ shows that the sought value $\hat{\theta}$ satisfies the equation (often called the *normal equation*)

$$\nabla\mathcal{J}(\hat{\theta}) = -\int_0^{t_f} F(t)C^{-1}(t)\left[z(t) - F^{\mathrm{T}}(t)\hat{\theta}\right] \mathrm{d}t = 0 \tag{3.5}$$

If the matrix

$$M = \int_0^{t_f} F(t)C^{-1}(t)F^{\mathrm{T}}(t)\,\mathrm{d}t \tag{3.6}$$

is non-singular, then there is a unique solution which can be expressed as

$$\hat{\theta} = M^{-1}\int_0^{t_f} F(t)C^{-1}(t)z(t)\,\mathrm{d}t \tag{3.7}$$

The estimator (3.7) is unbiased, since we have

$$\begin{aligned}\mathrm{E}\{\hat{\theta}\} &= M^{-1}\int_0^{t_f} F(t)C^{-1}(t)\,\mathrm{E}\{z(t)\}\,\mathrm{d}t \\ &= M^{-1}\underbrace{\int_0^{t_f} F(t)C^{-1}(t)F^{\mathrm{T}}(t)\,\mathrm{d}t}_{M}\,\theta = \theta\end{aligned} \tag{3.8}$$

provided that θ is the true parameter value. Moreover, its covariance is given by

$$\begin{aligned}\mathrm{cov}\{\hat{\theta}\} &= \mathrm{E}\{(\hat{\theta}-\theta)(\hat{\theta}-\theta)^{\mathrm{T}}\} \\ &= M^{-1}\int_0^{t_f}\int_0^{t_f} F(t)C^{-1}(t)\,\mathrm{E}\{\varepsilon(t)\varepsilon^{\mathrm{T}}(\tau)\}C^{-1}(\tau)F^{\mathrm{T}}(\tau)\,\mathrm{d}t\,\mathrm{d}\tau M^{-1} \\ &= M^{-1}MM^{-1} = M^{-1}\end{aligned} \tag{3.9}$$

The matrix M above plays the role of the Fisher information matrix, cf. (2.9). Let us observe that it does not depend on the observations z but it does depend on the parameters x^j, $j = 1, \ldots, N$. In practice, this means that we may attempt to adjust x^j's prior to any experiment so that they are (in terms of $\mathrm{cov}\{\hat{\theta}\}$) 'better' than others and the information provided by the experiment is maximized. This constitutes the main topic of the remainder of this section.

As was already mentioned (p. 18), a common procedure is to introduce a scalar cost function (design criterion) Ψ defined on the FIM, which permits the optimal experimental design to be cast as an optimization problem

$$\Psi\big[M(x^1, \ldots, x^N)\big] \longrightarrow \min \tag{3.10}$$

This leads to the so-called exact designs which can then be calculated with the use of numerous widely accessible non-linear programming solvers if N is not too large. Unfortunately, the problem quickly becomes computationally too demanding and intractable for larger N's. This predicament has been addressed in plentiful works on optimum experimental design and the most efficient solution is no doubt the introduction of the so-called continuous designs (Ermakov, 1983; Fedorov, 1972; Fedorov and Hackl, 1997; Goodwin and Payne, 1977; Pázman, 1986; Walter and Pronzato, 1997; Pukelsheim, 1993). Such an approach will also be adopted in what follows.

In order to relax the limitations of exact designs, it is necessary to orient the covariance C by the requirement that

$$C = \sigma^2 I \tag{3.11}$$

where I is the $N \times N$ identity matrix and σ plays the role of a constant standard deviation of the measurement errors (note that we might also assume that C is a diagonal matrix, but this will not be pursued for the sake of simplicity, since the corresponding changes are rather obvious). Such an assumption amounts to accepting the situation when the measurements are constantly independent of one another. Sometimes this is unrealistic (especially in most sensor location contexts), but the clear advantage of such a procedure, which outweighs all the shortcomings, is that the form of the FIM is then substantially simpler:

$$M = \frac{1}{\sigma^2} \int_0^{t_f} F(t) F^{\mathrm{T}}(t)\, \mathrm{d}t = \sum_{j=1}^{N} M_j \tag{3.12}$$

where

$$M_j = \frac{1}{\sigma^2} \int_0^{t_f} f(x^j, t) f^{\mathrm{T}}(x^j, t)\, \mathrm{d}t$$

As a result, the total FIM is the sum of the information matrices M_j for individual observations, which is crucial for the approach.

One more simplification comes in handy, but this time it involves no loss of generality. Since in practice all the design criteria satisfy the condition

$$\Psi(\beta M) = \gamma(\beta)\Psi(M), \quad \beta > 0 \tag{3.13}$$

γ being a positive function, we may set $\sigma = 1$. Similarly, operating on the so-called *average* (or *normalized*) FIM

$$\bar{M} = \frac{1}{N t_f} \sum_{j=1}^{N} \int_0^{t_f} f(x^j, t) f^{\mathrm{T}}(x^j, t)\, \mathrm{d}t \tag{3.14}$$

is slightly more convenient, so in the sequel we will constantly use it in lieu of M. For simplicity of notation, we will also drop the bar over M.

Since we admit of replicated measurements, i.e. some values x^j may appear several times in the optimal solution (this is an unavoidable consequence of independent measurements), it is sensible to distinguish only the components of the sequence $x^1, \ldots, x^N$ which are different and, if there are ℓ such components, to relabel them as $x^1, \ldots, x^\ell$ while introducing $r_1, \ldots, r_\ell$ as the corresponding numbers of replications. The redefined x^i's are said to be the *design* or *support* points. The collection of variables

$$\xi_N = \begin{Bmatrix} x^1, & x^2, & \ldots, & x^\ell \\ p_1, & p_2, & \ldots, & p_\ell \end{Bmatrix} \tag{3.15}$$

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

$$M(\xi_N) = \sum_{i=1}^{\ell} p_i \frac{1}{t_f} \int_0^{t_f} f(x^i, t) f^{\mathrm{T}}(x^i, t)\, \mathrm{d}t \tag{3.16}$$

Here the p_i's are rational numbers, since both r_i's and N are integers. Removing this constraint by assuming that they can be any real numbers

of the interval $[0,1]$ such that $\sum_{i=1}^{\ell} p_i = 1$, we may think of the designs as probability distributions on X. But if so, we may attempt to take one more step to widen the class of admissible designs a bit further, i.e. to all probability measures ξ over X which are absolutely continuous with respect to the Lebesgue measure and satisfy by definition the condition

$$\int_X \xi(\mathrm{d}x) = 1 \tag{3.17}$$

Such an extension of the design concept allows us to replace (3.16) by

$$M(\xi) = \int_X \Upsilon(x)\, \xi(\mathrm{d}x) \tag{3.18}$$

where

$$\Upsilon(x) = \frac{1}{t_f} \int_0^{t_f} f(x,t) f^{\mathrm{T}}(x,t)\, \mathrm{d}t$$

and the integration in (3.17) and (3.18) is to be understood in the Stieltjes-Lebesgue sense. This leads to the so-called *continuous* designs which constitute the basis of the modern theory of optimal experiments and originate in seminal works by Kiefer and Wolfowitz (1959). It turns out that such an approach drastically simplifies the design and the remainder of this section is devoted to this issue.

For clarity, we adopt the following notational conventions: Here and subsequently, we will use the symbol $\Xi(X)$ to denote the set of all probability measures on X. Let us also introduce the notation $\mathfrak{M}(X)$ for the set of all admissible information matrices, i.e.

$$\mathfrak{M}(X) = \big\{ M(\xi) : \xi \in \Xi(X) \big\} \tag{3.19}$$

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

$$\xi^\star = \arg \min_{\xi \in \Xi(X)} \Psi[M(\xi)] \tag{3.20}$$

In what follows, two basic assumptions are vital:

(A1) X is compact, and

(A2) $f \in C(X \times T; \mathbb{R}^m)$

We begin with certain convexity and representation properties of $M(\xi)$.

Lemma 3.1. *For any $\xi \in \Xi(X)$ the information matrix $M(\xi)$ is symmetric and non-negative definite.*

Proof. The first part is a direct consequence of the definition (3.18). The other results from the dependence

$$\begin{aligned} \forall\, b \in \mathbb{R}^m,\ b^{\mathrm{T}} M(\xi) b &= \int_X b^{\mathrm{T}} \Upsilon(x) b\, \xi(x) \\ &= \frac{1}{t_f} \int_X \left\{ \int_0^{t_f} [b^{\mathrm{T}} f(x,t)]^2 \,\mathrm{d}t \right\} \xi(\mathrm{d}x) \geq 0 \end{aligned} \tag{3.21}$$

■

Lemma 3.2. *$\mathfrak{M}(X)$ is compact and convex.*

Proof. Let us notice that by Assumption (A2) the function Υ is continuous in X (Kołodziej, 1979, Th. 22, p. 360). Helley's theorem (Ermakov and Zhigljavsky, 1987, Lem. 1.4, p. 91) then implies that $\Xi(X)$ is weakly compact, i.e. from any sequence $\{\xi_i\}_{i=1}^{\infty}$ of $\Xi(X)$ we can extract a subsequence $\{\xi_{i_j}\}_{j=1}^{\infty}$ which is weakly convergent to a probability measure $\xi_\star \in \Xi(X)$ in the sense that

$$\lim_{j\to\infty} \int_X g(x)\, \xi_{i_j}(\mathrm{d}x) = \int_X g(x)\, \xi_\star(\mathrm{d}x), \quad \forall\, g \in C(X) \tag{3.22}$$

Choosing g consecutively as the components of the matrix Υ, we get

$$\lim_{j\to\infty} M(\xi_{i_j}) = M(\xi_\star) \tag{3.23}$$

which establishes the first part of our claim. The other follows immediately from the implication

$$M[(1-\lambda)\xi_1 + \lambda\xi_2] = (1-\lambda)M(\xi_1) + \lambda M(\xi_2), \quad \forall\, \xi_1, \xi_2 \in \Xi(X) \tag{3.24}$$

valid for any $\lambda \in [0,1]$. ■

Remark 3.1. Let us observe that Assumption (A2) may be slightly weakened: For the continuity of Υ it suffices to require only $f(\,\cdot\,, t)$ to be continuous and to impose the condition

$$\forall\, x \in X,\ \|f(x,t)\| \leq h(t) \tag{3.25}$$

almost everywhere in T for some $h \in L^2(T)$.

Let us recall that the support of a function $g : X \to \mathbb{R}$ is defined to be the closure of the set of points in $\mathbb{R}^r$ at which g is non-zero. It turns out that, despite a rather abstract framework for continuous designs, the results obtained through their use are surprisingly closely related to discrete designs whose support consists of a finite number of x values. In other words, the optimal design can be chosen to be of the form

$$\xi^\star(x) = \left\{ \begin{matrix} x^1, & x^2, & \ldots, & x^\ell \\ \xi_1, & \xi_2, & \ldots, & \xi_\ell \end{matrix} ; \quad \sum_{i=1}^{\ell} \xi_i = 1 \right\} \tag{3.26}$$

where $\ell < \infty$, which concentrates $N\xi_1$ measurements at x_1, $N\xi_2$ at x_2, and so on. In fact, we have the following assertion.

Lemma 3.3. *For any $M_0 \in \mathfrak{M}(X)$ there always exists a purely discrete design ξ with no more than $m(m+1)/2+1$ support points such that $M(\xi) = M_0$. If M_0 lies on the boundary of $\mathfrak{M}(X)$, then the number of support points is less than or equal to $m(m+1)/2$.*

Proof. We first observe that due to the symmetry of FIM's, $\mathfrak{M}(X)$ can be identified with a closed convex set of $\mathbb{R}^{m(m+1)/2}$ (it suffices to use only the elements which are on and above the diagonals). It is easy to check that the average information matrices $M(\xi_x) = \Upsilon(x)$ which correspond to one-point designs $\xi_x = \{ \begin{smallmatrix} x \\ 1 \end{smallmatrix} \}$, i.e. the designs concentrated at a single point x, are the only extreme points of $\mathfrak{M}(X)$. Hence, from Carethéodory's theorem (Pázman, 1986, Prop. III.8, p. 57), the first part of our lemma follows (any point of a compact convex set A of $\mathbb{R}^{m(m+1)/2}$ can be expressed as a convex combination of $m(m+1)/2+1$ or less extreme points of A).

The second part is established based on the assertion that any boundary point of a compact convex set A of $\mathbb{R}^{m(m+1)/2}$ can be expressed as a convex combination of $m(m+1)/2$ or less extreme points of A (Ermakov and Zhigljavsky, 1987, Th. 1.4, p. 96). ■

The above lemma makes it justified to restrict our attention only to discrete designs with a limited number of supporting points, so the introduction of continuous designs, which may seem at first sight a superfluous complication, leads to very tangible results.

To make a step further, the following additional assumptions about the design criterion $\Psi : \mathbb{R}^{m\times m} \to \mathbb{R}$ will be needed:

(A3) Ψ is convex,

(A4) If $M_1 \leq M_2$, then $\Psi(M_1) \geq \Psi(M_2)$ (monotonicity),

(A5) There exists a finite real q such that

$$\big\{\xi : \Psi[M(\xi)] \leq q < \infty\big\} = \Xi(q) \neq \emptyset$$

(A6) For any $\xi \in \Xi(q)$ and $\bar{\xi} \in \Xi(X)$, we have

$$\begin{aligned}\Psi[M(\xi) + \lambda(M(\bar{\xi}) - M(\xi))] \\ = \Psi[M(\xi)] + \lambda \int_X \psi(x,\xi)\, \bar{\xi}(\mathrm{d}x) + o(\lambda;\xi,\bar{\xi})\end{aligned} \tag{3.27}$$

where o is the usual Landau symbol, i.e.

$$\lim_{\lambda \downarrow 0} \frac{o(\lambda;\xi,\bar{\xi})}{\lambda} = 0$$

Assumption (A3) is quite natural, since it allows us to stay within the framework of convex analysis, which greatly facilitates subsequent considerations. In turn, Assumption (A4) characterizes Ψ as a linear ordering of Ξ. (As regards the notation in (A4), we adopt that of the Loewner ordering of symmetric matrices, i.e. $M_1 \leq M_2$ iff $M_2 - M_1$ is non-negative definite.) As for Assumption (A5), it only states that there exist designs with finite values of Ψ, which constitutes a rather mild and quite logical requirement. At this juncture, only Assumption (A6) calls for an appropriate comment, as at first sight it may seem a bit odd. In practice, however, (A6) simply amounts to the existence of the directional derivative

$$\delta_+\Psi(M(\xi), M(\bar{\xi}) - M(\xi)) = \left.\frac{\partial \Psi[M(\xi) + \lambda(M(\bar{\xi}) - M(\xi))]}{\partial \lambda}\right|_{\lambda = 0^+} \tag{3.28}$$

whose form must be on one hand specific, i.e. $\int_X \psi(x,\xi)\, \bar{\xi}(\mathrm{d}x)$, 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 individual elements of its matrix argument, we obtain

$$\begin{aligned}&\delta_+\Psi(M(\xi), M(\bar{\xi}) - M(\xi)) \\ &\quad = \mathrm{trace}\Big[\overset{\circ}{\Psi}(\xi)(M(\bar{\xi}) - M(\xi))\Big] \\ &\quad = \int_X \mathrm{trace}\Big[\overset{\circ}{\Psi}(\xi)\Upsilon(x)\Big]\, \bar{\xi}(\mathrm{d}x) - \mathrm{trace}\Big[\overset{\circ}{\Psi}(\xi) M(\xi)\Big] \\ &\quad = \int_X \left\{\mathrm{trace}\Big[\overset{\circ}{\Psi}(\xi)\Upsilon(x)\Big] - \mathrm{trace}\Big[\overset{\circ}{\Psi}(\xi) M(\xi)\Big]\right\} \bar{\xi}(\mathrm{d}x)\end{aligned} \tag{3.29}$$

$\Psi[M(\xi)]$	$\phi(x,\xi)$	$c(\xi)$
$-\ln\det M(\xi)$	$\dfrac{1}{t_f}\int\limits_0^{t_f} f^{\mathrm{T}}(x,t)M^{-1}(\xi)f(x,t)\,\mathrm{d}t$	m
$\operatorname{trace} M^{-1}(\xi)$	$\dfrac{1}{t_f}\int\limits_0^{t_f} f^{\mathrm{T}}(x,t)M^{-2}(\xi)f(x,t)\,\mathrm{d}t$	$\operatorname{trace} M^{-1}(\xi)$

Table 3.1: Functions which define the directional derivatives of some most popular optimality criteria.

where

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

and therefore

$$\psi(x,\xi) = c(\xi) - \phi(x,\xi) \tag{3.30}$$

the functions c and φ being respectively defined as

$$c(\xi) = -\operatorname{trace}\Big[\overset{\circ}{\Psi}(\xi)M(\xi)\Big] \tag{3.31}$$

and

$$\phi(x,\xi) = -\operatorname{trace}\Big[\overset{\circ}{\Psi}(\xi)\Upsilon(x)\Big] = -\frac{1}{t_f}\int_0^{t_f} f^{\mathrm{T}}(x,t)\overset{\circ}{\Psi}(\xi)f(x,t)\,\mathrm{d}t \tag{3.32}$$

Table 3.1 lists specific forms of the foregoing mappings for most popular design criteria.

The next result provides a characterization of the optimal designs.

Theorem 3.1. *Let Assumptions (A1)–(A6) hold. Then:*

(i) An optimal design exists comprising not more than $m(m+1)/2$ points (i.e. one less than predicted by Lemma 3.3).

(ii) The set of optimal designs is convex.

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

$$\min_{x\in X}\psi(x,\xi^\star) = 0 \tag{3.33}$$

(iv) For any purely discrete optimal design $\xi^\star$, the function $\psi(\cdot, \xi^\star)$ has value zero at all support points.

Proof. The theorem can be established in exactly the same way as Theorem 2.3.2 of (Fedorov and Hackl, 1997, p. 31) as the explicit form of the FIM is not essential in the proof. ■

It is now clear that the function ψ is of paramount importance in our considerations, as it determines the location of the support points in the optimal design $\xi^\star$ (they are situated among its points of global minimum). Moreover, given any design ξ, it indicates points at which a new observation contributes to the greatest extent. Indeed, adding a new observation atomized at a single point x^+ amounts to constructing a new design

$$\xi^+ = (1 - \lambda)\xi + \lambda\xi_{x^+} \tag{3.34}$$

for some $\lambda \in (0, 1)$. If λ is sufficiently small, then from (3.27) it may be concluded that

$$\Psi[M(\xi^+)] - \Psi[M(\xi)] \approx \lambda\psi(x^+, \xi) \tag{3.35}$$

i.e. the resulting decrease in the criterion value is approximately equal to $-\lambda\psi(x^+, \xi)$. This fact also clarifies why the function $\phi(x, \xi) = -\psi(x, \xi) + c(\xi)$ is usually called the *sensitivity function* (this terminology is somewhat reminiscent of the sensitivity coefficients introduced in Section 2.6, but we hope that it will cause no confusion).

Analytical determination of optimal designs is possible only in simple situations and for general systems it is usually the case that some iterative design procedure will be required. The next theorem is useful in the checking for optimality of designs.

Theorem 3.2. *The following characterizations of an optimal design $\xi^\star$ are equivalent in the sense that each implies the other two:*

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

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

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

All the designs satisfying (i)–(iii) and their convex combinations have the same information matrix $M(\xi^\star)$.

Proof. With minor modifications, it may be adopted, e.g. from (Ermakov and Zhigljavsky, 1987, Th. 2.3, p. 109) and therefore it is omitted. ■

When formulated for a particular design criterion, Theorem 3.2 is usually called an *equivalence theorem* and the most famous is the Kiefer-Wolfowitz equivalence theorem corresponding to D-optimum designs. In our framework, this specializes to our next assertion.

Theorem 3.3. *The following conditions are equivalent:*

(i) the design $\xi^\star$ *maximizes* $\det M(\xi)$,

(ii) the design $\xi^\star$ *minimizes* $\max\limits_{x\in X} \dfrac{1}{t_f}\displaystyle\int_0^{t_f} f^{\mathrm{T}}(x,t)M^{-1}(\xi)f(x,t)\,\mathrm{d}t$, *and*

(iii) $\max\limits_{x\in X} \dfrac{1}{t_f}\displaystyle\int_0^{t_f} f^{\mathrm{T}}(x,t)M^{-1}(\xi^\star)f(x,t)\,\mathrm{d}t = m$

Let us give a thought to the integral expression which appears in the above formulation. Based on the calculated estimate $\hat{\theta}$ we may predict the response $\hat{y}(x_0,t) = f^{\mathrm{T}}(x_0,t)\hat{\theta}$ given a design point $x_0 \in X$ and a $t \in T$. We can then evaluate the prediction error variance according to the formula

$$\mathrm{var}\big\{\hat{y}(x_0,t)\big\} = \frac{1}{Nt_f} f^{\mathrm{T}}(x_0,t)M^{-1}(\xi^\star)f(x_0,t) \tag{3.36}$$

which implies the average variance per unit time in the form

$$\overline{\mathrm{var}}\big\{\hat{y}(x_0,t)\big\} = \frac{1}{Nt_f}\left\{\frac{1}{t_f}\int_0^{t_f} f^{\mathrm{T}}(x_0,t)M^{-1}(\xi^\star)f(x_0,t)\,\mathrm{d}t\right\} \tag{3.37}$$

where the expression in the braces is exactly the one which is used in Theorem 3.3. Hence we conclude that in a D-optimum design the observations must be taken at points where the average variance of the predicted response is the largest.

Remark 3.2. The equivalence theorems can also be extended to the case where a given optimality criterion depends on some parameters whose precise values are unknown and on which the experimenter cannot exert influence. Such a situation is rather common in the sensor location setting where the FIM elements usually depend on the parameters to be identified (cf. Section 2.4.4). At this moment, it is only worth pointing out that in general it is impossible to find a design which is the 'best' for all possible values of such parameters and consequently average- and minimax-optimality

designs are recommended. A detailed discussion of this topic is postponed to Chapter 5. As a by-product, some results delineated therein will permit us to find a solution to the problem of minimizing the E-optimality criterion. For now, a direct application of the methods which have just been introduced is rather difficult owing to some problems with differentiability in the presence of multiple eigenvalues of the FIM. An alternative approximation approach to circumvent this difficulty will be presented in the next chapter in the context of moving sensors.

The above results provide us with tests for the optimality of designs. In particular,

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

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

The interesting thing about these results is that in addition to revealing striking minimax properties of optimal designs, they also provide sequential numerical design algorithms. The underlying idea is quite simple. Suppose that we have an arbitrary (non-optimal) design ξ_k obtained after k iteration steps. Further, let $\phi(\,\cdot\,,\xi_k)$ attain its maximum (necessarily $> c(\xi_k)$) at $x = x_k^0$. Then the design

$$\xi_{k+1} = (1-\lambda_k)\xi_k + \lambda_k \xi_{x_k^0} \tag{3.38}$$

(recall that $\xi_{x_k^0}$ stands for the unit-weight design concentrated at x_k^0) leads to a decrease in the value of $\Psi[M(\xi_{k+1})]$ for a suitably small λ_k. This follows since the derivative with respect to λ_k is negative, i.e.

$$\frac{\partial}{\partial \lambda_k} \Psi[M(\xi_{k+1})]\Big|_{\lambda_k = 0^+} = c(\xi_k) - \phi(x_k^0, \xi_k) < 0 \tag{3.39}$$

The steps in using the outlined gradient method can be briefly summarized as follows (Fedorov and Hackl, 1997; Walter and Pronzato, 1997; Ermakov, 1983; Rafajłowicz, 1996):

Step 1. Guess a discrete non-degenerate starting design measure ξ_0 (we must have $\det M(\xi_0) \neq 0$). Choose some positive tolerance $\eta \ll 1$. Set $k = 0$.

Step 2. Determine $x_k^0 = \arg\max_{x \in X} \phi(x, \xi_k)$. If $\phi(x_k^0, \xi_k) < c(\xi_k) + \eta$, then *STOP*.

Step 3. For an appropriate value of $0 < \lambda_k < 1$, set

$$\xi_{k+1} = (1 - \lambda_k)\xi_k + \lambda_k \xi_k^0$$

increment k by one and go to Step 2.

In the same way as for the classical first-order algorithms in common use for many years, it can be shown that the above algorithm converges to an optimal design provided that the sequence $\{\lambda_k\}$ is suitably chosen. For example, the choices which satisfy one of the conditions below will yield the convergence:

(i) $\lim\limits_{k\to\infty} \lambda_k = 0$, $\sum\limits_{k=0}^{\infty} \lambda_k = \infty$ (Wynn's algorithm),

(ii) $\lambda_k = \arg\min\limits_{\lambda} \Psi[(1 - \lambda)M(\xi_k) + \lambda M(\xi_{x_k^0})]$ (Fedorov's algorithm),

(iii) $\lambda_k = \begin{cases} \lambda_{k-1} & \text{if } \Psi[(1 - \lambda_{k-1})M(\xi_k) + \lambda_{k-1}M(\xi_{x_k^0})] < \Psi[M(\xi_k)] \\ \gamma\lambda_{k-1} & \text{otherwise} \end{cases}$
for a suitably chosen $\gamma < 1$.

At this very moment, we should emphasize that the outlined numerical technique inherits all the drawbacks of its gradient counterparts from mathematical programming. In particular, it usually shows substantial improvments in the first few iterations, but has poor convergence characteristics as the optimal solution is approached.

Computationally, Step 2 is of crucial significance but at the same time it is the most time-consuming step in the algorithm. Complications arise, among other things, due to the necessity of calculating a global maximum of $\phi(\cdot, \xi_k)$ which is usually multimodal (getting stuck in one of local maxima leads to precocious termination of the algorithm). Therefore, while implementing this part of the computational procedure an effective global optimizer is essential. Based on numerous computer experiments it was found that the extremely simple adaptive random search (ARS) strategy from (Venot *et al.*, 1986; Walter and Pronzato, 1997, p. 216) is especially suited for that purpose if the design region X is a hypercube, i.e. the admissible range for x_i, $i = 1, \ldots, n$ is in the form

$$x_{i\,\min} \le x_i \le x_{i\,\max} \tag{3.40}$$

The routine choses the initial point x^0 at the centre of X. After q iterations, given the current best point x^q, a random displacement vector Δx is

generated and the trial point

$$x^+ = \Pi_X(x^q + \Delta x) \tag{3.41}$$

is checked, where Δx follows a multinormal distribution with zero mean and covariance

$$\mathrm{cov}\{\Delta x\} = \mathrm{diag}[\sigma_1, \ldots, \sigma_n] \tag{3.42}$$

Π_X being the projection onto X.

If $\phi(x^+, \xi^k) < \phi(x^q, \xi^k)$, then x^+ is rejected and consequently we set $x^{q+1} = x^q$, otherwise x^+ is taken as x^{q+1}. The adaptive strategy consists in repeatedly alternating two phases. During the first one (variance selection) $\mathrm{cov}\{\Delta x\}$ is selected from among the sequence ${}^1\sigma, {}^2\sigma, \ldots, {}^5\sigma$, where

$${}^1\sigma = x_{\max} - x_{\min} \tag{3.43}$$

and

$${}^i\sigma = {}^{(i-1)}\sigma/10, \quad i = 2, \ldots, 5 \tag{3.44}$$

With such a choice, ${}^1\sigma$ is large enough to allow for an easy exploration of X, whereas ${}^5\sigma$ is small enough for a precise localization of an optimal point. In order to allow a comparison to be drawn, all the possible ${}^i\sigma$'s are used $100/i$ times, starting from the same initial value of x. The largest ${}^i\sigma$'s, designed to escape local maxima, are therefore used more often than the smaller ones.

During the second (exploration) phase, the most successful ${}^i\sigma$ in terms of the criterion value reached during the variance selection phase is used for 100 random trials started from the best x obtained so far. The variance-selection phase then resumes, unless the decision to stop is taken.

As regards the choice of an optimal λ_k in Fedorov's variant of Step 3, it should be emphasized that the situation is a bit different from the well-known case of linear regression considered in classic textbooks for which it is possible to determine a closed-form solution. Since in our case the application of the matrix-inversion lemma by no means simplifies the problem, an optimal λ_k has to be determined numerically, e.g. with the use of the golden-section search.

Furthermore, while implementing the algorithms, numerous additional problems should be addressed. For instance, it may be possible to achieve a greater decrease in the value of Ψ by removing a measure from a point

already in the design ξ_k and distributing the measure removed among the most promising points of support. In this way, undesirable points of support which were included in the initial design can be eliminated. Another complication is the tendency of the points produced in Step 2 to cluster around support points of the optimal design. This can be avoided by checking whether the newly generated point is close enough to a point of the current support so as to qualify them as coinciding points. If so, the latter is replaced by the former with a simultaneous update of the weights of all the points according to the rule of Step 3. A cyclic removal of points with negligible weights is also suggested by Rafajłowicz (1996) in order to maintain a relatively small number of support points.

A detailed description of all the troubles and corresponding tricks which were invented to alleviate them so as to create efficient codes for constructing optimal experiments can no doubt constitute a subject for a separate monograph. Notwithstanding the fact that the problem outlined in this section is slightly different from the classical formulation, the problems encountered remain in principle the same and hence this topic will not be further discussed owing to a limited volume of this monograph. For a more comprehensive discussion, we refer the reader to the excellent specialized literature (Fedorov and Hackl, 1997; Walter and Pronzato, 1997; Ermakov, 1983; Rafajłowicz, 1996; Rafajłowicz, 1998; Skubalska-Rafajłowicz and Rafajłowicz, 1998; Torsney, 1988).

Example 3.1. To get a feel for Theorems 3.2 and 3.3, consider $X = [-1, 1]$ and the following vector of basis functions:

$$f(x,t) = \mathrm{col}[1, t\sin(\pi x), t^2\exp(-x)]$$

for which a D-optimal design was to be found. To generate a solution, Fedorov's version of the foregoing first-order algorithm was implemented and the design

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

such that $\det[M(\xi^0)] = 0.023928$, was adopted to launch the computational procedure. After nine cycles of the algorithm the following approximation of the optimal design was obtained:

$$\xi^\star = \begin{Bmatrix} -1.000000, & -0.512301, & 0.497145 \\ 0.370455, & 0.336952, & 0.292593 \end{Bmatrix}$$

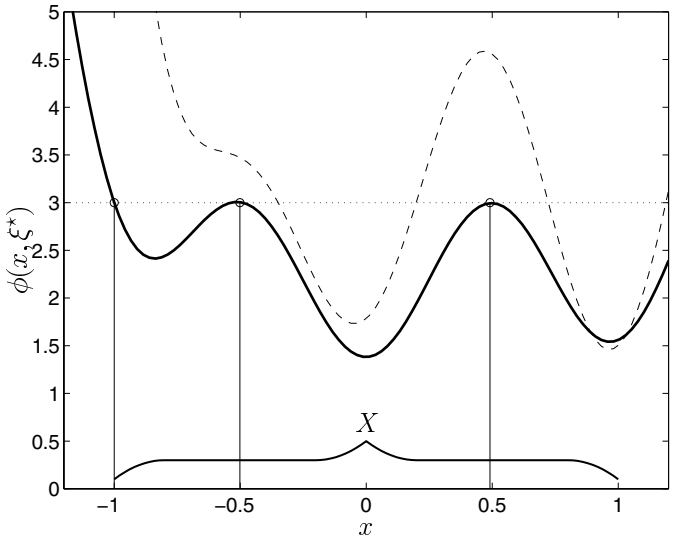


Figure 3.1: Sensitivity function for the D-optimal design of Example 3.1 (solid line). The same function for an exemplary non-optimal design is also shown (dashed line) for the sake of comparison.

which corresponds to $\det[M(\xi^\star)] = 0.080463$. This result is illustrated in Fig. 3.1, where a solid line represents the optimal sensitivity function. As can be seen, in the interval $[-1, 1]$ it attains the maximal value of $m = 3$ at the points supporting the design. For comparison, the dashed line represents an exemplary non-optimal design. Clearly, the maximal value of ϕ in the latter case exceeds the number of parameters. ♢

3.2 Continuous designs in measurement optimization

The introduction of continuous designs makes it possible, on one hand, to advance a very elegant theory based on convex optimization and, on the other hand, to develop very effective numerical algorithms which are implementable even on a low-cost PC. A natural question is therefore how to exploit all those benefits while designing a measurement system to estimate the unknown parameters of a given DPS as accurately as possible. Unfortunately, the answer is not as simple as that, since even if the model equation under consideration is linear in its parameters, the state depends linearly on

those parameters only in exceptional cases and the rule is that this dependence is highly non-linear, which causes severe difficulties and practically excludes direct analytical solutions in most interesting situations.

To settle this problem, it is customary to linearize the system response in the vicinity of a prior estimate θ^0 to the unknown parameter vector θ (Sun, 1994). As a result, observations may be represented approximately as

$$z(t) \approx y_{\mathrm{m}}(t;\theta^0) + \left.\frac{\partial y_{\mathrm{m}}(t;\theta)}{\partial\theta}\right|_{\theta=\theta^0}(\theta-\theta^0) + \varepsilon_{\mathrm{m}}(t) \tag{3.45}$$

where

$$y_{\mathrm{m}}(t;\theta^0) = \mathrm{col}[y(x^1,t;\theta^0),\ldots,y(x^N,t;\theta^0)] \tag{3.46}$$

$$\frac{\partial y_{\mathrm{m}}(t;\theta)}{\partial\theta} = \begin{bmatrix} \dfrac{\partial y(x^1,t;\theta)}{\partial\theta_1} & \cdots & \dfrac{\partial y(x^1,t;\theta)}{\partial\theta_m} \\ \vdots & & \vdots \\ \dfrac{\partial y(x^N,t;\theta)}{\partial\theta_1} & \cdots & \dfrac{\partial y(x^N,t;\theta)}{\partial\theta_m} \end{bmatrix} \tag{3.47}$$

the last quantity being the Jacobian of the observation vector y_{m} with respect to parameter vector θ. After an obvious rearrangement, (3.45) is expressed in the form

$$z(t) - y_{\mathrm{m}}(t;\theta^0) + \left.\frac{\partial y_{\mathrm{m}}(t;\theta)}{\partial\theta}\right|_{\theta=\theta^0}\theta^0 = \left.\frac{\partial y_{\mathrm{m}}(t;\theta)}{\partial\theta}\right|_{\theta=\theta^0}\theta + \varepsilon_{\mathrm{m}}(t) \tag{3.48}$$

so we loosely get the setting of (3.1) with $z(t)$ replaced by the left-hand side of (3.48) and

$$f(x^j,\,\cdot\,) = \left(\frac{\partial y(x^j,\,\cdot\,;\theta)}{\partial\theta}\right)^{\mathrm{T}}_{\theta=\theta^0} \tag{3.49}$$

Accordingly, from (3.16) it follows that the respective average 'FIM' which approximates (up to a constant multiplier) the dispersion matrix $\mathrm{cov}\{\hat{\theta}\}$ may be expressed as

$$M(\xi_N) = \sum_{i=1}^{\ell} p_i \frac{1}{t_f}\int_0^{t_f}\left(\frac{\partial y(x^i,t;\theta)}{\partial\theta}\right)^{\mathrm{T}}\left(\frac{\partial y(x^i,t;\theta)}{\partial\theta}\right)\Bigg|_{\theta=\theta^0}\mathrm{d}t \tag{3.50}$$

It goes without saying that (3.50) is valid as long as the approximation (3.45) is warranted. One way or another, it is now evident that the FIM

(3.50) will depend on the preliminary estimate θ^0 around which the model is linearized, so logically, the optimal sensor location can never be found at the design stage unless θ^0 is very close to the true parameters or the Jacobian (3.47) is insensitive to the values of the model parameters (in practice, the latter is unlikely in the considered applications).

It is worth pointing out that the delineated procedure is not only based in brute force and ignorance, as there have appeared many works regarding its statistical rationale. For more precise results on the consistency of least-squares estimates in DPS's and their asymptotic distributions, the interested reader should consult some painstaking works of Fitzpatrick (Banks and Fitzpatrick, 1990; Fitzpatrick, 1991; Fitzpatrick, 1995; Fitzpatrick and Yin, 1995; Yin and Fitzpatrick, 1992). At this juncture note that characterizing parameter uncertainty in a non-linear-in-parameters model by the inverse of the FIM involves approximations to which few alternatives exist (Walter and Pronzato, 1997; Gajda and Szyper, 1998).

If we assume that both $y(\cdot\,,\cdot\,;\theta^0)$ and $\partial y(\cdot\,,\cdot\,;\theta^0)/\partial\theta_i$, $i = 1,\ldots,m$ are continuous in $\bar{\Omega}\times T$ (for some relaxation of this requirement, see Remark 3.1), then all the results of Section 3.1, starting from the notion of a continuous design, through all the lemmas and theorems, and finally inclusive of the outlined algorithms of first-order, can be directly employed without any changes, bearing in mind (3.49). For example, the counterpart to the FIM of (3.18) is given in terms of the sensitivity coefficients as

$$M(\xi) = \int_X \Upsilon(x)\,\xi(\mathrm{d}x) \tag{3.51}$$

X being interpreted as an admissible region where we are allowed to place the sensors (a compact subset of $\bar{\Omega}$), and

$$\Upsilon(x) = \frac{1}{t_f}\int_0^{t_f} \left(\frac{\partial y(x,t;\theta)}{\partial\theta}\right)^{\mathrm{T}} \left(\frac{\partial y(x,t;\theta)}{\partial\theta}\right)\bigg|_{\theta=\theta^0} \mathrm{d}t$$

At this very moment, some interpretation of the resulting optimal design of the form (3.26) would be relevant. Since we manipulate continuous designs, the products $N\xi_i$, $i = 1,\ldots,\ell$ are not necessarily integers. In the spatial setting, however, the number of sensors may be quite large and the set of candidate points is continuous so that we can expect that some rounding procedures (Pukelsheim and Rieder, 1992) of the considered approximate designs calculated by the afore-mentioned algorithms will yield sufficiently good designs. Alternatively, some *exchange algorithms* can be adopted from the classical theory of optimal experiments if N is relatively

small, but such a procedure does not change the underlying idea and therefore it will not be pursued.

An interesting interpretation of continuous designs in terms of the randomized choice is given in (Rafajłowicz, 1986c). Namely, for ξ_N given by (3.15), if N sensors are randomly allocated to the points x^i, $i = 1, \ldots, \ell \leq N$ according to the distribution p_i, $i = 1, \ldots, \ell$ and such that the measurement process is repeated many times, then (3.50) is the expected value of the FIM. This justifies our results as theoretically exact from a slightly different point of view.

Some numerical examples have been solved to indicate the general nature of the results.

Example 3.2. The approach to the sensor placement developed in the previous section was applied to the optimal estimation of the spatially-varying parameter $\kappa = \kappa(x)$ in the heat-conduction process through a thin flat isotropic plate whose flat surfaces were insulated and which occupied the region $\Omega = [0, 1]^2$ with boundary Γ along which heat was lost to the surroundings. The unsteady state temperature $y = y(x, t)$ over the time horizon $T = (0, 1)$ was described by a linear parabolic equation of the form

$$\frac{\partial y(x,t)}{\partial t} = \frac{\partial}{\partial x_1}\left(\kappa(x)\frac{\partial y(x,t)}{\partial x_1}\right) + \frac{\partial}{\partial x_2}\left(\kappa(x)\frac{\partial y(x,t)}{\partial x_2}\right) \quad \text{in } \Omega \times T \tag{3.52}$$

The initial and boundary conditions of (3.52) were

$$y(x, 0) = 5 \qquad \text{in } \Omega \tag{3.53}$$

$$y(x, t) = 5(1 - t) \quad \text{on } \Gamma \times T \tag{3.54}$$

In our simulation study, the following true parameter was considered:

$$\kappa(x) = \theta_1 + \theta_2 x_1 + \theta_3 x_2 \tag{3.55}$$

where $\theta_1 = 0.1$, $\theta_2 = \theta_3 = 0.3$. On the basis of simulated data generated with the specified κ, we tried to determine a continuous design over $X = \bar{\Omega}$ such that the D-optimality criterion for $\theta = (\theta_1, \theta_2, \theta_3)$ would be minimized.

In order to numerically solve the measurement location problem, a computer programme was written in Essential Lahey Fortran 90 v.4.0 (Meissner, 1997) using a PC (Pentium II, 300 Mhz, 128 MB RAM) running Windows NT 4.0. The state and sensitivity equations were first solved using the finite-element method on an even grid (with 15 divisions along each space axis and 30 divisions of the time interval). The sensitivity coefficients were

then interpolated via tri-cubic spline interpolation (see Appendix C.2) and the corresponding spline parameters stored in computer memory. Finally, Fedorov's version of the first-order algorithm was applied with the ARS algorithm of p. 49 to maximize the determinant of the FIM. (The maximum number of evaluations for the performance index was 2000.)

Starting from the design

$$\xi_0 = \begin{Bmatrix} (0.6, 0.2), & (0.2, 0.5), & (0.1, 0.2) \\ 1/3 & 1/3 & 1/3 \end{Bmatrix}$$

after 13 iterations (which took about two minutes), the following approximation to the optimal design was obtained:

$$\xi^\star = \begin{Bmatrix} (0.65224, 0.26353), & (0.27083, 0.63834), & (0.14647, 0.15668) \\ 0.33570, & 0.33410, & 0.33019 \end{Bmatrix}$$

for the tolerance $\eta = 10^{-2}$.

The design is concentrated at three support points with approximately equal weights, which means that if we are to locate N sensors, then we should strive to distribute them as evenly as possible between the three calculated potential locations (as outlined before, sensor clusterization is inherent to the approach due to the assumption that the measurements are independent even though some of the sensors take measurements at the same point).

Let us observe that the diffusivity coefficient κ together with the system of boundary and initial conditions assume one axis of symmetry, i.e. the line $x_2 = x_1$. We feel by intuition that this symmetry should also be preserved in a way in the optimal design. In fact, this is confirmed in Fig. 3.2 where the optimal sensor positions are displayed. They are slightly shifted towards the lower-left part of the system, at which place the diffusivity coefficient is smaller and the system output is the most sensitive to changes in θ. $\diamondsuit$

Example 3.3. In another simulation experiment, the spatio-temporal domain was the same as in Example 3.2 (similarly, the introduced discretization for numerical calculations was retained). This time, however, the diffusion equation contained a driving force, i.e.

$$\begin{aligned} \frac{\partial y(x,t)}{\partial t} = \frac{\partial}{\partial x_1}\left(\kappa(x)\frac{\partial y(x,t)}{\partial x_1}\right) + \frac{\partial}{\partial x_2}\left(\kappa(x)\frac{\partial y(x,t)}{\partial x_2}\right) \\ + 30\exp(-30\|x-a\|^2) \quad \text{in } \Omega \times T \end{aligned} \tag{3.56}$$

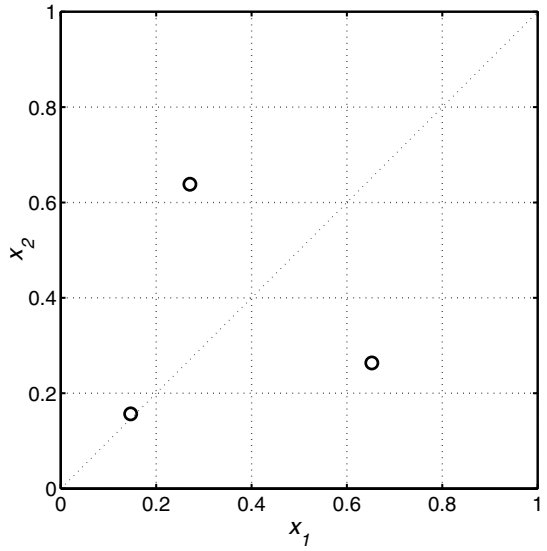


Figure 3.2: Optimal location of the support points in the problem of Example 3.2 (the axis of symmetry is represented by a sloping dotted line).

where $a = (0.75, 0.25)$, see Fig. 3.3. The boundary Γ was split into two subsets: $\Gamma_1 = \{(0, x_2) : 0 \leq x_2 \leq 1\}$ and $\Gamma_2 = \Gamma \setminus \Gamma_1$ so that the boundary conditions were

$$y(x,t) = \begin{cases} 6x_2(1-x_2) & \text{on } \Gamma_1 \times T \\ 0 & \text{on } \Gamma_2 \times T \end{cases} \tag{3.57}$$

The initial state was the same as before, i.e.

$$y(x,0) = 5 \quad \text{in } \Omega \tag{3.58}$$

Our task consisted in finding a best D-optimal design to identify a slightly changed diffusion coefficient

$$\kappa(x) = \theta_1 + \theta_2 x_1, \quad \theta_1 = 0.1, \quad \theta_2 = 0.3 \tag{3.59}$$

or, more precisely, the coefficients θ_1 and θ_2. All the other settings were the same as in Example 3.2.

Starting from the initial design

$$\xi_0 = \begin{Bmatrix} (0.6, 0.2), & (0.2, 0.5) \\ 1/2 & 1/2 \end{Bmatrix}$$

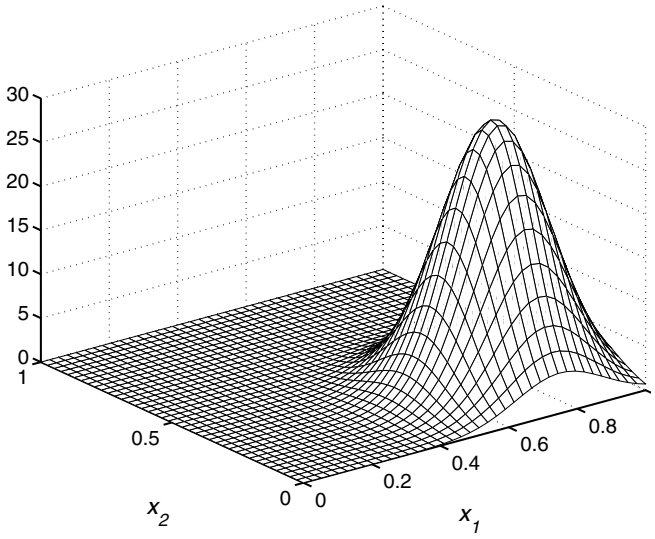


Figure 3.3: Driving force employed in Example 3.3.

after three iterations, we obtained the following approximation to the optimal design whose support is shown in Fig. 3.4:

$$\xi^\star = \begin{Bmatrix} (0.70166, 0.30929) & (0.16965, 0.53752) \\ 0.483938, & 0.516062 \end{Bmatrix}$$

On reflection, this result is not surprising. Indeed, in our system there exist two perturbations, i.e. the boundary excitation on Γ_1 and the impulse-like force concentrated around a, so logically the regions which provide most information about the system should lie in the vicinity of them. Since the corresponding weights are practically equal to each other, we should assign to each support point half of the available sensors. $\diamondsuit$

3.3 Clusterization-free designs

As pointed out in (Müller, 1998; Fedorov, 1996), two special features distinguish the spatial data collection schemes from classical regression designs. First of all, spatial observations are often affected by local correlations which are unaccounted for by standard techniques of optimum experimental design. What is more, there is usually no possibility of replicated measurements, i.e. different sensors cannot take measurements at one point without

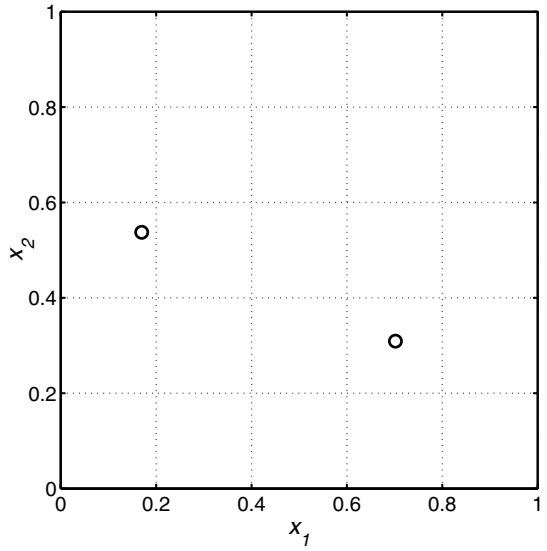


Figure 3.4: Optimal location of the support points in the problem of Example 3.3.

influencing one another. Anyway, several sensors situated in the close vicinity of one another usually do not give more information than a single sensor. The assumption of independent observations is advantageous from a theoretical point of view, since it allows for direct use of sublime results of convex optimization, but it can hardly be justified when in the optimal solution some sensors are to take measurements near one another. This generates interest in the so-called *clusterization-free* designs where the distances between the sensors are long enough in order to guarantee the independence of their measurements. This is reminiscent of the idea of replication-free designs which have emerged relatively late in the context of spatial statistics (see the monograph by Müller (1998), a survey by Fedorov (1996), and a seminal work by Brimkulov *et al.* (1986)).

In the literature, a typical motivation to work on replication-free designs is the situation when we observe the values of a random process or a random field at some times (at some points). When the mean of the process contains unknown parameters, we have a regression model, but typically without the possibility of replications, because just one realization of the process is allowed, and the experimental design consists in an adequate choice of times (points) of observation. This setup was considered e.g. in (Müller and Pázman, 1998) where the concept of continuous designs was extended by

the introduction of the so-called approximate information matrices. The preliminary results are quite promising, but the attendant derivations are rather awkward and lengthy, and the results themselves are obtained after a sequence of approximations.

An alternative approach to constructing replication-free designs was proposed by Fedorov (Fedorov and Hackl, 1997; Fedorov, 1996; Cook and Fedorov, 1995; Fedorov, 1989). In spite of its somewhat abstract assumptions, the resulting algorithm of exchange type is very easy to implement. It turns out that Fedorov's approach can be adapted to the problems considered in our monograph with relative ease.

The main idea is to operate on the density of sensors (i.e. the number of sensors per unit area), rather than on the sensors' locations, which is justified for a sufficiently large total number of sensors N. In contrast to the classical designs, however, we impose the crucial restriction that the density of sensor allocation must not exceed some prescribed level. For a design measure $\xi(\mathrm{d}x)$ this amounts to the condition

$$\xi(\mathrm{d}x) \leq \omega(\mathrm{d}x) \tag{3.60}$$

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

$$\int_X \omega(\mathrm{d}x) \geq 1 \tag{3.61}$$

Consequently, we are faced with the following optimization problem: Find

$$\xi^\star = \arg \min_{\xi \in \Xi(X)} \Psi(\xi) \quad \text{subject to} \quad \xi(\mathrm{d}x) \leq \omega(\mathrm{d}x) \tag{3.62}$$

The design $\xi^\star$ above is then said to be a (Ψ, ω)-*optimal design*.

Apart from Assumptions (A1), (A2) of p. 41 and (A3)–(A6) of p. 43, a proper mathematical formulation calls for the following proviso:

(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

$$\int_{\Delta X'} \omega(\mathrm{d}x) < \int_{\Delta X} \omega(\mathrm{d}x) \tag{3.63}$$

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

$$\xi(\Delta X) = \begin{cases} \omega(\Delta X) & \text{for } \Delta X \subset \operatorname{supp} \xi \\ 0 & \text{for } \Delta X \subset X \setminus \operatorname{supp} \xi \end{cases} \tag{3.64}$$

Given a design ξ, we will say that the function $\psi(\cdot\,,\xi)$ defined by (3.30) 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

$$\int_{\Delta X_1} \psi(x,\xi)\,\omega(\mathrm{d}x) \le \int_{\Delta X_2} \psi(x,\xi)\,\omega(\mathrm{d}x) \tag{3.65}$$

We can now formulate the main result which provides a characterization of (Ψ,ω)-optimal designs.

Theorem 3.4. *Let Assumptions (A1)–(A7) hold. Then:*

(i) There exists an optimal design $\xi^\star \in \bar{\Xi}$, 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 result may be proved in much the same way as Theorem 4.3.1 of (Fedorov and Hackl, 1997, p. 63), also see (Cook and Fedorov, 1995), since the explicit form of $\Upsilon(x)$ in the definition of the FIM is not substantial in the derivations. ■

From a practical point of view, the above theorem 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 $\psi(\cdot\,,\xi^\star)$ (let us note that for the D-optimality criterion this can be expressed as the situation when $\phi(\cdot\,,\xi^\star)$ is greater in $\operatorname{supp}\xi^\star$ than in the complement of $\operatorname{supp}\xi^\star$, which amounts to allocating observations to the points at which we know least of all about the system response, cf. the interpretation of $\phi(\cdot\,,\xi^\star)$ of p. 47).

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

$$N^\star(\Delta X_i) = \left\lceil N \int_{\Delta X_i} \xi^\star(\mathrm{d}x) \right\rceil \tag{3.66}$$

of sensors whose positions may coincide with nodes of some uniform grid (Fedorov and Hackl, 1997) (here $\lceil\zeta\rceil$ is the smallest integer greater than or equal to ζ). Additionally, bear in mind that we must also have $\xi^\star(\mathrm{d}x) = \omega(\mathrm{d}x)$ in $X^\star$.

Clearly, unless the considered design problem is quite simple, we must employ a numerical algorithm to make the outlined conceptions useful. 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 ξ_k. This is embodied by an iterative algorithm presented below:

Step 1. Guess an initial design $\xi_0 \in \bar{\Xi}$. Set $k = 0$.

Step 2. Set $X_{1k} = \operatorname{supp}\xi_k$ and $X_{2k} = X \setminus X_{1k}$. Determine

$$x_{1k} = \arg\max_{x\in X_{1k}} \psi(x,\xi_k), \quad x_{2k} = \arg\min_{x\in X_{2k}} \psi(x,\xi_k)$$

If $\psi(x_{1k},\xi_k) < \psi(x_{2k},\xi_k) + \eta$, where $\eta \ll 1$, then STOP. Else, find two sets $S_{1k} \subset X_{1k}$ and $S_{2k} \subset X_{2k}$ such that $x_{1k} \in S_{1k}$, $x_{2k} \in S_{2k}$ and

$$\int_{S_{1k}} \omega(\mathrm{d}x) = \int_{S_{2k}} \omega(\mathrm{d}x) = \alpha_k$$

(i.e. the measures of S_{1k} and S_{2k} must be identical) for some $\alpha_k > 0$.

Step 3. Construct ξ_{k+1} such that

$$\operatorname{supp}\xi_{k+1} = X_{1,k+1} = (X_{1k} \setminus S_{1k}) \cup S_{2k}$$

Increment k and to go Step 2.

Convergence is guaranteed if the sequence $\{\alpha\}_{k=0}^{\infty}$ satisfies the conditions (Fedorov, 1989)

$$\lim_{k\to\infty} \alpha_k = 0, \quad \sum_{k=0}^{\infty} \alpha_k = \infty \tag{3.67}$$

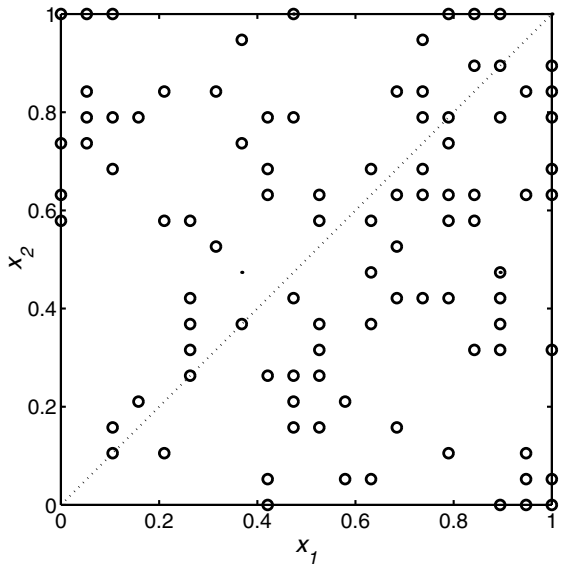
Within the framework of sensor placement, we usually have $\omega(\mathrm{d}x) = \varrho(x)\mathrm{d}x$, where ϱ is a density function. But in this situation we may restrict our attention to constant ϱ's (indeed, in any case we can perform an appropriate change of coordinates). Moreover, while implementing the algorithm

on a computer, all integrals are replaced by sums over some regular grid elements. Analogously, the sets X, X_{1k}, X_{2k}, S_{1k} and S_{2k} then simply consist of grid elements. 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_k is usually fixed and, what is more, one-point exchanges are most often adopted, i.e. $S_{1k} = \{x_{1k}\}$ and $S_{2k} = \{x_{2k}\}$, which substantially simplifies implementation. Let us note, however, that convergence to an optimal design is assured only for decreasing α_k'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).

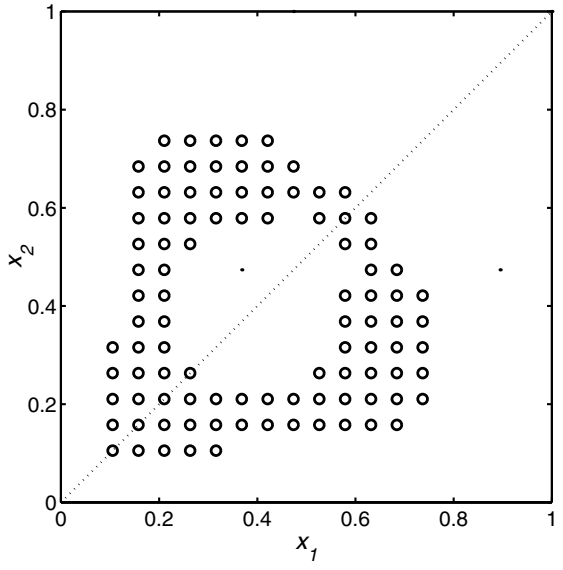
Example 3.4. Having developed the algorithm for calculation of clusterization-free designs, we go straight to a demonstrative example. To this end, for the setting of Example 3.2, consider the problem of locating $N = 97$ sensors. A (20×20)-point uniform grid was introduced to approximate the design space and an initial design was generated by randomly selecting its support points. This situation is shown in Fig. 3.5(a), where dots represent the grid points (these were potential sites where the sensors could be placed, but at most one sensor at one point) and open circles indicate the actual sensor positions.

In order to calculate a D-optimal design, a simple one-point correction algorithm was employed ($\eta = 10^{-2}$) which produced after only 83 iterations (practically, in the blink of an eye) the solution displayed in Fig. 3.5(b). The interesting thing about this solution is that the sensors tend to assemble round the points calculated based on the continuous-design approach. Finally, note that, as expected, symmetry is perfectly retained (cf. the axis of symmetry expressed by the sloping dotted line). ♢

Example 3.5. The setting of Example 3.3 served as another test of the algorithm. The grid and parameters of Example 3.4 were left without changes and only a slightly altered number of sensors ($N = 100$) were used. Similarly, the initial design presented graphically in Fig. 3.6(a) was generated by randomly selecting its support points. The optimal design obtained after 68 iterations is shown in Fig. 3.6(b). As can be seen, the sensors split into two groups: the first reacts to the perturbation on the left boundary, while the other takes measurements in the zone where the driving force acts as another perturbation. ♢

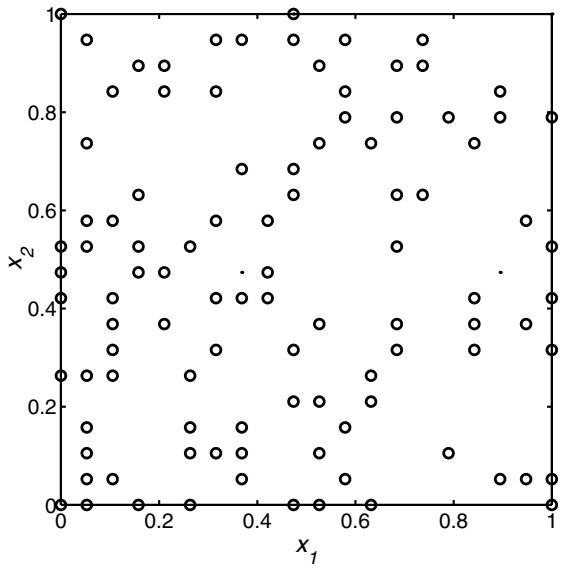


(a)

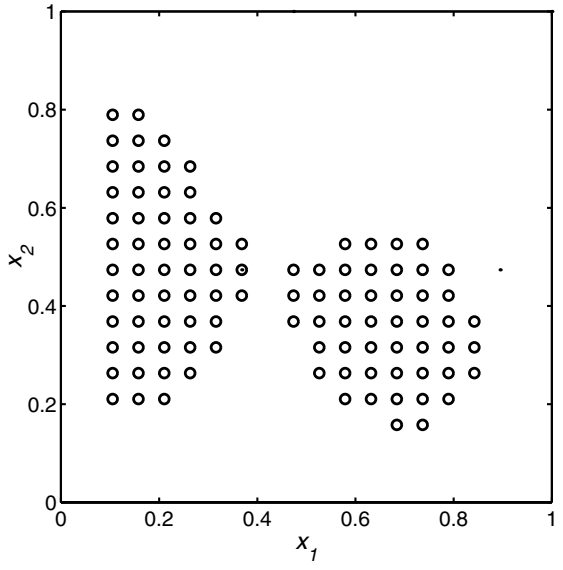


(b)

Figure 3.5: Calculation of the clusterization-free D-optimal design of Example 3.4: (a) Initial design (b) Optimal solution.



(a)



(b)

Figure 3.6: Calculation of the clusterization-free D-optimal design of Example 3.5: (a) Initial design (b) Optimal solution.

3.4 Non-linear programming approach

When the total number of sensors to be located in a given domain is moderate, the very first idea, which suggests itself, is to exploit numerous well-known numerical techniques of constrained optimization. In principle, such an approach is not difficult to apply (Uciński, 1998a) and only computation of the gradient of the design criterion necessitates some comments if gradient methods are to be employed.

As in (2.12), write

$$s = (x^1, \ldots, x^N) \tag{3.68}$$

Moreover, we denote $(\partial y/\partial\theta)^{\mathrm{T}}$ briefly by g. Accordingly, the design criterion to be minimized may be rewritten as

$$J(s) = \Psi[M(s)] \tag{3.69}$$

where

$$M(s) = \frac{1}{Nt_f} \sum_{j=1}^{N} \int_0^{t_f} g(x^j, t) g^{\mathrm{T}}(x^j, t)\, \mathrm{d}t \tag{3.70}$$

Using the chain rule, we get

$$\frac{\partial J(s)}{\partial s_r} = \operatorname{trace} \left\{ \overset{\circ}{\Psi}(s) \frac{\partial M(s)}{\partial s_r} \right\} \tag{3.71}$$

where s_r stands for the r-th component of s, and

$$\overset{\circ}{\Psi}(s) = \left. \frac{\partial \Psi(M)}{\partial M} \right|_{M=M(s)} \tag{3.72}$$

For most popular critera we have (see e.g. Ermakov and Zhigljavsky, 1987, Th. 3.3, p. 309 and Th. 3.4, p. 310):

- If $\Psi(M) = -\ln\det M$, then

$$\overset{\circ}{\Psi}(s) = -M^{-1}(s)$$

- If $\Psi(M) = \operatorname{trace} M^{-1}$, then

$$\overset{\circ}{\Psi}(s) = -M^{-2}(s)$$

- If $\Psi(M) = -\operatorname{trace} M$, then

$$\overset{\circ}{\Psi}(s) = -I$$

where I is the identity matrix.

As for computation of $\partial M/\partial s_r$, let us observe first that s_r appears at only one term of the sum in (3.70), since s_r is just a spatial coordinate of one of the sensors. If we use the symbol j_r to denote the index of the corresponding sensor, then obviously we have

$$\frac{\partial M}{\partial s_r} = \frac{1}{Nt_f} \int_0^{t_f} \left\{ \frac{\partial g(x^{j_r}, t)}{\partial s_r} g^{\mathrm{T}}(x^{j_r}, t) + g(x^{j_r}, t) \frac{\partial g^{\mathrm{T}}(x^{j_r}, t)}{\partial s_r} \right\} \mathrm{d}t \tag{3.73}$$

Hence, on account of the symmetry of $\overset{\circ}{\Psi}(s)$, it follows that

$$\frac{\partial J(s)}{\partial s_r} = \frac{2}{Nt_f} \operatorname{trace} \left\{ \overset{\circ}{\Psi}(s) \int_0^{t_f} \frac{\partial g(x^{j_r}, t)}{\partial s_r} g^{\mathrm{T}}(x^{j_r}, t)\, \mathrm{d}t \right\} \tag{3.74}$$

We see at once that calculation of $\nabla J(s)$ requires an efficient procedure to determine spatial derivatives of the sensitivity coefficients. Let us note, however, that this does not present a problem if we take advantage of spline interpolation (see Appendix C.2 for details).

Direct application of optimization techniques by no means excludes the phenomenon of clusterization. One way to attempt to avoid this undesirable effect is to include into the non-linear programming formulation appropriate constraints on the admissible distances between the sensors. Since such a solution will be discussed in the next chapter within a more general framework of moving sensors, here we focus our attention on an alternative approach, which consists in taking account of mutual correlations between the measurements made by different sensors. In other words, this time we assume that the covariance matrix C in (3.3) may not be diagonal. For example, its elements could be of the following isotropic form (Nychka and Saltzman, 1998):

$$c_{ij} = \sigma^2 \exp(-\|x^i - x^j\|/\beta) \tag{3.75}$$

Occasionally, its extension

$$c_{ij} = \sigma(x^i)\sigma(x^j) \exp(-\|x^i - x^j\|/\beta) \tag{3.76}$$

is also used, which allows for different marginal variances.

Let us note that if any two sensors are placed at one point, then the corresponding columns (and rows) of C are identical, which means that C becomes singular.

It is easy to check that the average FIM is then given by

$$M(s) = \frac{1}{Nt_f} \sum_{i=1}^{N} \sum_{j=1}^{N} \int_0^{t_f} d_{ij}(s) g(x^i, t) g^{\mathrm{T}}(x^j, t) \, \mathrm{d}t \tag{3.77}$$

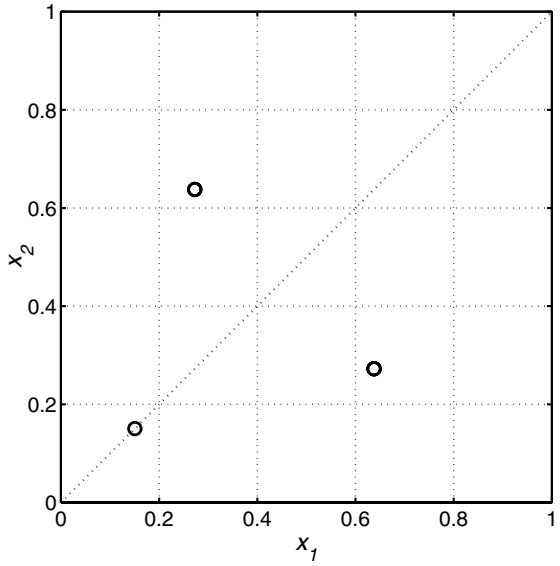
where d_{ij}'s are the elements if the inverse of C (i.e. $D = \left[d_{ij}\right] = C^{-1}$). A first inconvenience is that the form of $M(s)$ is much more cumbersome than in the case of independent measurements. But a more severe difficulty is that the functional dependence of M on s is much less regular owing to the occurence that C may be singular or nearly singular, which necessitates the notion of pseudo-inverses and involves serious problems with differentiability and numerical stability. Consequently, in practice it is much easier to simply impose additional constraints on the distances between the sensors which will warrant the assumption of independent measurements.

Example 3.6. Consider anew the setting of Example 3.2 for which six sensors were to be placed with the use of the direct non-linear programming approach. At first, the case of independent measurements was tested based on a sequential constrained quadratic programming (SQP) method (cf. Bertsekas, 1999; Spellucci, 1998a; Spellucci, 1998b; Miller, 1998). Starting from an initial solution generated via the ARS procedure of p. 49, the SQP algorithm found the approximate optimal solution

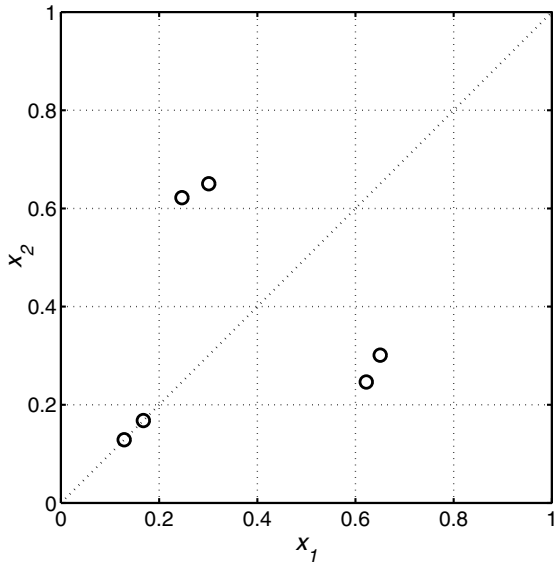
$$s^\star = \begin{pmatrix} 0.1505197, & 0.1505197, \ldots \\ 0.1505197, & 0.1505197, \ldots \\ 0.2724469, & 0.6376952, \ldots \\ 0.2724469, & 0.6376952, \ldots \\ 0.6376952, & 0.2724469, \ldots \\ 0.6376952, & 0.2724469 \end{pmatrix}$$

shown in Fig. 3.7(a). This means that we have three pairs of sensors and each of these pairs tends to measure the system state at the same point. In principle, this result should not be surprising, since it was already predicted in Example 3.2 where virtually the same support points were obtained. On the other hand, it tallies with some results on replications of D-optimal designs for non-linear models (Haines, 1993).

The case of correlated observations was also tested for the model (3.75) with $\beta = 10^{-2}$. Since the gradient algorithms are not appropriate for this



(a)



(b)

Figure 3.7: Optimal sensor location of Example 3.6 calculated via the direct approach: (a) Independent measurements (b) Correlated measurements.

type of performance indices, the ARS technique was employed to assess the optimal solution as

$$s^{\star}_{\text{corr}} = \begin{pmatrix} 0.128788, & 0.128788, \dots \\ 0.167856, & 0.167856, \dots \\ 0.246423, & 0.621963, \dots \\ 0.301227, & 0.650355, \dots \\ 0.621963, & 0.246423, \dots \\ 0.650355, & 0.301226 \end{pmatrix}$$

which is illustrated in Fig. 3.7(b). We see at once that the introduction of interrelations between the sensors results in removing the harmful clusterizaton. During experiments, however, some numerical instabilities were observed in addition to a considerably increased computational burden (three minutes versus half a minute for the correlation-free case). ♢

Example 3.7. Practically the same calculations as in the previous example were carried out for the setting of Example 3.3 and four sensors to be allocated. For independent measurements and the initial solution found with the use of the ARS algorithm, we obtained

$$s^{\star} = \begin{pmatrix} 0.176752, & 0.476745, \dots \\ 0.176752, & 0.476745, \dots \\ 0.701849, & 0.309336, \dots \\ 0.701849, & 0.309336 \end{pmatrix}$$

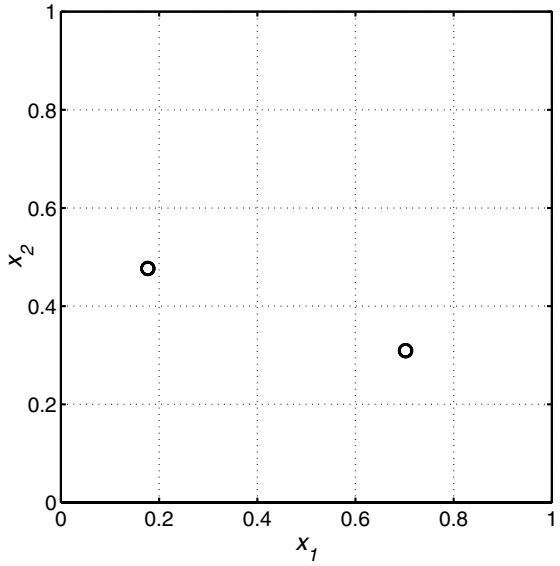
see Fig. 3.8(a), so we were faced again with the curse of clusterization. By allowing for correlations between the measurements of different sensors (according to the model (3.75) with $\beta = 10^{-2}$), this hurdle was avoided, since we got

$$s^{\star}_{\text{corr}} = \begin{pmatrix} 0.175956, & 0.511760, \dots \\ 0.176134, & 0.443545, \dots \\ 0.681270, & 0.330796, \dots \\ 0.718677, & 0.291468 \end{pmatrix}$$

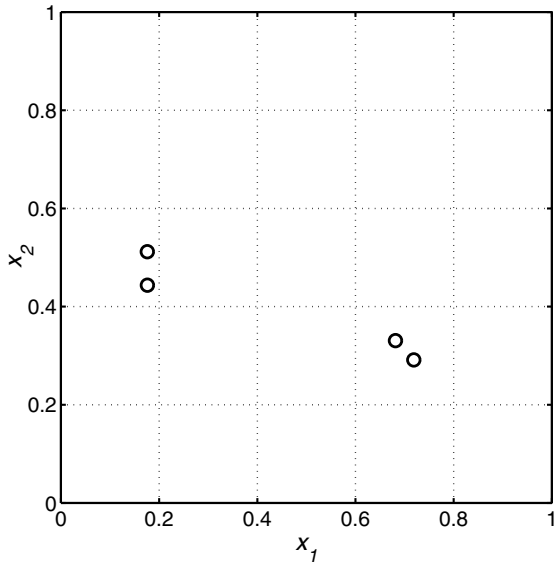
see Fig. 3.8(b). ♢

3.5 A critical note on some deterministic approach

Independently of any statistical motivations, it happens that some authors are interested in choosing sensor positions which make an approximation H



(a)



(b)

Figure 3.8: Optimal sensor location of Example 3.7 calculated via the direct approach: (a) Independent measurements (b) Correlated measurements.

to the Hessian of the estimation cost well-conditioned, as is pointed out in (Walter and Pronzato, 1997). More precisely, minimization with respect to s of the Frobenius condition number defined as

$$J(s) = \sqrt{\operatorname{trace}[H(s)] \operatorname{trace}[H^{-1}(s)]} \tag{3.78}$$

is considered. But as was already shown in Section 2.5, the second Gâteaux derivative at a global minimum $\hat{\theta}$ of the least-squares criterion is approximately equal, up to a constant multiplier, to the corresponding FIM.

In consequence, an optimal sensor location can equivalently be determined by choosing s which corresponds to a minimum of the criterion

$$\tilde{J}(s) = \frac{1}{m}\sqrt{\operatorname{trace}(M) \operatorname{trace}(M^{-1})} \tag{3.79}$$

This form of the criterion to be used while looking for optimum experimental designs was suggested in (Walter and Pronzato, 1990) under the name of *Turing's measure of conditioning*. It is used when it is desirable to obtain a confidence region for the parameters as spherical as possible. It is easy to check that its minimum value is 1 and it is obtained for spherical confidence regions.

It is a simple matter to show that for the criterion

$$\Psi(M) = \operatorname{trace}(M) \operatorname{trace}(M^{-1}) \tag{3.80}$$

whose minimization is equivalent to minimization of (3.79), we get

$$\overset{\circ}{\Psi} = -\operatorname{trace}(M) M^{-2} + \operatorname{trace}(M^{-1}) I \tag{3.81}$$

where, as usual, I stands for the identity matrix.

Unfortunately, in spite of its clear rationale, the approach should be used with great care, as it only guarantees that the condition number is close to unity and no more than that (Uciński and Korbicz, 1999b). This means that we might have a low value of J and at the same time little information about the parameters. This is confirmed by the following example.

Example 3.8. Let us consider again the situation of Example 3.3 with two sensors and criterion (3.79). Direct minimization yielded the solution (cf. Fig. 3.9)

$$s^\star = (0.050002, 0.115412, 0.936228, 0.234803)$$

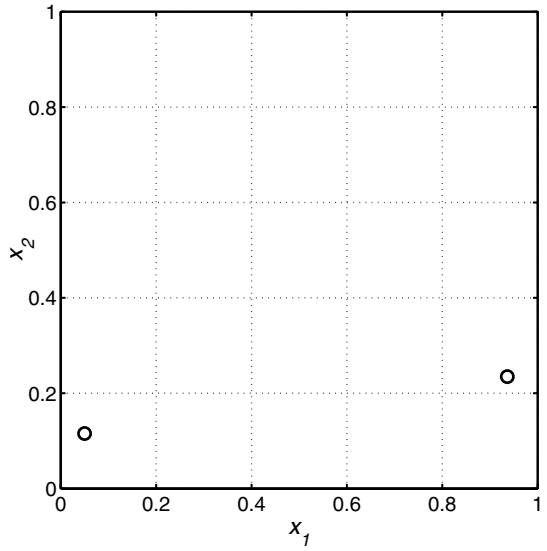


Figure 3.9: Optimal location of sensors for Turing's measure of conditioning of Example 3.8.

for which Turing's measure of conditioning was 1.739576, which is not bad if we recall that the smallest possible value is one (which is not always attainable). Nevertheless, let us note that those sensor positions are rather poor from the point of view of parameter accuracy, as e.g. the determinant of the FIM equals 1.7686, which is relatively small as compared to the value 157.438 obtained from the D-optimal solution for the same number of sensors. ♢

3.6 Summary

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 our sensor location problem. 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. Alternatively, we may seek to find an optimal

design, not within the class of all designs, but rather in a restricted subset of competing clusterization-free designs. To implement this idea, some recent advances in spatial statistics were employed, and in particular Fedorov's idea of directly constrained design measures was adapted to our framework. As a consequence, this led 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. If this is not the case, we can resort to standard optimization routines which ensure that the constraints on the design measure and region are satisfied (as indicated, computation of the gradient does not present a problem). Although the numerical examples presented here are clearly not real-world problems and their purpose is primarily to illustrate our considerations in an easily interpretable manner, they are complex enough to provide evidence for the effectiveness of the proposed approaches.

Chapter 4

Locally optimal location of moving internal observations

As was already emphasized, most of the contributions to the measurement optimization problem deal with the choice of stationary sensor positions. An alternative to such a strategy of taking measurements is to use movable sensors which offer additional degrees of freedom regarding optimality. Since systems with mobile observations are no doubt more flexible than those with non-mobile ones and their capabilities are wider, we can expect the minimal value of an adopted design criterion to be lower than the one for the stationary case. This is due to the fact that a non-mobile observation is a special case of a mobile one when all mobile observations are fixed (this implies, in turn, that the results of the theory for stationary observations must be contained in the more general mobile observation theory). Consequently, sensors are not assigned to positions which are optimal only on the average, but are capable of tracking points which provide at a given time moment the best information about the parameters to be identified.

A possibility of using moving observations does arise in a variety of applications, e.g. air polutants in the environment are often measured using data gathered by monitoring cars moving in an urban area and atmospheric variables are measured using instruments carried in a satellite (Nakano and Sagara, 1981; Nakano and Sagara, 1988). Other examples include scanning measurement of a surface temperature by optical pyrometers and measurement of vibrations and strains in materials using optical registration (Rafajłowicz, 1986c). The remainder of this chapter provides an exposition of basic systematic approaches to the design of moving sensor trajectories.

4.1 Adapting the idea of continuous designs

The very first idea, which suggests itself while attempting to address the problem of how to construct optimal sensor trajectories, is to establish a connection between this problem and the Kiefer-Wolfowitz theory of experimental design for regression problems. It goes without saying that its implementation is not straightforward as the main difficulty lies in the necessity of operating on mappings with values being Radon probability measures on the Borel sets of a given admissible compact set instead of the trajectories themselves, but nevertheless this can still be achieved and it is shown in what follows.

4.1.1 Optimal time-dependent measures

The approach outlined below was originally developed in (Rafajłowicz, 1986c) which has already become a classical reference work on moving sensors. As before, we will denote by $y = y(x,t;\theta)$ the scalar state of a DPS at a spatial point $x \in \bar{\Omega}$ (the closure of Ω) and time $t \in T = [0, t_f]$, which depends on a vector $\theta \in \mathbb{R}^m$ of unknown constant parameters. Furthermore, we will use the letter X to denote a compact set in which the observations of y can be made. Our main aim here is to study the optimal measurement scheduling problem for estimating θ in the case when the available observations are provided by N moving pointwise sensors, namely

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

where z^j_{m} is a scalar output, x^j stands for an observation curve (measurable in general) for the j-th sensor, so that

$$x^j(t) \in X \quad \text{a.e. on } T \tag{4.2}$$

Here ε signifies an additive disturbance being a realization of a white Gaussian random field whose statistics are given by

$$\mathrm{E}\{\varepsilon(x,t)\} = 0, \quad \mathrm{E}\{\varepsilon(x,t)\varepsilon(x',t')\} = \sigma^2\delta(x-x')\delta(t-t') \tag{4.3}$$

Our basic assumption is that the function $y(x,t;\,\cdot\,)$ is continuously differentiable in a neighbourhood of some known preliminary estimate θ^0 of θ. We then define

$$g(x,t) = \left(\frac{\partial y(x,t;\theta)}{\partial\theta}\right)^{\mathrm{T}}_{\theta=\theta^0} \tag{4.4}$$

and require g to be continuous in $\bar{Q} = \bar{\Omega} \times T$.

On the above assumptions, the average Fisher information matrix is of the form

$$M = \frac{1}{Nt_f} \sum_{j=1}^{N} \int_0^{t_f} g(x^j(t), t) g^{\mathrm{T}}(x^j(t), t)\, \mathrm{d}t \tag{4.5}$$

The independence of the measurements made by different sensors implies, however, that at some time moments we admit of clusterization, i.e. several sensors may measure the system state at the same points. We take account of this phenomenon through relabelling the sensors so that $x^i(t) \neq x^j(t)$ if $i \neq j$, where $1 \leq i, j \leq \ell(t)$, $\ell(t)$ being the number of sensors which are at different locations at time $t \in T$. Consequently, at a given time moment we may introduce the so-called exact design

$$\xi_N(t) = \begin{Bmatrix} x^1(t), & x^2(t), & \ldots, & x^{\ell(t)}(t) \\ p_1(t), & p_2(t), & \ldots, & p_{\ell(t)}(t) \end{Bmatrix} \tag{4.6}$$

where $p_i(t) = r_i(t)/N$ and $r_i(t)$ denotes the number of sensors which occupy the position $x^i(t)$. In terms of this modified notation, the FIM is

$$M(\xi_N) = \frac{1}{t_f} \int_0^{t_f} \left\{ \sum_{j=1}^{\ell(t)} p_i(t) g(x^i(t), t) g^{\mathrm{T}}(x^i(t), t) \right\} \mathrm{d}t \tag{4.7}$$

In much the same way as in Section 3.1, we may then extend the notion of the exact design to a more general concept of a randomized design which is to be understood as a mapping

$$\xi : T \ni t \mapsto \xi_t \in \Xi_t(X) \tag{4.8}$$

where $\Xi_t(X)$ is the set of all probability measures for all Borel sets of X including single points. Clearly, some measurability conditions about the mapping ξ must be imposed, but this topic is beyond the scope of this monograph and the interested reader is referred e.g. to (Warga, 1972), where a similar reasoning is conducted in the context of relaxed controls. In the sequel, $\Xi(X)$ denotes the set of all such mappings ξ.

It follows that the corresponding FIM is of the form

$$M(\xi) = \frac{1}{t_f} \int_0^{t_f} \int_X g(x, t) g^{\mathrm{T}}(x, t)\, \xi_t(\mathrm{d}x)\, \mathrm{d}t \tag{4.9}$$

A Ψ-optimal design will be a design $\xi^\star$ such that $\Psi[M(\xi)]$ is minimized at $\xi^\star$. We assume that Ψ satisfies (A3)–(A5) of p. 43 and, in place of (A6),

the following qualification:

(A6') For any $\xi \in \Xi(q) = \{\xi : \Psi[M(\xi)] \leq q < \infty\}$ and $\bar{\xi} \in \Xi(X)$, we have

$$\begin{aligned}&\Psi[M(\xi) + \lambda(M(\bar{\xi}) - M(\xi))] \\ &\quad = \Psi[M(\xi)] + \lambda \frac{1}{t_f} \int_0^{t_f} \int_X \psi(x,t,\xi)\, \bar{\xi}_t(\mathrm{d}x)\, \mathrm{d}t + o(\lambda; \xi, \bar{\xi}) \end{aligned} \tag{4.10}$$

where the scalar q is so chosen that $\Xi(q) \neq \emptyset$.

It turns out that (A6') is by no means restrictive, as for the differentiable criteria Ψ we have

$$\begin{aligned}&\delta_+ \Psi(M(\xi), M(\bar{\xi}) - M(\xi)) \\ &\quad = \operatorname{trace}\Big[\overset{\circ}{\Psi}(\xi)(M(\bar{\xi}) - M(\xi))\Big] \\ &\quad = \frac{1}{t_f} \int_0^{t_f} \int_X \left\{ g^{\mathrm{T}}(x,t) \overset{\circ}{\Psi}(\xi) g(x,t) - \operatorname{trace}\Big[\overset{\circ}{\Psi}(\xi) M(\xi)\Big] \right\} \bar{\xi}_t(\mathrm{d}x)\, \mathrm{d}t \end{aligned} \tag{4.11}$$

where

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

Hence

$$\psi(x,t,\xi) = g^{\mathrm{T}}(x,t) \overset{\circ}{\Psi}(\xi) g(x,t) - \operatorname{trace}\Big[\overset{\circ}{\Psi}(\xi) M(\xi)\Big] \tag{4.12}$$

or alternatively

$$\psi(x,t,\xi) = c(\xi) - \phi(x,t,\xi) \tag{4.13}$$

where

$$\phi(x,t,\xi) = -g^{\mathrm{T}}(x,t) \overset{\circ}{\Psi}(\xi) g(x,t) \tag{4.14}$$

and

$$c(\xi) = -\operatorname{trace}\Big[\overset{\circ}{\Psi}(\xi) M(\xi)\Big] \tag{4.15}$$

The next result provides a characterization of the optimal designs.

Theorem 4.1. *A design $\xi^\star$ is optimal iff*

$$\int_0^{t_f} \min_{x\in X} \psi(x,t,\xi^\star)\,\mathrm{d}t = 0 \tag{4.16}$$

Proof. From the convexity of Ψ it follows that a necessary and sufficient condition for optimality of $\xi^\star$ is

$$\inf_{\bar\xi\in\Xi(X)} \delta_+\Psi(M(\xi^\star), M(\bar\xi) - M(\xi^\star)) \geq 0 \tag{4.17}$$

or equivalently

$$\inf_{\bar\xi\in\Xi(X)} \delta_+\Psi(M(\xi^\star), M(\bar\xi) - M(\xi^\star)) = 0 \tag{4.18}$$

which is easy to check if we take $\bar\xi = \xi^\star$ on the left-hand side of (4.17).

If we set $x_0(t) = \arg\min_{x\in X} \psi(x,t,\xi^\star)$, then

$$\begin{aligned}
\int_0^{t_f} \psi(x_0(t),t,\xi^\star)\,\mathrm{d}t &= \int_0^{t_f}\int_X \psi(x,t,\xi^\star)\delta(x-x_0(t))\,\mathrm{d}x\,\mathrm{d}t \\
&\geq \inf_{\bar\xi} \int_0^{t_f}\int_X \psi(x,t,\xi^\star)\,\bar\xi_t(\mathrm{d}x)\,\mathrm{d}t \\
&\geq \inf_{\bar\xi} \int_0^{t_f}\int_X \min_{x\in X} \psi(x,t,\xi^\star)\,\bar\xi_t(\mathrm{d}x)\,\mathrm{d}t \\
&= \int_0^{t_f} \psi(x_0(t),t,\xi^\star)\,\mathrm{d}t
\end{aligned} \tag{4.19}$$

and therefore

$$\inf_{\bar\xi} \int_0^{t_f}\int_X \psi(x,t,\xi^\star)\,\bar\xi_t(\mathrm{d}x)\,\mathrm{d}t = \int_0^{t_f} \psi(x_0(t),t,\xi^\star)\,\mathrm{d}t \tag{4.20}$$

which gives (4.16) when combined with (4.11) and (4.18). ■

It is now a simple matter to deduce the respective form of the equivalence theorem:

Corollary 4.1. *The following are equivalent:*

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

(ii) $\xi^\star$ *minimizes* $\dfrac{1}{t_f}\displaystyle\int_0^{t_f} \max_{x\in X} \phi(x,t,\xi)\,\mathrm{d}t - c(\xi)$, *and*

(iii) $\dfrac{1}{t_f}\displaystyle\int_0^{t_f} \max_{x\in X} \phi(x,t,\xi^\star)\,\mathrm{d}t = c(\xi^\star)$

This constitutes a generalization of Theorem 1 of (Rafajłowicz, 1986c) where only D-optimal designs were considered. In that case Corollary 4.1 takes a particularly simple form:

Corollary 4.2. *Let $\xi^\star$ be a D-optimal design. Then the following are equivalent:*

(i) $\xi^\star$ *maximizes* $\det M(\xi)$,

(ii) $\xi^\star$ *minimizes* $\dfrac{1}{t_f}\displaystyle\int_0^{t_f} \max_{x\in X} g^{\mathrm{T}}(x,t)M^{-1}(\xi)g(x,t)\,\mathrm{d}t$, *and*

(iii) $\dfrac{1}{t_f}\displaystyle\int_0^{t_f} \max_{x\in X} g^{\mathrm{T}}(x,t)M^{-1}(\xi^\star)g(x,t)\,\mathrm{d}t = m$

In (Rafajłowicz, 1986c) some sufficient conditions for optimality are further given (e.g. a *quasi-maximum* principle). Owing to their use, the computational task reduces to solving at each time moment a separate optimization problem reminiscent of the classical D-optimum experimental design problem for which many numerical algorithms exist. The idea is very elegant, but from a practical point of view it can be applied only in relatively simple situations, as the attendant calculations are very time-consuming. Furthermore, only measurability of the resulting trajectories can be guaranteed, which may cause some difficulties when trying to apply the solutions in the setting of a real process. These complications can be sometimes avoided by suitably parametrizing the trajectories. The dimension of the optimization problem is thus reduced and we may impose any regularity conditions on the solutions. This constitutes the subject of the next section.

4.1.2 Parametrization of sensor trajectories

From now on we make the assumption that the trajectories of the available sensors can be represented as parametric curves of the form

$$x^j(t) = \eta(t,\beta^j), \quad t\in T \tag{4.21}$$

where η denotes a given function such that $\eta(\,\cdot\,,\beta^j)$ is continuous for each fixed β^j and $\eta(t,\,\cdot\,)$ is continuous for each fixed t, the constant parameter vector β^j ranging over a compact set $A\subset\mathbb{R}^p$. Since only the trajectories

lying entirely in an admissible compact set X are interesting, we introduce the set

$$B = \{\beta \in A : \eta(t,\beta) \in X, \forall\, t \in T\} \tag{4.22}$$

and assume that it is non-empty. A trivial verification shows that B is also compact.

If there are N sensors at our disposal and they move along the paths (4.21), then the resulting average FIM can be written down as

$$M = \frac{1}{Nt_f} \sum_{j=1}^{N} \int_0^{t_f} g(\eta(t,\beta^j),t) g^{\mathrm{T}}(\eta(t,\beta^j),t)\,\mathrm{d}t \tag{4.23}$$

Owing to the assumption of independent measurements, some trajectories may coincide and therefore we relabel the sensors so as to distinguish only $\ell \leq N$ different paths. Proceeding in this manner, we must also rewrite the FIM, which gives

$$M(\xi_N) = \sum_{i=1}^{\ell} p_i \left\{ \frac{1}{t_f} \int_0^{t_f} g(\eta(t,\beta^i),t) g^{\mathrm{T}}(\eta(t,\beta^i),t)\,\mathrm{d}t \right\} \tag{4.24}$$

where

$$\xi_N = \begin{Bmatrix} \beta^1, & \beta^2, & \ldots, & \beta^\ell \\ p_1, & p_2, & \ldots, & p_\ell \end{Bmatrix} \tag{4.25}$$

$p_i = r_i/N$, r_i is the number of sensors which follow the i-th path.

Accordingly, the experimental setting ξ_N can be interpreted as a discrete probability distribution. Removing the restriction that p_i's are multiples of $1/N$, we can extend the idea and think of a design as a probability measure ξ for all Borel sets of B including single points. With respect to such a modification, we can define the FIM analogous to (4.24) for a design ξ:

$$M(\xi) = \int_B \Upsilon(\beta)\,\xi(\mathrm{d}\beta) \tag{4.26}$$

where

$$\Upsilon(\beta) = \frac{1}{t_f} \int_0^{t_f} g(\eta(t,\beta),t) g^{\mathrm{T}}(\eta(t,\beta),t)\,\mathrm{d}t \tag{4.27}$$

The optimal design $\xi^\star$ is such that it minimizes the design criterion $\Psi[M(\xi)]$. It is easily seen that the form of this reformulated problem is

practically the same as that of the main problem of Section 3.1, p. 41 (it suffices to replace x, X and $f(x,t)$ with β, B and $g(\eta(t,\beta),t)$, respectively). Consequently, the corresponding results are also valid here. For instance, the probability measure $\xi(\mathrm{d}\beta)$ can be chosen to be purely discrete, i.e. non-zero for a finite number of β values (strictly speaking, this number is guaranteed to be less than or equal to $m(m+1)/2$). Similarly, the numerical schemes briefly delineated at the end of Section 3.1 can be employed to find approximations to the optimal solutions.

Let us note, however, that the simplicity of the presented approach is only limited to the applied idea and the resulting computational burden may be still quite heavy. Indeed, as was already emphasized, the most cumbersome part of the algorithm for obtaining Ψ-optimal designs consists in repeatedly solving a global non-linear programming problem with constraints. This problem can be settled with relative ease if stationary sensors are to be placed, as the dimension of the corresponding decision vector equals the number of space coordinates (i.e. 1, 2 or 3 in practical situations). In order for $\eta(\,\cdot\,,\beta)$ to be adjustable enough to approximate satisfactorily any trajectory x^j (i.e. to form a sufficiently rich family of feasible paths so as to be of any practical use), the size of β usually has to be much larger, which essentially complicates computations. But such a cost is unavoidable while attempting to increase the degree of freedom in solving any optimization problem (cf. parameter optimization problems versus optimization problems for dynamic systems).

4.2 Optimization of measurement schedules based on optimal-control techniques

If the number of moving sensors is imposed *a priori* (this is often encountered in practice and results from high costs of such measurement equipment), the dynamics of the vehicles carrying the sensors must be taken into account and various geometric constraints are put on sensor movements (induced e.g. by the admissible measurement regions and allowable distances between the sensors), then the only systematic and computationally tractable approach is to convert the problem to an optimal-control formulation and then to attempt to solve it numerically. Such an idea has already been successfully applied in the context of state estimation (Khapalov, 1992; Nakano and Sagara, 1981; Nakano and Sagara, 1988; Carotenuto *et al.*, 1987), but those results can hardly be exploited in the framework considered here as those authors make extensive use of some specific features of the ad-

dressed problem (e.g. the linear dependence of the current state on the initial state for linear systems). To the best of our knowledge, no approaches have been proposed so far as regards this line in the context of parameter estimation. Our purpose here is thus to describe some original results concerning numerical methods for the off-line determination of moving sensor positions which maximize parameter-identification accuracy subject to various constraints imposed on sensors' motions. The technique employed is to transform the problem to an optimal-control one in which both the control forces of the sensors and initial sensor positions are optimized.

4.2.1 Statement of the problem and notation

Equations of sensor motion

For simplicity of notation, let us write

$$s(t) = (x^1(t), x^2(t), \ldots, x^N(t)), \quad \forall\, t \in T = [0, t_f] \tag{4.28}$$

and set $n = \dim s(t)$. We assume that the sensors are conveyed by vehicles which are described by equations of motion of the form

$$\dot{s}(t) = f(s(t), u(t)) \quad \text{a.e. on } T, \quad s(0) = s_0 \tag{4.29}$$

where a given function $f : \mathbb{R}^n \times \mathbb{R}^r \to \mathbb{R}^n$ is required to be continuously differentiable, $s_0 \in \mathbb{R}^n$ defines an initial sensor configuration, and $u : T \to \mathbb{R}^r$ is a measurable control function which satisfies

$$u_l \leq u(t) \leq u_u \quad \text{a.e. on } T \tag{4.30}$$

for some constant vectors u_l and u_u. The last condition is quite sensible as in general the controls are limited for technical and/or economic reasons (strictly speaking, it is also of paramount importance in proving the existence of a solution to the optimal control problem described subsequently).

Given any initial sensor configuration s_0 and any control function, there is a unique absolutely continuous function $s : T \to \mathbb{R}^n$ which satisfies (4.29) a.e. on T. In what follows, we will call it the state trajectory corresponding to s_0 and u. Various particular choices are proposed for the 'state' equation (4.29), including the following:

- first-order linear equation (Khapalov, 1992)

$$\dot{s}(t) = C(t)s(t) + D(t)u(t), \quad s(0) = s_0$$

  where C and D are (continuous) matrices,

- second-order linear equation (Carotenuto *et al.*, 1987)

$$E\ddot{s}(t) + F\dot{s}(t) = Gu(t), \quad \dot{s}(0) = 0, \quad s(0) = s_0$$

where E and F are diagonal matrices, $E > 0$, $F \geq 0$ (this case reduces to (4.29) after extending the state vector and an obvious change of variables), and

- case where we do not attach importance to the dynamics of the vehicles carrying the sensors and the only interest is in the trajectories themselves (Nakano and Sagara, 1981)

$$\dot{s}(t) = u(t), \quad s(0) = s_0$$

Remark 4.1. Clearly, if the sensor dynamics is not of primary concern, in lieu of the last model above we might simply use the description

$$s(t) = u(t)$$

i.e. directly optimize sensor positions. Note, however, that such an approach necessitates additional assumptions about the regularity of s. Moreover, some supplementary constraints should also be introduced so as to guarantee a proper mathematical formulation and, as a consequence, the existence of solutions (e.g. constraints on the maximal lengths of the trajectories or on maximal speeds of sensor movements). In such a case, computational methods of calculus of variations can be exploited in order to find optimal trajectories. The optimal-control approach outlined in what follows is beyond doubt more general and flexible, and therefore we shall restrict our discussion only to this topic.

Induced pathwise state inequality constraints

If we intend to design sensor movements for a real application, some restrictions on the motions have to be inevitably included in our optimal-control formulation. First of all, all sensors should stay within an admissible region Ω_{ad} (a given compact set) where measurements can be made. In what follows, it is convenient to choose a quite general form

$$\Omega_{\text{ad}} = \{x \in \Omega : b_i(x) \leq 0,\ i = 1, \ldots, I\} \tag{4.31}$$

where b_i's are given continuously differentiable functions. Accordingly, the conditions

$$\alpha_{ij}(s(t)) = b_i(x^j(t)) \leq 0, \quad \forall\, t \in T \tag{4.32}$$

must be fulfilled, where $1 \le i \le I$ and $1 \le j \le N$.

Furthermore, to alleviate problems with sensor clusterization, we introduce constraints to restrict the admissible distances between the sensors. In the present approach, they are of the form

$$\beta_{ij}(s(t)) = R^2 - \|x^i(t) - x^j(t)\|^2 \le 0, \quad \forall\, t \in T \tag{4.33}$$

where $1 \le i < j \le N$ and R stands for a minimum allowable distance which guarantees that the measurements taken by the sensors can be considered as independent.

To shorten notation, after relabelling, we rewrite constraints (4.32) and (4.33) in the form

$$\gamma_\ell(s(t)) \le 0, \quad \forall\, t \in T \tag{4.34}$$

where γ_ℓ, $\ell = 1, \ldots, IN$ tally with (4.32), whereas γ_ℓ, $\ell = IN+1, \ldots, [I + (N-1)/2]N$ coincide with (4.33). In the sequel, $\bar{\nu}$ stands for the set of indices $\{1, \ldots, \nu\}$, $\nu = [I + (N-1)/2]N$.

Optimal measurement problem

The goal in the optimal measurement problem is to determine the forces (controls) applied to each vehicle conveying a sensor, which minimize a design criterion $\Psi[M(s)]$ defined on the set of all real-valued information matrices of the form

$$M(s) = \frac{1}{Nt_f} \sum_{j=1}^{N} \int_0^{t_f} g(x^j(t), t) g^{\mathrm{T}}(x^j(t), t)\, \mathrm{d}t \tag{4.35}$$

where g is defined in (4.4), under the constraints (4.30) on the magnitude of the controls and induced state constraints (4.34). In order to increase the degree of optimality, in our approach we will regard s_0 as a control parameter vector to be chosen in addition to the control function u.

Evidently, in order to guarantee the correctness of such a formulation and further derivations, it is necessary to put some restrictions on the sensitivity coefficients g. In the remainder of this chapter, we require g and $\partial g/\partial x$ to be continuous functions.

Since sensor trajectories s are unequivocally determined as solutions to the state equation (4.29), the above control problem can be interpreted as an optimization problem over the set of feasible pairs

$$\mathcal{P} = \big\{(s_0, u) : s_0 \in \Omega_{\mathrm{ad}}^N,\ u : T \to \mathbb{R}^r \text{ is measurable,} \\ u_l \le u(t) \le u_u \text{ a.e. on } T\big\} \tag{4.36}$$

Because of this, here and subsequently we will also make the following notational convention: if s appears without mention in a formula, it is always understood that a control u and initial condition s_0 have been specified and s is the trajectory corresponding to u and s_0 through (4.29).

Consequently, we wish to solve the following problem:

$$\min_{(s_0,u)\in\mathcal{P}} J(s_0,u) \tag{4.37}$$

subject to the inequality constraint

$$h(s_0,u) \leq 0 \tag{4.38}$$

where

$$J(s_0,u) = \Psi[M(s)] \tag{4.39}$$

$$h(s_0,u) = \max_{(\ell,t)\in\bar{\nu}\times T} \big\{\gamma_\ell(s(t))\big\} \tag{4.40}$$

Clearly, this highly non-linear problem is very complicated and we are not capable of finding closed-form formulae for its solution. Accordingly, we must resort to numerical techniques. A number of possibilities exist in this respect (Polak, 1997; Gruver and Sachs, 1980), but prior to the presentation of a pertinent method, let us notice that in spite of its non-classical form the resulting optimal-control problem can be easily cast as a classical Mayer problem where the performance index is defined only via terminal values of state variables (Fleming and Rishel, 1975).

4.2.2 Equivalent Mayer problem and existence results

To set forth our basic idea, define first the quantities

$$\chi_{ij}(s(t),t) = \frac{1}{Nt_f}\sum_{\ell=1}^{N} g_i(x^\ell(t),t)g_j(x^\ell(t),t) \tag{4.41}$$

and then the matrix $\Pi(t) = \big\{\varpi_{ij}(t)\big\} \in \mathbb{R}^{m\times m}$ with components

$$\varpi_{ij}(t) = \int_0^t \chi_{ij}(s(\tau),\tau)\,\mathrm{d}\tau \tag{4.42}$$

for $1 \leq i,j \leq m$. This clearly forces

$$M(s) = \Pi(t_f) \tag{4.43}$$

and

$$\dot{\varpi}_{ij}(t) = \chi_{ij}(s(t), t), \quad \forall\, t \in T \tag{4.44}$$

Hence introducing

$$v(t) = \begin{pmatrix} s(t) \\ \varpi_{11}(t) \\ \vdots \\ \varpi_{m1}(t) \\ \varpi_{12}(t) \\ \vdots \\ \varpi_{mm}(t) \end{pmatrix}, \quad v_0 = \begin{pmatrix} s_0 \\ 0 \\ \vdots \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \quad F(v(t), u(t), t) = \begin{pmatrix} f(s(t), u(t)) \\ \chi_{11}(s(t), t) \\ \vdots \\ \chi_{m1}(s(t), t) \\ \chi_{12}(s(t), t) \\ \vdots \\ \chi_{mm}(s(t), t) \end{pmatrix} \tag{4.45}$$

yields

$$\dot{v}(t) = F(v(t), u(t), t) \quad \text{a.e. on } T, \quad v(0) = v_0 \tag{4.46}$$

which allows us to treat v and (4.46) as a new extended state vector and a new state equation, respectively. Accordingly, the optimal control problem (4.37),(4.38) can be rewritten as

$$\min_{(v_0, u) \in \bar{\mathcal{P}}} \bar{J}(v_0, u) \tag{4.47}$$

subject to

$$\bar{h}(v_0, u) \leq 0 \tag{4.48}$$

where

$$\bar{\mathcal{P}} = \big\{(v_0, u) : v_0 = (v_{01}, \ldots, v_{0n}, \underbrace{0, \ldots, 0}_{m^2 \text{ times}}),\ (v_{01}, \ldots, v_{0n}, u) \in \mathcal{P}\big\}$$

$$\bar{J}(v_0, u) = G(v(t_f)) \stackrel{\text{def}}{=} \Psi(\Pi(t_f)), \quad \bar{h}(v_0, u) = h(v_{01}, \ldots, v_{0n}, u)$$

In this way, we are faced with a Mayer form of the performance index, which leads to a standard problem studied extensively in most works on optimal control in the presence of state inequality constraints. Moreover, a basic assertion is that the Mayer problem is equivalent to the Lagrange and Bolza ones in that each can be formulated as one of the other forms (Fleming and Rishel, 1975).

At this juncture, it should be underlined that optimal control problems with state-variable inequality constraints are not easy to solve and even the theory is not unambiguous, since there exist various forms of the necessary and sufficient optimality conditions (Hartl *et al.*, 1995). On rather strong regularity assumptions, standard existence theorems only provide the existence of an optimal *measurable* control. In our case such assumptions are not satisfied and measurable optimal solutions may fail to exist. This is because the set of admissible controls is not sequentially compact with respect to the L^∞ norm. A usual remedy to this predicament is to embed the considered set of controls into some larger topological space in which its closure is sequentially compact. This closure is usually called the class of *relaxed* (or *generalized*) controls (Teo and Wu, 1984). Relaxed optimal controls always exist in the setting of our Mayer problem (for details, see Hartl *et al.*, 1995; Pytlak and Vinter, 1998; Pytlak and Vinter, 1999).

4.2.3 Linearization of the optimal-control problem

Since at each iteration of the numerical algorithm delineated in the next section improvements of the current approximations to the optimal initial sensor configuration and optimal controls are calculated by solving an optimization problem in which the sensor dynamics, performance index and constraint functional are replaced by their first-order approximations around the current pair (s_0, u), in what follows we give some details about the technique of such a linearization.

Let us consider an initial state s_0 and a control u which is admissible in the sense of satisfying (4.30). The corresponding state vector is denoted by s. We assume that u is perturbated by a small function (variation) $\delta u \in L^\infty(T;\mathbb{R}^r)$ and s_0 is perturbated by a small vector $\delta s_0 \in \mathbb{R}^n$ such that $\|\delta u\|_{L^\infty(T;\mathbb{R}^r)}$ and $\|\delta s_0\|_{\ell_n^\infty}$ are sufficiently small, which warrants the correctness of the presented method. To shorten notation, here and subsequently, we write $\|\cdot\|$ instead of $\|\cdot\|_{L^\infty(T;\mathbb{R}^r)}$ and $\|\cdot\|_{\ell_n^\infty}$ when no confusion can arise.

From eqn. (4.29) which relates s to s_0 and u, we obtain the variational time-varying linear tangent system

$$\delta\dot{s}(t) = f_s(t)\delta s(t) + f_u(t)\delta u(t), \quad \delta s(0) = \delta s_0 \tag{4.49}$$

where

$$f_s(t) = \left(\frac{\partial f}{\partial s}\right)_{\substack{s=s(t)\\u=u(t)}}, \quad f_u(t) = \left(\frac{\partial f}{\partial u}\right)_{\substack{s=s(t)\\u=u(t)}}$$

which relates variations in s to variations in s_0 and u.

Based on the derivations presented in Appendix D.1, it may be concluded that the Fréchet differential of J at s_0 and u with increments δs_0 and δu, respectively, (the first variation of J due to variations in s_0 and u) is of the form

$$\delta J(s_0, u; \delta s_0, \delta u) = \langle \zeta(0), \delta s_0 \rangle + \int_0^{t_f} \langle f_u^{\mathrm{T}}(t)\zeta(t), \delta u(t) \rangle \, \mathrm{d}t \tag{4.50}$$

where the adjoint mapping ζ solves the Cauchy problem

$$\dot{\zeta}(t) + f_s^{\mathrm{T}}(t)\zeta(t) = -\sum_{i=1}^{m}\sum_{j=1}^{m} c_{ij} \left(\frac{\partial \chi_{ij}}{\partial s} \right)^{\mathrm{T}}_{s=s(t)}, \quad \zeta(t_f) = 0 \tag{4.51}$$

$\langle \cdot, \cdot \rangle$ stands for the inner product in the appropriate Euclidean space, χ_{ij}'s are defined in (4.41), and c_{ij}'s are the components of the matrix

$$\overset{\circ}{\Psi}(s) = \{c_{ij}\}_{m \times m} = \left. \frac{\partial \Psi(M)}{\partial M} \right|_{M=M(s)} \tag{4.52}$$

As for the state inequality constraints (4.38), owing to the fact that the functional h is not Fréchet differentiable (this is because the max function is nondifferentiable), in order to approximate its increments, we resort to the notion of the Gâteaux differential which is of the form (see Appendix D.2)

$$\begin{aligned} &\delta h(s_0^0, u^0; \delta s_0, \delta u) \\ &\qquad = \max_{(\ell,t)\in S} \left\{ \langle \zeta_h^\ell(0;t), \delta s_0 \rangle + \int_0^{t_f} \langle f_u^{\mathrm{T}}(\tau)\zeta_h^\ell(\tau;t), \delta u(\tau) \rangle \, \mathrm{d}\tau \right\} \end{aligned} \tag{4.53}$$

where $S = \{(\ell, t) \in \bar{\nu} \times T : \gamma_\ell(s(t)) = h(s_0, u)\}$ and $\zeta_h^\ell(\,\cdot\,; t)$ is the solution to the Cauchy problem

$$\frac{\mathrm{d}\zeta_h^\ell(\tau;t)}{\mathrm{d}\tau} + f_x^{\mathrm{T}}(\tau)\zeta_h^\ell(\tau;t) = -\left(\frac{\partial \gamma_\ell}{\partial s} \right)^{\mathrm{T}}_{s=s(\tau)} \delta(\tau - t), \quad \zeta_h^\ell(t_f;t) = 0 \tag{4.54}$$

4.2.4 A numerical technique of solving the optimal measurement problem

Owing to the complexity of the problem of minimizing the performance index (4.37) subject to pathwise inequality constraints (4.38), we have to resort to numerical techniques. Luckily, there exist numerous methods which

can be exploited here, as the problem is frequently encountered in applications, e.g. in mechanics, aerospace engineering, econometrics or robotics (Bryson, 1999; Bryson and Ho, 1975; Hartl *et al.*, 1995). In this context, we distinguish direct and indirect methods (Machielsen, 1987; Schwartz, 1996). With *direct* methods the optimal-control problem is treated directly as a minimization problem, i.e. the method is started with an initial approximation to the solution, which is improved iteratively by minimizing the performance index along a search direction, which is obtained via linearization of the problem. State constraints are often treated via a penalty function approach, i.e. a term which is a measure for the violation of the state constraints is added to the performance index. With *indirect* methods the optimality conditions, which must hold for a solution to the optimal-control problem, are used to derive a multi-point boundary-value problem. Solutions to the optimal-control problem will also be solutions to this multi-point boundary-value problem and hence the numerical solution to the multi-point boundary-value problem yields a candidate for the solution to the optimal-control problem (Machielsen, 1987). The main drawback to indirect methods is their extreme lack of robustness: the iterations of an indirect method must start close, sometimes very close, to a local solution in order to solve the pertinent boundary-value problem. Additionally, since first-order optimality conditions are satisfied by maximizers and saddle points as well as minimizers, there is no reason, in general, to expect solutions obtained by indirect methods to be minimizers.

A survey and comparison of numerical methods for state-constrained optimal-control problems can be found e.g. in (Polak, 1997; Bryson, 1999; Bryson and Ho, 1975; Machielsen, 1987; Pytlak and Vinter, 1998; Pytlak and Vinter, 1999; Holtz and Arora, 1997). As regards our measurement problem, in what follows we adopt a relatively unfamiliar method delineated long ago (Fedorenko, 1978; Dubovitskii and Milyutin, 1965), but implemented only recently (Galicki, 1998; Galicki and Uciński, 1998a; Galicki and Uciński, 1998b) for planning optimal motions of redundant manipulators. It is based on the so-called *negative formulation* of the Pontryagin Maximum Principle and leads to an iterative algorithm for improving estimates of the control histories u and initial states s_0 so as to decrease the value of the performance index J and to satisfy the imposed control and state constraints. Each iteration amounts, in turn, to linearization of the problem in the vicinity of the control approximation from the previous step and then solving the resulting linear-programming problem to modify the solution until a desired accuracy is achieved. It appears that this proced-

ure is extremely suited for numerically solving the sensor-location problem formulated in Section 4.2.1, as the Fréchet derivative of the performance index can be determined with reasonable computational burden and the state inequality constraints are taken into account by the method with relative ease, especially those induced by the conditions of preserving safe distances between the sensors (in the jargon of robotics, these are collision-avoidance conditions with moving obstacles).

The method is very similar to the feasible-direction algorithm proposed and thoroughly studied by Pytlak and Vinter (1998; 1999), as both the methods originate from ideas given by Fedorenko (1978). They also share the same characteristics which promote their efficient implementation, e.g. that the improvements generated by the algorithms drive state trajectories into the interior of the state constraint region (Pytlak and Vinter, 1998). Moreover, as opposed to the penalty-function method, the method presented here does nor require knowledge of an initial solution satisfying the constraint (4.38), which makes the implementation much easier.

For properly selected variations δs_0 and δu, the differentials of J and h can approximate the exact increments of these functionals with any desired accuracy. Given an initial state s_0^0 and a control u^0 satisfying (4.30), consider now the linearized problem: Find δs_0^1 and δu^1 to minimize the truncated functional

$$J(s_0^0, u^0) + \delta J(s_0^0, u^0; \delta s_0^1, \delta u^1) \quad (\approx J(s_0^0 + \delta s_0^1, u^0 + \delta u^1)) \tag{4.55}$$

subject to the constraints

$$\begin{cases} h(s_0^0, u^0) + \delta h(s_0^0, u^0; \delta s_0^1, \delta u^1) \leq 0 \\ u_l \leq u^0 + \delta u^1 \leq u_u \\ \|\delta u^1\| \leq \rho, \quad \|\delta s_0^1\| \leq \eta \end{cases} \tag{4.56}$$

where ρ and η are sufficiently small positive numbers.

According to the *negative formulation of the Pontryagin Maximum Principle* (Fedorenko, 1978; Galicki, 1998), the assumption of non-optimality of s_0^0 and u^0 implies the existence of an initial state $s_0^0 + \delta s_0^1$ and a control $u^0 + \delta u^1$ for (4.55), (4.56) such that $J(s_0^0 + \delta s_0^1, u^0 + \delta u^1) < J(s_0^0, u^0)$. A new initial state $s_0^1 = s_0^0 + \delta s_0^1$ and a new control $u^1 = u^0 + \delta u^1$ result in this way. The process of minimization is then rerun for s_0^1 and u^1 instead of s_0^0 and u^0, respectively. This procedure of linearization and minimization is thus repeated over and over. Sequences of pairs $\{(s_0^k, u^k)\}$ and the corresponding state trajectories $\{s^k\}$ are thus obtained. It is known that

$\{s^k\}$ is convergent (strictly speaking, it possesses a uniformly convergent subsequence). The corresponding proof proceeds on the same lines as in (Galicki, 1998).

As regards computational aspects of the problem (4.55), (4.56), its finite-dimensional approximation leads to a very effective and simple numerical procedure. The process of approximation can be accomplished by forming a partition on T by choosing points $t_k = kt_f/K$, $k = 0, 1, \ldots, K$ and then considering u^0 and δu^1 in the class of piecewise linear polynomials, i.e. we take

$$u^0(t) = \sum_{k=0}^{K} u_k^0 \varphi_k(t), \quad \delta u^1(t) = \sum_{k=0}^{K} \delta u_k^1 \varphi_k(t) \tag{4.57}$$

where the φ_k's can be e.g. piecewise linear spline basis functions. Accordingly, the problem of determining the variations δs_0^1 and δu^1 reduces to solving the finite-dimensional linear-programming problem

$$\begin{aligned} \mathfrak{J}(\delta s_0^1, \delta u_0^1, \ldots, \delta u_K^1) &= \langle \zeta(0), \delta s_0^1 \rangle \\ &\quad + \sum_{k=0}^{K} \delta u_k^1 \int_0^{t_f} \langle f_u^{\mathrm{T}}(t)\zeta(t), \varphi_k(t) \rangle \, \mathrm{d}t \longrightarrow \min \end{aligned} \tag{4.58}$$

subject to

$$h(s_0^0, u^0) + \langle \zeta_h^\ell(0; t_{k_i}), \delta s_0 \rangle + \sum_{k=0}^{K} \delta u_k^1 \int_0^{t_f} \langle f_u^T(t)\zeta_h^\ell(\tau; t_{k_i}), \varphi_k(\tau) \rangle \, \mathrm{d}\tau \leq 0 \tag{4.59}$$

for $(\ell, t_{k_i}) \in S_d$,

$$u_{l,k} \leq u_k^0 + \delta u_k^1 \leq u_{u,k}, \quad k = 0, \ldots, K \tag{4.60}$$

$$\|\delta u_k^1\| \leq \rho, \quad \|\delta s_0^1\| \leq \eta \tag{4.61}$$

where $S_d = \{(\ell, t_k) : \gamma_\ell(s^0(t_k)) \geq h(s_0^0, u^0) - \epsilon |h(s_0^0, u^0)|\}$, ϵ being a small positive number.

In spite of its simplicity, the method turns out to be extremely efficient, as was demonstrated while treating various aspects of the optimal measurement problem with moving sensors (see e.g. Uciński *et al.*, 1993; Korbicz and Uciński, 1994; Uciński, 1994; Uciński and Korbicz, 1995; Uciński, 1996a; Uciński and Korbicz, 1996; Uciński, 1997; Uciński and Korbicz, 1998; Uciński, 2000a; Uciński, 2000b).

Remark 4.2. Let us note that the same method (and, in particular, the same computer code) can be used to find optimal locations of stationary sensors. For that purpose, it suffices to set the initial control u^0 as zero and then to maintain the zero control variation (i.e. $\rho = 0$) during calculations. This forces the algorithm to improve the solution only by changing s_0.

Remark 4.3. The proposed method can also be generalized to consider more sophisticated dynamic models of the vehicles carrying the sensors and/or assume various constraints imposed on the sensor motions, e.g. the existing obstacles (fixed or mobile), sensors' geometrical dimensions, etc. As regards computational aspects, a considerable speed up can be achieved when the so-called upper-bounding version of the simplex algorithm, which exploits the special form of the constraints (4.56), is used to solve the linear-programming subproblems (Pierre, 1969). Furthermore, some decomposition-coordination techniques can also be applied to parallelize the computations (Malinowski, 1999; Galicki and Uciński, 1998b).

Example 4.1. The following numerical example serves as a vehicle to test the proposed solution technique. The point of departure is the two-dimensional diffusion equation

$$\frac{\partial y(x,t)}{\partial t} = \frac{\partial}{\partial x_1}\left(\kappa(x)\frac{\partial y(x,t)}{\partial x_1}\right) + \frac{\partial}{\partial x_2}\left(\kappa(x)\frac{\partial y(x,t)}{\partial x_2}\right) + 20\exp\bigl(-50(x-t)^2\bigr), \quad x \in \Omega = (0,1)\times(0,1), \quad t \in (0,1)$$

subject to the conditions

$$y(x,0) = 0, \quad x \in \Omega$$
$$y(x,t) = 0, \quad (x,t) \in \partial\Omega \times T$$

The diffusion coefficient to be identified has the form

$$\kappa(x) = \theta_1 + \theta_2 x_1 + \theta_3 x_2, \quad \theta_1 = 0.1, \quad \theta_2 = -0.05, \quad \theta_3 = 0.2$$

where the values θ_1, θ_2 and θ_3 are also treated as nominal and known to the experimenter prior to the identification itself.

As regards the forcing term in our model, it approximates the action of a line source whose support is constantly oriented along the x_2-axis and moves with constant speed from the left to the right boundary of Ω. Our purpose is to estimate κ (i.e. the parameters θ_1, θ_2 and θ_3) as accurately as possible based on the measurements made by three moving sensors. Accordingly, D- and A-optimum design criteria are primarily chosen as the measures of the

estimation accuracy, but to make a comparison, the sensitivity criterion is also considered.

Assuming that the sensor dynamics is not of primary concern, we adopt the simple model

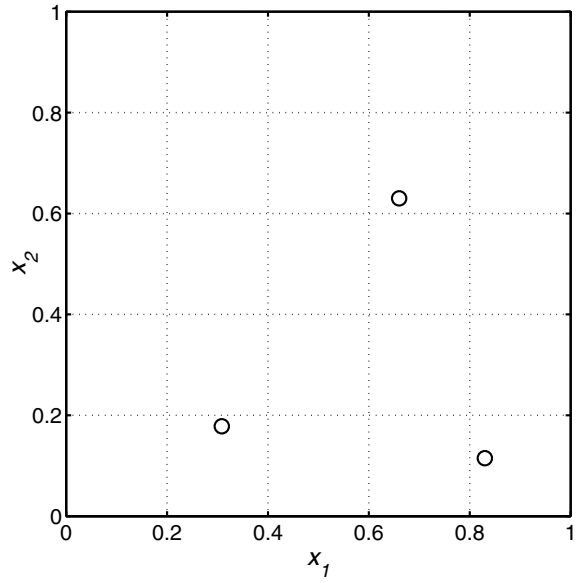
$$\dot{s}(t) = u(t), \quad s(0) = s_0$$

Moreover, we impose the following constraints on u:

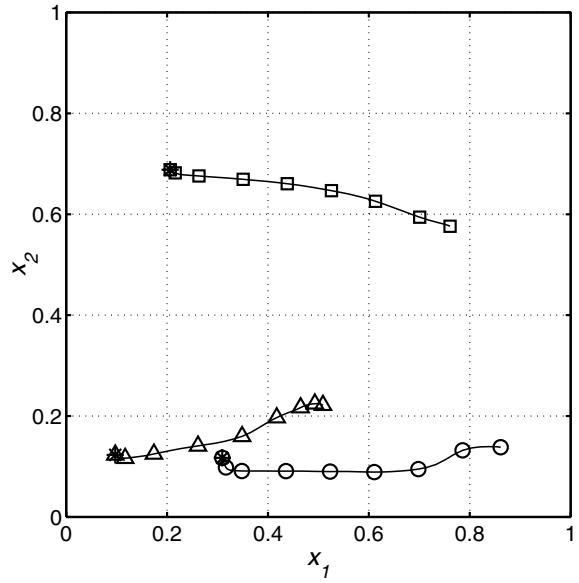
$$|u_i(t)| \leq 0.7, \quad \forall\, t \in T, \quad i = 1, \ldots, 6$$

As for technicalities, in order to numerically solve the measurement location problem, a computer programme was written in Essential Lahey Fortran 90 v.4.0 using a PC (Pentium II, 300 Mhz, 128 MB RAM) running Windows NT 4.0. During simulations the velocities themselves were considered in the class of piecewise linear polynomials ($K = 40$). On the other hand, the state and sensitivity equations were solved with the finite-element method. The sampling interval and coordinate divisions were $\Delta t = 0.0125$ and $\Delta x_1 = \Delta x_2 = 0.025$, respectively. The parameters ρ and η were gradually decreased from 0.05 to 0.01. The Cauchy convergence criterion for the sequence $J(s_0^k, u^k)$ was set as 10^{-3}. For simplicity, the constraints on the minimum allowable distance between the sensors were not considered and only the state constraints forcing the sensors to remain in Ω were imposed. On aggregate, approximately one hour of CPU time was used to complete the simulations.

Figures 4.1 and 4.2 shows the optimal sensor trajectories obtained after a couple of trials with different initial guesses regarding s_0^0 and u^0 (to escape entrapment in a local minimum). Symbols like circles, squares and triangles denote consecutive sensor positions. Furthermore, the sensors' positions at $t = 0$ are marked by the asterisks. Let us note that the diffusion coefficient values in the upper left of Ω are greater than those in the lower right. This means that the state changes during the system evolution are quicker when we move up and to the left (on the other hand, the system would have reached the steady state there earlier). This fact explains the form of the trajectories obtained—the sensors tend to measure the state in the regions where the distributed system is the most sensitive with respect to the unknown parameter κ, i.e. in the lower right. Figure 4.1(a) shows the D-optimum positions of stationary sensors ($\det M = 417.3$). A considerable gain in the accuracy of the parameter estimates is expected if moving observations are allowed, cf. Fig. 4.1(b), as in this case the value of the performance index is virtually four times as large as that for the stationary case, i.e.

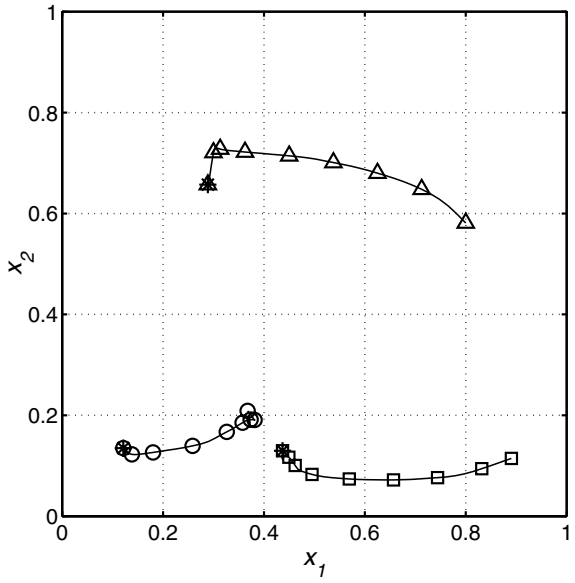


(a)

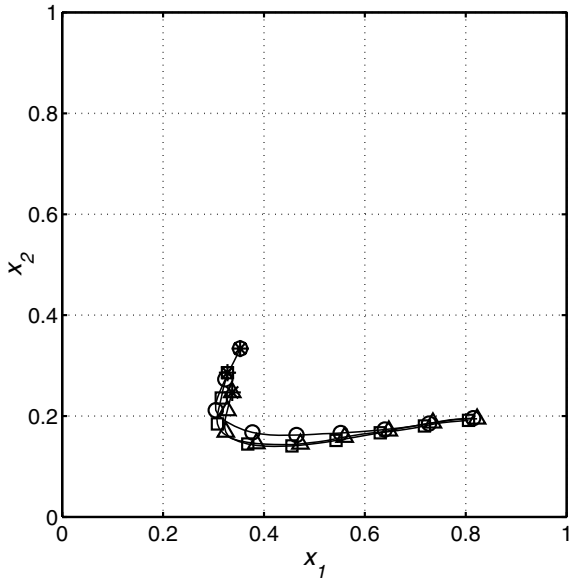


(b)

Figure 4.1: D-optimum positions of stationary sensors (a) versus D-optimum trajectories of moving sensors (b).



(a)



(b)

Figure 4.2: Optimum sensor trajectories: A-optimum criterion (a) versus sensitivity criterion (b).

we have $\det M = 1563$. In turn, Fig. 4.2(a) shows the calculated trajectories for the A-optimality criterion whose ultimate value is $\operatorname{trace} M^{-1} = 0.6101$. (In principle, the shapes of the trajectories are similar to those for the D-optimality counterpart.) On the other hand, Fig. 4.2(b) presents the results for the sensitivity criterion. In this case it turns out that the sensors strive to measure the system state very closely to one another and, in spite of a large value of the performance index ($\operatorname{trace} M = 258.82$), a comparatively low value of the FIM determinant is obtained ($\det M = 13.65$), which suggests that the resulting measurement setting may cause some problems regarding identifiability. ♢

4.2.5 Special cases

Optimal planning of sensor movements along given paths

Consider motion planning for sensors which can move only along prescribed paths being smooth curves parametrized e.g. by their lengths. A motivation to study this kind of problem is the situation when the sensors used in a system of monitoring and prediction of air pollution in a city may move only along given streets or roads. Accordingly, the motions of N sensors are restricted to given paths which are smooth curves $[0, \lambda^j_{\max}] \ni \lambda^j \mapsto \omega_j(\lambda^j) \in \bar{\Omega}$ parametrized by their lengths. Let $\lambda^j : T \to [0, \lambda^j_{\max}]$ be the trajectory of the j-th sensor. Without loss of generality we assume that the state can be measured directly, i.e. the observations are of the form

$$z^j_{\mathrm{m}}(t) = y(\omega_j(\lambda^j(t)), t; \theta) + \varepsilon(\omega_j(\lambda^j(t)), t), \quad t \in T, \tag{4.62}$$

for $j = 1, \ldots, N$.

Let the motion of the j-th sensor along the j-th trajectory be described by the equation

$$\dot{\lambda}^j(t) = u_j(t) \quad \text{a.e. on } T, \quad \lambda^j(0) = \lambda^j_0 \tag{4.63}$$

where u_j denotes the velocity of the j-th sensor, $j = 1, \ldots, N$. In the case considered here, the FIM can be written down as

$$M(\lambda_0, u) = \frac{1}{N t_f} \sum_{j=1}^{N} \int_0^{t_f} g(\omega_j(\lambda^j(t)), t) g^{\mathrm{T}}(\omega_j(\lambda^j(t)), t)\, \mathrm{d}t \tag{4.64}$$

where $\lambda_0 = \operatorname{col}[\lambda^1_0, \ldots, \lambda^N_0]$, $u(t) = \operatorname{col}[u_1(t), \ldots, u_N(t)]$. Optimal sensor trajectories for system identification can be found by choosing λ_0 and u so as to minimize some scalar function Ψ of the informations matrix.

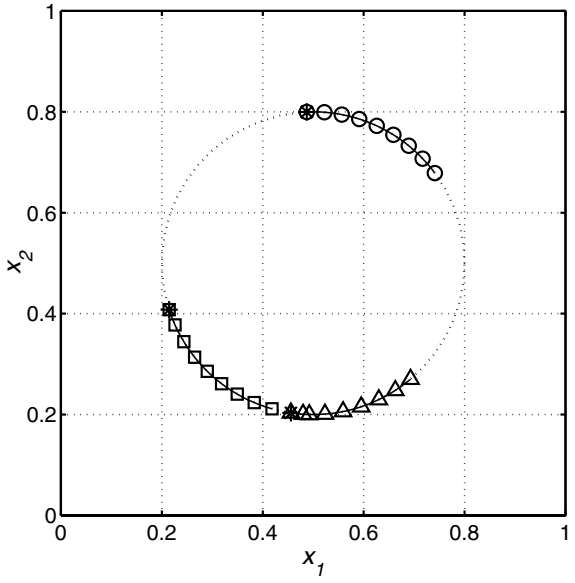


Figure 4.3: Optimal sensor trajectories along the circumference of a circle.

We see at once that the situation is by no means more difficult than in the setting of Section 4.2.1, as the only difference is that here the state is λ and g depends on λ only indirectly, via ω_j's. But while calculating the Fréchet derivative of J this complication is removed through the use of the Chain Rule (for details, see Uciński, 1996b).

Example 4.2. Consider the process of Example 4.1, but this time with the sensor motions restricted to the circumference of the circle with centre $(0.5, 0.5)$ and radius 0.3 (parametrized by its length). The sensor velocities (i.e. the control variables in the model (4.63)) were restricted so as to satisfy

$$|u_j(t)| \leq 0.3, \quad j = 1, 2, 3$$

When planning, the D-optimum design procedure was adopted. During the calculation, all the other numerical parameters of Example 4.1 were retained.

Figure 4.3 shows the optimal trajectories of the sensors obtained for several trials with different initial guesses regarding s_0^0 and u^0. Squares, circles and triangles denote consecutive sensor positions. Furthermore, sensors' positions at $t = 0$ are marked by the asterisks. The form of the trajectories is in agreement with our earlier findings, cf. Example 4.1. $\diamondsuit$

Measurement optimization with minimax criteria

In (Uciński and Korbicz, 1997) the outlined method of sensor motion planning was extended to include two widely-used minimax criteria, viz. those of MV- and E-optimality. As is well-known, they are not Fréchet differentiable (in general, only their directional derivatives exist), which highly complicates their use and hinders direct application of the foregoing algorithms.

The criteria are as follows:

- MV-optimality criterion

$$\Psi(M) = \max_{1 \le i \le m} d_{ii}(M) \tag{4.65}$$

- E-optimality criterion

$$\Psi(M) = \lambda_{\max}(M^{-1}) \tag{4.66}$$

where $d_{ii}(M)$ stands for the i-th element on the diagonal of M^{-1}, and $\lambda_{\max}(M^{-1})$ denotes the maximum eigenvalue of M^{-1}. Both the criteria have clear statistical interpretation. In the MV-optimum design, the maximal variance of the estimates $\hat{\theta}_1, \ldots, \hat{\theta}_m$ is minimized. On the other hand, while minimizing the E-optimality criterion, the length of the largest principal axis of the uncertainty ellipsoid of the estimates is suppressed.

The MV-optimality criterion is not Fréchet differentiable (this is because the max function is non-differentiable), which essentially complicates its minimization. To overcome this difficulty, an additional control parameter c is introduced and the equivalent problem of minimizing

$$J(s_0, u, c) = c \tag{4.67}$$

is considered subject to the additional inequality state constraint

$$\tilde{h}(s_0, u, c) = \max_{1 \le i \le m} d_{ii}(M) - c \le 0 \tag{4.68}$$

The following dependence is helpful while derivations of the expressions for the differentials:

$$\frac{\partial d_{ii}(M)}{\partial M} = -d^{(i)} d^{(i)\mathrm{T}} \tag{4.69}$$

where $d^{(i)}$ is the i-th column of M^{-1}.

In the case of minimizing the E-optimality criterion (4.66), we cannot use gradient methods, since in general the eigenvalues of M are not Fréchet differentiable. In fact, if an eigenvalue is repeated, then only its directional (Gâteaux) derivative exists which is strongly non-linear in δM (Haug *et al.*, 1986). To overcome this difficulty, we propose to make use of the dependence (Pázman, 1986)

$$\left(\text{trace } M^{-\mu}\right)^{1/\mu} \xrightarrow[\mu\to\infty]{} \lambda_{\max}(M^{-1}) \tag{4.70}$$

which is valid for any FIM and to replace minimization of (4.66) by that of the 'smooth' functional

$$J_\mu(s_0, u) = \text{trace } M^{-\mu} \tag{4.71}$$

for a sufficiently large μ. For such a regularized criterion, we have

$$\frac{\partial \,\text{trace}\, M^{-\mu}}{\partial M} = -\mu M^{-\mu-1} \tag{4.72}$$

Example 4.3. As an example of the application of the proposed algorithm, the two-dimensional heat equation

$$\frac{\partial y(x,t)}{\partial t} = \frac{\partial}{\partial x_1}\left(\kappa(x)\frac{\partial y(x,t)}{\partial x_1}\right) + \frac{\partial}{\partial x_2}\left(\kappa(x)\frac{\partial y(x,t)}{\partial x_2}\right),$$
$$x \in \Omega = (0,1)\times(0,1), \quad t \in (0,1)$$

is considered, subject to the conditions

$$\begin{aligned} y(x,0) &= 50, && x \in \Omega \\ y(x,t) &= 50\,(1-t), && (x,t) \in \partial\Omega \times T \end{aligned}$$

The diffusion coefficient to be identified has the form

$$\kappa(x) = \theta_1 + \theta_2 x_1 + \theta_3 x_2 + \theta_4 x_1 x_2$$
$$\theta_1 = 0.1, \quad \theta_2 = 0.3, \quad \theta_3 = 0.1, \quad \theta_4 = 0.3$$

where the values θ_1, θ_2 and θ_3 are also treated as nominal.

The problem is to estimate the thermal diffusivity coefficient κ (i.e. the parameters θ_i, $i = 1, \ldots, 4$) as accurately as possible, based on the measurements of the state made by four moving sensors. For that purpose,

the MV- and E-optimum design procedures are adopted. As regards the sensor dynamics, we consider the simple model

$$\dot{s}(t) = u(t), \quad s(0) = s_0$$

where the sensor velocities (controls) are limited according to

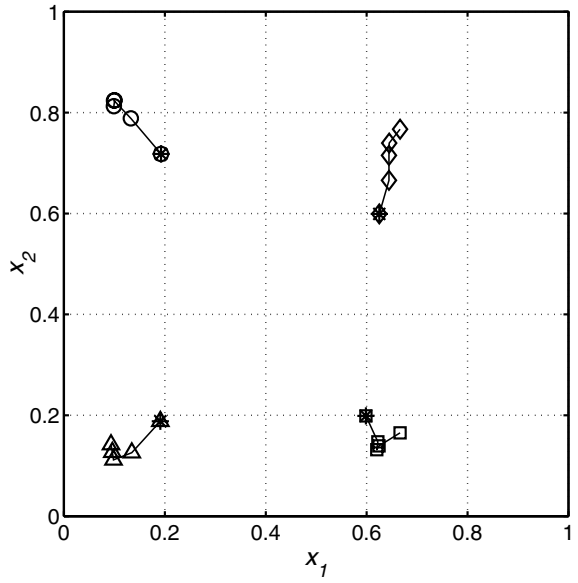
$$|u_i(t)| \leq 0.3, \quad i = 1, \ldots, 8$$

During simulations, the velocities were approximated by piecewise linear polynomials ($K = 40$). The parameters ρ, η and an additional parameter ς introduced to limit increments in c were changed to speed convergence in a manner similar to that used to adapt the learning rate in the training procedure for backpropagation neural networks (Korbicz *et al.*, 1994). The Cauchy convergence criterion for the sequence $J(s_0^k, u^k, c^k)$ equals 10^{-4}.

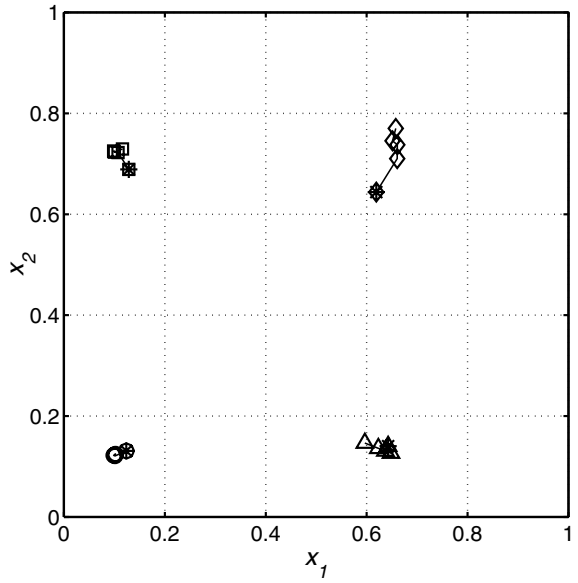
Figure 4.4(a) shows the MV-optimal trajectories of the sensors obtained after several trials with different initial guesses regarding s_0^0 and u^0 (to avoid getting stuck in a local minimum). Squares, circles, triangles and diamonds denote consecutive sensor positions. Furthermore, the sensors' positions at $t = 0$ are marked by the asterisks.

Let us note that the diffusion coefficient values in the upper right of Ω are greater than those in the lower left. This means that the state changes during the system evolution are quicker when we move up and to the right (on the other hand, the system reaches the steady state there earlier). This fact explains the form of the obtained trajectories—the sensors follow the regions where the distributed system is the most sensitive with respect to the unknown parameter κ. This region shifts to the lower left as time elapses and this is also reflected by the form of the trajectories. Let us note that one of the sensors practically stays at one point for most of the time and thus its behaviour is much like that of a stationary one.

For comparison, Fig. 4.4(b) shows the (sub-)optimal trajectories corresponding to the E-optimal criterion, which was in this case approximated by (4.71) with $\mu = 7$. The ultimate value of $\lambda_{\max}(M^{-1})$ was 0.4287. As can be seen, the results obtained for the MV- and E-optimality criteria are quite similar. In optimum experimental design for static linear regression models, some equivalence conditions for both the designs can even be formulated (Ermakov and Zhigljavsky, 1987), so it would be reasonable to expect some similarities also in the non-linear dynamic case. In this context, our results are not surprising. ♢



(a)



(b)

Figure 4.4: Optimal sensor trajectories: MV-optimality criterion (a) and approximated E-optimality criterion (b).

Minimal number of sensors

Since the number of sensors is generally governed by economic considerations, it is desirable to reduce their number to as few as possible provided that this new number of sensors still guarantees an acceptable level of precision for the estimates. The accuracy of parameter estimates for a fixed number of sensors is approximately described by the diagonal of the inverse of the FIM

$$M(s) = \frac{1}{\sigma^2} \sum_{j=1}^{N} \int_0^{t_f} \left(\frac{\partial y(x^j, t; \theta)}{\partial \theta} \right)^{\mathrm{T}} \left(\frac{\partial y(x^i, t; \theta)}{\partial \theta} \right) \Bigg|_{\theta=\theta^0} \mathrm{d}t \tag{4.73}$$

so we can define an error bound e.g. of the form

$$\mathfrak{J}(N) = \frac{1}{m} \sum_{i=1}^{m} \frac{d_{ii}}{\theta_i^0} \leq \epsilon \tag{4.74}$$

where d_{ii} denotes the i-th element of the diagonal of $D = M^{-1}$, θ_i^0 is a prior estimate of the i-th parameter (obtained e.g. from a preliminary experiment or by physical analysis), and ϵ stands for the desired estimation accuracy. This approach is similar to that used in the context of state estimation (Korbicz and Zgurowski, 1991; Azhogin *et al.*, 1988; Oh and No, 1994). Clearly, there exist many alternative choices of the criterion (4.74). The particular form presented here takes into account the relative errors of the estimates and improves the accuracy of the small parameters, which is of interest e.g. when parameters with very different magnitudes are to be found simultaneously.

The minimal number of sensors is equal to the minimum number N for which the condition (4.74) is satisfied. The fulfilment of (4.74) is checked after each optimization stage consisting in minimizing a selected design criterion for a given fixed number of sensors. If (4.74) is not satisfied, then a larger number of sensors should be used; otherwise, we should reduce the number of sensors to a value which has not been examined yet. Note that the right-hand side of (4.74) can be rewritten in the form $\mathrm{trace}(LM^{-1})$, where $L = \mathrm{diag}\{1/(m\theta_1^0), \ldots, 1/(m\theta_m^0)\}$, which corresponds to an L-optimal criterion (Pukelsheim, 1993; Uciński, 2000b).

Example 4.4. In order to study the applicability and performance of the proposed approach, let us consider the situation of Example 4.3 with a slightly changed diffusivity coefficient, i.e.

$$\kappa(x) = \theta_1 + \theta_2 x_1 + \theta_3 x_2, \quad \theta_1 = 0.1, \quad \theta_2 = 0.3, \quad \theta_3 = 0.1$$

Our purpose is to estimate κ (i.e. the parameters θ_1, θ_2 and θ_3) as accurately as possible based on the measurements made by N moving sensors. To this end, for each fixed N, the L-optimum design procedure is adopted, where L is selected as described above, i.e. the criteria J and $\mathfrak{J}$ are the same. Let us note that we could also select other design criteria at this stage. The criterion (4.74) is only used to validate the results after optimization of sensors' location for a given N. If the results are not satisfactory, we test another number of sensors.

It is required that the sensor velocities be bounded in accordance with the conditions

$$|u_j(t)| \leq 0.2, \quad j = 1, \ldots, 2N$$

As regards technicalities, during simulations the velocities were considered in the class of piecewise linear polynomials ($K = 50$). The parameters ρ and η were gradually decreased from 0.05 to 0.01. The Cauchy convergence criterion for the sequence $J(x_0^k, u^k)$ equals 10^{-4}. Furthermore, the minimum allowable distance between the sensors is $R = 0.1$.

In order to select a minimal number of sensors, we assume that $\sigma = 0.1$ and $\epsilon = 0.0025$ (this amounts to the average relative error for the parameters of about 5%). Figures 4.5 and 4.6 show the optimal sensor trajectories obtained for $N = 3, 4, 5, 6$ after several trials with different initial guesses regarding s_0^0 and u^0. As usual, symbols like circles, squares and triangles denote consecutive sensor positions. Furthermore, the sensors' positions at $t = 0$ are marked by the arrows.

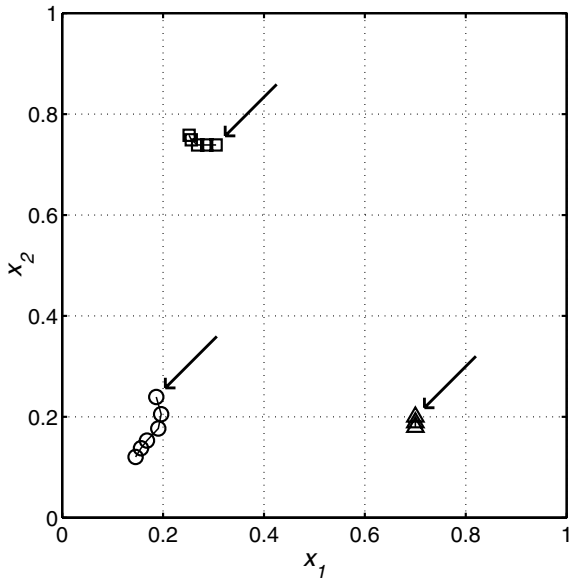
The following values of the criterion (4.74) were obtained:

$$\mathfrak{J}(3) = 0.0051, \quad \mathfrak{J}(4) = 0.004, \quad \mathfrak{J}(5) = 0.0029, \quad \mathfrak{J}(6) = 0.0024$$

which indicates that the minimum number of sensors is equal to six. $\diamondsuit$

4.3 Concluding remarks

In this chapter, the main principles of motion planning for mobile sensors have been presented. First, some fundamental results of modern optimum experimental design theory were extended to our framework following the ideas presented in the seminal paper (Rafajłowicz, 1986c). The implication is that the problem reduces to solving at each time moment a separate optimization task to which classical optimum-experimental design algorithms can be applied. Apart from the fact that the computing power necessary to



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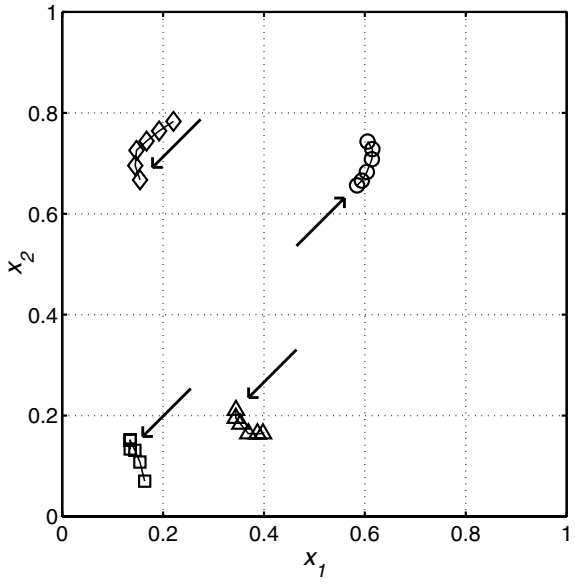
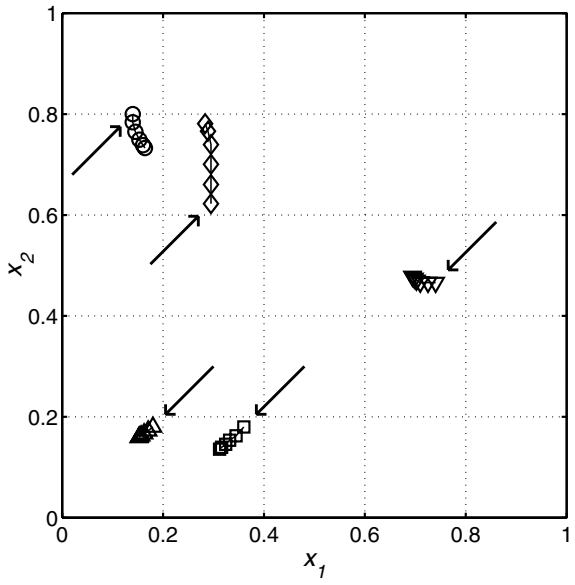
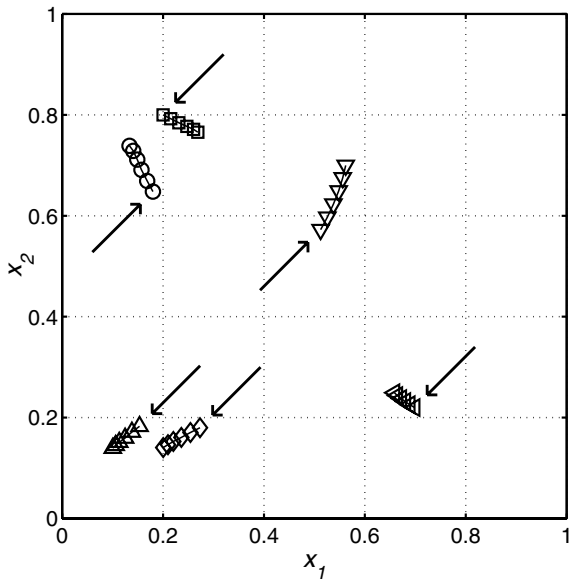


(b)

Figure 4.5: Optimum sensor trajectories of Example 4.4: (a) $N = 3$, (b) $N = 4$.



(a)



(b)

Figure 4.6: Optimum sensor trajectories of Example 4.4: (a) $N = 5$, (b) $N = 6$.

solve all the resulting subproblems is enormous, a major drawback to this method is that only measurability of the trajectories can be guaranteed. As was shown, these inconveniences can be somewhat alleviated by suitably parametrizing the trajectories, but the main disadvantage to the approaches based on continuous designs, i.e. sensor clusterization, still persists and restricts the spectrum of potential applications. On the other hand, the results obtained provide evidence for close relations between classical optimum experimental design for regression problems and motion planning for multiple sensors, and indicate some directions for future research (especially in connection with recent advances in spatial statistics).

Special attention has been paid to the problem of planning optimal motions for a given number of pointwise sensors which are to provide measurement data for parameter estimation of a general distributed system. Based on a scalar measure of performance defined on the Fisher information matrix related to the unknown parameters, the problem was formulated as an optimal-control one with state-variable inequality constraints representing geometric constraints induced by the admissible measurement regions and allowable distances between the sensors. Taking account of the dynamic models of the vehicles carrying the sensors, the problem was finally reduced to determination of both the control forces of the sensors and initial sensor positions. We showed that the resulting problem can be converted to an equivalent classical Mayer problem which is thoroughly treated in optimal control theory and for which numerous efficient algorithms exist. Accordingly, we applied one of them, i.e. a method of successive linearizations, to construct a quite efficient numerical scheme of determining optimal sensor trajectories. This scheme was verified through application to a two-dimensional parabolic equation. Simulation experiments validate the fact that making use of moving sensors may lead to dramatic gains in the values of the adopted performance indices, and hence to a much greater accuracy in the resulting parameter estimates.

The approach suggested here has the advantage that it is independent of a particular form of the partial-differential equation describing the considered distributed system. The only requirement is the existence of sufficiently regular solutions to the state and sensitivity equations, and consequently non-linear systems can also be treated within the same framework practically without any changes. Furthermore, the optimal-control approach proposed here allows for a variety of possible sensor motion models and motion constraints to be directly considered. Apart from the constraints preventing from clusterization and measurements outside the imposed ad-

missible zones, we might also include those induced by the existing obstacles (stationary or mobile), sensors' geometrical dimensions, etc. Moreover, the approach can be easily generalized to three spatial dimensions and the only limitation is the amount of required computations.

Clearly, the method of successive linearizations, which has been used to numerically calculate approximations to the optimal sensor trajectories, constitutes only one of many possible choices and other algorithms for problems with state inequality constraints could have been employed for that purpose. Its decided advantages, however, are that the improvements generated by the algorithm drive the state trajectories into the interior of the state constraint region and that it does not require knowledge of an initial solution satisfying the state constraints. Moreover, the specific form of the resulting linear-programming subtasks makes the method particularly suited for parallel implementations.

Chapter 5

Robustness of solutions to the sensor location problem

As was already emphasized (cf. Section 2.4.4), one of the main difficulties associated with optimization of sensor locations is the dependence of optimal solutions on the true values θ_{true} of the parameters to be estimated. Since these values are unknown, an obvious and common approach is to use one of the locally optimal designs described in previous chapters for some prior estimate θ^0 of θ_{true} in lieu of θ_{true} itself (it can be e.g. a nominal value for θ or a result of a preliminary experiment). But θ^0 may be far from θ_{true} and, simultaneously, properties of locally optimal designs can be very sensitive to changes in θ (Ford *et al.*, 1989). Such prior uncertainty on θ^0 is not taken into account by any optimization procedure to determine local designs and an experimental setting thus obtained may consequently be far from optimal. This has even raised some doubts among experimenters about the practical use of non-linear experimental design at all (Walter and Pronzato, 1990).

Several more cautious approaches have been proposed so far to attempt at surmounting this difficulty, but none of them is flawless and the problem still remains a real challenge for researchers. The aim of this chapter is to briefly outline the existing methods of making experimental designs independent of the true parameter values and to discuss how these methods can be adopted in the framework of the sensor location problem where, to the best of our knowledge, robust approaches have not been applied yet.

5.1 Sequential designs

Since a good choice of design depends on true parameter values, a very natural idea is to alternate experimentation and estimation steps. Accordingly, the total time horizon is divided into several contiguous parts and each of them is related to the corresponding stage of the experiment. At each stage, in turn, a locally optimal sensor location is determined based on the available parameter estimates (nominal parameter values can be assumed as initial guesses for the first stage), measurements are taken at the newly calculated sensor positions, and the data obtained are then analysed and used to update the parameter estimates (see Fig. 5.1). In this general scheme, it is intuitively supposed that each estimation phase improves our knowledge about the parameters and this knowledge can then be used to improve the quality of the next experiment to be performed.

Figure 5.1: A general scheme of sequential design.

Owing to its simplicity, sequential design is commonly considered as a universal panacea for the shortcomings of local designs. Let us note, however, that the following important questions are to be faced (Ford *et al.*, 1989) and the answers to them are by no means straightforward:

1. How many subintervals should be chosen?
2. How do the initial estimates of parameters influence the design?
3. What are the asymptotic properties of sequential procedures, i.e. does the generated design 'tend' in any sense to a design which would be optimal in terms of the true θ?

Some developments regarding a theoretical justification for the sequential approach can be found e.g. in (Ford *et al.*, 1989; Walter and Pronzato, 1990; Walter and Pronzato, 1997). But even though this technique can be

warranted to a certain extent, it is often impractical because the required exprimental time may be too long and the experimental cost may be too high.

In engineering practice it is sometimes known that θ_{true} belongs to a given compact set Θ_{ad}. In such a case, the following 'naïve' technique is often employed (Fedorov and Hackl, 1997): Θ_{ad} is covered with an appropriate grid $\bar{\Theta}_{\text{ad}}$ of a reasonable size and then the behaviour of $\Psi[M(s^\star(\theta^i),\theta^j)]$ is analysed for potential pairs $(\theta^i,\theta^j)\in\bar{\Theta}_{\text{ad}}^2$, where $M(s,\theta)$ stands for the FIM calculated at θ for a design s and $s^\star(\theta)=\arg\min_{s\in\mathcal{S}_{\text{ad}}}\Psi[M(s,\theta)]$. Consequently, a 'compromise' design can be determined such that it is good enough for any θ from the discretized set Θ_{ad}. Clearly, this may involve tremendeous calculations if the number of grid nodes is large. Nevertheless, this approach constitutes an origin for more systematic methods of robust design which are delineated in what follows.

5.2 Optimal designs in the average sense

5.2.1 Problem statement

If it is known that the range of possible θ values reduces to a given compact set Θ_{ad}, then a more cautious approach to the control of the properties of the sensor location over Θ_{ad} consists in a probabilistic description of the prior uncertainty in θ, characterized by a prior distribution ς which may have been inferred e.g. from previous observations collected on similar processes. The criterion to be minimized is then the expectation of the corresponding local optimality criterion J over Θ_{ad}, i.e.

$$J_{\text{E}}(s)=\mathop{\text{E}}_{\theta}\big\{J(s,\theta)\big\}=\mathop{\text{E}}_{\theta}\big\{\Psi[M(s,\theta)]\big\}=\int_{\Theta_{\text{ad}}}\Psi[M(s,\theta)]\,\varsigma(\text{d}\theta) \tag{5.1}$$

Using ς makes it possible to remove the dependence of the FIM on θ.

As for possible choices of ς, it is customary to assume that

$$\varsigma(\text{d}\theta)=p(\theta)\text{d}\theta \tag{5.2}$$

where p signifies the prior probability density function for θ. Some examples of p are as follows (Sun, 1994):

- If the true θ is known exactly as θ^0, then we have

  $$p(\theta)=\delta(\theta-\theta^0)$$

  where θ^0 is the Dirac delta function.

- If θ is limited to a region Θ_{ad}, but we have no other information, then we can assume a uniform distribution on Θ_{ad}, i.e.

$$p(\theta) = \begin{cases} 1/\operatorname{meas}(\Theta_{\mathrm{ad}}) & \text{if } \theta \in \Theta_{\mathrm{ad}} \\ 0 & \text{otherwise} \end{cases}$$

  where $\operatorname{meas}(\Theta_{\mathrm{ad}})$ stands for the Lebesgue measure of Θ_{ad}.

- If the expected value μ_θ and the covariance matrix V_θ of θ can be estimated, but we have no other information, we can assume that p is the probability density function for a multivariate normal distribution given by

$$p(\theta) = \frac{1}{(2\pi)^{m/2}(\det V_\theta)^{1/2}} \exp\left[-\frac{1}{2}(\theta - \mu_\theta)^{\mathrm{T}} V_\theta^{-1}(\theta - \mu_\theta)\right]$$

  where a cut-off and an appropriate normalization should be additionally imposed if this $p(\theta)$ does not diminish to a negligibly small value before the limits of Θ_{ad} are reached.

A notable feature of the approach is that the number of expectation criteria is greater than the number of their counterparts in the local case. Indeed, for the most popular D-optimal design we have e.g. the following choices (Walter and Pronzato, 1997):

- ED-optimal design which maximizes

$$J_{\mathrm{ED}}(s) = \mathop{\mathrm{E}}_{\theta}\{\det M(s,\theta)\} \tag{5.3}$$

- EID-optimal design which minimizes

$$J_{\mathrm{EID}}(s) = \mathop{\mathrm{E}}_{\theta}\{1/\det M(s,\theta)\} \tag{5.4}$$

- ELD-optimal design which maximizes

$$J_{\mathrm{ELD}}(s) = \mathop{\mathrm{E}}_{\theta}\{\ln\det M(s,\theta)\} \tag{5.5}$$

It turns out that the above criteria usually yield different optimal solutions and hence care must be exercised while adopting a particular option (their advantages and drawbacks are discussed in (Walter and Pronzato, 1997)). The other cost functions could be handled in a similar manner.

The extension of the approach to continuous designs of Section 3.2 does not present a problem, as we may introduce

$$\Psi_{\mathrm{E}}(\xi) = \int_{\Theta_{\mathrm{ad}}} \Psi[M(\xi,\theta)]\,\varsigma(\mathrm{d}\theta) \tag{5.6}$$

Since integrating acts as a linear operator, Theorem 3.1 of p. 45 and Theorem 3.2 of p. 46 can be rewritten in this new framework, practically without any changes by introducing

$$\psi(x,\xi) = \int_{\Theta_{\mathrm{ad}}} \hat{\psi}(x,\xi,\theta)\,\varsigma(\mathrm{d}\theta) \tag{5.7}$$

$$\phi(x,\xi) = \int_{\Theta_{\mathrm{ad}}} \hat{\phi}(x,\xi,\theta)\,\varsigma(\mathrm{d}\theta) \tag{5.8}$$

$$c(\xi) = \int_{\Theta_{\mathrm{ad}}} \hat{c}(\xi,\theta)\,\varsigma(\mathrm{d}\theta) \tag{5.9}$$

where $\hat{\psi}(x,\xi,\theta)$, $\hat{\phi}(x,\xi,\theta)$ and $\hat{c}(\xi,\theta)$ denote the respective quantities of Section 3.2 calculated for an indicated parameter vector θ. There are only two striking differences. First of all, Carethéodory's theorem cannot be directly applied since Ψ_{E} depends on different matrices $M(\xi,\theta)$ for different θ's, which implies in turn that the existence of an optimal design with not more than $m(m+1)/2$ support points is no longer guaranteed. Secondly, except for very special situations, an optimal design cannot be obtained analytically and algorithmic procedures are thus needed. Theorem 3.2 provides a basis for efficient numerical algorithms to determine approximations to optimal local designs. Unfortunately, its counterpart for an expectation criterion is conctructive only if the prior distribution ς is discrete with a moderate number of support points. Clearly, this remark pertains to any numerical scheme described in previous chapters, since the main intricacy remains the same: in order to directly minimize (5.1) or (5.6), we have to evaluate expectations, i.e. multi-dimensional integrals, which is extremely time-consuming. Luckily, it turns out that approximations to an optimal design can be determined without any evaluation of mathematical expectation. This constitutes the subject of the next subsection.

5.2.2 Stochastic-approximation algorithms

A direct minimization of (5.1) is highly complicated by the fact that an expected value of a local cost function has to be evalueated, which is plausible only when the prior distribution ς is discrete. Let us observe, however,

that the situation is by no means hopeless, as this framework is typical for the application of stochastic-approximation techniques. Indeed, it is standard for a stochastic optimization problem that the objective function is not explicitly known (Pflug, 1996), i.e. that there is no computer programme which finds its exact value at each value of the decision variable in a reasonable time (otherwise, we would just have to solve a deterministic non-linear optimization problem). Based on the validity of the law of large numbers, a stochastic optimization problem is approximated in such a way that the uncertain random quantities in the original problem are replaced by artificially generated random variables. If these random variables are produced in advance to construct an approximate empirical problem, then we deal with the so-called non-recursive methods being part of the broad family of Monte-Carlo methods. From a practical point of view, recursive methods are sometimes more interesting. In these methods random samples are drawn only at the moment when they are requested. The total number of such random draws does not have to be determined at the beginning, but it can be adaptively chosen during the progress of estimation (Pflug, 1996; Kushner and Yin, 1997).

In the context of a non-linear experimental design, the idea to employ algorithms of stochastic approximation was suggested and successfully applied to robust-design problems in (Pronzato and Walter, 1985; Walter and Pronzato, 1987; Walter and Pronzato, 1997). Owing to evident similarities of that setting to the sensor location problem considered in our monograph, the same technique can be put into execution in this slightly modified framework. A simple classical Robbins-Monro algorithm, also known as the stochastic-gradient algorithm, corresponds to the following iterative procedure:

$$s^{k+1} = \Pi_{\mathcal{S}_{\mathrm{ad}}}\left(s^k - \gamma_k \left(\frac{\partial \Psi[M(s,\theta^k)]}{\partial s} \right)^{\mathrm{T}}_{s=s^k} \right), \quad k = 0, 1, \ldots \tag{5.10}$$

where θ^k is randomly generated according to the prior distribution ς and $\Pi_{\mathcal{S}_{\mathrm{ad}}}$ denotes the orthogonal projection onto the set $\mathcal{S}_{\mathrm{ad}} = X^N$, where X signifies a spatial zone where the measurements are allowed (a compact subset of $\bar{\Omega}$). The sequence of decreasing scalar steps $\{\gamma_k\}$ must guarantee an implicit averaging of the outcomes of the simulation, which is attained if the following conditions are satisfied:

$$\gamma_k \geq 0, \quad \sum_{k=0}^{\infty} \gamma_k = \infty, \quad \sum_{k=0}^{\infty} \gamma_k^2 < \infty \tag{5.11}$$

The most common practice is to use the harmonic sequence

$$\gamma_k = \frac{b}{k+1}, \quad b > 0, \quad k = 0, 1, \ldots \tag{5.12}$$

The Robbins-Monro procedure requires the existence of unbiased estimates of the gradient $\partial \, \mathrm{E}_\theta \big\{ \Psi[M(s,\theta)] \big\} / \partial s$, but it is a simple matter to check that

$$\begin{aligned} \mathop{\mathrm{E}}_{\theta} \left\{ \frac{\partial \Psi[M(s,\theta)]}{\partial s} \right\} &= \int_{\Theta_{\mathrm{ad}}} \frac{\partial \Psi[M(s,\theta)]}{\partial s} \, \varsigma(\mathrm{d}\theta) \\ &= \frac{\partial}{\partial s} \int_{\Theta_{\mathrm{ad}}} \Psi[M(s,\theta)] \, \varsigma(\mathrm{d}\theta) = \frac{\partial}{\partial s} \mathop{\mathrm{E}}_{\theta} \{ \Psi[M(s,\theta)] \} \end{aligned} \tag{5.13}$$

provided that all derivatives $\partial^2 y / \partial x_i \partial \theta_j$ are continuous in $\bar{\Omega} \times T \times \Theta_{\mathrm{ad}}$. Consequently, the quantity $\partial \Psi[M(s,\theta^k)]/\partial s$ in (5.10) constitutes an unbiased estimate of the gradient of the expectation criterion (5.1).

Under some classical assumptions (Pflug, 1996; Kushner and Yin, 1997; Ermakov and Zhigljavsky, 1987) which are satisfied when the system state y is sufficiently smooth, convergence almost surely of the algorithm (5.10) is ensured. Note, however, that convergence to a global minimum is not guaranteed. As pointed out in (Pronzato and Walter, 1985), it can be accelerated by changing the value of s^k only when the angle between the gradients at iterations $k-1$ and k is greater than $\pi/2$.

Projection $\Pi_{\mathcal{S}_{\mathrm{ad}}}(s)$ denotes the closest point in $\mathcal{S}_{\mathrm{ad}}$ to s and is introduced to avoid the situations where s^{k+1} does not belong to $\mathcal{S}_{\mathrm{ad}}$. The uniqueness of such a mapping is guaranteed if $\mathcal{S}_{\mathrm{ad}}$ is convex. But if the closest point fails to be unique, a closest point should be selected such that the function $\Pi_{\mathcal{S}_{\mathrm{ad}}}(\,\cdot\,)$ is measurable (Kushner and Yin, 1997, p. 100). Let us recall that the projection can sometimes be performed without resorting to sophisticated optimization algorithms. For example, if $\mathcal{S}_{\mathrm{ad}}$ is a hyperrectangle, i.e. there are real numbers $a_i < b_i$, $i = 1, \ldots, n$ such that $\mathcal{S}_{\mathrm{ad}} = \big\{ s = (s_1, \ldots, s_n) : a_i \le s_i \le b_i, \ i = 1, \ldots, n \big\}$, then we have

$$\big[\Pi_{\mathcal{S}_{\mathrm{ad}}}(s) \big]_i = \begin{cases} b_i & \text{if } s_i > b_i \\ s_i & \text{if } a_i \le s_i \le b_i \\ a_i & \text{if } s_i < a_i \end{cases} \tag{5.14}$$

where $[\,\cdot\,]_i$ is the i-th component of a vector, $i = 1, \ldots, n$.

When solving sensor location problems, it is occasionally necessary to include additional constraints regarding e.g. the admissible distances between

the sensors since, as pointed out in (Walter and Pronzato, 1987), robust designs based on expectaton criteria inherit many properties of local designs, including replication of measurements, which in our context means that sensor clusterization may be observed. Formally, the corresponding constraints can be taken into account by an appropriate re-definition of the admissible set $\mathcal{S}_{\mathrm{ad}}$, but this would essentially complicate the projection. Note, however, that the constraints on the distances are merely a guide in that they should not be violated by much, but they *can* be violated, i.e. we simply deal with the so-called *soft* constraints. Such constraints can be added to the Robbins-Monro algorithm directly by adding appropriate penalty-function terms to the performance index (Kushner and Yin, 1997, p. 120). The idea is more or less obvious and therefore the corresponding details are omitted.

The convergence result tells us that we will get the desired point if we let the procedure run for a sufficiently long time. Clearly, such a statement is unsatisfactory for practical purposes. What is really needed is a statement about the precision of s^k for a finite k. This would allow us to make a decision whether or not the procedure should be terminated. But this topic is also classical and the corresponding results regarding stopping criteria and confidence regions for the solutions can be found in (Pflug, 1996, p. 297).

Another question is the optimum measurement problem for moving sensors. Of course, this case can be easily reduced to a static framework after a parametrization of the trajectories, but it turns out that the Robbins-Monro algorithm can also be generalized to minimizing noisy functionals in infinite-dimensional real separable Hilbert spaces. This requires operating on H-valued random variables and the theoretical results are scattered in the literature (see e.g. Dvoretzky, 1986; Kushner and Shwartz, 1985; Nixdorf, 1984; Shwartz and Berman, 1989; Walk and Zsidó, 1989; Yin and Zhu, 1990; Berger, 1986; Goldstein, 1988; Révész, 1973a; Révész, 1973b), but despite all that such a generalization can still be done. In (Uciński, 1998b; Uciński, 1998c; Uciński and Korbicz, 1999a; Uciński, 1999c) based on the general description of the sensor motions

$$\dot{s}(t) = f(s(t), u(t)) \quad \text{a.e. on } T, \quad s(0) = s_0 \tag{5.15}$$

the following general form of the performance index to be minimized was considered:

$$J_{\mathrm{E}}(s_0, u) = \mathop{\mathrm{E}}_{\theta}\bigl\{J(s_0, u, \theta)\bigr\} \tag{5.16}$$

where $J(s_0, u, \theta) = \Psi[M(s, \theta)]$. Here u is assumed to be an element in the set

$$\mathcal{U} = \left\{ u \in L^2(T; \mathbb{R}^r) : u_l \leq u(t) \leq u_u \text{ a.e. on } T \right\} \tag{5.17}$$

and $s_0 \in \mathcal{S}_{\text{ad}}$. This determines the set of feasible pairs (s_0, u) which will be denoted by $\mathcal{F} = \mathcal{S}_{\text{ad}} \times \mathcal{U}$. Clearly, $\mathcal{U}$ is a closed convex set of $L^2(T; \mathbb{R}^r)$ and if $\mathcal{S}_{\text{ad}}$ is convex (by assumption it is closed), then so is $\mathcal{F}$ treated as a subset of the separable Hilbert space $\mathcal{H} = \mathbb{R}^n \times L^2(T; \mathbb{R}^r)$.

The corresponding version of the Robbins-Monro stochastic-gradient algorithm is

$$(s_0^{k+1}, u^{k+1}) = \Pi_{\mathcal{F}}\big((s_0^k, u^k) - \gamma_k \nabla J(s_0^k, u^k, \theta^k)\big), \quad k = 0, 1, \ldots \tag{5.18}$$

where $\nabla J(s_0^k, u^k, \theta^k)$ stands for the gradient of $J(\,\cdot\,, \cdot\,, \theta^k)$ calculated at (s_0^k, u^k) and $\Pi_{\mathcal{F}}$ denotes the orthogonal projection onto $\mathcal{F}$ in $\mathcal{H}$. It follows easily that $\Pi_{\mathcal{F}}(s_0, u) = (\Pi_{\mathcal{S}_{\text{ad}}}(s_0), \Pi_{\mathcal{U}}(u))$ and

$$\left[\Pi_{\mathcal{U}}(u)\right]_i(t) = \begin{cases} u_{ui} & \text{if } u_i(t) > u_{ui} \\ u_i(t) & \text{if } u_{li} \leq u_i(t) \leq u_{ui} \\ u_{li} & \text{if } u_i(t) < u_{li} \end{cases} \tag{5.19}$$

As regards computation of $\nabla J(s_0^k, u^k, \theta^k) \in \mathcal{H}$, it may be easily concluded that

$$\nabla J(s_0^k, u^k, \theta^k) = (\zeta(0), f_u^{\mathrm{T}}(\,\cdot\,)\zeta(\,\cdot\,)) \tag{5.20}$$

where the adjoint mapping ζ solves the Cauchy problem

$$\dot{\zeta}(t) + f_s^{\mathrm{T}}(t)\zeta(t) = -\sum_{i=1}^{m}\sum_{j=1}^{m} c_{ij} \left(\frac{\partial \chi_{ij}}{\partial s}\right)^{\mathrm{T}}_{\substack{s=s(t) \\ \theta=\theta^k}}, \quad \zeta(t_f) = 0 \tag{5.21}$$

$\langle\,\cdot\,, \cdot\,\rangle$ stands for the inner product in the appropriate Euclidean space, χ_{ij}'s are defined in (4.41), and c_{ij}'s are the components of the matrix

$$\overset{\circ}{\Psi}(s) = \left\{c_{ij}\right\}_{m \times m} = \left.\frac{\partial \Psi(M)}{\partial M}\right|_{M = M(s, \theta^k)} \tag{5.22}$$

The derivations are in principle the same as in Appendix D.1, but a thorough proof necessitates additional assumptions on f and sensitivity coefficients $\partial y / \partial \theta_i$ (they should be Lipschitz continuously differentiable on bounded

sets), as well as an introduction of some supplementary notions and hence it is omitted. The interested reader is referred to Appendix 5.6 of (Polak, 1997), where analogous technicalities are exhaustively treated within the framework of a general optimal-control problem.

The above results suggest that solutions to robust sensor location problems with minimax criteria can be obtained almost as simply as those for classical local design criteria, which constitutes a sound argument for the delineated approach. Note, however, that this assertion concerns only the manner in which the computations are organized. The approach itself sometimes raises the objection that it is not clear that values of Ψ are directly comparable for different values of θ. Moreover, the locally optimal values of Ψ may vary considerably with θ. Hence the resulting robust designs may tend to look like locally optimal designs for θ values with large associated variances. Consequently, it is a good idea to have alternative approaches in order to compare and analyse the obtained solutions. An additional option is offered by minimax criteria.

5.3 Optimal designs in the minimax sense

5.3.1 Problem statement and characterization

An experiment which is good on the average may prove very poor for some particular values of the parameters associated with very low probability densities (Pronzato and Walter, 1988). If we do not accept such a situation, then a way out is to optimize the worst possible performance of the experiment over the prior admissible domain for the parameters Θ_{ad}, which leads to minimization of the criterion

$$J_{\mathrm{MM}}(s) = \max_{\theta \in \Theta_{\mathrm{ad}}} J(s, \theta) = \max_{\theta \in \Theta_{\mathrm{ad}}} \Psi[M(s, \theta)] \tag{5.23}$$

In other words, we provide maximum information to a parameter vector θ which is the most difficult to be identified in Θ_{ad}. For example, we may seek to maximize the MMD-optimality criterion (Walter and Pronzato, 1997)

$$J_{\mathrm{MMD}}(s) = \min_{\theta \in \Theta_{\mathrm{ad}}} \det M(s, \theta) \tag{5.24}$$

Thus the best experimental conditions in the worst circumstances are preferred to the best ones on the average.

Clearly, the same minimax approach can be taken in the case of continuous designs studied in Section 3.2, viz. we can consider minimization of

the performance index

$$J_{\mathrm{MM}}(\xi) = \max_{\theta \in \Theta_{\mathrm{ad}}} \Psi[M(\xi, \theta)] \tag{5.25}$$

and we shall start on this framework, as some non-obvious characterizations of the corresponding optimum designs can be derived prior to resorting to numerical methods. The main idea is to observe that this setting can be treated in much the same way as that of non-differentiable design criteria, where an optimal design

$$\xi^{\star}_{\mathrm{M}} = \arg \min_{\xi \in \Xi(X)} \max_{a \in A} \Psi[M(\xi), a] \tag{5.26}$$

is to be determined, A being a given compact set of parameters which cannot be controlled by the experimenter. Let $\Psi(\,\cdot\,,\,\cdot\,)$ and $\partial\Psi(\,\cdot\,,\,\cdot\,)/\partial M$ be continuous. Under Assumptions (A3)–(A5) of p. 43 together with the following qualification:

(A6") For any $\xi \in \Xi(q) = \big\{\xi : \Psi[M(\xi)] \le q < \infty\big\}$ and $\bar{\xi} \in \Xi(X)$, we have

$$\begin{aligned} &\Psi[M(\xi) + \lambda(M(\bar{\xi}) - M(\xi)), a] \\ &\qquad = \Psi[M(\xi), a] + \lambda \int_X \psi(x, \xi, a)\, \bar{\xi}(\mathrm{d}x) + o(\lambda; \xi, \bar{\xi}) \end{aligned} \tag{5.27}$$

where $o(\lambda; \xi, \bar{\xi})/\lambda \xrightarrow[\lambda \to 0]{} 0$ uniformly in A and the scalar q is so chosen that $\Xi(q) \neq \emptyset$,

in lieu of (A6), we can now formulate the following key result.

Theorem 5.1. *A design $\xi^{\star}_{\mathrm{M}}$ is optimal iff there exists a probability measure $\omega^{\star}$ defined on $A(\xi) = \big\{\hat{a} : \Psi[M(\xi), \hat{a}] = \max_{a \in A} \Psi[M(\xi), a]\big\}$ such that*

$$\min_{x \in X} \int_{A(\xi)} \psi(x, \xi^{\star}_{\mathrm{M}}, a)\, \omega^{\star}(\mathrm{d}a) \ge 0 \tag{5.28}$$

Proof. The proof is based on some properties of max functions (Polak, 1997, App. 5.4) and results of game theory (Dyubin and Suzdal, 1981, Th. 31, p. 108). It is omitted as the procedure is in principle the same as in the proof of Theorem 2.6.1 of (Fedorov and Hackl, 1997, p. 42), also see (Ermakov and Zhigljavsky, 1987, p. 113). ■

This theorem is indeed of utmost importance, as in the context of the linear regression model (3.1) it can be immediately used to determine necessary and sufficient E-optimality conditions for the design of the form

$$\hat{\Psi}[M(\xi)] = \lambda_{\max}[M^{-1}(\xi)] \tag{5.29}$$

where $\lambda_{\max}[M^{-1}(\xi)]$ denotes the maximal eigenvalue of $M^{-1}(\xi)$. To see this, recall that from the symmetry of $M^{-1}(\xi)$ we have (Bertsekas, 1999, Prop. A.18, p. 660)

$$\lambda_{\max}[M^{-1}(\xi)] = \max_{a \in A} a^{\mathrm{T}} M^{-1}(\xi) a \tag{5.30}$$

where $A = \{a : a^{\mathrm{T}} a = 1\}$, which means that, as a matter of fact, we deal with a problem of the form (5.26) for which $\Psi[M(\xi), a] = a^{\mathrm{T}} M^{-1}(\xi) a$.

By the formula (Ermakov and Zhigljavsky, 1987, Th. 3.3, p. 309)

$$\frac{\partial \Psi[M(\xi), a]}{\partial M} = \frac{\partial \operatorname{trace}\left(a a^{\mathrm{T}} M^{-1}\right)}{\partial M} = -M^{-1} a a^{\mathrm{T}} M^{-1} \tag{5.31}$$

and arguments similar to those in the derivation of (3.30), we get

$$\psi(x, \xi, a) = a^{\mathrm{T}} M^{-1}(\xi) a - \frac{1}{t_f} \int_0^{t_f} \left\{ f^{\mathrm{T}}(x,t) M^{-1}(\xi) a \right\}^2 \mathrm{d}t \tag{5.32}$$

Consequently, (5.28) amounts to the condition

$$\sum_{i=1}^{\mu} \omega_i^\star \frac{1}{t_f} \int_0^{t_f} \left\{ f^{\mathrm{T}}(x,t) a_{\max}^i \right\}^2 \mathrm{d}t \le \lambda_{\max}^{-1}[M^{-1}(\xi^\star)], \quad \forall x \in X \tag{5.33}$$

for some $\omega_i^\star \ge 0$, $i = 1, \ldots, \mu$, where

$$\sum_{i=1}^{\mu} \omega_i^\star = 1 \tag{5.34}$$

μ being the multiplicity of $\lambda_{\max}[M^{-1}(\xi^\star)]$ and $a_{\max}^i$, $i = 1, \ldots, \mu$ standing for the corresponding eigenvectors.

After this digression, consider now the problem of minimizing the criterion $\Psi[M(\xi, \theta)]$, where

$$M(\xi, \theta) = \int_X \Upsilon(x, \theta)\, \xi(\mathrm{d}x) \tag{5.35}$$

and

$$\Upsilon(x,\theta) = \frac{1}{t_f}\int_0^{t_f} f(x,t,\theta) f^{\mathrm{T}}(x,t,\theta)\,\mathrm{d}t$$

for the linear regression (3.1). As regards the regularity of f, assume that it is continuous in $X \times T \times \Theta_{\mathrm{ad}}$. The resulting design problem can be handled in much the same way as (5.26). For example, in the case of the D-optimality criterion analysis analogous to that in the proof of Theorem 5.1 implies that a necessary and sufficient condition for $\xi^\star$ to be optimal is the existence of a measure $\omega^\star$ such that

$$\max_{x\in X} \frac{1}{t_f}\int_{\Theta(\xi^\star)} \left\{\int_0^{t_f} f^{\mathrm{T}}(x,t,\theta) M^{-1}(\xi^\star,\theta) f(x,t,\theta)\,\mathrm{d}t\right\} \omega^\star(\mathrm{d}\theta) \le m \quad (5.36)$$

where

$$\Theta(\xi) = \left\{\hat\theta \in \Theta_{\mathrm{ad}} : \det M(\xi,\hat\theta) = \min_{\theta\in\Theta_{\mathrm{ad}}} \det M(\xi,\theta)\right\} \quad (5.37)$$

The Carathéodory theorem ensures the existence of $\omega^\star$ with not more than $m+1$ support points. Obviously, this conclusion remains the same if we replace $f(x,t,\theta)$ by the sensitivity coefficients $(\partial y(x,t;\theta)/\partial\theta)^{\mathrm{T}}$. Note, however, that implementation of the foregoing results in the form of a constructive computer algorithm is by no means straightforward.

Another drawback of minimax design is that criteria which are invariant with respect to transformations of θ for the calculation of locally optimal designs may no longer be invariant with respect to the minimax design criterion (Ford *et al.*, 1989).

5.3.2 Numerical techniques for exact designs

As regards exact designs for stationary sensors, let us observe first that the initial minimax optimization problem (5.23) can be viewed as the minimization of a scalar α, subject to the constraint

$$\max_{\theta\in\Theta_{\mathrm{ad}}} \Psi[M(s,\theta)] \le \alpha \quad (5.38)$$

which is, in turn, equivalent to the infinite set of constraints

$$\left\{\Psi[M(s,\theta)] \le \alpha, \quad \theta \in \Theta_{\mathrm{ad}}\right\} \quad (5.39)$$

This task can be solved with the use of some algorithms for inequality-constrained semi-inifinite optimization (Polak, 1997, Sec. 3.5), but in practice the simple relaxation algorithm proposed by Shimizu and Aiyoshi (1980) turns out to perform well in the considered non-linear experimental design problems, as is also suggested in (Pronzato and Walter, 1988; Walter and Pronzato, 1997). It consists in relaxing the problem by taking into account only a finite number of constraints (5.39). The relaxation procedure is represented by the following steps:

Step 1. Choose an initial parameter vector $\theta^1 \in \Theta_{\rm ad}$ and define the first set of representative values $Z^1 = \{\theta^1\}$. Set $k = 1$.

Step 2. Solve the current relaxed problem

$$s^k = \arg \min_{s \in \mathcal{S}_{\rm ad}} \left\{ \max_{\theta \in Z^k} \Psi[M(s, \theta)] \right\}$$

Step 3. Solve the maximization problem

$$\theta^{k+1} = \arg \max_{\theta \in \Theta_{\rm ad}} \Psi[M(s^k, \theta)]$$

Step 4. If

$$\Psi[M(s^k, \theta^{k+1})] \leq \max_{\theta \in Z^k} \Psi[M(s^k, \theta)] + \epsilon$$

where ϵ is a small predetermined positive constant, then s^k is a sought minimax solution, otherwise include θ^{k+1} into Z^k, increment k, and go to Step 2.

It can be proved (Shimizu and Aiyoshi, 1980) that the above algorithm terminates in a finite number of iterations for any given $\epsilon > 0$. The usefulness of the algorithm in planning sensor locations was confirmed in (Uciński, 1999b).

As for the case of moving sensors whose movements are given by (5.15), we may consider minimization of the functional

$$J_{\rm MM}(s_0, u) = \max_{\theta \in \Theta_{\rm ad}} J(s_0, u, \theta) \tag{5.40}$$

Clearly, this can be treated by some numerical algorithms of optimal control, but a much simpler approach consists in making use of the dependence (Banichuk, 1990, p. 33)

$$\left\{ \frac{1}{\operatorname{meas}(\Theta_{\rm ad})} \int_{\Theta_{\rm ad}} J^{\mu}(s_0, u, \theta) \, {\rm d}\theta \right\}^{1/\mu} \xrightarrow[\mu \to \infty]{} \max_{\theta \in \Theta_{\rm ad}} J(s_0, u, \theta) \tag{5.41}$$

where, without restriction of generality, it is assumed that J takes on only non-negative values. Hence we may write

$$J_{\mathrm{MM}}(s_0,u)=\max_{\theta\in\Theta_{\mathrm{ad}}}J(s_0,u,\theta)\approx\left\{\frac{1}{\mathrm{meas}(\Theta_{\mathrm{ad}})}\int_{\Theta_{\mathrm{ad}}}J^{\mu}(s_0,u,\theta)\,\mathrm{d}\theta\right\}^{1/\mu} \tag{5.42}$$

and replace minimization of (5.40) by minimization of the 'smooth' functional

$$J_{\mu}(x_0,u)=\frac{1}{\mathrm{meas}(\Theta_{\mathrm{ad}})}\int_{\Theta_{\mathrm{ad}}}J^{\mu}(s_0,u,\theta)\,\mathrm{d}\theta=\mathop{\mathrm{E}}_{\boldsymbol{\theta}}\{J^{\mu}(s_0,u,\theta)\} \tag{5.43}$$

for a sufficiently large μ, where the expectation is calculated for the uniform distribution on Θ_{ad}. The latter can be solved in much the same way as in Section 5.2.2.

Example 5.1. In what follows, our aim is to apply the delineated numerical algorithms to the two-dimensional heat equation

$$\begin{aligned}\frac{\partial y(x,t)}{\partial t}&=\frac{\partial}{\partial x_1}\left(\kappa(x)\frac{\partial y(x,t)}{\partial x_1}\right)+\frac{\partial}{\partial x_2}\left(\kappa(x)\frac{\partial y(x,t)}{\partial x_2}\right)\\&\quad+10[x_1+(1-x_1)t],\quad (x,t)\in\Omega\times T=(0,1)^3\end{aligned}$$

subject to the conditions

$$\begin{aligned}y(x,0)&=0,\quad x\in\Omega\\y(x,t)&=0,\quad (x,t)\in\partial\Omega\times T\end{aligned}$$

Let us assume the following form of the diffusion coefficient to be identified:

$$\kappa(x)=\theta_1+\theta_2x_1+\theta_3x_2$$

The objective is to estimate κ (i.e. the parameters θ_1, θ_2 and θ_3) as accurately as possible, based on the measurements made by three moving sensors. For this purpose, the ED- and approximated MMD-optimum design procedures have been implemented in Fortran 90 programming language and run on a PC (Pentium II, 300 Mhz, 128 MB RAM). During simulations, maximization of the criterion (5.24) was replaced by minimization of the smoothed functional (5.43) for $J(s_0,u,\theta)=1/\det M(s,\theta)$ and $\mu=5$. As

regards the prior knowledge about the parameters, we were working under the assumption that

$$0.05 \leq \theta_1 \leq 0.15$$
$$0.0 \leq \theta_2 \leq 0.2$$
$$0.0 \leq \theta_3 \leq 0.2$$

and that they were characterized by uniform distributions on the corresponding intervals.

As for the sensor dynamics, we assumed that it was not of primary concern, so we adopted the simple model

$$\dot{s}(t) = u(t), \quad s(0) = s_0$$

The sensor velocities were considered under the restrictions

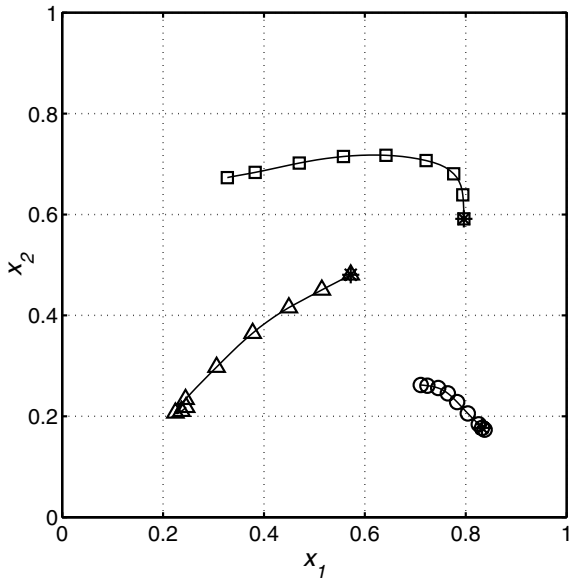
$$|u_i(t)| \leq 0.7, \quad i = 1, \ldots, 6$$

and approximated by piecewise linear polynomials (for 40 divisions of the interval $[0, t_f]$). In both the cases, the algorithm (5.18) started from

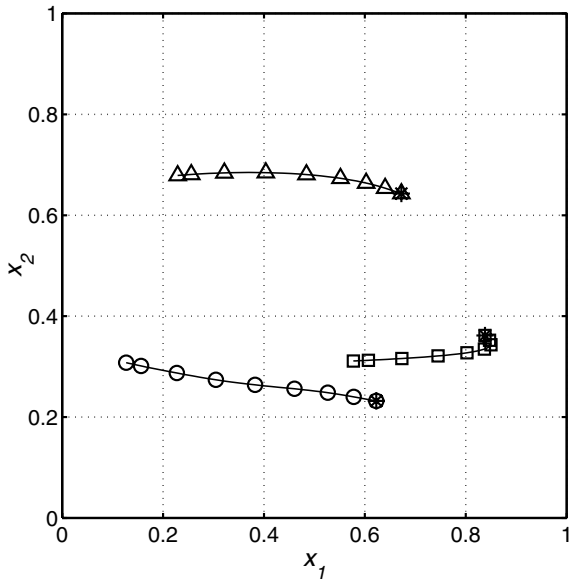
$$s_0^0 = (0.8, 0.2, 0.8, 0.4, 0.8, 0.6), \quad u^0 = 0$$

Moreover, the harmonic sequence (5.12) was employed for $b = 10^{-2}$.

Figure 5.2 shows the sensor trajectories obtained in 200 iterations (on aggregate, approximately fifty minutes of CPU time were used to run all the simulations). Circles, squares and triangles denote consecutive sensor positions. Furthermore, the sensors' positions at $t = 0$ are marked by the asterisks. Note that the form of the forcing term in our PDE implies that the 'snapshots' of the corresponding solution (i.e. the state of our DPS) at consecutive time moments resemble those of a hat-shaped surface whose maximum moves from the right to the left boundary of Ω. In addition, the diffusion coefficient values in the upper right of Ω are on the average greater than those in the lower left. This means that the state changes during the system evolution are quicker when we move up and to the right (on the other hand, the system reaches the steady state there earlier). This fact explains in a sense the form of the obtained trajectories (the sensors tend to measure the state in the regions where the distributed system is more sensitive with respect to the unknown parameter κ, i.e. in the lower part of Ω). As can be seen, the results obtained for the ED- and approximated MMD-optimality criteria are to some extent similar. $\diamondsuit$



(a)



(b)

Figure 5.2: Optimum sensor trajectories: ED-design criterion (a) and approximated MMD-design criterion (b).

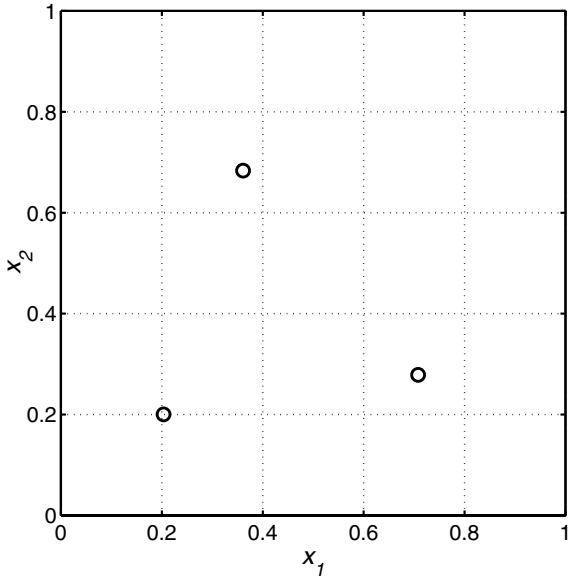


Figure 5.3: Optimum positions of stationary sensors for the MMD-design criterion.

Example 5.2. In the settings of Example 5.1 the problem of locating three stationary sensors was also solved through the direct maximization of the criterion (5.24) via the algorithm proposed by Shimizu and Aiyoshi, starting from $Z^1 = \{(0.1, 0.1, 0.1)\}$. The nonlinear-programming subtasks were solved using the adaptive random search strategy of p. 49 and a sequential constrained quadratic programming (SQP) method (Bertsekas, 1999; Spellucci, 1998a; Spellucci, 1998b; Miller, 1998). The convergence tolerance was set at $\epsilon = 5 \times 10^{-3}$.

Figure 5.3 shows the optimal sensor positions obtained in two iterations of the algorithm. They correspond to

$$s^\star = \begin{pmatrix} 0.203342, & 0.200193, \dots \\ 0.360944, & 0.683536, \dots \\ 0.707838, & 0.278700 \end{pmatrix}$$

and $\theta_1 = 0.15$, $\theta_2 = 0.2$ $\theta_3 = 0.2$, i.e. the largest admissible values of the parameters. $\diamondsuit$

5.4 Concluding remarks

We have shown that the difficulties created by the dependence of the solutions to the sensor location problem on the parameters to be identified can be cleared up to a certain extent by the introduction of robust designs, on the analogy of the common procedure in optimum experimental design for non-linear regression models. To the best of our knowledge, this issue has received no attention as yet in the context of parameter estimation for DPS's, in spite of the fact that it is of utmost importance while trying to find best sensor positions. In particular, optimal designs in the average and minimax senses were introduced, appropriate optimality conditions for continuous designs were derived and efficient algorithms to numerically obtain exact designs were discussed. Each choice between the two robust approaches has some advantages and some disadvantages. A final selection has to be made on the basis of secondary considerations. For example, if we are anxious to optimize the worst possible performances of the experiment designed, then optimal designs in the minimax sense are preferred. On the other hand, if the prior uncertainty on the parameters to be identified is characterized by some prior distribution, then the average experimental design is particularly suited for making the designs independent of the parameters.

The algorithms outlined in this chapter permit the application of any of the above policies at a reasonable computational cost. In particular, the use of the framework of stochastic approximation opens up the possibility of developing robust design strategies for moving sensors, since the corresponding solutions can be obtained almost as simply as the locally optimal designs discussed in the previous chapter.

Chapter 6

Conclusions and future research directions

From an engineering point of view it is clear that sensor placement is an integral part of control design, particularly in control of DPS's, e.g. flexible structures, air-pollution processes, oil and gas production from deposits, etc. Its choice is fundamental in the sense that it determines the accuracy of the system characteristics which are identified from an identification experiment. On the other hand, an engineering judgement and trial-and-error analysis are quite often used to determine spatial arrangements of measurement transducers, in spite of the fact that the problem has been attacked from various angles by many authors and a number of relevant results have already been reported in the literature. What is more, although it is commonly known that this area of research is difficult, since the non-linearity inherent in the sensor location problem precludes simple solution techniques, some systematic attempts at obtaining optimal sensor positions are still made and the progression is towards more general models, more realistic criteria and better understanding of the nature of the optimal locations. Logically, the number of applications should proliferate, yet this is not the case. It seems that two main reasons explain why strong formal methods are not accepted in engineering practice. First, with the use of the existing approaches, only relatively simple engineering problems can be solved without resorting to numerical methods. Second, the complexity of most sensor location algorithms does not encourage engineers to apply them in practice.

Bearing this in mind, the original goal of the research reported in this monograph was simply to develop computationally efficient methods to solve

practical sensor location problems for a wide class of DPS's. In the process of executing this task, we have developed a theoretical foundation for the adopted approach and constructed 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 optimal sensor location for parameter estimation in DPS's:

- Systematizes characteristic features of the problem and analyses the existing approaches based on the notion of the Fisher information matrix.

- Develops an effective method for computing sensitivity coefficients which are indispensable when determining the elements of the FIM. This scheme based on the direct-differentiation approach and tricubic spline interpolation enables us to implement the algorithms for finding optimal sensor positions in an extremely efficient manner.

- Provides characterizations of continuous (or approximated) designs for stationary sensors, which allows an easy testing of any given sensor setting for optimality, and then clarifies how to adapt well-known algorithms of optimum experimental design for finding numerical approximations to the solutions.

- Presents the concept of clusterization-free locations along with a practical algorithm being a modified version of the effective method proposed by Fedorov in the context of linear regression models.

- Extends Rafajłowicz's approach to constructing optimal trajectories of moving sensors and derives an alternative approach consisting in parametrization of sensor trajectories.

- Formulates and solves the problem of trajectory planning for moving sensors based on dynamic models of sensor motions and various constraints imposed on the movements. The line of development given here is original in that, to the best of our knowledge, there have been no approaches so far within such a framework in the context of parameter identification of DPS's. Specifically, it is shown how to reduce the problem to a state-constrained optimal-control problem. Then an effective method of successive linearizations is employed to solve it numerically. It is demonstrated that the proposed approach can tackle various challenging problems of vital importance, including motion

planning along specified paths, utilization of minimax criteria, or selection of a minimal number of sensors. Simulation experiments validate the fact that making use of moving sensors may lead to dramatic gains in the values of the adopted performance indices, and hence to a much greater accuracy in the resulting parameter estimates.

- Introduces the notion of robust design of sensor locations, characterizes the corresponding solutions for continuous designs, and indicates how to find numerical solutions for exact designs efficiently. The advantage of the suggested schemes based on stochastic approximation is that the solutions are obtained almost as simply as for local-optimality criteria. As a consequence, robust trajectories for moving sensors can be determined at a reasonable computational cost. Minimax designs are also discussed and it is shown that they might not be as difficult as it seems at first sight.

The approach suggested here has the advantage that it is independent of a particular form of the partial-differential equation describing the distributed system under consideration. The only requirement is the existence of sufficiently regular solutions to the state and sensitivity equations, and consequently non-linear systems can also be treated within the same framework practically without any changes. Moreover, it can easily be generalized to three spatial dimensions and the only limitation is the amount of required computations.

We believe that our approach has significant advantages which will make it, with sufficient development, a leading approach to solving sensor location problems facing engineers involved in applications. However, there still remain open problems regarding some important areas. What follows is a discussion of the areas for further investigation, besides applications.

Further development of robust approaches. Formally, robust sensor location is somewhat reminiscent of the problem of robustness analysis and design for uncertain control systems. In this respect, some ideas of statistical learning theory and randomized algorithms, which have already proved to be useful in robust controller design (Vidyasagar, 1997; Vidyasagar, 1998; Tempo and Dabbene, 1999), seem versatile enough so as to be exploited in the framework of the robust sensor location discussed in our monograph. Moreover, the potential results can be of significance in attempts at finding sensor positions which would guarantee an extended identifiability of a given DPS (this concept was introduced and thoroughly studied by Sun (1994)).

Coupled input and measurement system design. The problem of simultaneous optimum choice of the controls influencing a given DPS (including both the actuator location and the form of the input signals) and the locations to place the sensors was suggested in the survey paper (Mehra, 1974). Unfortunately, owing to the great complexity of the corresponding optimization problem, communications on this subject are rather limited. Some interesting preliminary results were reported in some early works of Rafajłowicz (1978; 1981; 1983) who then focused his attention solely on input optimization (Rafajłowicz, 1984; Rafajłowicz, 1986a; Rafajłowicz, 1986b; Rafajłowicz, 1989b; Rafajłowicz, 1990; Rafajłowicz and Myszka, 1986). The maturity of the optimal control theory of DPS's and the availability of more and more powerful computers encourage us to resume the research related to this idea.

Alternative objectives in the problem formulation. In this monograph, we have focused our attention only on determination of sensor locations which are optimal in the sense that they allow maximum information about the system parameters to be extracted from the identification experiments. In some applications, however, such as hydrology (Sun, 1994) or advanced process control (Lasiecka and Triggiani, 2000), the reliability of model predictions is sometimes more important than the accuracy of model parameters, because the ultimate objective in modelling is the prediction of the system states. In this case, the maximum over time of the output prediction variance should be minimized, which leads to the so-called G-optimal designs. This topic was discussed to some extent in (Sun, 1994, p. 201), where other design objectives were also considered, e.g. minimization of the risk of management decisions, minimization of experimental expenses, or experimental design for model discrimination. Some generalizations are still expected regarding e.g. moving sensors, robust designs, or efficient computational methods.

Further results on clusterization-free designs. In Section 3.3, Fedorov's algoritm based on the notion of directly constrained measures was extended to cover the case of locating a large number of stationary sensors. The results obtained are very promising and therefore the idea which suggests itself is to further extend this approach in a way to the case of moving sensors.

Modifications of the design procedures to allow for discrete-time measurements. The approach we have presented applies with minor

modifications to discrete-time measurements (e.g. some supplementary assumptions about the regularity of the solutions to a given PDE have to be appended and integration over time is to be replaced by summation). But if the data can be available in sampled data form and the choice of a sampling strategy is at our disposal, then the problem of selection of optimal measurement times can additionally be formulated. It has been considered only in the setting of lumped systems so far (Titterington, 1980).

Coupled parameter identification and experimental design. In the experiments discussed in this monographs, sensor allocation strategies are implemented off-line, before collecting the measurement data (though some kind of feedback is encountered in sequential designs). On the other hand, it would be interesting to investigate the problem of simultaneously taking measurements, identifying system parameters and updating locations of moving sensors. Unfortunately, the number of publications related to on-line parameter estimation for infinite-dimensional dynamical systems is very limited (cf. e.g. Baumeister *et al.*, 1997; Demetriou and Rosen, 1993; Aihara, 1997) and distributed measurements are only considered. In spite of that, owing to potential applications, further development of this line of research is desirable.

Appendices

Appendix A

Differentiation of non-linear operators

A.1 Gâteaux and Fréchet derivatives

The idea of derivative or differential of a scalar function of a scalar variable can be profitably extended to general mappings. The value of these abstract differentials and derivatives is both practical and theoretical. Practically, the theory allows for first-order approximation or 'linearization' of non-linear functionals. From a theoretical point of view, differentials and derivatives are frequently used to prove existence results and properties of dependence of state variables on system parameters (see Appendix B.2) (Haug *et al.*, 1986).

Let X and Y be two Banach spaces and F be an operator which maps an open subset V of X into Y. If given $x_0 \in V$ and $\delta x \in X$ the limit

$$\delta F(x_0; \delta x) = \lim_{\lambda \to 0} \frac{F(x_0 + \lambda \delta x) - F(x_0)}{\lambda} \tag{A1}$$

exists, then F is said to be Gâteaux differentiable and $\delta F(x_0; \delta x)$ is called the *Gâteaux differential* of F at x_0 in the direction δx.

We say that F is Gâteaux differentiable at x_0 if it is Gâteaux differentiable in every direction. If, additionally, the operator $U : X \ni \delta x \mapsto \delta F(x_0; \delta x) \in Y$ is linear and bounded, i.e. $U \in \mathcal{L}(X, Y)$, then U is called the *Gâteaux derivative* of F at x_0 and we write $U = F'(x_0)$. Accordingly,

$$\delta F(x_0; \delta x) = F'(x_0) \delta x \tag{A2}$$

Next, if the extra requirement that the convergence in (A1) is uniform for all $\delta x \in X$ from the unit sphere (i.e. $\|\delta x\|_X = 1$), then we call $F'(x_0)$ the *Fréchet derivative* of F at x_0 (in turn, F is said to be Fréchet differentiable at x_0). It is a simple matter to show that the existence of the Fréchet derivative is equivalent to the fulfilment of the conditions

$$F'(x_0) \in \mathcal{L}(X, Y) \tag{A3}$$

and

$$\lim_{\delta x \to 0} \frac{\|F(x_0 + \delta x) - F(x_0) - F'(x_0)\delta x\|_Y}{\|\delta x\|_X} = 0 \tag{A4}$$

A.2 Chain rule of differentiation

Let X, Y and Z be Banach spaces. Suppose that F is an operator which maps an open set $V \subset X$ into an open set $W \subset Y$ and G is an operator which maps W into Z. If G is Fréchet differentiable at $y_0 = F(x_0)$, $x_0 \in V$, and F is Gâteaux (resp. Fréchet) differentiable at x_0, then the composite $G \circ F$ is Gâteaux (resp. Fréchet) differentiable at x_0 and we have (Kantorovich and Akilov, 1984; Maurin, 1991)

$$\big[G \circ F\big]'(x_0) = G'(F(x_0))F'(x_0) \tag{A5}$$

A.3 Partial derivatives

Let X, Y and Z be Banach spaces. If F is an operator which maps an open subset $V \subset X \times Y$ into Z, then for a fixed $y_0 \in Y$ we may introduce the operator

$$F^{(y_0)} : x \mapsto F(x, y_0) \tag{A6}$$

which maps $V^{(y_0)} = \{x \in X : (x, y_0) \in V\}$ into Z. Similarly, for a given $x_0 \in X$ we may consider

$$F^{(x_0)} : y \mapsto F(x_0, y) \tag{A7}$$

which maps $V^{(x_0)} = \{y \in Y : (x_0, y) \in V\}$ into Z.

Obviously, if $x_0 \in X$ is an interior point of $V^{(y_0)}$, then we may speak of the (Gâteaux or Fréchet) derivative $F^{(y_0)\prime}(x_0, y_0) \in \mathcal{L}(X, Z)$ which we

call the *partial derivative* of F at (x_0, y_0) and write $F'_x(x_0, y_0)$. Similarly, we introduce the partial derivative with respect to y: $F^{(x_0)\prime}(x_0, y_0) = F'_y(x_0, y_0) \in \mathcal{L}(Y, Z)$.

If at least one of the partial Gâteaux (resp. Fréchet) derivatives is continuous in a neighbourhood of (x_0, y_0), then we have a very useful formula (Kantorovich and Akilov, 1984; Maurin, 1991)

$$F'(x_0, y_0)(\delta x, \delta y) = F'_x(x_0, y_0)\delta x + F'_y(x_0, y_0)\delta y \tag{A8}$$

where F' stands for the Gâteaux (resp. Fréchet) derivative of F. This permits calculations with individual variables and yields the differential of a mapping as the sum of its partial differentials.

A.4 Differentiability of mappings with one-dimensional domains

Let us assume now that Y is a Banach space and consider $U \in \mathcal{L}(\mathbb{R}, Y)$. We see at once that U may be rewritten as

$$U(t) = ty_0, \quad t \in \mathbb{R} \tag{A9}$$

where $y_0 = U(1) \in Y$. Moreover, from $\|U(t)\| = |t|\|y_0\|$ we obtain

$$\|U\| = \|y_0\| \tag{A10}$$

Conversely, for any $y_0 \in Y$, (A9) defines an operator $U \in \mathcal{L}(\mathbb{R}, Y)$. Clearly, the correspondence between the elements of Y and $\mathcal{L}(\mathbb{R}, Y)$ is one-to-one, linear and, based on (A10), it preserves the norm. Hence $\mathcal{L}(\mathbb{R}, Y)$ and Y are isometrically isomorphic and we may thus identify $\mathcal{L}(\mathbb{R}, Y)$ with Y.

Consider now an operator $F : \mathbb{R} \supset \Omega \to Y$. The existence of the Gâteaux derivative $F'(t_0) = y_0 \in Y$ means that for each $t \in \mathbb{R}$

$$\lim_{\lambda \to 0} \frac{F(t_0 + \lambda t) - F(t_0)}{\lambda} = ty_0 \tag{A11}$$

If we set $\Delta t = \lambda t$, then we may rewrite (A11) in the form

$$\lim_{\Delta t \to 0} \frac{F(t_0 + \Delta t) - F(t_0)}{\Delta t} = y_0 \tag{A12}$$

so in the case considered the definition of $F'(t_0)$ is the same as for the derivative of a real function of one real variable. Of course, (A12) implies that the Gâteaux derivative is also the Fréchet one, i.e. both the notions are equivalent (in general, this is not the case on higher-dimensional spaces, i.e. the Gâteaux derivative may exist, whereas the Fréchet one may not).

A.5 Second derivatives

When $F : X \to Y$ and both X, Y are Banach spaces, we have seen that the Gâteaux (or Fréchet) derivative of F is a bounded linear operator, i.e. $F'(x) \in \mathcal{L}(X, Y)$. But $\mathcal{L}(X, Y)$ itself is a Banach space and hence we may consider the derivative of $F'(\,\cdot\,) : X \to \mathcal{L}(X, Y)$ at a point $x_0 \in X$. If it exists, we call it the second derivative of F at x_0 and write $F''(x_0)$. It is clear that

$$F''(x_0) \in \mathcal{L}(X, \mathcal{L}(X, Y)) \tag{A13}$$

However, it can be shown that $\mathcal{L}(X, \mathcal{L}(X, Y))$ is isometrically isomorphic to $\mathcal{L}(X \times X, Y)$ (Curtain and Pritchard, 1977; Kantorovich and Akilov, 1984), so that we may think of $F''(x_0)$ as an element of $\mathcal{L}(X \times X, Y)$ and

$$F''(\,\cdot\,) : X \to \mathcal{L}(X \times X, Y) \tag{A14}$$

Interpreting $F''(x_0)$ as a bilinear operator, we obtain the following modified definition of the second Gâteaux derivative:

$$\lim_{\lambda \to 0} \frac{F'(x_0 + \lambda \delta x') - F'(x_0)}{\lambda} = F''(x_0)(\,\cdot\,, \delta x') \tag{A15}$$

Consequently, for any $\delta x \in X$ we get

$$F''(x_0)(\delta x, \delta x') = \lim_{\lambda \to 0} \frac{F'(x_0 + \lambda \delta x')\delta x - F'(x_0)\delta x}{\lambda} \tag{A16}$$

Note that (A15) and (A16) are not equivalent, i.e. it may happen that we have a bilinear operator $B \in \mathcal{L}(X \times X, Y)$ such that

$$\lim_{\lambda \to 0} \frac{F'(x_0 + \lambda \delta x')\delta x - F'(x_0)\delta x}{\lambda} = B(\delta x, \delta x'), \quad \forall\, \delta x, \delta x' \in X \tag{A17}$$

and yet $F''(x_0)$ does not exist. Nevertheless, it is straightforward to show that the necessary and sufficient condition for F to have the second Gâteaux derivative is that the convergence in (A16) is uniform on the unit sphere (i.e. for $\|\delta x\| = 1$). Moreover, the uniform convergence for both $\|\delta x\| = 1$ and $\|\delta x'\| = 1$ guarantees that B is also the second Fréchet derivative of F.

A.6 Functionals on Hilbert spaces

Given a real Hilbert space V with inner product $\langle\,\cdot\,, \cdot\,\rangle$, for any bounded linear functional $f : V \to \mathbb{R}$, there is a vector $y \in V$ such that

$$f(x) = \langle y, x \rangle, \quad \forall\, x \in V \tag{A18}$$

This result is known as the Riesz representation theorem.

Therefore, it follows that if $J : V \to \mathbb{R}$ possesses either a Fréchet or a Gâteaux derivative at $x_0 \in V$, then there exists a vector $\nabla J(x_0) \in V$ called the *gradient* of J at x_0, such that

$$J'(x_0)\delta x = \langle \nabla J(x_0), \delta x \rangle, \quad \forall \delta x \in V \tag{A19}$$

Next, for any continuous bilinear function $g : V \times V \to \mathbb{R}$, there exists a bounded linear operator $G : V \to V$, such that

$$g(x, y) = \langle x, Gy \rangle, \quad \forall\, x, y \in V \tag{A20}$$

Therefore, when $J : V \to \mathbb{R}$ has the second derivative, its second differential at $x_0 \in V$ is given by

$$J'(x_0)(\delta x, \delta x') = \langle \delta x, H(x_0)\delta x' \rangle \tag{A21}$$

where $H(x_0) \in \mathcal{L}(V)$ is called the *Hessian* of J at x_0.

A.7 Directional derivatives

At last, we introduce the notion of a directional derivative which may exist even when an operator fails to have a Gâteaux differential. Let X and Y be Banach spaces and suppose that $F : V \to Y$, where V is an open subset of X. We define the *one-sided directional differential* of F at a point $x_0 \in X$ in the direction $\delta x \in X$ by

$$\delta_+ F(x_0; \delta x) = \lim_{\lambda \downarrow 0} \frac{F(x_0 + \lambda \delta x) - F(x_0)}{\lambda} \tag{A22}$$

if this limit exists. We say that F is directionally differentiable at x_0 if the directional differential exists for all $\delta x \in X$. Clearly, when F is Gâteaux differentiable at x_0, then it is directionally differentiable at x_0 and $\delta_+ F(x_0; \delta x) = \delta F(x_0; \delta x)$ for all $\delta x \in X$.

Appendix B

Some accessory results for partial-differential equations

B.1 Green formulae

Let Ω be a bounded open domain in $\mathbb{R}^n$ with a Lipschitz boundary Γ. If $u, v \in H^1(\Omega)$, then we have the following integration-by-parts formula (Marcinkowska, 1993; Raviart and Thomas, 1992; Omatu and Seinfeld, 1989):

$$\int_\Omega \frac{\partial u}{\partial x_i} v \, \mathrm{d}x = -\int_\Omega u \frac{\partial v}{\partial x_i} \, \mathrm{d}x + \int_\Gamma uv\nu_i \, \mathrm{d}\sigma, \quad 1 \leq i \leq n \tag{B1}$$

where ν_i's signify the direction cosines of the unit outward normal to Γ which exist a.e. due to the Lipschitz assumption.

Moreover, if $u \in H^2(\Omega)$, then

$$-\int_\Omega (\Delta u) v \, \mathrm{d}x = \sum_{i=1}^{n} \int_\Omega \frac{\partial u}{\partial x_i} \frac{\partial v}{\partial x_i} \, \mathrm{d}x - \int_\Gamma \frac{\partial u}{\partial \nu} v \, \mathrm{d}\sigma \tag{B2}$$

where the normal derivative

$$\left.\frac{\partial u}{\partial \nu}\right|_\Gamma = \sum_{i=1}^{n} \nu_i \left.\frac{\partial u}{\partial x_i}\right|_\Gamma$$

is well-defined as a function of $L^2(\Gamma)$ since $\nu_i \in L^\infty(\Gamma)$, $1 \leq i \leq n$.

Now, let us introduce the second-order elliptic differential operator with spatially-varying coefficients

$$Au = -\sum_{i,j=1}^{n} \frac{\partial}{\partial x_i}\left\{a_{ij}\frac{\partial u}{\partial x_j}\right\} + a_0 u \tag{B3}$$

where $u \in H^2(\Omega)$, $a_0 \in L^\infty(\Omega)$, $a_{ij} \in C^1(\bar{\Omega})$, $1 \le i,j \le n$. The regularity of a_{ij}'s implies $\sum_{j=1}^{n} a_{ij}\partial u/\partial x_j \in H^1(\Omega)$, $1 \le i \le n$. Consequently, from (B1), we deduce that

$$\int_\Omega Au\, v\, \mathrm{d}x + \int_\Gamma \frac{\partial u}{\partial \nu_A}\, v\, \mathrm{d}\sigma = \int_\Omega \left\{\sum_{i,j=1}^{n} a_{ij}\frac{\partial u}{\partial x_j}\frac{\partial v}{\partial x_i} + a_0 uv\right\} \mathrm{d}x \tag{B4}$$

where

$$\frac{\partial u}{\partial \nu_A} = \sum_{i,j=1}^{n} a_{ij}\frac{\partial u}{\partial x_j}\nu_i$$

stands for the co-normal derivative associated with operator A.

B.2 Differentiability of the solution of a linear parabolic equation with respect to parameters

Let Ω be a bounded domain in $\mathbb{R}^n$ with a Lipschitz boundary Γ and T be the time horizon $]0, t_f[$. In this section we wish to investigate in detail the differentiability with respect to a functional parameter ϑ of the solution to the linear parabolic equation

$$\frac{\partial y}{\partial t}(x,t) - \sum_{i=1}^{n} \frac{\partial}{\partial x_i}\left\{\vartheta(x)\frac{\partial y}{\partial x_i}(x,t)\right\} = f(x,t) \quad \text{in } Q = \Omega \times T \tag{B5}$$

subject to the boundary conditions

$$y(x,t) = 0 \quad \text{on } \Sigma = \Gamma \times T \tag{B6}$$

and the initial condition

$$y(x,0) = y_0(x) \quad \text{in } \Omega \tag{B7}$$

At first, however, we have to clarify how the notion 'solution' is to be interpreted in our case. Indeed, we might look for the so-called classical

solution to (B5)–(B7) which is defined to be a function $y = y(x,t)$ such that all the derivatives which appear in (B5) exist, are continuous and boundary and initial conditions are all satisfied (Mikhailov, 1976; Renardy and Rogers, 1993; Reinhard, 1991; Curtain and Pritchard, 1977). It turns out, however, that the story is not quite so simple, as in many problems arising naturally in differential equations such requirements regarding regularity are too stringent. This prompts an introduction of generalized definitions of functions, derivatives, convergence, integrals, etc., and leads to the so-called variational formulation of problems described by PDE's with corresponding *weak* solutions.

In the case considered here, let us assume that $\vartheta \in C^1(\bar{\Omega})$, $f \in C(\bar{\Omega})$, and take a classical solution $y \in C^{2,1}(\bar{Q})$. We choose some $\psi \in H_0^1(\Omega)$ (called a *test* or *trial* function) arbitrarily, multiply (B5) by it and integrate the result on Ω. We thus get

$$\int_\Omega \frac{\partial y}{\partial t}(x,t)\psi(x)\,\mathrm{d}x - \int_\Omega \sum_{i=1}^{n} \frac{\partial}{\partial x_i}\left\{\vartheta(x)\frac{\partial y}{\partial x_i}(x,t)\right\}\psi(x)\,\mathrm{d}x = \int_\Omega f(x,t)\psi(x)\,\mathrm{d}x \quad \text{(B8)}$$

Making use of the Green formula (B4) and noticing that

$$\int_\Omega \frac{\partial y}{\partial t}(x,t)\psi(x)\,\mathrm{d}x = \frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega y(x,t)\psi(x)\,\mathrm{d}x$$

we conclude that

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega y(x,t)\psi(x)\,\mathrm{d}x + \sum_{i=1}^{n}\int_\Omega \vartheta(x)\frac{\partial y}{\partial x_i}(x,t)\frac{\partial \psi}{\partial x_i}(x)\,\mathrm{d}x = \int_\Omega f(x,t)\psi(x)\,\mathrm{d}x, \quad \forall \psi \in H_0^1(\Omega) \quad \text{(B9)}$$

which is called the *weak* or *variational* formulation of the problem.

Obviously, (B9) makes sense whenever weaker assumptions on data are made, i.e. $\vartheta \in L^\infty(\Omega)$ and $f \in L^2(Q)$, and the derivatives are interpreted in the distributional sense. The classical solution need not exist under these more general hypotheses, but when it exists, it coincides with the variational one. A proper mathematical statement of the weak formulation of (B5)–(B7) requires, however, rather profound knowledge of vector-valued distributions, generalized derivatives and Sobolev spaces (Lions, 1968; Dautray

and Lions, 1992; Omatu and Seinfeld, 1989; Renardy and Rogers, 1993), so the reader who is not familiar with those notions or is not interested in such technicalities may skip what follows and proceed directly with Theorem B.1 which is the main result of this section.

From now on, we make the folowing assumption regarding the set of admissible parameters $\Theta_{\rm ad}$:

$$\Theta_{\rm ad} = \Big\{ \vartheta \in L^\infty(\Omega) : \exists \alpha > 0,\ \vartheta(x) \geq \alpha > 0 \text{ a.e. in } \Omega \Big\} \tag{B10}$$

Furthermore, we introduce the notation $V = H_0^1(\Omega)$, $H = L^2(\Omega)$,

$$\begin{cases} ((\,\cdot\,,\,\cdot\,)) & \text{the scalar product,} \quad \|\cdot\| \quad \text{the norm in } V \\ (\,\cdot\,,\,\cdot\,) & \text{the scalar product,} \quad |\cdot| \quad \text{the norm in } H \end{cases}$$

We select H as the pivot space and therefore identify H with its dual H'. Denoting by V' the dual of V with norm $\|\cdot\|_\star$ (in our case $V' = H^{-1}(\Omega)$), we get

$$V \hookrightarrow H \hookrightarrow V' \tag{B11}$$

where $\hookrightarrow$ stands for a continuous and dense injection. The pairing between V' and V is denoted by $\langle w, v\rangle$ for $w \in V'$ and $v \in V$, and it coincides with the scalar product (w, v) if $w, v \in H$.

Additionally, we define a_ϑ to be the bounded bilinear form

$$a_\vartheta(u, v) = \sum_{i=1}^n \int_\Omega \vartheta \frac{\partial u}{\partial x_i} \frac{\partial v}{\partial x_i}\, {\rm d}x \quad \text{on } V \times V \tag{B12}$$

Let us note that a_ϑ defines a bounded linear operator $A_\vartheta : V \to V'$ according to the formula

$$\langle A_\vartheta u, v\rangle = a_\vartheta(u, v), \quad \forall\, u, v \in V \tag{B13}$$

We have

$$\begin{aligned} \|A_\vartheta\|_{\mathcal{L}(V,V')} &= \sup_{\|u\|=1} \|A_\vartheta u\|_\star = \sup_{\|u\|=1} \sup_{\|v\|=1} |\,\langle A_\vartheta u, v\rangle| \\ &= \sup_{\|u\|=1} \sup_{\|v\|=1} |\,a_\vartheta(u, v)| \leq \|\vartheta\|_{L^\infty(\Omega)} \end{aligned} \tag{B14}$$

Finally, we introduce the space

$$W(T) = \left\{ u \in L^2(T; V) : \frac{{\rm d}u}{{\rm d}t} \in L^2(T; V') \right\} \tag{B15}$$

where the derivative is understood in the vector-valued distributional sense. It is a Hilbert space when equipped with the norm

$$\begin{aligned} \|u\|_{W(T)} &= \left(\|u\|^2_{L^2(T;V)} + \|\frac{\mathrm{d}u}{\mathrm{d}t}\|^2_{L^2(T;V')} \right)^{1/2} \\ &= \left(\int_0^{t_f} \left[\|u(t)\|^2 + \|\frac{\mathrm{d}u}{\mathrm{d}t}(t)\|^2_\star \right] \mathrm{d}t \right)^{1/2} \end{aligned} \tag{B16}$$

If we assume that $y_0 \in H$ and $f \in L^2(T;V')$, then the following problem may be formulated:

Problem (P) Find y satisfying

$$y \in W(T) \tag{B17}$$

$$\begin{cases} \dfrac{\mathrm{d}}{\mathrm{d}t}(y(\,\cdot\,),\psi) + a_\vartheta(y(\,\cdot\,),\psi) = \langle f(\,\cdot\,),\psi\rangle \\ \text{in the sense of } \mathcal{D}'(T) \text{ for all } \psi \in V \end{cases} \tag{B18}$$

$$y(0) = y_0 \tag{B19}$$

It can be shown that it always possesses a unique solution (Dautray and Lions, 1992; Lions, 1968; Omatu and Seinfeld, 1989; Neittaanmäki and Tiba, 1994).

We remark that it is interesting to rewrite (B18) in the vector form

$$\frac{\mathrm{d}}{\mathrm{d}t}y(\,\cdot\,) + A_\vartheta y(\,\cdot\,) = f(\,\cdot\,) \quad \text{in the sense of } L^2(T;V') \tag{B20}$$

Theorem B.1. *The mapping* $\Theta_{\mathrm{ad}} \ni \vartheta \longmapsto y \in W(T)$ *defined by* (B17)–(B19) *is Fréchet differentiable and the variation* $\delta y \in W(T)$ *in* y *due to a variation* $\delta\vartheta$ *at a point* $\vartheta^0 \in \Theta_{\mathrm{ad}}$ *is the solution to the problem*

$$\frac{\mathrm{d}}{\mathrm{d}t}(\delta y(\,\cdot\,),\psi) + a_{\vartheta^0}(\delta y(\,\cdot\,),\psi) = -a_{\delta\vartheta}(y^0(\,\cdot\,),\psi), \quad \delta y(0) = 0 \tag{B21}$$

in the sense of $\mathcal{D}'(T)$ *for all* $\psi \in V$, *where* y^0 *is the solution to* (B17)–(B19) *for* $\vartheta = \vartheta^0$.

Proof. The main idea of the proof was suggested by Chavent (1974). We begin by introducing the mapping

$$P : \begin{cases} \Theta_{\mathrm{ad}} \times W(T) & \longrightarrow & L^2(T;V') \times H \\ (\vartheta, y) & \longmapsto & \left(\dfrac{\mathrm{d}y}{\mathrm{d}t} + A_\vartheta y - f, y(0) - y_0 \right) \end{cases} \tag{B22}$$

Let us take an arbitrary $\vartheta^0 \in \Theta_{\rm ad}$ and denote by y^0 the corresponding solution of (B17)–(B19). In this setting, the following conditions are satisfied:

(i) *P is continuous at (ϑ^0, y^0).*

Indeed, if $y \to y^0$ in $W(T)$, then $y(0) \to y^0(0)$ from the continuity of the trace operator (or, in other words, since $W(T)$ is continuously embedded in $C([0,t_f];H)$) and $\mathrm{d}y/\mathrm{d}t \to \mathrm{d}y^0/\mathrm{d}t$ in $L^2(T;V')$ from the definition of $W(T)$.

If we assume additionally that $\vartheta \to \vartheta^0$ in $L^\infty(\Omega)$, then from the estimate

$$\begin{aligned}
&\|A_\vartheta y - A_{\vartheta^0} y^0\|_{L^2(T;V')} \\
&\qquad \le \|A_\vartheta y - A_{\vartheta^0} y\|_{L^2(T;V')} + \|A_{\vartheta^0} y - A_{\vartheta^0} y^0\|_{L^2(T;V')} \\
&\qquad \le \|A_\vartheta - A_{\vartheta^0}\|_{\mathcal{L}(V,V')} \|y\|_{L^2(T;V)} + \|A_{\vartheta^0}\|_{\mathcal{L}(V,V')} \|y - y^0\|_{L^2(T;V)} \\
&\qquad \le \|\vartheta - \vartheta^0\|_{L^\infty(\Omega)} \|y\|_{L^2(T;V)} + \|\vartheta^0\|_{L^\infty(\Omega)} \|y - y^0\|_{L^2(T;V)}
\end{aligned}$$

we get $A_\vartheta y \to A_{\vartheta^0} y^0$ in $L^2(T;V')$, which completes the proof of the desired property.

(ii) *$P(\vartheta^0, y^0) = 0$.*

This is an immediate consequence of the definitions of y^0 and P.

(iii) *The partial Gâteaux derivative P'_y exists in $\Theta_{\rm ad} \times W(T)$ and is continuous at (ϑ^0, y^0).*

Given any $\bar\vartheta \in \Theta_{\rm ad}$ and any $\bar y \in W(T)$, consider an increment $\delta y \in W(T)$. As for the limit in formula (A1), we get

$$\begin{aligned}
P'_y(\bar\vartheta, \bar y)\delta y &= \lim_{\lambda \to 0} \frac{P(\bar\vartheta, \bar y + \lambda \delta y) - P(\bar\vartheta, \bar y)}{\lambda} \\
&= \left(\frac{\mathrm{d}\delta y}{\mathrm{d}t} + A_{\bar\vartheta} \delta y, \delta y(0) \right)
\end{aligned}$$

It follows immediately that $P'_y(\bar\vartheta, \bar y) \in \mathcal{L}(W(T), L^2(T;V') \times H)$, therefore it does define a partial Gâteaux derivative. From the estimate

$$\begin{aligned}
&\|P'_y(\bar\vartheta, \bar y) - P'_y(\vartheta^0, y^0)\|_{\mathcal{L}(W(T), L^2(T;V') \times H)} \\
&\qquad = \sup_{\|\delta y\|_{W(T)} = 1} \|A_{\bar\vartheta} \delta y - A_{\vartheta^0} \delta y\|_{L^2(T;V')} \\
&\qquad \le \|A_{\bar\vartheta} - A_{\vartheta^0}\|_{\mathcal{L}(V;V')} \sup_{\|\delta y\|_{W(T)} = 1} \|\delta y\|_{L^2(T;V)} \\
&\qquad \le \|A_{\bar\vartheta} - A_{\vartheta^0}\|_{\mathcal{L}(V;V')} \le \|\bar\vartheta - \vartheta^0\|_{L^\infty(\Omega)}
\end{aligned}$$

we conclude that this Gâteaux derivative is continuous at (ϑ^0, y^0).

(iv) $P'_y(\vartheta^0, y^0)$ *is invertible and*

$$\left[P'_y(\vartheta^0, y^0)\right]^{-1} \in \mathcal{L}(L^2(T;V') \times H, W(T))$$

The existence of the inverse results from the fact that for each $r \in L^2(T;V')$ and $\eta \in H$ the problem

$$\frac{\mathrm{d}\delta y}{\mathrm{d}t} + A_{\vartheta^0}\delta y = r, \quad \delta y(0) = \eta$$

has a unique solution in $W(T)$ (cf. (B17)–(B19)).

Clearly, $\left[P'_y(\vartheta^0, y^0)\right]^{-1}$ is linear and its continuity follows from that of the solution to (B17)–(B19) with respect to data, as there exists $C > 0$ depending only on ϑ^0 such that (Dautray and Lions, 1992, Th. 3, p. 520)

$$\|\delta y\|_{L^2(T;V)} \leq C \left\{ |\eta|^2 + \|r\|^2_{L^2(T;V')} \right\}^{1/2}$$

and we have

$$\begin{aligned} \left\|\frac{\mathrm{d}\delta y}{\mathrm{d}t}\right\|_{L^2(T;V')} &= \|r - A_{\vartheta^0}\delta y\|_{L^2(T;V')} \\ &\leq \|r\|_{L^2(T;V')} + \|A_{\vartheta^0}\|_{\mathcal{L}(V;V')}\|\delta y\|_{L^2(T;V)} \end{aligned}$$

An alternative proof of Property (iv) is based on the observation that the bounded linear operator $P'_y(\vartheta^0, y^0)$ is one-to-one and onto its range, so from the Banach Theorem (Rolewicz, 1974; Brezis, 1987, p. 19) it follows that its inverse is also a bounded linear operator.

(v) *The partial Gâteaux derivative* P'_ϑ *exists in* $\Theta_{\mathrm{ad}} \times W(T)$ *and is continuous at* (ϑ^0, y^0).

For arbitrary $\bar{\vartheta} \in \Theta_{\mathrm{ad}}$ and $\bar{y} \in W(T)$ consider an increment $\delta\vartheta \in L^\infty(\Omega)$. As regards formula (A1), we have

$$\begin{aligned} P'_\vartheta(\bar{\vartheta}, \bar{y})\delta\vartheta &= \lim_{\lambda \to 0} \frac{P(\bar{\vartheta} + \lambda\delta\vartheta, \bar{y}) - P(\bar{\vartheta}, \bar{y})}{\lambda} \\ &= \lim_{\lambda \to 0} \frac{1}{\lambda}\left(A_{\bar{\vartheta}+\lambda\delta\vartheta}\bar{y} - A_{\bar{\vartheta}}\bar{y}, 0\right) = (A_{\delta\vartheta}\bar{y}, 0) \end{aligned}$$

since the mapping $L : \vartheta \mapsto A_\vartheta y$ is linear and bounded. Moreover,

$$\|L\|_{\mathcal{L}(L^\infty(\Omega),L^2(T;V'))} \le \|y\|_{L^2(T;V)}$$

Consequently, $P'_\vartheta(\bar\vartheta,\bar y) \in \mathcal{L}(L^\infty(\Omega), L^2(T;V') \times H)$, i.e. indeed, we deal with a partial Gâteaux derivative.

From the estimate

$$\begin{aligned}\|P'_\vartheta(\bar\vartheta,\bar y) - P'_\vartheta(\vartheta^0,y^0)\|_{\mathcal{L}(L^\infty(\Omega),L^2(T;V')\times H)} &= \sup_{\|\delta\vartheta\|_{L^\infty(\Omega)}=1} \|A_{\delta\vartheta}(\bar y - y^0)\|_{L^2(T;V')} \\ &\le \|\bar y - y^0\|_{L^2(T;V)} \sup_{\|\delta\vartheta\|_{L^\infty(\Omega)}=1} \|A_{\delta\vartheta}\|_{\mathcal{L}(V;V')} \\ &\le \|\bar y - y^0\|_{L^2(T;V)}\end{aligned}$$

it follows that P'_ϑ is continuous at (ϑ^0, y^0).

Properties (i)–(v) constitute the assumptions of the Implicit Function Theorem (Kantorovich and Akilov, 1984, Th. 3, p. 673) from which we thus conclude that there exists an operator F defined in a neighbourhood $G \subset \Theta_{\text{ad}}$ of the point (ϑ^0, y^0), $F : G \to W(T)$, such that

(a) $P(\vartheta, F(\vartheta)) = 0 \quad (\vartheta \in G)$

(b) $F(\vartheta^0) = y^0$

(c) F is continuous at ϑ^0

(d) F is Fréchet differentiable at ϑ^0 (markedly, this implies (c) per se) and

$$F'(\vartheta^0) = -\left[P'_y(\vartheta^0, y^0)\right]^{-1} P'_\vartheta(\vartheta^0, y^0)$$

The last conclusion signifies that calculation of the variation $\delta y = F'_\vartheta(\vartheta^0)\delta\vartheta$ amounts to solving the problem

$$\frac{\mathrm{d}\delta y}{\mathrm{d}t} + A_{\vartheta^0}\delta y = -A_{\delta\vartheta} y^0, \quad \delta y(0) = 0$$

in the sense of $L^2(T;V')$. This completes the proof. ■

Let us consider now the case when $\vartheta \in L^\infty(\Omega)$ is parametrized by a parameter vector $\theta \in \mathbb{R}^m$, which is defined by a mapping $R : \mathbb{R}^m \to L^\infty(\Omega)$. Such a situation arises naturally in practice or is a consequence of applied parametrization which aims at simplifying the structure of an infinite- or a high-dimensional parameter space. Clearly, θ has to be chosen in such a way as to satisfy the imposed condition $\vartheta(\theta) \in \Theta_{\rm ad}$, so we introduce the set $\bar{\Theta}_{\rm ad} = R^{-1}(\Theta_{\rm ad})$. We wish to investigate the differentiability of the solution to (B17)–(B19) with respect to individual components θ_q, $1 \le q \le m$ of θ at θ^0. For that purpose, let us orient the mapping $Q = R|\,\bar{\Theta}_{\rm ad}$ by the requirement that it possess all the partial Fréchet derivatives at θ^0. Based on the remarks of Appendix A.4, $\mathcal{L}(\mathbb{R}, L^\infty(\Omega))$ is isometrically isomorphic to $L^\infty(\Omega)$ and therefore $Q'_{\theta_q}(\theta^0) \in \mathcal{L}(\mathbb{R}, L^\infty(\Omega))$ may be identified with an element $\vartheta_q(\theta^0) = Q'_{\theta_q}(\theta^0)(1) \in L^\infty(\Omega)$.

The variation s_q in y at y^0 produced by $\vartheta_q(\theta^0)$ is then given as the solution to the problem

$$\frac{\rm d}{{\rm d}t}(s_q(\,\cdot\,),\psi) + a_{Q(\theta^0)}(s_q(\,\cdot\,),\psi) = -a_{\vartheta_q(\theta^0)}(y^0(\,\cdot\,),\psi), \quad s_q(0) = 0 \qquad \text{(B23)}$$

in the sense of $\mathcal{D}'(T)$ for all $\psi \in V$, which results from the chain rule of differentiation (A5). Obviously, s_q is at the same time the element of $W(T)$ which is identified with the partial Fréchet derivative of the mapping assigning to each $\theta \in \bar{\Theta}_{\rm ad}$ the corresponding solution to (B17)–(B19).

Equations (B23), $1 \le q \le m$ are said to be the *sensitivity equations* and their solutions s_q's are called the *sensitivity coefficients*. A key step in finding an optimal sensor location is to solve both the state and sensitivity equations, so attention is now directed toward a technique to obtain their approximate solutions. To this end, we shall apply first the finite-element method in discretization of space variables (i.e. we apply the so-called semi-discrete Galerkin scheme).

Let us denote by V_h a finite-element subspace of V obtained e.g. after introducing a triangular mesh on Ω (for a detailed description of possible choices of V_h, see Neittaanmäki and Tiba, 1994; Raviart and Thomas, 1992; Johnson, 1987); a reader who has had no exposure to the finite-element method can interpret what follows in terms of a finite-dimensional approximation of V. To obtain the finite-element approximation of (B17)–(B19) simply amounts to finding $y_h = y_h(x,t)$ which belongs to V_h for every $t \in T$ and satisfies

$$\frac{\rm d}{{\rm d}t}(y_h(\,\cdot\,),v_h) + a_\vartheta(y_h(\,\cdot\,),v_h) = \langle f(\,\cdot\,),v_h\rangle, \quad \forall v_h \in V_h, \quad \text{a.e. in } T \qquad \text{(B24)}$$

Seeking y_h in the form

$$y_h(x,t) = \sum_{i=1}^{I} Y_i(t)\varphi_i(x) \tag{B25}$$

where $\{\varphi_i\}_{i=1}^{I}$ is a basis in V_h, we plug this expansion into (B24) and get the system of ODE's of first-order:

$$\sum_{j=1}^{I}(\varphi_i,\varphi_j)\frac{\mathrm{d}Y_j}{\mathrm{d}t} + \sum_{j=1}^{I} a_\vartheta(\varphi_i,\varphi_j)Y_j = \langle f,\varphi_i\rangle, \quad 1 \le i \le I, \quad \text{in } T \tag{B26}$$

for unknown functions $Y_1(\,\cdot\,),\ldots,Y_I(\,\cdot\,)$ ($I = \dim V_h$). Let us note that the boundary conditions are already included into this system via the space V. We have only to deal with the initial condition (B19). Writing $y_{0h}(x) = y_h(x,0)$, we set $y_{0h} = y_0$ when $y_0 \in V_h$. If $y_0 \notin V_h$, then y_{0h} may be the standard interpolant of y_0 (Neittaanmäki and Tiba, 1994; Raviart and Thomas, 1992) or a projection of y_0 onto V_h which can be determined e.g. by the set of linear equations

$$(y_{0h}, v_h) = (y_0, v_h), \quad \forall v_h \in V_h \tag{B27}$$

The initial values for Y_i are uniquely determined by the relation

$$\sum_{i=1}^{I} Y_i(0)\varphi_i(x) = y_{0h} \tag{B28}$$

since $\{\varphi_i\}_{i=1}^{I}$ is a basis of V_h. Introducing the vector of unknowns $Y = (Y_1,\ldots,Y_I)$, we rewrite (B26) in matrix form

$$M\frac{\mathrm{d}Y}{\mathrm{d}t} + KY = F \tag{B29}$$

where $F = (\langle f,\varphi_1\rangle,\ldots,\langle f,\varphi_I\rangle)$ is the *load vector*, $M = \big[(\varphi_i,\varphi_j)\big]_{i,j=1}^{I}$ is said to be the *mass matrix*, and $K = \big[a_\vartheta(\varphi_i,\varphi_j)\big]_{i,j=1}^{I}$ is termed the *stiffness matrix*. This method is traditionally called the *method-of-lines* semidiscretization.

As for the sensitivity equations, the procedure is exactly the same, i.e. each s_q is approximated by the quantity

$$s_{qh}(x,t) = \sum_{i=1}^{I} S_{qi}(t)\varphi_i(x) \tag{B30}$$

Setting $S_q = (S_{q1}, \ldots, S_{qI})$ as the vector of additional unknowns, we get the sets of ODE's in matrix form

$$M\frac{\mathrm{d}S_q}{\mathrm{d}t} + KS_q = -K_qY, \quad S_q(0) = 0, \quad 1 \le q \le m \tag{B31}$$

where $K_q = \left[a_{\vartheta_q(\theta^0)}(\varphi_i, \varphi_j)\right]_{i,j=1}^{I}$.

Equations (B29) and (B31) can be further discretized by forming a partition

$$0 = t_0 < t_1 < \cdots < t_N = t_f \tag{B32}$$

of the time interval $[0, t_f]$ with equidistant nodes $t_k = k\tau$ and time step $\tau = t_f/N$. Denoting by $f^{(k)}$ the value of F at the k-th time step, we can approximate (B29) e.g. with the use of the classical Crank-Nicolson scheme (Neittaanmäki and Tiba, 1994; Johnson, 1987; Korbicz *et al.*, 1991):

$$M\frac{Y^{(k+1)} - Y^{(k)}}{\tau} + K\frac{Y^{(k+1)} + Y^{(k)}}{2} = \frac{f^{(k+1)} + f^{(k)}}{2} \tag{B33}$$

where $Y^{(k)}$ signifies the vector of approximate values of Y at the k-th time step. Thus $Y^{(k+1)}$ can be calculated from the equation

$$\left(M + \frac{\tau K}{2}\right)Y^{(k+1)} = \left(M - \frac{\tau K}{2}\right)Y^{(k)} + \tau\frac{f^{(k+1)} + f^{(k)}}{2}, \quad k = 0, 1, \ldots, N-1 \tag{B34}$$

with the initial condition

$$Y^{(0)} = (Y_1(0), \ldots, Y_I(0)) \tag{B35}$$

Of course, equations (B31) can be treated in much the same way, which leads to solving the equations

$$\left(M + \frac{\tau K}{2}\right)S_q^{(k+1)} = \left(M - \frac{\tau K}{2}\right)S_q^{(k)} - \tau K_q\frac{Y^{(k+1)} + Y^{(k)}}{2}, \quad k = 0, 1, \ldots, N-1, \quad q = 1, \ldots, m \tag{B36}$$

subject to the initial condition

$$S_q^{(0)} = 0 \tag{B37}$$

A thorough error analysis of the method presented here can be made following standard textbooks on numerical methods for PDE's (Raviart and Thomas, 1992; Neittaanmäki and Tiba, 1994; Johnson, 1987) and is therefore omitted.

Finally, let us note that the form of the sensitivity problems (B36) is exactly the same as that of the simulation problem (B34), so we can use the same computer code to solve all of them.

Appendix C

Interpolation of tabulated sensitivity coefficients

The numerical treatment of the sensor location problem requires an efficient procedure to evaluate the sensitivity coefficents at arbitrarily picked points of the space-time domain. It is extremely costly to re-solve numerically the sensitivity equations whenever the afore-mentioned values are demanded (after all, this happens continually while planning). A more judicious approach is to solve those equations once and to store the solution in the form of a sequence of values on a finite grid resulting from the appropriate space-time discretization. But doing so, we also have to settle the problem of estimating, if necessary, the missing values at points out of the grid. Of course, the issue pertains to interpolation of functions in multidimensions and we can employ numerous well-developed techniques to deal with this task (see e.g. Press *et al.*, 1996). As partial derivatives of the sensitivities with respect to spatial variables will also be required while using gradient techniques to find optimal sensor locations, cubic spline interpolation seems especially efficient in achieving our aim. Since the topic of interpolation in multidimensions is usually limited in the literature to the case of two independent variables, below we delineate the procedure for trivariate functions, which is particularly suited for our purposes (two spatial variables and time). But before, some elementary notions regarding the one-dimensional situation are briefly recalled, because interpolation in three dimensions boils down to a sequence of univariate interpolations.

C.1 Cubic spline interpolation for functions of one variable

Given a tabulated function $f_i = f(x_i)$, $i = 0, \ldots, n$ on a set of points, called *nodes*, $a = x_0 \leq x_1 \leq \cdots \leq x_n = b$, a *natural cubic spline* interpolant g for f on the interval $[a, b]$ is a function which satisfies the following conditions (Burden and Faires, 1985; Marchuk, 1989):

(a) $g \in C^2([a, b])$,

(b) g is a (generally different) cubic polynomial on each of the subintervals $[x_{i-1}, x_i]$, $i = 1, \ldots, n$,

(c) $g(x_i) = f_i$, $i = 0, 1, \ldots, n$, and

(d) $g''(a) = g''(b) = 0$ (the so-called *free* boundary conditions).

Its graph approximates the shape which a long flexible rod would assume if forced to go through each of the data points $\{(x_i, f_i)\}$.

To construct the cubic-spline interpolant, let us observe that the second derivative g'' is to be continuous and piecewise linear. This clearly forces the conditions

$$g''(x) = m_{i-1}\frac{x_i - x}{\Delta x_i} + m_i\frac{x - x_{i-1}}{\Delta x_i} \quad \text{on } [x_{i-1}, x_i] \tag{C1}$$

where $\Delta x_i = x_i - x_{i-1}$, $m_i = g''(x_i)$, $1 \leq i \leq n$.

Integrating (C1) twice while bearing in mind Condition (c), we deduce that

$$\begin{aligned} g(x) = {} & m_{i-1}\frac{(x_i - x)^3}{6\Delta x_i} + m_i\frac{(x - x_{i-1})^3}{6\Delta x_i} \\ & + \left(f_{i-1} - \frac{m_{i-1}\Delta x_i^2}{6}\right)\frac{x_i - x}{\Delta x_i} + \left(f_i - \frac{m_i\Delta x_i^2}{6}\right)\frac{x - x_{i-1}}{\Delta x_i} \end{aligned} \tag{C2}$$

and

$$\begin{aligned} g'(x) = {} & -m_{i-1}\frac{(x_i - x)^2}{2\Delta x_i} + m_i\frac{(x - x_{i-1})^2}{2\Delta x_i} + \frac{f_i - f_{i-1}}{\Delta x_i} \\ & - \frac{m_i - m_{i-1}}{6}\Delta x_i \end{aligned} \tag{C3}$$

From (C3) and the postulated continuity of the first derivatives at points $x_1, \ldots, x_{n-1}$, we obtain the set of $n-1$ linear equations

$$\frac{\Delta x_i}{6} m_{i-1} + \frac{\Delta x_i + \Delta x_{i+1}}{3} m_i + \frac{\Delta x_{i+1}}{6} m_{i+1} = \frac{f_{i+1} - f_i}{\Delta x_{i+1}} - \frac{f_i - f_{i-1}}{\Delta x_i}, \quad 1 \le i \le n-1 \quad \text{(C4)}$$

in the $n-1$ unknowns m_i, $i = 1, \ldots, n-1$ (Condition (d) yields $m_0 = m_n = 0$). Its matrix of coefficients is tridiagonal and strictly diagonally dominant, so the linear system (C4) has a unique solution.

C.2 Tricubic spline interpolation

In the three-dimensional interpolation, we seek an estimate of a function $f = f(x, y, z)$ from a three-dimensional grid of tabulated values of f. For simplicity, we focus our attention only on the problem of interpolating on the so-called *Cartesian mesh*, i.e. the one which has tabulated function values at the vertices of a rectangular array.

Let $D = [a_l, a_u] \times [b_l, b_u] \times [c_l, c_u] \subset \mathbb{R}^3$ be a bounded cuboid. Given I, J, K and partitions

$$\begin{cases} a_l = x_0 < x_1 < \ldots < x_I = a_u \\ b_l = y_0 < y_1 < \ldots < y_J = b_u \\ c_l = z_0 < z_1 < \ldots < x_K = c_u \end{cases} \quad \text{(C5)}$$

we introduce the grid

$$D_h = \{(x_i, y_j, z_k) : 0 \le i \le I,\ 0 \le j \le J,\ 0 \le k \le K\} \quad \text{(C6)}$$

On such assumptions, tricubic spline interpolation of a function $f = f(x, y, z)$ represented by the values $f_{i,j,k}$ at the points of D_h consists in constructing a function $g : D \to \mathbb{R}$ which satisfies the following conditions (Marchuk, 1989):

(a) $g \in C^2(D)$,

(b) in each cell $[x_{i-1}, x_i] \times [y_{j-1}, y_j] \times [z_{k-1}, z_k]$, $(1 \le i \le I,\ 1 \le j \le J,\ 1 \le k \le K)$ g is a tricubic polynomial of the form

$$g(x, y, z) = g_{i,j,k}(x, y, z) = \sum_{p,q,r=0}^{3} a_{p,q,r}^{i,j,k} (x_i - x)^p (y_j - y)^q (z_k - z)^r$$

(c) $g(x_i, y_j, z_k) = f_{i,j,k}$, $0 \le i \le I$, $0 \le j \le J$, $0 \le k \le K$,

(d) if we denote by ν the vector outward normal to the boundary ∂D of D, then

$$\left.\frac{\partial^2 g}{\partial \nu^2}\right|_{\partial D} = 0$$

It can be shown that such an interpolatory function exists and is unique, but here we are interested above all in the practical problem of its determination. First of all, let us observe that it is a simple matter to calculate the values of the second derivatives g_{xx}, g_{yy} and g_{zz} on D_h. In fact, in Appendix C.1 (cf. (C1) and (C2)), we have shown how to obtain the values m_i's of the second derivative of the spline interpolant (let us recall that the affair boils down to solving a tridiagonal system of linear equations). The derivative g_{xx} on D_h here can be handled in much the same way, the only difference being the necessity of solving $(J+1)(K+1)$ linear systems of type (C4) while performing one-dimensional interpolations along the lines $\{y = y_j, z = z_k\}$, $0 \le j \le J$, $0 \le k \le K$ of the grid. Similarly, by solving $(I+1)(K+1)$ one-dimensional problems along the lines $\{x = x_i, z = z_k\}$, $0 \le i \le I$, $0 \le k \le K$ and $(I+1)(J+1)$ similar problems along the lines $\{x = x_i, y = y_j\}$, $0 \le i \le I$, $0 \le j \le J$, we obtain g_{yy} and g_{zz} on D_h, respectively.

Continuing in the same fashion, we calculate the arrays of g_{xxyy}, g_{yyzz} and g_{xxzz} on D_h based on the newly tabulated values of g_{xx} and g_{yy}. Finally, the delinated procedure permits determination of the values of the derivative g_{xxyyzz} on the grid, as may be readily guessed, from the tabulated values of g_{xxyy}. Consequently, seven three-dimensional arrays are formed. They can be precomputed and stored in computer memory.

Suppose now that it is necessary to determine the value of the interpolant g at a point (x, y, z) such that $x_{i-1} \le x \le x_i$, $y_{j-1} \le y \le y_j$ and $z_{k-1} \le z \le z_k$ for some i, j and k. First, let us take notice of the fact that this can be accomplished as a result of one-dimensional spline interpolation

$$\begin{aligned} g(x,y,z) = {} & g_{xx}(x_{i-1},y,z)\frac{(x_i - x)^3}{6\Delta x_i} + g_{xx}(x_i,y,z)\frac{(x - x_{i-1})^3}{6\Delta x_i} \\ & + \left(g(x_{i-1},y,z) - \frac{g_{xx}(x_{i-1},y,z)\Delta x_i^2}{6}\right)\frac{x_i - x}{\Delta x_i} \\ & + \left(g(x_i,y,z) - \frac{g_{xx}(x_i,y,z)\Delta x_i^2}{6}\right)\frac{x - x_{i-1}}{\Delta x_i} \end{aligned} \tag{C7}$$

But to make this formula useful, we have to indicate how to compute the missing quantities $g(x_i, y, z)$ and $g_{xx}(x_i, y, z)$ (more precisely, $g(x_{i-1}, y, z)$ and $g_{xx}(x_{i-1}, y, z)$ as well, but the corresponding alterations in the formulae for $g(x_i, y, z)$ and $g_{xx}(x_i, y, z)$ are obvious, so they are omitted for brevity; the same simplification is applied everywhere in what follows). For instance, $g(x_i, y, z)$ can be produced based on the following chain of dependences:

$$\begin{aligned} g(x_i, y, z) = {} & g_{yy}(x_i, y_{j-1}, z)\frac{(y_j - y)^3}{6\Delta y_j} \\ & + g_{yy}(x_i, y_j, z)\frac{(y - y_{j-1})^3}{6\Delta y_j} \\ & + \left(g(x_i, y_{j-1}, z) - \frac{g_{yy}(x_i, y_{j-1}, z)\Delta y_j^2}{6}\right)\frac{y_j - y}{\Delta y_j} \\ & + \left(g(x_i, y_j, z) - \frac{g_{yy}(x_i, y_j, z)\Delta y_j^2}{6}\right)\frac{y - y_{j-1}}{\Delta y_j} \end{aligned} \tag{C8}$$

in conjunction with

$$\begin{aligned} g(x_i, y_j, z) = {} & g_{zz}(x_i, y_j, z_{k-1})\frac{(z_k - z)^3}{6\Delta z_k} \\ & + g_{zz}(x_i, y_j, z_k)\frac{(z - z_{k-1})^3}{6\Delta z_k} \\ & + \left(g(x_i, y_j, z_{k-1}) - \frac{g_{zz}(x_i, y_j, z_{k-1})\Delta z_k^2}{6}\right)\frac{z_k - z}{\Delta z_k} \\ & + \left(g(x_i, y_j, z_k) - \frac{g_{zz}(x_i, y_j, z_k)\Delta z_k^2}{6}\right)\frac{z - z_{k-1}}{\Delta z_k} \end{aligned} \tag{C9}$$

and

$$\begin{aligned} g_{yy}(x_i, y_j, z) = {} & g_{yyzz}(x_i, y_j, z_{k-1})\frac{(z_k - z)^3}{6\Delta z_k} \\ & + g_{yyzz}(x_i, y_j, z_k)\frac{(z - z_{k-1})^3}{6\Delta z_k} \\ & + \left(g_{yy}(x_i, y_j, z_{k-1}) - \frac{g_{yyzz}(x_i, y_j, z_{k-1})\Delta z_k^2}{6}\right)\frac{z_k - z}{\Delta z_k} \\ & + \left(g_{yy}(x_i, y_j, z_k) - \frac{g_{yyzz}(x_i, y_j, z_k)\Delta z_k^2}{6}\right)\frac{z - z_{k-1}}{\Delta z_k} \end{aligned} \tag{C10}$$

Similarly, we can establish the formulae to calculate $g_{xx}(x_i, y, z)$:

$$\begin{aligned} g_{xx}(x_i, y, z) &= g_{xxyy}(x_i, y_{j-1}, z)\frac{(y_j - y)^3}{6\Delta y_j} \\ &+ g_{xxyy}(x_i, y_j, z)\frac{(y - y_{j-1})^3}{6\Delta y_j} \\ &+ \left(g_{xx}(x_i, y_{j-1}, z) - \frac{g_{xxyy}(x_i, y_{j-1}, z)\Delta y_j^2}{6}\right)\frac{y_j - y}{\Delta y_j} \\ &+ \left(g_{xx}(x_i, y_j, z) - \frac{g_{xxyy}(x_i, y_j, z)\Delta y_j^2}{6}\right)\frac{y - y_{j-1}}{\Delta y_j} \end{aligned} \tag{C11}$$

$$\begin{aligned} g_{xx}(x_i, y_j, z) &= g_{xxzz}(x_i, y_j, z_{k-1})\frac{(z_k - z)^3}{6\Delta z_k} \\ &+ g_{xxzz}(x_i, y_j, z_k)\frac{(z - z_{k-1})^3}{6\Delta z_k} \\ &+ \left(g_{xx}(x_i, y_j, z_{k-1}) - \frac{g_{xxzz}(x_i, y_j, z_{k-1})\Delta z_k^2}{6}\right)\frac{z_k - z}{\Delta z_k} \\ &+ \left(g_{xx}(x_i, y_j, z_k) - \frac{g_{xxzz}(x_i, y_j, z_k)\Delta z_k^2}{6}\right)\frac{z - z_{k-1}}{\Delta z_k} \end{aligned} \tag{C12}$$

$$\begin{aligned} g_{xxyy}(x_i, y_j, z) &= g_{xxyyzz}(x_i, y_j, z_{k-1})\frac{(z_k - z)^3}{6\Delta z_k} \\ &+ g_{xxyyzz}(x_i, y_j, z_k)\frac{(z - z_{k-1})^3}{6\Delta z_k} \\ &+ \left(g_{xxyy}(x_i, y_j, z_{k-1}) - \frac{g_{xxyyzz}(x_i, y_j, z_{k-1})\Delta z_k^2}{6}\right)\frac{z_k - z}{\Delta z_k} \\ &+ \left(g_{xxyy}(x_i, y_j, z_k) - \frac{g_{xxyyzz}(x_i, y_j, z_k)\Delta z_k^2}{6}\right)\frac{z - z_{k-1}}{\Delta z_k} \end{aligned} \tag{C13}$$

As regards the calculation of the derivative $g_x(x, y, z)$ (this is indispensable while using gradient techniques of sensor location outlined in this monograph), from (C3) it follows that

$$\begin{aligned} g_x(x, y, z) &= -g_{xx}(x_{i-1}, y, z)\frac{(x_i - x)^2}{2\Delta x_i} + g_{xx}(x_i, y, z)\frac{(x - x_{i-1})^2}{2\Delta x_i} \\ &+ \frac{g(x_i, y, z) - g(x_{i-1}, y, z)}{\Delta x_i} \\ &- \frac{g_{xx}(x_i, y, z) - g_{xx}(x_{i-1}, y, z)}{6}\Delta x_i \end{aligned} \tag{C14}$$

In order to evaluate the derivative $g_y(x,y,z)$, the most convenient approach is to employ the alternative form of (C7), i.e.

$$\begin{aligned} g(x,y,z) = {} & g_{yy}(x,y_{j-1},z)\frac{(y_j-y)^3}{6\Delta y_j} + g_{yy}(x,y_j,z)\frac{(y-y_{j-1})^3}{6\Delta y_j} \\ & + \left(g(x,y_{j-1},z) - \frac{g_{yy}(x,y_{j-1},z)\Delta y_j^2}{6}\right)\frac{y_j-y}{\Delta y_j} \\ & + \left(g(x,y_j,z) - \frac{g_{xx}(x,y_j,z)\Delta y_j^2}{6}\right)\frac{y-y_{j-1}}{\Delta y_j} \end{aligned} \tag{C15}$$

which yields

$$\begin{aligned} g_y(x,y,z) = {} & -g_{yy}(x,y_{j-1},z)\frac{(y_j-y)^2}{2\Delta y_j} + g_{yy}(x,y_j,z)\frac{(y-y_{j-1})^2}{2\Delta y_j} \\ & + \frac{g(x,y_j,z)-g(x,y_{j-1},z)}{\Delta y_j} \\ & - \frac{g_{yy}(x,y_j,z)-g_{yy}(x,y_{j-1},z)}{6}\Delta y_j \end{aligned} \tag{C16}$$

This is related to the additional formulae

$$\begin{aligned} g(x,y_j,z) = {} & g_{xx}(x_{i-1},y_j,z)\frac{(x_i-x)^3}{6\Delta x_i} + g_{xx}(x_i,y_j,z)\frac{(x-x_{i-1})^3}{6\Delta x_i} \\ & + \left(g(x_{i-1},y_j,z) - \frac{g_{xx}(x_{i-1},y_j,z)\Delta x_i^2}{6}\right)\frac{x_i-x}{\Delta x_i} \\ & + \left(g(x_i,y_j,z) - \frac{g_{xx}(x_i,y_j,z)\Delta x_i^2}{6}\right)\frac{x-x_{i-1}}{\Delta x_i} \end{aligned} \tag{C17}$$

and

$$\begin{aligned} g_{yy}(x,y_j,z) = {} & g_{yyxx}(x_{i-1},y_j,z)\frac{(x_i-x)^3}{6\Delta x_i} \\ & + g_{yyxx}(x_i,y_j,z)\frac{(x-x_{i-1})^3}{6\Delta x_i} \\ & + \left(g_{yy}(x_{i-1},y_j,z) - \frac{g_{yyxx}(x_{i-1},y_j,z)\Delta x_i^2}{6}\right)\frac{x_i-x}{\Delta x_i} \\ & + \left(g_{yy}(x_i,y_j,z) - \frac{g_{yyxx}(x_i,y_j,z)\Delta x_i^2}{6}\right)\frac{x-x_{i-1}}{\Delta x_i} \end{aligned} \tag{C18}$$

Let us note that $g_{yyxx} = g_{xxyy}$, so no additional calculations and storage are necessary.

Appendix D

Calculation of the differentials introduced in Section 4.2.3

D.1 Derivation of formula (4.50)

Setting $M(s) = \{\mu_{ij}\}_{m\times m}$ and $\overset{\circ}{\Psi}(s) = \{c_{ij}\}_{m\times m} = \partial\Psi(M)/\partial M\big|_{M=M(s)}$, we get

$$\delta J = \sum_{i=1}^{m}\sum_{j=1}^{m} c_{ij}\delta\mu_{ij} = \int_0^{t_f} \sum_{i=1}^{m}\sum_{j=1}^{m} c_{ij}\frac{\partial\chi_{ij}}{\partial s}\,\delta s\,\mathrm{d}t \tag{D1}$$

the last equality being a consequence of the dependence

$$\delta\chi_{ij} = \int_0^{t_f} \frac{\partial\chi_{ij}}{\partial s}\,\delta s\,\mathrm{d}t$$

with

$$\chi_{ij}(s(t),t) = \frac{1}{Nt_f}\sum_{\ell=1}^{N} g_i(x^\ell(t),t)g_j(x^\ell(t),t)$$

From (4.49) and the Lagrange identity (i.e. the integration-by-parts formula) of the form

$$\int_0^{t_f}\langle\zeta(t),\delta\dot{s}(t) - f_s(t)\delta s(t)\rangle\,\mathrm{d}t + \int_0^{t_f}\langle\dot{\zeta}(t) + f_s^{\mathrm{T}}(t)\zeta(t),\delta s(t)\rangle\,\mathrm{d}t$$
$$= \langle\zeta(t_f),\delta s(t_f)\rangle - \langle\zeta(0),\delta s(0)\rangle \tag{D2}$$

we deduce that

$$\delta J = \langle \zeta(0), \delta s_0 \rangle + \int_0^{t_f} \langle f_u^{\mathrm{T}}(t)\zeta(t), \delta u(t) \rangle \, \mathrm{d}t \tag{D3}$$

after setting ζ as the solution to the Cauchy problem

$$\dot{\zeta}(t) + f_s^{\mathrm{T}}(t)\zeta(t) = -\sum_{i=1}^{m}\sum_{j=1}^{m} c_{ij} \left(\frac{\partial \chi_{ij}}{\partial s} \right)^{\mathrm{T}}_{s=s(t)}, \quad \zeta(t_f) = 0 \tag{D4}$$

D.2 Derivation of formula (4.53)

For brevity, we omit all higher-order terms. The perturbed quantities yield

$$\begin{aligned} h(s_0 + \delta s_0, u + \delta u) &= \max_{(\ell,t)\in\bar{\nu}\times T} \{\gamma_\ell(s(t) + \delta s(t))\} \\ &= \max_{(\ell,t)\in\bar{\nu}\times T} \left\{ \gamma_\ell(s(t)) + \left\langle \left(\frac{\partial \gamma_\ell}{\partial s} \right)^{\mathrm{T}}_{s=s(t)}, \delta s(t) \right\rangle \right\} \end{aligned} \tag{D5}$$

Write $S = \{(\ell, t) \in \bar{\nu} \times T : \gamma_\ell(s(t)) = h(s_0, u)\}$. Consequently,

$$\begin{aligned} &h(s_0 + \delta s_0, u + \delta u) \\ &\quad = h(s_0, u) + \max_{(\ell,t)\in S} \left\{ \left\langle \left(\frac{\partial \gamma_\ell}{\partial s} \right)^{\mathrm{T}}_{s=s(t)}, \delta s(t) \right\rangle \right\} \\ &\quad = h(s_0, u) + \max_{(\ell,t)\in S} \left\{ \int_0^{t_f} \left\langle \left(\frac{\partial \gamma_\ell}{\partial s} \right)^{\mathrm{T}}_{s=s(\tau)}, \delta s(\tau) \right\rangle \delta(t-\tau) \, \mathrm{d}\tau \right\} \\ &\quad = h(s_0, u) + \max_{(\ell,t)\in S} \left\{ \langle \zeta_h^\ell(0;t), \delta s_0 \rangle + \int_0^{t_f} \langle f_u^{\mathrm{T}}(\tau)\zeta_h^\ell(\tau;t), \delta u(\tau) \rangle \, \mathrm{d}\tau \right\} \end{aligned} \tag{D6}$$

where δ is the Dirac delta function and $\zeta_h^\ell(\,\cdot\,;t)$ is the solution to the Cauchy problem

$$\frac{\mathrm{d}\zeta_h^\ell(\tau;t)}{\mathrm{d}\tau} + f_s^{\mathrm{T}}(\tau)\zeta_h^\ell(\tau;t) = -\left(\frac{\partial \gamma_\ell}{\partial s} \right)^{\mathrm{T}}_{s=s(\tau)} \delta(\tau - t), \quad \zeta_h^\ell(t_f;t) = 0 \tag{D7}$$

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