Optimal sensor placement in parameter estimation of distributed systems

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**Abstract**

The problem under consideration is to plan the spatial location of pointwise stationary sensors in such a way as to maximize the accuracy of parameter identification of a distributed system defined in a two-dimensional spatial domain. A general functional defined on the Fisher information matrix is used as the design criterion. The approach converts the problem to a classical experimental design one in which the idea of continuous designs is exploited. Its solution is obtained with the use of first-order numerical algorithms. Two simple numerical examples are presented which clearly demonstrate the ideas and trends presented in the paper.

**1 Introduction**

A fundamental problem underlying parameter identification of distributed systems is the selection of sensor locations. This problem comprises the arrangement of a limited number of measurement transducers over the spatial domain in such a way as to obtain the best estimates of the system 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.

Although it is well-known that the estimation accuracy of DPS parameters depends significantly on the choice of sensor locations, there have been relatively few contributions to the experimental design for those systems (for surveys, see[12, 27, 11, 29, 28]). Of course, one may argue that there exist a few works dealing with the problem of determining sensor positions for optimal state estimation [12, 1]. At this point, however, it should be noted that the state estimation problem is essentially different from the optimal measurement problem for parameter identification since in the latter case the current state depends strongly non-linearly on unknown parameters, while its dependence on the initial state is linear.

In the present work, some iterative first-order algorithms for determining pointwise sensor positions maximizing parameter identification accuracy for two-dimensional distributed systems are developed. Measurements at the sensors are assumed to be available continuously in time, and the design criterion is the minimization of a scalar measure of the Fisher Information Matrix related to the identified parameters. This paper is close in spirit to the classical optimum experimental design theory for lumped systems [7, 14, 15, 31] and the approach delineated in [21].

**2 Optimal measurement problem based on pointwise observations**

Let \( \Omega \subset \mathbb{R}^2 \) be a bounded simply-connected open domain with sufficiently smooth boundary \( \partial \Omega \). As our fundamental state system we consider the scalar distributed system

\[
\frac{\partial y}{\partial t} = F \left( x, t, y, \frac{\partial y}{\partial x_1}, \frac{\partial y}{\partial x_2}, \frac{\partial^2 y}{\partial x_1^2}, \frac{\partial^2 y}{\partial x_2^2}, \theta \right),
\]

\( x \in \Omega, \ t \in T \) \hspace{1cm} (1)

where \( x = (x_1, x_2) \in \tilde{\Omega} = \Omega \cup \partial \Omega \) is the corresponding spatial coordinate vector, \( t \) stands for time, \( T = (0, t_f) \), \( y = y(x, t) \) denotes the state variable with values in \( \mathbb{R} \) and \( F \) 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 (1) is accompanied by the boundary condition of the general form

\[
E \left( x, t, y, \frac{\partial y}{\partial x_1}, \frac{\partial y}{\partial x_2}, \theta \right) = 0, \quad x \in \partial \Omega, \ t \in T \]

and the initial condition

\[
y(x, 0) = y_0(x), \quad x \in \Omega \]

(3)

where \( E \) and \( y_0 \) denote some known functions.

We assume the existence of a unique solution to (1)–(3), which is sufficiently regular. The system model above contains an unknown constant parameter vector denoted by
of the model with respect to its parameters is mild and the

\((FIM)\) \[25, 21\] which is widely

the right-hand side of (6). This fact suggests that we may at-

the parameter estimates to be obtained from the data col-

ness’ of particular locations is required. A logical approach

of different locations, a quantitative measure of the ‘good-

of the system parameters. To form a basis for the comparison

data criterion

\(z(t) = y_m(t) + \varepsilon_m(t), \quad t \in T\) (4)

where

\(y_m(t) = \text{col}[y(x_1^j, t), \ldots, y(x_N^j, t)]\)

\(\varepsilon_m(t) = \text{col}[\varepsilon(x_1^j, t), \ldots, \varepsilon(x_N^j, t)]\)

\(z(t)\) is the \(N\)-dimensional observation vector, \(x_j^j \in \tilde{\Omega},\)

\(j = 1, \ldots, N\) denote the pointwise and stationary sensor lo-

cations, and \(\varepsilon = \varepsilon(x, t)\) is a white Gaussian noise process (a

formal time derivative of a Wiener process) whose statistics are

\[\begin{align*}
E\{\varepsilon(x, t)\} &= 0 \\
E\{\varepsilon(x, t)\varepsilon(x', t')\} &= \delta(t-t')
\end{align*}\]

\(\delta\) being the Dirac delta function concentrated at the origin.

Mathematically, the problem is usually cast as an opti-
mization 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)

\[
\mathcal{J}(\theta) = \frac{1}{2} \int_T \|z(t) - \hat{y}_m(t; \theta)\|^2_{Q^{-1}(t)} \, dt
\] (6)

where \(Q(t) = \{q(x^j_i, x^j_j, t)\}_{i,j=1}^N \in \mathbb{R}^{N \times N}\) is assumed to be

positive definite,

\[
\|a\|^2_{Q^{-1}(t)} = a^T Q^{-1}(t) a, \quad \forall a \in \mathbb{R}^N
\]

\(\hat{y}_m(t; \theta) = \text{col}[\hat{y}(x_1^j, t; \theta), \ldots, \hat{y}(x_N^j, t; \theta)]\)

and \(\hat{y}(\cdot, \cdot; \theta)\) stands for the solution to (1)-(3) corre-
ing to a given parameter \(\theta\).

Clearly, the parameter estimate \(\hat{\theta}\) resulting from min-

imization of the fit-to-data criterion depends on the sensor posi-
tions since one can observe the quantity \(z\) in the integrand on

the right-hand side of (6). This fact suggests that we may at-
ttempt to select sensor locations which lead to best estimates of

the system parameters. To form a basis for the comparison

different locations, a quantitative measure of the ‘good-
ness’ 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 col-

lected. Such a measure is usually based on the concept of the

Fisher Information Matrix (FIM) [25, 21] which is widely

used in optimum experimental design theory for lumped sys-

tems [32, 7]. 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 ap-

proximation of the covariance matrix for the estimate of \(\theta\)

[32, 7]. Derivation of this fundamental property is centred

on the use of the Cramér-Rao inequality\(^2\) \[8\]

\[
\text{cov} \hat{\theta} \geq M^{-1}
\] (7)

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 ef-
ficient (minimum-variance) in the sense that the parameter

covariance matrix achieves the lower bound, i.e. (7) becomes

an equality, which is justified in many situations [20]. This

leads to a great simplification since the minimum variance

given by the Cramér-Rao lower bound can be easily com-

puted in a number of estimation problems, even though the

exact covariance matrix of a particular estimator is very dif-

icult to obtain.

It is customary to restrict investigations to spatial uncor-

correlated observations, i.e.

\[
E\{\varepsilon(x^j_i, t)\varepsilon(x'^j_i, t')\} = \sigma^2 \delta_{ij}\delta(t-t')
\] (8)

where \(\delta_{ij}\) denotes the Kronecker delta function and \(\sigma > 0\)

is the standard deviation of the measurement noise. The rea-

son obviously lies in the simplicity of a subsequent analysis.

Such an assumption yields the following explicit form of the

FIM [19]:

\[
M = \frac{1}{\sigma^2} \sum_{j=1}^N \int_0^{t_f} f(x^j_i, t) f(x^j_i, t) \, dt
\] (9)

which is encountered in the bulk of the literature on sensor lo-

cation (we shall also adopt this approach in the remainder of

this paper). Here

\[
f(x^j_i, t) = \left(\frac{\partial y(x^j_i, t; \theta)}{\partial \theta}\right)^T_{\theta=\theta^0}
\] (10)

stands for the so-called sensitivity vector, \(\theta^0\) being a prior

estimate to the unknown parameter vector \(\theta\) [25]. 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 \(\Omega \times T\).

Optimal sensor positions for system identification can be

found by choosing \(x^j_i, j = 1, \ldots, N\) so as to minimize some

scalar measure of performance \(\Psi\) based on the FIM. Various

choices exist for such a function [32, 7, 17, 15], including e.g. the following:

- The D-optimality (determinant) criterion

\[
\Psi(M) = - \log \det M
\] (11)

- The A-optimality (trace) criterion

\[
\Psi(M) = \text{trace } M^{-1}
\] (12)

\(^2\)Recall that (7) should be interpreted in terms of the Loewner ordering

of symmetric matrices, i.e. the matrix \(\text{cov} \hat{\theta} - M^{-1}\) is required to be non-

negative definite.
The sensitivity criterion
\[ \Psi(M) = - \text{trace } M \]  
(13)

A D-optimum design minimizes the volume of the uncertainty ellipsoid for the estimates. 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 [33], so in principle it should be used only to obtain startup locations for one of the above criteria. The introduction of the design criterion \( \Psi \) defined on the FIM
\[ \Psi(\beta M) = \gamma(\beta) \Psi(M), \quad \beta > 0 \]  
(14)

\( \gamma \) being a positive function, we may set \( \gamma = 1 \). Similarly, operating on the so-called average (or normalized) FIM
\[ \bar{M} = \frac{1}{Nt_f} \sum_{j=1}^{N} \int_{0}^{t_f} f(x^j, t) f^T(x^j, t) \, dt \]  
(15)
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 \( M \).

### 3 Continuous designs in measurement optimization

The introduction of the design criterion \( \Psi \) defined on the FIM permits the optimal experimental design to be cast as an optimization problem
\[ \Psi[M(x^1, \ldots, x^N)] \to \min \]  
(16)

where \( x^j, j = 1, \ldots, N \) belong to a given compact set \( X \subset \bar{\Omega} \) in which the measurements are allowed. 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 [3, 5, 7, 8, 15, 32, 17]. Such an approach will also be adopted in what follows.

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 \( \ell \) 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
\[ \xi_N = \{ x^1, x^2, \ldots, x^\ell \} \]  
(17)

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
\[ M(\xi_N) = \sum_{i=1}^{\ell} \frac{1}{t_f} \int_{0}^{t_f} f(x^i, t) f^T(x^i, t) \, dt \]  
(18)

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 \( \xi \) over \( X \) which are absolutely continuous with respect to the Lebesgue measure and satisfy by definition the condition
\[ \int_X \xi(dx) = 1 \]  
(19)

Such an extension of the design concept allows us to replace (18) by
\[ M(\xi) = \int_X \Upsilon(x) \xi(dx) \]  
(20)

where
\[ \Upsilon(x) = \frac{1}{t_f} \int_{0}^{t_f} f(x, t) f^T(x, t) \, dt \]

and the integration in (19) and (20) 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 [9]. 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 \( \mathcal{M}(X) \) for the set of all admissible information matrices, i.e.
\[ \mathcal{M}(X) = \{ M(\xi) : \xi \in \Xi(X) \} \]  
(21)

Then we may redefine an optimal design as a solution to the optimization problem
\[ \xi^* = \arg \min_{\xi \in \Xi(X)} \Psi[M(\xi)] \]  
(22)
In what follows, two basic assumptions are vital:

(A1) \( X \) is compact, and

\[
\text{\textbf{(A2)} \quad f \in C(X \times T; \mathbb{R}^m)}
\]

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

**Lemma 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 (20). The other results from the dependence

\[
b^T M(\xi) b = \int_X b^T \Upsilon(x) b \xi(x)
\]

\[
= \frac{1}{t_f} \int_X \left\{ \int_0^{t_f} \| b^T f(x, t) \|^2 d t \right\} \xi(dx) \geq 0
\]

valid for any \( b \in \mathbb{R}^m \).

\[\blacksquare\]

**Lemma 2.** \( \mathcal{M}(X) \) is compact and convex.

**Proof.** Let us notice that by Assumption (A2) the function \( \Upsilon \) is continuous in \( X \) [10, Th. 22, p. 360]. Helley’s theorem [4, 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 \( \xi_* \in \Xi(X) \) in the sense that

\[
\lim_{j \to \infty} \int_X g(x) \xi_{i_j}(dx) = \int_X g(x) \xi_*(dx), \quad \forall g \in C(X)
\]

Choosing \( g \) consecutively as the components of the matrix \( \Upsilon \), we get

\[
\lim_{j \to \infty} M(\xi_{i_j}) = M(\xi_*)
\]

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

\[
M[(1 - \lambda)\xi_1 + \lambda \xi_2] = (1 - \lambda)M(\xi_1) + \lambda M(\xi_2),
\]

\[\forall \xi_1, \xi_2 \in \Xi(X)\]

valid for any \( \lambda \in [0, 1] \).

\[\blacksquare\]

**Remark 1.** Let us observe that Assumption (A2) may be slightly weakened: For the continuity of \( \Upsilon \) it suffices to require only \( f(\cdot, t) \) to be continuous and to impose the condition

\[
\forall x \in X, \| f(x, t) \| \leq h(t)
\]

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 \( \mathbb{R}^m \) 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

\[
\xi^*(x) = \begin{cases}
  x^1, & x^2, \ldots, x^\ell \\
  \xi_1, \xi_2, \ldots, \xi_\ell \\
  \sum_{i=1}^{\ell} \xi_i = 1
\end{cases}
\]

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.** For any \( M_0 \in \mathcal{M}(X) \) there always exists a purely discrete design \( \xi \) 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 \( \mathcal{M}(X) \), 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 \( \text{FIM's} \), \( \mathcal{M}(X) \) 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 \( M(\xi) = \bar{\Upsilon}(x) \) which correspond to one-point designs \( \xi = \{ x \} \), i.e. the designs concentrated at a single point \( x \), are the only extreme points of \( \mathcal{M}(X) \). Hence, from Carethodory’s theorem [15, 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 \( A \) [4, 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) \( \Psi \) 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

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

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

\[
\Psi[M(\xi) + \lambda(M(\tilde{\xi}) - M(\xi))] = \Psi[M(\xi)] + \lambda \int_X \psi(x, \xi, \tilde{\xi}) \xi(dx) + o(\lambda; \xi, \tilde{\xi})
\]

where \( o \) is the usual Landau symbol, i.e.

\[
\lim_{\lambda \to 0} \frac{o(\lambda; \xi, \tilde{\xi})}{\lambda} = 0
\]
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 $\Psi$ as a linear ordering of $\mathbb{Z}$. (As regards the notation in (A4), we adopt that of the Loewner ordering of symmetric matrices, i.e. $M_1 \preceq M_2$ iff $M_2 - M_1$ is non-negative definite.) As for Assumption (A5), it only states that at first sight it may seem a bit odd. In practice, however, (A6) 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

$$\delta_+ \Psi(M(\xi), M(\xi) - M(\xi)) = \left. \frac{\partial \Psi(M(\xi) + \lambda(M(\xi) - M(\xi)))}{\partial \lambda} \right|_{\lambda=0^+}$$ (30)

whose form must be on one hand specific, i.e. $\int_X \psi(x, \xi) \xi(dx)$, but on the other hand, for most practical criteria such a condition is not particularly restrictive.

In fact, requiring $\Psi$ to be differentiable with respect to individual elements of its matrix argument, we obtain

$$\delta_+ \Psi(M(\xi), M(\xi) - M(\xi)) = \text{trace} \left[ \frac{\partial \Psi(M(\xi))}{\partial M} (M(\xi) - M(\xi)) \right]$$

$$= \int_X \text{trace} \left[ \frac{\partial \Psi(M(\xi))}{\partial M} \right] \bar{\Psi}(x) \xi(dx) \quad \text{(31)}$$

where

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

and therefore

$$\psi(x, \xi) = c(\xi) - \phi(x, \xi)$$ (32)

the functions $c$ and $\varphi$ being respectively defined as

$$c(\xi) = -\text{trace} \left[ \frac{\partial \Psi(M(\xi))}{\partial M} \right]$$ (33)

and

$$\phi(x, \xi) = -\text{trace} \left[ \frac{\partial \Psi(M(\xi))}{\partial M} \right] \bar{\Psi}(x)$$

$$= -\frac{1}{t_f} \int_0^{t_f} f^T(x, t) \Psi(\xi)f(x, t) \, dt$$ (34)

The next result provides a characterization of the optimal designs.

**Theorem 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).

(ii) The set of optimal designs is convex.

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

$$\min_{x \in X} \psi(x, \xi^*) = 0 \quad \text{(35)}$$

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

**Proof.** The theorem can be established in exactly the same way as Theorem 2.3.2 of [7, p. 31] as the explicit form of the FIM is not essential in the proof.

It is now clear that the function $\psi$ is of paramount importance in our considerations, as it determines the location of the support points in the optimal design $\xi^*$ (they are situated among its points of global minimum). Moreover, given any design $\xi$, 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

$$\xi^+ = (1 - \lambda)\xi + \lambda x^*$$ (36)

for some $\lambda \in (0, 1)$. If $\lambda$ is sufficiently small, then from (29) it may be concluded that

$$\Psi[M(\xi^+)] - \Psi[M(\xi)] \approx \lambda \psi(x^*, \xi)$$ (37)

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 (10), 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 2.** The following characterizations of an optimal design $\xi^*$ are equivalent in the sense that each implies the other two:

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

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

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

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

**Proof.** With minor modifications, it may be adopted, e.g. from [4, Th. 2.3, p. 109] and therefore it is omitted.

When formulated for a particular design criterion, Theorem 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. The following conditions are equivalent:

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

(ii) The design $\xi^*$ minimizes

$$\max_{x \in X} \frac{1}{t_f} \int_0^{t_f} f^T(x, t) M^{-1}(\xi) f(x, t) \, dt,$$

and

(iii) $\max_{x \in X} \frac{1}{t_f} \int_0^{t_f} f^T(x, t) M^{-1}(\xi^*) f(x, t) \, dt = m$

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 $\xi$ is optimal.

2. If the sensitivity function $\phi(x, \xi)$ exceeds $c(\xi)$, then $\xi$ 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 $\xi_k$ 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

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

(recall that $\xi_k^0$ 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 $\lambda_k$. This follows since the derivative with respect to $\lambda_k$ is negative, i.e.

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

The steps in using the outlined gradient method can be briefly summarized as follows [7, 32, 22, 23, 24, 26]:

Step 1. Guess a discrete non-degenerate starting design measure $\xi_0$ (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) $\lim_{k \to \infty} \lambda_k = 0$, $\sum_{k=0}^{\infty} \lambda_k = \infty$ (Wynn’s algorithm),

(ii) $\lambda_k = \arg \min_\Lambda \Psi[(1 - \lambda) M(\xi_k) + \lambda M(\xi_k^0)]$ (Fedorov’s algorithm).

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 [30, 32, p. 216] is especially suited for that purpose if the design region $X$ is a hypercube.

Notwithstanding the fact that the problem outlined in this section is slightly different from the classical formulation encountered in works on optimum experimental design, the details regarding implementations of the corresponding algorithms remain in principle the same and hence this topic will not be further discussed. Instead, we refer the reader to the excellent specialized literature [7, 32, 22, 23, 24, 26].

Let us note that the FIM will depend on the preliminary estimate $\theta^0$ around which the model is linearized, so logically, the optimal sensor location can never be found at the design stage unless $\theta^0$ is very close to the true parameters or the sensitivity vector $f$ is insensitive to the values of the model parameters (in practice, the latter is unlikely in the considered applications). But this problem is unavoidable in non-linear optimum experimental design [16].

At this very moment, some interpretation of the resulting optimal design of the form (28) 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 [18] 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 [21]. Namely, for $\xi_N$ given by (17), 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 (18) is the expected value of the FIM. This justifies our results as theoretically exact from a slightly different point of view.

4 Simulation examples

Some numerical examples have been solved to indicate the general nature of the results.
Example 1. 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 $\Gamma$ 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

$$\frac{\partial y(x, t)}{\partial t} = \frac{\partial}{\partial x_1} \left( \kappa(x) \frac{\partial y(x, t)}{\partial x_1} \right) + \frac{\partial}{\partial x_2} \left( \kappa(x) \frac{\partial y(x, t)}{\partial x_2} \right)$$

in $\Omega \times T$ \hspace{1cm} (40)

The initial and boundary conditions of (40) were

$$y(x, 0) = 5 \quad \text{in} \quad \Omega \hspace{1cm} (41)$$

$$y(x, t) = 5(1 - t) \quad \text{on} \quad \Gamma \times T \hspace{1cm} (42)$$

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

$$\kappa(x) = \theta_1 + \theta_2 x_1 + \theta_3 x_2 \hspace{1cm} (43)$$

where $\theta_1 = 0.1$, $\theta_2 = \theta_3 = 0.3$. On the basis of simulated data generated with the specified $\kappa$, we tried to determine a continuous design over $X = \Omega$ 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 program was written in Essential Lahey Fortran 90 v.4.0 [13] 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 evenly spaced grid (with 15 divisions along each spatial axis and 30 divisions of the time interval). The sensitivity coefficients were then interpolated via tri-cubic spline interpolation and the corresponding spline parameter values were stored in computer memory. Finally, Fedorov’s version of the first-order algorithm was applied to maximize the determinant of the FIM. (The maximum number of evaluations for the performance index was 2000.)

Starting from the design

$$\xi_0 = \left\{ \begin{array}{c} (0.6, 0.2), \ 0.2, 0.5, \ 0.1, 0.2) \ 1/3 \ 1/3 \ 1/3 \end{array} \right\}$$

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

$$\xi^* = \left\{ \begin{array}{c} (0.65224, 0.26353), \ (0.27083, 0.63834), \ldots \ 0.33570, \ 0.33410, \ldots \ (0.14647, 0.15668) \ 0.33019 \end{array} \right\}$$

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 $\kappa$ 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. 1 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 $\theta$.

Example 2. In another simulation experiment, the spatio-temporal domain was the same as in Example 1 (similarly, the introduced discretization for numerical calculations was retained). This time, however, the diffusion equation contained a driving force, i.e.

$$\frac{\partial y(x, t)}{\partial t} = \frac{\partial}{\partial x_1} \left( \kappa(x) \frac{\partial y(x, t)}{\partial x_1} \right) + \frac{\partial}{\partial x_2} \left( \kappa(x) \frac{\partial y(x, t)}{\partial x_2} \right) + 30 \exp(-30||x - a||^2)$$

in $\Omega \times T$ \hspace{1cm} (44)

where $a = (0.75, 0.25)$, see Fig. 2. The boundary $\Gamma$ 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

$$y(x, t) = \begin{cases} 6x_2(1 - x_2) & \text{on} \ \Gamma_1 \times T \\ 0 & \text{on} \ \Gamma_2 \times T \end{cases} \hspace{1cm} (45)$$

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

$$y(x, 0) = 5 \quad \text{in} \quad \Omega \hspace{1cm} (46)$$

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

$$\kappa(x) = \theta_1 + \theta_2 x_1, \ \theta_1 = 0.1, \ \theta_2 = 0.3 \hspace{1cm} (47)$$

Figure 1: Optimal location of the support points in the problem of Example 1 (the axis of symmetry is represented by a sloping dotted line).
or, more precisely, the coefficients $\theta_1$ and $\theta_2$. All the other settings were the same as in Example 1.

Starting from the initial design

$$\xi_0 = \left\{ \frac{1}{2}, \frac{1}{2} \right\}$$

after three iterations, we obtained the following approximation to the optimal design whose support is shown in Fig. 3:

$$\xi^* = \left\{ \frac{(0.70166, 0.30929)}{0.483938}, \frac{(0.16965, 0.53752)}{0.516062} \right\}$$

On reflection, this result is not surprising. Indeed, in our system there exist two perturbations, i.e. the boundary excitation on $\Gamma_1$ 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.

### 5 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 the sensor location problem for DPS’s. The advantage of introducing continuous designs lies in the fact that the problem dimensionality is dramatically reduced. Moreover, with some minor changes, sequential numerical design algorithms, which have been continually refined since the early 1960s, can be employed here. Unfortunately, this approach does not prevent sensors from clustering which is a rather undesirable phenomenon in potential applications. 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 can be employed, and in particular the idea of replication-free designs which have emerged relatively late in the context of spatial statistics (see the monograph by Müller [14], a survey by Fedorov [6], and a seminal work by Brimkulov et al. [2]). But this will constitute the subject of a separate paper.

If the number of sensors is not large, 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.

### References


