Optimal Design of Experiments for linear, elliptic PDEs

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Abstract

We've discussed Optimal Design of Experiments for linear, elliptic PDEs. Many chemical processes can be modelled by equations depending on unknown parameters, e.g. heat capacities, which can not be measured directly. However, often it is possible to take measurements of other quantities, like the temperature, which depend on those parameters. Due to technical limitations those measurements are peturbed by random measurement errors. Therefore an estimate for the true parameters can be determined by Maximum likelihood estimation from the obtained mesurements. The quality of such an estimate corresponds to the size of the confidence domains of the Maximum likelihood estimator. By the optimal placement of the sensors we can design experiments that lead to Maximum likelihood estimators with minimized confidence domains. Our main contribution to this topic is a formulation of this sensor placement problem as a nonlinear optimization problem over the set of all positive measures in the unit ball in $M(\Omega)$, the space of finite Radon measures. We proved existence of optimal designs, derived optimality conditions and characterized their structure for a model problem with one unknown parameter.

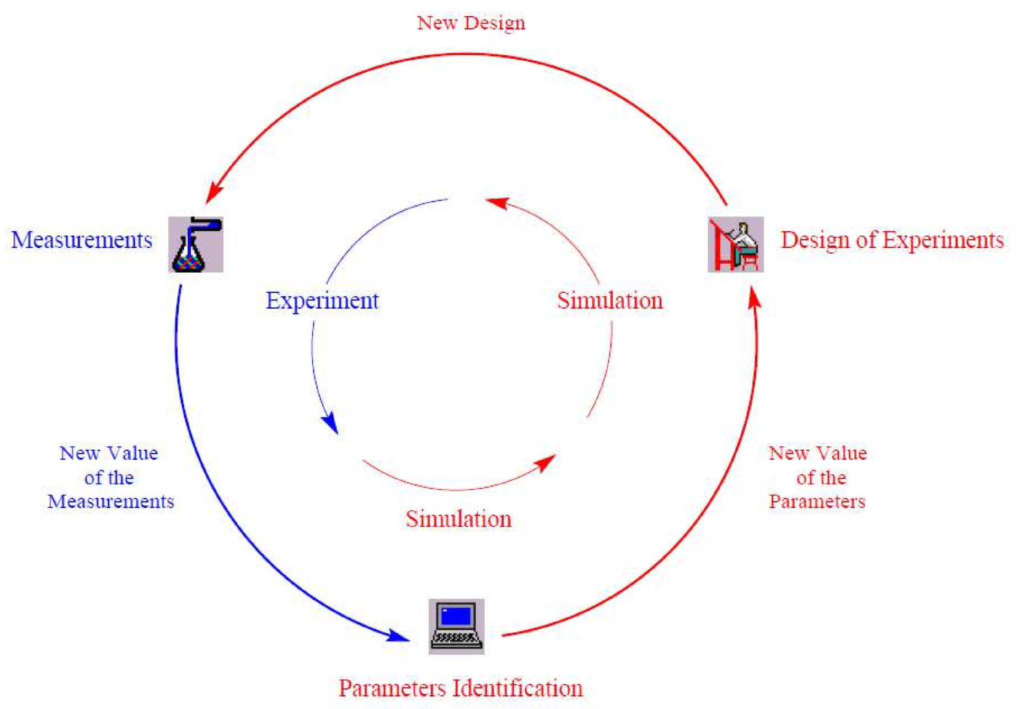
Model Problem and Setting

As a model problem we consider a linear, elliptic PDE, given in its weak form by

$$\text{find } y \in H_0^1(\Omega): \quad \int_\Omega (\nabla y \cdot \nabla \varphi + q y \varphi)\mathrm{d}x = \int_\Omega f \varphi \mathrm{d}x \;\forall \varphi \in H_0^1(\Omega) \qquad (1)$$

where Ω denotes an open and bounded subset of $\mathbb{R}^d$, $d \in \{2,3\}$. Furthermore we assume that it is a convex polygon or polyhedron, respectively. f is a given $L^2(\Omega)$ function and $q \in Q_{ad} := [\epsilon, \infty)$ for an $\epsilon > 0$.
We considered experiments in which the underlying chemical/physical process can be modelled by an equation of the form (1) and q takes the role of the unknown parameter. For the "true" value of the parameter we write q^*.

Procedure



Optimal Design of Experiments [3].

From a data set $\{\tilde{y}_{d_i}\}_{i=1}^n$ collected in an experiment at a **fixed** set of sensor locations $\{x_i\}_{i=1}^n$ an estimate for the parameter q^* is determined in the **Parameter Identification problem** by Maximum likelihood estimation.
In the **Design problem** the parameter is **fixed** and the sensor locations are subject to optimization.

Approximation of the Confidence Intervals

We define the Parameter-to-State operator S by

$$S: \; Q_{ad} \to H^2(\Omega) \cap H_0^1(\Omega) \quad q \to S(q)$$

where $S(q)$ denotes the unique solution of (1).
For a detailed discussion of Parameter Identification with Maximum likelihood we refer to [1]. Due to the nonlinearity of S the confidence interval $G(q^*, \alpha)$ to the niveau α is hard to calculate. Therefore we approximate it by the confidence interval $G(\tilde{q}_{mean}, \alpha)$ of a random variable $\tilde{q}$, $\tilde{q} \sim \mathcal{N}(\tilde{q}_{mean}, C_q)$, where

$$C_q = \frac{1}{\langle S'(\bar{q})(1)^2, \omega\rangle} \quad \tilde{q}_{mean} = \bar{q} + C_q \langle S'(\bar{q})(1)(S(q^*) - S(\bar{q})), \omega\rangle$$

where $S'(\bar{q})(1)$ denotes the directional derivative of S in the direction 1 at a point $\bar{q}$, given as solution to

$$\min_{q \in Q_{ad}} \frac{1}{2} \sum_{i=1}^n \lambda_i (S(q)(x_i) - \tilde{y}_{d_i})^2$$

and $\omega = \sum_{i=1}^n \lambda_i \delta_{x_i}$. The boundary points of $G(\tilde{q}_{mean}, \alpha)$ are given by

$$p_{1/2} = \tilde{q} \pm \frac{\gamma(\alpha)}{\sqrt{\langle S'(\bar{q})(1)^2, \omega\rangle}}$$

with an α-dependent constant $\gamma(\alpha)$. λ_i denotes the number of measurements taken at x_i.

References

1. S. Körkel. Numerische Methoden für Optimale Versuchsplanungsprobleme bei nichtlinearen DAE-Modellen. IWR, 2002
2. E. Casas, C. Clason, and K. Kunisch. Approximation of elliptic control problems in measure spaces with sparse solutions. SIAM J. Control and Optimization, $50(4): 1735\text{˘}1752$, 2012.
3. T. Carraro. Parameter estimation and optimal experimental design in flow reactors, 2005.

Design Problem

For a given estimate $\bar{q}$ of q^* an optimal placement of the measurements $\bar{\omega}$ fulfills

$$\bar{\omega} \in \arg\min_{\omega \in \bar{W}_{ad}} \frac{1}{\langle S'(\bar{q})(1)^2, \omega\rangle} = \arg\min_{\omega \in \bar{W}_{ad}} \phi(\omega) \qquad (2)$$

,i.e. it minimizes the variance of $\tilde{q}$. The admissible set $\bar{W}_{ad}$ is defined as

$$\bar{W}_{ad} = \{\omega \in M(\Omega) | \; \omega \geq 0, \|\omega\|_{M(\Omega)} \leq 1\}.$$

Radon measures in $\bar{W}_{ad}$ tell you where to measure and how much "experimental effort" should be spent at every spatial point.

Discretization and Main Results

We consider a shape regular and quasi-uniform family $\{T_h\}_{h>0}$ of triangulations of Ω and discretize (1) by piecewise linear finite elements. For the Design problem we consider a semi-discretization

$$\min_{\omega \in \bar{W}_{ad}} \phi_h(\omega) = \min_{\omega \in \bar{W}_{ad}} \frac{1}{\langle S_h'(\bar{q})(1)^2, \omega\rangle}, \qquad (3)$$

where S_h denotes the discrete Parameter-to-State map. For fixed $h > 0$ small enough we obtain:

Theorem 1: Let ϕ in (2) be proper. Then there exists a solution $\bar{\omega}_h$ to (3) and there holds the equivalence
1.: ω_h is optimal for (3).
2.: $\|\omega_h\|_{M(\Omega)} = 1$ und $supp\ \omega_h \subset \left\{ x \in \Omega | \; S_h'(\bar{q})(1)^2(x) = \|S_h'(\bar{q})(1)^2\|_\infty \right\}$.

Corollary 1: There exists an inner node x of T_h so that δ_x is optimal.

Numerical Results

We considered (1) on the unit sqare in $\mathbb{R}^2$ with

$$f(x_1, x_2) = (\pi^2 + 2)^2 \sin(\pi x_1) \sin(\pi x_2) \quad q^* = 2$$

We proceeded as followed:

- In Exp. 1 an estimate from 3 randomly placed measurements was determined.
- In Exp. 2 we took 3 additional randomly place measurements.
- In Exp 3. we took the 3 measurements from Exp. 1 and performed 3 additional measurements at a computed, optimal sensor location.

To compare the quality of the obtained estimates, we computed realizations of the confidence intervals to the level 0.95 as well as the locations of the measurements.

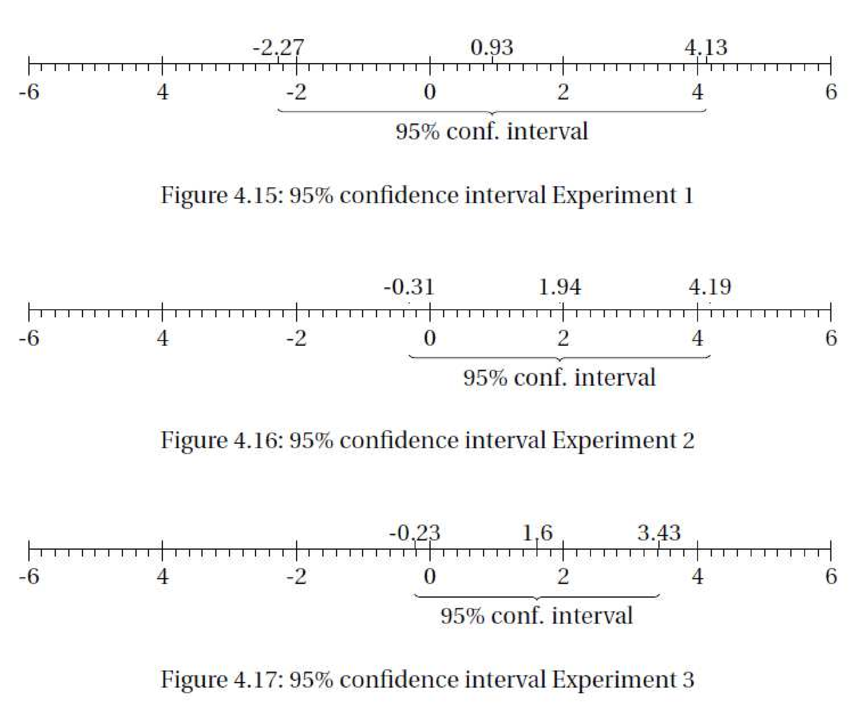


Figure 4.15: 95% confidence interval Experiment 1

Figure 4.16: 95% confidence interval Experiment 2

Figure 4.17: 95% confidence interval Experiment 3