Optimal Experimental Design for Finding Optimally Located Boreholes in Geothermal Engineering

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ABSTRACT
An obstacle for further commercial utilization of deep geothermal resources is the high cost for deep drilling in regard to the productivity risk of a well. Minimizing the risk by optimizing the location of a well is thus a question of primary importance. For a given geological model of a reservoir, we demonstrate how this problem may be tackled by a mathematical optimization approach called optimal experimental design. We show how this problem can be mathematically derived, numerically formulated, and practically implemented using distributed computing. We discuss an example for a sedimentary geothermal reservoir with multiple lithological units. We show how optimized positions of boreholes can be determined such that uncertainty of estimating the hydraulic permeability of a target rock unit from temperature measurements is minimized.

1. INTRODUCTION
Optimal experimental design (OED) refers to a set of methods developed in statistics since the 1970s. These techniques are also known as design of experiments; see Atkinson and Donev (1992), Pronzato (2008) and Pukelsheim (2006) for a thorough introduction to these methods. In general, OED can be understood as a technique to extract the most useful information from data to be collected. Therefore, it is considered to be a central method in occasions where unknown quantities are estimated and the choice for estimation is open. Even so the method has been developed originally in the field of mathematical statistics, application to problems governed by differential equations are quite recent. Many open problems are still to be discussed, in particular for complex flows.

In the present extended abstract, we apply OED to obtain “good” model-based parameter estimates. Thus, the main objective of OED is to present a reliable (and at least for simple problems provable) method to minimize errors in the parameter estimation. To explain the basic procedure we first formulate an abstract problem in Section 2 before turning to a particular geothermal forward problem in Section 3. In Section 4, we formulate an OED problem that is based on this forward problem. Finally, we draw some conclusions in Section 5.

2. OPTIMAL EXPERIMENTAL DESIGN (OED)
In an abstract setting, we consider a mathematical model $A$ that depends on unknown parameters $\theta$ and further on experimental conditions $F$. The output of the model is denoted by the symbol $y$ and therefore we may formally write

$$ y = A(\theta, F) $$

Here, we assume that we observe the output without any error. Suppose now that there are some experimental conditions $F^*$ given. Suppose further that the output of the model $A$ under these experimental conditions $y^*$ is known. Then, the classical parameter estimation problem is given by

$$ \min_{\theta} \left\| y^* - A(\theta, F^*) \right\| $$

Assume that this parameter estimation problem has a solution $\theta^*$. Then those parameters are the optimal ones under the experimental condition $F^*$. The OED problem tries to answer the following question: Suppose you can choose the experimental condition $F$ freely. Suppose further that the model output $y$ is only available up to some unknown error. Which experimental condition $F$ should be chosen such that the resulting error in determining the parameter $\theta$ is minimal?

One possibility to answer the previous question is to study the variation of the model output $y$ with respect to the experimental conditions $F$. Mathematically, this is described by certain measures of the Fisher matrix

$$ M(\theta, F) = \begin{bmatrix} \frac{\partial y}{\partial F} \\ \frac{\partial y}{\partial \theta} \end{bmatrix}^T \begin{bmatrix} \frac{\partial y}{\partial \theta} \\ \frac{\partial y}{\partial F} \end{bmatrix} $$

where $y = A(\theta, F)$. A typical example of a measure of the Fisher matrix is the so-called D-optimality design, which is given by the optimality criterion
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\[ D (\theta, F) = \frac{1}{2} \log(\det(M(\theta, F))) - \theta^T (\Delta \theta) \]

Other possibilities for optimality criteria include computing eigenvalues of or traces of the Fisher matrix \( M \). Finally, OED answers the previously raised question as follows: The optimal experimental conditions \( \hat{F} \) are given as the solution to the min-max problem

\[
\min_{\theta} \max_{F} D (\theta, F).
\]

In this extended abstract, we consider the D-optimality design criterion for a particular geothermal OED problem. For this problem, we obtain similar results for other optimality criteria.

3. A PARTICULAR GEOTHERMAL FORWARD PROBLEM

Before discussing an OED problem we introduce the underlying forward model. The mathematical model \( A \) describes geothermal processes in a geological reservoir. Parameters \( \theta \) of the model include the hydraulic permeability \( \kappa \), the thermal conductivity \( \lambda \), and the porosity \( \psi \). Furthermore, the subsurface model includes several different layers. We assume for simplicity that, within each layer, the previous mentioned parameters are constant, but unknown. The model describes the evolution of the temperature distribution \( T(t, x) \) at a three-dimensional position \( x \) and time \( t > 0 \) as well as the evolution of the hydraulic pressure \( P(t, x) \). We use the following notations. Let \( \rho_f \) denote the fluid density. The symbols \( \alpha \) and \( \beta \) are used for compressibilities of rock and fluid phase, respectively. The symbol \( \mu_f \) denotes the fluid viscosity whereas \( (dc) \) and \( (dc)_f \) are used for the heat capacity of the porous medium and fluid, respectively. The symbol \( g \) stands for the gravitational constant. Then, the model \( A \) is given by the following coupled system of differential equations:

\[
\rho_f (\alpha + \beta \psi) \frac{\partial P}{\partial t} + \nabla \cdot (\rho_f \frac{\partial P}{\partial t}) = \nabla \cdot (\rho_f g \nabla x_j) + W, \]

\[
(\rho c) \frac{\partial x_j}{\partial t} - \nabla \cdot (\alpha \nabla T) - (\rho c) a \cdot \nabla T = H, \]

\[
a = \frac{K}{\mu_f} (\nabla P + \rho_f g \nabla x_j).
\]

Here, \( W \) and \( H \) are source terms due to inflowing water and possible heat, respectively. The model is numerically solved using appropriate initial and boundary conditions. To this end, we use the software package SHEMAT-Suite; see Bartels, Kühn, and Clauser (2003) and Rath, Wolf, and Bückler (2006). The subsurface model including the different layers is depicted in Figure 1 where each color represents a different geophysical layer with possibly different parameters.

Figure 1: Multilayer geothermal model where different colors refer to different permeability values. This figure shows a two-dimensional cut in the \( x_2 \) (location) and \( x_3 \) (depth) direction.

4. A PARTICULAR GEOTHERMAL OED PROBLEM

Even so more general computations are possible we consider an OED problem under the following additional assumptions: We assume that only the hydraulic permeability in zone \( j \) is an unknown parameter; hence \( \theta = \kappa_j \). Here, the symbol \( \kappa_j \) refers to the permeability in the fault zone. Furthermore, the experimental condition \( F \) is the location of the borehole on the surface \( (\zeta_1, \zeta_2) \) in the two-dimensional space. Different experimental conditions therefore correspond to different possible boreholes or drilling locations. Finally, as model output, we consider only the temperature along the depth of the reservoir at terminal time \( \tau \) within the single borehole described by \( F \), i.e., located at coordinates \( (\zeta_1, \zeta_2) \). Hence, the model output is given by \( y = T(\tau, \zeta_1, \zeta_2, \cdot) \) and we may formally write \( y = A(\theta, F) \) where the evaluation of the model \( A \) for given parameter \( \theta = \kappa_j \) and given experimental condition \( F \) described by the location \( (\zeta_1, \zeta_2) \) requires to solve the coupled system of differential equations.

Finally, we numerically solve the min-max problem introduced in Section 2. Note that every evaluation of the D-optimality criterion \( D(\theta, F) \) corresponds to at least solving the coupled system of differential equations and the numerical evaluation of the gradient. The latter is obtained using a combination of numerical and automatic differentiation. More precisely, we compute the derivatives of the model with respect to the experimental condition, \( \partial y/\partial F \), via automatic differentiation and approximate the mixed second-order derivatives, \( \partial^2 y/(\partial F \partial \theta) \), using divided differences on the code generated automatically via automatic differentiation.
Due to the highly nonlinear structure, a direct method to solve the min-max problem is not yet available. The evaluation of equation using only a one-dimensional unknown parameter and borehole positions with fixed coordinate $x_1$ is computationally expensive. Therefore, we employ the EFCOSS framework for the solution of OED problems; see Rasch und Bücker (2010). EFCOSS uses a combination of distributed and parallel computing which is capable of reducing the computing time to a reasonable limit. A graph of the function

$$O(F) = \max_{\theta} D(\theta, F)$$

for varying borehole position $x_2$ is shown in Figure 2. When solving the min-max problem we are interested in the minimum of the graph with respect to $x_2$. The permeability $\theta = \kappa_j$ in the fault zone $j$ is unknown. A borehole location can be freely chosen, but only along the $x_2$ direction. We observe that the minimum is located in between the interval $x_2 = 7$ km to 10 km. This coincides well with the intuition since the fault zone is precisely in this area.

![Figure 2: Plot of the function $O(F) := \max_\theta D(\theta, F)$ for varying experimental conditions $F$.](image)

5. CONCLUSIONS
Finding the location of a borehole is an important task in geothermal engineering. We formulate this task mathematically using concepts from optimal experimental design. Here, the solution of the underlying forward problem is already computationally expensive. We showed that the solution of a corresponding optimal experimental design problem, which is even more time-consuming, is indeed possible and computationally feasible. Moreover, the borehole location computed by this approach is physically plausible and coincides with the intuition of a geothermal engineer.

REFERENCES