Optimal Experimental Design for the Large-Scale Nonlinear Ill-posed Problem of Impedance Imaging

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0.1 Introduction

Many theoretical and practical problems in science involve acquisition of data via indirect observations of a model or phenomena. Naturally, the observed data are determined by the physical properties of the model sought, as well as by the physical laws that govern the problem, however, they also depend on the experimental configuration. Unlike the model and the physical laws, the latter can be controlled by the experimenter. It is this possibility of controlling the experimental setup that leads to optimal experimental design (OED).

Optimal experimental design of well-posed inverse problems is a well-established field (e.g., Fedorov (1972); Pukelsheim (2006) and references therein), yet, despite the practical necessity, experimental design of ill-posed inverse problems and in particular ill-posed nonlinear problems has remained largely unexplored. We
discuss some of the intrinsic differences between well- and ill-posed experimental designs, and propose an efficient and generic framework for optimal experimental design of nonlinear ill-posed problems in the context of impedance tomography.

We use discrete data modeled as

\[ d = F(m; y) + \varepsilon, \]

where \( d \) is a vector of observed data, \( m \) is a vector of the model to be recovered, \( F \) is an observation operator (aka the forward operator), \( y \) is a vector (or matrix) of experimental design parameters, and \( \varepsilon \) is a random noise vector. The design parameters \( y \) determine the experimental configuration. In the context of tomography these may define, for example, source and receiver positions, source frequencies or amplitudes. In other contexts such parameters may be ambient temperature, pressure, or any other controllable experimental setting. We assume that the problem is ill-posed in the usual sense (e.g., Hansen (1998)). In particular, there is no unique stable solution for the problem of finding \( m \) such that \( F(m; y) = d \). Regularization techniques are used for finding stable and meaningful solution of such ill-posed problems. We consider a generalized Tikhonov regularization approach where the solution \( \hat{m} \) is recovered by an optimization problem of the form

\[ \hat{m} = \arg\min_m \left\{ \frac{1}{2} \| F(m; y) - d \|^2 + R(m) \right\}, \]

with \( R \) being a regularization functional utilized for the incorporation of a-priori information.

Most efforts in the field of inverse problems have been primarily devoted to the development of either numerical methods (Biros & Ghattas 2005; Haber & Ascher 2001; Vogel 2001) for the solution of the optimization problem (2), or methods for prescribing regularization functionals and selecting their regularization parameters (Claerbout & and Muir 1973; Wahba et al. 1979; Hanke & Hansen 1993; Hansen 1998; Rudin 1992; Tikhonov & Arsenin 1977). Little work has addressed the selection strategy of the experimental settings \( y \) even though a proper design inherently offers improved information extraction and bias control. Figure 1 demonstrates the importance of experimental design in impedance tomography. The images display three recovered models; each corresponds to a particular experimental design setting, but are conducted over the very same true model. If these models were acquired for presurgical assessment of brain tumor removal, for instance, the neurosurgeon would be faced with the serious problem of deciding which region to operate.

While optimal experimental design for well-posed (over-determined) problems is well established (Pukelsheim 2006), the authors are aware of very few publications (e.g., Bardow (2008); Curtis (1999); Haber et al. (2008)) that address ill-posed (under-determined) problems and of even fewer that consider nonlinear problems. Still, many practical problems in biomedical imaging, geophysics, engineering as well as other physical sciences are intrinsically ill-posed and nonlinear.

In this paper we propose a formulation for optimal experimental design of ill-posed, nonlinear inverse problems and demonstrate its application to impedance
tomography. The rest of the paper is organized as follows: In Section 0.2 we introduce the basic impedance tomography problem. In Section 0.3 we briefly review different optimal experimental design formulations for linear ill-posed problems and describe the shortcomings of these approaches in overcoming the unique difficulties that arise in nonlinear ill-posed problems. In Section 0.4 we provide the rationale for our proposed formulation that is based on statistical considerations. In Section 0.5 we describe the mathematical formulation of the suggested approach and explain the optimization framework developed for its solution. Section 0.6 provides numerical results for a realistic impedance tomography model problem. In Section 0.7 we discuss the numerical results as well as various technical matters related to the implementation of such formulation. We close with some comments regarding future research.

**0.2 Impedance Tomography**

The inverse impedance tomography problem aims at the recovery of an impedance distribution in a domain given a set of boundary potential measurements for a known configuration of sources and receivers (Holder 2005). Acquisition is based on injection of low frequency currents from multiple sources while boundary potentials are recorded by a set of receivers. Typically, the sources and receivers are both deployed over the boundary of the domain. In the context of the estimate defined by (2), the model \( m \) stands for the conductivity (or admittivity) distribution in the domain and the data vector \( d \) corresponds to the electric potentials measured on the boundary.

The observation (forward) model under consideration is derived from Maxwell’s equations in the low frequency domain. Under these considerations these entail the
partial differential equation
\[
\nabla \cdot (m \nabla u) = 0 \quad u \in \Omega \\
\n
m \nabla u = Q \quad u \in \partial \Omega,
\]
where the model \(m\) is the conductivity, \(u\) the electric potential and \(Q\) are the sources.

Standard finite volume or finite element discretization (Ascher 2008; Vauhkonen et al. 1999; Vavasis 1996) leads to the construction of a discrete linear system. This system is solved for \(u\) given the conductivity model \(m\):
\[
A(m)u = D^\top M(m)D = PQQ,
\]
where \(D\) is a sparse matrix holding the gradients of the basis functions (shape gradients) and \(M(m)\) is a diagonal matrix that holds the conductivity values multiplied by the support (volumes) of the elements.

The forward model can be written as
\[
F(m, V, Q) = V^\top P_V^\top A(m)^{-1} P_Q Q,
\]
where the matrices \(P_Q\) and \(P_V\) map the source and measurement distributions onto the model grid.

In the context of the specific given forward model, another important physical restriction is current conservation. We assume that there is no dissipation of energy through the medium, and therefore the total amount of current driven in is equal to the total amount of current drained out. This constraint implies that \(e^\top Q = 0\), where \(e\) is a vector of ones.

### 0.3 Optimal Experimental Design - Background

We briefly review the basic framework of OED in the context of discrete linear well-posed inverse problems where \(F(m; y) = K(y)m\).

#### 0.3.1 Optimal Experimental Design for Well-Posed Linear Problems

The data are modeled as
\[
d = K(y)m + \varepsilon,
\]
where \(K(y)\) is an \(\ell \times k\) matrix representation of the forward operator that acts on the model \(m\) and depends on a vector of experimental parameters \(y\). The noise vector \(\varepsilon\) is assumed to be zero mean with independent entries of known variance \(\sigma^2\). The objective of experimental design is the selection of \(y\) that leads to an optimal estimate of \(m\).

In the well-posed case, the matrix \(K(y)^\top K(y)\) is nonsingular and for fixed \(y\) the least squares (LS) estimate \(\hat{m} = (K^\top K)^{-1}K^\top d\) is unbiased with covariance
matrix $\sigma^2 C(y)^{-1}$, where $C(y) = K(y)\top K(y)$. One can then choose $y$ so as to obtain a good LS estimate of $m$. Since $\hat{m}$ is unbiased, it is common to assess its performance using different characteristics of its covariance matrix. For example, an $A$-optimal type experiment design prescribes a choice of $y$ that minimizes the trace of $C(y)^{-1}$. If instead of the trace, the determinant or the $\ell_2$-norm of $C(y)^{-1}$ is used, then the design is known as $D$- or $E$-optimal, respectively (see Pukelsheim (2006) and references therein). Unsurprisingly, each optimality criterion corresponds to a different statistical interpretation: the $A$-optimal criterion minimizes the average variance, the $D$-optimality relates to the volume of an uncertainty ellipsoid (confidence region) (Beck & Arnold 1977), and the $E$-optimality criterion corresponds to a minimax approach. Other than the aforementioned optimality criteria, almost a complete alphabet of criteria can be found in the literature.

0.3.2 Optimal Experimental Design for Linear Ill-Posed Problems

Designs that are solely based on the covariance matrix are unsuitable for ill-posed problems where estimators of $m$ are most likely biased. In fact, the bias may be the dominant component of the error.

Assume now that $K(y)^\top K(y)$ is singular or ill-conditioned. A regularized estimate of $m$ can be obtained using penalized LS (Tikhonov regularization) with a smoothing penalty matrix $L$

$$
\hat{m} = \arg\min \frac{1}{2} (K(y)m - d)^\top (K(y)m - d) + \frac{a}{2} \| Lm \|^2,
$$

where $a > 0$ is a fixed regularization parameter that controls the balance between the data misfit and the smoothness penalty. Assuming that $K(y)^\top K(y) + aL^\top L$ is nonsingular, the estimator is

$$
\hat{m} = (K(y)^\top K(y) + aL^\top L)^{-1} K(y)^\top d, \quad (7)
$$

whose bias can be written as

$$
\text{Bias}(\hat{m}) = E\hat{m} - m = -a (K(y)^\top K(y) + aL^\top L)^{-1} L^\top Lm. \quad (8)
$$

Since the bias is independent of the noise level, it cannot be reduced by averaging repeated observations. The noise level affects the variability of $\hat{m}$ around its mean $E\hat{m}$. Thus, this variability and the bias ought to be taken into account when choosing an estimator of $m$.

Define $B(y,m) := \| \text{Bias}(\hat{m}) \|^2$ and $V(y) = E \| \hat{m} - E\hat{m} \|^2 / \sigma^2$. The sum of these two error terms provides an overall measure of the expected performance of $\hat{m}$. This is essentially the mean squared error (MSE) of $\hat{m}$. More precisely, the MSE of $\hat{m}$ is defined as $E \| m - \hat{m} \|^2$, which can also be written as

$$
\text{MSE}(\hat{m}) = E \| \hat{m} - E\hat{m} + E\hat{m} - m \|^2 = E \| m - \hat{m} \|^2 + E \| \hat{m} - E\hat{m} \|^2 = \| \text{Bias}(\hat{m}) \|^2 + E \| \hat{m} - E\hat{m} \|^2 = a^2 B(y,m) + \sigma^2 V(y). \quad (9)
$$
The overall idea is then to define optimization problems so as to control a measure of the performance of $\hat{m}$ that takes into account its bias and stochastic variability. A natural choice would be the MSE, nevertheless, this measure depends on the unknown $m$ itself. However, in many practical applications it is possible to obtain examples of plausible models. For example, there are geostatistical methods to generate realizations of a given media from a single image (Journel & Kyriakidis 2004; Sarma et al. 2007). Also, in many applications, and in particular in medical imaging, it is possible to obtain a set of likely example models $\mathcal{M} = \{m_1, ..., m_s\}$. In medical imaging such models can be proposed based on prognosis studies. These studies provide useful statistics of common pathologies and their classes, and therefore can be used for the construction of models associated with likely pathologies. Basically, this set of example models enables one to implicitly define regions of interest and similarly regions of lack of interest; either of which provides valuable guidance for the experimental setup. For some applications, the designer may even feel comfortable assigning a prior distribution to the models. This would be a natural approach in the context of experimental design as it is performed prior to data collection.

Let $\mathcal{M} = \{m_1, ..., m_s\}$ be examples of plausible models which will be henceforth called training models. As with Bayesian optimal designs (Chaloner & Verdinelli 1995), these models are assumed to be iid samples from an unknown multivariate distribution $\pi$. We use the following sample average of the MSE

$$\hat{R}(y) = \alpha^2 \hat{E}_\pi B(y, m) + \sigma^2 V(y).$$

(10)

where

$$\hat{E}_\pi B(y, m) = \frac{1}{s} \sum_{i=1}^{s} B(y, m_i).$$

(11)

$\hat{R}(y)$ is an unbiased estimator of the Bayes risk $E_{\pi} \text{MSE}(\hat{m})$. This type of empirical approach is commonly used in machine learning, where estimators are trained using iid samples.

### 0.4 Optimal Experimental Design for Nonlinear Ill-Posed Problems

Nonlinear problems are inherently more difficult. For example, there is no closed form solution of the Tikhonov estimate $\hat{m}$ and its MSE cannot be easily separated into bias and variance components $B$ and $V$; linearity allowed us to find closed expressions for the expected value over the noise distribution. This time we estimate such expected value in two stages. First, we generate a noise sample $\varepsilon_j$ that is added to $F(m_i; y)$; second, we solve the inverse problem and obtain an estimate $\hat{m}_{i,j}$, which is then compared to $m_i$. We repeat this procedure for multiple noise realizations and for each training model. This sequence defines an empirical estimate of
\[
\hat{R}(y) = \sum_{i=1}^{n} \sum_{j=1}^{s} \| \hat{m}_{i,j}(y) - m_{i} \|^2. 
\] (12)

Since the design problem may still be under-determined, the design parameter \( y \) might oscillate wildly and may generate designs that overfit the training set. It is therefore important to introduce additional constraints or preferences related to the design parameters.

Numerous desirable properties may be considered for favoring one design over another. Depending on the application, some reasonable and popular preferences may be: to shorten acquisition time, to reduce the number of sources/receivers or to achieve higher resolution and promote spatial selectiveness. All these preferences pursue, of course, the final objective of finding the best model estimate given the available resources.

For most geophysical problems as well as medical applications, control over the number of sources and/or receivers is desirable. Let \( Q \) and \( V \) be, respectively, the vectors of sources and receivers and set \( y = \{Q, V\} \). A sparsity preference for the number of active sources and receivers can be formulated by the addition of an \( \ell_1 \)-norm penalty to the empirical risk

\[
\hat{R}_1(y; M, \hat{m}) = \frac{1}{2ns} \sum_{i=1}^{n} \sum_{j=1}^{s} \| \hat{m}_{i,j}(y) - m_{i} \|^2 + \beta \| y \|_1. 
\] (13)

The idea of sparsifying by \( \ell_1 \) penalty in optimal-control is analyzed in Stadler (2006). The design problem dictates the minimization of this regularized empirical risk while retaining the conventional inverse problem (2) and forward model feasible. This requirement can be formulated as a bi-level optimization problem (Alexandrov 1994; Bard 2006; Colson et al. 2007; Dempe & Gadhi 2007) that reads as follows

\[
\min_y \quad \frac{1}{2ns} \sum_{i=1}^{n} \sum_{j=1}^{s} \| \hat{m}_{i,j}(y) - m_{i} \|^2 + \beta \| y \|_1 
\text{s.t.} \quad \hat{m}_{i,j} = \arg\min_m \frac{1}{2} \| F(m; y) - d_{i,j}(m_{i}; y) \|^2 + R(m), 
\] (14)

where \( d_{i,j}(m_{i}; y) = F(m_{i}; y) + \varepsilon_j \). With a slight abuse of notation, we shall henceforth denote \( R_1 \) by \( R \), and write

\[
\psi(m; m_{i}, y) = \frac{1}{2} \| F(m; y) - d_{i,j}(m_{i}; y) \|^2 + R(m).
\]

Before we proceed with discussing an appropriate optimization framework for the solution of the above problem, we would like to make an important distinction. Beyond the fundamental difference between linear and nonlinear inversion that distinguishes this work from our previous work (Haber et al. 2008), another important difference is related to the design mechanism itself. In the previous work, the aim
was finding the best subset out of a given set of excitation and measurement vectors, while here their number is predefined, while their content is controlled by inducing sparsity. The current mechanism typically requires larger number of parameters, which, on the one hand offers greater solution flexibility and optimality but on the other hand, introduces higher computational demands.

In principle, it is also possible to employ Bayesian OED (Chaloner & Verdinelli 1995) for handling nonlinear OED problems of this sort. However, given the complexity of the nonlinear problem, one will most likely end up sampling models from the prior and follow the approach we propose here.

0.5 Optimization Framework

0.5.1 General Scheme

General bi-level optimization problems are difficult because the inner optimization problem may have multiple solutions and/or may be non-convex. Here, we make the assumption that the inner level is convex (or at least convex over the set of \( y \)'s of interest). This leads to simpler algorithms (Alexandrov 1994). Thus, we replace the inner optimization problem by the necessary conditions for a minimum solving

\[
\begin{align*}
\min_{y, m=(m_{i,j})} \quad & R(y; \mathcal{M}) = \frac{1}{2n} \sum_{i=1}^{s} \sum_{j=1}^{n} ||m_{i,j} - m_i||^2 + \beta ||y||_1 \quad (16) \\
\text{s.t.} \quad & c_{i,j}(m_{i,j}, y) := \frac{\partial \psi_{i,j}(m; m_i, y)}{\partial m_{i,j}} = 0. \quad (17)
\end{align*}
\]

The necessary conditions for a minimum are (Ito & Kunisch 2008)

\[
\begin{align*}
R_{m_{i,j}} + (c_{i,j})^\top_{m_{i,j}} \lambda_{i,j} &= 0 \quad (18a) \\
R_y + \sum_{i,j} (c_{i,j})^\top_y \lambda_{i,j} &= 0 \quad (18b) \\
c_{i,j}(m_{i,j}, y) &= 0, \quad (18c)
\end{align*}
\]

where \( \lambda_{i,j} \) are Lagrange multipliers. Although it is possible to develop an efficient method to solve the system for \( m_{i,j} \) and \( y \) simultaneously, we have chosen an unconstrained optimization approach. This approach is advantageous for two reasons: first, the infrastructure of the forward simulator can be reused to solve the adjoint equation and therefore major implementation issues associated with solution of the optimality conditions as one system are avoided. Second, since the storage of all \( m_{i,j} \)'s and \( \lambda_{i,j} \)'s is not required, the complete optimization procedure can be executed by solving each inverse problem separately. More precisely, we first solve the \( s \times n \) decoupled nonlinear systems (18c) for \( m_{i,j} \) given \( y \), then we solve the other \( s \times n \) decoupled linear systems (18a) for \( \lambda_{i,j} \). For each \( m_{i,j} \) and \( \lambda_{i,j} \) computed, the
reduced gradient (18b) is updated. Thus, even when the number of training models and noise realizations is excessively large, such a design process can be conducted over modest computational architectures.

In order to avoid the non-differentiability nature of the $\ell_1$-norm at zero, we use the Iterated Re-weighted Least Squares (IRLS) approximation (O’Leary 1990; Street et al. 1988). This approach has been successfully used for $\ell_1$ inversion in many practical scenarios (Sacchi & Ulrych 1995; Vogel 2001; Whittall & Oldenburg 1992). In the IRLS approximation, the $\ell_1$-norm is replaced by a smoothed version $\|x\|_{1,\epsilon}$ of the absolute value function defined as:

$$|t|_\epsilon := \sqrt{t^2 + \epsilon} \quad \text{and} \quad \|x\|_{1,\epsilon} := \sum_i |x_i|_\epsilon.$$  

As discussed in Haber et al. (2000), obtaining the sensitivities of $m_{i,j}$ with respect to $y$ is straightforward; they can be written as

$$J = -\sum_{i,j} (c_{i,j})^{-1} (c_{i,j})_y.$$  

The sensitivities are then used with IRLS (O’Leary 1990) to obtain an approximation of the Hessian

$$H = J^T J + \beta \text{diag}\left(\min(\|y\|^{-1}, \epsilon^{-1})\right),$$

which in turn is used to define the update

$$y \leftarrow y - \tau H^{-1} g,$$  

where $\tau$ is a line search step size and $H^{-1} g$ is computed using the conjugate gradient method. Note that computation of the update step can be performed without the explicit construction of either the matrix $(c_{i,j})_{m_{i,j}}$ or its inverse. These matrices are only accessed implicitly via matrix vector products.

0.5.2 Application to Impedance Tomography

We now discuss a specific application of the design strategy to impedance tomography. As previously discussed, we consider an experimental design problem of placing and activating sources and receivers over a predefined region of permissible locations. Such region could be the entire boundary $\partial \Omega$ of a domain $\Omega$ as often occurs in medical imaging or, alternatively, any sub-domain $\Omega_r \subseteq \Omega$.

We consider the Tikhonov regularized estimate (2) with $F(m; y)$ representing the forward operator (5) and $R(m) = \alpha \|Lm\|^2$, with $L$ a discrete derivative operator that penalizes local impedance inhomogeneities.

At this point we comment on the choice of the regularization parameters $\alpha$ and $\beta$. The parameter $\alpha$ is chosen prior to the inversion process; we choose it so as to balance the expected misfit with the norm of $R(m)$. For iid Gaussian noise the expected value of $\|d - F(m; y)\|^2$ is $\ell \sigma^2$. Choosing $\alpha \approx \ell \sigma^2 / R(m)$ yields reasonable model reconstructions. The choice of $\beta$ is user-dependant. The designer may
tune this parameter according to some sparsity preferences. The higher the sparsity of the active sources and receivers, the larger the value of $\beta$. Conversely better model recovery can be achieved with lower levels of $\beta$ at the expense of lower sparsity. Further discussion regarding the choice of $\beta$ for OED of linear problems can be found in Haber et al. (2008).

For our impedance tomography design problem, the optimality criterion prescribes the construction of an experimental design that minimizes the number of active sources and receivers, as well as minimizing the description error between the recovered and given training models. This configuration must comply with a feasible forward model and an inverse solution, and should be consistent with the acquisition noise level. Such design can be obtained with a sparsity requirement imposed over the source and measurement vectors in the form of $\ell_1$-norm penalty. Thus, we set $y := \{V, Q\}$ and accordingly denote the forward operator by $F(m; V, Q)$. We assume that a collection of feasible, representing models $\mathcal{M} = \{m_1, \ldots, m_s\}$ is at our disposal, for which we can compute a measurement set using the forward model $F(m; V, Q)$.

The design problem given in (14) - (15) can be formulated as follows

$$\min_{V, Q} \mathcal{R}(V, Q; \mathcal{M}, \hat{m}) \quad (20a)$$
$$\text{s.t. } \hat{m} = \arg\min_m \psi(m; V, Q), \quad (20b)$$

where the objective function (i.e., the regularized empirical risk $\mathcal{R}$) and the linearized constraints $c$, as in (16) and (17) respectively, are given by

$$\mathcal{R}(V, Q; \mathcal{M}, m) = \frac{1}{2} \sum_{i,j}^s \sum_{n} \|m_{i,j} - m_i\|^2 + \beta_1 \|V\|_1 + \beta_2 \|Q\|_1$$

$$c_{i,j}(m_{i,j}; V, Q) = S_{i,j}^T V^T P_V \left( (A(m_{i,j})^{-1} - A(m_i)^{-1}) P_Q Q - \epsilon_j \right) + \alpha L^T L m_{i,j},$$

where $S_{i,j}$ is the sensitivity matrix, that is the Fréchet derivative of the forward operator. This operator represents the sensitivity of the acquired data to small changes in the model $S_{i,j} := \partial d_{i,j}/\partial m$. For this formulation, $S_{i,j}$ can be derived by implicit differentiation using the relation (5) (Haber et al. 2000).

In order to solve (16) - (17), we shall now evaluate the remaining components of (18a) - (18b). Since the empirical risk is convex on $m_{i,j}$, we have $R_{m_{i,j}} = m_{i,j} - m_i$. The derivatives of the risk with respect to the design parameters $P$ and $Q$ are obtained using the IRLS relation given in (0.5.1)

$$R_V = \beta_1 \text{diag} \left( \frac{1}{\|V\|_{1, \epsilon}} \right) V, \quad R_Q = \beta_2 \text{diag} \left( \frac{1}{\|Q\|_{1, \epsilon}} \right) Q.$$

The derivative of the linearized constraint $c_{i,j}$ with respect to the model $m_{i,j}$ is in fact the conventional Hessian of the inverse problem (2)

$$(c_{i,j})_{m_{i,j}} = S_{i,j}^T S_{i,j} + \alpha L^T L + M_{i,j},$$
where \( M_{i,j} \) stands for the second order derivatives that can be computed implicitly (Haber et al. 2000). The derivatives \((c_{i,j})_V\) and \((c_{i,j})_Q\) can be calculated from the structures of \( S_{i,j} \) and \( M_{i,j} \). The reduced space gradients \( g(V) \) and \( g(Q) \) are obtained using the relations

\[
g(V) = R_V + \sum_{i,j}^{n,n} (c_{i,j})_V^\top (c_{i,j})_V^{m_{i,j}} R_{m_{i,j}}
\]

\[
g(Q) = R_Q + \sum_{i,j}^{n,n} (c_{i,j})_Q^\top (c_{i,j})_Q^{m_{i,j}} R_{m_{i,j}}.
\]

Next, the reduced Hessians \( H_V \) and \( H_Q \) can be derived as in (0.5.1) and, similarly, the updates for \( V \) and \( Q \) at each iteration of the reduced space IRLS as in (19).

**Remark.** We have used a conventional reparametrization of the model space in order to comply with the broad dynamic range requirement and therefore set \( m := \log(\gamma) \), where \( \gamma \) is the conductivity.

### 0.6 Numerical Results

We now show results of applying the optimal experimental design framework described in Section 0.5.2 to a realistic design problem of placing and activating sources and receivers for impedance imaging of a human head.

The setup involves two stages. In the first stage the source and receiver vectors are optimized to comply with the sparsity requirement using a set of given training models. In the second stage, several unseen (test) models are used to assess the performance of the obtained design.

For training purposes, three example models of impedance perturbations in the mid, left and right parietal brain lobe (marked in red on the head diagrams in Figure 4) are considered. The design problem consists of 16 receiver vectors \( V \) and 16 source vectors \( Q \) that were initialized at random.

Figure 2 shows the behavior of the empirical risk and MSE as a function of iteration number. The regularized empirical risk is reduced by an order of magnitude in the first six iterations, while the MSE itself was reduced by a factor of about two. On the 6th iteration the MSE starts to increase. At this point the tradeoff between sparsity and reconstruction accuracy begins to be evident. We stopped the optimization process when the relative change in the risk dropped below 1%.

Figure 3 shows the ensemble of source \( Q \) and measurement vectors \( V \) for the initial and optimized designs. The figure shows that the optimized vectors are clearly sparser than those obtained with the initial design. Another way to visualize the difference in the designs is shown in Figure 4, where 4 out of the 16 source vectors are plotted as colored circles at the active source locations. Again, it can be clearly observed that the optimized design requires the deployment of a smaller number of active sources, and thereby complies with our original intent.
Figure 2  Experimental design of 16 receiver and 16 source vectors for three models. Left: Empirical risk convergence; Right: MSE convergence.

Figure 3  Sparsity pattern of 16 receiver vectors $V$ (above) and 16 source vectors $Q$ (below) for three training models. Left: Initial experimental design. Right: Optimized design after six iterations.
While the first three figures illustrate the performance of the design procedure at the learning stage, the performance of the obtained design for an unseen (testing) model is shown in Figure 5. It presents a comparison between a 3D impedance tomography model that was recovered using the initial and optimal designs. The impedance intensities of the perturbations recovered with the optimized design are distinctly better than those obtained with the initial design. The quantitative results for models obtained with the optimized design indicate that the recovered models were almost identical to the true model. Moreover, while models recovered using the initial design were cluttered with artifacts, models recovered with the optimized design show higher qualitative structural similarity with the true models.

Figure 4  Human-head-shaped training models from a transversal projection. The red objects inside the head represent impedance perturbations as provided by the training example models. The colored dots located on vertices of the head mesh represent dominant locations for positioning sources (Only 4 out of the 16 vectors (colors) were presented here to avoid over-cluttering). Left: Initial design. Right: Optimized design.

0.7 Discussion and Conclusions

We have presented a statistical formulation for optimal experimental design of non-linear ill-posed problems. Such problems frequently arise in medical imaging and geophysics, but also in many other fields such as chemistry and aerospace engineering. For each of the different applications, the construction of an effective design procedure requires careful thought. Nevertheless, the rationale presented in this study is generic and therefore transferable to a broad range of important applications.

The numerical results have shown that the proposed optimal experimental design can provide substantial improvement in image quality, on both the quantitative and qualitative levels. But there are several outstanding issues that still need to be addressed.
The first of which is the choice of regularized empirical risk measure. This choice is crucial for obtaining an effective design. We have used an $\ell_2$-norm discrepancy between training and recovered models for the empirical risk measure, and an $\ell_1$-norm penalty on $y$ to promote sparsity. These choices may seem natural for the impedance design problem considered here but in general this choice will depend on the specific application.

Obviously, the choice of regularized estimate of the inverse problem is also important. We have chosen Tikhonov regularization with an $\ell_2$ data misfit and smoothness penalty to promote smooth model estimates. Such smoothness may not be appropriate in some applications. In the numerical examples above, all model examples comprised sharp parameter changes, which may have impaired, to some extent, the overall performance of the design procedure.

One defining feature of the proposed formalism is that the choice of inversion method is embedded in the design problem. Thus, different inversion frameworks will inherently result in different designs. The fact that the design reflects the inversion settings may be regarded as a hindrance, as one may expect the design to be solely related to the physical properties of the problem. Yet, in reality the choice of an inversion framework is mandatory. Moreover, since each inversion framework introduces distinctive a-priori information and individual degrees of belief one has attributed to the solution, the incorporation of such knowledge (if justified) into the design is essential.

Another fundamental issue is the source of training models. We have deliberately avoided a discussion about the retrieval of proper training examples as it is very much problem dependent issue. It was assumed that these were provided by a trusted source and as such were representative of the type of model to be recovered.

In addition to the source of models, their number is an important variable that determines how well the empirical risk approximates the true risk. A careful study of this question will require empirical process theory as in Vapnik (1995) and Rakhlin
Since several nonlinear inversion procedures are required at each design iteration, the design process is time consuming. Apart from the explicit construction of the forward model discretization matrix, the implementation of a bi-level optimization framework in this study relied on implicit calculation of matrices and parallel processing of the inversions of independent example models. This implementation enabled the processing of large-scale models despite memory limitations. Nevertheless, the overall design process is still computationally intensive and time consuming. For several applications, such as geophysical surveys, offline processing time of several hours or even a few days prior to a survey is certainly acceptable but, for some medical applications, development of faster design procedures may be essential.

Another issue that needs to be addressed is sensitivity analysis. A better insight into the interplay between the design requirement and the sensitivity gain/loss can be obtained by observing changes in the sensitivity map that evolves throughout the design process. Such analysis can illustrate and explain how sensitivity and independence of measurable information originating in regions of interest (i.e., where perturbations are expected) form higher local sensitivity compared with irrelevant areas.

The practical aim of this work is mainly to help improve current designs and, therefore, whenever the designer is able to provide a good initial design, the formulation provided here will yield an improved experimental design. In many practical settings improvement over a design at hand may suffice and, therefore, an exhaustive solution of the design problem may not be needed.

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