

# ADAPTIVE A-OPTIMAL EXPERIMENTAL DESIGN FOR DYNAMIC TARGETS

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**Abstract.** The optimal collection of data required to infer the dynamic model parameters which govern a partial differential equation(PDE) through the inversion process is important to many applications. One method of optimally collecting data is to control the number of measurements required for a given experiment. Popular methods of optimal data collection, or optimal experimental design, minimize the mean square error (mse) of the estimated model parameters to determine an optimal experimental design. However, these methods do not include any historic data collected at early times.

To optimally design future experiments we reformulate the model estimation inverse problem to include both the dynamic PDE and historic data. We present two formulations, one which does not consider error in the dynamic PDE and a second formulation which does include this error. We then define adaptive optimal design, which minimizes the adaptive mean square error (amse) of the estimated model. The amse is defined such that historic model estimates are included through a monitor function. In this way, minimizing the amse in the design optimization problem results in designs where historic data and the dynamics contribute to the design of the future experiment.

We demonstrate our method for a two dimensional target whose motion is governed by a tracer advection model, and whose imaging with seismic borehole tomography experiment is used to image the motion of the target.

**1. Introduction.** While there exists a vast area of research and development in optimal experimental design for well posed inverse problems with static targets, there is little in the way of optimal design algorithms for ill-posed inverse problems with dynamic targets. Although static methods can be applied to time dependent PDE's [?], this approach results in an 'all at once' recovery of experimental designs which are dependent only on prior information provided in the form of a regularization to the ill posed problem. In reality, after an experiment is conducted the available data contain valuable information about the current target. This information should thus be included in the design algorithm for the future target. In this paper we present an adaptive method to determine a future optimal experimental design for a dynamic target given historic data.

There are several considerations to be made when developing an optimal experimental design method. One such item is what exactly is meant by an 'optimal experiment'. In our context we refer to the problem of determining the optimal placement of sensors to infer model parameters through the inversion of data. Although there are several design criteria for such inverse problems, standard references for optimal experimental designs include [?], we focus on A-optimal design in our work [?].

The A-optimal design method minimizes the mean squared error (mse) of the posterior model estimator, or the trace of the posterior covariance matrix (from the Bayesian perspective), associated with the posterior probability law for the parameter field solution to a governing linear partial differential equation. Here our work builds on A-optimal design algorithms presented in [?] for large-scale ill-posed inverse problems, and on work presented in [?] where both a static imaging PDE and the dynamic PDE describing the motion of a target were combined such that the dynamic model parameters could be inferred from imaging data.

One major challenge when combining PDEs to formulate an inverse problem is how to deal with the error. One approach, as in [?] is to group or ignore the error in the dynamic PDE and formulate the problem as a PDE constrained optimization problem. A second approach is to consider a formulation where the error in the dynamics are accounted for [?, ?]. We will address both cases in this work. However, in either case the mse of the inferred model parameters does not depend on historic data, only on a priori information. To incorporate historic data into the A-optimal design algorithm we will instead compute a post priori design, where we define the adapted means square error (amse) by introducing a monitor function dependent on historic estimates of the target.

The paper is outlined as follows. In section 2 we derive from first principals the mse of a linear estimator, then present the adapted mse and define its monitor functions. In section 3 we briefly outline the two methods for combining two different PDEs governing the imaging technique and the dynamic motion, and present the adaptive design algorithms. In section 4 we present the numerical optimization method for solving the design problem, and finally in section ?? we present numerical examples demonstrating the adaptive A-optimal design method.

**2. Adaptive experimental design .** In this section we discuss A-optimal design from first principals and present the adaptive A-optimal design method.

Consider the case where we have a time dependent measurement of the form

$$\mathbf{F}_1 \mathbf{m} + \boldsymbol{\epsilon} = \mathbf{d}_1 \quad \text{and} \quad \mathbf{F}_2 \mathbf{m} + \boldsymbol{\epsilon} = \mathbf{d}_2 \quad (2.1)$$

where  $\mathbf{F}_1$  is the forward operator at time  $t_1$  and  $\mathbf{F}_2$  is the forward operator at time  $t_2$ . Our goal is to design the experiments at times  $t_1$  and  $t_2$  such that we obtain the “best” recovery by some criteria.

Two different designs can be considered. First, it is possible to perform *a priori* design, that is, to design the experiments  $\mathbf{F}_1$  and  $\mathbf{F}_2$  prior to the data collection. This is the case when the time between  $t_1$  and  $t_2$  is much shorter than the time for the processing of the data. A second approach is to use *post priori* design. The idea here is to use the results obtained from the first experiment in order to design a “better” second experiment. The idea of a-priori versus post-priori estimators is not new. For example, when numerically solving partial differential equations one often uses a-priori estimates in order to solve the problem on one mesh and then refines the mesh in order to obtain a more accurate solution.

In a similar spirit, our goal is to first obtain an a-priori design for the first experiment and then, after the data is collected and processed, use the estimator obtained at  $t_1$  in order to design the data collection at time  $t_2$ .

Before we discuss the design of the data acquisition for time  $t_2$  we review the a priori design of the experiment at time  $t_1$ . Our approach is based on the A-optimal design criteria, which is now derived from first principles.

Consider the estimation of  $\mathbf{m}$  given  $\mathbf{d}_1$ , which is done by solving the ill-posed optimization problem

$$\frac{1}{2} \|\mathbf{F}_1 \mathbf{m} - \mathbf{d}_1\|_{\mathbf{W}_1}^2 + \frac{\alpha}{2} \|\mathbf{L}(\mathbf{m} - \hat{\mathbf{m}}_0)\|^2. \quad (2.2)$$

where  $\mathbf{W}_1 = \text{diag}(\mathbf{w}_1)$  is a matrix of inverse standard deviations, that is, the inverse covariance of the noise. Minimizing the optimization problem yields the estimator

$$\hat{\mathbf{m}}_1 = (\mathbf{F}_1^\top \mathbf{W}_1 \mathbf{F}_1 + \alpha \mathbf{L}^\top \mathbf{L})^{-1} (\mathbf{F}_1^\top \mathbf{W}_1 \mathbf{d}_1 + \alpha \mathbf{L}^\top \mathbf{L} \hat{\mathbf{m}}_0). \quad (2.3)$$

Defining the matrix  $\mathbf{C} = (\mathbf{F}_1^\top \mathbf{W}_1 \mathbf{F}_1 + \alpha \mathbf{L}^\top \mathbf{L})$ , and recalling that  $\mathbf{F}_1 \mathbf{m} + \boldsymbol{\epsilon} = \mathbf{d}_1$  we can write the error in the recovery as

$$\hat{\mathbf{m}}_1 - \mathbf{m} = \mathbf{C}^{-1} \mathbf{F}_1^\top \mathbf{W}_1 \mathbf{F}_1 \mathbf{m} + \mathbf{C}^{-1} \mathbf{F}_1^\top \mathbf{W}_1 \boldsymbol{\epsilon} + \alpha \mathbf{C}^{-1} \mathbf{L}^\top \mathbf{L} \hat{\mathbf{m}}_0 \quad (2.4)$$

$$+ (\alpha \mathbf{C}^{-1} \mathbf{L}^\top \mathbf{L} \mathbf{m} - \alpha \mathbf{C}^{-1} \mathbf{L}^\top \mathbf{L} \mathbf{m}) - \mathbf{m}. \quad (2.5)$$

Collecting terms and using the definition of  $\mathbf{C}$  we obtain

$$\hat{\mathbf{m}}_1 - \mathbf{m} = \mathbf{C}^{-1} \mathbf{F}_1^\top \mathbf{W}_1 \boldsymbol{\epsilon} + \alpha \mathbf{C}^{-1} \mathbf{L}^\top \mathbf{L} (\hat{\mathbf{m}}_0 - \mathbf{m}). \quad (2.6)$$

Squaring and taking the expectation over  $\boldsymbol{\epsilon}$  and recalling that  $\boldsymbol{\epsilon} \sim N(\mathbf{0}, \text{cov}(\boldsymbol{\epsilon}) = \mathbf{W}_1^{-1})$ , we obtain that the mean square error is

$$\text{mse}(\mathbf{w}, \mathbf{m}) = \mathbf{E} \|\hat{\mathbf{m}}_1 - \mathbf{m}\|^2 = \text{trace}(\mathbf{F}_1 \mathbf{C}^{-2} \mathbf{F}_1^\top \mathbf{W}_1) + \alpha^2 \mathbf{E} \|\mathbf{C}^{-1} \mathbf{L}^\top \mathbf{L} (\hat{\mathbf{m}}_0 - \mathbf{m})\|^2. \quad (2.7)$$

If we assume that  $\mathbf{m} - \mathbf{m}_0$  is Gaussian with a zero mean and a covariance  $(\alpha \mathbf{L}^\top \mathbf{L})^{-1}$  then we obtain that

$$\phi(\mathbf{w}_1) = \text{mse}(\mathbf{w}_1) = \text{trace}(\mathbf{C}^{-2} \mathbf{F}_1^\top \mathbf{W}_1 \mathbf{F}_1) + \alpha \text{trace}(\mathbf{C}^{-2} \mathbf{L}^\top \mathbf{L}). \quad (2.8)$$

Finally, using the linearity of the trace and the definition of  $\mathbf{C}$  we obtain that

$$\phi_1(\mathbf{w}_1) = \text{trace} [(\mathbf{F}_1^\top \mathbf{W}_1 \mathbf{F}_1 + \alpha \mathbf{L}^\top \mathbf{L})^{-1}]. \quad (2.9)$$

In the design problem we seek to obtain a better estimate for  $\mathbf{m}$  and therefore we minimize  $\phi_1(\mathbf{w}_1)$  with an additional cost on  $\mathbf{w}_1$ , for example, in our previous work we proposed to minimize the function

$$\phi_1^\beta(\mathbf{w}_1) = \text{trace} [(\mathbf{F}_1^\top \mathbf{W}_1 \mathbf{F}_1 + \alpha \mathbf{L}^\top \mathbf{L})^{-1}] + \beta \sum \mathbf{w}_1 \quad 0 \leq \mathbf{w} \quad (2.10)$$

which balances the minimization of the least square error and the cost of the experiment [?].

Consider now using the design problem of estimating  $\mathbf{m}$  given the estimated model  $\hat{\mathbf{m}}_1$ . One could rewrite the recovery problem in a similar way, that is

$$\frac{1}{2}\|\mathbf{F}_1\mathbf{m} - \mathbf{d}_1\|_{\mathbf{W}_1}^2 + \frac{1}{2}\|\mathbf{F}_2\mathbf{m} - \mathbf{d}_2\|_{\mathbf{W}_2}^2 + \frac{\alpha}{2}\|\mathbf{L}(\mathbf{m} - \hat{\mathbf{m}}_0)\|^2. \quad (2.11)$$

which leads to the estimate

$$\hat{\mathbf{m}}_2(\mathbf{w}_2) = (\mathbf{F}_1^\top \mathbf{W}_1 \mathbf{F}_1 + \mathbf{F}_2^\top \mathbf{W}_2 \mathbf{F}_2 + \alpha \mathbf{L}^\top \mathbf{L})^{-1} (\mathbf{F}_1^\top \mathbf{W}_1 \mathbf{d}_1 + \mathbf{F}_2^\top \mathbf{W}_2 \mathbf{d}_2 + \alpha \mathbf{L}^\top \mathbf{L} \hat{\mathbf{m}}_0) \quad (2.12)$$

Note that we assume that  $\mathbf{w}_1$  is fixed and therefore the new estimate is a function of  $\mathbf{w}_2$  alone. If we repeat the steps above then we obtain that the A-optimal design for time  $t_2$  yields the minimization of the function

$$\phi_2(\mathbf{w}_2) = \text{trace} [(\mathbf{F}_1^\top \mathbf{W}_1 \mathbf{F}_1 + \mathbf{F}_2^\top \mathbf{W}_2 \mathbf{F}_2 + \alpha \mathbf{L}^\top \mathbf{L})^{-1}]. \quad (2.13)$$

While this design optimization problem can be solved, it does not take into consideration the fact that we already have an estimate of the model,  $\hat{\mathbf{m}}_1$  and therefore, does not include the information we have already obtained at time  $t_1$  in order to plan a better design. It is easy to verify that any linear estimator of the data yields a covariance matrix that is independent of  $\mathbf{d}_1$ , and therefore the approach above does not yield a post-priori estimator.

In order to use the information obtained at time  $t_1$  for the design of the experiment at time  $t_2$  we now present the concept of *adaptive dynamic design*.

Assume that the model,  $\hat{\mathbf{m}}_1$  has some “interesting” features and some “boring” features. For example, assume that the difference

$$\boldsymbol{\delta}_1 = \hat{\mathbf{m}}_1 - \hat{\mathbf{m}}_0 \quad (2.14)$$

is small in some norm over some region and large in others. The goal then is to better estimate the new features that appear in the model. It may also be the case that we wish to design for only  $\mathbf{m}_1$  itself. In this case

$$\boldsymbol{\delta}_k = \mathbf{m} \quad (2.15)$$

To this end, we introduce a **monitor function**,  $\boldsymbol{\tau}(\boldsymbol{\delta})$  that measures the change in the model. Examples for this function are

$$\boldsymbol{\tau}_s = \boldsymbol{\delta}_1 \odot \boldsymbol{\delta}_1 \quad (2.16a)$$

$$\boldsymbol{\tau}_N = \boldsymbol{\delta}_k > 0 == 1 \quad (2.16b)$$

but other functions can be used. The first monitor function,  $\boldsymbol{\tau}_s$ , simply measures the change in the estimator compared to the a-priori information in a 2-norm, while the second,  $\boldsymbol{\tau}_L$ , measures the change in the “natural” norm of the problem.

Given the monitor function, rather than minimizing the mean square error, we propose to minimize the adaptive mean square error, **amse** defined by

$$\text{amse}(\mathbf{w}, \mathbf{m}) = \|\hat{\mathbf{m}}_2 - \mathbf{m}\|_{\boldsymbol{\tau}_1}^2 = (\hat{\mathbf{m}}_2 - \mathbf{m})^\top \text{diag}(\boldsymbol{\tau}_1)(\hat{\mathbf{m}}_2 - \mathbf{m}). \quad (2.17)$$

The idea behind the **amse** is to obtain a tighter bound on the model where the estimator exhibits large changes compared to the known a-priori estimator.

Starting from (2.6), modifying it to deal with the **amse** and repeating the calculation above we obtain that the expectation over the **amse** is

$$\phi_2(\mathbf{w}_2) = \text{trace} (\text{diag}(\boldsymbol{\tau})(\mathbf{F}_1^\top \mathbf{W}_1 \mathbf{F}_1 + \mathbf{F}_2^\top \mathbf{W}_2 \mathbf{F}_2 + \alpha \mathbf{L}^\top \mathbf{L})^{-1}). \quad (2.18)$$

Similar to the non-adaptive case, the adaptive design is obtained by minimizing the (penalized) function  $\phi_2(\mathbf{w}_2)$ .

In general, the design for the  $k^{th}$  experiment given data collected for times  $t_1, ..t_{k-1}$  is

$$\phi_k(\mathbf{w}_k) = \text{tr} \left( \text{diag}(\boldsymbol{\tau}_{k-1}) \left( \sum_{j=1}^k \mathbf{F}_j^\top \mathbf{W}_j \mathbf{F}_j + \alpha \mathbf{L}^\top \mathbf{L} \right)^{-1} \right) \quad (2.19)$$

$$\boldsymbol{\tau}_{k-1}(\hat{\mathbf{m}}_{k-1} - \hat{\mathbf{m}}_{k-2}) \quad (2.20)$$

$$\hat{\mathbf{m}}_{k-1} = \text{argmin} \frac{1}{2} \sum_{j=1}^{k-1} \|\mathbf{F}_j \mathbf{m} - \mathbf{d}_j\|^2 + R(\mathbf{m}). \quad (2.21)$$

If the model  $\mathbf{m}$  is a dynamic target, then some consideration must be made as to how the dynamics are incorporated.

**3. Dynamic target.** In the previous section we presented a formulation for adaptive A-optimal experimental design that incorporates historic data, given a set of measurements. However, we did not distinguish between a static model  $\mathbf{m}$  or a model that is changing over time. To design for a moving target, we must address how the dynamics describing its motion are defined. Consider the discrete dynamic process and imaging described by the following set of linear equations

$$\mathbf{m}_k = \mathbf{T} \mathbf{m}_{k-1} + \boldsymbol{\eta}_k, \quad (3.1a)$$

$$\mathbf{d}_k = \mathbf{F} \mathbf{m}_k + \boldsymbol{\epsilon}_k, \quad (3.1b)$$

where the transport matrix  $\mathbf{T} : \mathbb{R}^N \rightarrow \mathbb{R}^N$  is a discretization of the PDE governing the dynamics in the system. The noise vectors  $\boldsymbol{\eta}$  and  $\boldsymbol{\epsilon}$  are assumed to be Gaussian normal,  $\boldsymbol{\eta} \sim N(\boldsymbol{\eta}_0, \mathbf{Q})$  and  $\boldsymbol{\epsilon} \sim N(\boldsymbol{\epsilon}_0, \mathbf{W}^{-1})$ .

In combining equations (3.1a) and (3.1b) there are two instances of the dynamics that result in different formulations, whether there is noise in the equations describing the motion or not. That is, is  $\boldsymbol{\eta}_k \stackrel{?}{=} \mathbf{0}$ ? We will present differing formulations for  $\boldsymbol{\eta} = \mathbf{0}$ , and  $\boldsymbol{\eta} \neq \mathbf{0}$  in the following sections.

**3.1. Noiseless model dynamics.** Setting  $\boldsymbol{\eta}_k = \mathbf{0}$ , allows us to write the model at time  $t_k$  as linear mapping of the initial model  $\mathbf{m}_0$ ,

$$\begin{aligned} \mathbf{m}_k &= \mathbf{T} \mathbf{m}_{k-1}, \quad \text{or} \\ \mathbf{m}_k &= \mathbf{T}^{k-1} \mathbf{m}_0. \end{aligned}$$

To this end the data for time step  $t_k$  can be written in terms of the initial model

$$\mathbf{d}_k = \mathbf{F}_k \mathbf{m}_0 + \boldsymbol{\epsilon}_k \quad (3.2)$$

where  $\mathbf{F}_k = \mathbf{F} \mathbf{T}^{k-1}$ , and the estimation of the initial model,  $\mathbf{m}_0$  given  $k$  data sets is

$$\hat{\mathbf{m}}_{0,k} = \text{argmin} \frac{1}{2} \sum_{j=1}^k \|\mathbf{F} \mathbf{T}^{j-1} \mathbf{m}_0 - \mathbf{d}_j\|_{\mathbf{W}_j}^2 + \frac{\alpha}{2} \|\mathbf{L} \mathbf{m}_0\|_2^2. \quad (3.3)$$

Substituting the definition of  $\mathbf{F}_k$  into the amse leads to the amse design functional,

$$\phi_k(\mathbf{w}_k) = \text{tr} \left[ \text{diag}(\boldsymbol{\tau}) \left( \sum_{j=1}^k (\mathbf{F} \mathbf{T}^{j-1})^\top \mathbf{W}_j \mathbf{F} \mathbf{T}^{j-1} + \alpha \mathbf{L}^\top \mathbf{L} \right)^{-1} \right]. \quad (3.4)$$

In minimizing equation (3.4) a sparsity penalty,  $\beta \|\mathbf{w}_k\|_1$ , is imposed on the weight vector to guarantee a design with a minimal number of measurements. Additionally we require that the weights all be positive, as

it does not make sense to have negative variances. This results in the adaptive design optimization problem is given by

$$\begin{aligned} \min_{\mathbf{w}_k} \quad & \left\{ \text{tr} \left[ \text{diag}(\boldsymbol{\tau}) \left( \sum_{j=1}^k \mathbf{F}_j^\top \mathbf{W}_j \mathbf{F}_j + \alpha \mathbf{L}^\top \mathbf{L} \right)^{-1} \right] + \beta \mathbf{e}^\top \mathbf{w}_k \right\} \\ \text{s.t.} \quad & 0 \geq \omega_i, \end{aligned} \quad (3.5)$$

where  $\mathbf{e}$  is a vector of ones (the constraint allows us to write the 1-norm as a sum).

The adaptive design method is outlined in the following algorithm 1 below. Note that in step 5 of the

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**Algorithm 1** Adaptive Optimal Design: Noiseless dynamics

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| 1: Given a prior $\hat{\mathbf{m}}_0$ for $\mathbf{m}$ , set $\boldsymbol{\tau}(\hat{\mathbf{m}}_0)$   | ▷ if there is no prior, $\boldsymbol{\tau} = \mathbf{I}$ |
| 2: <b>for</b> $k = 1$ to $n$ <b>do</b>   | ▷ $n$ time points  |
| 3: $\mathbf{w}_k = \text{argmin} \quad \phi_k(\mathbf{w}_k) + \beta \mathbf{e}^\top \mathbf{w}_k$  | ▷ design using equation (3.4)                            |
| 4:     Given $\mathbf{w}_k$ collect data $\mathbf{d}_k$  |  |
| 5: $\hat{\mathbf{m}}_{0,k} = \text{argmin} \quad \frac{1}{2} \sum_{j=1}^k \ \mathbf{F} \mathbf{T}^{j-1} \mathbf{m}_0 - \mathbf{d}_j\ _2^2 + R(\mathbf{m}_0)$ | ▷ re-estimate $\mathbf{m}_0$                             |
| 6: $\boldsymbol{\tau}(\hat{\mathbf{m}}_{0,k})$   | ▷ Recompute the monitor function $\boldsymbol{\tau}$     |
| 7: <b>end for</b>  |  |
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algorithm we have left the regularization as an arbitrary function even though the design functional was derived for a linear regularization. The regularization adjusts the ill-posed inverse problem such that the solutions best estimate the true model parameter distributions, so when calculating the monitor function it is imperative to get a best estimate since this directly effects the experimental design. For example, one could choose total variation as a regularization to promote sharper edges then say the smoothing gradient operator if this is expected of the model.

**3.2. Noisy model dynamics.** To include the noise inherent in the dynamic model we begin by considering three measurements of the dynamic target  $\mathbf{m}_k$ ,

$$\begin{aligned} \mathbf{F} \mathbf{m}_1 - \mathbf{d}_1 &= \boldsymbol{\epsilon}_1, \\ \mathbf{F} \mathbf{m}_2 - \mathbf{d}_2 &= \boldsymbol{\epsilon}_2, \quad \mathbf{m}_2 - \mathbf{T} \mathbf{m}_1 = \boldsymbol{\eta}_2 \\ \mathbf{F} \mathbf{m}_3 - \mathbf{d}_3 &= \boldsymbol{\epsilon}_3, \quad \mathbf{m}_3 - \mathbf{T} \mathbf{m}_2 = \boldsymbol{\eta}_3. \end{aligned}$$

It is assumed in this case that the first experiment will either be estimated in the regular way with no prior estimate or will be conducted in a naive way. In either case it is assumed that  $\mathbf{W}_1 = \text{diag}(\mathbf{w}_1)$  is known. Also note that if  $\boldsymbol{\eta} = \mathbf{0}$  we end up with the previous formulation for no noise.

To estimate  $\mathbf{m}_1, \dots, \mathbf{m}_3$  given  $\mathbf{d}_1, \dots, \mathbf{d}_3$  we minimize the following system with respect to  $(\mathbf{m}_1, \dots, \mathbf{m}_3)^\top$

$$\begin{aligned} & \frac{1}{2} \left\| \begin{pmatrix} \mathbf{W}_1 & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{W}_2 & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{W}_3 \end{pmatrix}^{\frac{1}{2}} \left( \begin{pmatrix} \mathbf{F} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{F} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{F} \end{pmatrix} \begin{pmatrix} \mathbf{m}_1 \\ \mathbf{m}_2 \\ \mathbf{m}_3 \end{pmatrix} - \begin{pmatrix} \mathbf{d}_1 \\ \mathbf{d}_2 \\ \mathbf{d}_3 \end{pmatrix} \right) \right\|_2^2 \\ & + \frac{1}{2} \left\| \begin{pmatrix} \mathbf{Q}_1^{-1} & \mathbf{0} \\ \mathbf{0} & \mathbf{Q}_2^{-1} \end{pmatrix}^{\frac{1}{2}} \begin{pmatrix} -\mathbf{T} & \mathbf{I} & \mathbf{0} \\ \mathbf{0} & -\mathbf{T} & \mathbf{I} \end{pmatrix} \begin{pmatrix} \mathbf{m}_1 \\ \mathbf{m}_2 \\ \mathbf{m}_3 \end{pmatrix} \right\|_2^2 \end{aligned} \quad (3.6)$$

Taking the gradient of (3.6), setting it equal to zero, and solving for  $(\mathbf{m}_1, \mathbf{m}_2, \mathbf{m}_3)^\top$  results in the following estimator  $(\hat{\mathbf{m}}_1, \hat{\mathbf{m}}_2, \hat{\mathbf{m}}_3) =$

$$\begin{pmatrix} (\mathbf{F}^\top \mathbf{W}_1 \mathbf{F} + \mathbf{T}^\top \mathbf{Q}_1^{-1} \mathbf{T} + \alpha \mathbf{L}^\top \mathbf{L}) & -\mathbf{T}^\top \mathbf{Q}_1^{-1} & \mathbf{0} \\ -\mathbf{Q}_1^{-1} \mathbf{T} & (\mathbf{F}^\top \mathbf{W}_2 \mathbf{F} + \mathbf{Q}_1^{-1} + \mathbf{T}^\top \mathbf{Q}_2^{-1} \mathbf{T} + \alpha \mathbf{L}^\top \mathbf{L}) & -\mathbf{T}^\top \mathbf{Q}_2^{-1} \\ \mathbf{0} & -\mathbf{Q}_2^{-1} \mathbf{T} & \mathbf{F}^\top \mathbf{W}_3 \mathbf{F} + \mathbf{Q}_2^{-1} + \alpha \mathbf{L}^\top \mathbf{L} \end{pmatrix}^{-1} \begin{pmatrix} \hat{\mathbf{d}}_1 \\ \hat{\mathbf{d}}_2 \\ \hat{\mathbf{d}}_3 \end{pmatrix}$$

where  $\hat{\mathbf{d}}_k = \mathbf{F}^\top \mathbf{W}_k^{\frac{1}{2}} \mathbf{d}_k$ . The mse of  $(\hat{\mathbf{m}}_1, \hat{\mathbf{m}}_2, \hat{\mathbf{m}}_3)$  is then

$$\text{tr} \left[ \begin{pmatrix} (\mathbf{F}^\top \mathbf{W}_1 \mathbf{F} + \mathbf{T}^\top \mathbf{Q}_1^{-1} \mathbf{T} + \alpha \mathbf{L}^\top \mathbf{L}) & -\mathbf{T}^\top \mathbf{Q}_1^{-1} & \mathbf{0} \\ -\mathbf{Q}_1^{-1} \mathbf{T} & (\mathbf{F}^\top \mathbf{W}_2 \mathbf{F} + \mathbf{Q}_1^{-1} + \mathbf{T}^\top \mathbf{Q}_2^{-1} \mathbf{T} + \alpha \mathbf{L}^\top \mathbf{L}) & -\mathbf{T}^\top \mathbf{Q}_2^{-1} \\ \mathbf{0} & -\mathbf{Q}_2^{-1} \mathbf{T} & \mathbf{F}^\top \mathbf{W}_3 \mathbf{F} + \mathbf{Q}_2^{-1} + \alpha \mathbf{L}^\top \mathbf{L} \end{pmatrix}^{-1} \right]$$

Now, consider that we wish to find the design  $\mathbf{w}_3$  after having already carried out experiments  $\mathbf{w}_1$  and  $\mathbf{w}_2$ . In the tradition of A-optimal design we would again minimize the mse. However, as is evident the mse does not depend on the data  $\mathbf{d}_1$ , and thus we will again introduce the amse and scale the mse by the available estimates of  $\mathbf{m}_k$ ,

$$\begin{pmatrix} \text{diag}(\boldsymbol{\tau}_1(\hat{\mathbf{m}}_1)) & & \\ & \text{diag}(\boldsymbol{\tau}_2(\hat{\mathbf{m}}_2)) & \\ & & \text{diag}(\boldsymbol{\tau}_3(\mathbf{T}\hat{\mathbf{m}}_2)) \end{pmatrix}.$$

Note that since the objective is to design for experiment 3, an estimate for  $\mathbf{m}_3$  does not yet exist, thus to approximate  $\hat{\mathbf{m}}_3$  we use the dynamics to propagate  $\hat{\mathbf{m}}_2$  forward one time step.

Defining  $\mathbf{S}_k = \mathbf{F}^\top \mathbf{W}_k \mathbf{F} + \mathbf{Q}_{k-1}^{-1} + \mathbf{T}^\top \mathbf{Q}_k^{-1} \mathbf{T} + \mathbf{L}^\top \mathbf{L}$  and  $\mathbf{A}_k = -\mathbf{Q}_k^{-1} \mathbf{T}$ , the design for the  $k^{\text{th}}$  experiment minimizes the general amse  $\Phi_k(\mathbf{w}_k)$ , given by

$$\text{tr} \left[ \text{diag} \begin{pmatrix} \boldsymbol{\tau}_1(\hat{\mathbf{m}}_1) \\ \boldsymbol{\tau}_2(\hat{\mathbf{m}}_2) \\ \vdots \\ \boldsymbol{\tau}_k(\mathbf{T}\hat{\mathbf{m}}_{k-1}) \end{pmatrix} \begin{pmatrix} (\mathbf{F}^\top \mathbf{W}_1 \mathbf{F} + \mathbf{T}^\top \mathbf{Q}_1^{-1} \mathbf{T} + \alpha \mathbf{L}^\top \mathbf{L}) & \mathbf{A}_1^\top & 0 \\ \mathbf{A}_1 & \mathbf{S}_2 & \mathbf{A}_2^\top & 0 \\ 0 & \ddots & \ddots & \ddots \\ 0 & \mathbf{A}_{k-1} & (\mathbf{F}^\top \mathbf{W}_k \mathbf{F} + \mathbf{Q}_{k-1}^{-1} + \alpha \mathbf{L}^\top \mathbf{L}) \end{pmatrix}^{-1} \right] \quad (3.7)$$

The noisy design optimization problem is constructed in exactly the same fashion as the noiseless case, by minimizing the amse for  $\mathbf{w}_k$  with a sparsity penalty on  $\mathbf{w}_k$ .

$$\begin{aligned} \min_{\mathbf{w}_k} \quad & \left\{ \text{tr} \left[ \text{diag} \begin{pmatrix} \boldsymbol{\tau}_1(\hat{\mathbf{m}}_1) \\ \boldsymbol{\tau}_2(\hat{\mathbf{m}}_2) \\ \vdots \\ \boldsymbol{\tau}_k(\mathbf{T}\hat{\mathbf{m}}_{k-1}) \end{pmatrix} \begin{pmatrix} \mathbf{S}_1 & \mathbf{A}_1^\top & 0 \\ \mathbf{A}_1 & \mathbf{S}_2 & \mathbf{A}_2^\top & 0 \\ 0 & \ddots & \ddots & \ddots \\ 0 & \mathbf{A}_{k-1} & \mathbf{S}_k(\mathbf{w}_k) \end{pmatrix}^{-1} \right] + \beta \mathbf{e}^\top \mathbf{w}_k \right\} \\ \text{s.t.} \quad & 0 \geq \omega_i. \end{aligned}$$

where  $\mathbf{e}$  is a vector of ones.

This formulation provides an alternate method of designing for a future experiment given historic data, where the error in the dynamics is now propagated in time. The adaptive design method for noisy dynamics is outlined in algorithm 2 below.

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**Algorithm 2** Adaptive Optimal Design: Noisy dynamics

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- 1: Given a design for experiment 1,  $\mathbf{w}_1$  for  $\mathbf{m}_1$  ▷ A naive design with no dynamics included
  - 2: **for**  $k = 2$  to  $n$  **do** ▷  $n$  time points
  - 3:    $\mathbf{w}_k = \text{argmin} \quad \Phi_k(\mathbf{w}_k) + \beta \mathbf{e}^\top \mathbf{w}_k$  ▷ design using equation (3.7)
  - 4:   Given  $\mathbf{w}_k$  collect data  $\mathbf{d}_k$
  - 5:    $\hat{\mathbf{m}}_k = \text{argmin} \quad \frac{1}{2} \|\mathbf{F}\hat{\mathbf{m}}_k - \mathbf{d}_k\|_2^2 + R(\hat{\mathbf{m}}_k)$  ▷ estimate  $\mathbf{m}_k$
  - 6:    $\boldsymbol{\tau}_{k+1}(\mathbf{T}\hat{\mathbf{m}}_k)$  ▷ Propagate the estimator to compute the monitor function  $\boldsymbol{\tau}_{k+1}$
  - 7: **end for**
- 

**4. Numerical optimization.** In this section we present the calculation of the gradients required to solve the design optimization problems for both the noiseless and noisy dynamics.

**4.1. Noiseless dynamics.** Finding an optimal design for time step  $k$  involves minimizing the objective functional (3.4). This is a difficult task for large problems, particularly due to the presence of the trace of a large dense matrix and the computation of the derivative of the trace. To this end, several actions can be taken to reduce the computational costs.

To avoid computing the trace explicitly, a stochastic Hutchinson trace estimator is used such that Equation (3.4) can be written as

$$\phi_k(\mathbf{w}_k) = \mathbf{v}^\top \text{diag}(\boldsymbol{\tau}) \left( \mathbf{F}_k^\top \mathbf{W}_k \mathbf{F}_k + \mathbf{G} \right)^{-1} \mathbf{v},$$

where  $\mathbf{G} = \sum_{j=1}^{k-1} \mathbf{F}_j^\top \mathbf{W}_j \mathbf{F}_j + \alpha \mathbf{L}^\top \mathbf{L}$  and  $\mathbf{v}$  is a random vector with equally distributed values of 1 and  $-1$  [?].

The calculation of the gradient of  $\phi_k(\mathbf{w}_k)$  involves computing the derivative of an inverse matrix times a vector,

$$\text{grad}_{\mathbf{w}_k} \phi_k(\mathbf{w}_k) = \mathbf{v}^\top \text{diag}(\boldsymbol{\tau}) \text{grad}_{\mathbf{w}_k} \left( \left( \mathbf{F}_k^\top \mathbf{W}_k \mathbf{F}_k + \mathbf{G} \right)^{-1} \mathbf{v} \right). \quad (4.1)$$

This calculation can easily be carried out by defining  $\mathbf{z}$  such that

$$\mathbf{z} = (\mathbf{F}_k^\top \mathbf{W}_k \mathbf{F}_k + \mathbf{G})^{-1} \mathbf{v} \quad \Leftrightarrow \quad (\mathbf{F}_k^\top \mathbf{W}_k \mathbf{F}_k + \mathbf{G}) \mathbf{z} = \mathbf{v}, \quad (4.2)$$

recalling that  $\mathbf{W}_k = \text{diag}(\mathbf{w}_k)$ , and differentiating implicitly to obtain

$$\mathbf{F}_k^\top \text{diag}(\mathbf{F}_k \mathbf{z}) + (\mathbf{F}_k^\top \text{diag}(\mathbf{w}_k) \mathbf{F}_k + \mathbf{G}) \text{grad}_{\mathbf{w}_k} \mathbf{z} = \mathbf{0}.$$

The gradient of  $\mathbf{z}$  is then given by

$$\nabla_{\mathbf{w}} \mathbf{z} = -(\mathbf{F}_k^\top \text{diag}(\mathbf{w}_k) \mathbf{F}_k + \mathbf{G})^{-1} \mathbf{F}_k^\top \text{diag}(\mathbf{F}_k \mathbf{z}).$$

Transposing, defining  $\mathbf{C} = \mathbf{F}_k^\top \mathbf{W}_k \mathbf{F}_k + \mathbf{G}$ , and  $\mathbf{C} \mathbf{y} = \text{diag}(\boldsymbol{\tau}) \mathbf{v}$ , the gradient of the design objective function, equation (3.4), is then

$$-\text{diag}(\mathbf{F}_k \mathbf{z}) \mathbf{F}_k \mathbf{y} + \beta \mathbf{e}, \quad (4.3)$$

where  $\mathbf{F}_k = \mathbf{F} \mathbf{T}^{k-1}$ . The computation of the Hessian of  $\phi$  is fairly straight forward if one notes that the gradient  $\nabla \mathbf{y} = \nabla \mathbf{z}$ ,

$$\mathbf{H}(\mathbf{w}_k) = -\text{diag}(\mathbf{F}_k(\mathbf{z} - \mathbf{y})) \mathbf{F}_k \nabla \mathbf{z}. \quad (4.4)$$

Unfortunately due to the inclusion of the monitor function  $\boldsymbol{\tau}$ , the gradient is not as a "nice" as in the classic A-optimal design since we must now solve two linear systems,  $\mathbf{C} \mathbf{z} = \mathbf{v}$  and  $\mathbf{C} \mathbf{y} = \text{diag}(\boldsymbol{\tau}) \mathbf{v}$ . However, we can make use of the conjugate gradient method to solve the systems to avoid ever forming  $\mathbf{C}$  since only matrix vector products are required.

Since the design problem is nonlinear with respect to  $\mathbf{w}_k$ , a Newton type iterative method (steepest descent) is used with a backtracking line search.

**4.2. Noisy dynamics.** Computing the gradient of equation (3.7) is somewhat more involved then for the noiseless case. First, to approximate the trace operation and reduce computational cost we will again apply a Hutchinson trace estimator,

$$\Phi(\mathbf{w}_k) = \begin{pmatrix} \mathbf{v}_1 \\ \mathbf{v}_2 \\ \vdots \\ \mathbf{v}_k \end{pmatrix}^\top \text{diag} \begin{pmatrix} \boldsymbol{\tau}_1(\hat{\mathbf{m}}_1) \\ \boldsymbol{\tau}_2(\hat{\mathbf{m}}_2) \\ \vdots \\ \boldsymbol{\tau}_k(\mathbf{T} \hat{\mathbf{m}}_{k-1}) \end{pmatrix} \begin{pmatrix} \mathbf{S}_1 & \mathbf{A}_1^\top & 0 & 0 \\ \mathbf{A}_1 & \mathbf{S}_2 & \mathbf{A}_2^\top & 0 \\ 0 & \ddots & \ddots & \ddots \\ 0 & 0 & \mathbf{A}_{k-1} & \mathbf{S}_k \end{pmatrix}^{-1} \begin{pmatrix} \mathbf{v}_1 \\ \mathbf{v}_2 \\ \vdots \\ \mathbf{v}_k \end{pmatrix}. \quad (4.5)$$

To compute the gradient of  $\Phi$  we define the vector  $(\mathbf{z}_1, \mathbf{z}_2, \dots, \mathbf{z}_k)^\top$  such that

$$\begin{pmatrix} \mathbf{S}_1 & \mathbf{A}_1^\top & 0 & \\ \mathbf{A}_1 & \mathbf{S}_2 & \mathbf{A}_2^\top & 0 \\ 0 & \ddots & \ddots & \ddots \\ & 0 & \mathbf{A}_{k-1} & \mathbf{S}_k \end{pmatrix} \begin{pmatrix} \mathbf{z}_1 \\ \mathbf{z}_2 \\ \vdots \\ \mathbf{z}_k \end{pmatrix} = \begin{pmatrix} \mathbf{v}_1 \\ \mathbf{v}_2 \\ \vdots \\ \mathbf{v}_k \end{pmatrix} \quad (4.6)$$

and note that the gradient of equation (3.7) requires the gradient of  $(\mathbf{z}_1, \mathbf{z}_2, \dots, \mathbf{z}_k)^\top$ . We then implicitly differentiate to obtain  $\nabla_{\mathbf{w}_k}(\mathbf{z}_1, \mathbf{z}_2, \dots, \mathbf{z}_k)^\top$ . Recalling that  $\mathbf{S}_k = \mathbf{F}^\top \mathbf{W}_k \mathbf{F} + \mathbf{Q}_{k-1}^{-1} + \mathbf{T}^\top \mathbf{Q}_k^{-1} \mathbf{T} + \alpha \mathbf{L}^\top \mathbf{L}$  and  $\mathbf{A}_k = -\mathbf{Q}_k^{-1} \mathbf{T}$ , and that only  $\mathbf{S}_k(\mathbf{w}_k)$  depends on  $\mathbf{w}_k$  it is easy to show that the gradient is given by

$$\underbrace{\begin{pmatrix} \mathbf{S}_1 & \mathbf{A}_1^\top & 0 & \\ \mathbf{A}_1 & \mathbf{S}_2 & \mathbf{A}_2^\top & 0 \\ 0 & \ddots & \ddots & \ddots \\ & 0 & \mathbf{A}_{k-1} & \mathbf{S}_k \end{pmatrix}}_{\mathbf{E}} \begin{pmatrix} \text{grad } \mathbf{z}_1 \\ \text{grad } \mathbf{z}_2 \\ \vdots \\ \text{grad } \mathbf{z}_k \end{pmatrix} = \underbrace{\begin{pmatrix} \mathbf{0} \\ \mathbf{0} \\ \vdots \\ -\mathbf{F}^\top \text{diag}(\mathbf{F} \mathbf{z}_k) \end{pmatrix}}_{\mathbf{B}} \quad (4.7)$$

Note that the gradient of  $\mathbf{z}$  is a matrix with dimensions  $kN \times N$ .

Defining the large matrix as  $\mathbf{E}$  and the right hand side as  $\mathbf{B}$ , we can write the gradient of  $\mathbf{z}$  is

$$\begin{pmatrix} \text{grad } \mathbf{z}_1 \\ \text{grad } \mathbf{z}_2 \\ \vdots \\ \text{grad } \mathbf{z}_k \end{pmatrix} = \mathbf{E}^{-1} \mathbf{B}, \quad (4.8)$$

and thus the gradient of  $\Phi$  as

$$\nabla \Phi(\mathbf{w}_k) = \mathbf{B}^\top \mathbf{E}^{-\top} (\mathbf{v} \odot \bar{\mathbf{v}}) \quad (4.9)$$

where  $\mathbf{v}$  is the vector of all  $\tau_k$ 's and  $\bar{\mathbf{v}}$  is the vector of all  $\mathbf{v}_k$ 's. Because the matrix  $\mathbf{E}$  is not symmetric, gmres was used to solve the system  $\mathbf{E}^{-\top} (\mathbf{v} \odot \bar{\mathbf{v}})$  without having to explicitly form the big matrix  $\mathbf{E}$ .

**5. Numerical Examples .** To demonstrate the adaptive dynamic design we begin with a toy problem designed to fully demonstrate the ability of the methods to track the motion of a target. The toy model problem consists of a circular target of constant concentration which is moved vertically in a whole space of constant background. The motion of the target is governed by a time invariant velocity field generated by a simple source-sink system with no diffusion. To image the target we chose a geophysical borehole seismic tomography method since it is linear with respect to  $\mathbf{m}$  and tends to cover a large area.

The partial differential equations governing both the imaging and the transport of the target are discretized on a 2D computational domain  $\Omega = [0, 400] \times [0, 100]$  meters, divided into  $m = [100, 50]$  cells of width  $h = [4, 2]$  meters.

**5.1. Imaging: seismic borehole tomography.** Borehole seismic tomography measures the travel time of an acoustic wave traveling between sources  $n_s$  and receivers  $n_r$ . Travel times are given by integrating the slowness  $m(t, \vec{\mathbf{x}})$  or inverse acoustic velocity of the media along a linear ray path  $\Gamma$ ,

$$\mathbf{d}_{j,k}(t) = \int_{\Gamma_{j,k}} m(t, \vec{\mathbf{x}}) d\ell.$$

Assuming the data are noisy and measured at times  $(t_0, \dots, t_n)$  the tomography problem is given by

$$\mathcal{F}m(t_k, \vec{\mathbf{x}}) + \epsilon_k = \mathbf{d}(t_k).$$

Equation (5.1) is discretized on a standard staggered 2D grid using a finite volume scheme placing  $s$  and  $\mathbf{d}$  at the cell centers, see figure 5.1 below.



The discrete tomography experiment in matrix form is then,

$$\mathbf{F}\mathbf{m}_k = \mathbf{d}_k, \text{ for } k = 1, \dots, n. \quad (5.1)$$

The initial survey setup is pictured in figure 5.2, and includes 2 boreholes with 20 sources in the east borehole and 30 receivers in the west borehole. The initial design was chosen to overly cover all the area in the flow domain, with the goal of significantly reducing the number of data required to image the moving target.

**5.2. Dynamics: Tracer advection.** The subsurface dynamics are described by the tracer advection equations as presented in [?], which characterize the transport of a solute in a fully saturated porous media,

$$\begin{aligned} \frac{\partial(c\rho)}{\partial t} + \nabla \cdot c\rho\vec{\mathbf{u}} &= 0, \\ \text{subject to } c\rho(0, \vec{\mathbf{x}}) &= c_0\rho(\vec{\mathbf{x}}), \end{aligned} \quad (5.2a)$$

with hydraulic conductivity  $\mathbf{K}$ , and tracer concentration  $c$  in a fluid of density  $\rho$ . The fluid velocity field  $\vec{\mathbf{u}}$  satisfies a simple source-sink ( $q$ ) flow model

$$\nabla \cdot \vec{\mathbf{u}} = q \quad (5.2b)$$

$$\vec{\mathbf{u}} = \mathbf{K}(\vec{\mathbf{x}}) \text{grad } p \quad (5.2c)$$

$$p(0, \vec{\mathbf{x}}) = p_0(\vec{\mathbf{x}}), \quad (5.2d)$$

with either Dirichlet or Neumann boundary conditions on the pressure  $p$ .

With the goal being to image the motion of the tracer,  $c(t, \vec{\mathbf{x}})$ , we assume that changes in  $c$  amount to changes in geophysical properties. This implies that  $m(c)$  exists and is linear, and that the motion of  $m$  is governed by Equation (5.2a). From now on we will refer only to  $\mathbf{m}$ .

To discretize the advection of the tracer, a particle in cell discretization was chosen such that equation (5.2a) is then given by,

$$\mathbf{m}_k = \mathbf{T}(\mathbf{u})\mathbf{m}_{k-1}.$$

The matrix  $\mathbf{T}(\mathbf{u})$  is the transpose of a bi-linear interpolation matrix which pushes mass from a cell center along the path  $\mathbf{u}\Delta t$  and spreads it to the 4 neighboring cells accordingly.

The remainder of the flow equations were discretized on a staggered grid using the finite volume method, with the components of the velocity field located on the cell edges and the tracer concentration at the cell centers.

The fluid velocity field  $\mathbf{u}$  was computed by solving equations (5.2b) and (5.2c) with a constant hydraulic conductivity for  $1\text{e-}03 \text{ kg/s}^2\text{m}^2$ .

**5.3. Regularization.** We chose a gradient operator for the linear regularization operator  $\mathbf{L} = \text{GRAD}$ , which maps from cell centers to edges with Dirichlet boundary conditions to promote smoothness in the recovered models.

Two different inversions were carried out to recover models  $\mathbf{m}_k$ . First a linear inversion was performed with the gradient operator, and second a non-linear inversion was performed with smoothed total variation as the regularization [?, ?] because it is possible that the models can have discontinuities or sharp boundaries. This is particularly valid for our experiment since we have chosen advection without any diffusion term to transport a concentration of tracer. In this ideal case there should be no diffusion of the tracer.

In continuous space smoothed total variation is described by the following relation,

$$R(m) = \alpha \int \phi(|\text{grad } m|) d\vec{\mathbf{x}}. \quad (5.3)$$

A standard discrete approximation for the smoothed total variation regularization found in [?] is,

$$R(\mathbf{m}) = \alpha h^2 \mathbf{e}^\top \sqrt{\mathbf{A}_f^c ((\text{GRAD } \mathbf{m}) \odot (\text{GRAD } \mathbf{m}))} + \epsilon, \quad (5.4)$$

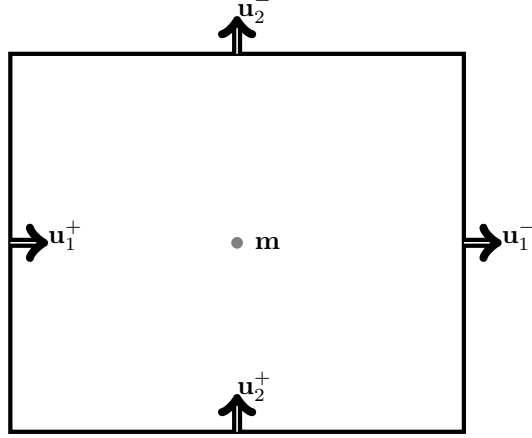


FIG. 5.1. An example of a staggered grid cell with model parameters at the cell center and fluid velocity field on the edges.

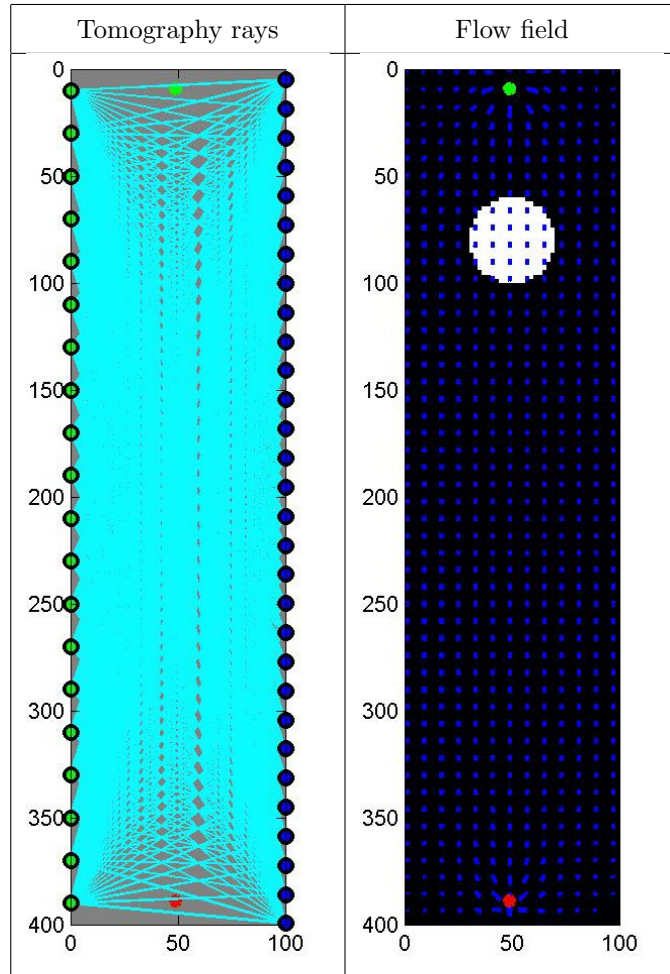


FIG. 5.2. Initial experiment setup. Sources are pictured in green on the left and receivers in blue on. The initial setup covers the entire flow domain with 20 sources and 30 receivers.

where the GRAD gradient operator again maps from cell centers to cell faces, and the averaging matrix  $\mathbf{A}_f^c$  maps from faces to cell centers. Although we have formulated the optimal design based on a linear estimation

of  $\mathbf{m}$ , it is not unreasonable to estimate  $\mathbf{m}_k$  or  $\mathbf{m}_0$  with a non-linear regularization, provided that this will contribute to recovering the best estimate of  $\mathbf{m}_k$ . As you can see in figure 5.3 below, the overall relative model error is significantly lower than that of the models recovered using the linear regularization.

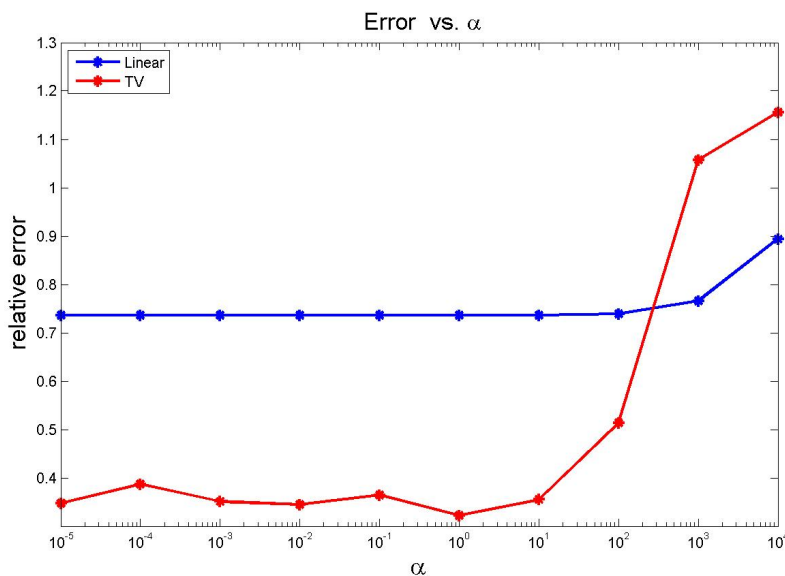


FIG. 5.3. Plot of the relative error ( $\|\mathbf{m}_1^{true} - \hat{\mathbf{m}}_1\|/(\|\mathbf{m}_1^{true}\|)$ ) versus the regularization paramtere  $\alpha$  for both the linear regularization and smoothed total variation.

**6. Results: Noiseless dynamics.** To generate data, the initial tracer concentration was marched along in time for time steps of 25 days, and measured by conducting a tomography survey. Gaussian noise was added to each data set. In total 9 experiments were conducted.

The initial design for time point  $t_0$  did not include the dynamics, which amounts to setting  $\tau = 1$  in algorithm 1. The design algorithm is therefore identical to the static case and produces an optimal design based on the physics and that of the linear regularization operator  $\mathbf{L}$ , without any historic data. This is apparent in both the plot of the weights for experiment 1 at time  $t_0$  in figure 6.1 and the image of the rays in figure 7.1.

For each experiment the  $\text{mse}$  was plotted versus the number of nonzero weights for a set of regularization parameters  $\beta$ , see figure 6.1 for images for times  $t_0, t_2, t_4$ . From these curves, the best set of weights were chosen such that the weights were sparse, but also so the  $\text{mse}$  was kept reasonably small. The experiment weights are also plotted.

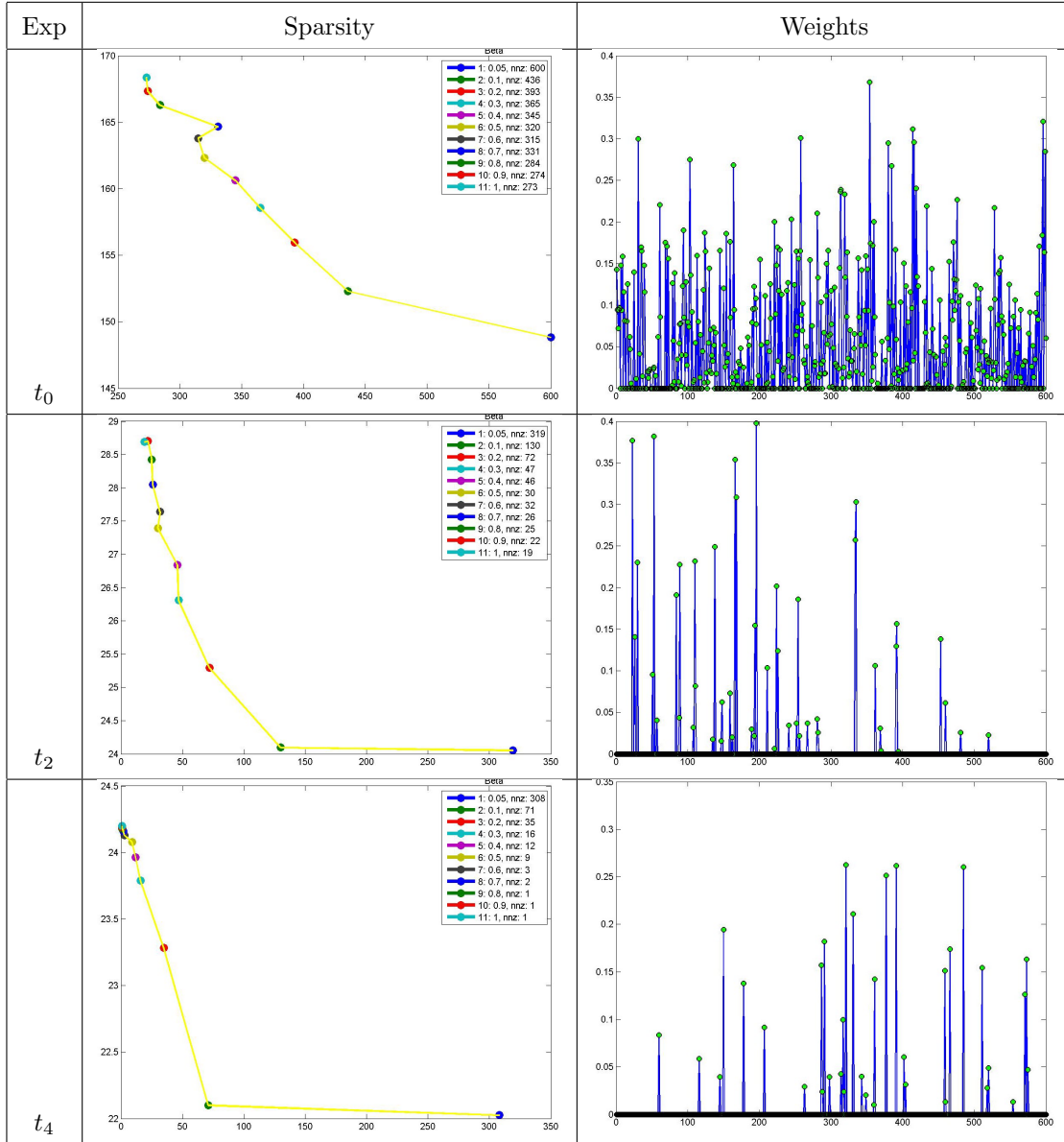


FIG. 6.1. Noiseless dynamics: Plots of the  $\text{mse}$  vs. the number of nonzero weights (left column), and the weights used to conduct the experiment for experiments 1,3, and 5, at times  $t_0, t_2, t_4$ .

After each experimental design was determined, both  $\mathbf{m}_0$  and the current model  $\mathbf{m}_k$  were reconstructed from the reduced set of data corresponding to the optimal experimental design. The new estimate for  $\mathbf{m}_0$  was then used to compute  $\tau$ . In figure 7.1 the rays corresponding to the optimal experimental design data used to estimate the current models are pictured in blue over an image of the model. Note that the rays tend to follow the model as it moves through the domain. The total number of data required to image the models is significantly reduced. In most cases the number of data are approximately 40 of a possible 600. There do appear to be rays that do not pass through the target, and thus would not contribute to the image reconstruction. However, since the reconstruction of  $\mathbf{m}_0$  is never perfect and there is noise in the data, these spurious rays are somewhat expected.

It is also apparent in the reconstructions of  $\mathbf{m}_k$  that the smoothed total variation does a better job, even when the optimal design was computed for the linear regularization when estimating the target. Again, this is to be expected since we have chosen a model with discontinuous edges, and are transporting the target only by advection.

**7. Results: Noisy dynamics.** To demonstrate the formulation presented in section 3.2, we again march the tracer along in time while determining an optimal survey design for the future experiment, given a current data. Models  $\mathbf{m}_k$  are reconstructed at each time step again using the reduced data sets, for the non-linear regularization, and again for the linear regularization.

## 8. Conclusions.

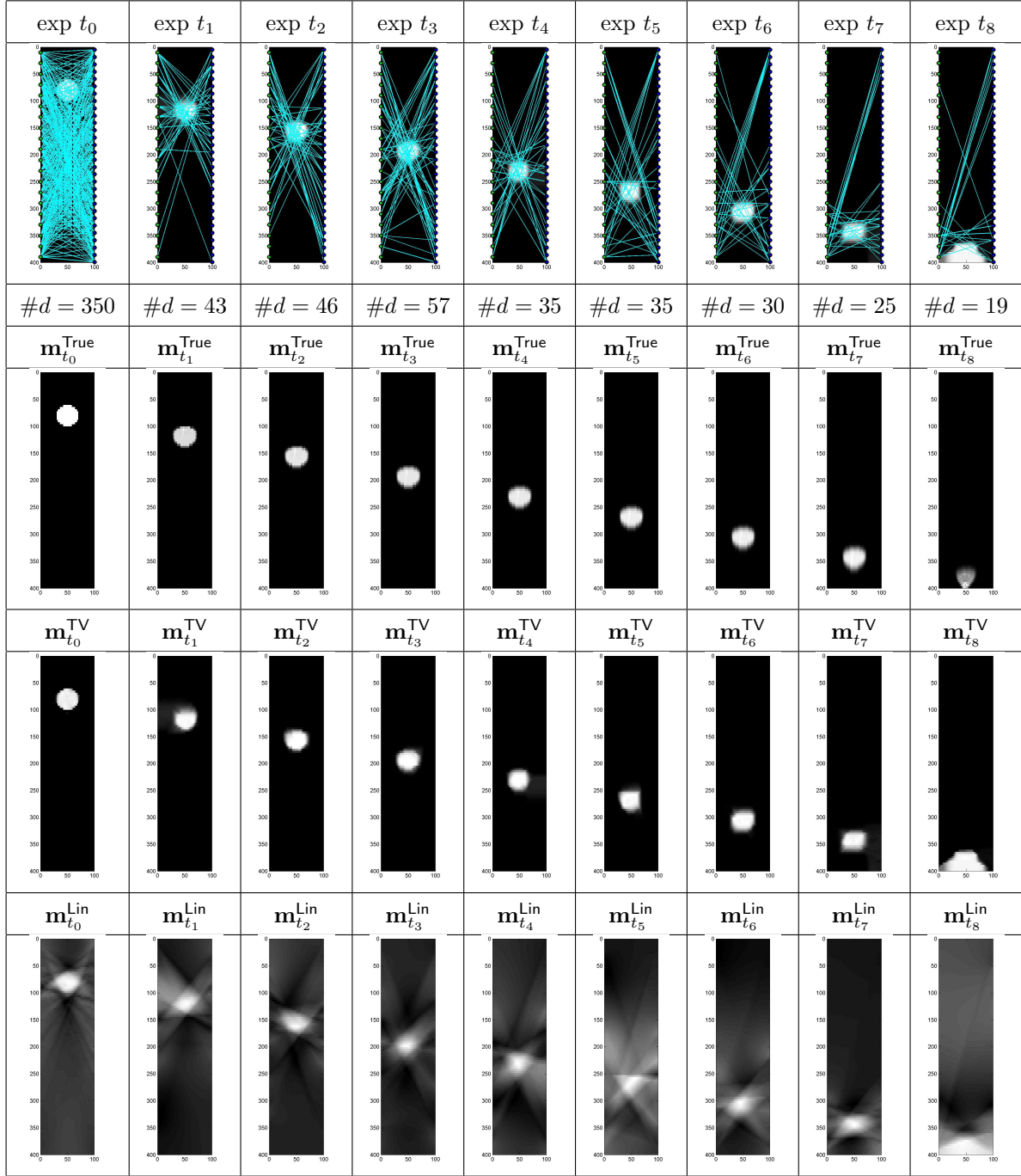


FIG. 6.2. Noiseless dynamics: Optimal designs and recovered models for 9 experiments. The top row shows the rays and the recovered model, with the number of rays ( $\#d = 350$ ) given below, followed by the true models, the models recovered using total variation, and finally the models recovered using the linear gradient regularization.

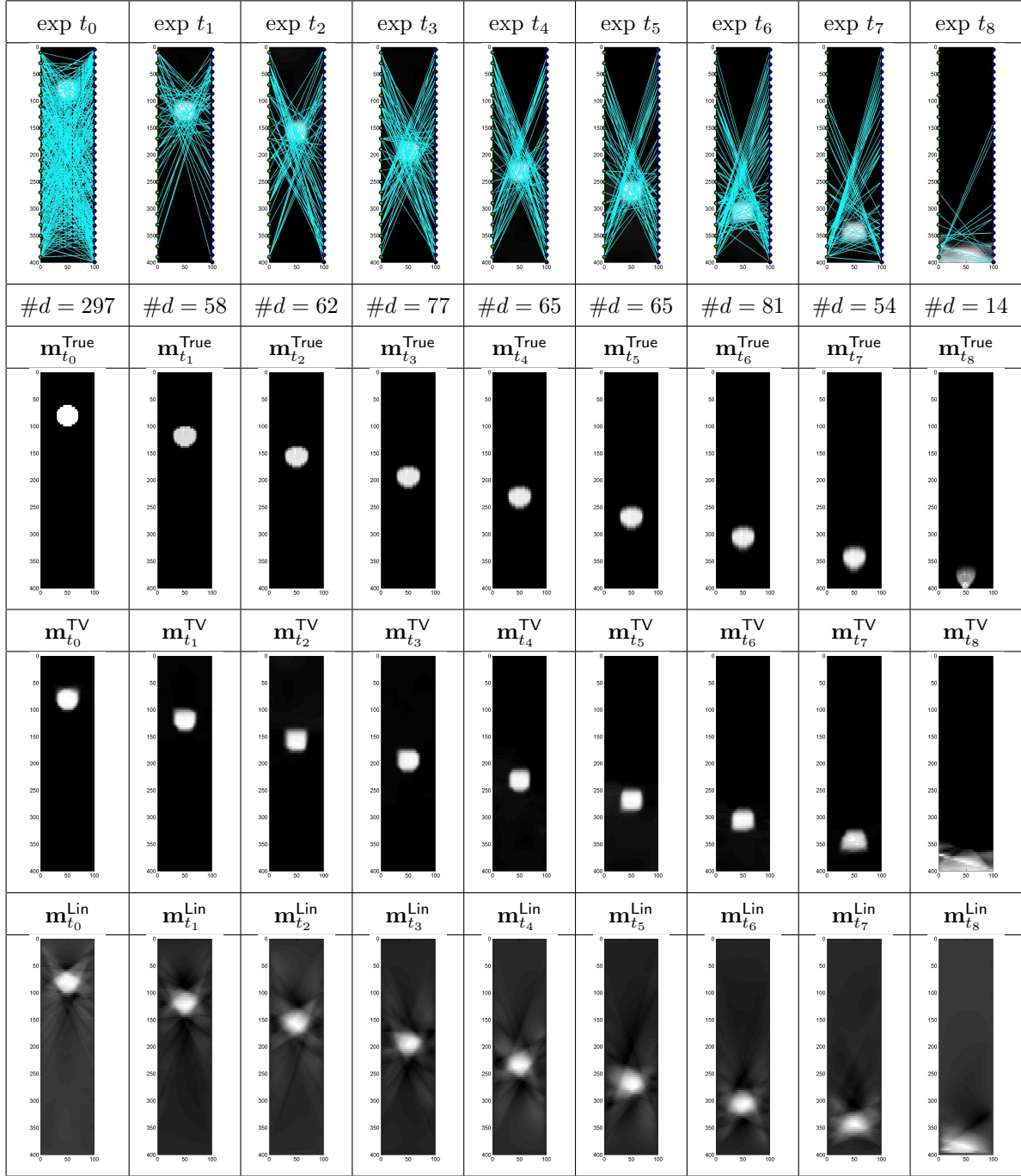


FIG. 7.1. Noisy dynamics: Optimal designs and recovered models for 9 experiments. The top row shows the rays and the recovered model, with the number of rays (ex.  $\#d = 297$ ) given below. The second row pictures true models, the third shows the models recovered using total variation, and finally the bottom shows models recovered using the linear gradient regularization.