SENSOR CLUSTERIZATION IN D-OPTIMAL DESIGN IN INFINITE DIMENSIONAL BAYESIAN INVERSE PROBLEMS

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Abstract. We investigate the problem of sensor clusterization in optimal experimental design for infinite-dimensional Bayesian inverse problems. We suggest an analytically tractable model for such designs and reason how it may lead to sensor clusterization in the case of iid measurement noise. We also show that in the case of spatially correlated measurement error clusterization does not occur. As a part of the analysis we prove a matrix determinant lemma analog in infinite dimensions, as well as a lemma for calculating derivatives of \( \log \det \) of operators.

1. Introduction

Experimental design is an important part of many scientific investigations. When considering an inverse problem, one can often specify sensor locations (e.g. in geophysics and oceanography applications), certain wavelengths (e.g. in MRI) or wave reflections from the ground (e.g. searching for oil or using a radar). Whatever the allowed set of measurements is, one should select the optimal measurements to take, in order to increase accuracy, reduce costs, or both.

Designing experiments is usually done by optimizing some design criterion and this is true both for frequentists \cite{13, 17} as well as for Bayesians \cite{4}, see \cite{4} for an investigation of the analogy between the two approaches. Although there is a plethora of design criteria, in the current work we will focus on just one of these, commonly referred to as D-optimal design. It has a simple and appealing motivation in the Bayesian context as explained in \cite{4}: for a linear model, a D-optimal design seeks to maximize the expected information gain (KL divergence \cite{5, 11}) between posterior and prior. In finite dimensions, maximizing the expected information gain amounts to minimizing the determinant of the posterior covariance matrix. In a frequentist settings, an optimal design minimizes the volume of the uncertainty ellipsoid \cite[page 16]{17}, but this is done for the Fisher information matrix and not the posterior covariance. However, \cite{4} shows that the latter is just a regularized version of the former.

The previous discussion is classical for experimental design when inference is to take place over a finite (not too large) number of parameters. The subject of optimal experimental design for function inference in a Bayesian context was pioneered by \cite{1-3}. Similarly to the finite dimensional case, it can be shown that a D-optimal design arises naturally for linear models when one wishes to maximize the KL divergence between posterior and prior and this amounts to minimizing the
determinant of the posterior covariance operator (understood as a product of its eigenvalues). Some difficulties arise in the process, but remedies can be found as shown in [1].

It seems counter intuitive that when one computes an optimal design using the D-optimal criterion (and others that will not be investigated here), the optimization process results in measurements that are very similar. For example, if a measurement is thought of as measuring some function value at \( x \in \Omega \subseteq \mathbb{R}^d, d = 1, 2, 3 \) (with added error) then the optimization procedure sometimes places sensors in close proximity to each other (as can be seen in figure 1.3). Following [17], we refer to this phenomenon as sensor clusterization.

1.1. Related Work. The phenomenon of sensor clusterization seems to be known in several different contexts. In a frequentist and finite-dimensional context, [7] and [17, chapter 2.4.3] discuss this phenomenon and suggest an approach called clusterization-free design, where the user enforces measurement locations to be far from each other. One way to do this is by introducing correlated errors which, philosophically, accounts for both measurement error and model error. Another method considered is imposing distance constraints between measurements. A somewhat different approach is suggested in [8, page 49], where close by design measurements are merged — a procedure which obviously does not avoid clusterization. The same problem arises in time-series analysis for pharmacokinetic experiments. The authors of [9] suggest modeling auto-correlation time in the noise model, which is equivalent to the correlated errors mentioned above.

Any of the above mentioned approaches might serve as a remedy and push sensors away from each other. Yet, none offers any insight as to why clusterization occurs. Also, as better models are employed, model error is decreased and the clusterization phenomenon will eventually reappear. While these approaches are practical and help us avoid the problem, they do not provide insight as to why sensors are clustering.

1.2. Contribution. We propose and thoroughly study an analytically tractable model for understanding D-optimal designs. In this model, an optimal design arises as a solution to a constrained optimization problem, formulated using Lagrange multipliers (section 3). In the case of no model error we show this problem is in fact a set of eigenvector-eigenvalue problems (equation (4.1)). We then characterize an optimal design as one that reduces the highest uncertainties, and show how that can give rise to repeated measurements (section 4.2 and figure 2).

In the process we generalize several lemmas from linear algebra to infinite-dimensional settings — the Matrix Determinant Lemma and a lemma for calculating the derivative of determinants. We also provide other tools for understanding D-optimal designs in infinite-dimensional Bayesian inverse problems, including lemmas for calculating the increase in the design criterion per observation — Lemmas B.1 and Corollary 2. The arguments presented are completely generic and apply equally to any of the scenarios mentioned in the introduction.

1.3. An Example of Clusterization. In section 2.1 we present a more abstract and general formulation of the problem, but for the purpose of illustration, we present the problem via a toy model — the 1D heat equation in \([0, \pi]\) with homogeneous Dirichlet boundary conditions.

The 1D heat equation is:

\[
\begin{align*}
(1.1a) & \quad u_t = \Delta u \quad \text{in} \ [0, \pi] \times [0, \infty), \\
(1.1b) & \quad u = 0 \quad \text{on} \ {0, \pi} \times [0, \infty), \\
(1.1c) & \quad u = u_0 \quad \text{on} \ [0, \pi] \times \{0\}.
\end{align*}
\]
Figure 1. Shown are pointwise posterior standard deviations for various numbers of sensors, and location of these sensors for the 1D heat equation with homogeneous Dirichlet boundary described in section 1.3. Note the clusterization that occurs when 6 sensors are used — only 4 measurement locations are included. Observed data does not influence the pointwise variances, hence it is omitted.

We would like to infer the initial condition \( u_0 \). For that purpose, we measure \( u \) at some set of locations \( x_j \in [0, \pi], j = 1, \ldots, m \) and a final time \( T > 0 \). We assume centered Gaussian measurement error, so we can observe \( v(x_j, T) = u(x_j, T) + \epsilon(x_j) \) with \( \epsilon(x_j) \sim N(0, \sigma^2) \), \( \sigma > 0 \) iid. We model the initial condition as \( u_0 \sim N(0, \Gamma_{pr}) \), for \( \Gamma_{pr} = (-\Delta)^{-1} \) with homogeneous Dirichlet boundary condition. It is well known [16] that for linear problems, with Gaussian prior and error, the posterior is also Gaussian with a covariance that does not depend on the observed data. The posterior covariance \( \Gamma_{post} \) is known to have a closed form formula, even in infinite dimensions [15]. If we denote by \( \mathcal{F} \) the dynamics operator, so that \( u(\cdot, T) = \mathcal{F}u_0 \), and the observation operator \( \mathcal{O} \) so that \( u(x_j, T) = (\mathcal{O}u)_j, j = 1, \ldots, m \), then the posterior covariance is known and depends on \( \Gamma_{pr}, \mathcal{F}, \mathcal{O} \) and \( \sigma^2 \) (see section 2.1 and (2.6) specifically).

We will consider generalization of the information-theoretic design criterion presented in section 1 to infinite dimensions (section 2.2). We choose \( x_j, j = 1, \ldots, m \) so as to minimize an expression analogous to the log-determinant of the posterior covariance operator (corresponding to a D-optimal design). We can see the clusterization effect in figure 1.3 — the design criterion suggests placing sensors in locations that are extremely close.

1.4. Remarks to the Reader. The Lagrange multipliers problem for iid measurement noise is discussed in section 4. In that section, it is shown how sensor clusterization can occur. The reader
may skip if they are constrained by time. It is advised that a reader less comfortable with Hilbert and Banach spaces mostly ignore these terms and consider $\mathcal{H}$ and $\mathcal{B}$ finite dimensional vector spaces.

2. Preliminaries and Notation

The theoretical foundations for inverse problems over function spaces can be found in [15]. This section is mostly devoted to setting notation. At this point, it is useful to record a known result regarding the posterior covariance operator of our inverse problem, namely

$$\Gamma_{\text{post}} = (\Gamma_{\text{pr}}^{-1} + \mathcal{F}^* O^* \Sigma^{-1} O \mathcal{F})^{-1}. \quad (2.1)$$

2.1. Bayesian Inverse Problems. Let $\mathcal{H}$ be a Hilbert space and $\mathcal{B}$ a Banach space, both infinite-dimensional. Consider $\mathcal{F} : \mathcal{H} \to \mathcal{B}$, a linear operator (the “forward operator”). We are interested in forward operators that are strongly smoothing (have fast decaying singular values — the heat operator from section 1.3 is a prime example).

We want to infer $m \in \mathcal{H}$, some parameter of the dynamics given noisy observations of $\mathcal{F} m$. We model $m \sim N(0, \Gamma_{\text{pr}})$ with some appropriate covariance operator $\Gamma_{\text{pr}}$ [15]. Observations (measurements) are taken via the linear observation operator $\mathcal{O} \in (\mathcal{B}^*)^m$, where $m$ is the number of observations allowed (e.g. sensors at our disposal). In an analogy with linear algebra (where row vectors are thought of as linear functionals), we think of $\mathcal{O}$ as having “rows” $o_j, j = 1, \ldots, m$.

$$\mathcal{O} = (o_1, \ldots, o_m)^t, o_j \in \mathcal{B}^*, j = 1, \ldots, m. \quad (2.2)$$

This way, for $u \in \mathcal{B}$ we have $\mathcal{O} u = (o_1(u), \ldots, o_m(u))^t \in \mathbb{R}^m$. A few observations regarding $\mathcal{O}$ are in order. First, it is good to keep in mind that $(\mathcal{B}^*)^m$ is a Banach space with norm $\|\mathcal{O}\| = \sum_{j=1}^m \|o_j\|$. Next, for $u \in \mathcal{B}$ and $v \in \mathbb{R}^m$:

$$\langle \mathcal{O}^* v, u \rangle_{\mathbb{R}^m} = \sum_{j=1}^m v_j o_j(u) = v^t (\mathcal{O} u) = (v^t \mathcal{O})(u),$$

and thus:

$$\mathcal{O}^* v = \sum_{j=1}^m v_j o_j = v^t \mathcal{O}. \quad (2.3)$$

Observation 2.1. It is best to think of $o_j, j = 1, \ldots, m$ as row vectors and of $\mathcal{O}$ as a matrix with rows $o_j$.

Each measurement consists of a linear functional, chosen from an allowed set of linear functionals in $\mathcal{B}^*$. Data is acquired via noisy measurements

$$d := \mathcal{O}(\mathcal{F} m + \varepsilon') + \varepsilon = \mathcal{O} \mathcal{F} m + \mathcal{O} \varepsilon' + \varepsilon$$

with $d \in \mathbb{R}^m$ and $\varepsilon, \varepsilon'$ defined next. Measurement error consists of two parts. First, there is spatially correlated error $\varepsilon' \sim N(0, \Gamma_{\text{model}})$, modeled as a centered Gaussian measure on $\mathcal{B}$ with covariance operator $\Gamma_{\text{model}} : \mathcal{B}^* \to \mathcal{B}$ (see [15, section 6] for some details on Gaussian measures on Banach spaces). Then there is measurement / independent error $\varepsilon \sim N(0, \sigma^2 I_m)$, with $I_m$ the $m \times m$ identity. Both error terms and the prior are assumed independent of each other. Let us now understand the terms present in the above expression.
2.1. Dynamics and Observation Operators. One can think of \((\mathcal{O}\mathcal{F}\mathbf{m})_j\) as pointwise evaluations of a continuous function if \(\mathcal{B}\) is some appropriate function space, e.g. \(C(\Omega)\), the Banach space of real-valued continuous functions over a compact \(\mathcal{O}\) with the \(\|\cdot\|_\infty\) norm. These measurements can be represented using the linear functionals \(\delta_{x_j} \in C(\Omega)^*\). In a different setting, we may be able to measure other quantities, e.g. some Fourier coefficients as is the case in MRI applications. Either way, the rows of \(\mathcal{O}\) are linear functionals and we refer to these as measurement vectors. Note that we cannot choose every measurement vector we want, though. For example, we may be restricted only to pointwise evaluations of \(\mathcal{F}\mathbf{m}\) by the sensors at our disposal, in which case measuring the mean \(\ell(u) = \int_{\Omega} u \) (or any non-atomic measure) of a function is not possible.

2.1.2. Error Terms. Considering the sum of the error terms it is easy to see that \(\mathcal{O}\varepsilon' + \varepsilon \in \mathbb{R}^m\). It is a centered Gaussian random vector and its covariance matrix is

\[
\Sigma(O) := \mathbb{E}[(\mathcal{O}\varepsilon' + \varepsilon)(\mathcal{O}\varepsilon' + \varepsilon)^\mathsf{T}] = \mathcal{O}\Gamma_{\text{model}}\mathcal{O}^* + \sigma^2 I,
\]

where

\[
[\mathcal{O}\Gamma_{\text{model}}(\mathcal{O}^*)]_{ij} = \varepsilon_i^* \mathcal{O}\Gamma_{\text{model}}\mathcal{O}^* \varepsilon_j = \mathbf{m}_i(\mathcal{O}\Gamma_{\text{model}}\mathcal{O}^*)_j,
\]

where the first equality in (2.5) holds by definition and the second by (2.3). The explicit dependence on \(\mathcal{O}\) will be mostly dropped for notational convenience, so \(\Sigma(O) = \Sigma\). Thus, for a fixed \(\mathcal{O}\) (i.e. a fixed set of measurements) we can equivalently write \(\mathbf{d} = \mathcal{O}\mathbf{F}\mathbf{m} + \bar{\varepsilon}\) with \(\bar{\varepsilon} \sim \mathcal{N}(0, \Sigma)\). At this point, it is useful to rewrite the posterior covariance operator of our inverse problem from (2.1)

\[
\Gamma_{\text{post}} = (\Gamma_{\text{pr}}^{-1} + \mathcal{F}\mathcal{O}^*\Sigma^{-1}\mathcal{O}\mathcal{F})^{-1}.
\]

Taking \(\Gamma_{\text{model}} = 0\) is common practice [10, 16, 18] and then we are reduced to the case where we take iid observations and \(\Sigma = \sigma^2 I\) is simply a scalar matrix that does not depend on \(\mathcal{O}\). Note that taking an error model with a non-scalar covariance as we do here allows us to consider model error (modeled by \(\Gamma_{\text{model}}\)) as well as measurement error (modeled by \(\sigma^2\)). For example, say we believe our forward model does not capture some small scale phenomenon. Then we may express this belief by saying \(\mathcal{F}_{\text{True}} = \mathcal{F} + \mathcal{F}_{\text{Error}}\), with \(\mathcal{F}\) depending on \(\mathbf{m}\) and \(\mathcal{F}_{\text{Error}}\) depending on \(\mathbf{m}_{\text{SmallScale}}\), and \(\mathbf{m} \perp \mathbf{m}_{\text{SmallScale}}\). We do not know much about this effect but it is reasonable to assume it changes continuously in our domain. We (may choose to) model it as \(\mathcal{N}(0, \Gamma_{\text{model}})\) and take \(\Gamma_{\text{model}}\) to reflect the spatial (or other) variability we imagine \(\mathcal{F}_{\text{Error}}\mathbf{m}_{\text{SmallScale}}\) has. Such small scale phenomenon can arise as a modeling issue, where we might not model the system in its entirety. It can also arise from a numerical source, where our discretization of the system is not fine enough to capture all small scale phenomena. We will see that assuming some correlation in the error may reduce the clusterization phenomenon, as is also reported in the literature [17].

2.2. D-Optimal Design in Infinite Dimensions. The meaning of D-optimal design in infinite-dimensional Hilbert spaces was investigated in [1]. Note that the authors make assumptions that amount to \(\Sigma = I\) (implied by \(\Gamma_{\text{model}} = 0, \sigma^2 = 1\)), but we choose not to take these simplification here. This is because \(\Sigma\) can determine “how much” clusterization we see. As stated [1, pp. 681], the results hold for more general covariance matrices. The conclusion is that in infinite-dimensions, a D-optimal design is well-defined as maximizing the expected KL divergence between posterior and prior and is summarized, using our notation, in the following theorem:

**Theorem 2.2** (Slightly modified Theorem 1 from [1]). Let \(\mu_{\text{pr}} = \mathcal{N}(0, \Gamma_{\text{pr}})\) be a centered Gaussian prior on \(\mathcal{H}\) and let \(\mu_{\text{post}} = \mathcal{N}(\mathbf{m}_{\text{post}}, \Gamma_{\text{post}})\) the posterior measure on \(\mathcal{B}\) for the Bayesian linear
We find the inverse problem \( d = \mathcal{O} F m + \mathcal{O} \varepsilon + \varepsilon \) discussed above. Then

\[
\Psi(O) := E_d \left[ D_{KL}(\mu_{\text{post}} || \mu_{\text{pr}}) \right] \\
= \frac{1}{2} \log \det(I + \Gamma_{\text{pr}}^{1/2} \mathcal{F}^* \mathcal{O}^* \Sigma^{-1} \mathcal{O} \mathcal{F}^{\top} \Gamma_{\text{pr}}^{1/2}).
\]

### 3. The Constrained Optimization Problem of D-Optimal Design

From (2.7) we wish to characterize solution(s) of the following optimization problem for \( \Psi \).

\[
\mathcal{O}^* := \arg \max_O \Psi(O) = \arg \max_O \frac{1}{2} \log \det(I + \Gamma_{\text{pr}}^{1/2} \mathcal{F}^* \mathcal{O}^* \Sigma^{-1} \mathcal{O} \mathcal{F}^{\top} \Gamma_{\text{pr}}^{1/2}),
\]

where \( \mathcal{O} \) is constrained to some allowed set of measurements (e.g. pointwise evaluations on \([0, \pi]\)). We seek a formulation of the optimal design using Lagrange multipliers. In section 3.1 we find the gradient of \( \Psi \). In section 3.2 we relax the constraints on \( \mathcal{O} \) so that the optimization problem in (3.1) and find gradients for the new constraints.

#### 3.1. The Objective and its Gradient

In order to use Lagrange multipliers, we need to find the gradient of \( \Psi \). This section is mostly technical and devoted to calculating said gradient. The result is recorded in (3.2).

We start by calculating the first variation. Some calculations are delegated to Lemma B.3 in the appendix. Also, we use the following lemma whose proof is also delegated to the appendix:

**Lemma 3.1** (Generalized from [12]). Let \( Y(t) \) be a differentiable operator-valued function. Assume \( I + Y(t) \) is invertible, \( Y(t) \) self-adjoint and trace-class. Then

\[
\frac{d \log \det(I + Y(t))}{dt} = \text{tr} (I + Y(t))^{-1} \dot{Y}(t).
\]

First variation of \( \Psi(O) \) in the direction \( V \) is:

\[
\delta \Psi(O)V := \frac{d}{d\tau} \bigg|_{\tau=0} \Psi(O + \tau V) \quad \text{(by definition of variation)}
\]

\[
= \frac{1}{2} \frac{d}{d\tau} \bigg|_{\tau=0} \log \det(I + \Gamma_{\text{pr}}^{1/2} \mathcal{F}^* T(O + \tau V) \mathcal{F}^{\top} \Gamma_{\text{pr}}^{1/2}) \quad \text{(by definition (2.7))}
\]

\[
= \frac{1}{2} \text{tr} \left( I + \Gamma_{\text{pr}}^{1/2} \mathcal{F}^* O^* \Sigma^{-1} \mathcal{O} \mathcal{F}^{\top} \Gamma_{\text{pr}}^{1/2} \right)^{-1} \frac{d}{d\tau} \bigg|_{\tau=0} \Gamma_{\text{pr}}^{1/2} \mathcal{F}^* T(O + \tau V) \mathcal{F}^{\top} \Gamma_{\text{pr}}^{1/2} \quad \text{(by A.1)}
\]

\[
= \frac{1}{2} \text{tr} \Gamma_{\text{post}} \mathcal{F}^* (V^* \Sigma^{-1} O - O^* \Sigma^{-1} V \Gamma_{\text{model}} O^* \Sigma^{-1} O) \quad \text{(by B.3)}
\]

\[
- O^* \Sigma^{-1} \Omega \Gamma_{\text{model}} V^* \Sigma^{-1} O + O^* \Sigma^{-1} V \mathcal{F}
\]

\[
= \text{tr} \Gamma_{\text{post}} \mathcal{F}^* (O^* \Sigma^{-1} V - O^* \Sigma^{-1} V \Gamma_{\text{model}} O^* \Sigma^{-1} O) \mathcal{F}
\]

\[
= \text{tr} \Gamma_{\text{post}} \mathcal{F}^* O^* \Sigma^{-1} V (I - \Gamma_{\text{model}} \mathcal{O}^* \Sigma^{-1} \mathcal{O}) \mathcal{F}
\]

\[
= \text{tr} V(I - \Gamma_{\text{model}} \mathcal{O}^* \Sigma^{-1} \mathcal{O}) \mathcal{F} \Gamma_{\text{post}} \mathcal{F}^* O^* \Sigma^{-1}.
\]

Denote

\[
\nabla \Psi(O) := (I - \Gamma_{\text{model}} \mathcal{O}^* \Sigma^{-1} \mathcal{O}) \mathcal{F} \Gamma_{\text{post}} \mathcal{F}^* O^* \Sigma^{-1},
\]
the gradient of \( \Psi(\mathcal{O}) \) and we now justify this definition. Since the trace of \( A := V \nabla \Psi(\mathcal{O}) \in \mathbb{R}^{m \times m} \) is just \( \text{tr} A = \sum_{j=1}^{m} e_j^t A e_j \) (with \( e_j \) the \( j \)th standard basis vector), we see that
\[
\delta \Psi(\mathcal{O}) V = \text{tr} \ V \nabla \Psi(\mathcal{O}) = \sum_{j=1}^{m} V_j (\nabla \Psi(\mathcal{O})_j),
\]
with \( V_j \in B^* \) and \( \nabla \Psi(\mathcal{O})_j \in B^{**} \subseteq B, j = 1, \ldots, m \). Thus, \( \nabla \Psi(\mathcal{O}) \in (B^{**})^m \subseteq B^m \) is indeed the correct gradient and the notation (3.2) is justified. Note that by the comment following (2.3), we view \( V \) (defined on the same space as \( \mathcal{O} \)) as a column vector. Then the gradient \( \nabla \Psi(\mathcal{O}) \) should be viewed as a row vector, as the product \( V \nabla \Psi \) is in \( \mathbb{R}^{m \times m} \). This will prove important in section 3.3.

3.2. Unit Length Constraints and their Gradients. In this section we suggest relaxed constraints in (3.3) and derive their gradient in (3.4), for the purpose of using them in a Lagrange multipliers problem.

As mentioned before, we cannot choose any \( \mathcal{O} \) when maximizing \( \Psi(\mathcal{O}) \). Recall \( \mathcal{O} = (o_1, \ldots, o_m)^t \in (B^*)^m \) and each \( o_j, j = 1, \ldots, m \) must be chosen from some allowed set of functionals in \( B^* \). This set differs based on the kind of sensors we have at our disposal and the properties of \( B \), as discussed in section 2.1.1. The following proposition will give us better understanding of the constraints.

**Proposition 1.** Let \( \mathcal{O} = (o_1, \ldots, o_m)^t, j \in \{1, \ldots, m\}, \sigma^2 > 0 \) and \( \lambda > 1 \). Then \( \Psi(\mathcal{O}) \) increases if we use \( \lambda o_j \) in \( \mathcal{O} \) instead of \( o_j \).

Proof of Proposition 2 is delegated to the appendix but the idea behind it is simple: making rows of \( \mathcal{O} \) large is equivalent to making \( \sigma^2 \) small. This can be understood easily from the formulation of the inverse problem \( \mathbf{d} = \mathcal{O} \mathbf{F}^\dagger + \mathcal{O} e' + \varepsilon \), where \( e' \) can be taken as model error and \( \varepsilon \) is iid measurement error.

We now suggest a more convenient-to-work-with set of constraints. By Proposition 2, we cannot just take all \( B^* \) to be the allowed set of measurement vectors, since this would effectively eliminate measurement error entirely. We note that for point evaluations, the norm of the measurement is always one:
\[
\|\delta_x\| = \sup_{0 \neq u \in \mathcal{C}(\Omega)} \left| \int_{\Omega} u(y) \delta_x(y) \, dy \right| \cdot \frac{\sup_{0 \neq u \in \mathcal{C}(\Omega)} \|u\|}{\sup_{0 \neq u \in \mathcal{C}(\Omega)} \|u\|} = 1, \forall x \in \Omega.
\]
Following this, we also restrict the norm of our measurement vectors to be one. But the norm on functionals is hard to work with. Instead, we assume there exists a Hilbert space \( \mathcal{H} \subseteq B^* \) and take measurements \( o_j \in \mathcal{H}^* = \mathcal{H} \) such that \( \|o_j\| = 1, j = 1, \ldots, m \). Recall that we think of \( B \) as a somewhat restricted space (\( C(\bar{\Omega}) \) with the sup-norm over a bounded domain \( \Omega \), for example) and so \( B^* \) can be thought of as large. Then \( B^* \) can accommodate a reasonable Hilbert space \( \mathcal{H} \). For example, if \( B = C(\bar{\Omega}) \), we take \( \mathcal{H} = L^2(\Omega) \subseteq B^* \). Then
\[
B \subseteq \mathcal{H} \subseteq B^* 
\]
since members of \( C(\bar{\Omega}) \) are bounded, hence square integrable. The unit norm constraint can be written using (2.3) as a series of \( m \) equality constraints (one for each measurement) on \( \mathcal{O} \) as
\[
\phi_j(\mathcal{O}) := \frac{1}{2} \|O^* e_j\|_{\mathcal{H}^*}^2 - \frac{1}{2} = 0, j = 1, \ldots, m
\]
with \( e_j \in \mathbb{R}^m \) the \( j \)th standard basis vector. The first variations are:

\[
\delta \phi_j(O)V = \frac{1}{2} \lim_{\tau \to 0} \tau^{-1}(\| (O + \tau V)^* e_j \|^2_H - \| O^* e_j \|^2_H) = \frac{1}{2} \lim_{\tau \to 0} \tau^{-1}(\langle (O + \tau V)^* e_j, (O + \tau V)^* e_j \rangle_H - \langle O^* e_j, O^* e_j \rangle_H)
\]

\[
= \frac{1}{2} \lim_{\tau \to 0} \tau^{-1}(2\tau \langle O^* e_j, V^* e_j \rangle_H + \tau^2 \langle V^* e_j, V^* e_j \rangle_H)
\]

\[
= \langle O^* e_j, V^* e_j \rangle_H
= \langle V O^* e_j, e_j \rangle_{\mathbb{R}^m}
= e_j^t V O^* e_j
= \text{tr } V O^* e_j e_j^t.
\]

Using the same arguments we used to justify the definition of (3.2), we conclude that

\[
(3.4) \quad \nabla \phi_j(O) = O^* e_j e_j^t = o_j e_j^t, j = 1, \ldots, m,
\]

with \( \nabla \phi_j(O) \in \mathcal{H}_m \subseteq B^m \) and where the last equality follows since \( O^* e_j = o_j \) by (3.3). As we noted at the end of section 3, the gradient \( \nabla \phi_j(O) \) is a row vector.

3.3. Necessary Conditions for Optimal Design. Necessary conditions for optimality are found using Lagrange multipliers:

\[
(3.5) \quad \nabla \Psi(O) = \sum_{j=1}^m \xi_j \nabla \phi_j(O)
\]

\[
(3.6) \quad \phi_j(O) = 0, j = 1, \ldots, m.
\]

Recall where the objects involved are defined: the observation operator, \( O \in \mathcal{H}_m \subseteq (B^*)^m \). The objective \( \Psi: (B^*)^m \to \mathbb{R} \) and its gradient is \( \nabla \Psi(O) \in B^m \). The constraints are defined similarly — \( \phi_j: (B^*)^m \to \mathbb{R} \) and \( \nabla \phi_j(O) \in B^m \).

Focusing on (3.5) and using the gradients of the objective and constraints (3.2) and (3.4) we have:

\[
(I - \Gamma_{\text{model}} O^* \Sigma^{-1} O) \mathcal{F} \Gamma_{\text{post}}^* O^* \Sigma^{-1} = \sum_{j=1}^m \xi_j O^* e_j e_j^t = (\xi_1 o_1, \ldots, \xi_m o_m).
\]

If we let \( \Xi = \text{diag}(\xi_j) \), then with some abuse of notation, we can write this more compactly as:

\[
(3.7) \quad (I - \Gamma_{\text{model}} O^* \Sigma^{-1} O) \mathcal{F} \Gamma_{\text{post}}^* O^* \Sigma^{-1} = O^* \Xi.
\]

4. Analysis of Optimal Designs — Vanishing Model Error

When \( \Gamma_{\text{model}} = 0 \), then \( \Sigma = \sigma^2 I \). The necessary first-order condition for optimality (3.7) becomes

\[
(4.1) \quad \sigma^{-2} \mathcal{F} \Gamma_{\text{post}}^* O^* = O^* \Xi,
\]

with \( \Xi \) diagonal. This is an eigenvalue problem for the self-adjoint operator \( \sigma^{-2} \mathcal{F} \Gamma_{\text{post}}^* \mathcal{F}^* \) where the rows of \( O \), namely \( o_j, j = 1, \ldots, m \), are the eigenvectors. If \( \mathcal{F} \) is invertible, then we may write:

\[
O^* \Xi = \sigma^{-2} \mathcal{F} \Gamma_{\text{post}}^* O^* O^* = \sigma^{-2} \mathcal{F} \Gamma_{\text{post}}^* (\Gamma_{\text{pr}}^{-1} + \sigma^{-2} \mathcal{F}^* O^* O \mathcal{F})^{-1} \mathcal{F}^* O^* = \sigma^{-2} ((\mathcal{F} \Gamma_{\text{pr}} \mathcal{F}^*)^{-1} + \sigma^{-2} O^* O)^{-1} O^*.
\]
which presents the optimal design problem as a problem on \( B \) and not on \( \mathcal{H} \) — the term \((\mathcal{F} \Gamma_{pr} \mathcal{F}^*)^{-1}\) is the prior precision in \( B \) and the big parentheses enclose the posterior precision in \( B \). This expression makes sense even if \( \mathcal{F} \) is not invertible — consider instead \( \mathcal{F} \) restricted to \( \text{ker} \mathcal{F}^\perp \). This does not change the optimal design problem at all, since we will never take measurements that have a component in \( \text{ker} \mathcal{F} \) (this can be understood from Corollary 2).

**4.1. Characterizing D-Optimal Designs.** In light of (4.2), let us denote eigenvalues of \( \mathcal{F} \Gamma_{pr} \mathcal{F}^* \) by \( \lambda_1 \geq \lambda_2 \geq \ldots \) and its eigenvectors \( \{e_i\}_{i=1}^\infty \). The following lemma will be useful:

**Lemma 4.1** (Proved as lemma B.4 in the appendix). Let \( C : \mathcal{H} \to \mathcal{H} \) self-adjoint and let \( a_1, \ldots, a_m \in \mathcal{H} \). Denote \( a^* \) the element \( a \) acting as a linear functional. If

\[
(C + \sum_{j=1}^m a_j a_j^*) a_k = \xi_k a_k, k = 1, \ldots, m
\]

then \( C \) and \( \sum_{j=1}^m a_j a_j^* \) are simultaneously diagonalizable.

Thus, if we take \( a_j^* = o_j \) and \( C := (\mathcal{F} \Gamma_{pr} \mathcal{F}^*)^{-1} \) in the above lemma, we conclude from the eigenproblem (4.2) that \( \mathcal{O}^* \mathcal{O} \) has the same eigenvectors as \( \mathcal{F} \Gamma_{pr} \mathcal{F}^* \), namely \( \{e_i\}_{i=1}^\infty \) (infinitely many of them with zero eigenvalue, since \( \mathcal{O}^* \mathcal{O} \) is finite-rank). Denote the corresponding non-zero eigenvalues of \( \mathcal{O}^* \mathcal{O} \) by \( \{\eta_i\}_{i=1}^k \) and let \( \eta_i = 0 \) for \( i \geq k + 1 \). By the argument in the paragraph following (4.2):

\[
I + \sigma^{-2} \Gamma_{pr}^{1/2} \mathcal{F}^* \mathcal{O}^* \mathcal{O} \Gamma_{pr}^{1/2} = \Gamma_{pr}^{1/2} (\Gamma_{pr}^{-1} + \sigma^{-2} \mathcal{F}^* \mathcal{O}^* \mathcal{O}) \Gamma_{pr}^{1/2}
\]

\[
= \Gamma_{pr}^{1/2} \mathcal{F}^* (\mathcal{F}^{-1} \Gamma_{pr}^{-1} \mathcal{F}^{-1} + \sigma^{-2} \mathcal{O}^* \mathcal{O}) \mathcal{F} \Gamma_{pr}^{1/2}
\]

\[
= \Gamma_{pr}^{1/2} \mathcal{F}^* ((\mathcal{F} \Gamma_{pr} \mathcal{F}^*)^{-1} + \sigma^{-2} \mathcal{O}^* \mathcal{O}) \mathcal{F} \Gamma_{pr}^{1/2}.
\]

By definition of the objective (2.7) and using (4.3):

\[
\Psi(\mathcal{O}) = \frac{1}{2} \log \det (I + \sigma^{-2} \Gamma_{pr}^{1/2} \mathcal{F}^* \mathcal{O}^* \mathcal{O} \Gamma_{pr}^{1/2})
\]

\[
= \frac{1}{2} \log \det (\mathcal{F} \Gamma_{pr} \mathcal{F}^* (\mathcal{F} \Gamma_{pr} \mathcal{F}^*)^{-1} + \sigma^{-2} \mathcal{O}^* \mathcal{O}) \mathcal{F} \Gamma_{pr} \mathcal{F}^*
\]

\[
= \frac{1}{2} \log \left( \prod_{i=1}^\infty (\lambda_i^{-1} + \sigma^{-2} \eta_i) \prod_{i=1}^\infty \lambda_i \right)
\]

\[
= \frac{1}{2} \log \left( \prod_{i=1}^k (\lambda_i^{-1} + \sigma^{-2} \eta_i) \prod_{i=1}^k \lambda_i \right).
\]

Therefore, an optimal design maximizes

\[
\sum_{i=1}^k \log(\lambda_i^{-1} + \sigma^{-2} \eta_i),
\]

with the norm constraints on \( o_j, j = 1, \ldots, m \). We show in the appendix (Lemma B.2) we can find \( o_1, \ldots, o_m \) such that \( \{\eta_i\}_{i=1}^k \) have any value we desire, subject only to the restriction that we do not change the trace of \( \mathcal{O}^* \mathcal{O} \), so that \( \sum_{i=1}^k \eta_i = m \). By concavity of \( \log \), the fastest increase in the design criterion (equation (4.5)) is gained by increasing \( \lambda_i^{-1} + \sigma^{-2} \eta_i \) where it is smallest. So, no weight should be given to (i.e. measurement taken of) the \( k \)th eigenvector before \( \lambda_i^{-1} + \sigma^{-2} \eta_i \geq \ldots \)
Figure 2. Posterior precision per eigenvector, after taking a measurement \( o_i \).
Each \( o_i \) increases precision uniformly across the lowest precision eigenvectors. We see that \( o_2 \) and \( o_3 \) are repeated measurements, as well as \( o_5 \) and \( o_6 \).

\[ \lambda_k^{-1}, \forall i \neq k. \] Thus, we should choose \( \{ \eta_i \}_{i=1}^k \) as follows. We would increase \( \lambda_1^{-1} + \sigma^{-2} \eta_i \) until it equals \( \lambda_2^{-1} \). Then, \( \lambda_i^{-1} + \sigma^{-2} \eta_i, i = 1, 2 \) are increased until \( \lambda_2^{-1} + \sigma^{-2} \eta_i = \lambda_3^{-1}, i = 1, 2 \) and so forth.

The argument above has the important consequence that the eigenvalues in (4.1) are all equal! This makes perfect sense. First, we know the Lagrange multipliers tell us how much we gain by relaxing the constraints and there is no reason for any measurement to give us more than any other (otherwise we would put more weight on the better measurement, as can be understood from the discussion in the following paragraph). We are also used to symmetric optimization problems having symmetric solutions \([19]\), so symmetric and identical Lagrange multipliers definitely make sense in this context.

4.2. Sensor Clusterization. The way clusterization can occur is best understood from figure 2. We see that each measurement increases precision (reduces uncertainty) only for the eigenvectors of lowest precision. If the precision in these is lower than the precision for the next eigenvector, a repeated measurement is optimal.

5. Analysis of Optimal Designs — Non-Vanishing Model Error

Denote \( O = (o_1, \ldots, o_m)^t \) and \( \tilde{O} := (o_1, \ldots, o_{m-1})^t \). The following corollary is proved in the appendix.

**Corollary 1** (Proved as corollary 3 in the appendix). If \( o_m = o_j \) for some \( 1 \leq j \leq m - 1 \), then

\[ \Psi(O) - \Psi(\tilde{O}) = \log \left( 1 + \frac{\sigma^2 (\mathcal{F}^* \mathcal{F}^* \hat{\Sigma}_j \hat{\Sigma}_j^{-1} e_j, \hat{\Sigma}_j \hat{\Sigma}_j^{-1} e_j)}{2 - \sigma^2 e_j^t \Sigma_j^{-1} e_j} \right). \]

In contrast to the previous case of vanishing model error, we will see that if \( \Gamma_{\text{model}} \neq 0 \) clustering will not occur. From Corollary 3 we can observe that as \( \sigma^2 \to 0 \), the increase in the design
criterion gained by taking a measurement identical to a previous one approaches zero. We may conclude that for small measurement error levels, the clusterization effect will be mitigated by the presence of a non-zero model error. Since the design criterion is not defined for $\sigma^2 = 0$ and identical measurements, we cannot make a statement regarding $\sigma^2 = 0$, except in the limiting sense described above.

6. Conclusion

Our relaxed model gives us insight to D-optimal designs. We see that in our setting, uncertainty is not reduced in any direction (eigenvector) before it is the largest uncertainty present. We show how and why repeated measurements can give rise to a D-optimal design. There is more work to be done in understanding exactly what causes such designs to be strictly better than others.

7. Acknowledgements

This study is a part of my PhD thesis [6] which was written under the instruction of Prof. Georg Stadler in New York University’s Courant Institute. I would like to thank him for his great mentorship.

Appendix A. Widely Applicable Lemmas

The following lemma is generalized from [12, Chapter 9, Theorem 4, pp. 127]

Lemma A.1. Let $Y(t)$ be a differentiable operator-valued function. Assume $I + Y(t)$ is invertible, $Y(t)$ self-adjoint and trace-class. Then

$$\frac{d \log \det(I + Y(t))}{dt} = \text{tr} \left( I + Y(t) \right)^{-1} Y(t).$$

Proof. Consider a differentiable operator-valued function $X(t)$ such that $X(0) = 0$ and $X(t)$ is positive, self-adjoint and trace-class for every $t \in \mathbb{R}$. We denote the eigenvalues of this operator by $\lambda_k(X(t))$ and sometimes drop the dependence on $X(t)$, so $\lambda_k = \lambda_k(X(t))$. Then $\det(I + X(t)) = \prod_{k=1}^{\infty} (1 + \lambda_k) < \infty$ where the bound holds by the arguments given in [1]. The full derivative is

$$\frac{d \det(I + X(t))}{dt} = \sum_{k=1}^{\infty} \frac{\partial \det(I + X(s))}{\partial (1 + \lambda_k)} \bigg|_{s=t} \frac{d(1 + \lambda_k)}{dt}$$

$$= \sum_{k=1}^{\infty} \frac{\partial \prod_{l=1}^{\infty} (1 + \lambda_l(s))}{\partial (1 + \lambda_k)} \bigg|_{s=t} \frac{d(1 + \lambda_k)}{dt}$$

$$= \sum_{k=1}^{\infty} \frac{\prod_{l=1}^{\infty} (1 + \lambda_l(s))}{(1 + \lambda_k)} \lambda_k(X(t))$$

$$= \sum_{k=1}^{\infty} \frac{\det(I + X(t))}{1 + \lambda_k} \lambda_k(X(t)).$$

The assumption $X(0) = 0$ means $\lambda_k(X(0)) = 0$, $\forall k \geq 1$. Thus:

$$\left. \frac{d(I + \det X(t))}{dt} \right|_{t=0} = \sum_{k=1}^{\infty} \lambda_k(X(0)) = \frac{d}{dt} \text{tr} X(0) = \text{tr} \dot{X}(0),$$
where the second equality follows by monotone convergence. Let \( Y(t) \) a trace-class self-adjoint operator such that \( I + Y(t) \) is invertible. Define \( X(t) \) via \( I + X(t) = (I + Y(0))^{-1/2}(I + Y(t))(I + Y(0))^{-1/2} \). We show \( X(t) \) satisfies the conditions above. It is trace-class:

\[
\text{tr } X(t) = \text{tr } ((I + Y(0))^{-1}(I + Y(t)) - I) \leq \text{tr } (I + Y(t) - I) < \infty,
\]
since \( Y(t) \) is trace-class. It is also clear that \( X(0) = 0 \) and \( X(t) \) is self-adjoint. \( I + Y(t) = (I + Y(0))^{1/2}(I + X(t))(I + Y(0))^{1/2} \), so

\[
\begin{align*}
\frac{d\det(I + Y(t))}{dt}|_{t=0} &= \det(I + Y(0)) \frac{d\det(I + X(t))}{dt}|_{t=0} \\
&= \det(I + Y(0)) \text{tr } X(0) \\
&= \det(I + Y(0)) \text{tr } (I + Y(0))^{-1}\dot{Y}(0).
\end{align*}
\]

Consequently, by the one-variable chain rule:

\[
\frac{d\log \det(I + Y(t))}{dt}|_{t=0} = \frac{1}{\det(I + Y(0))} \frac{d\det(I + Y(t))}{dt}|_{t=0} \\
&= \text{tr } (I + Y(t))^{-1}\dot{Y}(t)|_{t=0}.
\]

Since there is nothing special about \( t = 0 \), the relation holds for all \( t \). \( \square \)

**Lemma A.2** (Matrix Determinant Lemma in Hilbert Spaces). Let \( \mathcal{H} \) a separable Hilbert space, \( u, v \in \mathcal{H} \) and \( A : \mathcal{H} \to \mathcal{H} \) an invertible linear operator such that \( \text{tr } A - I < \infty \). Then \( \det A \) and \( \det A + uv^* \) are well defined and

\[
\det(A + uv^*) = (1 + \langle A^{-1}u, v \rangle) \det A,
\]

where \( (A + uv^*)w := Aw + \langle v, w \rangle u \).

**Proof.** In this proof we rely on definitions and results from [14]. First, consider \( B := I + xy^* \) for some \( x, y \in \mathcal{H} \). We construct an eigenbasis for \( B \) and use that to show \( \det B = 1 + \langle x, y \rangle \). First let \( x_1 := x \). Now, if \( x \parallel y \), take \( \{x_n\}_{n=2}^\infty \) an orthogonal basis for \( \text{span}\{x_1\}^\perp \). If, on the other hand, \( x \parallel y \), let

\[
x_2 := x - \frac{\langle x, y \rangle}{\|y\|^2} y
\]

and it is easy to verify that \( x_2 \perp y \) and \( \text{span}\{x, y\} = \text{span}\{x_1, x_2\} \). Take \( \{x_n\}_{n=3}^\infty \) an orthogonal basis for \( \text{span}\{x_1, x_2\}^\perp \). In both cases,

\[
Bx_n = \begin{cases} 
(1 + \langle x, y \rangle)x_n & n = 1 \\
\langle x, y \rangle x_n & n \neq 1,
\end{cases}
\]

and so \( \det B = 1 + \langle x, y \rangle \).

It is easy to verify that \( uv^* \) is trace-class and since \( \text{tr } A - I < \infty \), also \( \text{tr } A + uv^* - I < \infty \) (sum of two trace-class operators is trace-class). Thus \( \det A \) and \( \det(A + uv^*) \) are well defined. Let \( x := A^{-1}u \) and \( y := v \):

\[
\det(A + uv^*) = \det A \det(I + A^{-1}uv^*) = (1 + \langle A^{-1}u, v \rangle) \det A.
\]

\( \square \)
APPENDIX B. SPECIFIC LEMMAS

Lemma B.1 (Increase due to a Measurement). Let $O = (o_1, \ldots, o_m)^t$ and $\hat{O} := (o_1, \ldots, o_{m-1})^t$. Then

$$\Psi(O) - \Psi(\hat{O}) = \frac{1}{2} \log \left( 1 + \frac{(F_{\text{post}}^\top F^* (\hat{O}^\top \Sigma^{-1} \Gamma_{\text{model}} - I) o_m, (\hat{O}^\top \Sigma^{-1} \Gamma_{\text{model}} - I) o_m)^t}{\sigma^2 + o_m \Gamma_{\text{model}} o_m - o_m \Gamma_{\text{model}} \hat{O}^\top \Sigma^{-1} \hat{O} \Gamma_{\text{model}} o_m} \right).$$

Proof. We use the Schur complement to write one inverse in terms of the other and introduce notations to make the derivation cleaner. Note that we think of $\hat{O}$ and $\hat{O}^*$ as column and row vectors (respectively).

$$\Sigma(O) = \Sigma = \begin{bmatrix} \Sigma(\hat{O}) & \hat{O} \Gamma_{\text{model}} o_m \\ o_m \Gamma_{\text{model}} \hat{O}^* & \sigma^2 + o_m \Gamma_{\text{model}} o_m \end{bmatrix} = \begin{bmatrix} \hat{\Sigma} & w \\ w^t & c \end{bmatrix}$$

$$\Sigma^{-1} = \begin{bmatrix} \hat{\Sigma}^{-1} + \hat{\Sigma}^{-1} w (c - w^t \hat{\Sigma}^{-1} w)^{-1} w^t \hat{\Sigma}^{-1} & -\hat{\Sigma}^{-1} w (c - w^t \hat{\Sigma}^{-1} w)^{-1} \\ -(c - w^t \hat{\Sigma}^{-1} w)^{-1} w^t \hat{\Sigma}^{-1} & (c - w^t \hat{\Sigma}^{-1} w)^{-1} \end{bmatrix}$$

$$= \begin{bmatrix} \hat{\Sigma}^{-1} & 0 \\ 0 & (c - w^t \hat{\Sigma}^{-1} w)^{-1} \end{bmatrix} [w^t \hat{\Sigma}^{-1} -1]$$

Further, define

$$M(O) := \Gamma_{\text{pr}}^{1/2} F^* O^* \Sigma^{-1} O F_{\text{pr}}^{1/2}$$

and note that, using our understanding of what is a column vector and what is a row vector:

$$M(O) = \Gamma_{\text{pr}}^{1/2} F^* O^* \Sigma^{-1} O F_{\text{pr}}^{1/2}$$

$$= \Gamma_{\text{pr}}^{1/2} F^* O^* \left\{ \begin{bmatrix} \hat{\Sigma}^{-1} & 0 \\ 0 & (c - w^t \hat{\Sigma}^{-1} w)^{-1} \end{bmatrix} [w^t \hat{\Sigma}^{-1} -1] \right\} O F_{\text{pr}}^{1/2}$$

$$= M(\hat{O}) + (c - w^t \hat{\Sigma}^{-1} w)^{-1} \Gamma_{\text{pr}}^{1/2} F^* O^* \left[ \begin{bmatrix} \hat{\Sigma}^{-1} w \\ -1 \end{bmatrix} [w^t \hat{\Sigma}^{-1} -1] \right] O F_{\text{pr}}^{1/2}$$

Now, denote:

$$u := (c - w^t \hat{\Sigma}^{-1} w)^{-1/2} \Gamma_{\text{pr}}^{1/2} F^* O^* \left[ \begin{bmatrix} \hat{\Sigma}^{-1} w \\ -1 \end{bmatrix} \right]$$

(B.1)

$$u^* := (c - w^t \hat{\Sigma}^{-1} w)^{-1/2} (\Gamma_{\text{pr}}^{1/2} F^* O^* \Sigma^{-1} \Gamma_{\text{model}} o_m - \Gamma_{\text{pr}}^{1/2} F^* o_m)$$

so that

(B.2) $$I + M(O) = I + M(\hat{O}) + uu^*.$$ 

Note that

(B.3) $$\Gamma_{\text{pr}}^{1/2} \left( I + M(\hat{O}) \right)^{-1} = \Gamma_{\text{post}}^{1/2}.$$
The increase in the design criterion gained by including $o_m$ in the design is found by using Lemma A.2 the above results:

$$\Psi(\mathcal{O}) - \Psi(\hat{\mathcal{O}}) = \frac{1}{2} \log \det \left( I + M(\mathcal{O}) \right) / \det \left( I + M(\hat{\mathcal{O}}) \right)$$

$$= \frac{1}{2} \log \det \left( I + M(\hat{\mathcal{O}}) + uu^* \right) / \det \left( I + M(\hat{\mathcal{O}}) \right)$$

$$= \frac{1}{2} \log \left( 1 + \langle (I + M(\hat{\mathcal{O}}))^{-1} u, u \rangle \right).$$

Using (B.1):

$$\left\langle (I + M(\hat{\mathcal{O}}))^{-1} u, u \right\rangle$$

$$= (\hat{F} \hat{\Gamma}_{\text{post}} F^{\ast} o_m, o_m)$$

$$= \sigma^2 + o_m \Gamma_{\text{model}} o_m - o_m \Gamma_{\text{model}} \hat{\Sigma}^{-1}$$

and the conclusion follows. □

Lemma B.1 implies the following two corollaries.

**Corollary 2** (Gain for No Model Error). If $\Gamma_{\text{model}} = 0$, then

$$\Psi(\mathcal{O}) - \Psi(\hat{\mathcal{O}}) = -\frac{1}{2} \log \left( 1 - \sigma^{-2} \langle \hat{F} \hat{\Gamma}_{\text{post}}^{\ast} o_m, o_m \rangle \right).$$

**Proof.** Note that this is not immediate by substituting $\Gamma_{\text{model}} = 0$ in the conclusion of Lemma B.1, since we make a claim for $\hat{\Gamma}_{\text{post}}$, and not $\Gamma_{\text{post}}$. Let us first review (B.1) and note that since $\Gamma_{\text{model}} = 0$ the covariance $\hat{\Sigma} = \sigma^2 I_{m-1}$ and $w = 0$, so $c - w^t \hat{\Sigma}^{-1} w = \sigma^2$:

$$u : = -\sigma^{-1} \Gamma^{1/2}_{\text{pr}} F^{\ast} o_m$$

$$u^* : = -\sigma^{-1} o_m \Gamma^{1/2}_{\text{pr}}.$$

From (B.2):

$$I + M(\hat{\mathcal{O}}) = I + M(\mathcal{O}) - uu^*,$$

and thus:

$$\left\langle (I + M(\mathcal{O}))^{-1} u, u \right\rangle = \sigma^{-2} \langle \hat{F} \hat{\Gamma}_{\text{post}}^{\ast} o_m, o_m \rangle.$$

Analogously to (B.3) we note that

$$\Gamma^{1/2}_{\text{pr}} (I + M(\mathcal{O}))^{-1} \Gamma^{1/2}_{\text{pr}} = \hat{\Gamma}_{\text{post}}.$$
Using Lemma A.2 we conclude
\[
\Psi(O) - \Psi(\widehat{O}) = \frac{1}{2} \log \det (I + M(O)) / \det (I + M(\widehat{O})) \\
= \frac{1}{2} \log \det (I + M(O)) / \det (I + M(O) - uu^*) \\
= -\frac{1}{2} \log (1 - \langle (I + M(O))^{-1}u, u \rangle) \\
= -\frac{1}{2} \log(1 - \sigma^{-2}(F\Gamma_{post}^*o_m, o_m)).
\]

\[\square\]

**Corollary 3** (Gain for Identical Measurement). If \(o_m = o_j\) for some \(1 \leq j \leq m - 1\), then
\[
\Psi(O) - \Psi(\widehat{O}) = \log \left( 1 + \frac{\sigma^2(F\Gamma_{post}^*\hat{\Sigma}^{-1}e_j, \hat{\Sigma}^{-1}e_j)}{2 - \sigma^2 e_j^t\hat{\Sigma}^{-1}e_j} \right).
\]

**Proof.** Denote \(A := O\Gamma_{model}O^*\) and \(v_j\) the \(j\)th column of \(A\). Note that \(v_j = \hat{\Gamma}_{model}o_m\), since \((\hat{\Gamma}_{model}\hat{\Sigma}e_j)_{ij} = o_i(\Gamma_{model}o_j)\), as explained in (2.5). One can now verify that
\[
\hat{\Sigma}^{-1}\hat{\Gamma}_{model}o_m = \hat{\Sigma}^{-1}v_j = (A + \sigma^2I_{m-1})^{-1}v_j = e_j - \sigma^2\hat{\Sigma}^{-1}e_j.
\]
Using (B.4):
\[
o_m\Gamma_{model}\hat{\Sigma}^{-1}\hat{\Gamma}_{model}o_m = o_m\Gamma_{model}\hat{\Gamma}^* (e_j - \sigma^2\hat{\Sigma}^{-1}e_j)
\]
\[
= o_m\Gamma_{model}o_j - \sigma^2 o_m\Gamma_{model}\hat{\Sigma}^{-1}e_j
\]
\[
= o_m\Gamma_{model}o_j - \sigma^2 (e_j - \sigma^2\hat{\Sigma}^{-1}e_j) e_j
\]
\[
= o_m\Gamma_{model}o_m - \sigma^2 + \sigma^4 e_j^t\hat{\Sigma}^{-1}e_j.
\]
We use (B.4) to simplify the terms in the enumerator of the conclusion of Lemma B.1:
\[
(\hat{\Gamma}^*\hat{\Sigma}^{-1}\hat{\Gamma}_{model} - I)o_m = \hat{\Gamma}^*\hat{\Sigma}^{-1}\hat{\Gamma}_{model}o_m - o_m
\]
\[
= \hat{\Gamma}^*(e_j - \sigma^2\hat{\Sigma}^{-1}e_j) - o_j
\]
\[
= -\sigma^2\hat{\Gamma}^*\Sigma^{-1}e_j.
\]
Substitute (B.6) and (B.5) to the enumerator and denominator (respectively) of the conclusion of Lemma B.1:
\[
\Psi(O) - \Psi(\widehat{O}) = \log \left( 1 + \frac{\langle F\Gamma_{post}^*\hat{\Gamma}^*\hat{\Sigma}^{-1}\Gamma_{model} - I \rangle o_m, (\hat{\Gamma}^*\hat{\Sigma}^{-1}\Gamma_{model} - I) o_m \rangle}{\sigma^2 + o_m\Gamma_{model}o_m - o_m\Gamma_{model}\hat{\Gamma}^*\hat{\Sigma}^{-1}\hat{\Gamma}_{model}o_m} \right)
\]
\[
= \log \left( 1 + \frac{\sigma^2 \langle F\Gamma_{post}^*\hat{\Sigma}^{-1}e_j, \hat{\Sigma}^{-1}e_j \rangle}{2\sigma^2 - \sigma^4 e_j^t\hat{\Sigma}^{-1}e_j} \right)
\]
\[
= \log \left( 1 + \frac{\sigma^2 \langle F\Gamma_{post}^*\hat{\Sigma}^{-1}e_j, \hat{\Sigma}^{-1}e_j \rangle}{2 - \sigma^2 e_j^t\hat{\Sigma}^{-1}e_j} \right).
\]

\[\square\]

**Lemma B.2.** Let \(M \in \mathbb{R}^{k \times k}\) symmetric positive definite with \(\text{tr } M = m, m > k\). Then we can find \(a_j \in \mathbb{R}^k, j = 1, \ldots, m\) with \(\|a_j\| = 1\) and \(A = (a_1, \ldots, a_m)\) such that \(AA^t = M\).
such that rows and columns

Note that conjugating a matrix by $R$ This quadratic in

and it suffices to choose $\theta$ such that $A$ also satisfies the unit norm constraints we are done. These constraints are, for $j = 1, \ldots, m$:

$$(B.7) \quad 1 = [A' A]_{jj} = [V S' S V']_{jj},$$

and we can expect to do this since we assumed $\text{tr} D = m$.

Define $C = S' S - I \in \mathbb{R}^{m \times m}$. Note that $\text{tr} C = 0$ and $C$ is diagonal with non-zero entries $d_i - 1, i = 1, \ldots, k$. It suffices to find $V$ orthogonal such that $V C V^t$ has zero diagonal. We construct such $V$ by sequentially inserting zeros in the diagonal and not destroying zeros we already introduced, starting from the last diagonal entry and moving to the first. If $c_{kk} \neq 0$, let $p < k$ such that $c_{pp} c_{kk} < 0$ (such $p$ exists because the trace is zero) and let $\theta \in (0, \pi)$. Define a Givens rotation $R^{(k)} \in \mathbb{R}^{m \times m}$ by

$$r_{ab}^{(k)} := \begin{cases} 1 & a = b \neq p \text{ or } a = b \neq k \\ \cos \theta & a = b = p \\ -\sin \theta & a = p, b = k \\ \cos \theta & a = b = k \\ \sin \theta & a = k, b = p \\ 0 & \text{o.w} \end{cases}$$

Note that conjugating a matrix by $R^{(k)}$ changes only its $k$ and $p$ rows and columns. Specifically, it leaves rows and columns $k + 1, \ldots, m$ unchanged. We want to choose $\theta$ such that

$$(B.8) \quad 0 = [R^{(k)} C (R^{(k)})^t]_{kk} = \cos^2 \theta c_{kk} + 2 \cos \theta \sin \theta c_{kp} + \sin^2 \theta c_{pp},$$

and it suffices to choose $\theta$ such that

$$c_{kk} \cot^2 \theta + 2 c_{kp} \cot \theta + c_{pp} = 0.$$ 

This quadratic in $\cot \theta$ has a real solution, since $c_{pp} c_{kk} < 0$ by assumption and we can find $\theta \in (0, \pi)$ such that (B.8) is satisfied. We continue to find $R^{(k-1)}$ that leaves rows and columns $k, \ldots, m$ unchanged and continue introducing zeros to the diagonal. The assumption $\text{tr} D = m \Rightarrow \text{tr} C = 0$ guarantees we can do this. Taking $V := R^{(1)} R^{(2)} \ldots R^{(k-1)} R^{(k)}$ completes the proof. \hfill \Box

**Lemma B.3** (Auxilliary Calculations). Let $T(\mathcal{O}) := \mathcal{O}^* \Sigma^{-1} (O) \mathcal{O}$, with $\Sigma(\mathcal{O})$ defined as in (2.4). Then:

$$\delta T(\mathcal{O}) V = V^* \Sigma^{-1} \mathcal{O} - \mathcal{O}^* \Sigma^{-1} V \Gamma_{\text{model}} \mathcal{O}^* \Sigma^{-1} \mathcal{O} - \mathcal{O}^* \Sigma^{-1} \mathcal{O} \Gamma_{\text{model}} V^* \Sigma^{-1} \mathcal{O} + \mathcal{O}^* \Sigma^{-1} V.$$

**Proof.** We need a few supplementary calculations. First:

$$(B.9) \quad \frac{d}{d\tau} \bigg|_{\tau=0} \Sigma(\mathcal{O} + \tau V) = \frac{d}{d\tau} \bigg|_{\tau=0} (\mathcal{O} + \tau V) \Gamma_{\text{model}} (\mathcal{O} + \tau V)^* + \sigma^2 I = V \Gamma_{\text{model}} \mathcal{O}^* + \mathcal{O} \Gamma_{\text{model}} V^*.$$
By the standard trick for the derivative of an operator:

\[
0 = \left. \frac{d}{d\tau} I \right|_{\tau=0} = \left. \frac{d}{d\tau} \left( \Sigma(\mathcal{O} + \tau V)^{-1}\Sigma(\mathcal{O} + \tau V) \right) \right|_{\tau=0} = \left. \frac{d\Sigma(\mathcal{O} + \tau V)^{-1}}{d\tau} \right|_{\tau=0} + \left. \Sigma^{-1} \frac{d\Sigma(\mathcal{O} + \tau V)}{d\tau} \right|_{\tau=0}
\]

\[
= \left. \frac{d\Sigma(\mathcal{O} + \tau V)^{-1}}{d\tau} \right|_{\tau=0} \Sigma + \Sigma^{-1}(\mathcal{V}_{\text{model}}\mathcal{O}^* + \mathcal{O}\mathcal{V}_{\text{model}}V^*) \Sigma^{-1},
\]

by (B.9).

Now we can write the variation of \(\Sigma^{-1}\):

\[
\left. \frac{d\Sigma(\mathcal{O} + \tau V)^{-1}}{d\tau} \right|_{\tau=0} = -\Sigma^{-1}(\mathcal{V}_{\text{model}}\mathcal{O}^* + \mathcal{O}\mathcal{V}_{\text{model}}V^*) \Sigma^{-1}.
\]

Finally, we can do the calculation we need to. By Leibnitz (product) rule and (B.10):

\[
\delta T(\mathcal{O})V = \left. \frac{dT(\mathcal{O} + \tau V)}{d\tau} \right|_{\tau=0} = V^*\Sigma^{-1}\mathcal{O} - \mathcal{O}^*\Sigma^{-1}\mathcal{V}_{\text{model}}\mathcal{O}^*\Sigma^{-1}\mathcal{O} - \mathcal{O}^*\Sigma^{-1}\mathcal{O}\mathcal{V}_{\text{model}}V^*\Sigma^{-1}\mathcal{O} + \mathcal{O}^*\Sigma^{-1}V,
\]
as required.

**Lemma B.4.** Let \(C : \mathcal{H} \to \mathcal{H}\) self-adjoint and let \(a_1, \ldots, a_m \in \mathcal{H}\). Denote \(a^*\) the element \(a\) acting as a functional. If

\[
(C + \sum_{j=1}^{m} a_j a_j^*)a_k = \xi_k a_k, \quad k = 1, \ldots, m
\]

then \(C\) and \(\sum_{j=1}^{m} a_j a_j^*\) are simultaneously diagonalizable.

**Proof.** First, enumerate the eigenvalues of \(C + \sum_{j=1}^{m} a_j a_j^*\) as \(\xi_1, \ldots, \xi_\ell\). Denote the indices of the eigenvectors corresponding to \(\xi_i\)

\[
S_i := \{1 \leq k \leq m | (C + \sum_{j=1}^{m} a_j a_j^*)a_k = \xi_k a_k \}.
\]

Define further

\[
A_i := \sum_{k \in S_i} a_k a_k^*,
\]

which is self-adjoint. Two observations are in order. First, \(\sum_{j=1}^{m} a_j a_j^* = \sum_{i=1}^{\ell} A_i\). Second, \(A_i a_k = 0\) if \(k \not\in S_i\), since eigenvectors of different eigenvalue are orthogonal. For \(k \in S_i\)

\[
\xi_i a_k = (C + \sum_{j=1}^{m} a_j a_j^*)a_k = (C + A_i)a_k.
\]

Let \(V_i := \text{span}\{a_k\}_{k \in S_i}\). Observe that \(V_i\) is invariant under \(A_i\), by definition, and under \(C\), by (B.11). Using (B.11) again, we conclude that on \(V_i\), \(A_i = \xi_i I - C\). This immediately implied \(A_i\) and \(C\) have the same eigenvectors on \(V_i\). This holds for every \(1 \leq i \leq \ell\) and we conclude that \(C\) and \(A_i\) have the same eigenvectors. \(\Box\)
Proposition 2. Let \( O = (o_1, \ldots, o_m)^t, j \in \{1, \ldots, m\}, \sigma^2 > 0 \) and \( \lambda > 1 \). Then \( \Psi(O) \) increases if we use \( \lambda o_j \) in \( O \) instead of \( o_j \).

Proof. Fix an arbitrary \( j = 1, \ldots, m \) and take \( V := e_j e_j^t O \). We see that for \( u \in B \)

\[
V u = e_j e_j^t (o_1(u), \ldots, o_m(u))^t = e_j o_j(u) = (0, \ldots, 0, o_j(u), 0, \ldots, 0)^t.
\]

This way, \( V \) has the same \( j \)th entry as \( O \) while the rest are set to zero. We calculate the variation in this direction and show it is positive — \( \delta \Psi(O)V > 0 \). This means that increasing the magnitude of the \( j \)th measurement functional increases \( \Psi(O) \). We start with the last line of (3.3), and denote \( G := \mathcal{F} \Gamma_{post} \mathcal{F}^* : B^* \rightarrow B \):

\[
\delta \Psi(O)V = \text{tr} \, V(I - \Gamma_{model} O^* \Sigma^{-1} O) \mathcal{G} O^* \Sigma^{-1} = \text{tr} \, e_j e_j^t O(I - \Gamma_{model} O^* \Sigma^{-1} O) \mathcal{G} O^* \Sigma^{-1} e_j
\]

\[
= e_j^t O(I - \Gamma_{model} O^* \Sigma^{-1} O) \mathcal{G} O^* \Sigma^{-1} e_j = e_j^t (I - \mathcal{O}_j \Gamma_{model} O^* \Sigma^{-1} O) \mathcal{G} O^* \Sigma^{-1} e_j
\]

\[
= e_j^t (\Sigma - \mathcal{O}_j \Gamma_{model} O^*) \Sigma^{-1} O \mathcal{G} O^* \Sigma^{-1} e_j = \sigma^2 e_j^t \Sigma^{-1} O \mathcal{G} O^* \Sigma^{-1} e_j \text{ by (2.4)}
\]

\[
= \sigma^2 e_j^t \Sigma^{-1} O \mathcal{F} \Gamma_{post} \mathcal{F}^* O^* \Sigma^{-1} e_j.
\]

Since \( \Gamma_{post} \) is positive definite, \( \delta \Psi(O)V > 0 \). \( \square \)

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