

# Computational Advances in Data-Consistent Inversion: Measure-Theoretic Methods for Improving Predictions

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*The one where we describe why any of this matters.*

Broad Goals of Uncertainty Quantification:

- Make inferences and predictions
- Quantify and reduce uncertainty (aleatoric, epistemic)
- Be *accurate* and *precise*
- Design “efficient” experiments
- Collect and use data “intelligently”



The one where we define the letters we use and what they mean.

- State variable:  $u$  (e.g. heat, energy, pressure, deflection)
- Parameters:  $\lambda$  (e.g. source term, diffusion, boundary data)
- Deterministic model:  $\mathcal{M}(u, \lambda) = 0,$

$$\mathcal{M} : \lambda \rightarrow u(\lambda)$$

- Quantity of Interest map (QoI) - at least pcw differentiable

- » Functional of the solution

$$q : u(\lambda) \rightarrow \mathbb{R}$$

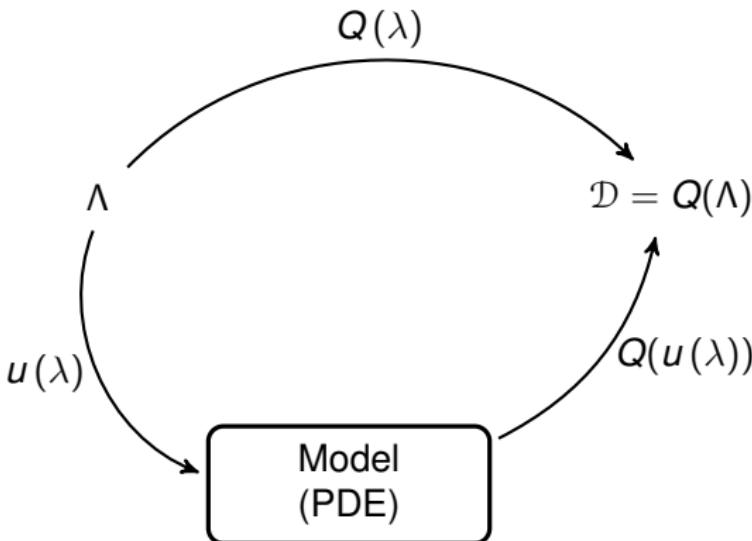
- » Can be vector valued

$$Q = \begin{bmatrix} q_1 \\ q_2 \\ \vdots \\ q_d \end{bmatrix}$$

- »  $Q(\lambda) := Q(u(\lambda))$



*The one where we illustrate how a QoI map relates inputs to outputs.*



*Defining the Quantity of Interest Map*

## Definition (Stochastic Forward Problem (SFP))

Given a probability measure  $\mathbb{P}_\Lambda$  on  $(\Lambda, \mathcal{B}_\Lambda)$ , and QoI map  $Q$ , the *stochastic forward problem* is to determine a measure,  $\mathbb{P}_{\mathcal{D}}$ , on  $(\mathcal{D}, \mathcal{B}_{\mathcal{D}})$  that satisfies

$$\mathbb{P}_{\mathcal{D}}(E) = \mathbb{P}_\Lambda(Q^{-1}(E)), \quad \forall E \in \mathcal{B}_{\mathcal{D}}. \quad (1.1)$$



## Definition (Stochastic Inverse Problem (SIP))

Given a probability measure,  $\mathbb{P}_{\mathcal{D}}$ , on  $(\mathcal{D}, \mathcal{B}_{\mathcal{D}})$  the *stochastic inverse problem* is to determine a probability measure,  $\mathbb{P}_{\Lambda}$ , on  $(\Lambda, \mathcal{B}_{\Lambda})$  satisfying

$$\mathbb{P}_{\Lambda}(Q^{-1}(E)) = \mathbb{P}_{\mathcal{D}}(E), \quad \forall E \in \mathcal{B}_{\mathcal{D}}. \quad (1.2)$$

The above is known as the *consistency condition*.

## Definition (Observed Distribution)

When the measure  $\mathbb{P}_{\mathcal{D}}$  in (1.2) quantifies the characterization of uncertainty in the QoI data, it is referred to as the *observed measure*,  $\mathbb{P}_{\text{ob}}$ .

If a dominating measure  $\mu_{\mathcal{D}}$  exists on  $(\mathcal{D}, \mathcal{B}_{\mathcal{D}})$ , the *observed density*  $\pi_{\text{ob}}$  is given by the Radon-Nikodym derivative of  $\mathbb{P}_{\text{ob}}$  with respect to the measure  $\mu_{\mathcal{D}}$ .



## Definition (Consistent Solution)

Any probability measure  $\mathbb{P}_\Lambda$  satisfying (1.2) is referred to as a *consistent solution* to the inverse problem, and (1.2).

If  $\mathbb{P}_\Lambda$  or  $\mathbb{P}_\mathcal{D}$  absolutely continuous w.r.t  $\mu_\Lambda$  or  $\mu_\mathcal{D}$ , resp, then we write

$$\pi_\Lambda := \frac{d\mathbb{P}_\Lambda}{d\mu_\Lambda} \text{ or } \pi_\mathcal{D} := \frac{d\mathbb{P}_\mathcal{D}}{d\mu_\mathcal{D}}$$

to denote the Radon-Nikodym derivatives of  $\mathbb{P}_\Lambda$  and  $\mathbb{P}_\mathcal{D}$ , resp.

In such a case, we can rewrite (1.1) and (1.2) using these pdfs:

$$\mathbb{P}_\Lambda(Q^{-1}(E)) = \int_{Q^{-1}(E)} \pi_\Lambda(\lambda) d\mu_\Lambda = \int_E \pi_\mathcal{D}(Q(\lambda)) d\mu_\mathcal{D} = \mathbb{P}_\mathcal{D}(E)$$



## Definition (Initial Distribution)

When  $\mathbb{P}_\Lambda$  in (1.1) quantifies the characterization of uncertainty in parameter variability before observations on QoI are taken into account, it is referred to as the *initial measure*  $\mathbb{P}_{in}$ .

If a dominating measure  $\mu_\Lambda$  exists on  $(\Lambda, \mathcal{B}_\Lambda)$ , the *initial distribution*  $\pi_{in}$  is given by the Radon-Nikodym derivative of  $\mathbb{P}_{in}$  w.r.t the measure  $\mu_\Lambda$ .

## Definition (Predicted Distribution)

The *predicted distribution* (or density) is the push-forward density of  $\pi_{in}$  under the map  $Q$ , and is denoted as  $\pi_{pr}$ .

Given as the Radon-Nikodym derivative (w.r.t  $\mu_{\mathcal{D}}$ ) of the pushforward measure

$$\mathbb{P}_{pr}(E) = \mathbb{P}_{in}(Q^{-1}(E)), \forall E \in \mathcal{B}_{\mathcal{D}}. \quad (1.3)$$



*The one where we define the solution to the SIP.*

We now have all of the definitions required to summarize the density-based solution to the SIP, known as the *updated density* as:

$$\pi_{\text{up}}(\lambda) := \pi_{\text{in}}(\lambda) \frac{\pi_{\text{ob}}(Q(\lambda))}{\pi_{\text{pr}}(Q(\lambda))}. \quad (1.4)$$



## Practical Considerations

- We approximate  $\pi_{\text{pr}}$  using density estimation on forward propagation of samples from  $\pi_{\text{in}}$
- May evaluate  $\pi_{\text{up}}$  directly for any sample of  $\Lambda$  (one model solve)
- Accuracy of the computed updated density is proportional to accuracy of approximation of the predicted density
- We (currently) use Gaussian KDE
  - » Let  $D$  be the dimension of  $\mathcal{D}$
  - » Let  $N$  be the number of samples from  $\pi_{\text{in}}$  propagated through  $Q$
  - » Converges at a rate of  $\mathcal{O}(N^{-4/(4+D)})$  in mean-squared error
  - » Converges at a rate of  $\mathcal{O}(N^{-2/(4+D)})$  in  $L^1$ -error



*The one where we distinguish ourselves from the Bayesian Inverse Problem.*

Bayesian approach: modeling epistemic uncertainties in data on a QoI obtained from a true, but unknown, parameter value,  $\lambda^\dagger$ .

### Definition (Deterministic Forward Problem (DFP))

Given a space  $\Lambda$ , and QoI map  $Q$ , the *deterministic forward problem* is to determine the values,  $q \in \mathcal{D}$  that satisfy

$$q = Q(\lambda), \forall \lambda \in \Lambda. \quad (1.5)$$



*The one where we distinguish ourselves from the Bayesian Inverse Problem.*

### Definition (Deterministic Inverse Problem (DIP) Under Uncertainty)

Given a noisy datum (or data-vector)  $d = q + \xi$ ,  $q \in \mathcal{D}$ , the *deterministic inverse problem* is to determine the parameter  $\lambda \in \Lambda$  which minimizes

$$\|Q(\lambda) - d\| \quad (1.6)$$

where  $\xi$  is a random variable (or vector) drawn from a distribution characterizing the uncertainty in observations due to measurement errors.

In the above definition,  $\xi$  is some unobservable perturbation to the true output, arising from epistemic uncertainty (e.g. the precision of available measurement equipment).



*The one where we distinguish ourselves from the Bayesian Inverse Problem.*

The *posterior* is a conditional density, denoted by  $\pi_{\text{post}}(\lambda | d)$ , proportional to the product of the prior and data-likelihood function [3, 2, 1, 4]:

$$\pi_{\text{post}}(\lambda) := \pi_{\text{prior}}(\lambda) \frac{L_{\mathcal{D}}(q|\lambda)}{C}, \quad (1.7)$$

where we emphasize the use of  $\pi_{\text{post}}$  to distinguish the *posterior* from the updated density  $\pi_{\text{up}}$  in (1.4).

evidence term  $C$  ensures the posterior density integrates to one; given by

$$C = \int_{\Lambda} \pi_{\text{prior}}(\lambda) L_{\mathcal{D}}(q|\lambda) d\lambda.$$

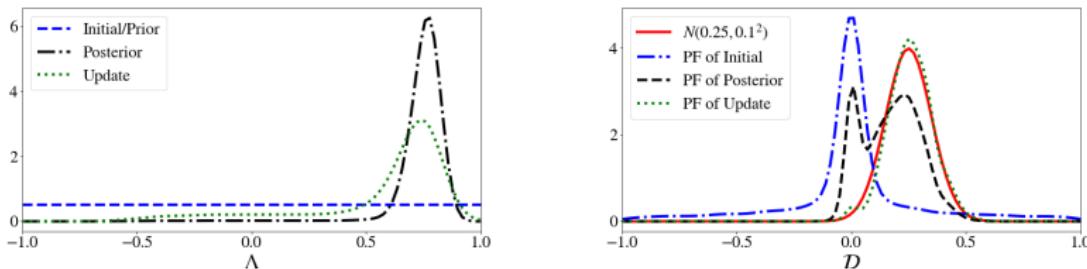


*The one where we provide an illustrative example.*

- Suppose  $\Lambda = [-1, 1] \subset \mathbb{R}$  and  $Q(\lambda) = \lambda^5$  so that  $\mathcal{D} = [-1, 1]$
- $\pi_{\text{in}} \sim \mathcal{U}([-1, 1])$  and  $\pi_{\text{ob}} \sim N(0.25, 0.1^2)$
- $d \in \mathcal{D}$  with  $d = Q(\lambda^\dagger) + \xi$  where  $\xi \sim N(0, 0.1^2)$
- We then construct  $\pi_{\text{post}}(\lambda | d)$  for this example assuming a uniform prior (to match the initial density) with an assumed observed value of  $d = 0.25$  so that the data-likelihood function matches the observed density.



*The one where we provide an illustrative example.*



**Figure:** (Left) The initial/prior PDF  $\pi_{\text{in}}$  (blue solid curve), updated PDF  $\pi_{\text{up}}$  (black dashed curve), and posterior PDF  $\pi_{\text{post}}$  (green dashed-dotted curve) on  $\Lambda$ . (Right) The push-forward (PF) of the initial/prior PDF  $\pi_{\text{pr}}$  (blue solid curve), observed/likelihood PDF (red solid curve), PF of the updated PDF  $\pi_{\text{up}}$  (black dashed curve), and the PF of the posterior PDF  $\pi_{\text{post}}$  (green dashed-dotted curve) for the QoI.

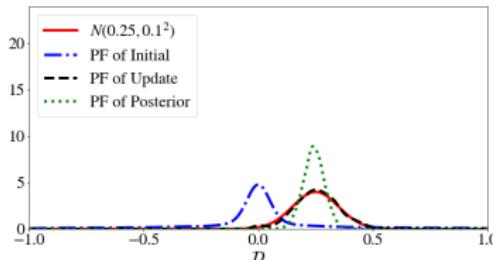
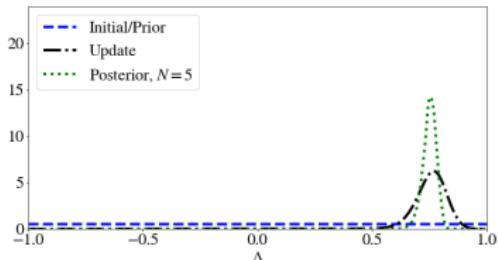
*The one where we provide an illustrative example.*

*What happens as we collect more data?*

One approach:

SIP: Use  $N$  to estimate mean of observed

DIP: likelihood function incorporates more data



SIP and DIP solutions for varying  $N$  for comparison.

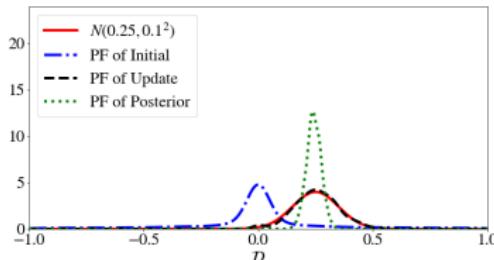
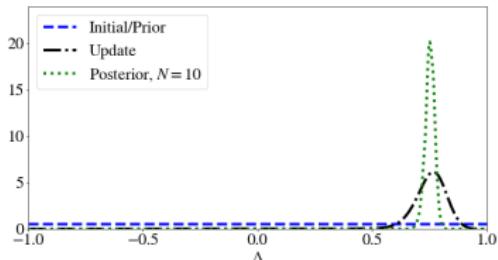
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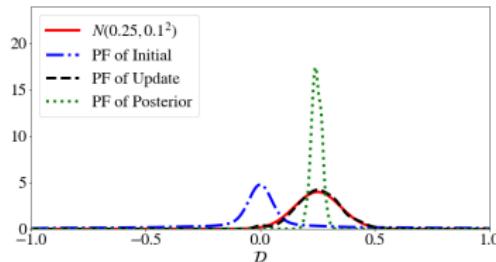
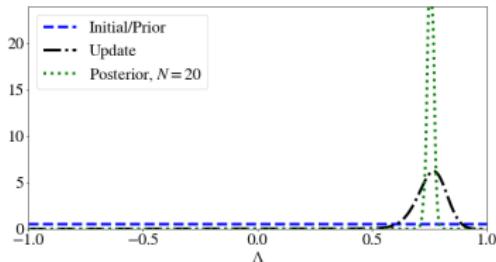
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SIP and DIP solutions for varying  $N$  for comparison.

We formally define the maximal updated density (MUD) point as

$$\lambda^{\text{MUD}} := \arg \max \pi_{\text{up}}(\lambda). \quad (2.1)$$

We motivate the use of the MUD point as an alternative to the MAP point for parameter estimation problems.



Let  $\|\mathbf{x}\|_C^2 := (\mathbf{x}, \mathbf{x})_C = \mathbf{x}^\top C \mathbf{x}$ .

Inverse covariances associated with non-degenerative multivariate Gaussian distributions will play the role of  $C$ .

Suppose that the initial and prior densities are both given by the same  $\mathcal{N}(\lambda_0, \Sigma_{\text{init}})$  distribution.

Additionally, suppose the map  $Q$  is linear and that the data-likelihood and observed densities are both given by the same  $\mathcal{N}(\mathbf{y}, \Sigma_{\text{obs}})$  distribution.

The linearity of  $Q$  implies that  $Q(\lambda) = A\lambda$  for some  $A \in \mathbb{R}^{d \times p}$ , and that the predicted density follows a  $\mathcal{N}(Q(\lambda_0), \Sigma_{\text{pred}})$  distribution where

$$\Sigma_{\text{pred}} := A\Sigma_{\text{init}}A^\top. \quad (2.2)$$



*The one with the regularization equations.*

$\pi_{\text{up}}(\lambda) = \pi_{\text{in}}(\lambda) \frac{\pi_{\text{ob}}(Q(\lambda))}{\pi_{\text{pr}}(Q(\lambda))}$	$\pi_{\text{post}}(\lambda   d) = \frac{\pi_{\text{prior}}(\lambda) \pi_{\text{like}}(d   \lambda)}{\int_{\Lambda} \pi_{\text{like}}(d   \lambda) \pi_{\text{prior}}(\lambda) d\mu_{\Lambda}}$
Tikhonov	$T(\lambda) := \ Q(\lambda) - \mathbf{y}\ _{\Sigma_{\text{obs}}^{-1}}^2 + \ \lambda - \lambda_0\ _{\Sigma_{\text{init}}^{-1}}^2$
Data-Consistent	$J(\lambda) := T(\lambda) - \ Q(\lambda) - Q(\lambda_0)\ _{\Sigma_{\text{pred}}^{-1}}^2$

**Table:** The  $\lambda$  which minimizes these functionals also maximizes the updated PDF (left) and the Bayesian posterior PDF (right).

$T(\lambda)$  is the typical functional often associated with Tikhonov regularization. The  $J(\lambda)$  has an additional term subtracted from  $T(\lambda)$  coming from the predicted density that serves as “unregularization” in data-informed directions.

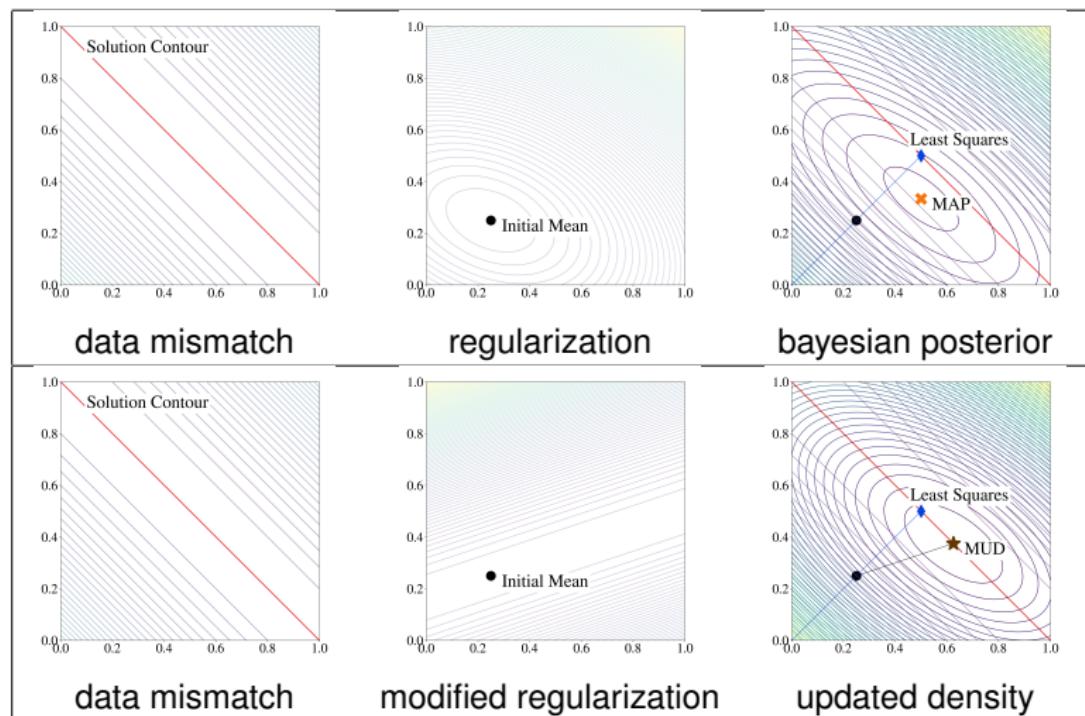
*The one where an example highlights a key difference.*

Consider a linear QoI map is defined by  $A = [ \begin{array}{cc} 1 & 1 \end{array} ]$ .  
2-D input, 1-D output  $\implies$  rank-deficient

Parameters in the initial and observed densities are given by

$$\lambda_0 = [ \begin{array}{cc} 0.25 & 0.25 \end{array} ]^\top,$$
$$\Sigma_{\text{init}} = [ \begin{array}{cc} 1 & -0.25 \\ -0.25 & 0.5 \end{array} ],$$
$$\mathbf{y} = 1, \text{ and } \Sigma_{\text{obs}} = [ \begin{array}{c} 0.25 \end{array} ]$$





**Figure:** Gaussian data mismatch for a 2-to-1 linear map (left plots). Gaussian initial/prior induce different regularization terms (middle plots), which leads to different optimization functions (right plots) and parameter estimates.

The posterior covariance is formally given by

$$\Sigma_{\text{post}} := (A^\top \Sigma_{\text{obs}}^{-1} A + \Sigma_{\text{init}}^{-1})^{-1}. \quad (2.3)$$

Applying Woodbury identity and (2.2), we rewrite the posterior covariance:

$$\Sigma_{\text{post}} = \Sigma_{\text{init}} - \Sigma_{\text{init}} A^\top [\Sigma_{\text{pred}} + \Sigma_{\text{obs}}]^{-1} A \Sigma_{\text{init}} \quad (2.4)$$

Can now interpret  $\Sigma_{\text{post}}$  as a rank  $d$  correction (or update) of  $\Sigma_{\text{init}}$ .  
 $\Sigma_{\text{pred}} + \Sigma_{\text{obs}}$  is invertible because it is the sum of two s.p.d matrices.  
We rewrite the closed form expression for the MAP point given in [5] as

$$\lambda^{\text{MAP}} = \lambda_0 + \Sigma_{\text{post}} A^\top \Sigma_{\text{obs}}^{-1} (\mathbf{y} - b - A\lambda_0). \quad (2.5)$$



We define

$$R := \Sigma_{\text{init}}^{-1} - A^\top \Sigma_{\text{pred}}^{-1} A. \quad (2.6)$$

Using this  $R$ , rewrite  $J(\lambda)$  as

$$J(\lambda) := \|\mathbf{y} - Q(\lambda)\|_{\Sigma_{\text{obs}}^{-1}}^2 + \|\lambda - \lambda_0\|_R^2. \quad (2.7)$$

In this form, we identify  $R$  as the *effective regularization* in  $J(\lambda)$  due to the formulation in the data-consistent framework.

$$\Sigma_{\text{up}} := \left( A^\top \Sigma_{\text{obs}}^{-1} A + R \right)^{-1}. \quad (2.8)$$

Since  $R$  is not invertible, Woodbury's identity cannot be applied (yet).



We derive using several identities

$$\Sigma_{\text{up}} = \Sigma_{\text{init}} - \Sigma_{\text{init}} A^\top \Sigma_{\text{pred}}^{-1} [\Sigma_{\text{pred}} - \Sigma_{\text{obs}}] \Sigma_{\text{pred}}^{-1} A \Sigma_{\text{init}}. \quad (2.9)$$

Substitute  $\Sigma_{\text{up}}$  for  $\Sigma_{\text{post}}$  in (2.5) to write the point that minimizes  $J$  as:

$$\lambda^{\text{MUD}} = \lambda_0 + \Sigma_{\text{up}} A^\top \Sigma_{\text{obs}}^{-1} (\mathbf{y} - b - A\lambda_0). \quad (2.10)$$

Substituting (2.9) into (2.10) and simplifying, we have

$$\lambda^{\text{MUD}} = \lambda_0 + \Sigma_{\text{init}} A^\top \Sigma_{\text{pred}}^{-1} (\mathbf{y} - b - A\lambda_0). \quad (2.11)$$



Predictability assumption:  
smallest predicted > largest observed (eigenvalues of covariances)

## Theorem

Suppose  $Q(\lambda) = A\lambda + b$  for some full rank  $A \in \mathbb{R}^{d \times p}$  with  $d \leq p$  and  $b \in \mathbb{R}^d$ . If  $\pi_{\text{in}} \sim N(\lambda_0, \Sigma_{\text{init}})$ ,  $\pi_{\text{ob}} \sim N(\mathbf{y}, \Sigma_{\text{obs}})$ , and the predictability assumption holds, then

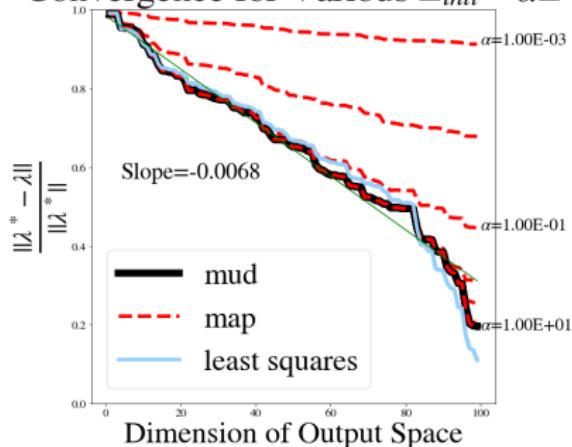
- (a) There exists a unique parameter, denoted by  $\lambda^{\text{MUD}}$ , that maximizes  $\pi_{\text{up}}$ .
- (b)  $Q(\lambda^{\text{MUD}}) = \mathbf{y}$ .
- (c) If  $d = p$ ,  $\lambda^{\text{MUD}}$  is given by  $A^{-1}$ . If  $d < p$ ,  $\lambda^{\text{MUD}}$  is given by (2.11) and the covariance associated with this point is given by (2.9).



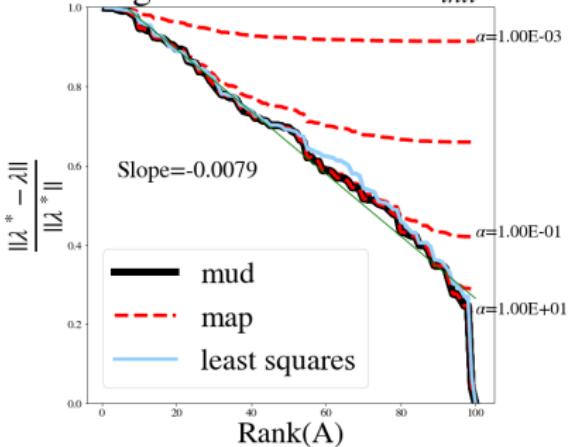
*The one where we show how rank and dimension impact our solutions.*

Example: scaling random diagonal initial covariances

Convergence for Various  $\Sigma_{init} = \alpha \Sigma$



Convergence for Various  $\Sigma_{init} = \alpha \Sigma$



**Figure:** Relative errors between  $\lambda^\dagger$  and (i) the least squares solution obtained through numpy's linalg.pinv module, (ii) the closed-form solution for the MUD point given in Eq (2.11), and (iii) the MAP point. (Left): Error for increasing dimensions of  $D$  for  $A$  taken to be a Gaussian Random Map. (Right): Error for increasing row-rank of  $A$ , generated with Gaussian vectors and a SVD.

The one where we leverage this framework for general streams of data.

Suppose  $\exists d$  measurement devices generating repeated noisy data.

For each  $1 \leq j \leq d$ , denote by  $\mathcal{M}_j(\lambda^\dagger)$  the  $j$ th measurement device.  
 $N_j$  is number of noisy data obtained for  $\mathcal{M}_j(\lambda^\dagger)$ .

$d_{j,i}$  is the  $i$ th noisy datum for the  $j$ th measurement, where  $1 \leq i \leq N_j$ .

Assume an unbiased additive error model for the measurement noise,  
with independent identically distributed (i.i.d.) Gaussian errors so that

$$d_{j,i} = M_j(\lambda^*) + \xi_i, \quad \xi_i \sim N(0, \sigma_j^2), \quad 1 \leq i \leq N_j. \quad (2.12)$$

We now construct a  $d$ -dimensional vector-valued map from data  
obtained on the  $d$  measurement devices.



*The one with the Weighted Mean Error (WME) map.*

The weighted mean error (WME) map, denoted by  $Q_{\text{WME}}(\lambda)$  has  $j$ th component, denoted by  $Q_{\text{WME},j}(\lambda)$ , given by

$$Q_{\text{WME},j}(\lambda) := \frac{1}{\sqrt{N_j}} \sum_{i=1}^{N_j} \frac{M_j(\lambda) - d_{j,i}}{\sigma_j}. \quad (2.13)$$

$Q_{\text{WME},j}(\lambda^\dagger)$  is the sample avg of  $N_j$  random draws from an i.i.d.  $N(0, N_j)$ . By assumption, the observed data are generated according to the fixed true physical parameter vector given by  $\lambda^\dagger$  in (2.12).

Subsequently, each component of  $Q_{\text{WME}}(\lambda^\dagger)$  is a random draw from an  $N(0, 1)$  distribution.

Therefore, with this choice of data-defined QoI map, we specify  $\pi_{\text{ob}}$  as a  $N(\mathbf{0}_{d \times 1}, \mathbf{I}_{d \times d})$  distribution.

*The one where measurements impact the predictability assumption.*

The  $j$ th diagonal component of the predicted covariance matrix is given by the predicted variance associated with using the scalar-valued

$$Q_{\text{WME},j}.$$

Then, the associated predicted variance is given by

$$\frac{N_j}{\sigma_j^2} M_j \Sigma_{\text{init}} M_j^\top \quad (2.14)$$

Since  $\Sigma_{\text{init}}$  is assumed to be non-degenerative and  $M_j$  is a non-trivial row vector, this predicted variance grows linearly with  $N_j$ .

In other words, the  $j$ th diagonal component of the predicted covariance has the form  $\beta_j N_j$  for some  $\beta_j > 0$ .



Let  $N_{\min,j}$  denote the minimum  $N_j$  for  $1 \leq j \leq N$  necessary to make the  $j$ th diagonal components sufficiently large so that the smallest eigenvalue of the predicted covariance is larger than 1.

The following result is now an immediate consequence of Theorem 2.1:

### Corollary

If  $\pi_{\text{in}} \sim N(\lambda_0, \Sigma_{\text{init}})$  and data are obtained for  $d$  linearly independent measurements on  $\Lambda$  with an additive noise model with i.i.d. Gaussian noise for each measurement, then **there exists a minimum number of data points obtained for each of the measurements such that there exists a unique  $\lambda^{\text{MUD}}$  and  $Q_{\text{WME}}(\lambda^{\text{MUD}}) = 0$ .**

*The one where we violate some assumptions.*

Consider the exponential decay problem with uncertain decay rate  $\lambda$ :

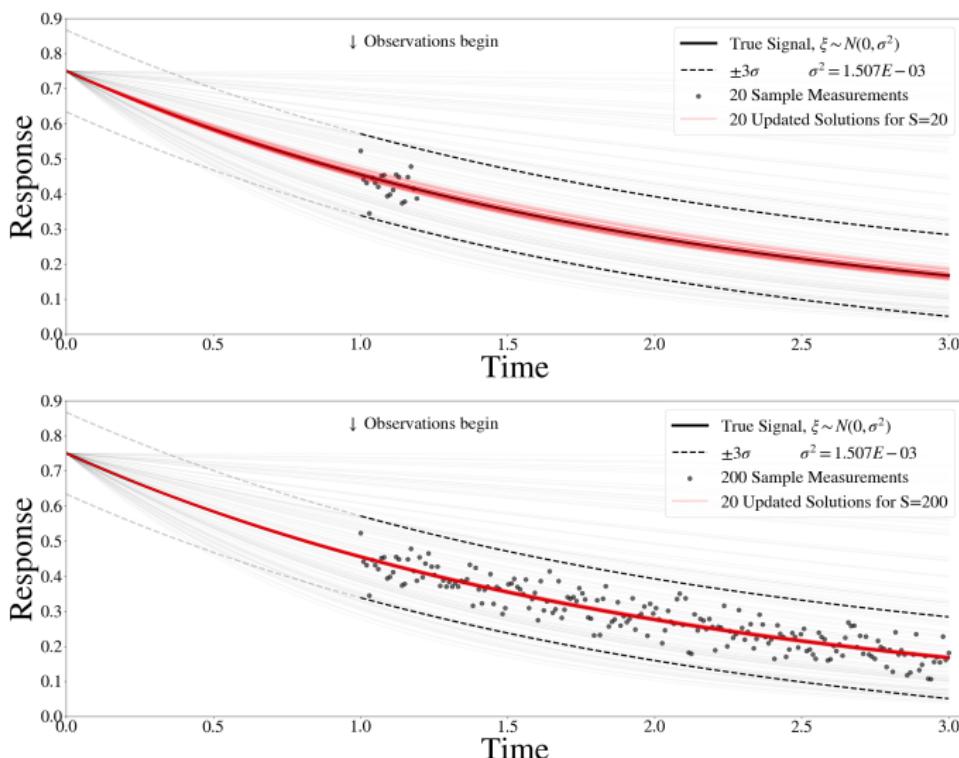
$$\begin{cases} \frac{\partial u}{\partial t} = \lambda u(t), & 0 < t \leq 3, \\ u(0) = 0.75, \end{cases}$$

with solution

$$u(t; \lambda) = u_0 \exp(-\lambda t), \quad u_0 = 0.75, \tag{2.15}$$

and measurements begin at  $t = 1$ .

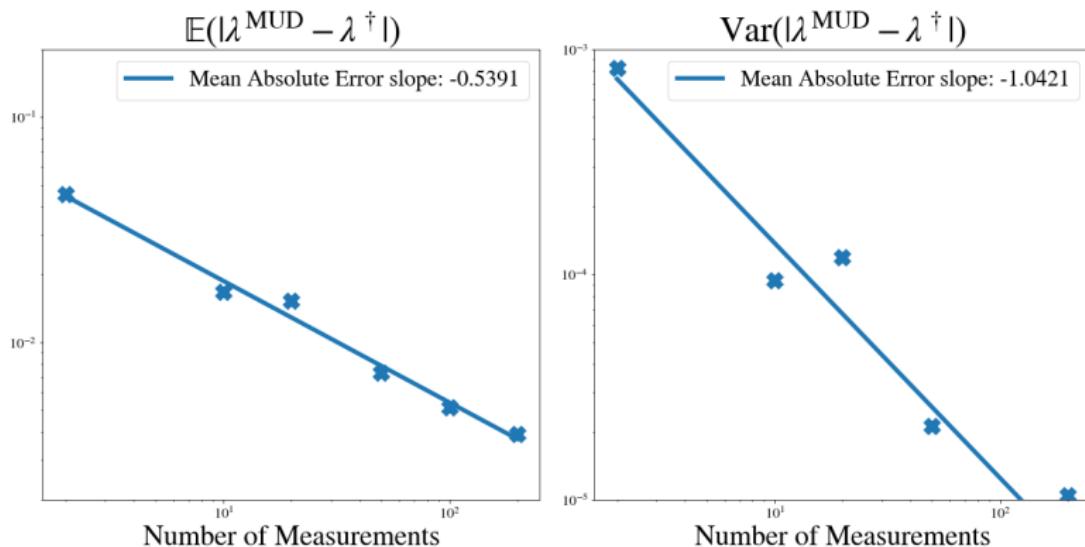




**Figure:** Curves for exponential decay model with various decay coefficients. Dashed curves denote 99% probability intervals for noise. The true signal is



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**Figure:** The mean (left) and variance (right) of absolute errors in MUD estimates as a function of the number of data points used. These statistics are computed over 20 trials.

*The one where we violate some assumptions.*

Consider the Poisson problem:

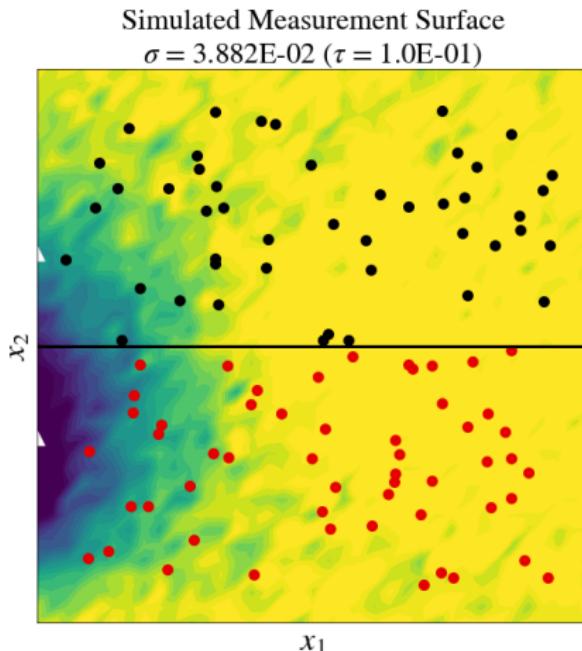
$$\begin{cases} -\nabla \cdot \nabla u = f(x), & \text{on } x \in \Omega, \\ u = 0, & \text{on } \Gamma_T \cup \Gamma_B, \\ \frac{\partial u}{\partial \mathbf{n}} = g(x_2), & \text{on } \Gamma_L, \\ \frac{\partial u}{\partial \mathbf{n}} = 0, & \text{on } \Gamma_R, \end{cases} \quad (2.16)$$

where  $x = (x_1, x_2) \in \Omega = (0, 1)^2$  is the spatial domain.

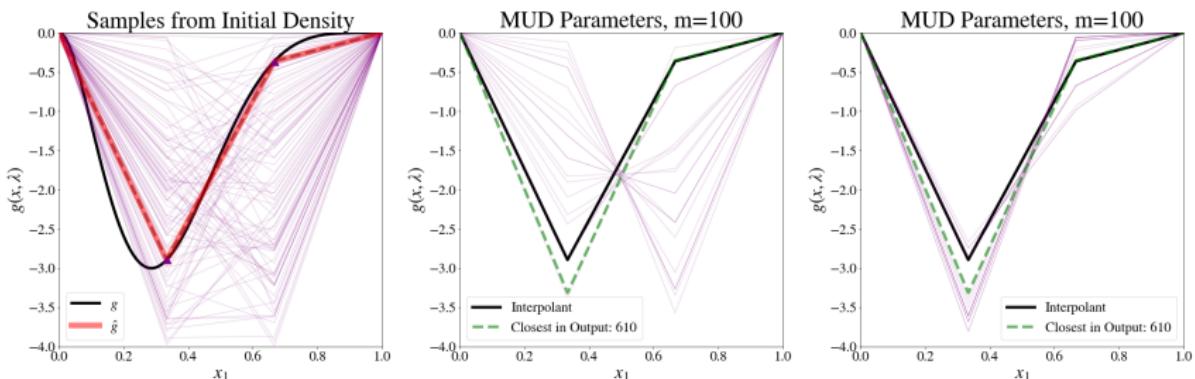
- $\Gamma_T$ ,  $\Gamma_B$ ,  $\Gamma_L$ , and  $\Gamma_R$ , denote the top, bottom, left, and right boundaries of this domain
- $\frac{\partial u}{\partial \mathbf{n}}$  denotes the usual outward normal derivative.
- The forcing function  $f$  is taken to be  $10 \exp\left(\|x - 0.5\|^2 / 0.02\right)$ .



- $g(x_2)$  is unknown, and the goal is to use noisy data to estimate this unknown boundary data.
- In other words, the parameter  $\lambda$  now represents an uncertain function.
- To generate the noisy data, we use  $g(x_2) \propto x_2^2(x_2 - 1)^5$
- Constant of proportionality chosen so  $\min g = -3$  at  $x_2 = \frac{2}{7}$ .
- Piecewise-linear finite elements on a triangulation of a  $36 \times 36$  mesh.
- 100 randomly placed sensors in the subdomain  $(0.05, 0.95)^2 \subset \Omega$ .
- Repeated 20 times to study the subsequent variation in MUD points due to different realizations of noisy data.



**Figure:** A representative noisy perturbation of the reference response surface. Locations of the randomly chosen spatial data used to construct both  $Q_{1D}$  and  $Q_{2D}$  are shown as black and red dots.



**Figure:** In the left plot, the reference  $g(x_2)$  is shown as the solid black curve with its interpolant onto the spline basis shown as a dotted red curve. The dashed blue line represents the sample from parameter space which most closely predicts noiseless data, which we refer to as the projection of  $g$ . The purple curves in the center and right plots show the variability in MUD estimates of  $g(x_2)$  for the 20 different realizations of noisy data. The center plot uses  $Q_{1D}$  and the right plot uses  $Q_{2D}$  to construct the MUD estimates.

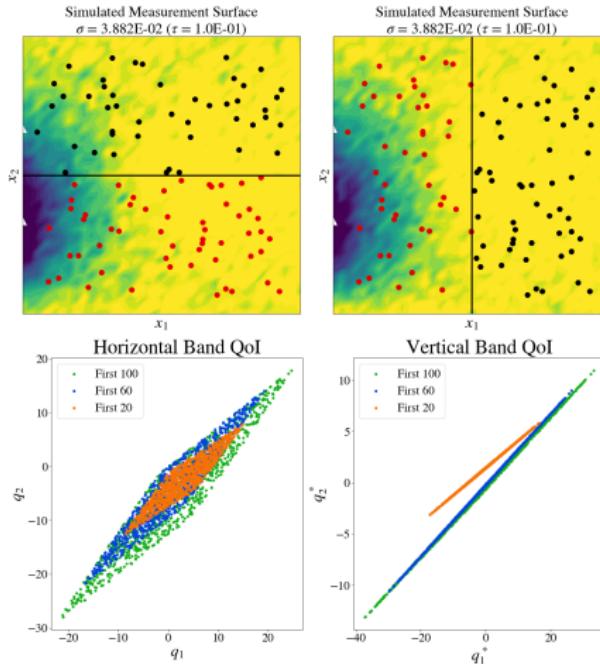
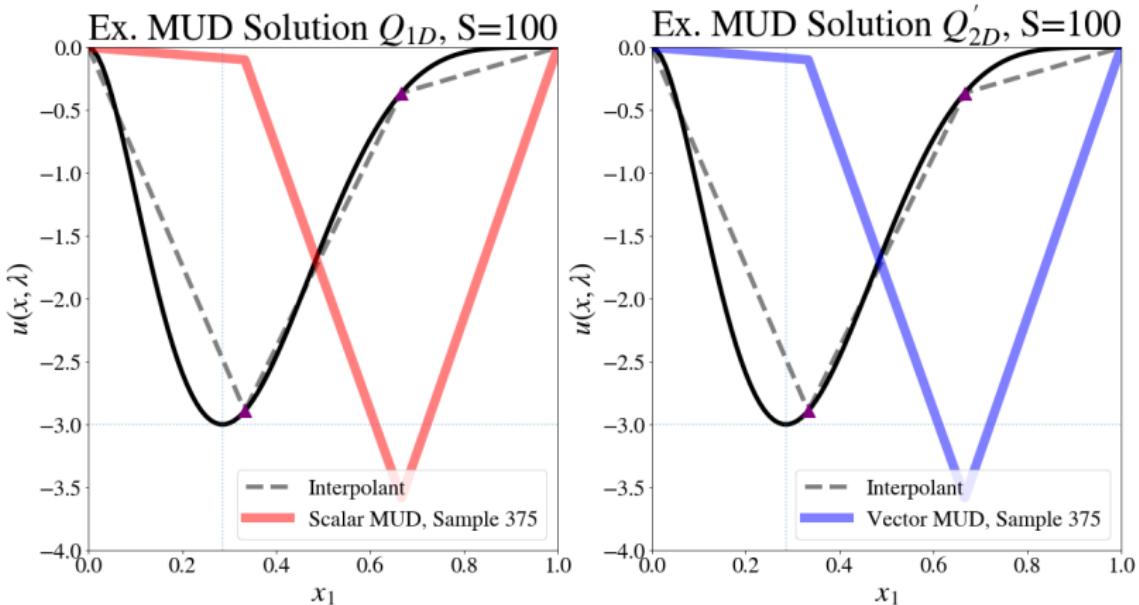


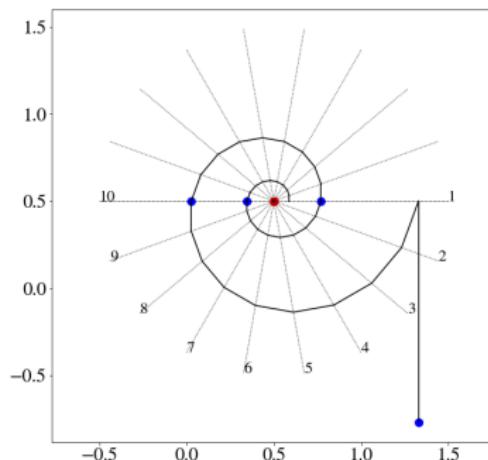
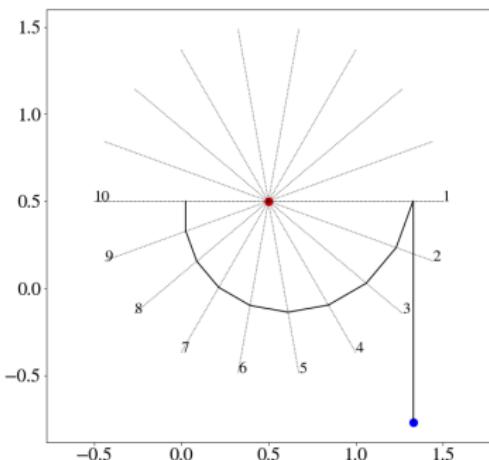
Figure:  $N = 1000$  parameter evaluations for both methods of partitioning  $\Omega$ .



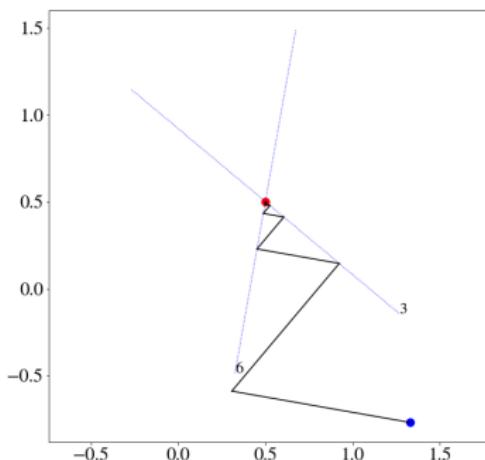
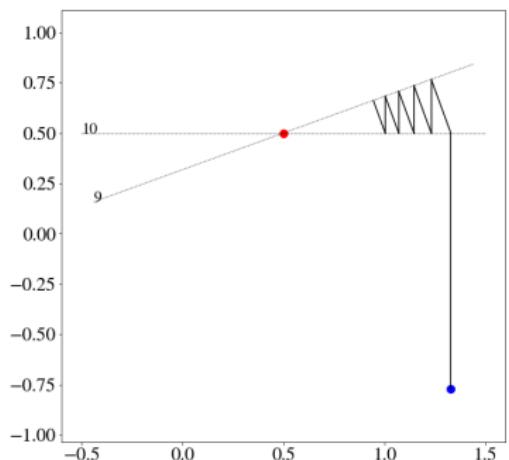
**Figure:** Side-by-side comparison of an example solution to the SIP using  $Q_{1D}$  (left) compared to using  $Q'_{2D}$ , juxtaposed against a plot of  $g$ .

The one with the small problems in many batches.

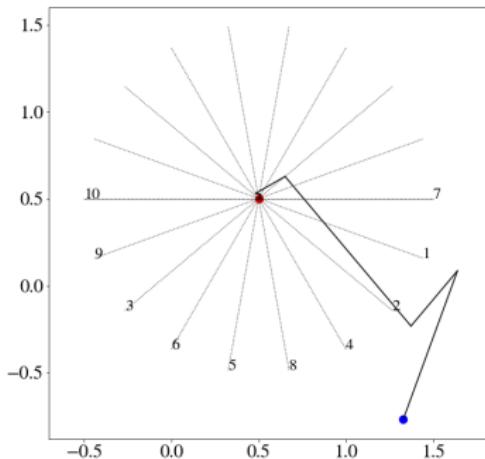
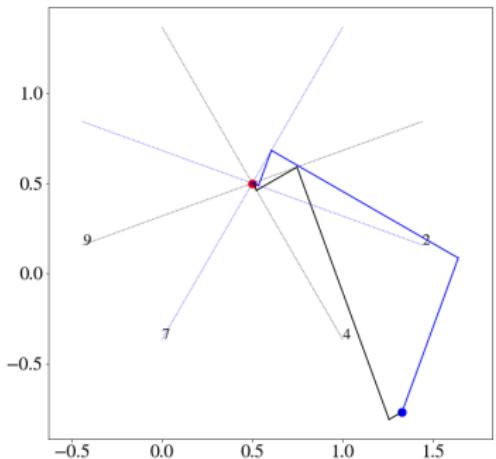
QoI defined by 10 equispaced rotations of the unit vector  $[0, 1]$  through the first two Euclidean quadrants



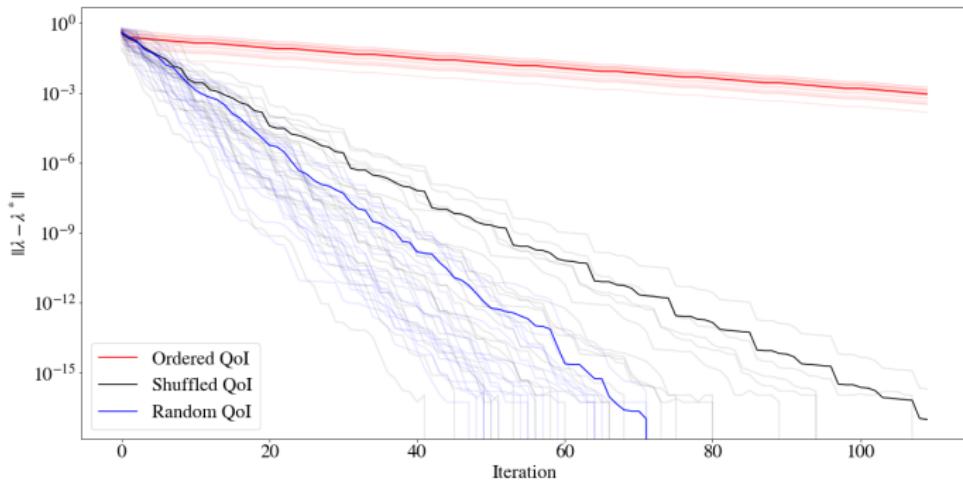
**Figure:** Dotted lines show the solution contours for each row of the operator  $A$ . (Left): First epoch for iterating through 10 QoI. (Right): Three more epochs allows our estimate to get much closer to the true value.



**Figure:** Iterating through five epochs of two QoI, each formed by picking two of the ten available rows of  $A$  at random. The random directions chosen on the left exhibit more redundancy than those on the right, so the same amount of iteration results in less accuracy.



**Figure:** (Left): Subsets of available QoI components can be chosen to exhibit minimal redundancy and lead to expedited convergence. (Right): Random components of the QoI map used for each iterative step. This leads to an overall similar level of precision in this example, without the need to use gradients.



**Figure:** 20 initial means are chosen and iterated on for three approaches for ordering QoI. Individual experiments are transparent and the mean error is shown as a solid line for each approach.

*How do I know I can trust you?*

You don't. But I enabled you to check for yourself.

- Public repository hosted on Github.com  
(github.com/mathematicalmichael/thesis)
- Github Actions implements Continuous Integration / Deployment
- Each change is validated for reproducibility
- makefile for convenience (make <filename>)
  - » dissertation + presentation (L<sup>A</sup>T<sub>E</sub>X, themes, style files)
  - » every example, convergence result (Python)
  - » every image in every figure
- PyPi published implementation of main methods: pip install mud
- Unit tests aid in ensuring integrity of functions
- Docker guarantees software runtime (ran on x86 and arm)  
docker pull mathematicalmichael/python:thesis(latex:thesis)



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