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 (aleotoric, 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: λ (e.g. source term, diffusion, boundary data)
- Deterministic model: $\mathcal{M}(u, \lambda) = 0$,

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

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

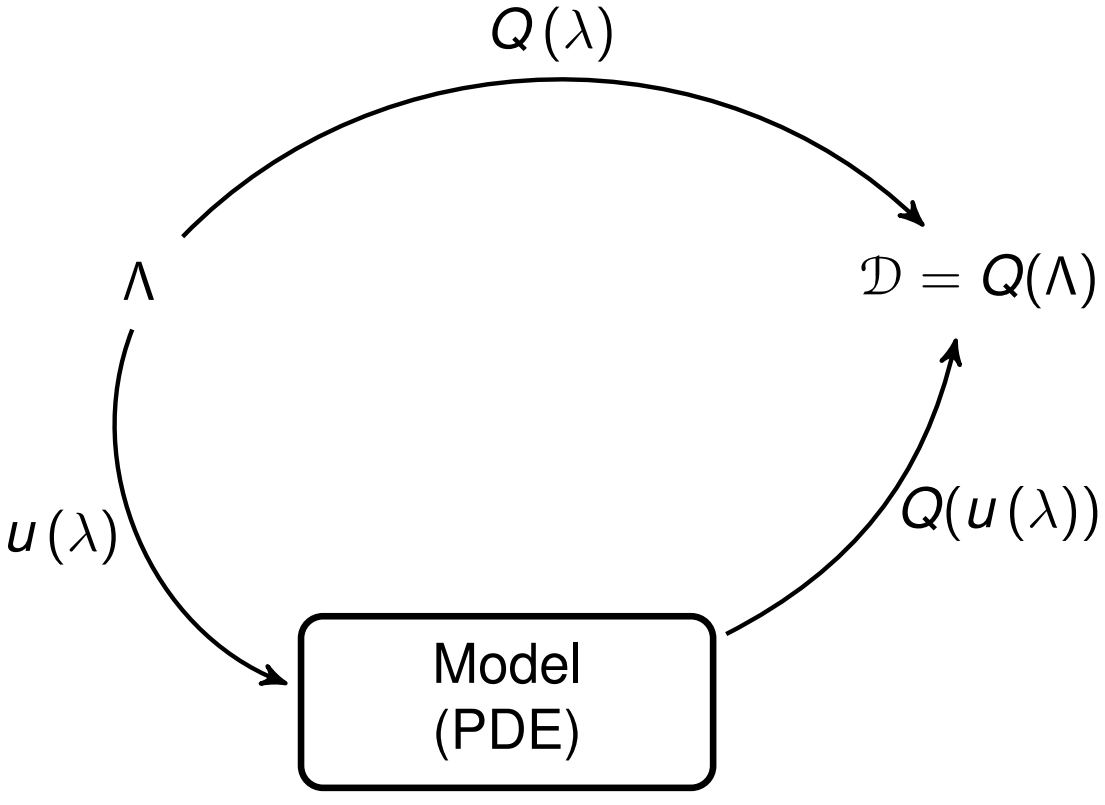
$$q : u(\lambda) \to \mathbb{R}$$

  - 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

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

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

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

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* π_{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 μ_Λ or $\mu_\mathcal{D}$, resp, then we write

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

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

Definition (Predicted Distribution)

The *predicted distribution* (or density) is the push-forward density of π_{in} under the map Q, and is denoted as π_{pr}.
Given as the Radon-Nikodym derivative (w.r.t $\mu_\mathcal{D}$) of the pushforward measure

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

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:

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

Practical Considerations

- We approximate π_{pr} using density estimation on forward propagation of samples from π_{in}
- May evaluate π_{up} directly for any sample of Λ (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 π_{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 Λ, and QoI map Q, the *deterministic forward problem* is to determine the values, $q \in \mathcal{D}$ that satisfy

$$q = Q(\lambda), \ \forall \ \lambda \in \Lambda. \tag{1.5}$$

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

$$\|Q(\lambda) - d\| \tag{1.6}$$

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

In the above definition, ξ 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 $\pi_{\text{post}}(\lambda \mid d)$, proportional to the product of the prior and data-likelihood function [3, 2, 1, 4]:

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

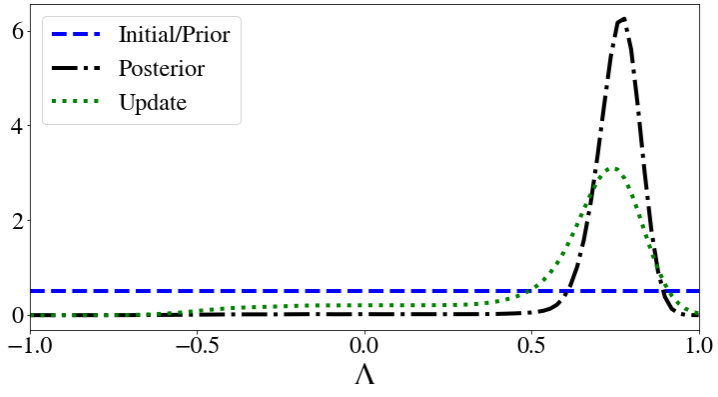
where we emphasize the use of π_{post} to distinguish the *posterior* from the updated density π_{up} in (1.4).
evidence term C ensures the posterior density integrates to one; given by

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

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 $\pi_{\text{post}}(\lambda \mid d)$ 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.



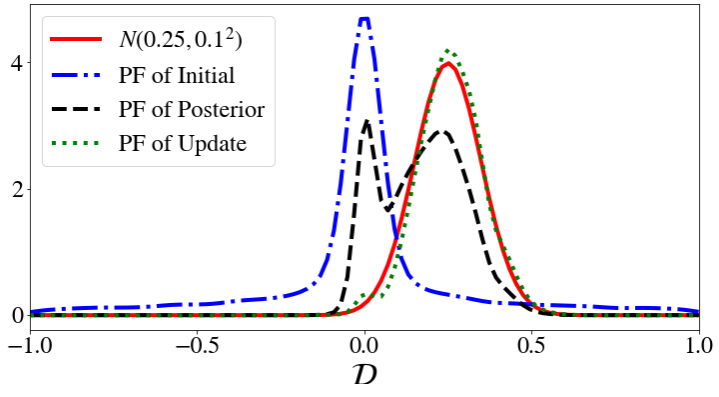
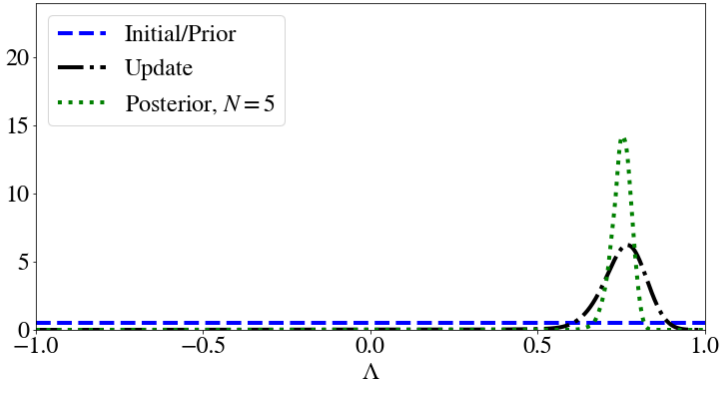


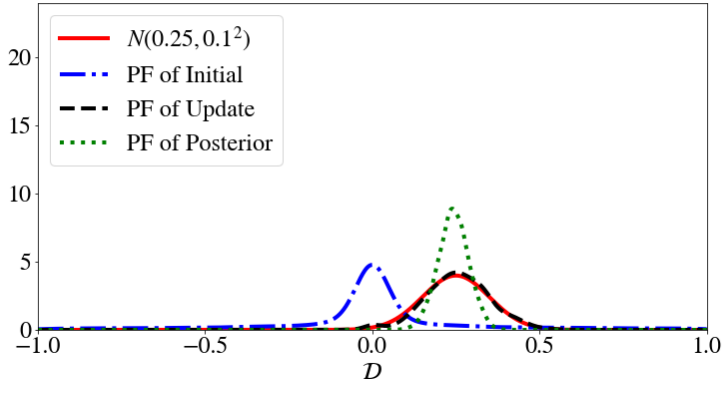
Figure: (Left) The initial/prior PDF π_{in} (blue solid curve), updated PDF π_{up} (black dashed curve), and posterior PDF π_{post} (green dashed-dotted curve) on Λ. (Right) The push-forward (PF) of the initial/prior PDF π_{pr} (blue solid curve), observed/likelihood PDF (red solid curve), PF of the updated PDF π_{up} (black dashed curve), and the PF of the posterior PDF π_{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.

The one where we provide an illustrative example.

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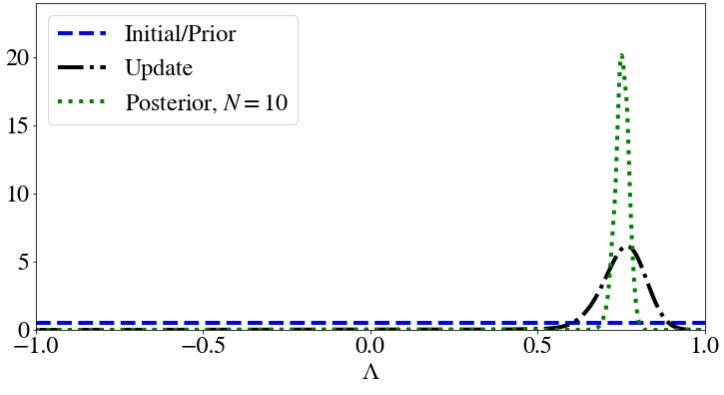

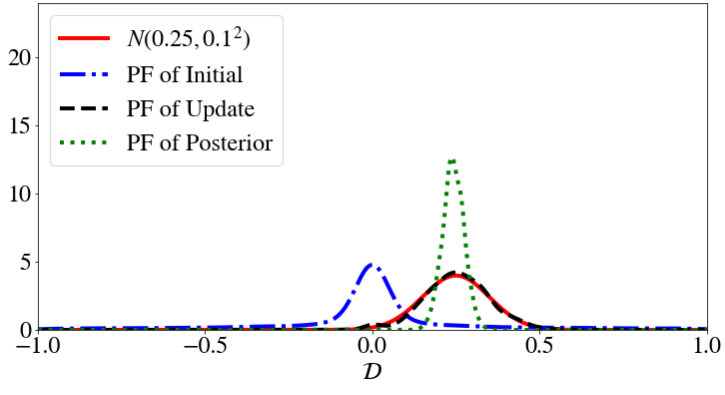

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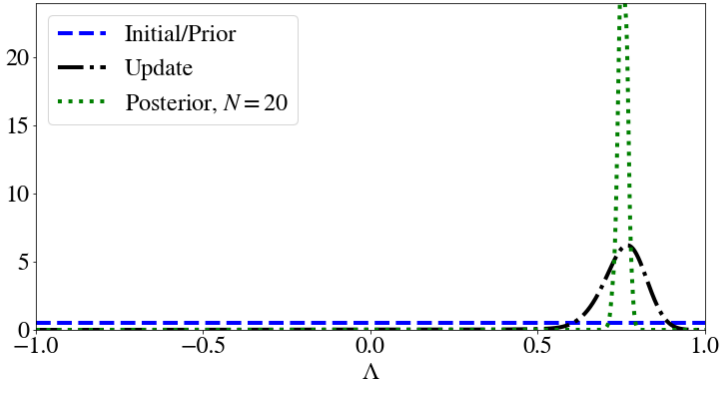

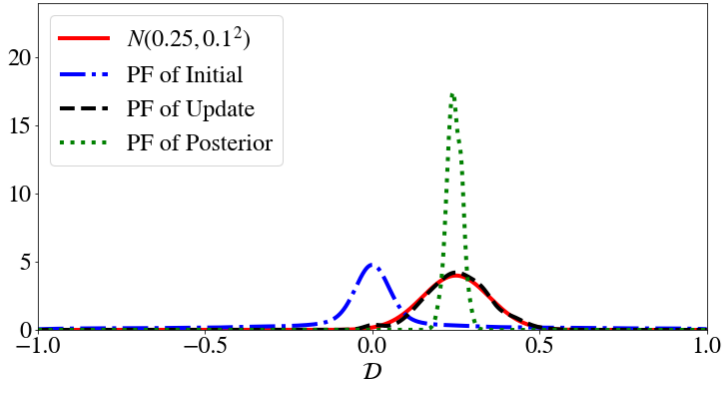

SIP and DIP solutions for varying N for comparison.

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

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

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

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

$$\Sigma_{\text{pred}} := A\Sigma_{\text{init}}A^\top. \tag{2.2}$$

The one with the regularization equations.

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

Table: The λ 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 $A = \begin{bmatrix} 1 & 1 \end{bmatrix}$.

2-D input, 1-D output $\implies$ rank-deficient

Parameters in the initial and observed densities are given by

$$\lambda_0 = \begin{bmatrix} 0.25 & 0.25 \end{bmatrix}^\top,$$

$$\Sigma_{\text{init}} = \begin{bmatrix} 1 & -0.25 \\ -0.25 & 0.5 \end{bmatrix},$$

$$\mathbf{y} = 1, \text{ and } \Sigma_{\text{obs}} = \begin{bmatrix} 0.25 \end{bmatrix}$$

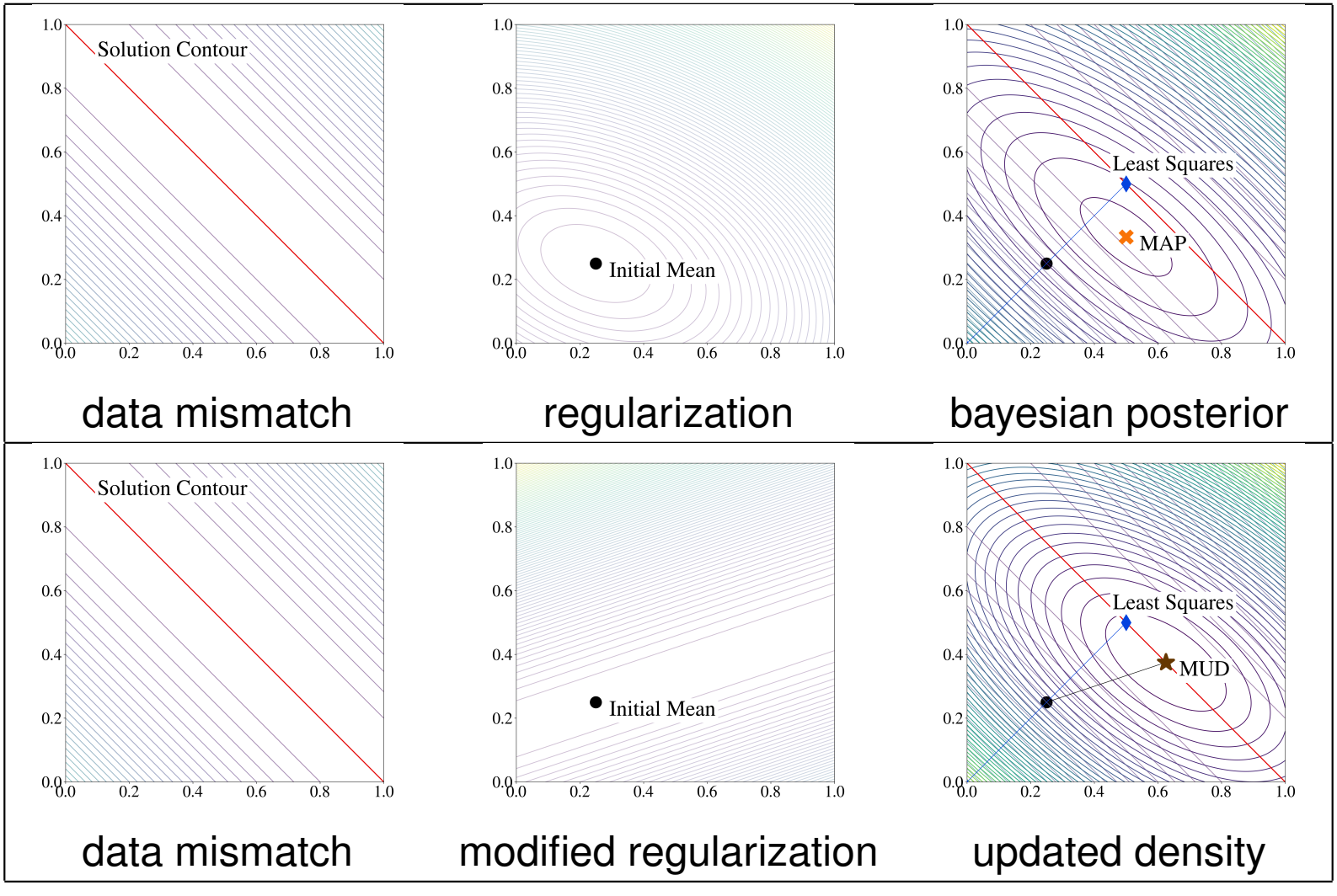

Figure: Gaussian data mismatch for a 2-to-1 linear map (left plots). Gaussian initial/prior induce different regularization terms (middle plots), which leads to different optimization functions (right plots) and parameter estimates.

The posterior covariance is formally given by

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

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

$$\Sigma_{\text{post}} = \Sigma_{\text{init}} - \Sigma_{\text{init}} A^\top \left[\Sigma_{\text{pred}} + \Sigma_{\text{obs}}\right]^{-1} A \Sigma_{\text{init}} \tag{2.4}$$

Can now interpret Σ_{post} as a rank d correction (or update) of Σ_{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 poing given in [5] as

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

We define

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

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

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

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

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

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

We derive using several identities

$$\Sigma_{up} = \Sigma_{init} - \Sigma_{init} A^\top \Sigma_{pred}^{-1} \left[\Sigma_{pred} - \Sigma_{obs}\right] \Sigma_{pred}^{-1} A \Sigma_{init}. \tag{2.9}$$

Substitute Σ_{up} for Σ_{post} in (2.5) to write the point that minimizes J as:

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

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

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

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* $\pi_{\text{in}} \sim N(\lambda_0, \Sigma_{init})$, $\pi_{\text{ob}} \sim N(\mathbf{y}, \Sigma_{obs})$, *and the predictability assumption holds, then*

(a) *There exists a unique parameter, denoted by* λ^{MUD}, *that maximizes* π_{up}.

(b) $Q(\lambda^{MUD}) = \mathbf{y}$.

(c) *If* $d = p$, λ^{MUD} *is given by* A^{-1}. *If* $d < p$, λ^{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

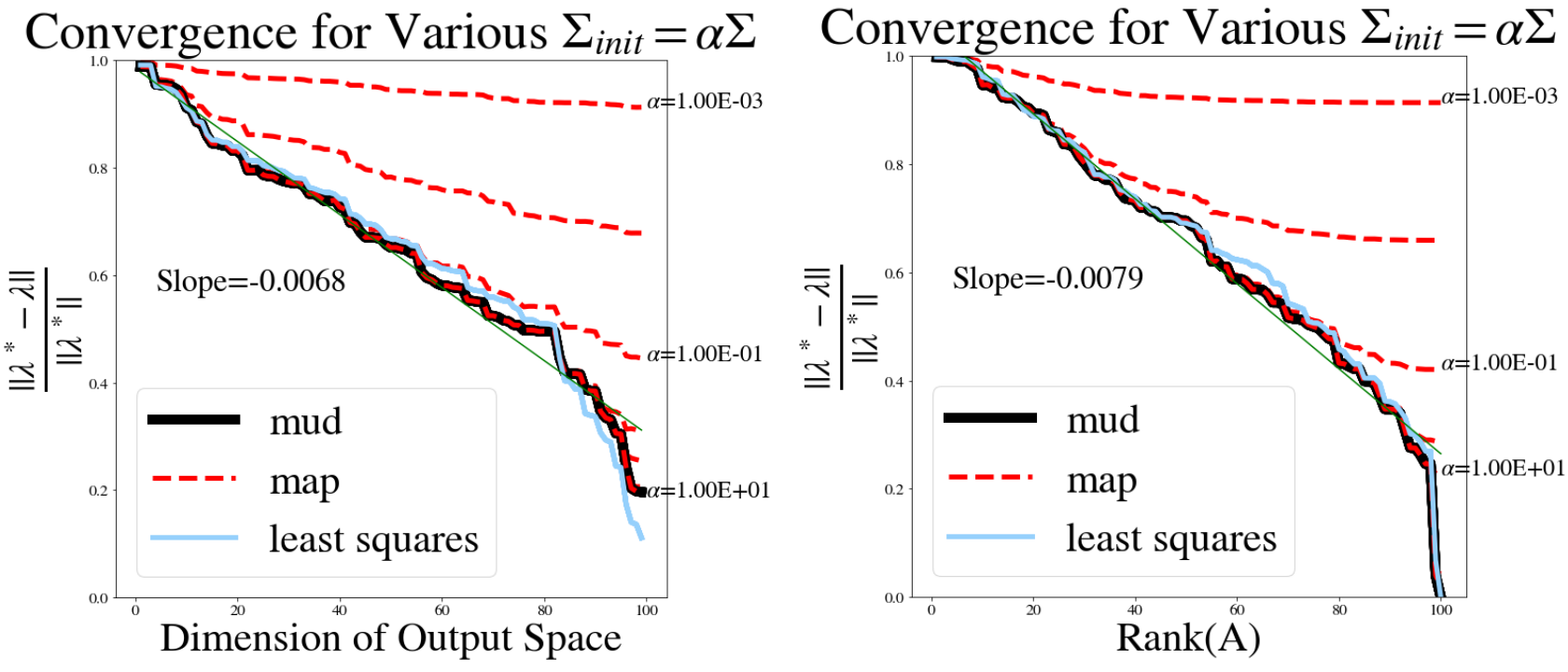

Figure: Relative errors between $\lambda^\dagger$ and (i) the least squares solution obtained through `numpy`'s `linalg.pinv` module, (ii) the closed-form solution for the MUD point given in Eq (2.11), and (iii) the MAP point. (Left): Error for increasing dimensions of D for A taken to be a Gaussian 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 jth measurement device.
N_j is number of noisy data obtained for $\mathcal{M}_j(\lambda^\dagger)$.

$d_{j,i}$ is the ith noisy datum for the jth 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

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

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 jth component, denoted by $Q_{\text{WME},j}(\lambda)$, given by

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

$Q_{\text{WME},j}(\lambda^\dagger)$ 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 π_{ob} as a $N(\mathbf{0}_{d\times 1}, \mathbf{I}_{d\times d})$ distribution.

The one where measurements impact the predictability assumption.

The jth 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

$$\frac{N_j}{\sigma_j^2} M_j \Sigma_{\text{init}} M_j^\top \tag{2.14}$$

Since Σ_{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 jth 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 jth 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 $\pi_{\text{in}} \sim N(\lambda_0, \Sigma_{init})$ and data are obtained for d linearly independent measurements on Λ 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 λ^{MUD} and $Q_{WME}(\lambda^{MUD}) = 0$.*

The one where we show that our approach works even when some assumptions are violated.

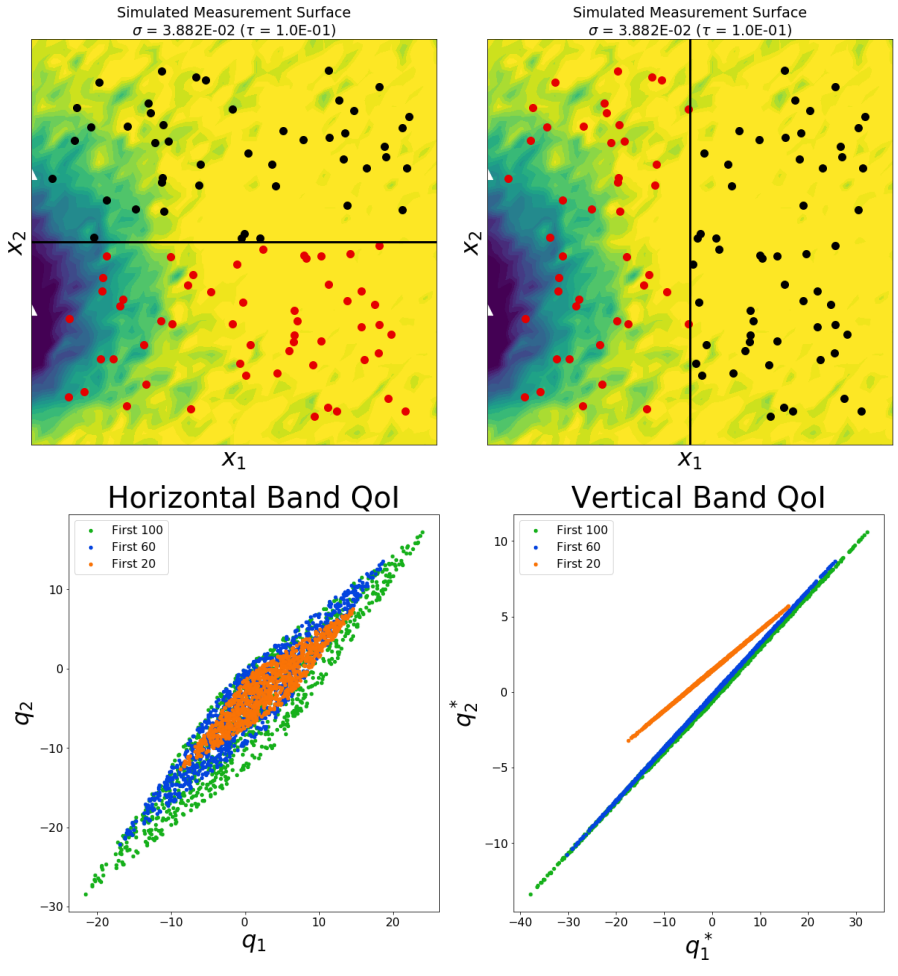

Figure: $N = 1000$ parameter evaluations for both methods of partitioning Ω.

The one with the small problems in many batches.

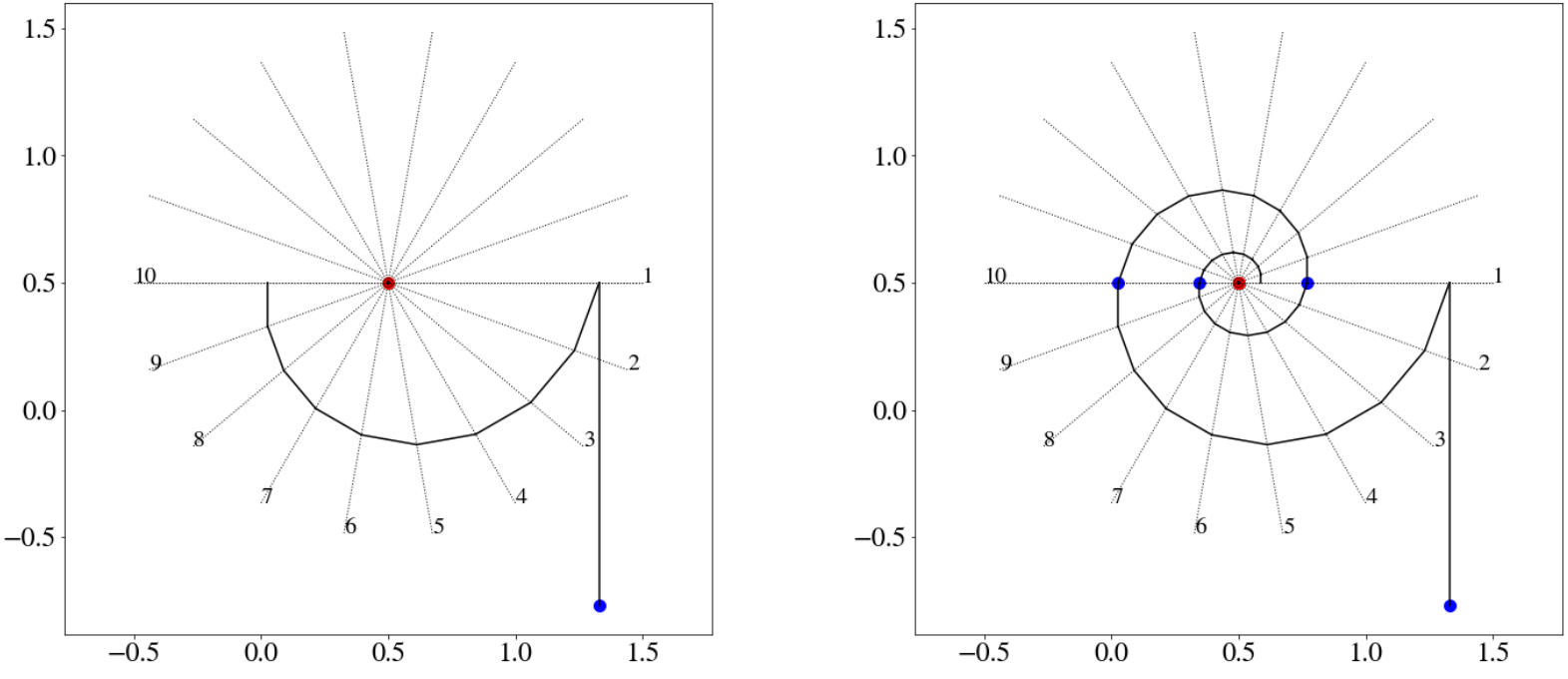

Figure: Dotted lines show the solution contours for each row of the operator A. (Left): First epoch for iterating through 10 QoI. (Right): Three more epochs allows our estimate to get much closer to the true value.

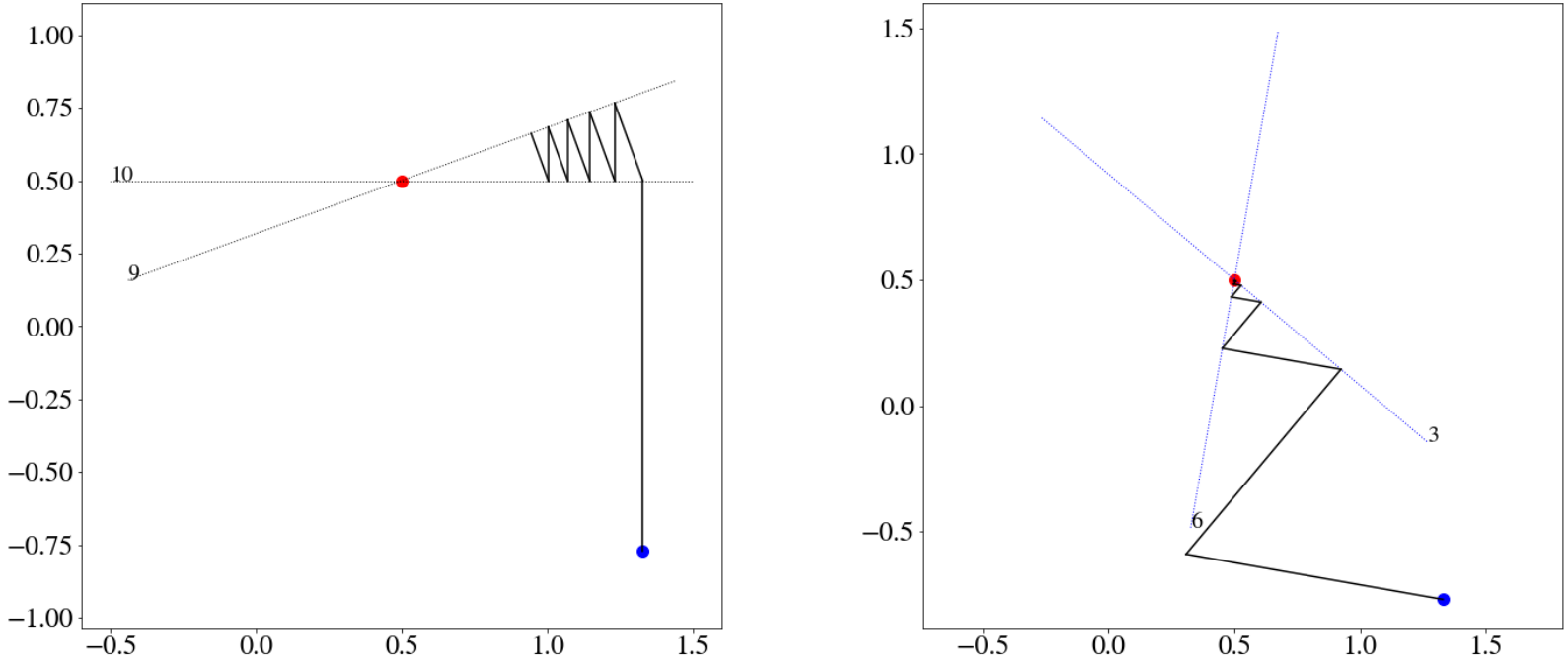

Figure: Iterating through five epochs of two QoI, each formed by picking two of the ten available rows of A at random. The random directions chosen on the left exhibit more redundancy than those on the right, so the same amount of iteration results in less accuracy.

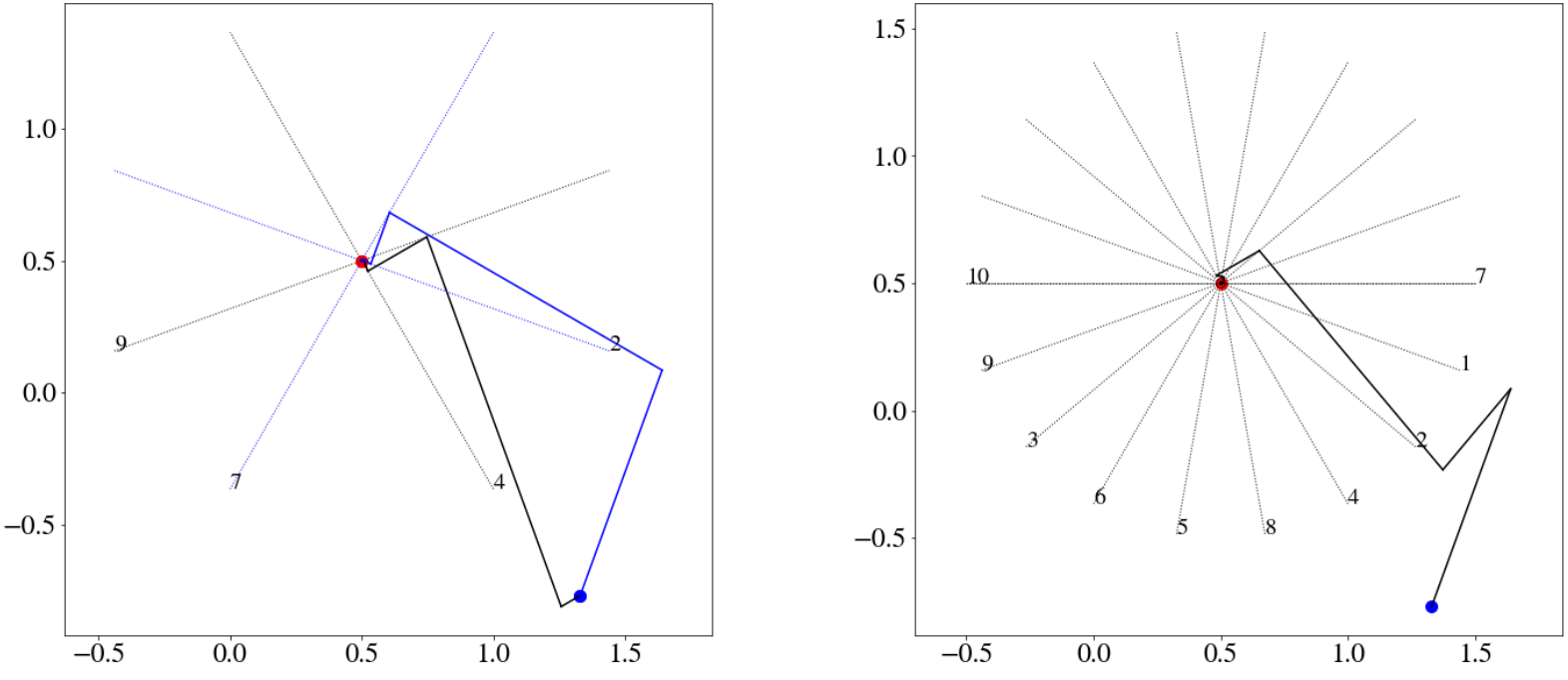

Figure: (Left): Subsets of available QoI components can be chosen to exhibit minimal redudancy and lead to expedited convergence. (Right): Random components of the QoI map used for each iterative step. This leads to an overall similar level of precision in this example, without the need to use gradients.

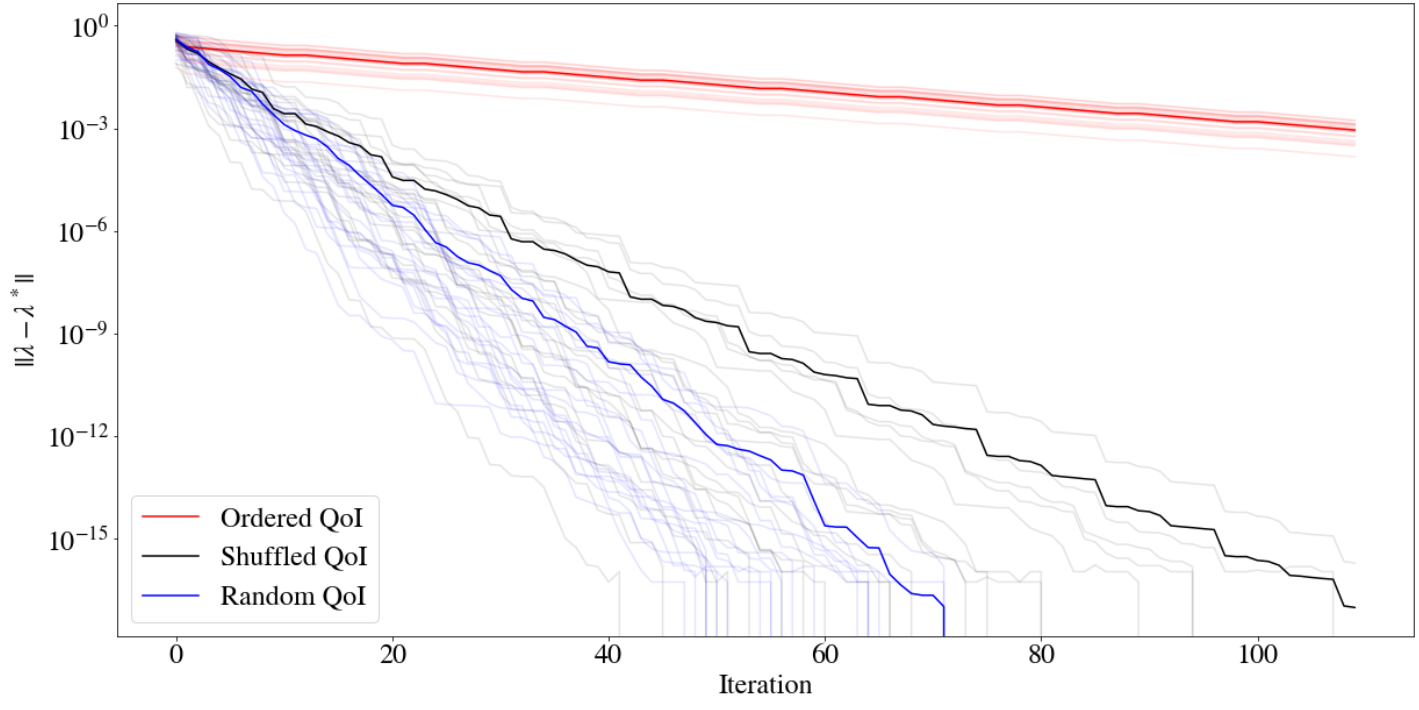

Figure: 20 initial means are chosen and iterated on for three approaches for ordering QoI. Individual experiments are transparent and the mean error is shown as a solid line for each approach.

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 (LaTeX, 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`)

M. Allmaras, W. Bangareth, J.M. Linhart, J. Polanco, F. Wang, K. Wang, J. Webster, and S. Zedler.
Estimating parameters in physical models through Bayesian inversion: A complete example.
2013.

J.O. Berger.
Statistical Decision Theory and Bayesian Analysis.
Springer-Verlag, 1985.

S. Myers R. Walpole, R. Myers and K. Ye.
Probability & Statistics for Engineers & Scientists.
Pearson Education, 2007.

Ralph C. Smith.
Uncertainty Quantification: Theory, Implementation, and Applications.
Society for Industrial and Applied Mathematics, Philadelphia, PA, USA, 2013.

Albert Tarantola.

Inverse Problem Theory and Methods for Model Parameter Estimation.
siam, 2005.