

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

Michael Pilosov

Advisor: Troy Butler

University of Colorado Denver

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Department of Mathematical
& Statistical Sciences

UNIVERSITY OF COLORADO DENVER

The one where we describe why any of this matters.

Broad Goals of Uncertainty Quantification

- Make inferences and predictions
- Quantify and reduce uncertainties (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.

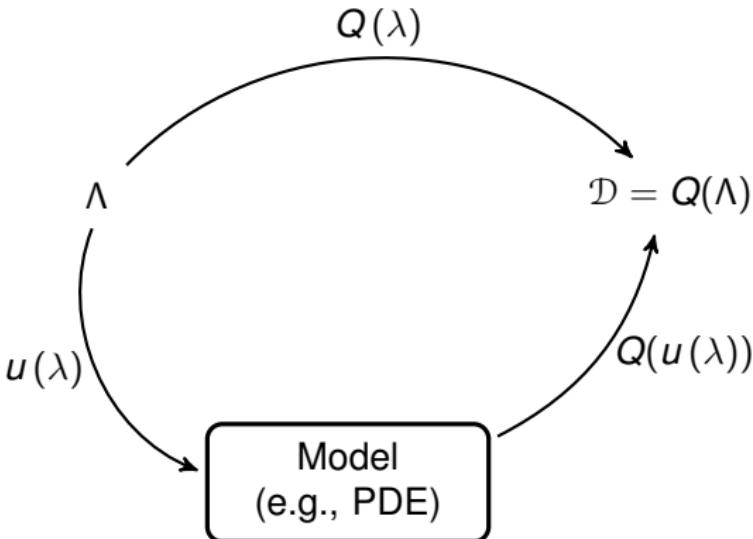
- State variable: u (e.g. heat, energy, pressure, deflection)
- Parameters: λ (e.g. source term, diffusion, boundary data)
- Model: $\mathcal{M}(u, \lambda) = 0$, so $u(\lambda)$
- Quantity of Interest (QoI) map, (piecewise smooth):

$$Q = \begin{bmatrix} q_1 \\ q_2 \\ \vdots \\ q_D \end{bmatrix}, \text{ where } q_i : u(\lambda) \rightarrow \mathbb{R}$$

- We write $Q(\lambda) := Q(u(\lambda))$ to make the dependence on λ explicit.



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



Definition (Stochastic Forward Problem (SFP))

Given a probability measure \mathbb{P}_Λ 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

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



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

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}_Λ , on $(\Lambda, \mathcal{B}_\Lambda)$ satisfying

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

Equation (1.3) is referred to as the *consistency condition*.



Definition (Consistent Solution and Density)

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

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

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

In such a case, we can rewrite (1.2) and (1.3) 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}_Λ in (1.2) 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 μ_Λ exists on $(\Lambda, \mathcal{B}_\Lambda)$, the *initial distribution* π_{in} is given by the Radon-Nikodym derivative of \mathbb{P}_{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

$$\mathbb{P}_{\text{pr}}(E) = \mathbb{P}_{\text{in}}(Q^{-1}(E)), \quad \forall E \in \mathcal{B}_{\mathcal{D}}. \quad (1.4)$$



Definition (Observed Distribution)

When $\mathbb{P}_{\mathcal{D}}$ in (1.3) quantifies the characterization of uncertainty in the QoI data, it is referred to as the *observed measure*, \mathbb{P}_{ob} .

Given a dominating $\mu_{\mathcal{D}}$ on $(\mathcal{D}, \mathcal{B}_{\mathcal{D}})$, the Radon-Nikodym derivative \mathbb{P}_{ob} w.r.t. $\mu_{\mathcal{D}}$ is referred to as the *observed density* π_{ob} .



The one where we define the solution to the Stochastic Inverse Problem.

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

$$\pi_{\text{up}}(\lambda) := \pi_{\text{in}}(\lambda) \frac{\pi_{\text{ob}}(Q(\lambda))}{\pi_{\text{pr}}(Q(\lambda))}. \quad (1.5)$$



The one with some practical considerations.

- Approximate π_{pr} using density estimation using samples from π_{in} .
- May evaluate π_{up} directly for any sample of Λ (one model solve).
- Accuracy proportional to that of approximation to 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.
- Stable w.r.t. perturbations in the Total Variation metric.



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

Bayesian approach:

- Modeling epistemic uncertainties in data.
- Data obtained from a true, but unknown, parameter value, λ^\dagger .
- Fundamentally solving a different problem.

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

$$q = Q(\lambda), \forall \lambda \in \Lambda. \quad (1.6)$$



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

$$\|Q(\lambda) - d\| \tag{1.7}$$

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

- ξ is some unobservable perturbation to the true output.
- ξ arises 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 $\pi_{\text{post}}(\lambda | d)$.
- π_{post} proportional to the product of π_{prior} and $L_{\mathcal{D}}$ [3, 2, 1, 4]:

$$\pi_{\text{post}}(\lambda) := \pi_{\text{prior}}(\lambda) \frac{L_{\mathcal{D}}(q|\lambda)}{C}. \quad (1.8)$$

- The *evidence* term C ensures integration to unity. Given by:

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

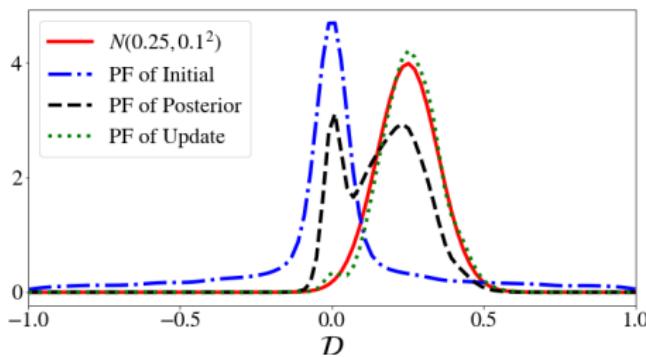
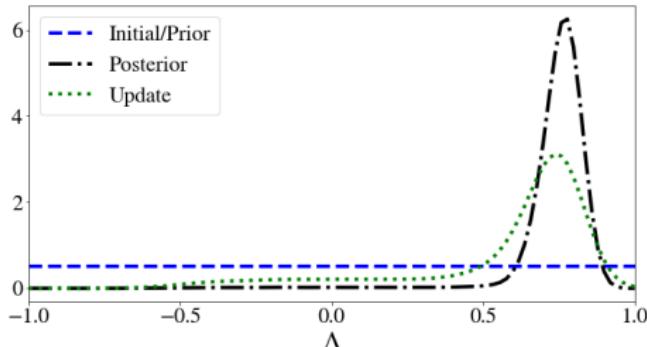


The one where we provide an illustrative example.

- 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 $\xi \sim N(0, 0.1^2)$
- $\pi_{\text{prior}} = \pi_{\text{in}}$ and $d = 0.25$ so $L_{\mathcal{D}} = \pi_{\text{ob}}$



The one where we provide an illustrative example.



The one where we provide an illustrative example.

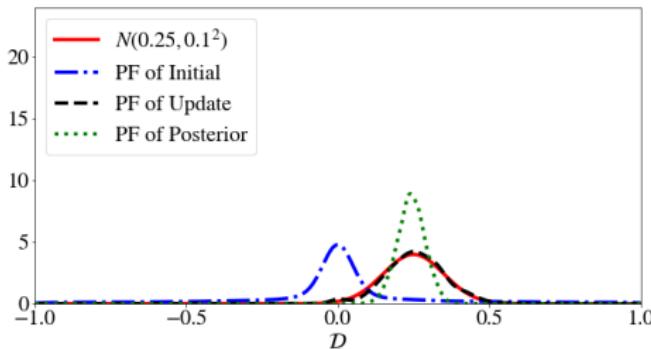
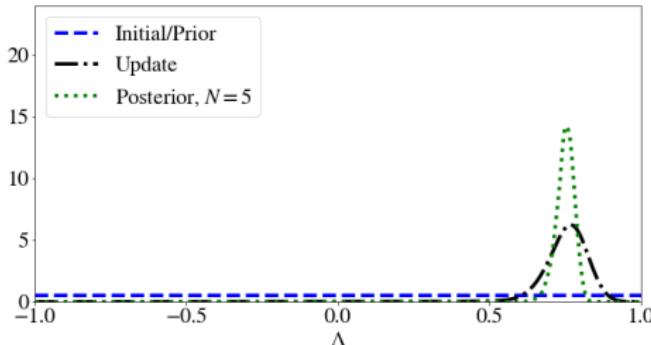
What happens as we collect more data?

SIP: Use N to estimate mean of observed

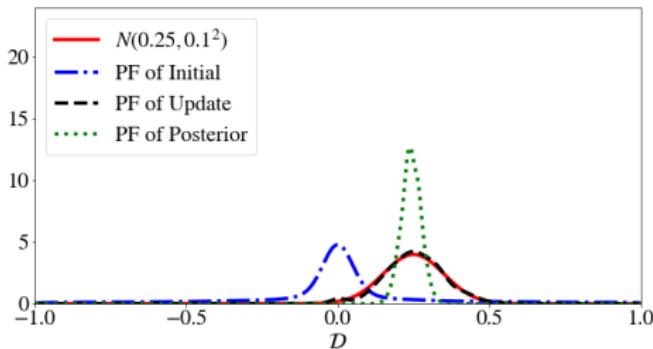
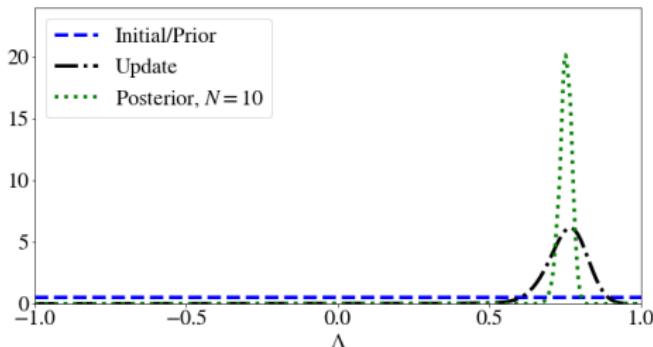
DIP: likelihood function incorporates more data



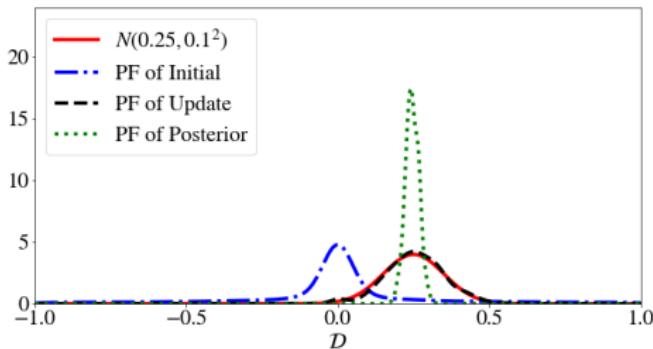
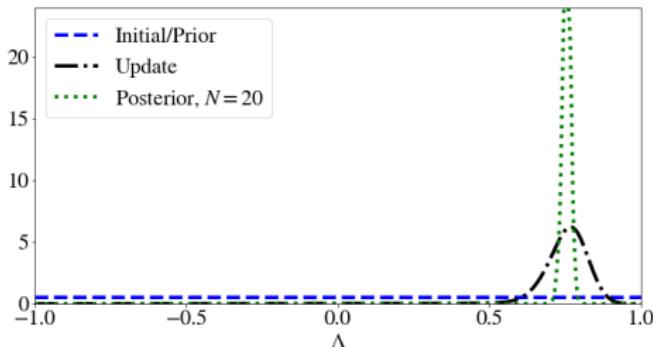
The one where we provide an illustrative example.



The one where we provide an illustrative example.



The one where we provide an illustrative example.



The one where we define the Maximal Updated Density (MUD) point.

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



The one where we create a unifying framework.

- Recall $\|\mathbf{x}\|_C^2 := (\mathbf{x}, \mathbf{x})_C = \mathbf{x}^T C \mathbf{x}$.
- Non-degenerative $\Sigma_{\text{pred}}^{-1}$, Σ_{obs}^{-1} , $\Sigma_{\text{init}}^{-1}$ play the role of C .
- Suppose that $\pi_{\text{in}} = \pi_{\text{prior}} \sim \mathcal{N}(\lambda_0, \Sigma_{\text{init}})$.
- Suppose Q is linear and that $\pi_{\text{ob}} = \pi_{\text{like}} \sim \mathcal{N}(\mathbf{y}, \Sigma_{\text{obs}})$.
- Linearity of Q implies that $Q(\lambda) = A\lambda$ for some $A \in \mathbb{R}^{d \times p}$, and that $\pi_{\text{pr}} \sim \mathcal{N}(Q(\lambda_0), \Sigma_{\text{pred}})$, 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	$J(\lambda) := T(\lambda) - \ Q(\lambda) - Q(\lambda_0)\ _{\Sigma_{\text{pred}}^{-1}}^2$



The one where an example highlights a key difference.

- $A = \begin{bmatrix} 1 & 1 \end{bmatrix}$
- 2-D input, 1-D output \implies rank-deficient
- Details:

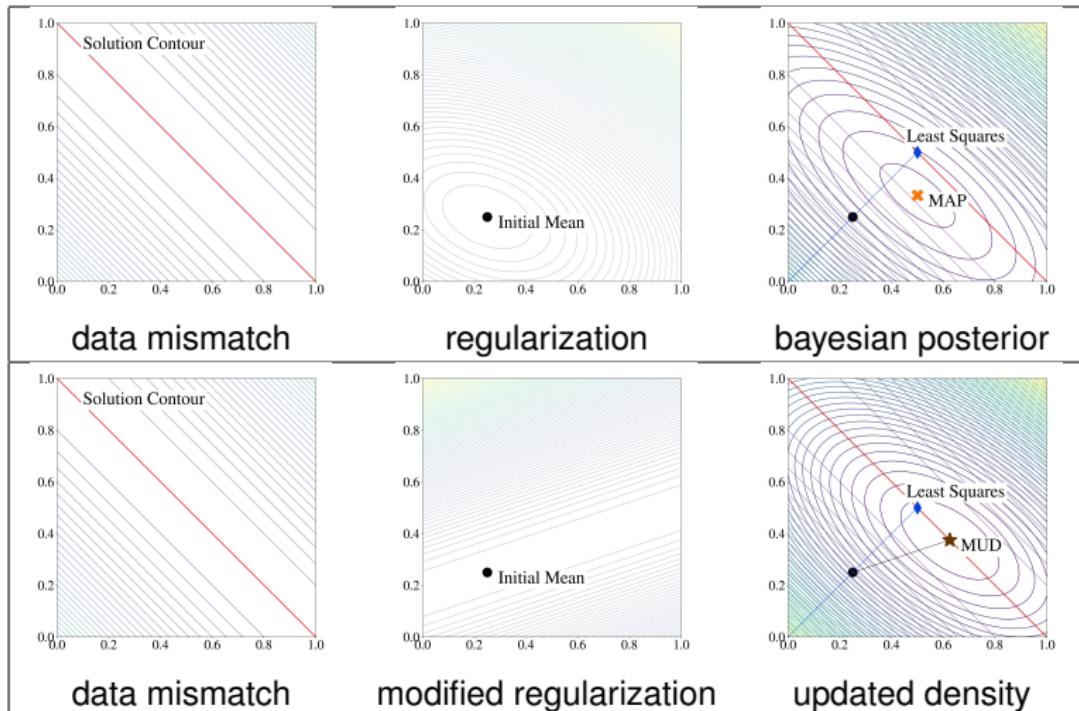
$$\lambda_0 = \begin{bmatrix} 0.25 & 0.25 \end{bmatrix}^\top$$

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

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



The one that kind of says it all.



- Posterior covariance:

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

- Using Woodbury identity and (2.2):

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

- Interpretation: Σ_{post} is 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.
- Rewrite using analytical expression for the MAP point:

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

The one where we make some convenient manipulations.

- Let

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

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

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

- R is the *effective regularization* in $J(\lambda)$ in the DCI 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).

The one where we make some convenient manipulations.

- *Using linear algebra ...*

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

- Substitute Σ_{up} for Σ_{post} in (2.5):

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

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

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



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



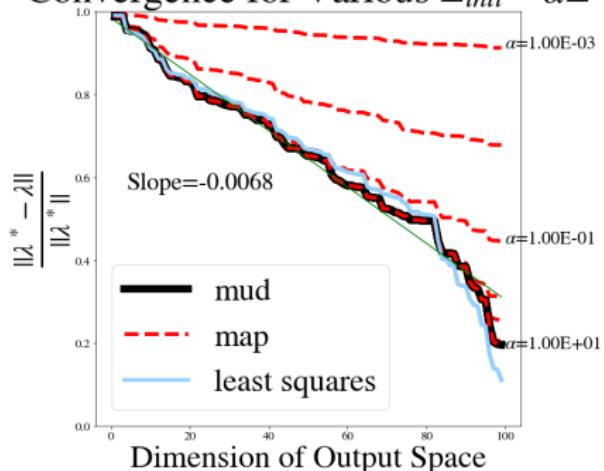
The one where we address a key assumption

- Predictability Assumption: π_{pr} is a dominating measure for π_{ob}
- Linear case: involves eigenvalues of covariances:
 - » min eigenvalue $\Sigma_{\text{pred}} >$ max eigenvalue Σ_{obs}

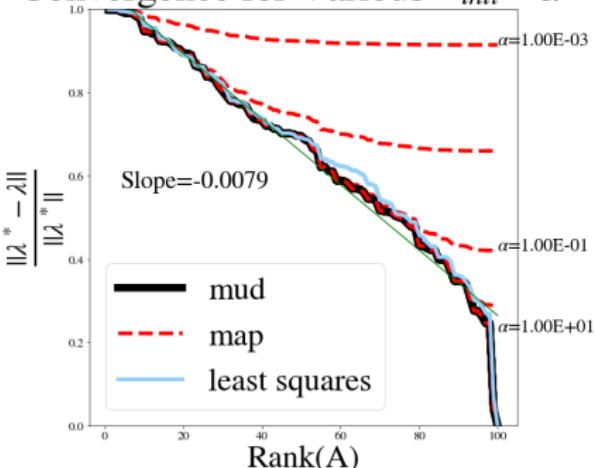


The one where we show how rank and dimension impact our solutions.

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



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



Example: scaling random diagonal initial covariances

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 $1 \leq i \leq N_j$.
- Unbiased additive error model for the measurement noise.
- Noise is independent identically distributed (i.i.d.) Gaussian errors, so

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

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 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 λ^\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 j th diagonal component of Σ_{pred} is given by the predicted variance associated with using the scalar-valued $Q_{\text{WME},j}$.
- The associated predicted variance is given by

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

- Σ_{init} non-degenerative and M_j non-trivial row vector, which implies that the **predicted variance grows linearly** with N_j .

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 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 $Q_{\text{WME}}(\lambda^{\text{MUD}}) = 0$.**



The one where we violate some assumptions (and see what happens).

Consider the exponential decay problem with uncertain decay rate λ :

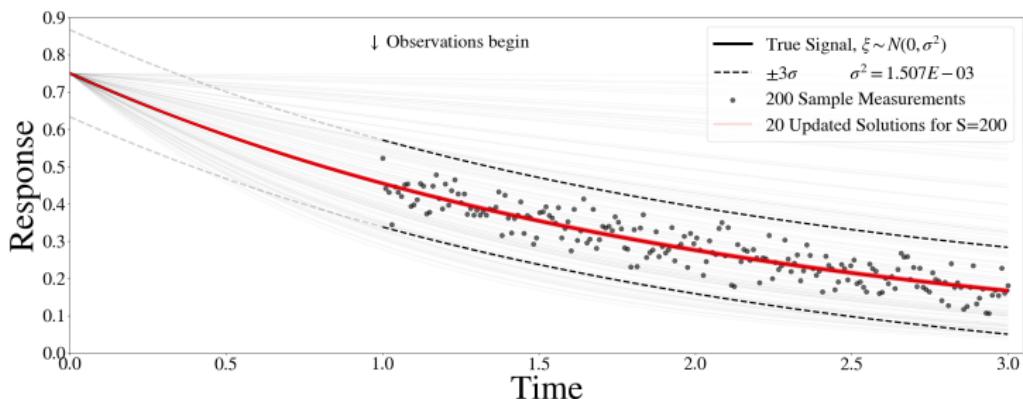
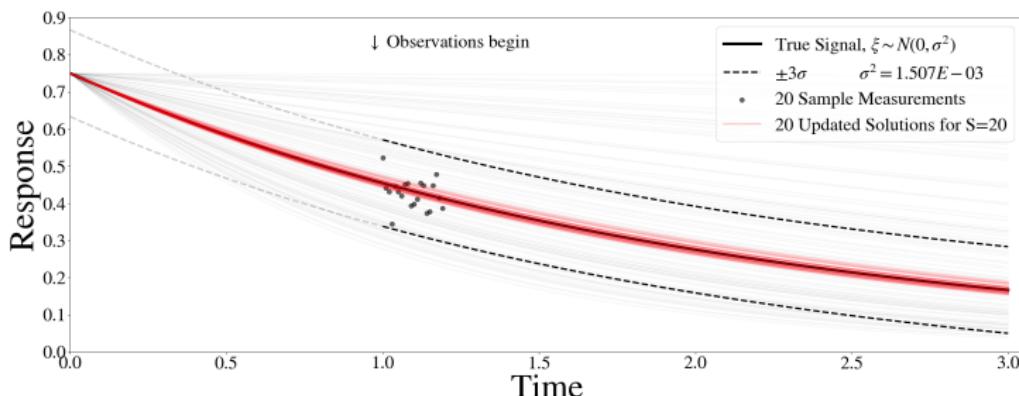
$$\begin{cases} \frac{\partial u}{\partial t} &= \lambda u(t), \quad 0 < t \leq 3, \\ u(0) &= 0.75, \end{cases}$$

with solution

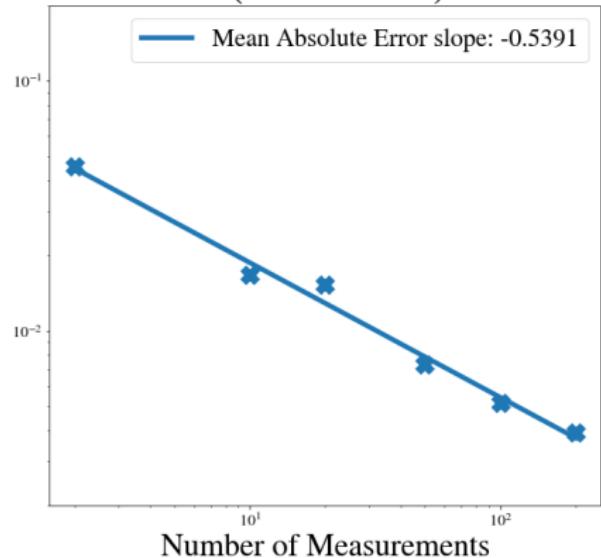
$$u(t; \lambda) = u_0 \exp(-\lambda t), \quad u_0 = 0.75, \tag{2.15}$$

and measurements begin at $t = 1$, continuing until $t = 3$.

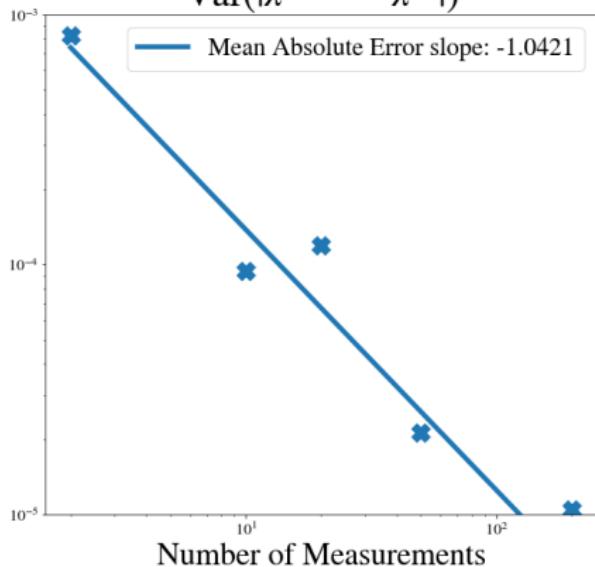




$$\mathbb{E}(|\lambda^{\text{MUD}} - \lambda^\dagger|)$$



$$\text{Var}(|\lambda^{\text{MUD}} - \lambda^\dagger|)$$



The one where we violate some assumptions (and see what happens).

Consider the Poisson problem:

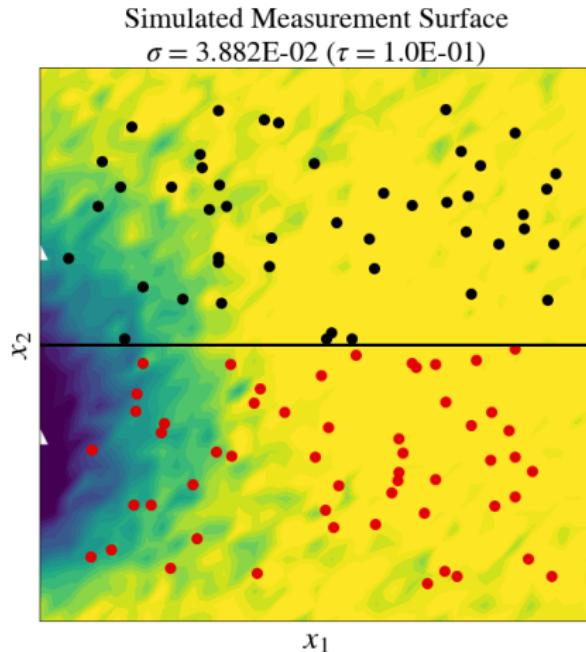
$$\begin{cases} -\nabla \cdot \nabla u = f(x), & \text{on } x \in \Omega, \\ u = 0, & \text{on } \Gamma_T \cup \Gamma_B, \\ \frac{\partial u}{\partial \mathbf{n}} = g(x_2), & \text{on } \Gamma_L, \\ \frac{\partial u}{\partial \mathbf{n}} = 0, & \text{on } \Gamma_R, \end{cases} \quad (2.16)$$

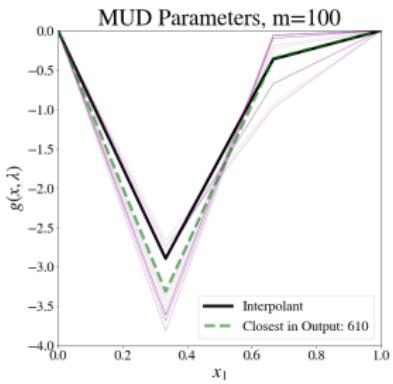
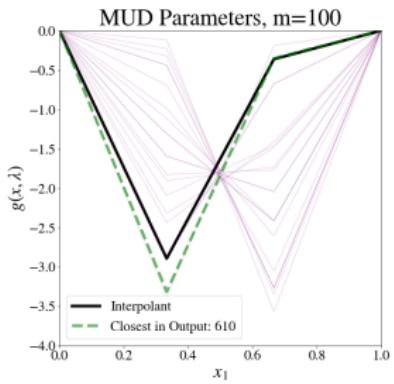
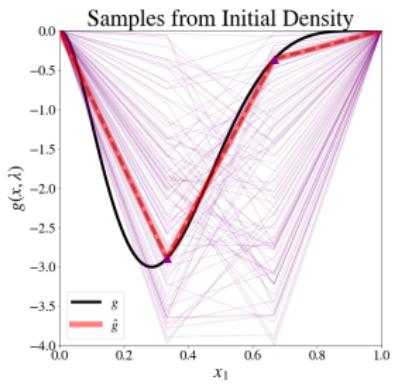
where $x = (x_1, x_2) \in \Omega = (0, 1)^2$ is the spatial domain.

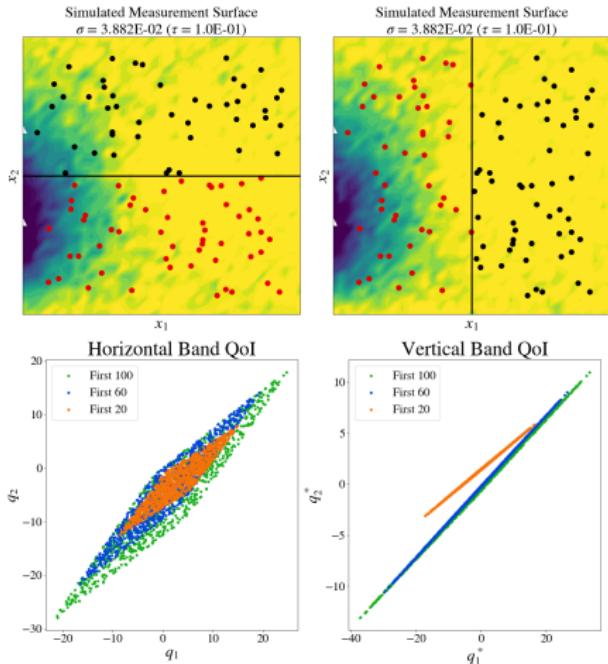
- Γ_T , Γ_B , Γ_L , and Γ_R , denote the top, bottom, left, and right boundaries.
- The outward normal derivative is denoted by $\frac{\partial u}{\partial \mathbf{n}}$.
- The forcing function is $f = 10 \exp \left(\|x - 0.5\|^2 / 0.02 \right)$.

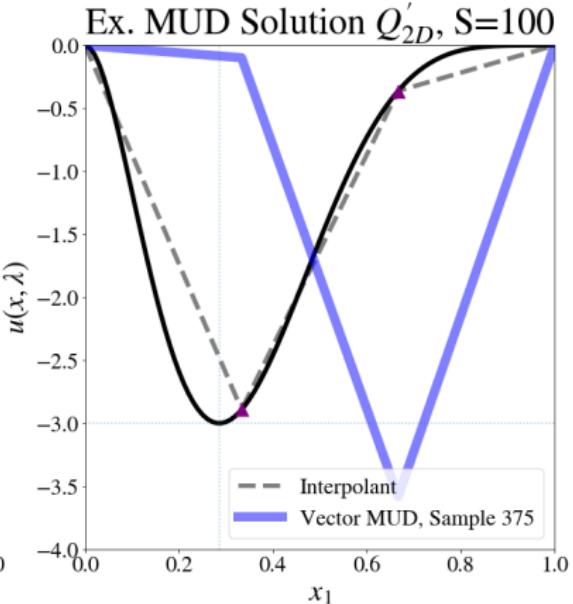
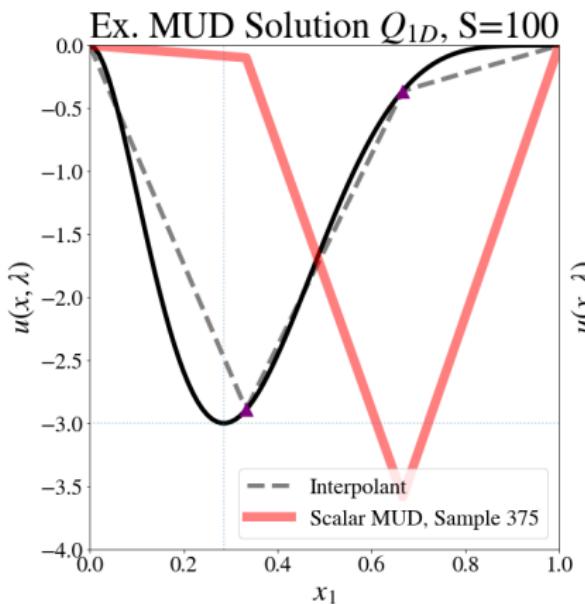


- $g(x_2)$ is uncertain parameter, i.e., λ defines an uncertain function.
- To generate the noisy data, we use $g(x_2) \propto x_2^2(x_2 - 1)^5$.
- Constant of proportionality chosen so $\min g = -3$ at $x_2 = \frac{2}{7}$.
- Piecewise-linear finite elements on a triangulation of a 36×36 mesh.
- 100 randomly placed sensors in the subdomain $(0.05, 0.95)^2 \subset \Omega$.
- Repeated 20 times to study variation due to realizations of noisy data.
- Limited to $N = 1000$ samples from initial density.

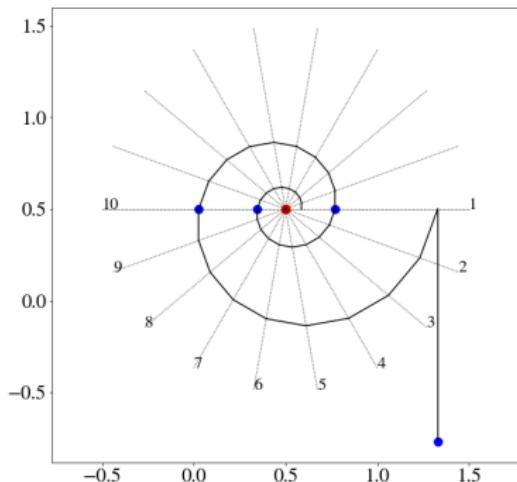
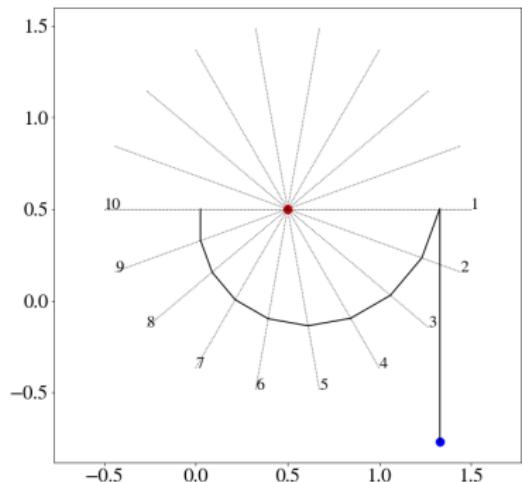






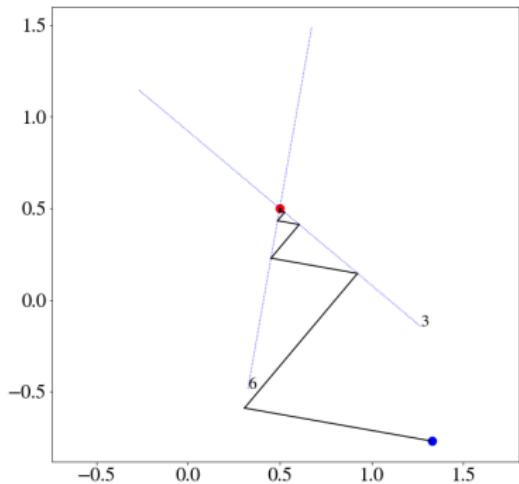
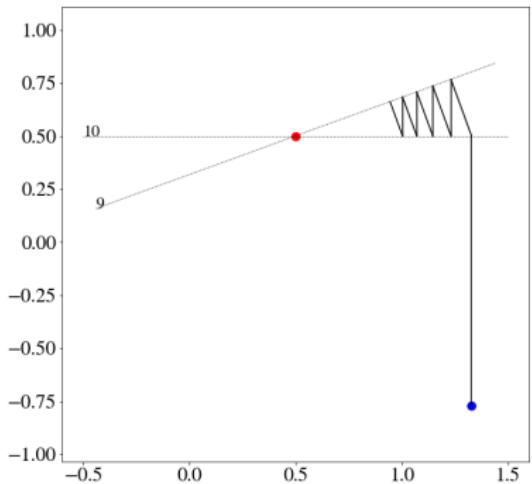


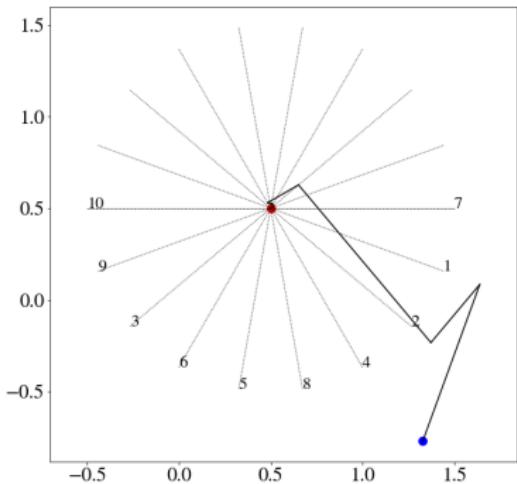
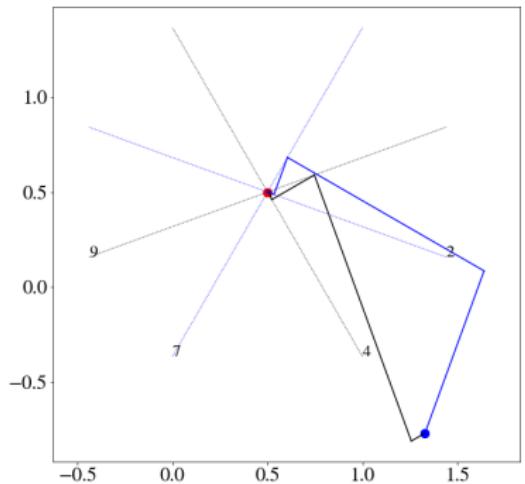
The one with the small problems in many batches.

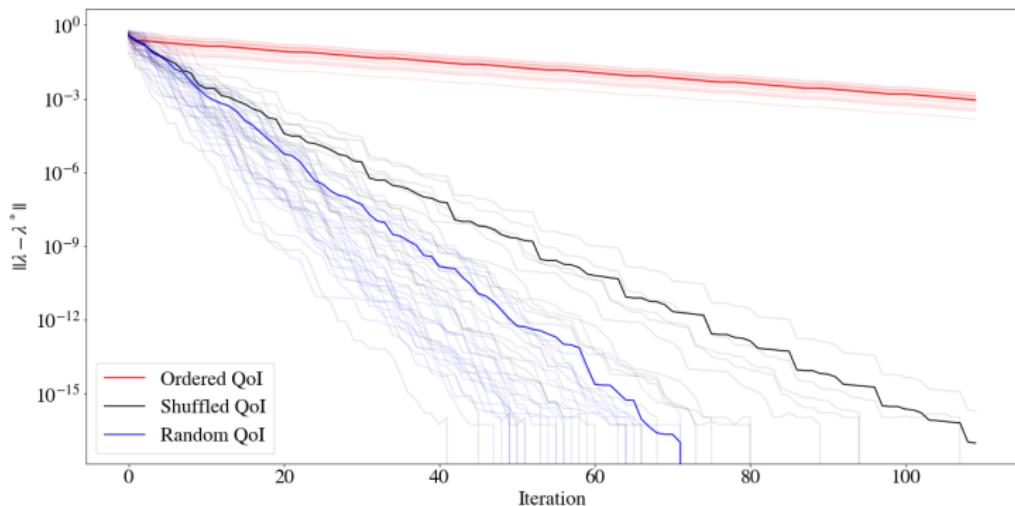


QoI defined by 10 equispaced rotations of the unit vector $[0, 1]$ through the first two Euclidean quadrants.









The one where we convince you to trust our numerics.

- 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^AT_EX, 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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