

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 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.

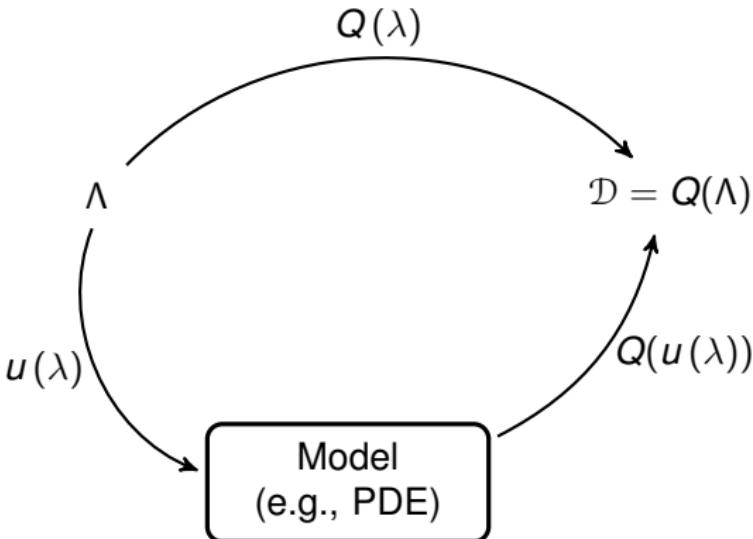
- State variable: u (e.g. heat, energy, pressure, deflection)
- Parameters: λ (e.g. source term, diffusion, boundary data)
- Model: $\mathcal{M}(u, \lambda) = 0$, so $u(\lambda)$
- Quantity of Interest (QoI) map, (piecewise smooth):

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

- 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} .

Given a dominating μ_Λ on $(\Lambda, \mathcal{B}_\Lambda)$, the Radon-Nikodym derivative π_{in} w.r.t μ_Λ is referred to as the *initial distribution*.



Definition (Predicted Distribution)

The *predicted distribution* is the push-forward of π_{in} under the map Q , and is denoted as π_{pr} .

Given as Radon-Nikodym derivative (w.r.t $\mu_{\mathcal{D}}$) of 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 distribution* π_{ob} .



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

We now have all of the definitions required for the *updated distribution* which solves the SIP:

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



The one with some practical considerations.

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



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

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



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

$$\|Q(\lambda) - d\| \quad (1.7)$$

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:

$$\pi_{\text{post}}(\lambda | d)$$

- π_{post} proportional to the product of π_{prior} and $L_{\mathcal{D}}$ [3, 2, 1, 4]:

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

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

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

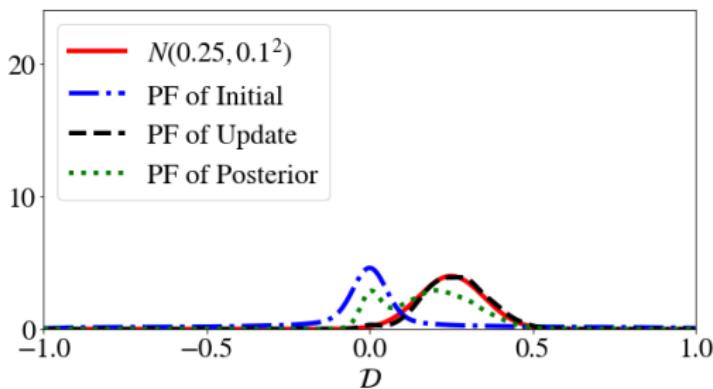
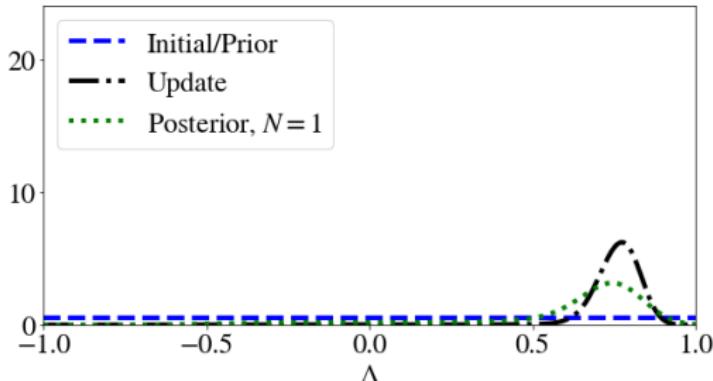


The one where we provide an illustrative example.

- Suppose $\Lambda = [-1, 1] \subset \mathbb{R}$ and $Q(\lambda) = \lambda^5$ so that $\mathcal{D} = [-1, 1]$
- $\pi_{\text{in}} \sim \mathcal{U}([-1, 1])$
- $\pi_{\text{ob}} \sim N(0.25, 0.1^2)$
- $d \in \mathcal{D}$ 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.

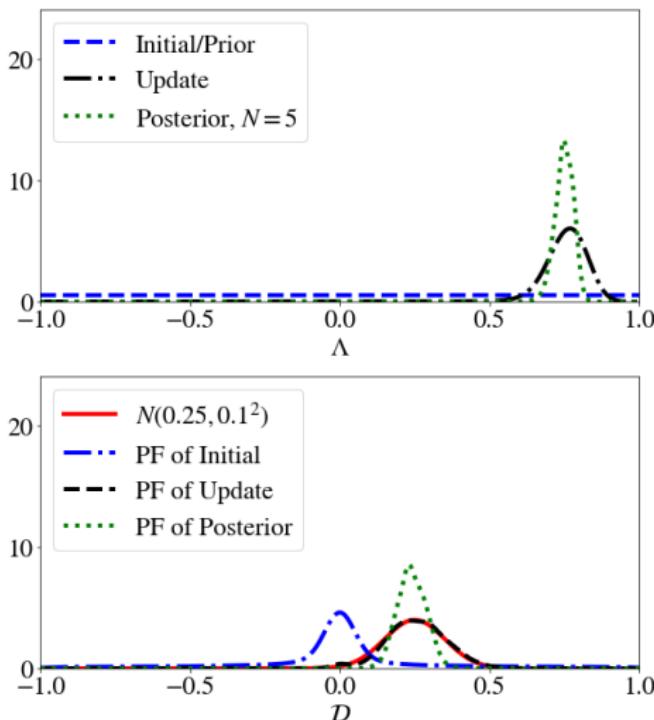
What happens as we collect more data?

SIP: Use N to estimate mean of observed.

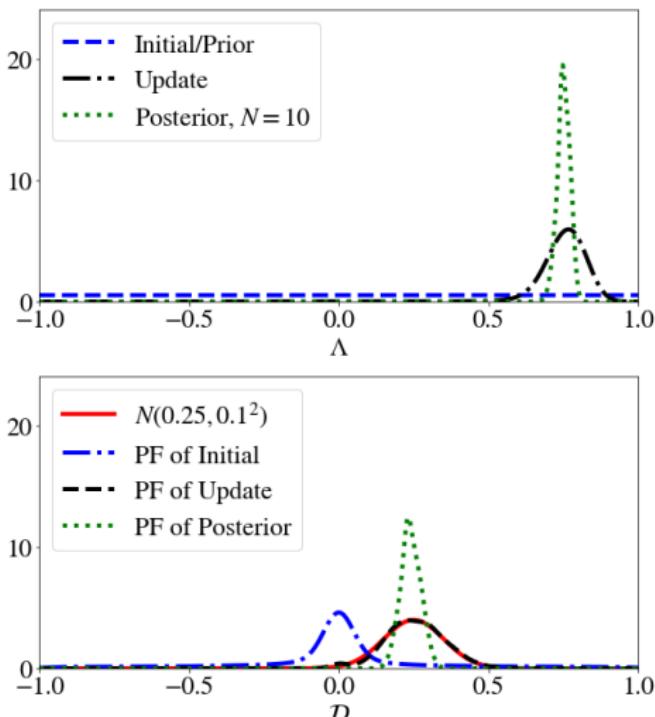
DIP: Likelihood function incorporates more terms.



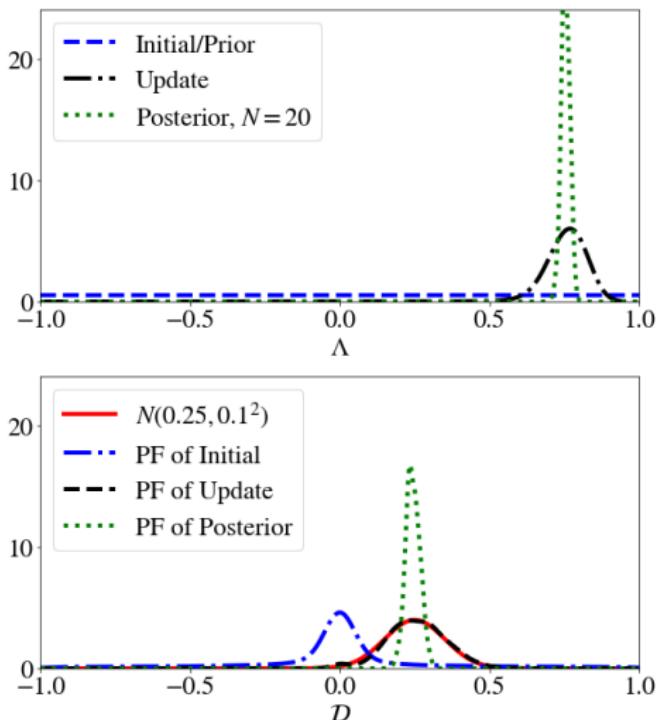
The one where we provide an illustrative example.



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.

$$\pi_{\text{post}}(\lambda \mid d) = \frac{\pi_{\text{prior}}(\lambda) \pi_{\text{like}}(d \mid \lambda)}{\int_{\Lambda} \pi_{\text{like}}(d \mid \lambda) \pi_{\text{prior}}(\lambda) d\mu_{\Lambda}}$$

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

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:

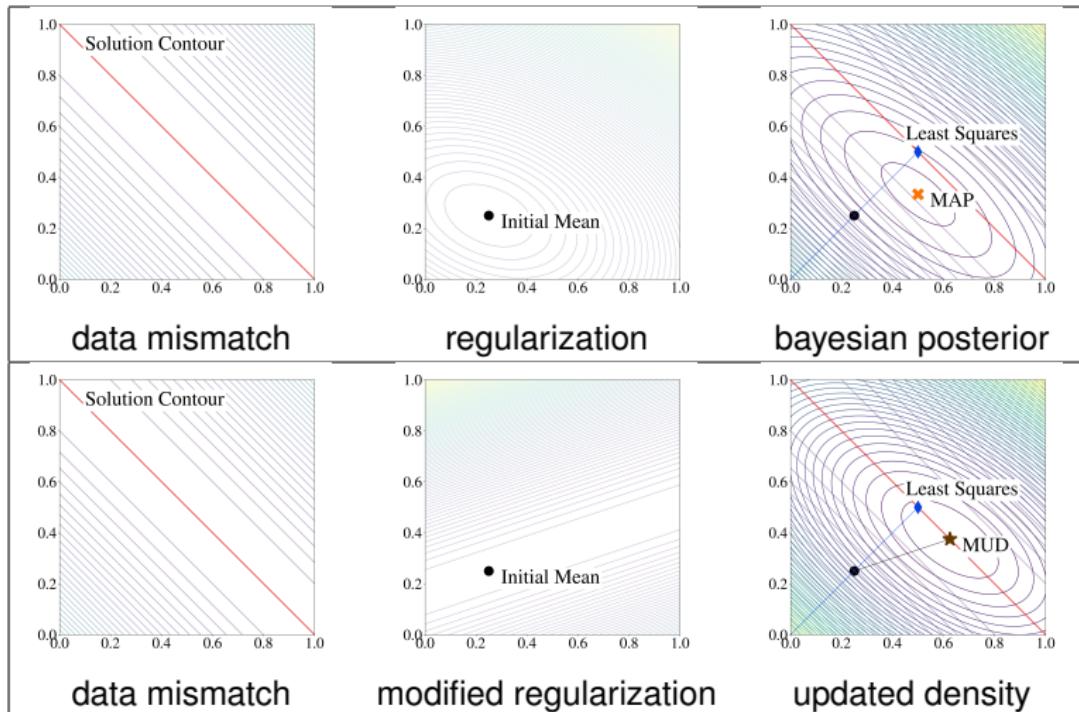
$$\lambda_0 = \begin{bmatrix} 0.25 & 0.25 \end{bmatrix}^\top$$

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

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



The one that kind of says it all.



- Posterior covariance:

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

- Using Woodbury identity and (2.2):

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

- 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:

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

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).



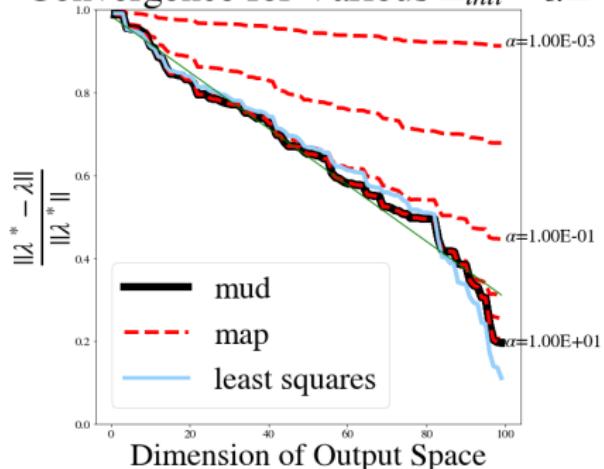
The one where we address a key assumption

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

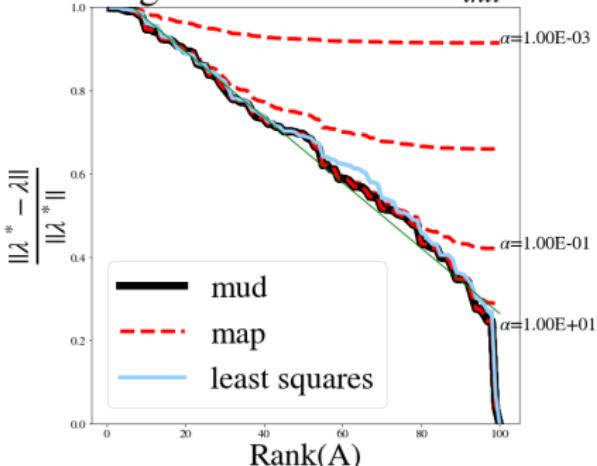


The one where we show how rank and dimension impact our solutions.

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.

- Measurement devices M_j generating repeated noisy data, $1 \leq j \leq d$.
- $d_{j,i}$ 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:

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

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 $Q_{WME}(\lambda)$.

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

- $Q_{WME,j}(\lambda^\dagger)$ is the sample avg of N_j draws from an i.i.d. $N(0, N_j)$.
- Observed data are generated according to fixed (truth) λ^\dagger in (2.12).
- For each component, $Q_{WME,j}(\lambda^\dagger) \sim N(0, 1)$.
- π_{ob} is a $N(\mathbf{0}_{d \times 1}, \mathbf{I}_{d \times d})$ due to the structure of $Q_{WME}(\lambda)$.



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 for the j th component 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 :

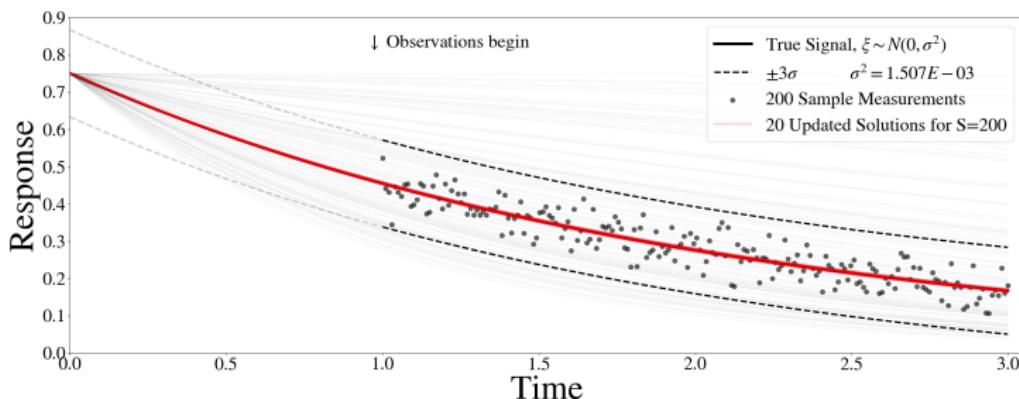
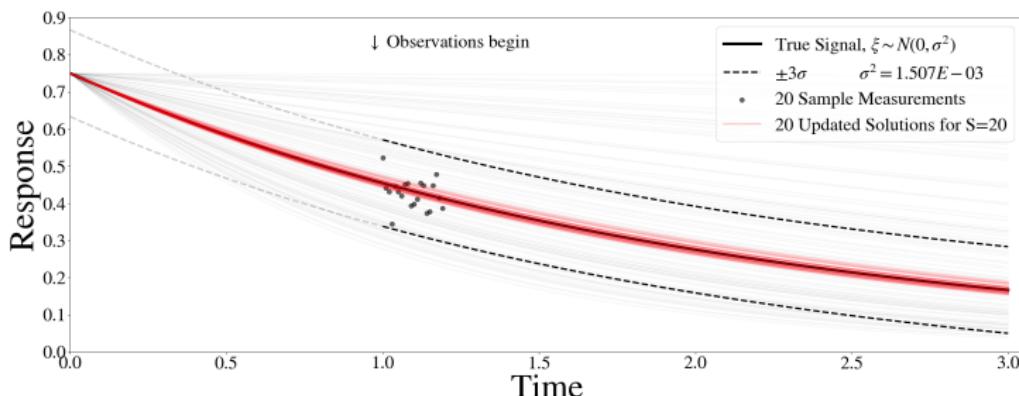
$$\begin{cases} \frac{\partial u}{\partial t} = \lambda u(t), & 0 < t \leq 3, \\ u(0) = 0.75, \end{cases}$$

with solution

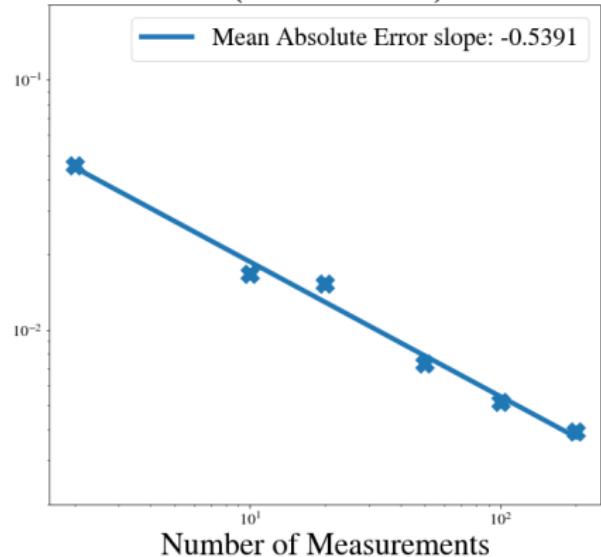
$$u(t; \lambda) = u_0 \exp(-\lambda t), \quad u_0 = 0.75, \quad (2.15)$$

and measurements occur from $t = 1$ until $t = 3$ at rate of 100Hz.

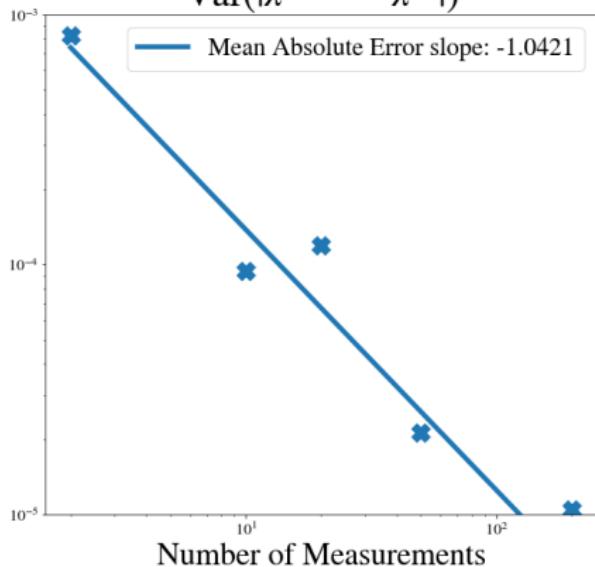




$$\mathbb{E}(|\lambda^{\text{MUD}} - \lambda^\dagger|)$$



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



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

Consider the Poisson problem:

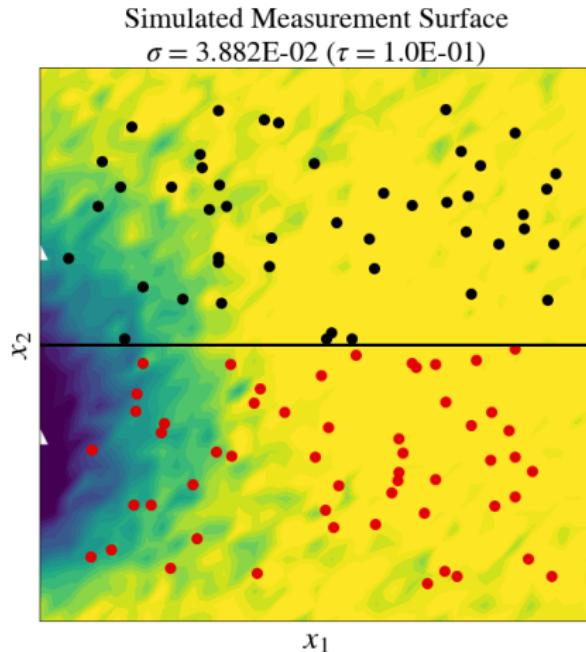
$$\begin{cases} -\nabla \cdot \nabla u = f(x), & \text{on } x \in \Omega, \\ u = 0, & \text{on } \Gamma_T \cup \Gamma_B, \\ \frac{\partial u}{\partial \mathbf{n}} = g(x_2), & \text{on } \Gamma_L, \\ \frac{\partial u}{\partial \mathbf{n}} = 0, & \text{on } \Gamma_R, \end{cases} \quad (2.16)$$

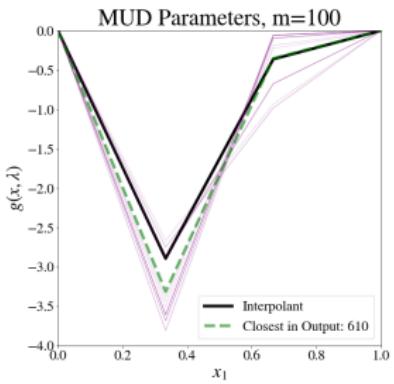
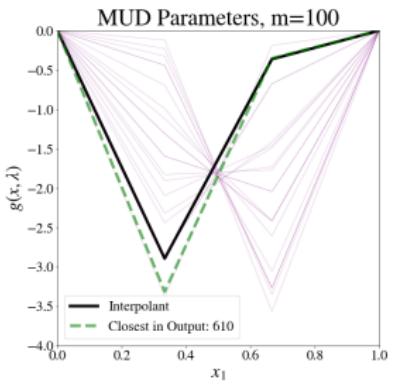
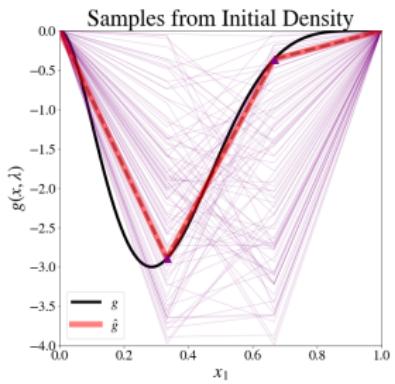
where $x = (x_1, x_2) \in \Omega = (0, 1)^2$ is the spatial domain.

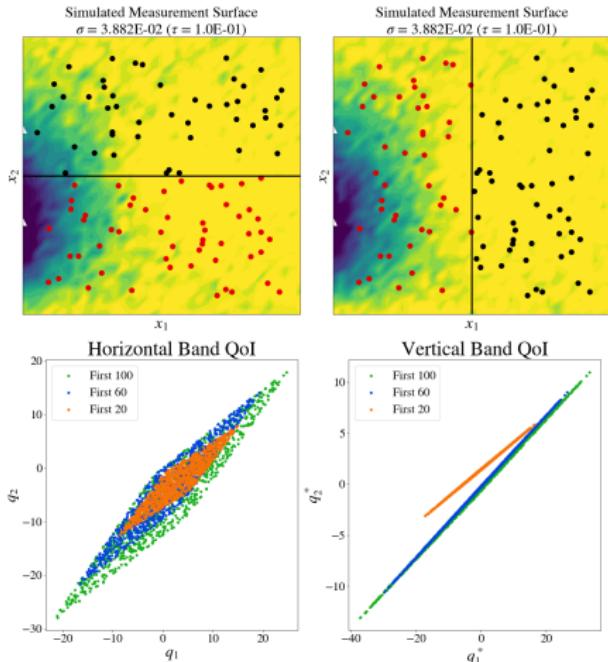
- Γ_T , Γ_B , Γ_L , and Γ_R , denote the top, bottom, left, and right boundaries.
- The outward normal derivative is denoted by $\frac{\partial u}{\partial \mathbf{n}}$.
- The forcing function is $f = 10 \exp \left(\|x - 0.5\|^2 / 0.02 \right)$.

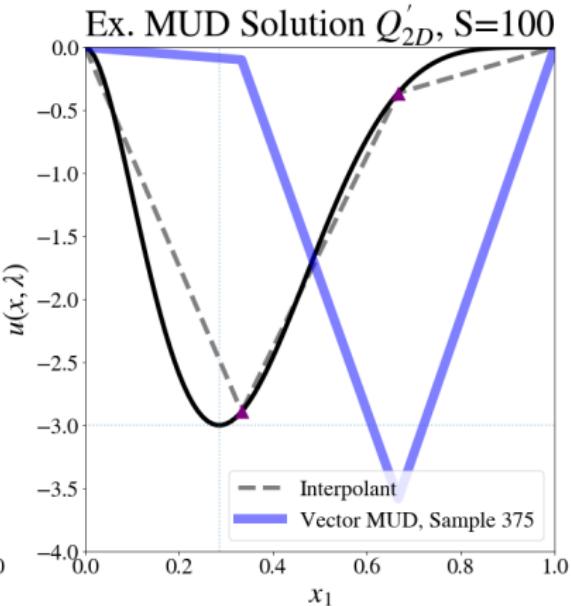
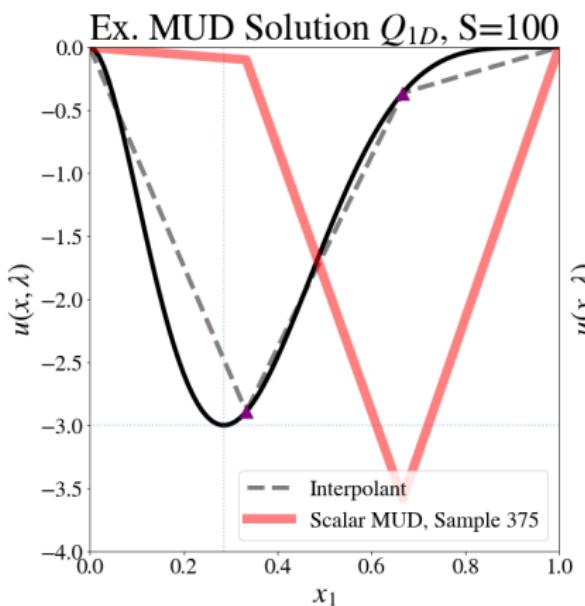


- $g(x_2)$ is uncertain parameter, i.e., λ defines an uncertain function.
- To generate the noisy data, we use $g(x_2) \propto x_2^2(x_2 - 1)^5$.
- Constant of proportionality chosen so $\min g = -3$ at $x_2 = \frac{2}{7}$.
- Piecewise-linear finite elements on a triangulation of a 36×36 mesh.
- 100 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.

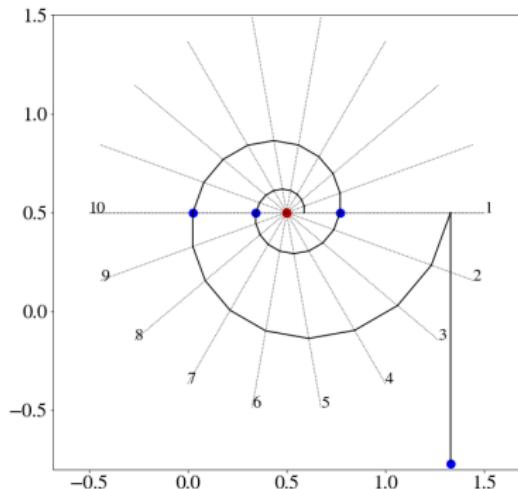
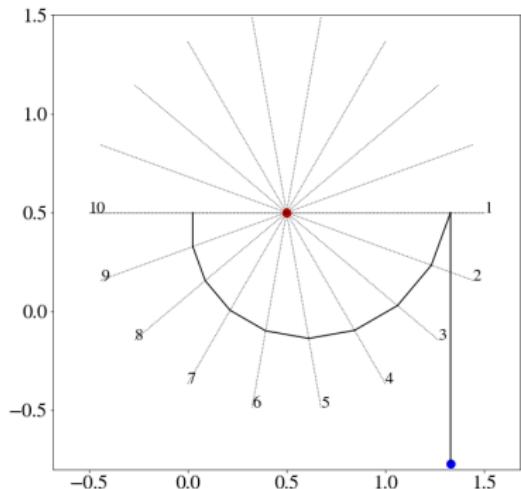




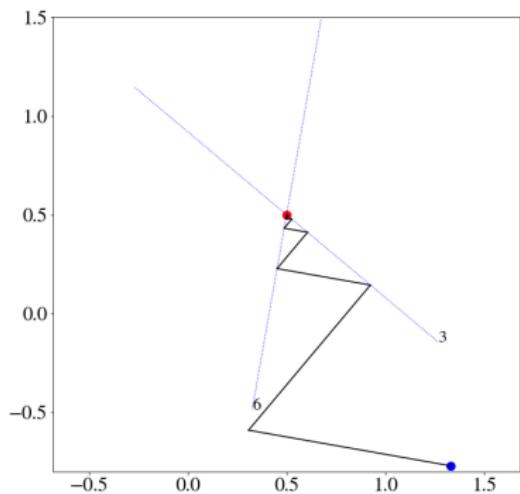
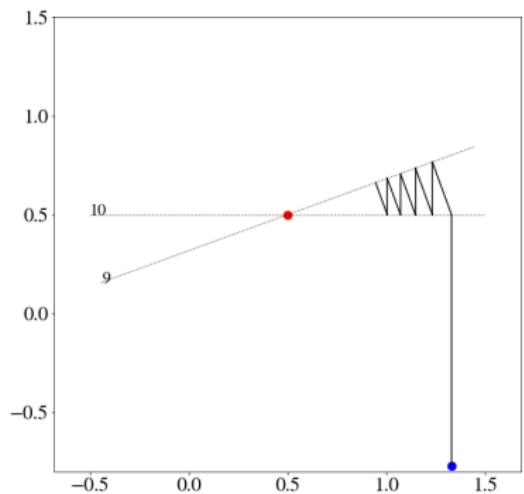


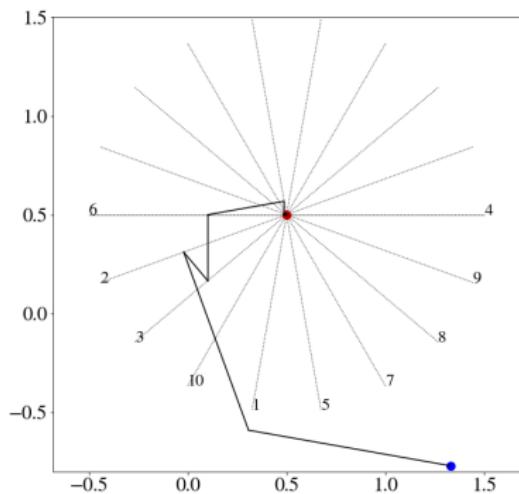
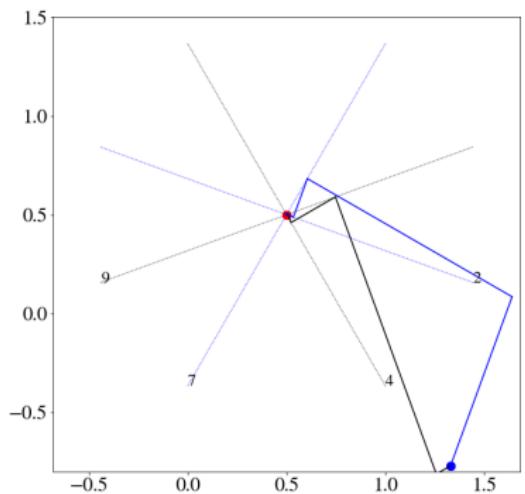


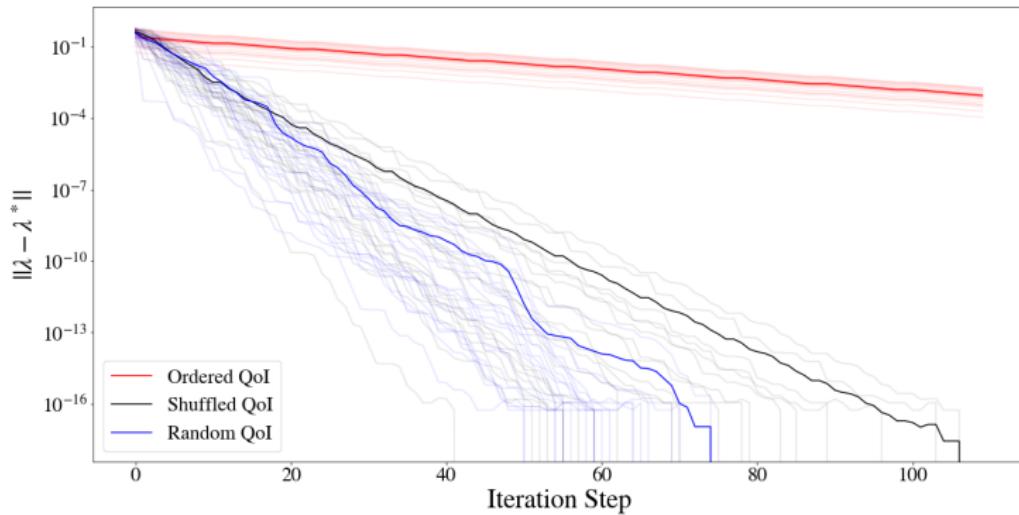
The one with the small problems in many batches.



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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