

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

- Notation and background
- Demonstrate differences: aleatoric v epistemic
- Motivation: How to incorporate arbitrary streams of data
- Theory: Parameter Identification in a DCI framework
- Practice: Computational Examples
- Extensions

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.

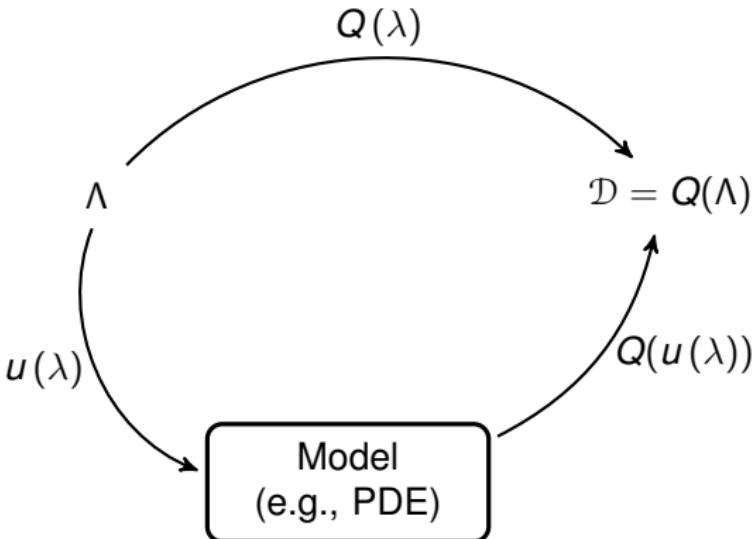
- State variable: u (e.g. heat, energy, pressure, deflection)
- Parameters: λ (e.g. source term, diffusion, boundary data)
- Model: $\mathcal{M}(u, \lambda) = 0$, so $u(\lambda)$
- Quantity of Interest (QoI) map, (piecewise smooth):

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

- 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

$$\mathbb{P}_{\mathcal{D}}(E) = \mathbb{P}_\Lambda(Q^{-1}(E)), \quad \forall E \in \mathcal{B}_{\mathcal{D}}. \quad (2.1)$$



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$$\mathbb{P}_{\mathcal{D}}(E) = \mathbb{P}_\Lambda(Q^{-1}(E)), \quad \forall E \in \mathcal{B}_{\mathcal{D}}. \quad (2.2)$$

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

$$\mathbb{P}_\Lambda(Q^{-1}(E)) = \mathbb{P}_{\mathcal{D}}(E), \quad \forall E \in \mathcal{B}_{\mathcal{D}}. \quad (2.3)$$

Equation (2.3) 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 (2.2) and (2.3) 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 (2.2) 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:

$$\mathbb{P}_{\text{pr}}(E) = \mathbb{P}_{\text{in}}(Q^{-1}(E)), \quad \forall E \in \mathcal{B}_{\mathcal{D}}. \quad (2.4)$$



Definition (Observed Distribution)

When $\mathbb{P}_{\mathcal{D}}$ in (2.3) 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:

$$\pi_{\text{up}}(\lambda) := \pi_{\text{in}}(\lambda) \frac{\pi_{\text{ob}}(Q(\lambda))}{\pi_{\text{pr}}(Q(\lambda))}. \quad (2.5)$$



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

$$q = Q(\lambda), \forall \lambda \in \Lambda. \quad (2.6)$$



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

$$\|Q(\lambda) - d\| \quad (2.7)$$

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]:

$$\pi_{\text{post}}(\lambda | d) := \pi_{\text{prior}}(\lambda) \frac{L_{\mathcal{D}}(q|\lambda)}{C} \quad (2.8)$$

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

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

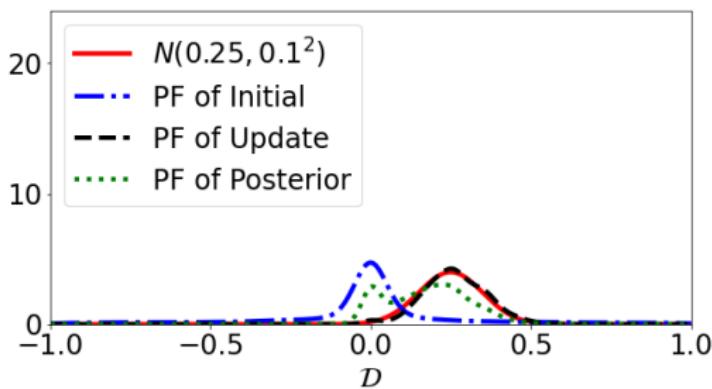
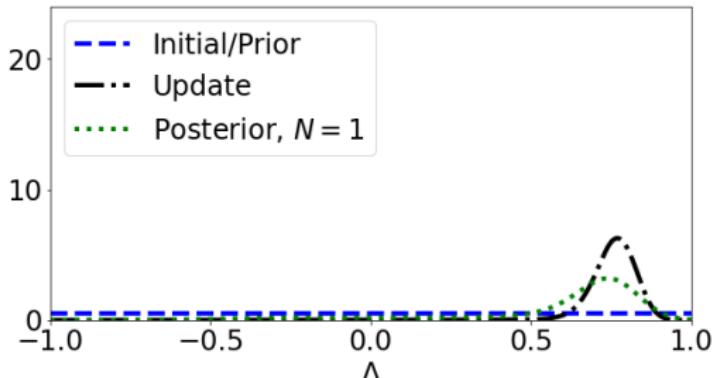


The one where we provide an illustrative example.

- 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.

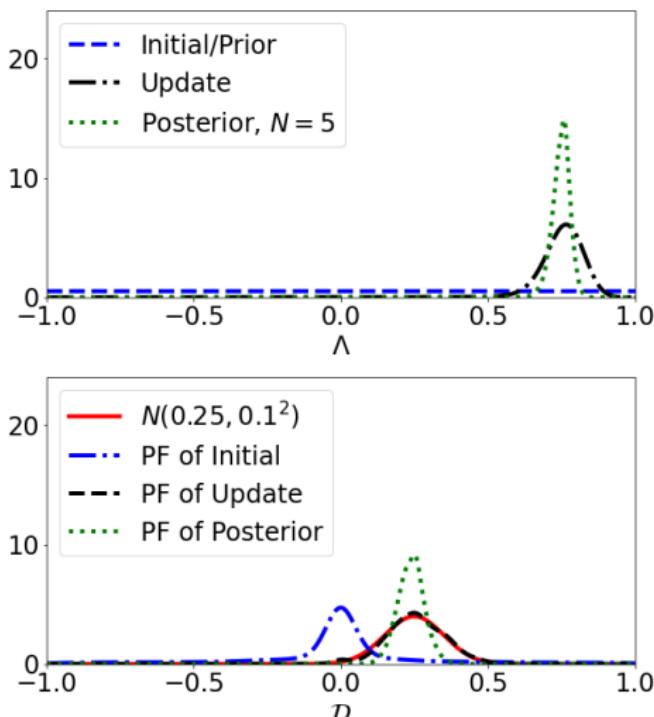
What happens as we collect more data?

SIP: Use N to estimate mean of observed.

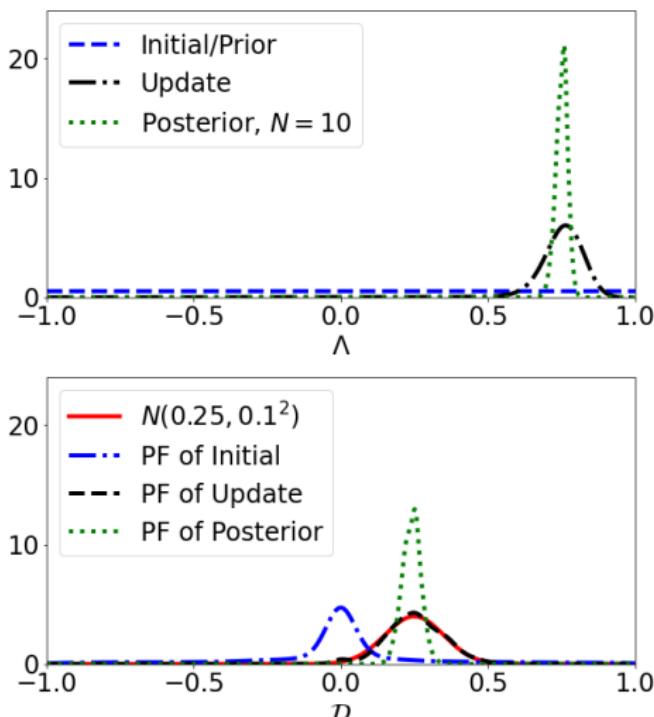
DIP: Likelihood function incorporates more terms.



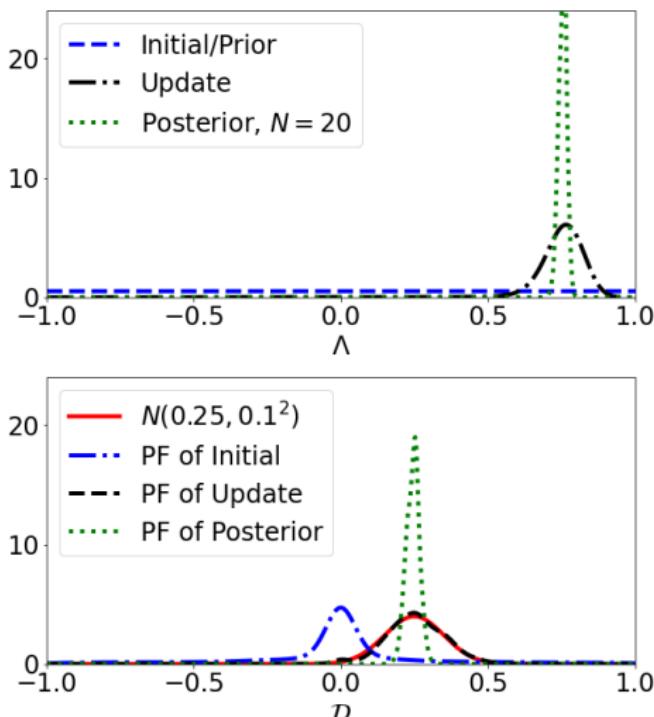
The one where we provide an illustrative example.



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The one where we provide an illustrative example.



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

$$\lambda^{\text{MUD}} := \arg \max \pi_{\text{up}}(\lambda) \quad (3.1)$$



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

$$\Sigma_{\text{pred}} := A \Sigma_{\text{init}} A^\top. \quad (3.2)$$



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:

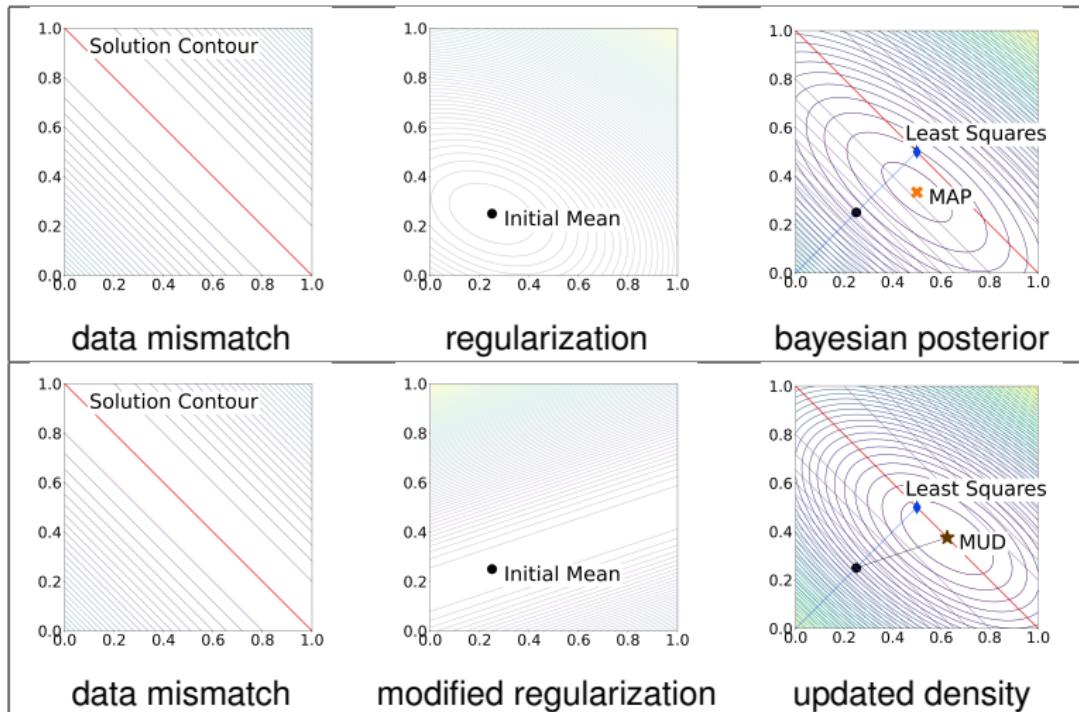
$$\lambda_0 = \begin{bmatrix} 0.25 & 0.25 \end{bmatrix}^\top$$

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

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



The one that kind of says it all.



- Posterior covariance:

$$\Sigma_{\text{post}} := (\mathbf{A}^{\top} \Sigma_{\text{obs}}^{-1} \mathbf{A} + \Sigma_{\text{init}}^{-1})^{-1} \quad (3.3)$$

- Using Woodbury identity and (3.2):

$$\Sigma_{\text{post}} = \Sigma_{\text{init}} - \Sigma_{\text{init}} \mathbf{A}^{\top} [\Sigma_{\text{pred}} + \Sigma_{\text{obs}}]^{-1} \mathbf{A} \Sigma_{\text{init}} \quad (3.4)$$

- 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:

$$\lambda^{\text{MAP}} = \lambda_0 + \Sigma_{\text{post}} \mathbf{A}^{\top} \Sigma_{\text{obs}}^{-1} (\mathbf{y} - \mathbf{b} - \mathbf{A} \lambda_0). \quad (3.5)$$



The one where we make some convenient manipulations.

- Let

$$R := \Sigma_{\text{init}}^{-1} - A^\top \Sigma_{\text{pred}}^{-1} A. \quad (3.6)$$

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

$$J(\lambda) := \|\mathbf{y} - Q(\lambda)\|_{\Sigma_{\text{obs}}^{-1}}^2 + \|\lambda - \lambda_0\|_R^2. \quad (3.7)$$

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

$$\Sigma_{\text{up}} := \left(A^\top \Sigma_{\text{obs}}^{-1} A + R \right)^{-1} \quad (3.8)$$

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

The one where we make some convenient manipulations.

- *Using linear algebra ...*

$$\Sigma_{\text{up}} = \Sigma_{\text{init}} - \Sigma_{\text{init}} A^\top \Sigma_{\text{pred}}^{-1} [\Sigma_{\text{pred}} - \Sigma_{\text{obs}}] \Sigma_{\text{pred}}^{-1} A \Sigma_{\text{init}}. \quad (3.9)$$

- Substitute Σ_{up} for Σ_{post} in (3.5):

$$\lambda^{\text{MUD}} = \lambda_0 + \Sigma_{\text{up}} A^\top \Sigma_{\text{obs}}^{-1} (\mathbf{y} - b - A\lambda_0). \quad (3.10)$$

- Substituting (3.9) into (3.10) and simplifying, we have

$$\lambda^{\text{MUD}} = \lambda_0 + \Sigma_{\text{init}} A^\top \Sigma_{\text{pred}}^{-1} (\mathbf{y} - b - A\lambda_0). \quad (3.11)$$



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 (3.11) and the covariance associated with this point is given by (3.9).

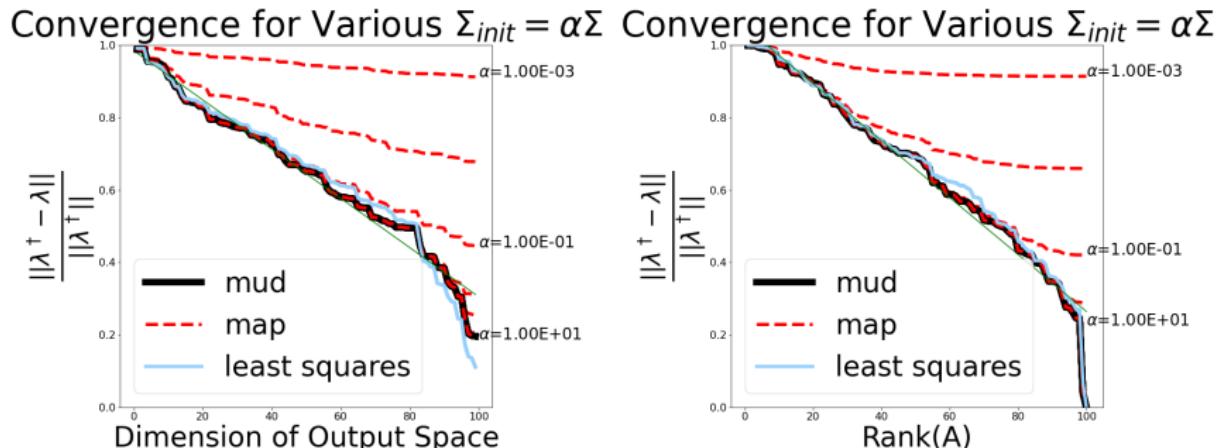


The one where we address a key assumption

- 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.



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:

$$d_{j,i} = M_j(\lambda^\dagger) + \xi_i, \quad \xi_i \sim N(0, \sigma_j^2), \quad 1 \leq i \leq N_j. \quad (3.12)$$

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 $Q_{WME}(\lambda)$.

$$Q_{WME,j}(\lambda) := \frac{1}{\sqrt{N_j}} \sum_{i=1}^{N_j} \frac{M_j(\lambda) - d_{j,i}}{\sigma_j}. \quad (3.13)$$

- $Q_{WME,j}(\lambda^\dagger)$ 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 (3.12).
- 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:

$$\frac{N_j}{\sigma_j^2} M_j \Sigma_{\text{init}} M_j^\top. \quad (3.14)$$

- 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 3.1.



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 :

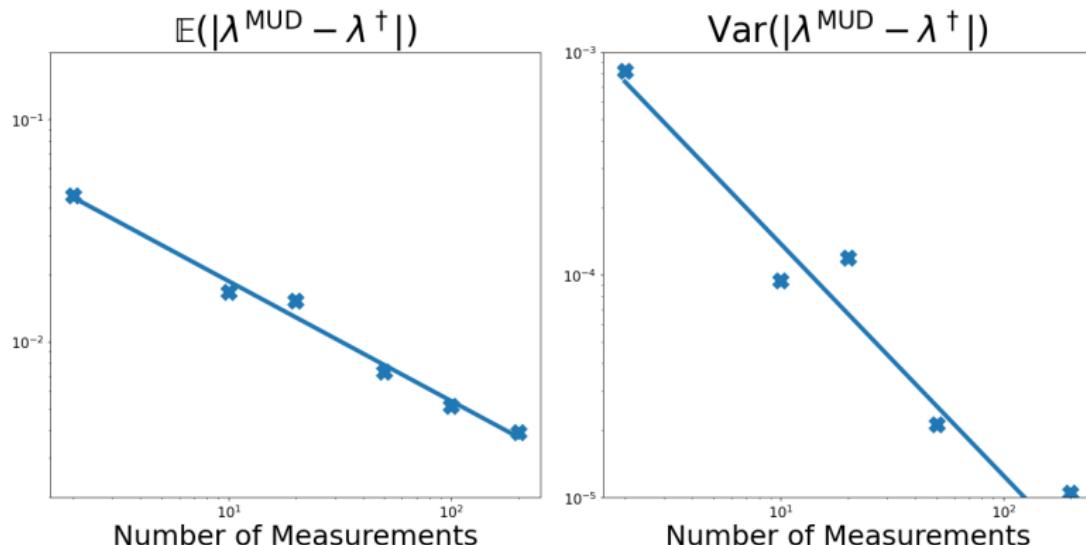
$$\begin{cases} \frac{\partial u}{\partial t} = \lambda u(t), & 0 < t \leq 3, \\ u(0) = 0.75, \end{cases}$$

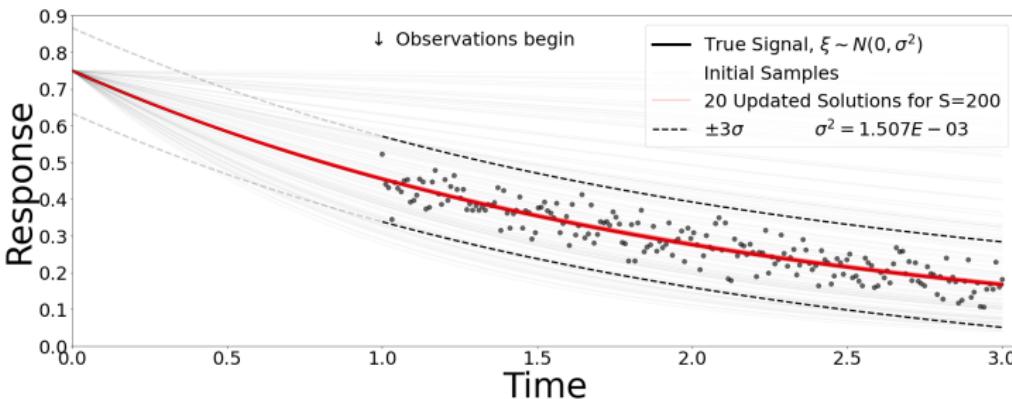
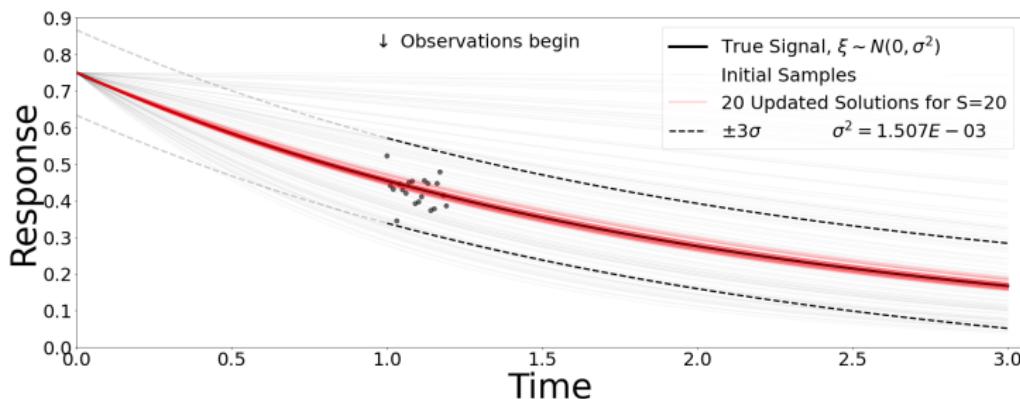
with solution

$$u(t; \lambda) = u_0 \exp(-\lambda t), \quad u_0 = 0.75, \quad (3.15)$$

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







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

Consider the Poisson problem:

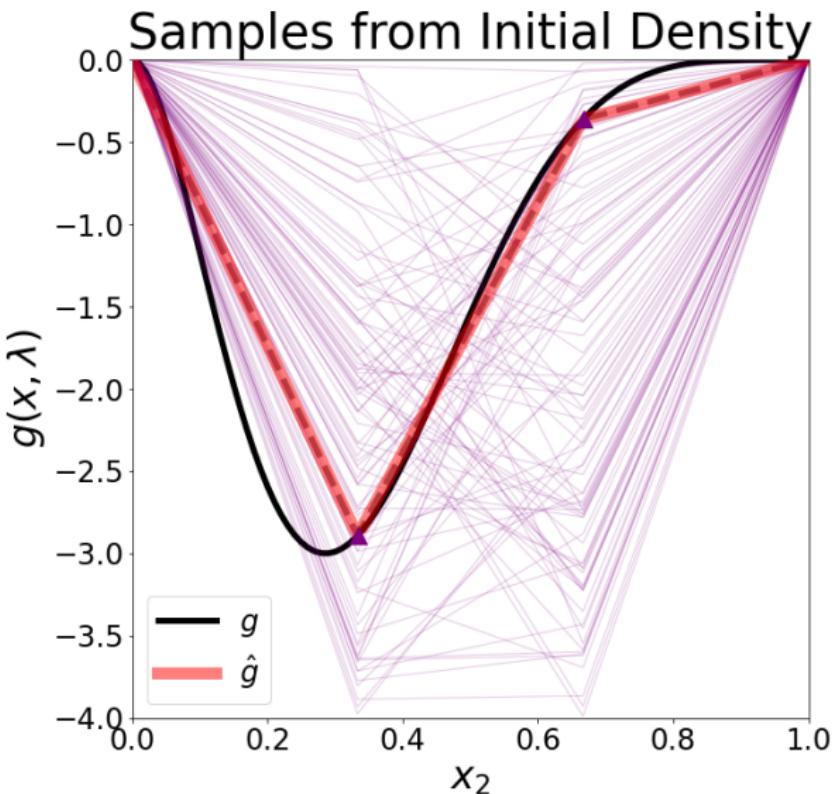
$$\begin{cases} -\nabla \cdot \nabla u = f(x), & \text{on } x \in \Omega, \\ u = 0, & \text{on } \Gamma_T \cup \Gamma_B, \\ \frac{\partial u}{\partial \mathbf{n}} = g(x_2), & \text{on } \Gamma_L, \\ \frac{\partial u}{\partial \mathbf{n}} = 0, & \text{on } \Gamma_R, \end{cases} \quad (3.16)$$

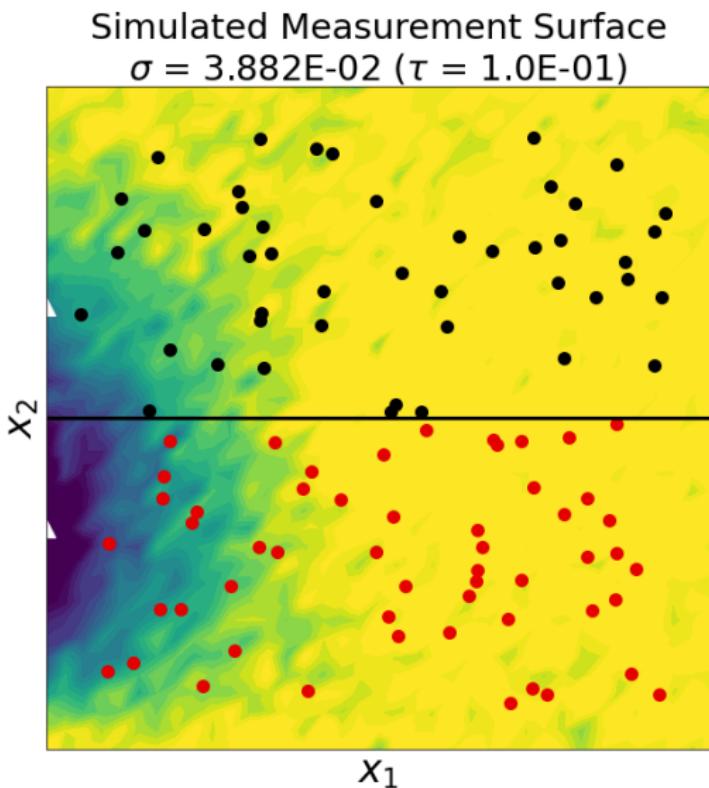
where $x = (x_1, x_2) \in \Omega = (0, 1)^2$ is the spatial domain.

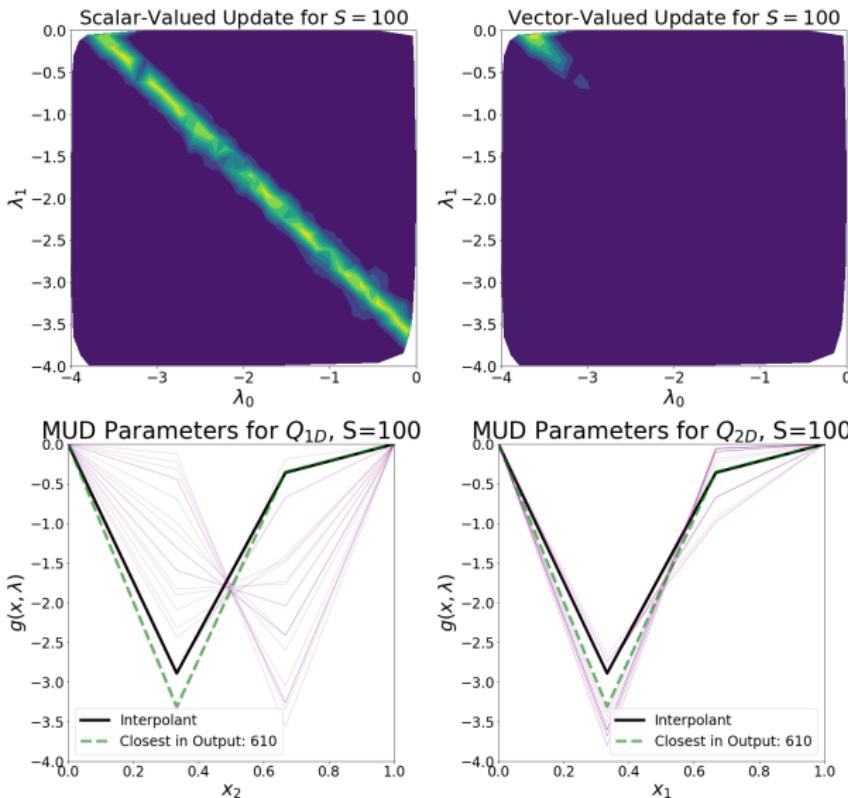
- Γ_T , Γ_B , Γ_L , and Γ_R , denote the top, bottom, left, and right boundaries.
- The outward normal derivative is denoted by $\frac{\partial u}{\partial \mathbf{n}}$.
- The forcing function is $f = 10 \exp \left(\|x - 0.5\|^2 / 0.02 \right)$.

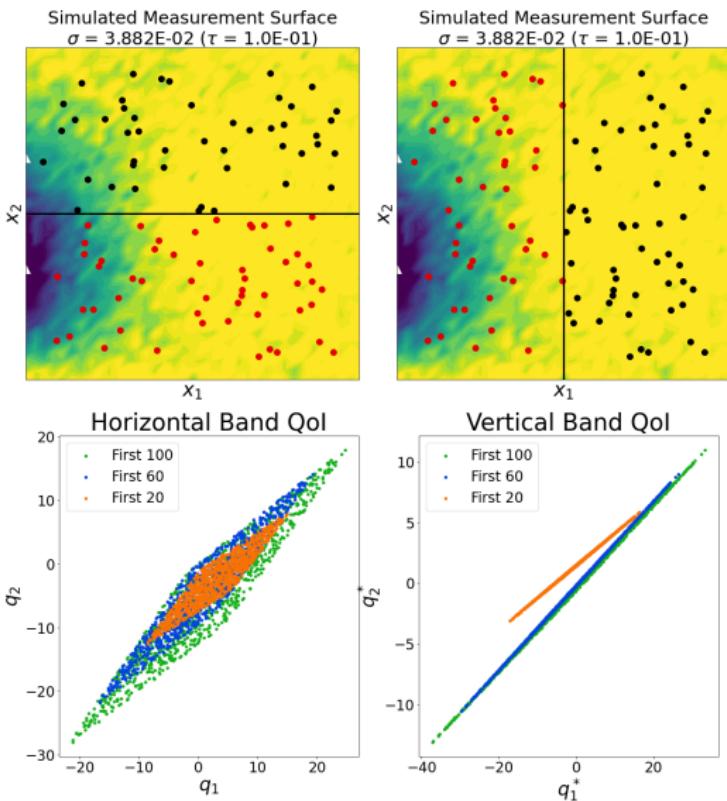


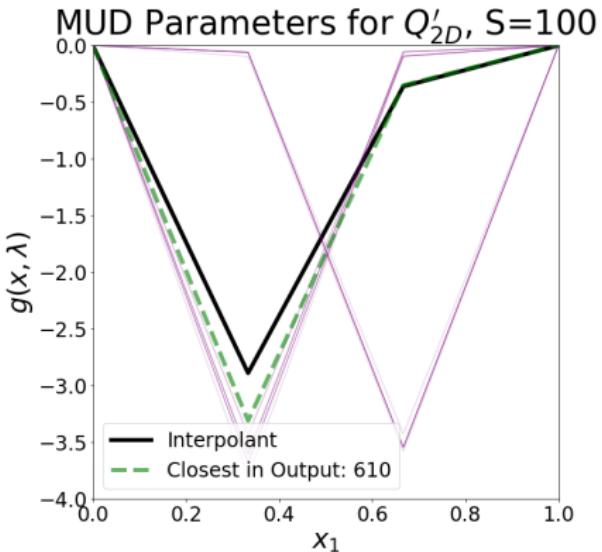
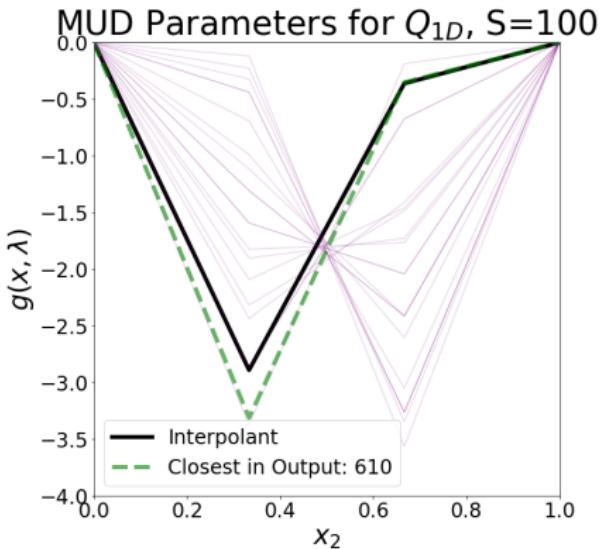
- $g(x_2)$ is uncertain parameter, i.e., λ defines an uncertain function.
- To generate the noisy data, we use $g(x_2) \propto x_2^2(x_2 - 1)^5$.
- Constant of proportionality chosen so $\min g = -3$ at $x_2 = \frac{2}{7}$.
- Piecewise-linear finite elements on a triangulation of a 36×36 mesh.
- $S =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



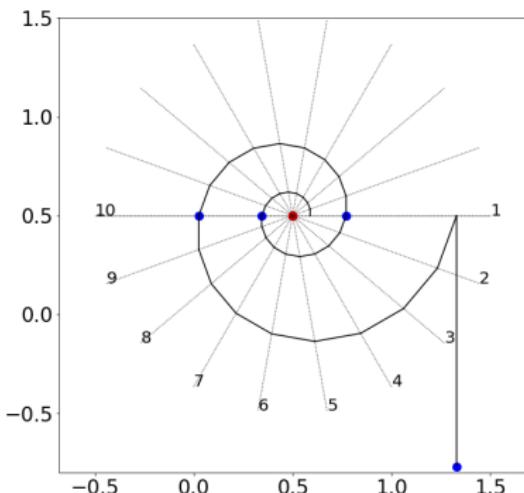
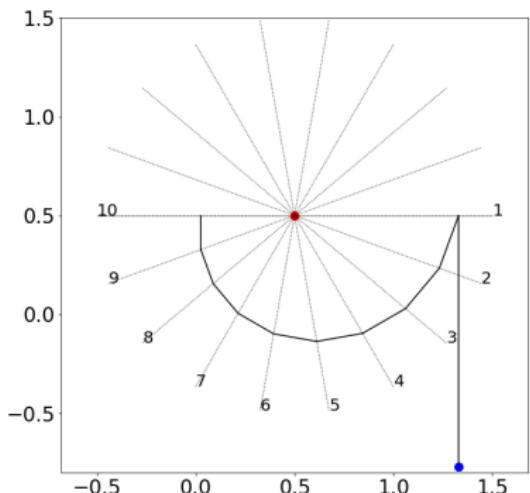




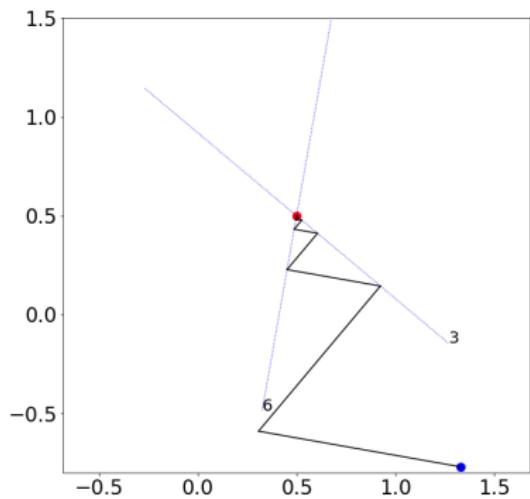
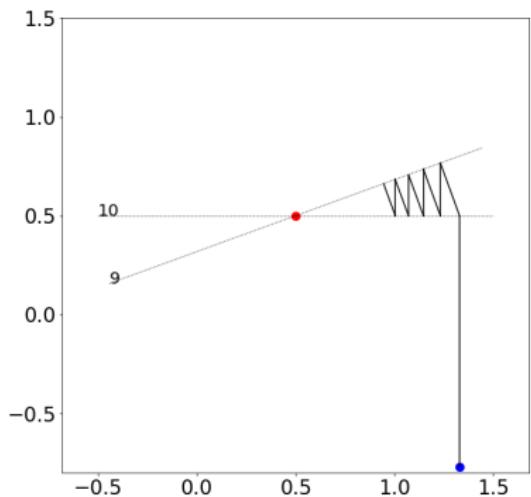


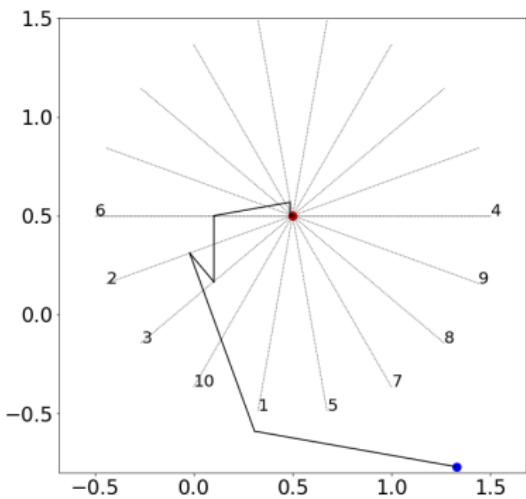
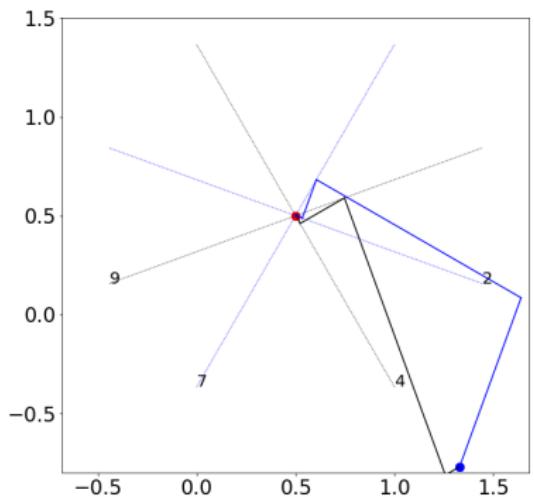


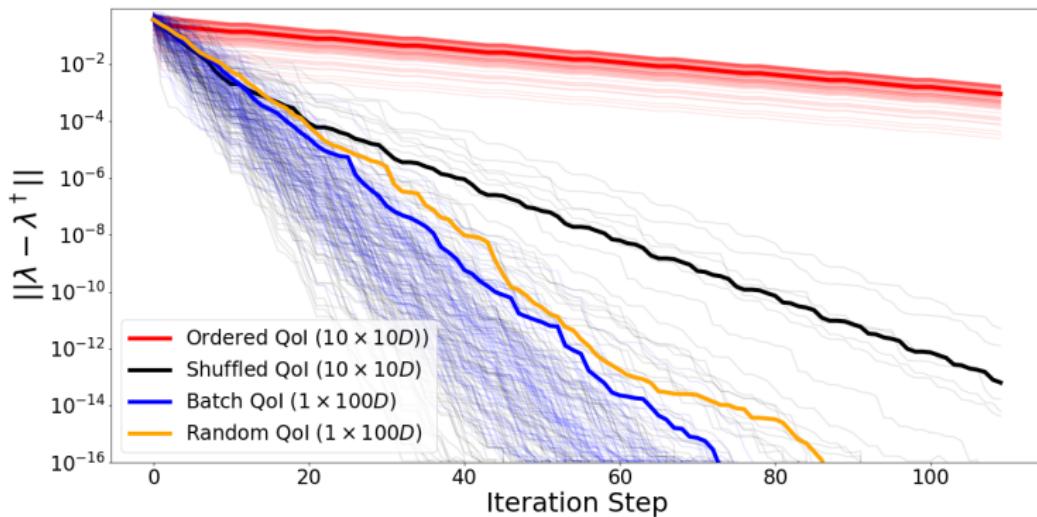
The one with the small problems in many batches.



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







Same model evaluation budget and final usage of QoL components.

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)`



 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.