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 (aleotoric, epistemic)
- Be *accurate* and *precise*
- Design “efficient” experiments
- Collect and use data “intelligently”

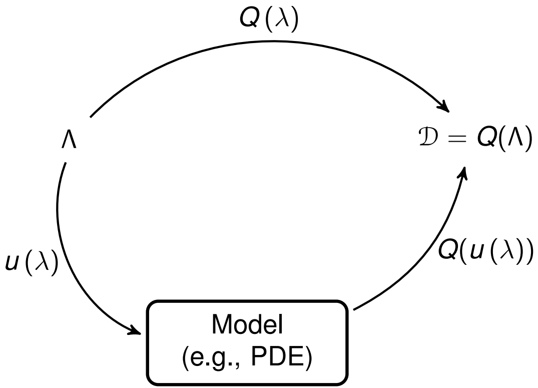
The one where we define the letters we use and what they mean.

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

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

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

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



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

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

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

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

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

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

Definition (Consistent Solution and Density)

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

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

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

In such a case, we can rewrite (1.2) 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 $\mathbb{P}_\Lambda$ 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* $\mathbb{P}_{\text{in}}$.

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:

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

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*, $\mathbb{P}_{\text{ob}}$.

Given a dominating $\mu_{\mathcal{D}}$ on $(\mathcal{D}, \mathcal{B}_{\mathcal{D}})$, the Radon-Nikodym derivative $\mathbb{P}_{\text{ob}}$ 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:

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

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, $\lambda^\dagger$.
- 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

$$q = Q(\lambda), \; \forall \, \lambda \in \Lambda. \tag{1.6}$$

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

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

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:

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

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

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

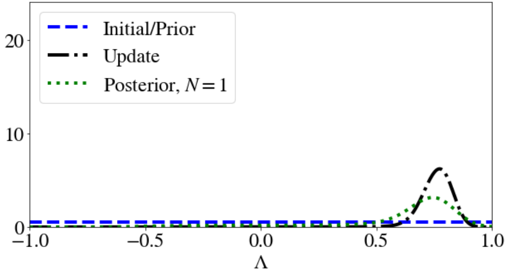
- The *evidence* term C ensures integration to unity. Given by:

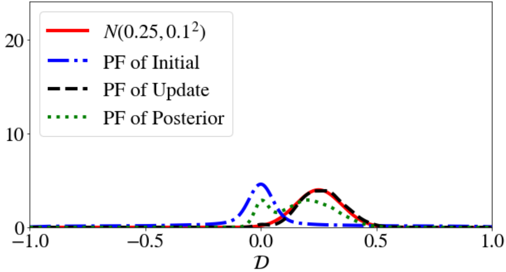
$$C = \int_{\Lambda} \pi_{\text{prior}}(\lambda) \, L_{\mathfrak{D}}(q|\lambda) \, d\lambda$$

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.





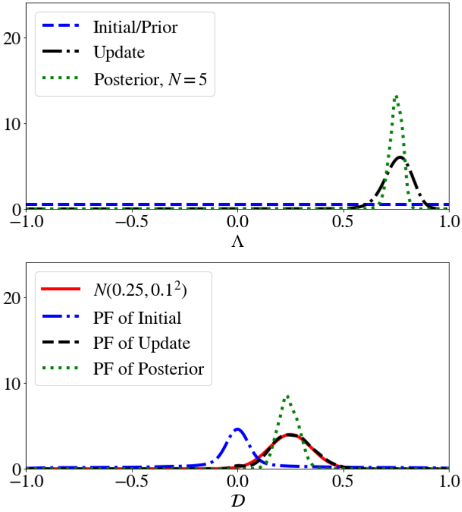
The one where we provide an illustrative example.

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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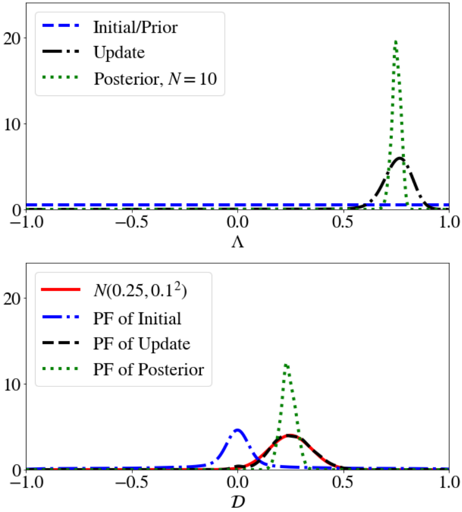
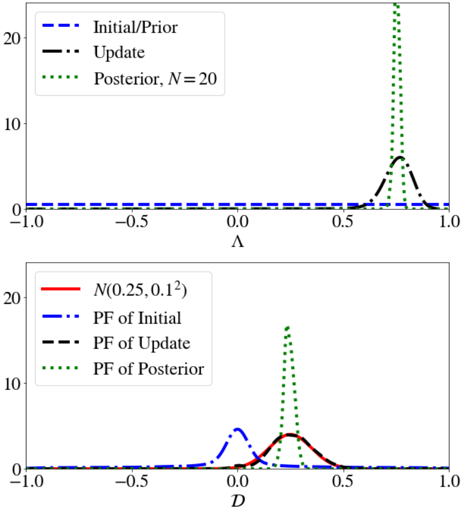


The one where we provide an illustrative example.



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

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

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

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

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	$T(\lambda) := \lVert Q(\lambda) - \mathbf{y} \rVert^2_{\Sigma_{\text{obs}}^{-1}} + \lVert \lambda - \lambda_0 \rVert^2_{\Sigma_{\text{init}}^{-1}}$
Data-Consistent	$J(\lambda) := T(\lambda) - \lVert Q(\lambda) - Q(\lambda_0) \rVert^2_{\Sigma_{\text{pred}}^{-1}}$

The one where an example highlights a key difference.

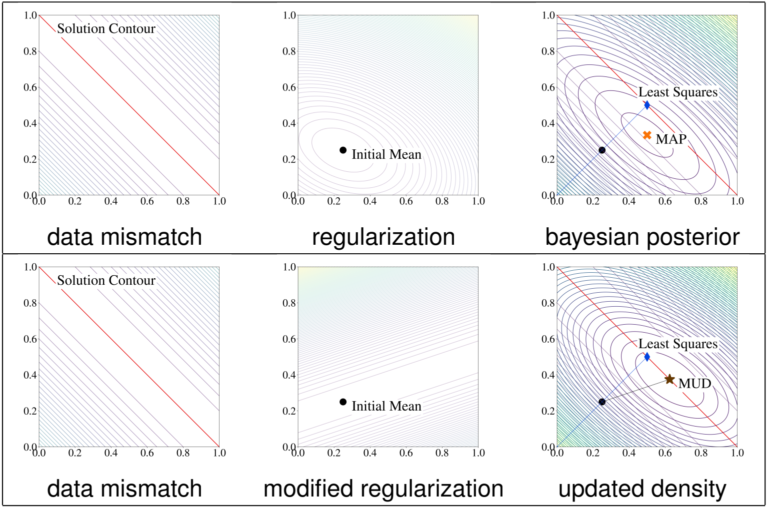
- $A = \begin{bmatrix} 1 & 1 \end{bmatrix}$
- 2-D input, 1-D output $\implies$ rank-deficient
- Details:

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

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

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

The one that kind of says it all.



- Posterior covariance:

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

- Using Woodbury identity and (2.2):

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

- 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:

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

The one where we make some convenient manipulations.

- Let

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

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

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

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

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

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

The one where we make some convenient manipulations.

- *Using linear algebra ...*

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

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

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

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

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

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

(a) *There exists a unique* λ^{MUD}.

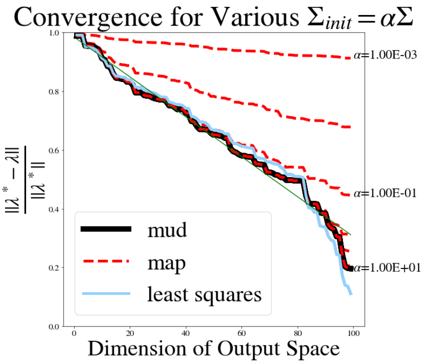
(b) $Q(\lambda^{MUD}) = \mathbf{y}$.

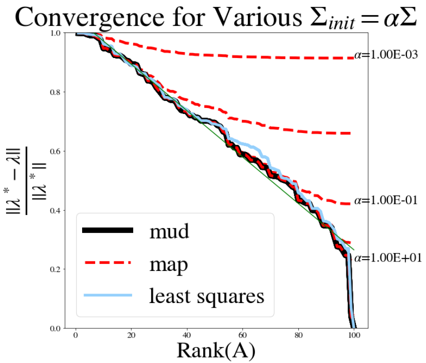
(c) *If* $d = p$, λ^{MUD} *is given by* A^{-1}. *If* $d < p$, λ^{MUD} *is given by* (2.11) *and the covariance associated with this point is given by* (2.9).

The one where we address a key assumption

- Predictability Assumption: π_{pr} is a dominating measure for π_{ob}
- Linear case: involves eigenvalues of covariances:
  - min eigenvalue Σ_{pred} > max eigenvalue Σ_{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 ith noisy datum for the jth measurement, where $1 \leq i \leq N_j$.
- Unbiased additive error model for the measurement noise:

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

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 $Q_{WME}(\lambda)$.

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

- $Q_{\mathrm{WME},j}(\lambda^\dagger)$ 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) $\lambda^\dagger$ in (2.12).
- For each component, $Q_{\mathrm{WME},j}(\lambda^\dagger) \sim N(0, 1)$.
- π_{ob} is a $N(\mathbf{0}_{d\times 1}, \mathbf{I}_{d\times d})$ due to the structure of $Q_{\mathrm{WME}}(\lambda)$.

The one where measurements impact the predictability assumption.

- The jth 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 jth component is given by:

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

- 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 $\pi_{\text{in}} \sim N(\lambda_0, \Sigma_{init})$ *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 violate some assumptions (and see what happens).

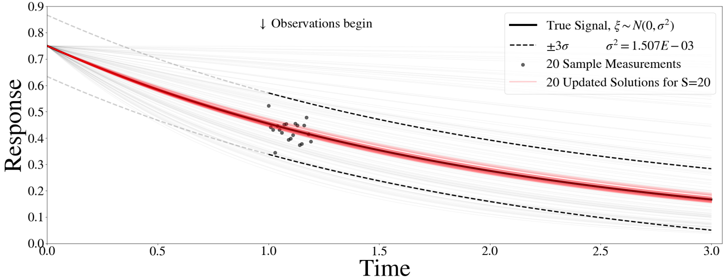
Consider the exponential decay problem with uncertain decay rate λ:

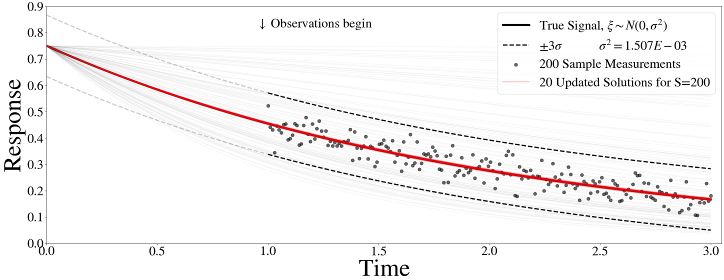
$$\begin{cases} \frac{\partial u}{\partial t} & = \lambda u(t),\ 0 < t \leq 3, \\ u(0) & = 0.75, \end{cases}$$

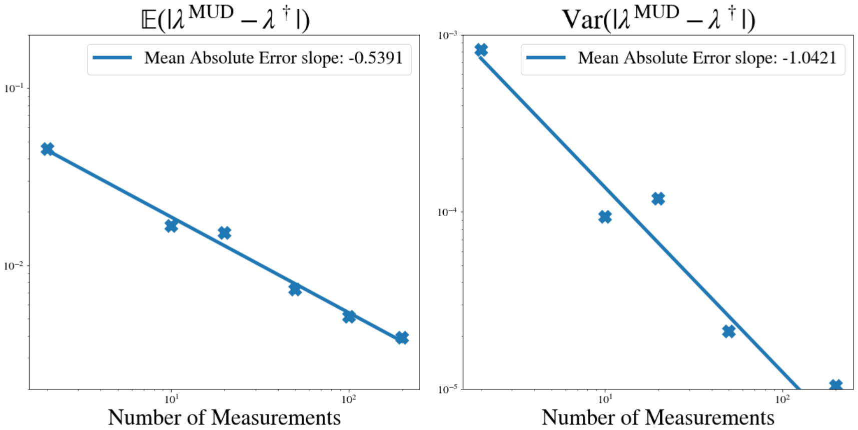
with solution

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

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


↓ Observations begin
True Signal, $\xi \sim N(0, \sigma^2)$
$\pm 3\sigma$ $\sigma^2 = 1.507E-03$
20 Sample Measurements
20 Updated Solutions for S=20
Response
Time


↓ Observations begin
True Signal, $\xi \sim N(0, \sigma^2)$
$\pm 3\sigma$ $\sigma^2 = 1.507E-03$
200 Sample Measurements
20 Updated Solutions for S=200
Response
Time


$\mathbb{E}(|\lambda^{MUD} - \lambda^{\dagger}|)$
Mean Absolute Error slope: -0.5391
10^{-1}
10^{-2}
10^{1}
10^{2}
Number of Measurements
$\mathrm{Var}(|\lambda^{MUD} - \lambda^{\dagger}|)$
Mean Absolute Error slope: -1.0421
10^{-3}
10^{-4}
10^{-5}
10^{1}
10^{2}
Number of Measurements

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

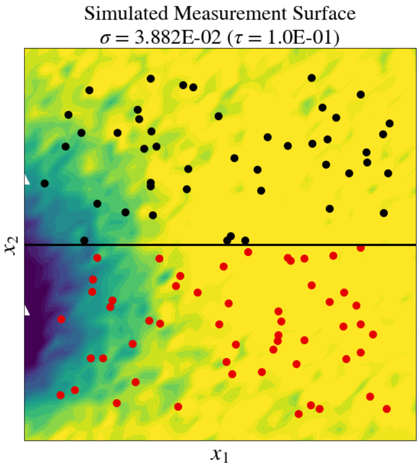
Consider the Poisson problem:

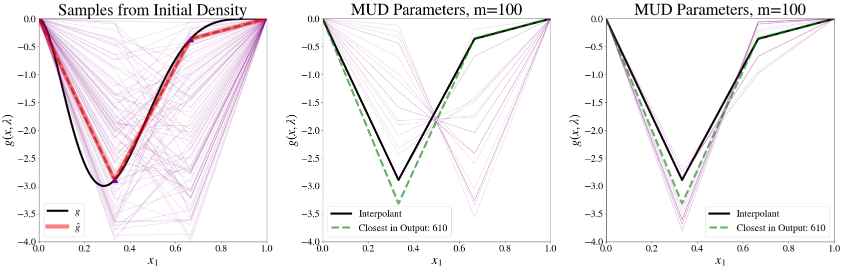
$$\begin{cases} -\nabla \cdot \nabla u &= f(x), \quad \text{on } x \in \Omega, \\ u &= 0, \quad \text{on } \Gamma_T \cup \Gamma_B, \\ \frac{\partial u}{\partial \mathbf{n}} &= g(x_2), \quad \text{on } \Gamma_L, \\ \frac{\partial u}{\partial \mathbf{n}} &= 0, \quad \text{on } \Gamma_R, \end{cases} \tag{2.16}$$

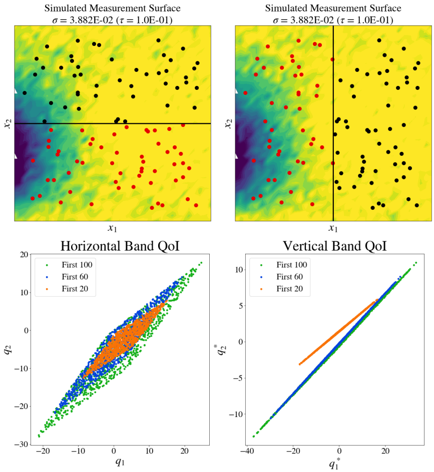
where $x = (x_1, x_2) \in \Omega = (0,1)^2$ is the spatial domain.

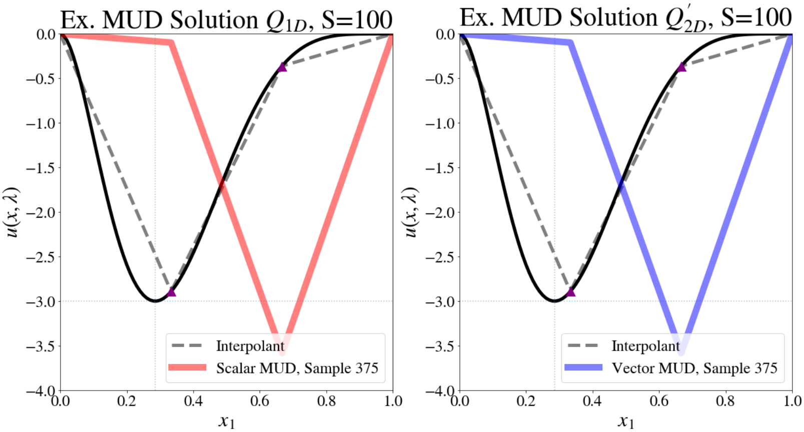
- Γ_T, Γ_B, Γ_L, and Γ_R, denote the top, bottom, left, and right boundaries.
- The outward normal derivative is denoted by $\frac{\partial u}{\partial \mathbf{n}}$.
- The forcing function is $f = 10 \exp\left(\|x - 0.5\|^2 / 0.02\right)$.

- $g(x_2)$ 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.

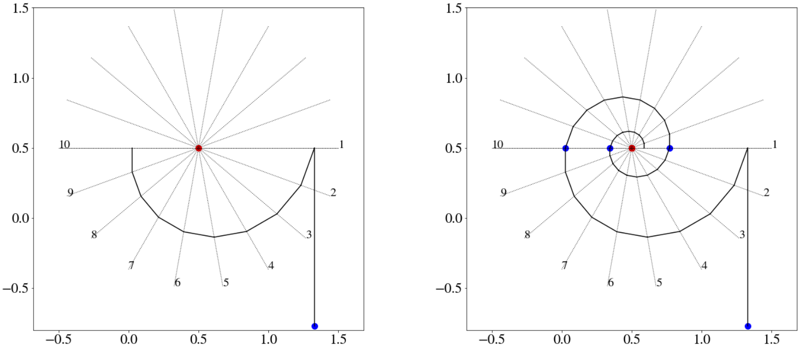

Simulated Measurement Surface
σ = 3.882E-02 (τ = 1.0E-01)
x2
x1


Samples from Initial Density
g
$\hat{g}$
MUD Parameters, m=100
Interpolant
Closest in Output: 610
MUD Parameters, m=100
Interpolant
Closest in Output: 610
$g(x, \lambda)$
x_1
0.0
−0.5
−1.0
−1.5
−2.0
−2.5
−3.0
−3.5
−4.0
0.2
0.4
0.6
0.8
1.0

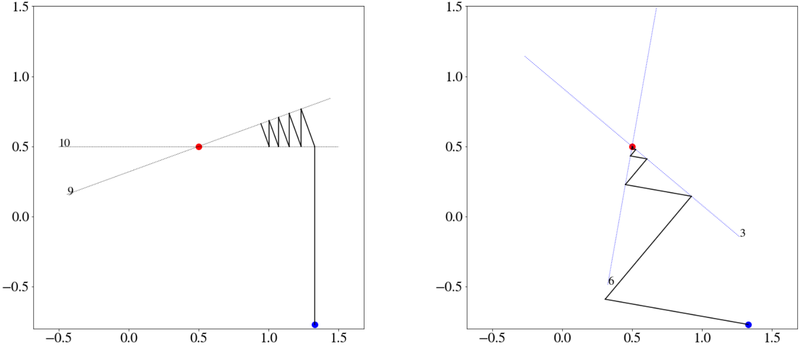

Simulated Measurement Surface
$\sigma = 3.882E\text{-}02$ ($\tau = 1.0E\text{-}01$)
x_1
x_2
Horizontal Band QoI
Vertical Band QoI
First 100
First 60
First 20
q_1
q_2
q_1^*
q_2^*

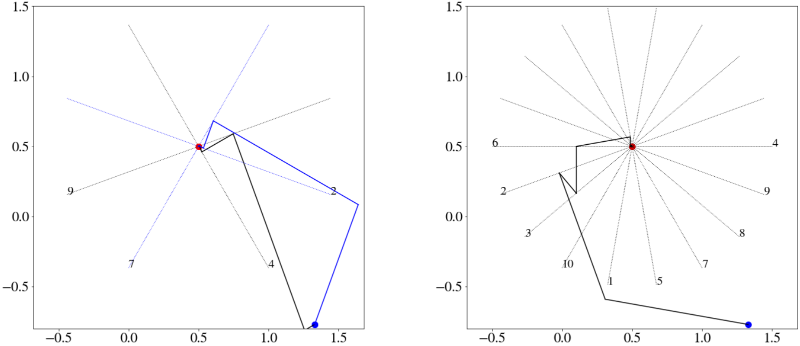

Ex. MUD Solution Q_{1D}, S=100
Ex. MUD Solution Q'_{2D}, S=100
$u(x, \lambda)$
x_1
0.0
−0.5
−1.0
−1.5
−2.0
−2.5
−3.0
−3.5
−4.0
0.0
0.2
0.4
0.6
0.8
1.0
Interpolant
Scalar MUD, Sample 375
Vector MUD, Sample 375

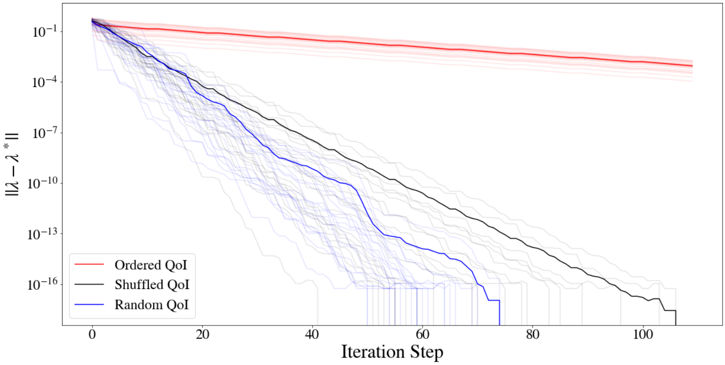
The one with the small problems in many batches.



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


1.5
1.0
0.5
0.0
−0.5
−0.5
0.0
0.5
1.0
1.5
10
9
3
6


1.5
1.0
0.5
0.0
−0.5
−0.5
0.0
0.5
1.0
1.5
9
2
7
4
1.5
1.0
0.5
0.0
−0.5
−0.5
0.0
0.5
1.0
1.5
6
4
2
9
3
8
10
7
1
5



10^{-1}
10^{-4}
10^{-7}
10^{-10}
10^{-13}
10^{-16}
$\|\lambda - \lambda^*\|$
Ordered QoI
Shuffled QoI
Random QoI
0
20
40
60
80
100
Iteration Step

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 (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)`

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