# Combining Measure Theory and Bayes' Rule to Solve a Stochastic Inverse Problem

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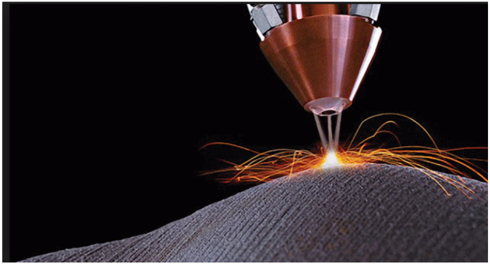
# Motivation



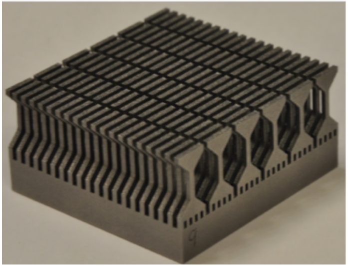
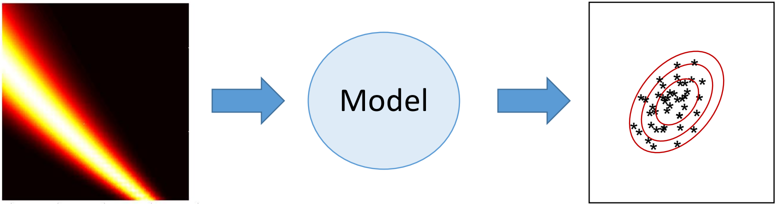


Figure: Additive manufacturing and high-throughput testing provides new data science challenges.

# A Stochastic Inverse Problem




## Problem

Given a probability density on observations, find a probability density on X such that the push-forward matches the given density on the observed data.

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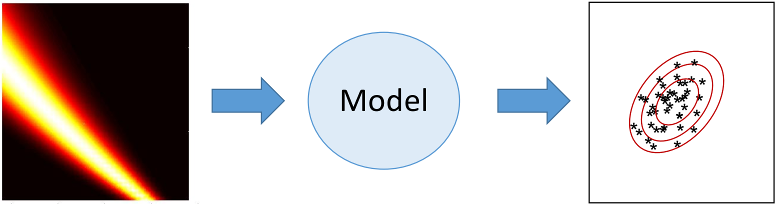


## Problem

Given a probability density on observations, find a probability density on X such that the push-forward matches the given density on the observed data.

- Solutions may not be unique without additional assumptions.
- **We only need to solve a single stochastic forward problem.**

# Notation

## We assume we are given:

1. A finite-dimensional **parameter space**, $\mathrm{X}$.
2. A **parameter-to-observation/data map**, $f : \mathrm{X} \to \mathcal{D} = f(\mathrm{X})$
3. An **observed probability measure** on $(\mathcal{D}, \mathcal{B}_{\mathcal{D}})$, denoted $\mathbb{P}_{\mathcal{D}}^{\text{obs}}$, that has a density, $\pi_{\mathcal{D}}^{\text{obs}}$.
4. An **initial probability measure** on $(\mathrm{X}, \mathcal{B}_{\mathrm{X}})$, denoted $\mathbb{P}_{\mathrm{X}}^{\text{init}}$, that has a density, $\pi_{\mathrm{X}}^{\text{init}}$.

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## We need to compute:

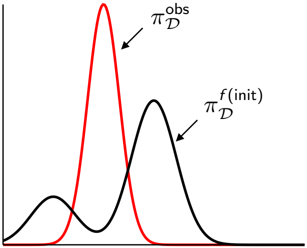
1. The **push-forward of the initial density** through the model.

- In other words, **we need to solve a forward UQ problem using the initial.**
- We use $\pi_{\mathcal{D}}^{f(\text{init})}$ to denote this push-forward density.

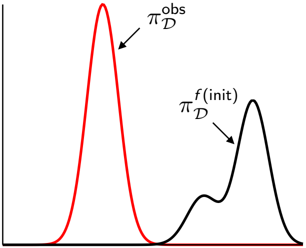
# A Key Assumption

## Predictability Assumption

We assume that the observed probability measure, $\mathbb{P}_{\mathcal{D}}^{\text{obs}}$, is absolutely continuous with respect to the push-forward of the initial, $\mathbb{P}_{\mathcal{D}}^{f(\text{init})}$.




Good Initial




Bad Initial
(Cannot predict all observations)

# A Solution to the Stochastic Inverse Problem

## Theorem

*Given an initial probability measure,* $\mathbb{P}_{\mathsf{X}}^{init}$ *on* $(\mathsf{X}, \mathcal{B}_{\mathsf{X}})$ *and an observed probability measure,* $\mathbb{P}_{\mathcal{D}}^{obs}$*, on* $(\mathcal{D}, \mathcal{B}_{\mathcal{D}})$*, the probability measure* $P_{\mathsf{X}}^{up}$ *on* $(\mathsf{X}, \mathcal{B}_{\mathsf{X}})$ *defined by*

$$\mathbb{P}_{\mathsf{X}}^{up}(A) = \int_{\mathcal{D}} \left( \int_{A \cap f^{-1}(q)} \pi_{\mathsf{X}}^{init}(x) \frac{\pi_{\mathcal{D}}^{obs}(f(x))}{\pi_{\mathcal{D}}^{f(init)}(f(x))} d\mu_{\mathsf{X},q}(x) \right) d\mu_{\mathcal{D}}(q), \; \forall A \in \mathcal{B}_{\mathsf{X}}$$

*solves the stochastic inverse problem.*

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*Given an initial probability measure, $\mathbb{P}_{\mathsf{X}}^{init}$ on $(\mathsf{X}, \mathcal{B}_{\mathsf{X}})$ and an observed probability measure, $\mathbb{P}_{\mathcal{D}}^{obs}$, on $(\mathcal{D}, \mathcal{B}_{\mathcal{D}})$, the probability measure $P_{\mathsf{X}}^{up}$ on $(\mathsf{X}, \mathcal{B}_{\mathsf{X}})$ defined by*

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*The updated measure of $\mathsf{X}$ is 1.*

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*$\mathbb{P}_X^{up}$ is stable with respect to perturbations in $\mathbb{P}_{\mathcal{D}}^{obs}$ and in $\mathbb{P}_X^{init}$.*

For details: [Combining Push-forward Measures and Bayes' Rule to Construct Consistent Solutions to Stochastic Inverse Problems, BJW. SISC 40 (2), 2018.]

# A Solution to the Stochastic Inverse Problem

## Theorem

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The updated density is:

$$\pi_{\mathrm{X}}^{\mathrm{up}}(x) = \pi_{\mathrm{X}}^{\mathrm{init}}(x) \frac{\pi_{\mathcal{D}}^{\mathrm{obs}}(f(x))}{\pi_{\mathcal{D}}^{f(\mathrm{init})}(f(x))}.$$

- Both $\pi_{\mathrm{X}}^{\mathrm{init}}$ and $\pi_{\mathcal{D}}^{\mathrm{obs}}$ are given.
- Computing $\pi_{\mathcal{D}}^{f(\mathrm{init})}$ requires a forward propagation of the initial density.

# A Parameterized Nonlinear System

## Example

Consider a parameterized nonlinear system of equations:

$$\begin{aligned} x_1 u_1^2 + u_2^2 &= 1, \\ u_1^2 - x_2 u_2^2 &= 1 \end{aligned}$$

- The quantity of interest is the second component: $f(x) = u_2$.
- Assume that we observe $\pi_{\mathcal{D}}^{\text{obs}} \sim N(0.3, 0.025^2)$.
- We consider a uniform initial density.
- We use 10,000 samples from the initial and a standard KDE to approximate the push-forward.

# A Parameterized Nonlinear System

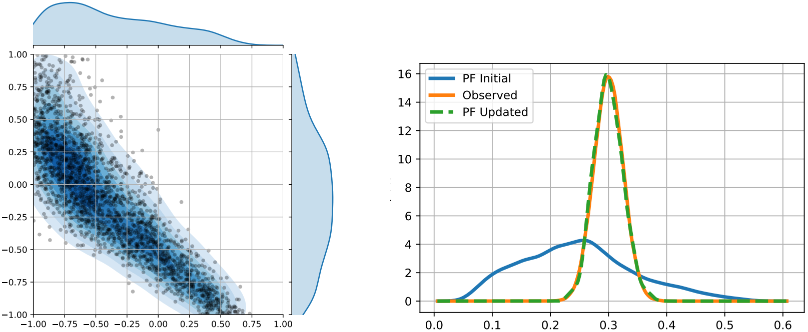


Figure: Samples from the updated density (left) and a comparison of $\pi_{\mathcal{D}}^{\text{obs}}$, $\pi_{\mathcal{D}}^{f(\text{init})}$ and $\pi_{\mathcal{D}}^{f(\text{up})}$ (right).

Additional demonstrations and interactive lecture materials can be found at https://github.com/eecsu/SIAM-AN18-Tutorial.

# Relationship with Statistical Bayesian Inference

Using Bayes theorem we can define a different posterior density [Stuart 2010; Gelman et al 2013; Jaynes 1998, ...]:

$$\tilde{\pi}_{\mathsf{X}}^{\text{post}}(\lambda|q) = \pi_{\mathsf{X}}^{\text{init}}(\lambda)\frac{\pi(q|\lambda)}{C}.$$

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## Example

Let $\mathrm{X} = [-1, 1]$ and consider the simple nonlinear map

$$q(\lambda) = \lambda^p, \quad p = 1, 3, 5, \ldots.$$

Here, $p$ is not uncertain and are used to vary the nonlinearity.

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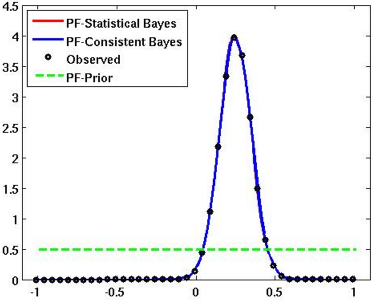
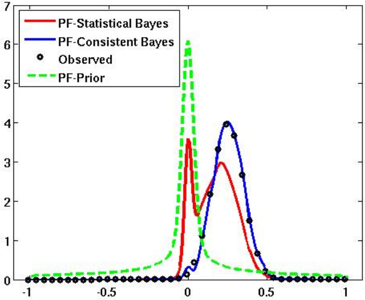
- Assume a uniform prior and the observed density is given by $\pi_{\mathcal{D}}^{\text{obs}} \sim N(0.25, 0.1^2)$.
- For the statistical Bayesian approach, we use an observed value of $\hat{q} = 0.25$ and assume a Gaussian noise model $\eta \sim N(0, 0.1^2)$.

# Comparing Push-forwards for Linear and Nonlinear Maps




Linear map ($p = 1$)




Nonlinear map ($p = 5$)

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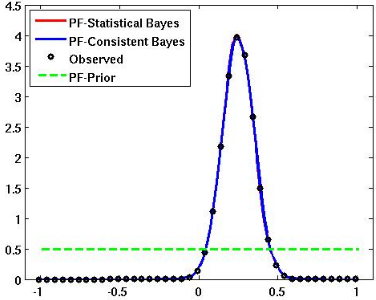


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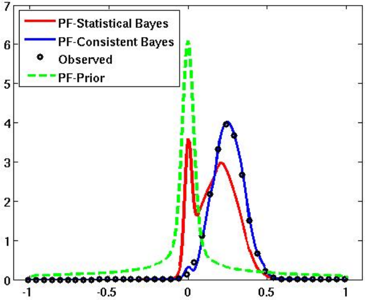


Nonlinear map ($p = 5$)

The Bayesian and measure-theoretic formulations **solve different problems**, **have different posteriors** and **make different predictions**.

# A Computational Mechanics Example

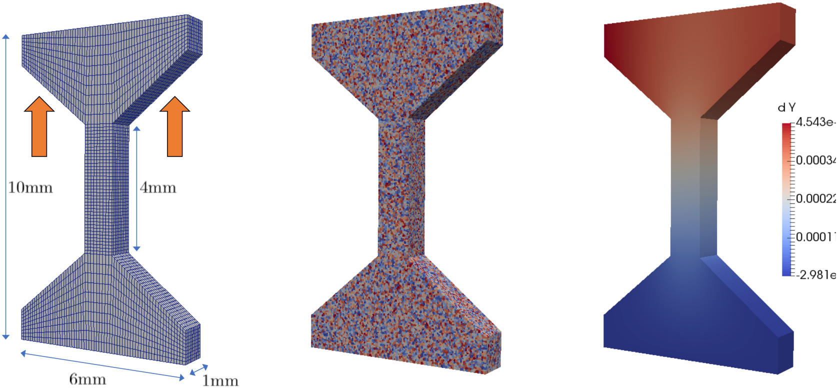


Figure: On the left, an illustration of the computational model on a coarse mesh (16,600 elements). In the middle, the granular microstructure on a finer mesh ($\approx$ 17 million elements). On the right, the vertical displacement using the high-fidelity model and nominal parameter values.

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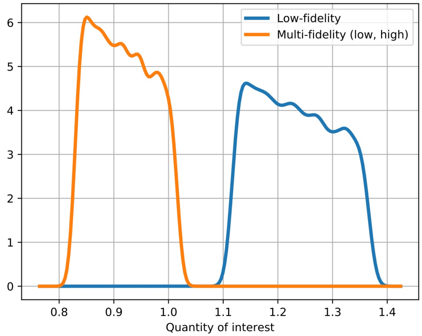

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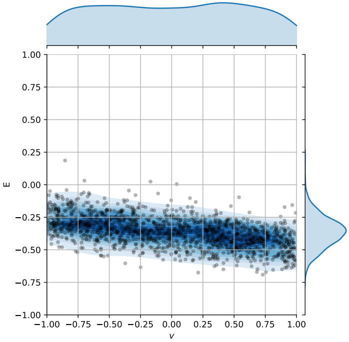


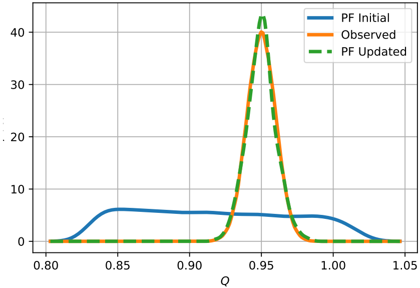
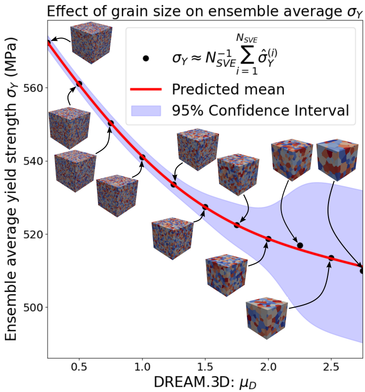




Figure: Samples from the updated density (left) and the comparison of $\pi_{\mathcal{D}}^{\text{obs}}$, $\pi_{\mathcal{D}}^{f(\text{init})}$ and $\pi_{\mathcal{D}}^{f(\text{up})}$ (right) using a 1-dimensional active subspace with $N = 100$ and $M = 10,000$.

# A Stochastic Inverse Problem in Structure-Property Linkages




For details: [Solving stochastic inverse problems for property-structure linkages using data-consistent inversion and machine learning, A. Tran and T. Wildey, JOM, 2020.]

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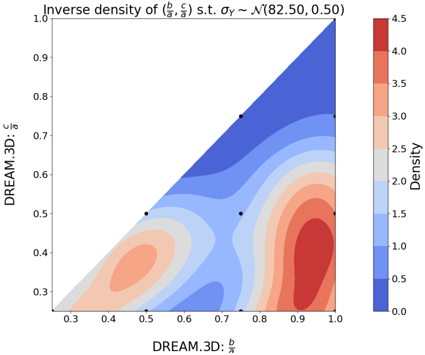


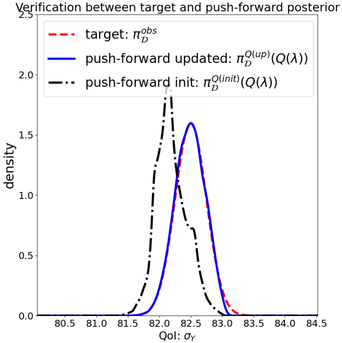

# Conclusions

- Our goal is to develop **data-informed physics-based** models.
- Many approaches exist for incorporating data into a model.
  - Deterministic optimization, Bayesian methods, OUU, data assimilation, etc.
- Our approach provides a solution to a specific stochastic inverse problem.
- Main computational expense is the forward UQ problem to obtain the push-forward of the initial density.

# Thanks! Questions?

**Acknowledgments**

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Thank you for your attention!

Questions?