

Probabilistic Meshless Methods for Bayesian Inverse Problems

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What is PN?

Many problems in mathematics have no analytical solution, and must be solved numerically.

In Probabilistic Numerics we phrase such problems as **inference problems** and construct a **probabilistic description** of this error.

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This is not a new idea¹!

Lots of recent development on Integration, Optimization, ODEs, PDEs... see <http://probnum.org/>

²[Kadane, 1985, Diaconis, 1988, O'Hagan, 1992, Skilling, 1991]

PN for PDEs

A “widely used” linear PDE. Given g , κ , b find u

$$\begin{aligned}-\nabla \cdot (\kappa(\mathbf{x}) \nabla u(\mathbf{x})) &= g(\mathbf{x}) \quad \text{in } D \\ u(\mathbf{x}) &= b(\mathbf{x}) \quad \text{on } \partial D\end{aligned}$$

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The majority of PDE solvers produce an approximation like:

$$\hat{u}(\mathbf{x}) = \sum_{i=1}^N w_i \phi_i(\mathbf{x})$$

We want to quantify the error from finite N probabilistically.

PN for PDEs

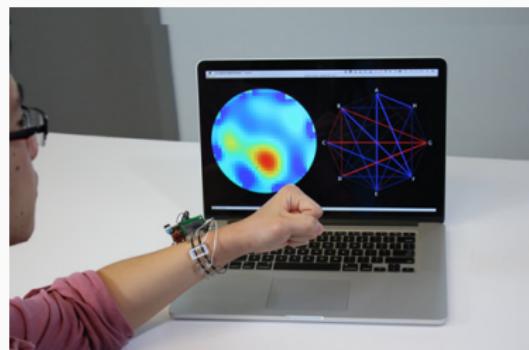
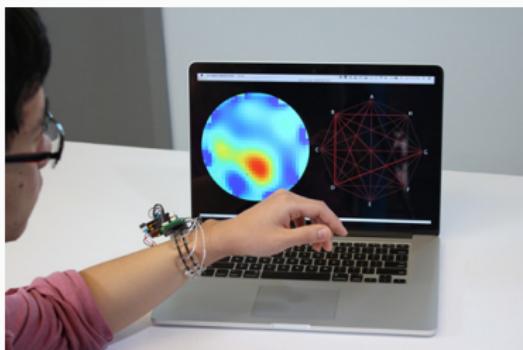
Inverse Problem: Given **partial information of g, b, u** find κ

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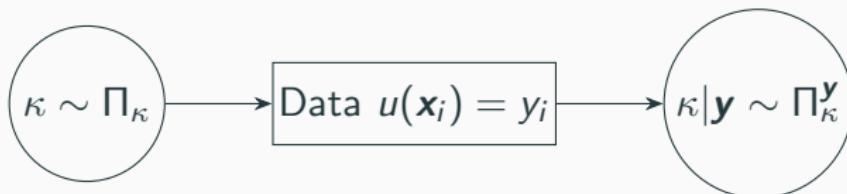


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Bayesian Inverse Problem:



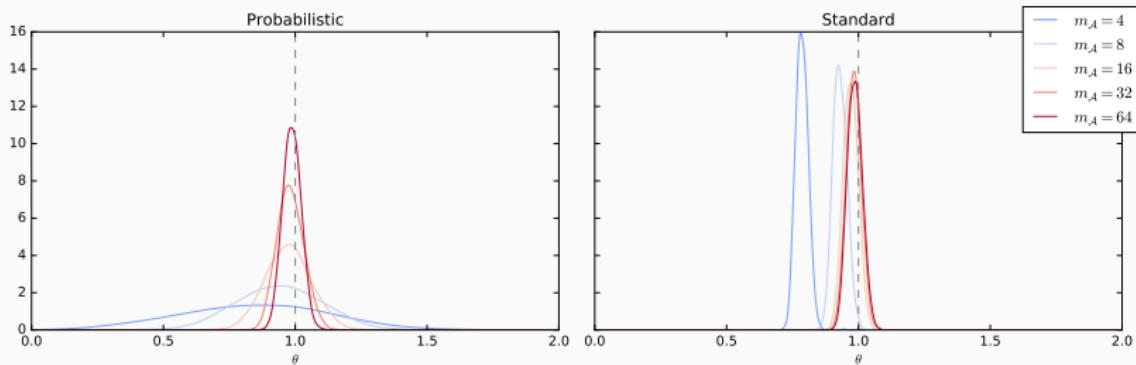
We want to account for an inaccurate forward solver in the inverse problem.

Why do this?

Using an inaccurate forward solver in an inverse problem can produce **biased** and **overconfident** posteriors.

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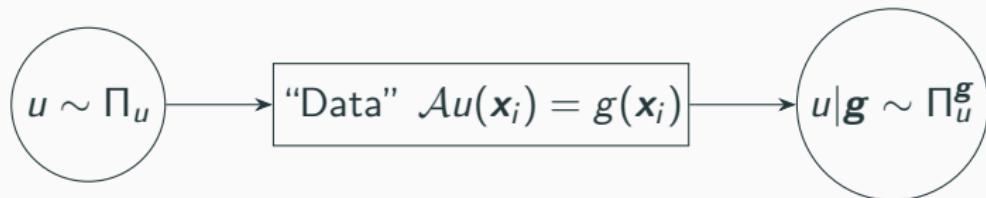
Comparison of inverse problem posteriors produced using the Probabilistic Meshless Method (PMM) vs. symmetric collocation.

Forward Problem

Abstract Formulation

$$\mathcal{A}u(\mathbf{x}) = g(\mathbf{x}) \quad \text{in } D$$

Forward inference procedure:



Posterior for the forward problem

Use a Gaussian Process prior $u \sim \Pi_u = \mathcal{GP}(0, k)$. Assuming linearity, the posterior Π_u^g is available in closed-form².

²[Cockayne et al., 2016, Särkkä, 2011, Cialenco et al., 2012, Owhadi, 2014]

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$$\Pi_u^g \sim \mathcal{GP}(m_1, \Sigma_1)$$

$$m_1(\mathbf{x}) = \bar{\mathcal{A}}K(\mathbf{x}, X) [\mathcal{A}\bar{\mathcal{A}}K(X, X)]^{-1} \mathbf{g}$$

$$\Sigma_1(\mathbf{x}, \mathbf{x}') = k(\mathbf{x}, \mathbf{x}') - \bar{\mathcal{A}}K(\mathbf{x}, X) [\mathcal{A}\bar{\mathcal{A}}K(X, X)]^{-1} \mathcal{A}K(X, \mathbf{x}')$$

$\bar{\mathcal{A}}$ the adjoint of \mathcal{A}

Observation: The mean function is the same as in symmetric collocation!

²[Cockayne et al., 2016, Särkkä, 2011, Cialenco et al., 2012, Owhadi, 2014]

Theoretical Results

Theorem (Forward Contraction)

For a ball $B_\epsilon(u_0)$ of radius ϵ centered on the true solution u_0 of the PDE, we have

$$1 - \Pi_u^g[B_\epsilon(u_0)] = \mathcal{O}\left(\frac{h^{2\beta-2\rho-d}}{\epsilon}\right)$$

- h the fill distance
- β the smoothness of the prior
- $\rho < \beta - d/2$ the order of the PDE
- d the input dimension

Toy Example

$$\begin{aligned}-\nabla^2 u(x) &= g(x) & x \in (0, 1) \\ u(x) &= 0 & x = 0, 1\end{aligned}$$

To associate with the notation from before...

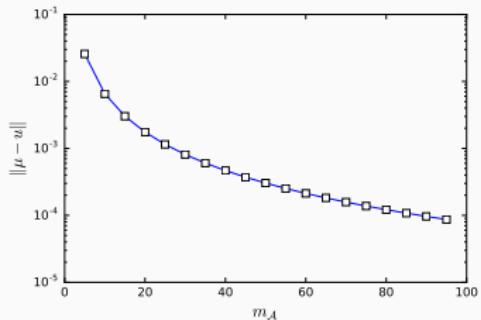
$$\Pi_u \sim \mathcal{GP}(0, k(x, y))$$

$$\mathcal{A} = -\frac{d^2}{dx^2} \quad \bar{\mathcal{A}} = -\frac{d^2}{dy^2}$$

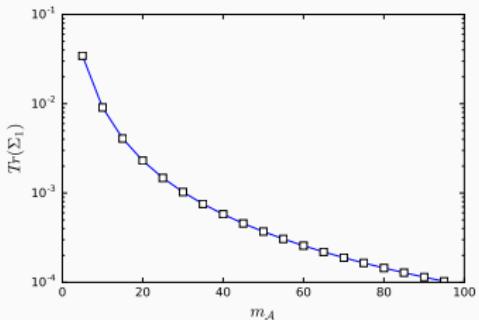
Forward problem: posterior samples

$$g(x) = \sin(2\pi x)$$

Forward problem: convergence



(a) Mean error from truth



(b) Trace of posterior covariance

Figure 1: Convergence

Inverse Problem

Recap

$$\begin{aligned}-\nabla \cdot (\kappa(\mathbf{x}) \nabla u(\mathbf{x})) &= g(\mathbf{x}) \quad \text{in } D \\ u(\mathbf{x}) &= b(\mathbf{x}) \quad \text{on } \partial D\end{aligned}$$

Now we need to incorporate the forward posterior measure Π_u^g into the posterior measure for the inverse problem, κ

Incorporation of Forward Measure

Assuming the data in the inverse problem is:

$$y_i = u(x_i) + \xi_i \quad i = 1, \dots, n$$

$$\xi \sim N(\mathbf{0}, \Gamma)$$

implies the **standard** likelihood:

$$p(y|\kappa, u) \sim N(y; u, \Gamma)$$

But we don't know u

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But we don't know u

Marginalise the forward posterior Π_u^g to obtain a “**PN**” likelihood:

$$\begin{aligned} p_{\text{PN}}(y|\kappa) &\propto \int p(y|\kappa, u) d\Pi_u^g \\ &\sim N(y; m_1, \Gamma + \Sigma_1) \end{aligned}$$

Inverse Contraction

Denote by Π_κ^y the posterior for κ from likelihood p , and by $\Pi_{\kappa,PN}^y$ the posterior for κ from likelihood p_{PN} .

Theorem (Inverse Contraction)

Assume $\Pi_\kappa^y \rightarrow \delta(\kappa_0)$ as $n \rightarrow \infty$.

Then $\Pi_{\kappa,PN}^y \rightarrow \delta(\kappa_0)$ *provided*

$$h = o(n^{-1/(\beta - \rho - d/2)})$$

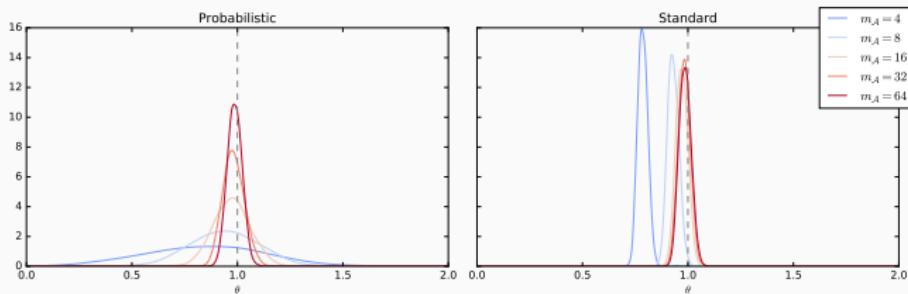
Back to the Toy Example

$$\begin{aligned}-\nabla \cdot (\kappa \nabla u(x)) &= \sin(2\pi x) & x \in (0, 1) \\ u(x) &= 0 & x = 0, 1\end{aligned}$$

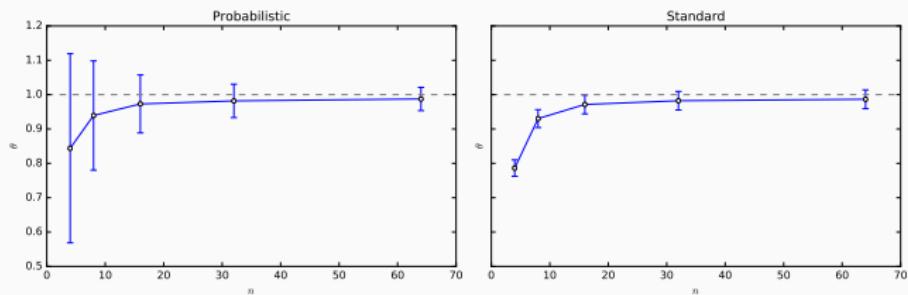
Infer $\kappa \in \mathbb{R}^+$; data generated for $\kappa = 1$ at $x = 0.25, 0.75$.

Corrupted with independent Gaussian noise $\xi \sim N(0, 0.01^2)$

Posteriors for κ



(a) Posterior Distributions for different numbers of design points.



(b) Convergence of posterior distributions with number of design points.

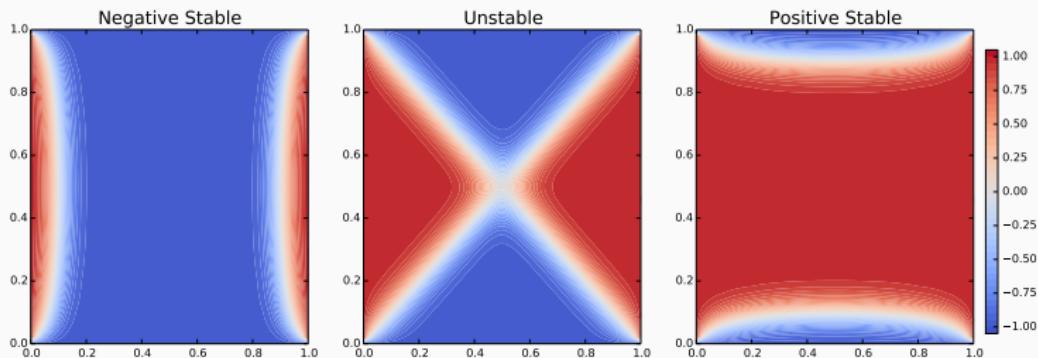
Nonlinear Example: Steady-State Allen–Cahn

Allen–Cahn

A prototypical nonlinear model.

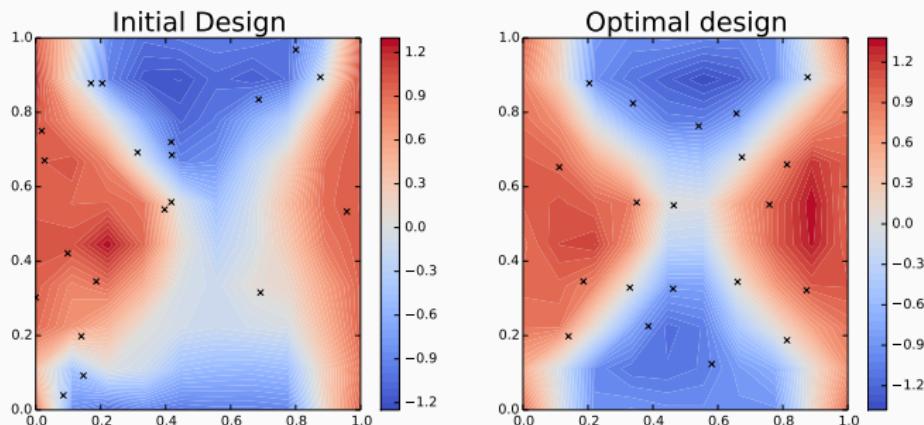
$$\begin{aligned} -\delta \nabla^2 u(\mathbf{x}) + \delta^{-1}(u(\mathbf{x})^3 - u(\mathbf{x})) &= 0 & \mathbf{x} \in (0, 1)^2 \\ u(\mathbf{x}) &= 1 & x_1 \in \{0, 1\}; 0 < x_2 < 1 \\ u(\mathbf{x}) &= -1 & x_2 \in \{0, 1\}; 0 < x_1 < 1 \end{aligned}$$

Goal: infer δ from 16 equally spaced observations of $u(\mathbf{x})$ in the interior of the domain.

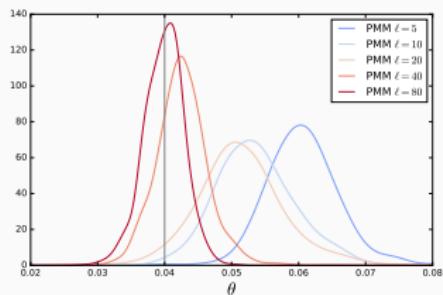


Allen–Cahn: Forward Solutions

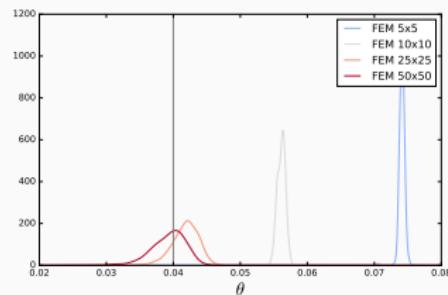
Nonlinear PDE - non-GP posterior sampling schemes required, see [Cockayne et al., 2016].



Allen–Cahn: Inverse Problem



(a) PMM



(b) FEA

Comparison of posteriors for δ with different solver resolutions, when using the PMM forward solver with PN likelihood, vs. FEA forward solver with Gaussian likelihood.

Conclusions

We have shown...

- How to build probability measures for the forward solution of PDEs.
- How to use this to make robust inferences in PDE inverse problems, even with inaccurate forward solvers.

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Coming soon...

- Evolutionary problems ($\partial/\partial t$).
- More profound nonlinearities.
- Non-Gaussian priors.

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