Probabilistic Meshless Methods for Partial Differential Equations and Bayesian Inverse Problems

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What is PN?

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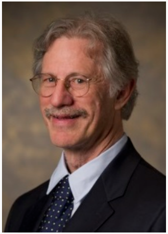
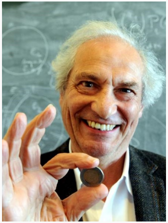
In Probabilistic Numerics we phrase such problems as inference problems and construct a probabilistic description of the discretisation error.



Joseph Kadane
Kadane [1985]



Persi Diaconis
Diaconis [1988]

Tony O'Hagan
O'Hagan [1992]

John Skilling
Skilling [1991]

This is not a new idea!

www.probnum.com

PN for PDEs

Darcy's law: given g, θ, b find u

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

For general D, $\theta(x)$ this cannot be solved analytically.

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The majority of PDE solvers produce an approximation like:

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

We want to quantify the error from finite N probabilistically.

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

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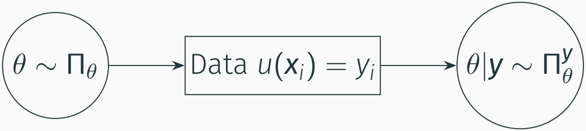
Bayesian Inverse Problem:



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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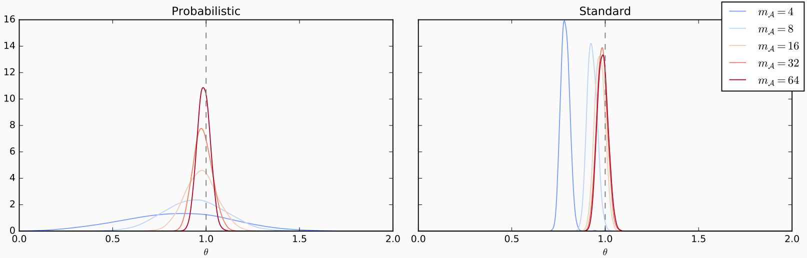


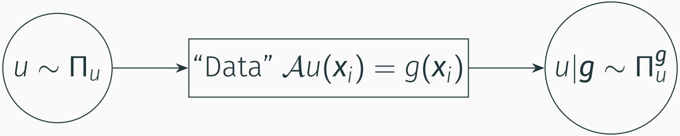
Comparison of inverse problem posteriors produced using the Probabilistic Meshless Method (PMM) vs. symmetric collocation.

Forward Problem

Abstract Formulation

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

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-form[1].

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

Posterior for the forward problem

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$$\begin{aligned} \Pi_u^{\boldsymbol{g}} &\sim \mathcal{GP}(m_1, \Sigma_1) \\ m_1(\boldsymbol{x}) &= \bar{\mathcal{A}} K(\boldsymbol{x}, X) \left[\mathcal{A}\bar{\mathcal{A}} K(X, X) \right]^{-1} \boldsymbol{g} \\ \Sigma_1(\boldsymbol{x}, \boldsymbol{x}') &= k(\boldsymbol{x}, \boldsymbol{x}') - \bar{\mathcal{A}} K(\boldsymbol{x}, X) \left[\mathcal{A}\bar{\mathcal{A}} K(X, X) \right]^{-1} \mathcal{A} K(X, \boldsymbol{x}') \end{aligned}$$

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

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

[1] [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

Poisson's Equation:

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

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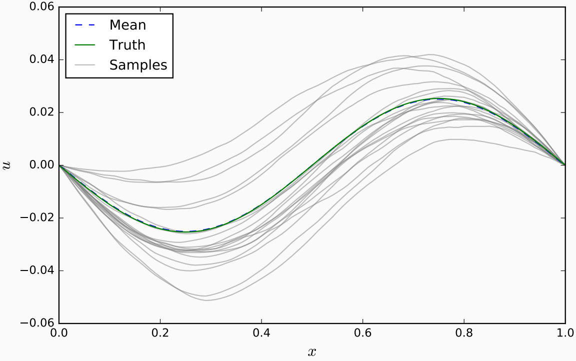

Inverse Problem

Recap

$$-\nabla \cdot (\theta(x)\nabla u(x)) = g(x) \quad \text{in } D$$
$$u(x) = b(x) \quad \text{on } \partial D$$

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

Incorporation of Forward Measure

Assuming the data in the inverse problem is:

$$y_i = u(\mathbf{x}_i) + \xi_i \quad i = 1, \dots, n$$
$$\boldsymbol{\xi} \sim N(\mathbf{0}, \Gamma)$$

implies the standard likelihood:

$$p(\mathbf{y}|\theta, u) \sim N(\mathbf{y}; \mathbf{u}, \Gamma)$$

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Marginalise the forward posterior $\Pi_u^{\mathbf{g}}$ to obtain a "PN" likelihood:

$$p_{\mathrm{PN}}(\mathbf{y}|\theta) \propto \int p(\mathbf{y}|\theta, u) d\Pi_u^{\mathbf{g}}$$
$$\sim N(\mathbf{y}; \mathbf{m}_1, \Gamma + \Sigma_1)$$

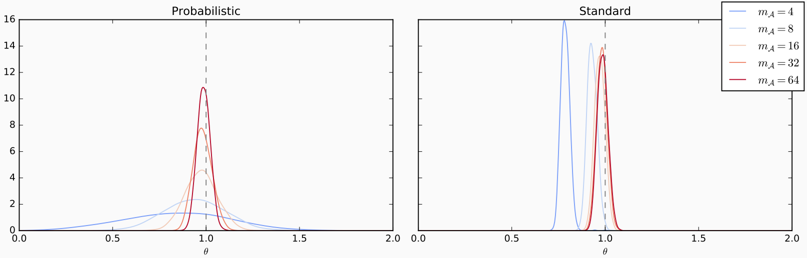
Back to the Toy Example

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

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

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

Posteriors for θ



Nonlinear Example: Steady-State Allen–Cahn

Allen–Cahn

A prototypical nonlinear model.

$$
\begin{aligned}
-\theta\nabla^2 u(\mathbf{x}) + \theta^{-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 \\
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Goal: infer θ from 16 equally spaced observations of $u(\mathbf{x})$ in the interior of the domain.

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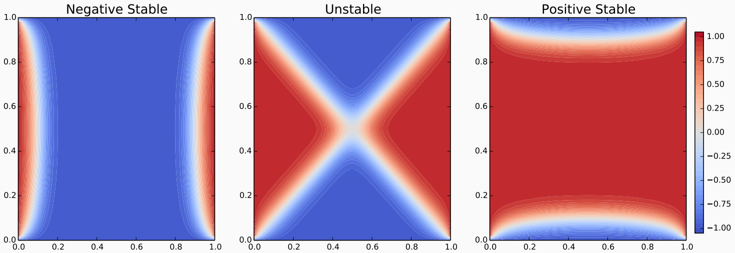
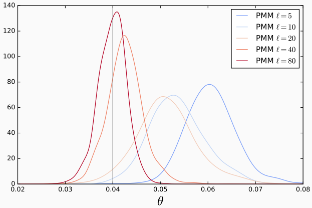
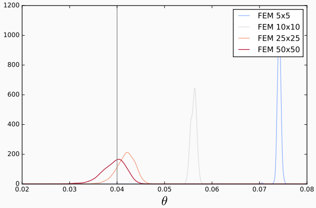


Allen–Cahn: Inverse Problem



(a) PMM



(b) FEA

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

Conclusions

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We have shown...

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

“Bayesian Probabilistic Numerical Methods”

http://www.joncockayne.com/papers/pn_foundations

Questions?

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