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.

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

This is not a new idea[1]!

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

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

What does this mean for PDEs?

A prototypical linear PDE. Given g, κ, b find u

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

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The majority of PDE solvers produce an approximation like:

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

We want to quantify the error from finite N probabilistically.

What does this mean for PDEs?

Inverse Problem: Given partial information of $\boldsymbol{g}, \boldsymbol{b}, \boldsymbol{u}$ find κ

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Bayesian Inverse Problem:

$$\kappa \sim \Pi_\kappa \longrightarrow \boxed{\text{Data } u(\boldsymbol{x}_i) = y_i} \longrightarrow \kappa | \boldsymbol{y} \sim \Pi_\kappa^{\boldsymbol{y}}$$

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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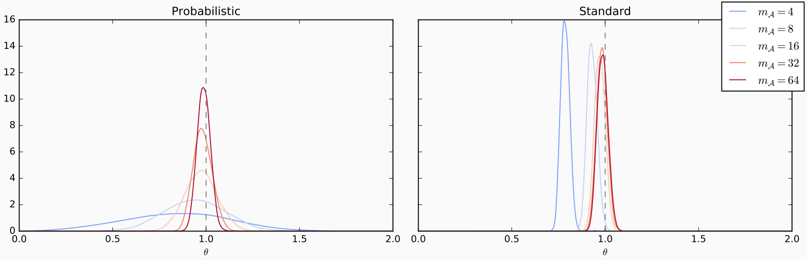

Comparison of inverse problem posteriors produced using the Probabilistic Meshless Method (PMM) vs. symmetric collocation.

Forward Problem

Abstract Formulation

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

Forward inference procedure:

$$u \sim \Pi_u \longrightarrow \boxed{\text{“Data” } \mathcal{A}u(\boldsymbol{x}_i) = g(\boldsymbol{x}_i)} \longrightarrow u|\boldsymbol{g} \sim \Pi_u^{\boldsymbol{g}}$$

Posterior for the forward problem

Use a Gaussian Process prior $u \sim \Pi_u = \mathcal{GP}(0, k)$. Assuming linearity, the posterior $\Pi_u^{\boldsymbol{g}}$ is available in closed-form[2].

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

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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!

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

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

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

- *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

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

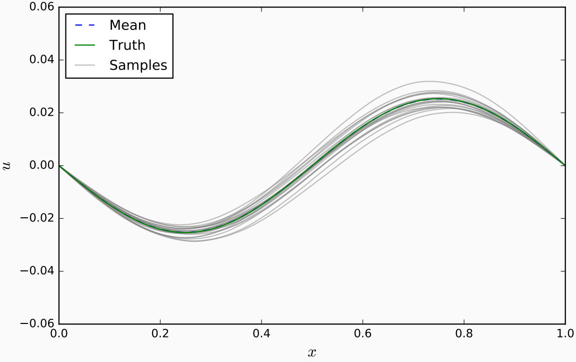
To associate with the notation from before...

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

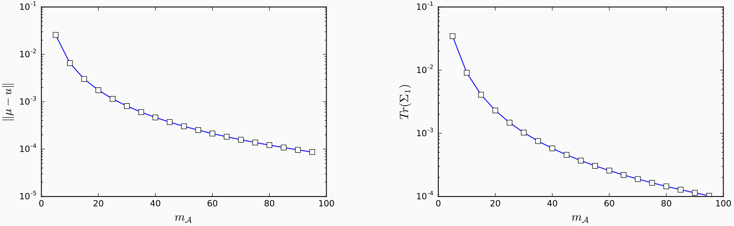
$$\mathcal{A} = \frac{d^2}{dx^2} \quad \bar{\mathcal{A}} = \frac{d^2}{dy^2}$$

Forward problem: posterior samples

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



Forward problem: convergence



(a) Mean error from truth **(b)** Trace of posterior covariance

Figure 2: Convergence

Inverse Problem

Recap

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

Now we need to incorporate the forward posterior measure $\Pi_u^{\boldsymbol{g}}$ into the posterior measure for the inverse problem, κ

Incorporation of Forward Measure

Assuming the data in the inverse problem is:

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

implies the standard likelihood:

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

But we don't know u

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

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

Inverse Contraction

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

Theorem (Inverse Contraction)

Assume $\Pi_\kappa^{\boldsymbol{y}} \to \delta(\kappa_0)$ *as* $n \to \infty$.

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

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

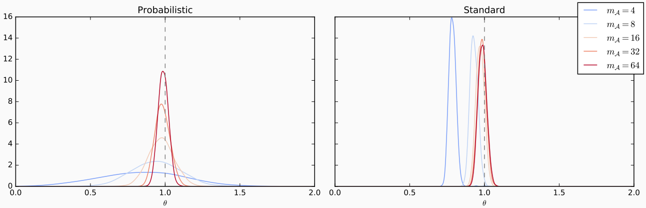
Back to the Toy Example

$$-\nabla \cdot (\kappa \nabla u(x)) = \sin(2\pi x) \qquad x \in (0,1)$$
$$u(x) = 0 \qquad x = 0,1$$

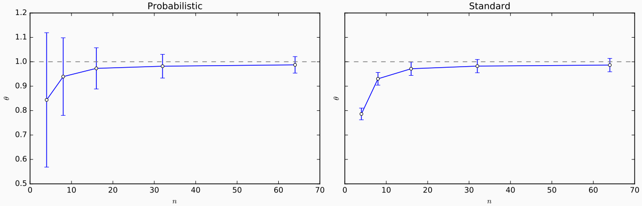
Infer $\kappa \in \mathbb{R}^+$; data generated for $\kappa = 1$ at $x = 0.25, 0.75$.

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.

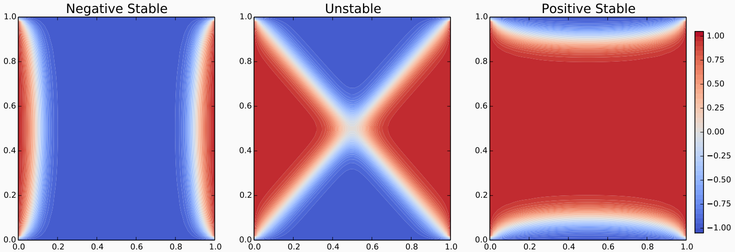
Nonlinear Example: Steady-State Allen–Cahn

Allen–Cahn

A prototypical nonlinear model.

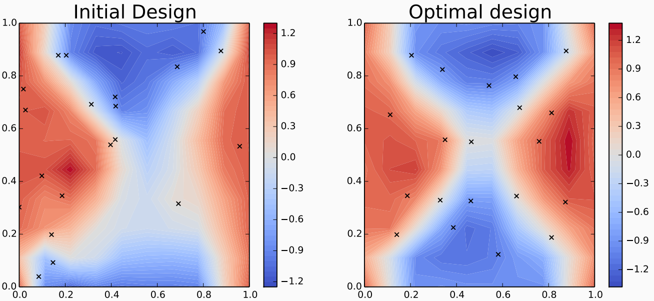
$$
\begin{aligned}
-\delta \nabla^2 u(\boldsymbol{x}) + \delta^{-1}(u(\boldsymbol{x})^3 - u(\boldsymbol{x})) &= 0 && \boldsymbol{x} \in (0,1)^2 \\
u(\boldsymbol{x}) &= 1 && x_1 \in \{0,1\}\,; 0 < x_2 < 1 \\
u(\boldsymbol{x}) &= -1 && x_2 \in \{0,1\}\,; 0 < x_1 < 1
\end{aligned}
$$

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

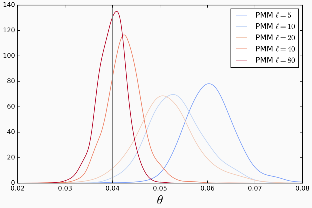


Allen–Cahn: Forward Solutions

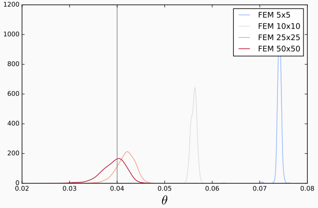
Nonlinear PDE - non-GP posterior sampling schemes required, see [Cockayne et al., 2016].



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 rhobust 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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