Bayesian Inference for Latent Gaussian Models Governed by PDEs

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Goal

Characterize the posterior of a linear PDE-governed Bayesian inverse problem with Gaussian prior, marginalizing out hyperparameters.

Latent Gaussian Models (LGMs)

Hierarchical model with Gaussian prior:

$$\begin{aligned} \boldsymbol{\theta} &\sim \pi_{\text{hyp}}(\boldsymbol{\theta}) && \text{low-dim hyperparameter} \\ \boldsymbol{m}|\boldsymbol{\theta} &\sim \mathcal{N}(\boldsymbol{\mu}_{\text{pr}}(\boldsymbol{\theta}), \boldsymbol{Q}_{\text{pr}}^{-1}(\boldsymbol{\theta})) && \text{high-dim latent variable} \\ \boldsymbol{y}|\boldsymbol{m},\boldsymbol{\theta} &\sim \pi_{\text{like}}(\boldsymbol{y}|\boldsymbol{m},\boldsymbol{\theta}) && \text{observed data} \end{aligned}$$

Linear Gaussian Bayesian inverse problem as LGM:

$$\boldsymbol{y} = \boldsymbol{A}\boldsymbol{m} + \boldsymbol{\varepsilon} \quad \text{with} \quad \boldsymbol{\varepsilon} \sim \mathcal{N}(0, \boldsymbol{Q}_{\varepsilon}^{-1}(\boldsymbol{\theta})),$$

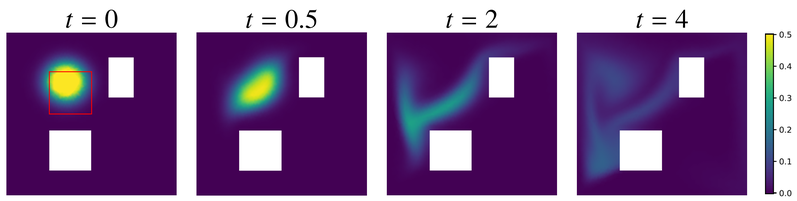
with $\boldsymbol{A}$ a discretization of a linear PDE. Want to characterize $\pi(\boldsymbol{m}|\boldsymbol{y})$.

Example: Initial Condition Inference

Infer distribution of initial condition of advection diffusion equation

$$\begin{cases} u_t - \kappa\Delta u + v\cdot\nabla u = 0 & \text{in} \quad \Omega\times[0,T] \\ u(x,0) = m(x) & \text{in} \quad \Omega \\ \kappa\nabla u\cdot n = 0 & \text{on} \quad \partial\Omega, \end{cases}$$

from solution evaluated at points x_i and times $t_i > 0$.



$u(x,t)$ for various times t.

- Data: $y_i = u(x_i, t_i) + \varepsilon_i$
- Latent var.: initial condition $\boldsymbol{m}$
- Forward map: discretized PDE $\boldsymbol{A}$
- Prior: Matérn GRF with precision $(\delta I - \gamma\Delta)^2$
- Likelihood: $\mathcal{N}(\boldsymbol{A}\boldsymbol{m}, \lambda^{-2}\boldsymbol{I})$
- Hyperparam. $\boldsymbol{\theta}$: $(\delta, \gamma, \lambda)$
- Hyperprior: independent gamma distributions
- QoI: q = avg. of $m(x)$ in red box

Sampling & Integration by Marginalization

Sampling: sample $\boldsymbol{m}^* \sim \pi(\boldsymbol{m}|\boldsymbol{y})$ by

1. sampling $\boldsymbol{\theta}^* \sim \pi(\boldsymbol{\theta}|\boldsymbol{y})$ (low-dimensional, so can use MCMC)
2. sampling $\boldsymbol{m}^* \sim \pi_{\text{post}}(\boldsymbol{m}|\boldsymbol{\theta}^*, \boldsymbol{y})$ (Gaussian, posterior of a linear IP)

Integration: (low-dim quadrature)

$$\int f(\boldsymbol{m})\pi(\boldsymbol{m}|\boldsymbol{y})\,d\boldsymbol{m} = \int\left(\int f(\boldsymbol{m})\pi_{\text{post}}(\boldsymbol{m}|\boldsymbol{\theta},\boldsymbol{y})\,d\boldsymbol{m}\right)\pi(\boldsymbol{\theta}|\boldsymbol{y})\,d\boldsymbol{\theta}$$

Find max of $\pi(\boldsymbol{\theta}|\boldsymbol{y})$ and quadrature points around max.

Fast Computation of Marginal: Low Rank Approx

Both require many evaluations of $\pi(\boldsymbol{\theta}|\boldsymbol{y})$ with different $\boldsymbol{\theta}$:

$$\begin{aligned} \pi(\boldsymbol{\theta}|\boldsymbol{y}) &\propto \frac{\pi(\boldsymbol{m},\boldsymbol{\theta},\boldsymbol{y})}{\pi_{\text{post}}(\boldsymbol{m}|\boldsymbol{\theta},\boldsymbol{y})} = \frac{\pi_{\text{like}}(\boldsymbol{y}|\boldsymbol{m},\boldsymbol{\theta})\pi_{\text{pr}}(\boldsymbol{m}|\boldsymbol{\theta})\pi_{\text{hyp}}(\boldsymbol{\theta})}{\pi_{\text{post}}(\boldsymbol{m}|\boldsymbol{\theta},\boldsymbol{y})} \\ &\propto \left(\frac{|\boldsymbol{Q}_{\text{pr}}||\boldsymbol{Q}_{\varepsilon}|}{|\boldsymbol{Q}_{\text{post}}|}\right)^{1/2} \exp\left(-\frac{1}{2}\left[\|\boldsymbol{y}\|_{\boldsymbol{Q}_{\varepsilon}} + \|\boldsymbol{\mu}_{\text{pr}}\|_{\boldsymbol{Q}_{\text{pr}}} - \|\boldsymbol{\mu}_{\text{post}}\|_{\boldsymbol{Q}_{\text{post}}}\right]\right)\pi_{\text{hyp}}(\boldsymbol{\theta}) \end{aligned}$$

Each new $\boldsymbol{\theta}$ requires solving a linear BIP. Cost is dominated by forward and adjoint PDE solve in the prior-to-posterior precision update:

$$\boldsymbol{Q}_{\text{post}} = \boldsymbol{Q}_{\text{pr}} + \underbrace{\boldsymbol{A}^T\boldsymbol{Q}_{\varepsilon}\boldsymbol{A}}_{\text{update}}$$

Instead, precompute rank-r approximation to update. Requires $2r$ PDE solves up front, but avoids most PDE solves for each $\boldsymbol{\theta}$ (a few are needed in practice to improve accuracy of $\boldsymbol{\mu}_{\text{post}}$).

✗ Prior Preconditioned Approximation

Standard approach: use randomized eigensolver to find

$$\boldsymbol{Q}_{\text{pr}}^{-1/2}(\boldsymbol{\theta})\boldsymbol{A}^T\boldsymbol{Q}_{\varepsilon}\boldsymbol{A}\boldsymbol{Q}_{\text{pr}}^{-1/2}(\boldsymbol{\theta}) \approx \boldsymbol{V}_r\boldsymbol{\Lambda}_r\boldsymbol{V}_r^T,$$

since $\boldsymbol{Q}_{\text{pr}}^{-1/2}$ is smoothing, it lowers required r and we have a natural bound on truncation error. *But:* $\boldsymbol{Q}_{\text{pr}}$ depends on $\boldsymbol{\theta}$!

✓ Weakest Prior Preconditioned Approximation

Instead,

$$\boldsymbol{Q}_{\text{pr}}^{-1/2}(\boldsymbol{\theta}_0)\boldsymbol{A}^T\boldsymbol{Q}_{\varepsilon}\boldsymbol{A}\boldsymbol{Q}_{\text{pr}}^{-1/2}(\boldsymbol{\theta}_0) \approx \boldsymbol{V}_r\boldsymbol{\Lambda}_r\boldsymbol{V}_r^T$$

for some fixed $\boldsymbol{\theta}_0$ and convert for each $\boldsymbol{\theta}$:

$$\boldsymbol{Q}_{\text{pr}}^{-1/2}(\boldsymbol{\theta})\boldsymbol{A}^T\boldsymbol{Q}_{\varepsilon}\boldsymbol{A}\boldsymbol{Q}_{\text{pr}}^{-1/2}(\boldsymbol{\theta}) \approx \boldsymbol{Q}_{\text{pr}}^{-1/2}(\boldsymbol{\theta})\boldsymbol{Q}_{\text{pr}}^{1/2}(\boldsymbol{\theta}_0)\boldsymbol{V}_r\boldsymbol{\Lambda}_r\boldsymbol{V}_r^T\boldsymbol{Q}_{\text{pr}}^{1/2}(\boldsymbol{\theta}_0)\boldsymbol{Q}_{\text{pr}}^{-1/2}(\boldsymbol{\theta}).$$

Choose $\boldsymbol{\theta}_0$ to be the parameters of the least smoothing, "weakest" prior to avoid amplifying truncation error.

✓ Unpreconditioned Approximation

Alternatively,

$$\boldsymbol{A}^T\boldsymbol{Q}_{\varepsilon}\boldsymbol{A} \approx \boldsymbol{V}_r\boldsymbol{\Lambda}_r\boldsymbol{V}_r^T.$$

Higher rank needed, and no principled way to choose rank, but simplest.

Computational Complexity

Main computational cost in evaluating $\pi(\boldsymbol{\theta}|\boldsymbol{y})$ comes from forward/adjoint PDE solves and prior precision solves. The table below reports the complexity of N evaluations in terms of these operations.

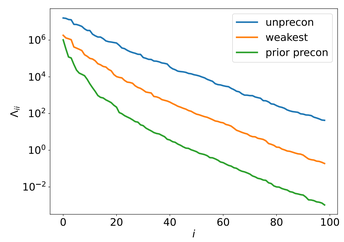
	prior preconditioned	weakest	unpreconditioned
$\boldsymbol{A}$, $\boldsymbol{A}^T$ applies	$2Nr_p + 2N\ell$	$2r_w + 2N\ell$	$2r_u + 2N\ell$
$\boldsymbol{Q}_{\text{pr}}$ solves	$N(r_p + \ell)$	$r_w + N(r_w + \ell)$	$N(r_u + \ell)$
rank	$r_p = 57$	$r_w = 66$	$r_u = 84$
time for $N = 100$	1167 s	167 s	182 s

Number of most expensive operations (first two rows) for the low-rank approximation methods above (columns); numerical rank used in each method (3rd row); and time for $N = 100$ evaluations in the initial-condition inference example (4th row); ℓ = num. of CG iterations to find $\boldsymbol{\mu}_{\text{post}}$.

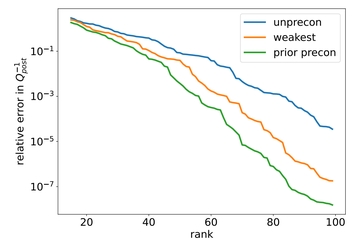
Numerical Results: Initial Condition Inference

Comparison of low rank approximations

- Fastest decay when preconditioned with $\boldsymbol{Q}_{\text{pr}}(\boldsymbol{\theta})$ (as expected)
- Preconditioning with weakest $\boldsymbol{Q}_{\text{pr}}(\boldsymbol{\theta}_0)$ improves over no precond
- Error plot allows for comparison of unpreconditioned method
- Using weakest $\boldsymbol{Q}_{\text{pr}}(\boldsymbol{\theta}_0)$ may be a good tradeoff between up-front and online computation



Eigenvalue spectrum of update, by type of preconditioning.



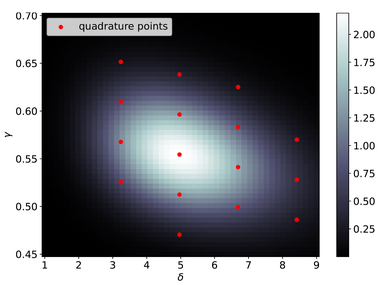
Error in norm of pointwise posterior variance as a function of rank.

Hyperparameter marginal $\pi(\boldsymbol{\theta}|\boldsymbol{y})$

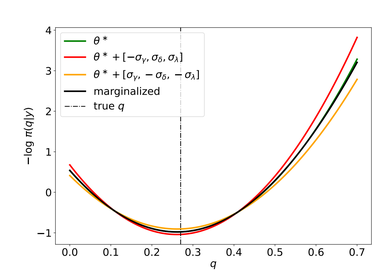
- Argmax γ^*, δ^* approximate smoothness and variance of true IC
- Unimodal, easy to sample and to integrate using quadrature

Quantity of Interest distribution

- With quadrature, can approximate $\pi(q|\boldsymbol{y})$ for any quantity of interest q that is a linear function of $\boldsymbol{m}$ (here, avg. of $m(x)$ in a region)
- In this case $\pi(q|\boldsymbol{y})$ is close to $\pi(q|\boldsymbol{y}, \boldsymbol{\theta}^*)$, but other choices of $\boldsymbol{\theta}$ change the variance significantly.



$\pi(\boldsymbol{\theta}|\boldsymbol{y})$ (only γ, δ shown) in gray scale, with tailored quadrature points in red.



$\pi(q|\boldsymbol{y})$ compared to $\pi(q|\boldsymbol{y}, \boldsymbol{\theta})$ evaluated at $\boldsymbol{\theta}^* = \arg\max \pi(\boldsymbol{\theta}|\boldsymbol{y})$ and other quadrature points.

Next Steps

- Use various discretizations of PDE to speed up MCMC
- Find a way to adapt low rank approximation when $\boldsymbol{A}$ depends on $\boldsymbol{\theta}$
- Extend to nonlinear PDEs using ideas from Integrated Nested Laplace Approximation

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