Bayesian Inversion: Applications and Mathematical Foundations

Andrew M Stuart¹

¹Mathematics Institute and Centre for Scientific Computing University of Warwick

Woudshoten Lectures 2013 October 2nd 2013

Funded by EPSRC, ERC and ONR



http://homepages.warwick.ac.uk/~masdr/

A.M. Stuart. Inverse Problems: a Bayesian Perspective. Acta Numerica 19(2010). ~masdr/BOOKCHAPTERS/stuart15c.pdf

- M. Hairer, A.M. Stuart, J. Voss, *Signal Processing Problems on Function Space: Bayesian formulation*.... The Oxford Handbook of Nonlinear Filtering, editors D. Crisan and B. Rozovsky, OxfordUniversity Press, 2011. ~masdr/BOOKCHAPTERS/stuart16c.pdf
- S.L.Cotter, M. Dashti, A.M.Stuart. Approximation of Bayesian Inverse Problems. SINUM 48(2010), 322–345. ~masdr/JOURNALPUBS/stuart81.pdf
- Y. Marzouk, D. Xiu. A Stochastic Collocation Approach to Bayesian Inference in Inverse Problems. Comm. Comp. Phys. 6(2009), 836–847.



Outline

BAYESIAN INVERSION: PDE INVERSE PROBLEMS

2 BAYESIAN INVERSION: CONDITIONED DIFFUSIONS

3 COMMON STRUCTURE





Outline

BAYESIAN INVERSION: PDE INVERSE PROBLEMS

2 BAYESIAN INVERSION: CONDITIONED DIFFUSIONS

- **3 COMMON STRUCTURE**
- 4 CONCLUSIONS



Motivation

- Aim: to solve $y = \mathcal{G}(u) + \text{noise}$ for *u* given *y*.
- LSQ: minimize $\Phi(u; y) := \frac{1}{2} ||y \mathcal{G}(u)||^2$.
- Bayesian: u and y|u random variables then find u|y.



Lagrangian Data Assimilation

• Find $u \in H = L^2_{\text{div}}(\Omega, \mathbb{R}^2)$ initial condition for Navier-Stokes:

$$\frac{dv}{dt} + \nu Av + B(v, v) = f, v(0) = u$$

• Given noisy Lagrangian data $y = \{z_j(t_k) + \eta_{j,k}\}$:

$$\frac{dz_j}{dt} = v(z_j, t), \, z_j(0) = z_{j,0}$$

• Abstractly: for $\mathcal{G} : X \subseteq H \mapsto Y = \mathbb{R}^{JK}$ find *u* given

$$y = \mathcal{G}(u) + \eta$$
, noise.



Eulerian Data Assimilation

• Find $u \in H = L^2_{div}(\Omega, \mathbb{R}^2)$ initial condition for Navier-Stokes:

$$\frac{dv}{dt} + \nu Av + B(v, v) = f, v(0) = u$$

• Given noisy Eulerian data $y = \{v(x_j, t_k) + \eta_{j,k}\}$:

$$\mathbf{y}_{j,k} = \mathbf{v}(\mathbf{x}_j, \mathbf{t}_k) + \eta_{j,k}$$

• Abstractly: for $\mathcal{G} : X \subset H \mapsto Y = \mathbb{R}^{JK}$ find *u* given

$$y = \mathcal{G}(u) + \eta$$
, noise.



Groundwater Flow Inversion

• Let $f \in H^{-1}(D)$. Find log permeability $u \in X = L^{\infty}(D)$:

$$-
abla \cdot \left(e^{u}
abla p
ight) = f, \quad x \in D$$

 $p = 0, \quad x \in \partial D$

• Given, for
$$j = 1, \ldots, J$$
,

$$y_j = \ell_j(p) + \eta_j, \ \ell_j \in H^{-1}(D), \ \eta_j$$
 noise.

• Abstractly: for $\mathcal{G} : X \mapsto Y = \mathbb{R}^J$ find *u* given

$$y = \mathcal{G}(u) + \eta$$
, noise.



Outline

BAYESIAN INVERSION: PDE INVERSE PROBLEMS

2 BAYESIAN INVERSION: CONDITIONED DIFFUSIONS

3 COMMON STRUCTURE

4 CONCLUSIONS



Motivation

• Aim: to find $u \in L^2([0, T]; \mathbb{R}^p)$ solving

$$du = f(u)dt + \Sigma dB$$
, $u(0) = u^{-}$.

Conditioned on:

$$u(T)=u^+.$$

• Or conditioned on $y \in L^2([0, T]; \mathbb{R}^q)$ solving

 $dy = h(u)dt + \Gamma dW$, y(0) = 0.



Molecular Dynamics

• Find
$$u \in H = L^2([0, 1], \mathbb{R}^{Nd})$$
:

$$du = -
abla V(u)dt + \sqrt{rac{2}{eta}}dB.$$

• Conditioned on red atom moving into vacancy:





Signal Processing

• Find
$$u \in H = L^2([0, 1], \mathbb{R})$$
:

$$du = u - u^3 + dB, u(0) = -1$$

• Conditioned on: $y \in L^2([0,1],\mathbb{R})$ where

$$y(t) = \int_0^t u(s) ds + \Gamma W(t).$$



Outline

BAYESIAN INVERSION: PDE INVERSE PROBLEMS

2 BAYESIAN INVERSION: CONDITIONED DIFFUSIONS

3 COMMON STRUCTURE

4 CONCLUSIONS



Common Probabilistic Framework

- There is a simple probability measure μ_0 on *H*.
- The complicated measure of interest is μ^{y} , also on *H*.
- μ^{y} is related to μ_{0} by

$$rac{d\mu^y}{d\mu_0}(u) = rac{1}{Z} \exp\Bigl(-\Phi(u)\Bigr).$$

• Since $\mu^{y}(du) = Z^{-1} \exp(-\Phi(u))\mu_{0}(du)$ we have

$$\mathbb{E}^{\mu^{y}}f(u)=\frac{1}{Z}\mathbb{E}^{\mu_{0}}\Big(\exp\bigl(-\Phi(u)\bigr)f(u)\Big).$$

• Here Z is the normalization:

$$Z = \mathbb{E}^{\mu_0} \Big(\exp(-\Phi(u)) \Big).$$



PDE Inverse Problems

- Unknown $u \in H$.
- Data $y \in \mathbb{R}^J$.
- Prior $\mathbb{P}(u)$: $u \sim \mu_0(du)$.
- Likelihood $\mathbb{P}(y|u)$: $y|u \sim N(\mathcal{G}(u), \Gamma)$.
- Bayes' Theorem: $\mathbb{P}(u|y) \propto \mathbb{P}(y|u) \times \mathbb{P}(u)$.
- Posterior: $\mu^{y}(du) \propto \exp(-\Phi(u; y))\mu_{0}(du)$.
- Potential: $\Phi(u; y) := \frac{1}{2} \| \Gamma^{-\frac{1}{2}}(y \mathcal{G}(u)) \|^2$.



Priors for Permeability









Hellinger Distance

For μ and ν which have density with respect to μ₀ we define the *Hellinger distance*

$$d_{\text{Hell}}(\mu,\nu) = \sqrt{\left(\frac{1}{2}\int_{X}\left[\left(\frac{d\mu}{d\mu_{0}}\right)^{\frac{1}{2}} - \left(\frac{d\nu}{d\mu_{0}}\right)^{\frac{1}{2}}\right]^{2}d\mu_{0}(u)\right)}.$$

Distance good because, for f ∈ L²_µ(H; S), L²_ν(H; S):

$$\|\mathbb{E}^{\mu}f(u) - \mathbb{E}^{\nu}f(u)\|_{\mathcal{S}} \leq 2\Big(\mathbb{E}^{\mu}\|f(u)\|_{\mathcal{S}}^{2} + \mathbb{E}^{\nu}\|f(u)\|_{\mathcal{S}}^{2}\Big)^{\frac{1}{2}}d_{\textit{Hell}}(\mu, \nu).$$



The Well-Posedness Theorem

POTENTIAL CONDITIONS: $\Phi : X \times Y \to \mathbb{R}$ locally Lipschitz with appropriate growth conditions on Lipschitz constant.

Theorem

(S, Acta Numerica, 2010.) Assume that

• POTENTIAL CONDITIONS; $X \subseteq H$.

• $\mu_0(X) = 1$ *plus* INTEGRABILITY CONDITIONS.

Then μ^{y} well-defined and there is $C = C(|y_{1}|, |y_{2}|) > 0$:

$$d_{\textit{Hell}}(\mu^{y_1},\mu^{y_2}) \leq C|y_1-y_2|.$$



Implications

• Mean:
$$\left\| \mathbb{E}^{\mu^{y_1}} u - \mathbb{E}^{\mu^{y_2}} u \right\|_H \le C |y_1 - y_2|.$$

Covariance

$$\left\|\mathbb{E}^{\mu^{y_1}} u \otimes u - \mathbb{E}^{\mu^{y_2}} u \otimes u\right\|_{H \to H} \leq C|y_1 - y_2|.$$



Forward Error Gives Inverse Error

Write $\mu = \mu^{y}$; let μ^{N} denote approximation in finite dimensions.

Theorem

(Cotter, Dashti and S, SINUM, 2010). Assume that $X \subseteq H$

• Φ and Φ^N satisfy POTENTIAL CONDITIONS, uniformly in N;

• forward approximation error satisfies

$$|\Phi(u) - \Phi^{N}(u)| \leq M(\|u\|_X)\psi(N)$$

where $\psi(N) \rightarrow 0$ as $N \rightarrow \infty$;

• $\mu_0(X) = 1$ *plus* INTEGRABILITY CONDITIONS.

Then there is a constant *C*, independent of *N*, and such that the **inverse** approximation error is

$$d_{\text{Hell}}(\mu,\mu^N) \leq C\psi(N).$$



Implications

• Mean:

$$\left\|\mathbb{E}^{\mu}u-\mathbb{E}^{\mu^{N}}u\right\|_{H}\leq C\psi(N).$$

• Covariance

$$\left\|\mathbb{E}^{\mu} u \otimes u - \mathbb{E}^{\mu^{N}} u \otimes u\right\|_{H \to H} \leq C\psi(N)$$

(Marzouk/Xiu used Kullback-Leibler divergence instead of Hellinger distance to prove a similar result.)



Outline

BAYESIAN INVERSION: PDE INVERSE PROBLEMS

2 BAYESIAN INVERSION: CONDITIONED DIFFUSIONS

3 COMMON STRUCTURE





What We Have Shown

We have shown that:

- **Applications:** Many inverse problems in partial and stochastic differential equations can be formulated in the framework of Bayesian statistics on function space.
- **Common Structure:** These problems share a common mathematical structure leading to *well-posed* inverse problems for measures.
- **Approximation:** This well-posedness leads to a transfer of approximation properties from the forward problem to the inverse problem, in the Hellinger metric.
- Algorithms: Good algorithms follow from this infinite dimensional perspective on Bayes' Theorem – next lecture.



http://homepages.warwick.ac.uk/~masdr/

A.M. Stuart. Inverse Problems: a Bayesian Perspective. Acta Numerica 19(2010). ~masdr/BOOKCHAPTERS/stuart15c.pdf

- M. Hairer, A.M. Stuart, J. Voss, *Signal Processing Problems on Function Space: Bayesian formulation*.... The Oxford Handbook of Nonlinear Filtering, editors D. Crisan and B. Rozovsky, OxfordUniversity Press, 2011. ~masdr/BOOKCHAPTERS/stuart16c.pdf
- S.L.Cotter, M. Dashti, A.M.Stuart. Approximation of Bayesian Inverse Problems. SINUM 48(2010), 322–345. ~masdr/JOURNALPUBS/stuart81.pdf
- Y. Marzouk, D. Xiu. A Stochastic Collocation Approach to Bayesian Inference in Inverse Problems. Comm. Comp. Phys. 6(2009), 836–847.

