Probabilistic Numerical Methods for Deterministic Differential Equations

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Outline

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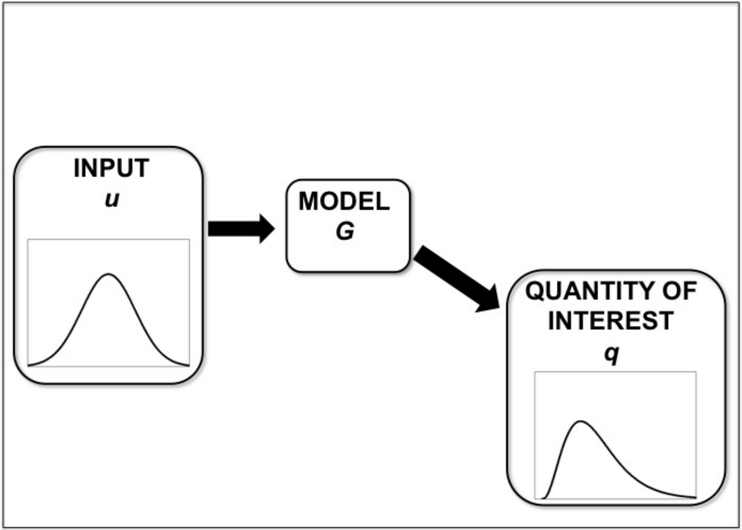
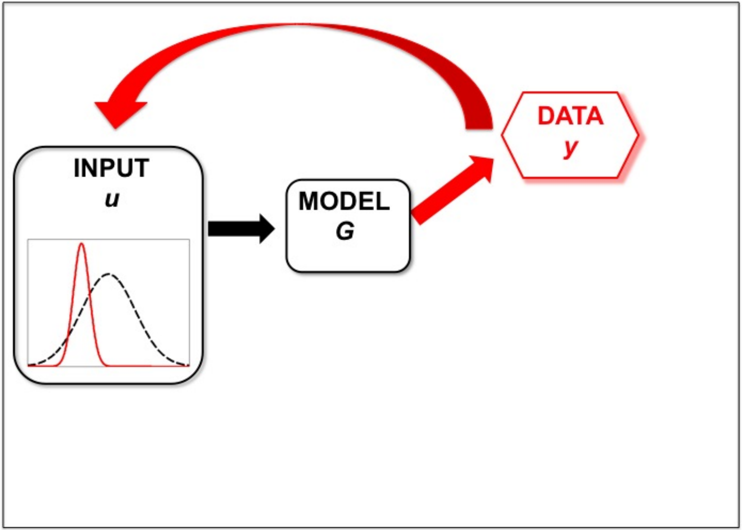
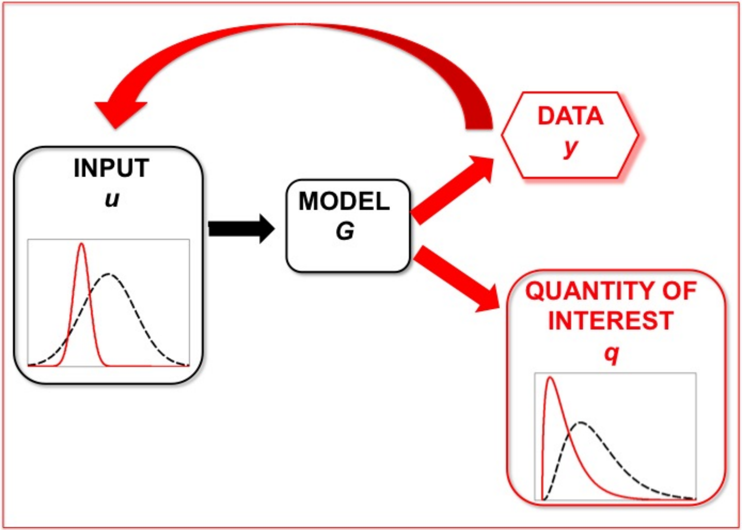
Uncertainty Quantification (UQ)



Bayesian Inverse Problem (BIP)



BIP and UQ



Deterministic Approach to Numerical Approximation of G

Assumption on Numerical Integrator

Approximate forward map G by a numerical method to obtain G^N:

$$\|G(u) - G^N(u)\| \le \psi(N) \to 0$$

as $N \to \infty$. Leads to approximate posterior measure μ^N in place of μ.

Theorem

For appropriate class of test functions $f : X \to S$:

$$\|\mathbb{E}^{\mu} f(u) - \mathbb{E}^{\mu^N} f(u)\|_S \le C\psi(N).$$

S.L. Cotter, M. Dashti and A. M . Stuart
Approximation of Bayesian Inverse Problems.
SINUM 2010 **48**(2010) 322–345.

Probabilistic Approach to Numerical Approximation of G

- Approximate G by a random map $G^{N,\omega}$.
- Ensure that: $\mathbb{E}\|G(u) - G^{N,\omega}(u)\| \le \psi(N)$.
- Vanilla UQ: infer scale parameter σ in $G^{N,\omega}(u)$.
- BIP UQ: augment unknown input parameters u by ω.

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Bayesian solution of ordinary differential equations
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Outline

Set-Up

Consider the ODE:

$$\frac{du}{dt} = f(u), \quad u(0) = u_0.$$

One-step numerical method

For $U_k \approx u(kh)$:

$$U_{k+1} = \Psi_h(U_k), \quad U_0 = u_0.$$

Randomized numerical method

For $U_k \approx u(kh)$:

$$U_{k+1} = \Psi_h(U_k) + \xi_k(h), \quad U_0 = u_0,$$

where $\xi_k(\cdot)$ is a Gaussian random field defined on $[0, h]$.

Derivation (Euler)

Integral equation

For $u_k = u(kh)$ and for $t \in [t_k, t_{k+1}]$:

$$\begin{aligned} u(t) &= u_k + \int_{t_k}^{t_{k+1}} f\big(u(s)\big)ds \\ &= u_k + \int_{t_k}^{t} g(s)ds. \end{aligned}$$

Uncertain g

We do not know $g(s)$. Assume that g is a Gaussian random field conditioned to satisfy $g(t_k) = f(U_k)$. This gives approximation $U(t)$ for $t \in [t_k, t_{k+1}]$:

$$\begin{aligned} U(t) &= U_k + (t - t_k)f(U_k) + \xi_k(t - t_k). \\ U_{k+1} &= U_k + hf(U_k) + \xi_k(h). \end{aligned}$$

Assumptions

Assumption 1 (Uncertain Approximation)

Let $\xi(t) := \int_0^t \chi(s)ds$ with $\chi \sim N(0, C^h)$. Then there exists $K > 0, p \geq 1$ such that, for all $t \in [0, h]$, $\mathbb{E}|\xi(t)\xi(t)^T|_{\mathrm{F}}^2 \leq Kt^{2p+1}$; in particular $\mathbb{E}|\xi(t)|^2 \leq Kt^{2p+1}$. Furthermore we assume the existence of matrix Q, independent of h, such that $\mathbb{E}\xi(h)\xi(h)^T = Qh^{2p+1}$.

Assumption 2 (Underlying Deterministic Integrator)

The function f and a sufficient number of its derivatives are bounded uniformly in $\mathbf{R}^n$ in order to ensure that f is globally Lipschitz and that the numerical flow-map Ψ_h has uniform local truncation error of order $q+1$ with respect to the true flow-map Φ_h:

$$\sup_{u \in \mathbf{R}^n} |\Psi_t(u) - \Phi_t(u)| \leq Kt^{q+1}.$$

Theorem

Theorem

Under Assumptions 1 and 2 it follows that there is $K > 0$ such that

$$\sup_{0 \le kh \le T} \mathbb{E}|u_k - U_k|^2 \le K h^{2\min\{p,q\}}.$$

Furthermore

$$\sup_{0 \le t \le T} \mathbb{E}|(u(t) - U(t)| \le K h^{\min\{p,q\}}.$$

Scaling of Noise

- Optimal scaling of noise is $p = q$.
- Then deterministic rate of convergence is unaffected.
- But maximal noise is added to the system.
- Fit constant σ in scale matrix $Q = \sigma I$ to an error estimator.

ODE Example

FitzHugh-Nagumo Model

We illustrate the randomized ODE solvers on the FitzHugh-Nagumo model two-species (V, R) non-linear oscillator, with parameters (a, b, c).

Governing Equations

$$\frac{dV}{dt} = c\left(V - \frac{V^3}{3} + R\right), \tag{1}$$

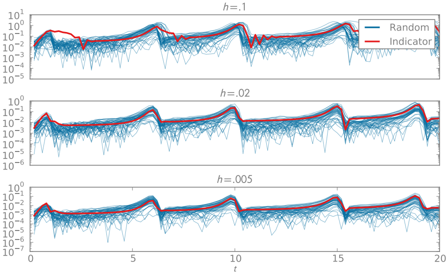
$$\frac{dR}{dt} = -\frac{1}{c}\left(V - a + bR\right). \tag{2}$$

Parameter Values

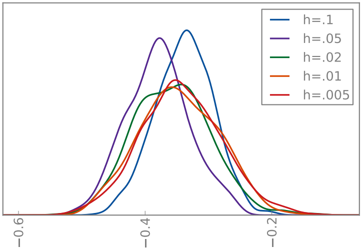
For numerical results, we choose fixed initial conditions $V(0) = -1, R(0) = 1$, and parameter values $(.2, .2, 3)$.

Derivation

Standard basis

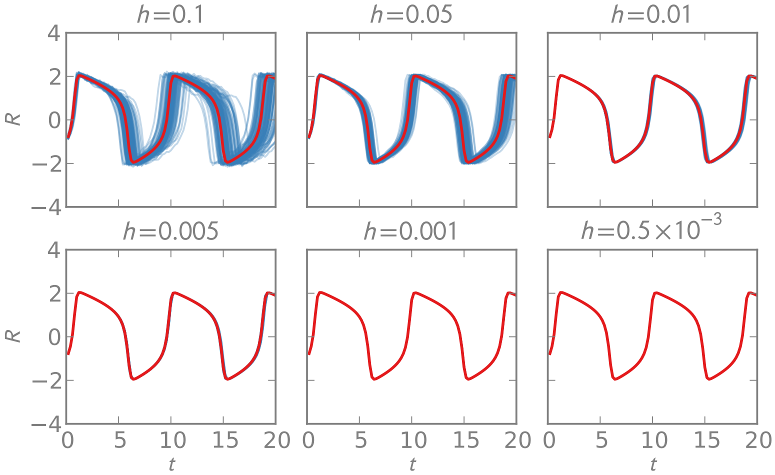


Randomized basis



Convergence of Random Solutions

Draws from the random solver for fixed σ



Backward Error Analysis

Modified (Stochastic Differential) Equation

$$\frac{du^h}{dt} = f(u^h) + h^q \sum_{l=0}^{q} h^\ell f_\ell(u^h) + \sqrt{Qh^{2q}}\frac{dW}{dt}, \quad u^h(0) = u_0$$

Theorem

Under Assumptions 1 and 2, for Φ a C^∞ function with all derivatives bounded uniformly on $\mathbf{R}^n$, there is a choice of $\{f_\ell\}_{\ell=0}^{q}$ such that weak error for true equation si given by

$$\Big|\Phi\big(u(T)\big) - \mathbb{E}\Phi\big(U_k\big)\Big| \leq Kh^q, \quad kh = T.$$

whilst weak error from the modified equation is given by

$$\Big|\mathbb{E}\Phi\big(u^h(T)\big) - \mathbb{E}\Phi\big(U_k\big)\Big| \leq Kh^{2q+1}, \quad kh = T.$$

Statistical Inference: find $\theta = (a, b, c)$ from noisy observations

Inverse Problem

$$y_j = u(t_j) + \eta_j, \quad y = \mathcal{G}(\theta) + \eta.$$

Deterministic Solver

Simply replace $u(\cdot)$ by deterministic approximation to obtain

$$y = \mathcal{G}^h(\theta) + \eta.$$

Use MCMC to compute $\mathbb{P}(\theta|y)$.

Randomized Solver

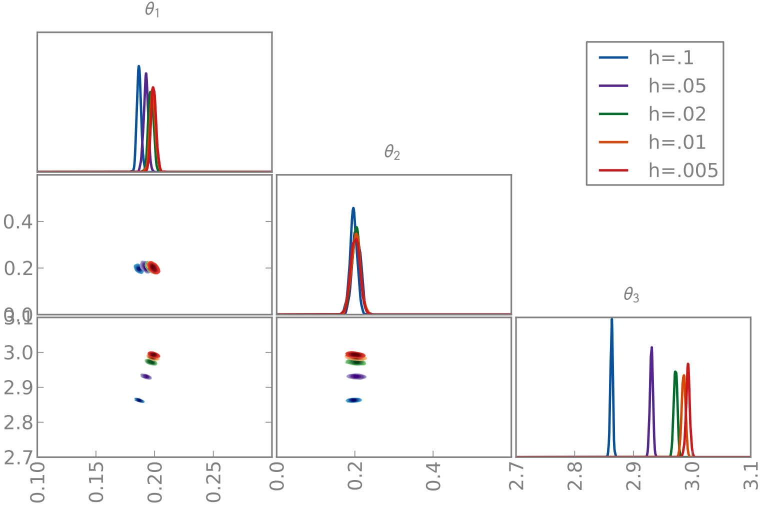
Replace $u(\cdot)$ by random approximation to obtain

$$y = \mathcal{G}^h(\theta, \xi) + \eta.$$

Use MCMC to compute $\int \mathbb{P}(\theta, \xi|y) d\xi$.

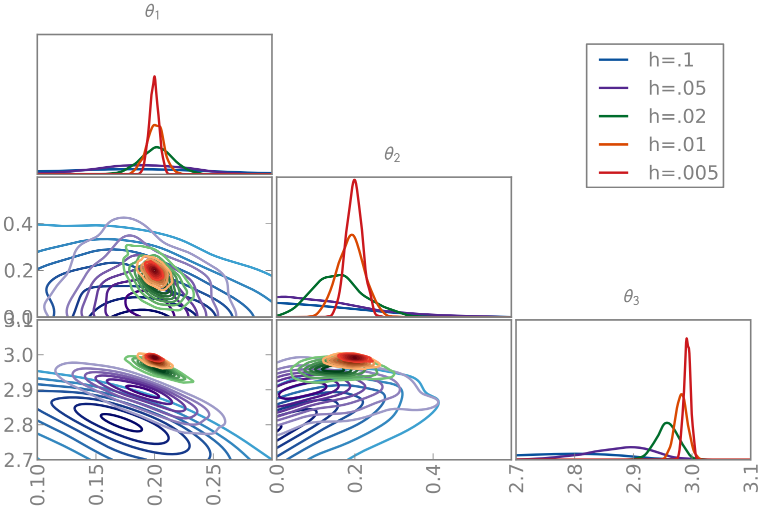
FitzHugh-Nagumo Parameter Posterior (Deterministic Solver)

Posterior is over-confident at finite *h* values



FitzHugh-Nagumo Parameter Posterior (Random Solver)

Posterior still contains bias, but posterior width reflects error



Outline

Set-Up

Weak Form

$$u \in \mathcal{V} : \; a(u, v) = r(v), \quad \forall v \in \mathcal{V}.$$

Galerkin Method

$$u^h \in \mathcal{V}^h : a(u^h, v) = r(v), \quad \forall v \in \mathcal{V}^h.$$

Then

$$\mathcal{V}^h = \mathrm{span}\{\Phi_j = \Phi_j^{\mathrm{s}}\}_{j=1}^{J}.$$

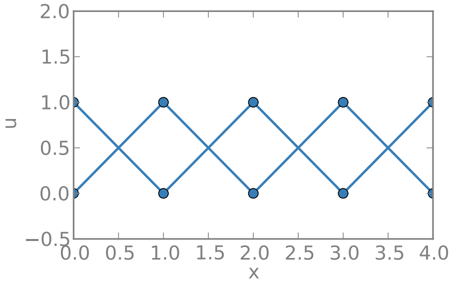
Randomized Galerkin Method

$\mathcal{V}^h$ comprises small randomized perturbations of the standard Galerkin method:

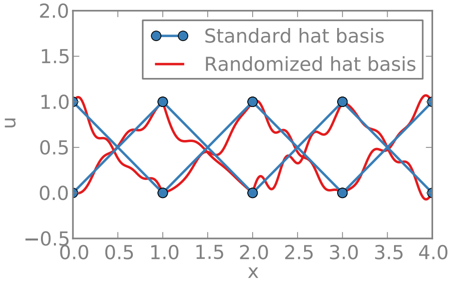
$$\mathcal{V}^h = \mathrm{span}\{\Phi_j = \Phi_j^{\mathrm{s}} + \Phi_j^{\mathrm{r}}\}_{j=1}^{J}.$$

Derivation

Standard basis



Randomized basis



Assumptions

Assumption 1 (Uncertain Approximation)

The $\{\Phi_j^{\mathrm{r}}\}_{j=1}^J$ are independent, mean zero, Gaussian random fields, with the same support as the $\{\Phi_j^{\mathrm{s}}\}$, and satisfying

$$\Phi_j^{\mathrm{r}}(x_k) = 0 \;\forall \{j,k\}, \quad \sum_{j=1}^{J} \mathbb{E}\|\Phi_j^{\mathrm{r}}\|_a^2 \le Ch^{2q}.$$

Assumption 2 (Underlying Deterministic FEM)

The true solution u is in $L^\infty(D)$. Furthermore the standard deterministic interpolant of the true solution, defined by

$$v^{\mathrm{s}} := \sum_{j=1}^{J} u(x_j)\Phi_j^{\mathrm{s}},$$

satisfies $\|u - v^{\mathrm{s}}\|_a \le Ch^p$.

Theorem

Theorem

Under Assumptions 1 and 2 it follows that the random approximation u^h satisfies

$$\mathbb{E}\|u - u^h\|_a^2 \le Ch^{2\min\{p,q\}}.$$

Corollary (Aubin-Nitsche Duality)

Consider the Poisson equation with Dirichlet boundary conditions and a random perturbation of the piecewise linear FEM approximation, with $p = q = 1$. Under Assumptions 1 and 2 it follows that the random approximation u^h satisfies

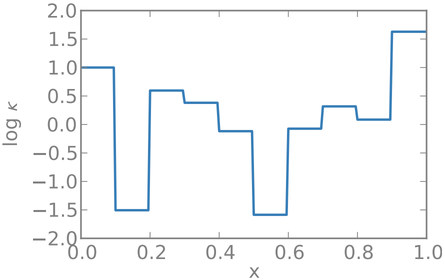
$$\mathbb{E}\|u - u^h\|_{L^2} \le Ch^2.$$

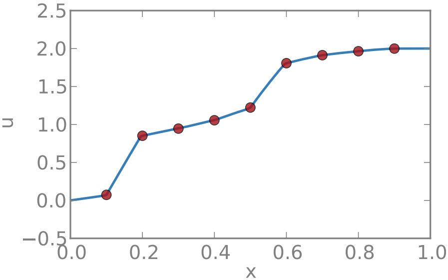
PDE Example

Standard elliptic inversion problem:

$$-\nabla \cdot (\kappa(x)\nabla u(x)) = -4x$$

$$u(0) = 0, u(1) = 2$$





$$\kappa(x) = \sum_{n=1}^{N} \theta_i \mathbb{I}_i(x).$$

Statistical Inference: find θ from noisy observations

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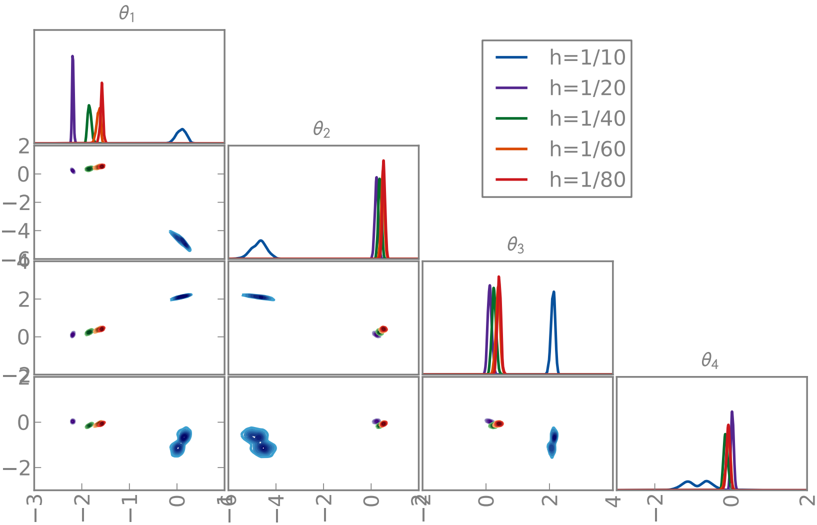
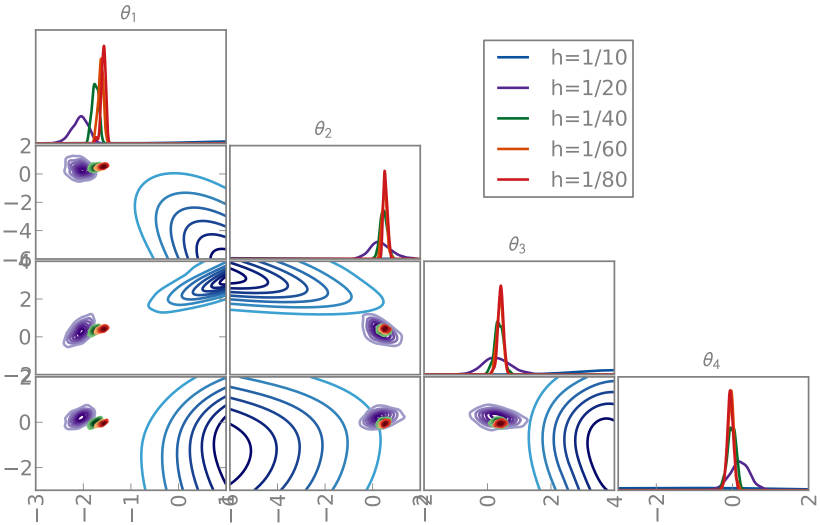
Use MCMC to compute $\int \mathbb{P}(\theta, \xi|y) d\xi$.

Elliptic Inference (Deterministic Solver)



Elliptic Inference (Random Solver)



Outline

Summary

- Numerical methods are inherently uncertain.
- Classical numerical anaysis upper bounds this uncertainty.
- Our approach treats it as a random variable.
- Mean square rates of convergence are derived, consistent with classical numerical analysis.
- Backward error analysis gives universal interpretation of the methods as solving stochastic or random problems.
- In forward modelling scale parameter is set using classical error indicators.
- In inverse modelling, the random parameters augment the unknown inputs.

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S.L. Cotter, M. Dashti and A. M . Stuart
Approximation of Bayesian Inverse Problems.
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