Probabilistic Numerical Methods for Deterministic Differential Equations

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Outline

1 Introduction

2 Ordinary Differential Equations

3 Elliptic PDE

4 Conclusions
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1 Introduction

2 Ordinary Differential Equations

3 Elliptic PDE

4 Conclusions
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 $G^N$:

\[ \| G(u) - G^N(u) \| \leq \psi(N) \to 0 \]

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

**Theorem**

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

\[ \| \mathbb{E}^\mu f(u) - \mathbb{E}^{\mu^N} f(u) \|_S \leq C\psi(N). \]

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S.L. Cotter, M. Dashti and A. M. Stuart
Approximation of Bayesian Inverse Problems.
Approximate $G$ by a random map $G^{N,\omega}$.
Ensure that: $\mathbb{E}\|G(u) - G^{N,\omega}(u)\| \leq \psi(N)$.
Vanilla UQ: infer scale parameter $\sigma$ in $G^{N,\omega}(u)$.
BIP UQ: augment unknown input parameters $u$ by $\omega$.

J. Skilling
Bayesian solution of ordinary differential equations

O.A. Chkrebtii, D.A. Campbell, M.A. Girolami, B. Calderhead
Bayesian uncertainty quantification for differential equations
*arxiv.1306.2365*

M. Schober, D.K. Duvenaud and P. Hennig
Probabilistic ODE solvers with Runge- Kutta means

P. Conrad, M. Girolami, S. Sarkka, A.M. Stuart and K. Zygalakis
*arxiv.1506.04592.*
Outline

1. Introduction

2. Ordinary Differential Equations

3. Elliptic PDE

4. Conclusions
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 $t \in [t_k, t_{k+1}]$:

$$u(t) = u_k + \int_{t_k}^{t_{k+1}} f(u(s)) \, ds$$

$$= u_k + \int_{t_k}^{t} g(s) \, ds.$$

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 $t \in [t_k, t_{k+1}]$:

$$U(t) = U_k + (t - t_k)f(U_k) + \xi_k(t - t_k).$$

$$U_{k+1} = U_k + hf(U_k) + \xi_k(h).$$
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 $t \in [0, h]$, $\mathbb{E}|\xi(t)\xi(t)^T|^2 \leq Kt^{2p+1}$; 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 $\mathbb{R}^n$ in order to ensure that $f$ is globally Lipschitz and that the numerical flow-map $\Psi_h$ has uniform local truncation error of order $q + 1$ with respect to the true flow-map $\Phi_h$:

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

Under Assumptions 1 and 2 it follows that there is \( K > 0 \) such that

\[
\sup_{0 \leq kh \leq T} \mathbb{E} |u_k - U_k|^2 \leq Kh^{2 \min\{p, q\}}.
\]

Furthermore

\[
\sup_{0 \leq t \leq T} \mathbb{E} |(u(t) - U(t))| \leq Kh^{\min\{p, q\}}.
\]

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 \( \sigma \) 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

\[
\begin{align*}
\frac{dV}{dt} &= c \left( V - \frac{V^3}{3} + R \right), \\
\frac{dR}{dt} &= -\frac{1}{c} \left( V - a + bR \right).
\end{align*}
\]

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

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Convergence of Random Solutions
Draws from the random solver for fixed $\sigma$

![Graphs showing convergence of random solutions](image)
Backward Error Analysis

Modified (Stochastic Differential) Equation

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

Theorem

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

\[
\left| \Phi(u(T)) - \mathbb{E}\Phi(U_k) \right| \leq K h^q, \quad kh = T.
\]

whilst weak error from the modified equation is given by

\[
\left| \mathbb{E}\Phi(u^h(T)) - \mathbb{E}\Phi(U_k) \right| \leq K h^{2q+1}, \quad kh = T.
\]
**Statistical Inference:** find $\theta = (a, b, c)$ from noisy observations

### Inverse Problem

\[
y_j = u(t_j) + \eta_j, \quad y = G(\theta) + \eta.
\]

### Deterministic Solver

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

\[
y = G^h(\theta) + \eta.
\]

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

### Randomized Solver

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

\[
y = G^h(\theta, \xi) + \eta.
\]

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

\[ \mathcal{V}^h = \text{span}\{\Phi_j = \Phi_j^s\}_{j=1}^J \]

**Randomized Galerkin Method**

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

\[ \mathcal{V}^h = \text{span}\{\Phi_j = \Phi_j^s + \Phi_j^r\}_{j=1}^J \]
Derivation

Standard basis

Randomized basis

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Assumptions

Assumption 1 (Uncertain Approximation)

The $\{\Phi^r_j\}_{j=1}^J$ are independent, mean zero, Gaussian random fields, with the same support as the $\{\Phi^s_j\}$, and satisfying

$$\Phi^r_j(x_k) = 0 \forall \{j, k\}, \quad \sum_{j=1}^J \mathbb{E} \|\Phi^r_j\|_a^2 \leq Ch^{2q}.$$ 

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

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

satisfies $\|u - v^s\|_a \leq Ch^p$. 
Theorem

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

\[
\mathbb{E}\| u - u^h \|^2_a \leq Ch^2 \min\{p,q\}.
\]

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

\[
\mathbb{E}\| u - u^h \|_{L^2} \leq Ch^2.
\]
PDE Example

Standard elliptic inversion problem:

\[-\nabla \cdot (\kappa(x) \nabla u(x)) = -4x\]

\[u(0) = 0, \ u(1) = 2\]

\[\kappa(x) = \sum_{n=1}^{N} \theta_i \Pi_i(x).\]
Statistical Inference: find $\theta$ 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 $\int \mathbb{P}(\theta, \xi|y) d\xi$. 

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Elliptic Inference (Deterministic Solver)

$\theta_1$

$\theta_2$

$\theta_3$

$\theta_4$

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Elliptic Inference (Random Solver)

$\theta_1$

$\theta_2$

$\theta_3$

$\theta_4$

- $h = 1/10$
- $h = 1/20$
- $h = 1/40$
- $h = 1/60$
- $h = 1/80$

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Numerical methods are inherently uncertain.

Classical numerical analysis 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.
P. Diaconis
Bayesian numerical analysis.

M. Dashti and A.M. Stuart
The Bayesian approach to inverse problems.
Handbook of Uncertainty Quantification
arXiv:1302.6989

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

P. Conrad, M. Girolami, S. Sarkka, A.M. Stuart and K. Zygalakis
arxiv.1506.04592.