Random time steps geometric integrators of ordinary differential equations for uncertainty quantification of numerical errors

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Outline

Probabilistic methods – why?

Consider Lorenz equation (atmospheric convection)

$$\begin{aligned} x' &= \sigma(y - x), && x(0) = -10, \\ y' &= x(\rho - z) - y, && y(0) = -1, \\ z' &= xy - \beta z, && z(0) = 40. \end{aligned}$$

For $\rho = 28$, $\sigma = 10$, $\beta = 8/3$ chaotic behaviour.

$\Longrightarrow$ Numerical integration gives unreliable solutions.

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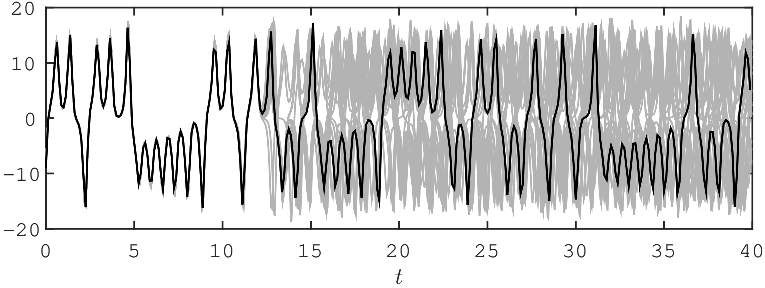
Goal

Establish a probability measure over the numerical solution given by classical methods.

Probabilistic methods – why?



Time evolution of the first component of Lorenz equation

Black line $\rightarrow$ deterministic solution

Gray lines $\rightarrow$ family of perturbed solutions.

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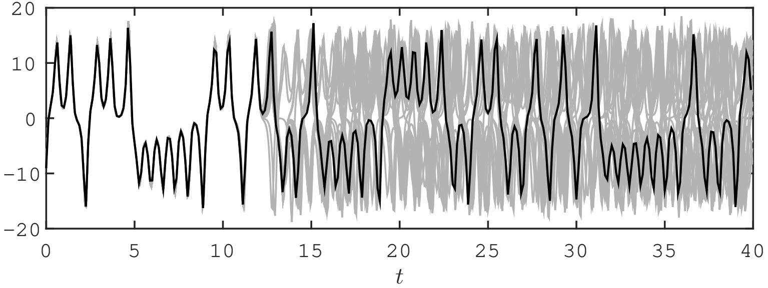

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Chaotic behaviour appears frequently in nonlinear differential equations.

Notation

Autonomous dynamical system, function $f\colon \mathbb{R}^d \to \mathbb{R}^d$ and the ODE

$$y' = f(y), \quad y(0) = y_0.$$

Flow of the equation $\varphi_t\colon \mathbb{R}^d \to \mathbb{R}^d$ such that

$$y(t) = \varphi_t(y_0).$$

One-step method (e.g. Runge Kutta): numerical flow Ψ_h such that

$$y_{n+1} = \Psi_h(y_n).$$

Probabilistic methods for ODEs

Filtering methods for ODEs: fix a prior on $y(t)$ (Gaussian process), update with evaluations of $f(y)$
[Kersting and Hennig, 2016, Chkrebtii et al., 2016]

Randomised methods for ODEs: random perturbation of deterministic numerical solutions $\rightarrow$ sampling

- Additive noise [Conrad et al., 2016],
- Random time steps [Abdulle and Garegnani, 2018].

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Additive noise method

Stochastic process $\{Y_n\}_{n=1,2,\ldots}$ with recurrence

$$Y_{n+1} = \underbrace{\Psi_h(Y_n)}_{\text{deterministic}} + \underbrace{\xi_n(h)}_{\text{random}}.$$

Main assumption: $\{\xi_n\}_{n=0,1,\ldots}$ iid such that for $p > 1$ and $Q \in \mathbb{R}^{d\times d}$

$$\mathbb{E}\,\xi_n(h) = 0, \quad \mathbb{E}\,\xi_n(h)\xi_n(h)^T = Qh^{2p+1}.$$

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Properties

If Ψ_h is of order q and for $\Phi\colon \mathbb{R}^d \to \mathbb{R}$ smooth

- Strong convergence: $\mathbb{E}\|y(hn) - Y_n\| \leq Ch^{\min\{p,q\}}$,
- Weak convergence: $|\Phi\big(y(hn)\big) - \mathbb{E}\,\Phi(Y_n)| \leq Ch^{\min\{2p,q\}}$,
- Good qualitative behavior in Bayesian inverse problems.

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Issues

- Robustness: $\Psi_h(Y_{n-1}) > 0 \;\not\Rightarrow\; \mathbb{P}(Y_n < 0) = 0$,
- Geometric properties are not conserved from Ψ_h. For example if $I(y) = y^T S y$ and $I(\Psi_h(y_0)) = I(y_0)$

$$I(Y_1) = I(y_0) + 2\xi_0(h)^T S \Psi_h(y_0) + \xi_0(h)^T S \xi_0(h).$$

Random time steps

Intrinsic noise: Random time-stepping Runge-Kutta (RTS-RK)

$$Y_{n+1} = \Psi_{H_n}(Y_n),$$

Main assumption: $\{H_n\}_{n=0,1,\dots}$ iid such that for $h, C > 0$ and $p > 1$

$$H_n > 0 \text{ a.s.}, \quad \mathbb{E}\, H_n = h, \quad \operatorname{Var} H_n = Ch^{2p}.$$

Example: $H_n \overset{\text{iid}}{\sim} \mathcal{U}(h - h^p, h + h^p)$.

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Properties (Geometric)

- Conservation of (polynomial) first integrals is inherited by Ψ_h,
- Flow map is symplectic if Ψ_h is symplectic,
- Long-time conservation of energy in Hamiltonian systems.

Numerical experiment – Geometric properties

Consider the perturbed Kepler equation (model for two-body problem)

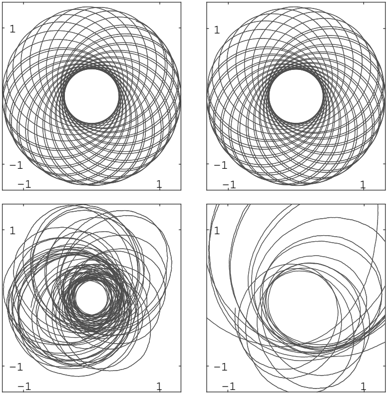
$$q_1' = p_1, \quad p_1' = -\frac{q_1}{\|q\|^3} - \frac{\delta q_1}{\|q\|^5},$$
$$q_2' = p_2, \quad p_2' = -\frac{q_2}{\|q\|^3} - \frac{\delta q_2}{\|q\|^5}.$$

The angular momentum is conserved (quadratic first integral)

$$I(p, q) = q_1 p_2 - q_2 p_1$$

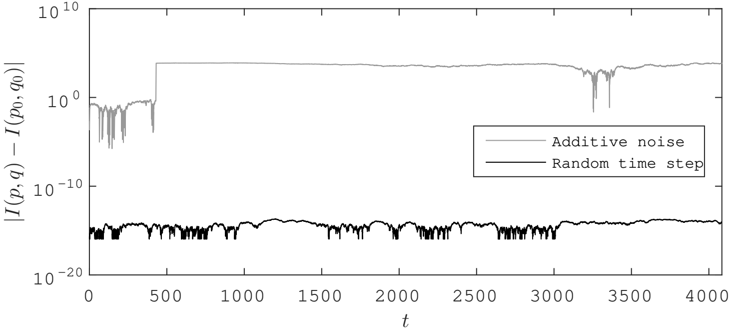
$\rightarrow$ employ a Gauss method (implicit midpoint rule).

Numerical experiment – Geometric properties



RTS-RK (first row), Additive noise (second row). Time $0 \leq t \leq 200$ and $200 \leq t \leq 400$ (left and right)

Numerical experiment – Geometric properties



Conservation of the angular momentum (quadratic first integral)

Bayesian inverse problems

Goal

Given $\vartheta \in \mathbb{R}^n$, $f_\vartheta \colon \mathbb{R}^d \to \mathbb{R}^d$ and the ODE

$$y' = f_\vartheta(y), \quad y(0) = y_{0,\vartheta} \in \mathbb{R}^d,$$

retrieve the true value ϑ^* from observations of $y(t)$, $t > 0$.

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Bayesian setting: fix prior $\pi_{\mathrm{prior}}(\vartheta)$, consider the forward operator $\mathcal{G}$ and model observations as

$$\underbrace{\mathcal{Y}}_{\text{observations}} = \underbrace{\mathcal{G}(\vartheta^*)}_{\text{forward}} + \underbrace{\varepsilon}_{\text{noise}}, \quad \varepsilon \sim \pi_{\mathrm{noise}},$$

then the posterior distribution (density) is

$$\pi(\vartheta \mid \mathcal{Y}) \propto \pi_{\mathrm{prior}}(\vartheta)\pi_{\mathrm{noise}}(\mathcal{Y} - \mathcal{G}(\vartheta)).$$

Bayesian inverse problems

The posterior $\pi(\vartheta \mid \mathcal{Y})$ is not computable, approximate with

$$\pi^h(\vartheta \mid \mathcal{Y}) \propto \pi_{\mathrm{prior}}(\vartheta)\pi_{\mathrm{noise}}(\mathcal{Y} - \mathcal{G}^h(\vartheta)).$$

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Properties

$\pi^h \to \pi$ for $h \to 0$ (in the Hellinger distance).

Issue

- π^h concentrated around values "far" from $\vartheta^* \to$ non-predictive posterior

Bayesian inverse problems

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$$\pi^{\boldsymbol{h},\mathrm{RTS}}(\vartheta \mid \mathcal{Y}) \propto \pi_{\mathrm{prior}}(\vartheta)\mathbb{E}^{\mathbf{H}}\pi_{\mathrm{noise}}(\mathcal{Y} - \mathcal{G}^{\mathbf{H}}(\vartheta)),$$

where $\mathbf{H} = (H_0, H_1, \dots)$ is the vector of all time steps chosen in one run.

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Properties

- $\pi^{h,\mathrm{RTS}} \to \pi$ for $h \to 0$ (in the Hellinger distance). [Lie et al., 2017]
- "correct" the non-predictive behaviour of deterministic approximations

Warning

- Approximation of $\mathbb{E}^{\mathbf{H}}\,\pi_{\mathrm{noise}}(\mathcal{Y} - \mathcal{G}^{\mathbf{H}}(\vartheta))$ is required

Numerical experiment – Bayesian inverse problems

Consider the Hénon-Heiles system (motion of a star around a galactic center), Hamiltonian with energy

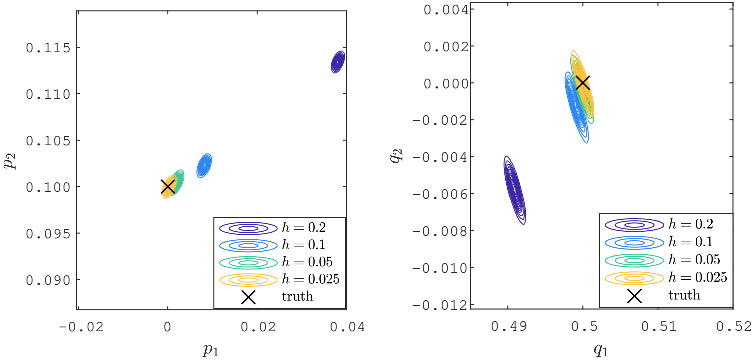
$$E(p, q) = \frac{1}{2}\|p\|^2 + \frac{1}{2}\|q\|^2 + q_1^2 q_2 - \frac{1}{3} q_2^3.$$

Chaotic problem for certain levels of energy.

Goal

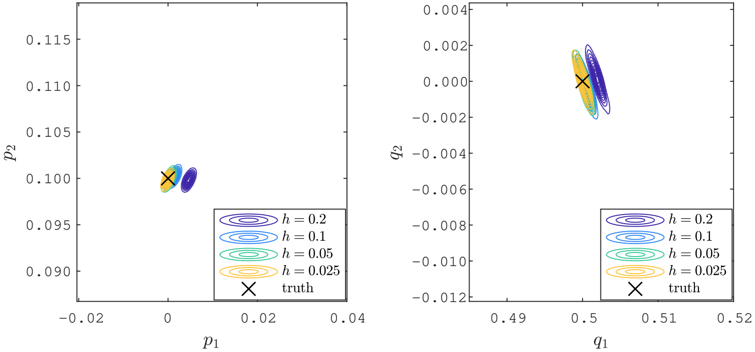
Find posterior $\pi((p_0, q_0) \mid \mathcal{Y})$ over the initial condition from a single observation of $(p(10), q(10))$

Numerical experiment – Bayesian inverse problems



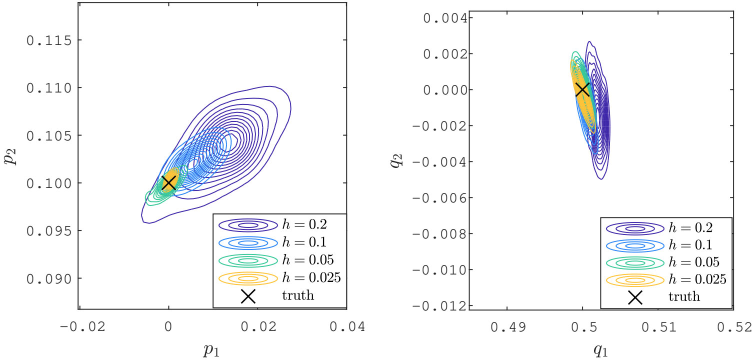
Posterior distributions given by deterministic Heun method.

Numerical experiment – Bayesian inverse problems



Posterior distributions given by deterministic Störmer-Verlet method.

Numerical experiment – Bayesian inverse problems



Posterior distributions given by RTS-RK Störmer-Verlet method.

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