Probabilistic Runge-Kutta methods for ODEs

Chaotic problems and geometric properties

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Motivation

Example

Lorenz system ($\sigma = 10$, $\rho = 28$, $\beta = 8/3$)

$$\begin{aligned} y_1' &= \sigma(y_2 - y_1), & y_1(0) &= -10, \\ y_2' &= y_1(\rho - y_3) - y_2, & y_2(0) &= -1, \\ y_3' &= y_1 y_2 - \beta y_3, & y_3(0) &= 40. \end{aligned} \tag{1}$$

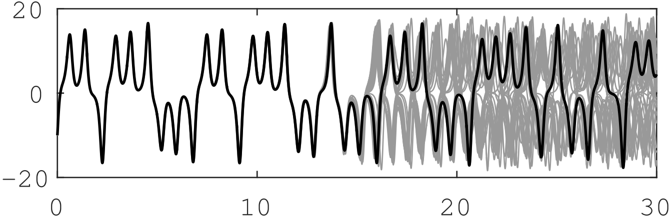

Figure: Deterministic (black) and probabilistic (grey) numerical solutions of (1)

Problem statement

Consider $f: \mathbb{R}^d \to \mathbb{R}$ and the ODE

$$y' = f(y), \quad y(0) = y_0. \tag{2}$$

Flow of the equation φ_t: for any $y_0 \in \mathbb{R}^d$

$$y(t) = \varphi_t(y_0). \tag{3}$$

One-step Runge-Kutta method: numerical flow Ψ_h such that

$$y_{n+1} = \Psi_h(y_n). \tag{4}$$

Problem

Modify (4) in order to give a probabilistic numerical solution.

Existing method

Additive noise [Conrad et al., 2016]. Build stochastic process $\{Y_n\}_{n=1,2,\dots}$

$$Y_{n+1} = \underbrace{\Psi_h(Y_n)}_{\text{deterministic}} + \underbrace{\xi_n(h)}_{\text{random}}, \tag{5}$$

where $\{\xi_n\}_{n=1,2,\dots}$ i.i.d. random variables s.t. for $p > 1$ and $Q \in \mathbb{R}^{d\times d}$

$$\mathbb{E}\,\xi_n(h) = 0, \quad \mathbb{E}\,\xi_n(h)\xi_n(h)^T = Qh^{2p+1}. \tag{6}$$

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

$$I(Y_1) = I(y_0) + 2\xi_0(h)^T S\Psi_h(y_0) + \xi_0(h)^T S\xi_0(h). \tag{7}$$

Method proposal

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

$$Y_{n+1} = \Psi_{H_n}(Y_n), \tag{8}$$

where $\{H_n\}_{n=1,2,\dots}$ i.i.d. random variables s.t. for $h, C > 0$ and $p > 1$

$$H_n > 0 \text{ a.s.}, \quad \mathbb{E}\, H_n = h, \quad \operatorname{Var} H_n = Ch^{2p}. \tag{9}$$

For example $H_n \overset{\text{i.i.d.}}{\sim} \mathcal{U}(h - h^p, h + h^p)$ is a suitable choice.

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- Strong and weak convergence equivalent to additive noise method,
- Good qualitative behavior in Bayesian inverse problems,
- If Ψ_h conserves an invariant $I(y)$, then so do RTS-RK,
- Simplecticity is guaranteed for Ψ_h symplectic.

Numerical example

Hénon-Heiles problem [Hénon and Heiles, 1964]. Hamiltonian function $(p, q \in \mathbb{R}^2)$

$$H(p,q) = \frac{1}{2}\|p\|^2 + \frac{1}{2}\|q\|^2 + q_1^2 q_2 - \frac{1}{3}q_2^3, \tag{10}$$

Corresponding system of ODEs

$$\begin{aligned} p' &= -\nabla_q H(p,q), \quad & p(0) = p_0 \in \mathbb{R}^2, \\ q' &= \nabla_p H(p,q), \quad & q(0) = q_0 \in \mathbb{R}^2. \end{aligned} \tag{11}$$

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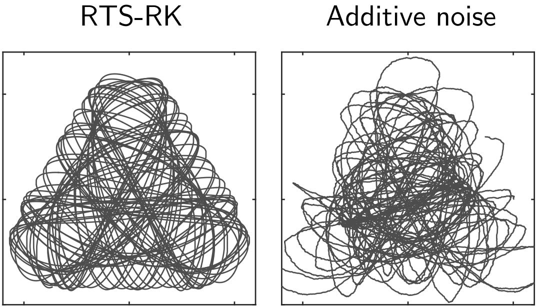
Problem properties [Hairer et al., 2006]

- Chaotic regime for $H(p,q) > 1/8$,
- Hamiltonian is conserved $\implies$ use symplectic integrator.

Numerical results



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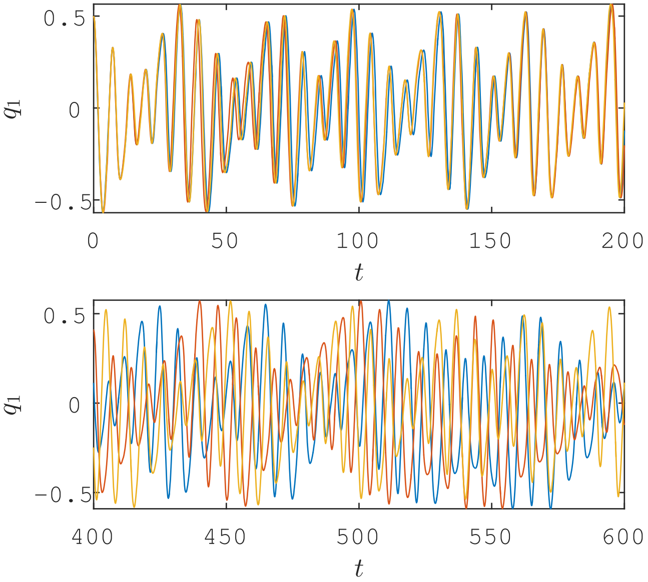

References I

[Conrad et al., 2016] Conrad, P. R., Girolami, M., Särkkä, S., Stuart, A., and Zygalakis, K. (2016).
Statistical analysis of differential equations: introducing probability measures on numerical solutions.
Stat. Comput.

[Hairer et al., 2006] Hairer, E., Lubich, C., and Wanner, G. (2006).
Geometric Numerical Integration. Structure-Preserving Algorithms for Ordinary Differential Equations.
Springer Series in Computational Mathematics 31. Springer-Verlag, Berlin, second edition.

[Hénon and Heiles, 1964] Hénon, M. and Heiles, C. (1964).
The applicability of the third integral of motion: Some numerical experiments.
Astronom. J., 69:73–79.