Probabilistic Runge-Kutta methods for uncertainty quantification of numerical errors in geometric integration

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Outline

Motivation – Chaotic equations

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.

$\implies$ Numerical integration gives unreliable solutions.

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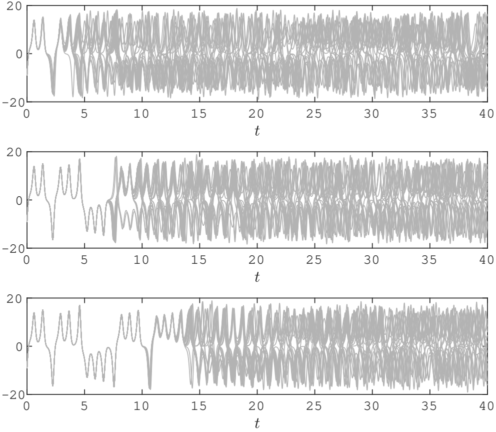
$\implies$ Numerical integration gives unreliable solutions.

Goal: Understand reliability of numerical solutions.
Idea: Perturb the initial data e.g. with Gaussian noise on $x(0)$

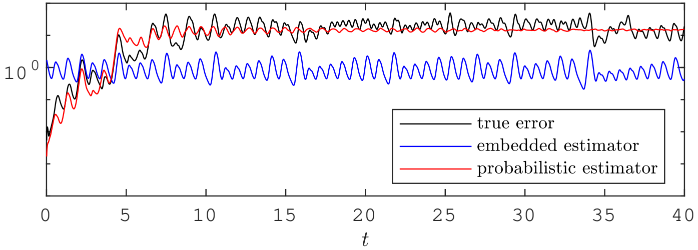
Motivation – Chaotic equations



Solutions of the Lorenz system (x component) – different perturbations

Which one has the correct magnitude wrt numerical error?

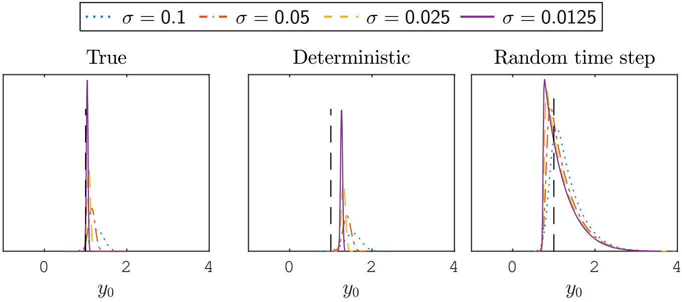
Motivation – Error estimators



Error estimators for Lorenz given by
Probabilistic solution: use $\|\mathrm{Var}\, Y_n\|^{1/2}$ where Y_n is a probabilistic family
Classical embedded couple: Local errors don't show the true behaviour!

Goal: A posteriori error estimator $\mathrm{err}_n \approx \|\mathrm{Var}\, Y_n\|^{1/2} \rightsquigarrow$ Work in progress!

Motivation – Bayesian inverse problems



Posterior distributions (analytic) on y_0 for $y' = -y$, $y(0) = y_0$. One observation corrupted by noise $\mathcal{N}(0, \sigma^2)$ with truth y_0^*.

For $\sigma \to 0$:

- True solution: Posterior converging to $\delta_{y_0^*}$ $\to$ good
- Runge-Kutta: Posterior converging to Dirac delta on wrong value $\to$ bad
- Probabilistic method: Posterior variance $\approx$ numerical error

Outline

Notation

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

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

Flow of the equation φ_t

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

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

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

Geometric numerical integration

Goal

Develop numerical methods that preserve geometric properties of certain dynamical systems.

First integral of motion $I \colon \mathbb{R}^d \to \mathbb{R}$

$$I(\varphi_t(y_0)) = I(y_0), \quad \forall t > 0.$$

Example: quadratic first integral, given $S \in \mathbb{R}^{d \times d}$, $v \in \mathbb{R}^d$

$$I(y) = y^\top S y + v^\top y,$$

conserved by all Gauss collocation methods (e.g., implicit midpoint, ...).

Theorem (Polynomial first integrals)

No Runge-Kutta method can conserve all polynomial first integrals of degree $\mathrm{Deg}(I) \geq 3$.

Geometric numerical integration

Goal

Develop numerical methods that preserve geometric properties of certain dynamical systems.

Hamiltonian systems: Given $Q\colon \mathbb{R}^{2d} \to \mathbb{R}$, define

$$y'(t) = J^{-1}\nabla Q(y), \qquad y(0) = y_0$$

$$J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}, \qquad I \text{ identity in } \mathbb{R}^{d\times d}$$

The flow φ_t is symplectic

$$\varphi_t'(y)^\top J \varphi_t'(y) = J \implies \text{Conservation of volumes}$$

Symplectic numerical methods

$$\Psi_h'(y)^\top J \Psi_h'(y) = J$$

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Theorem

For a symplectic integrator of order q, there exist $C, \kappa > 0$, independent of h such that

$$\mathbb{E}|Q(y_n) - Q(y_0)| \leq C_1 h^q,$$

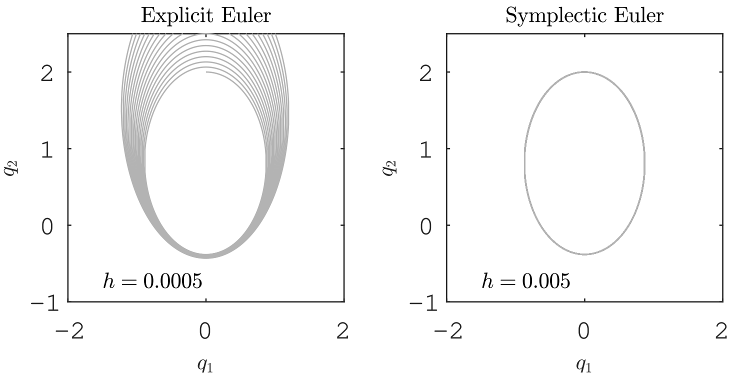
for time intervals of length $nh = \mathcal{O}(e^{\kappa/h})$.

Geometric numerical integration

Example

Two-body problem (planetary orbits), $y = (p, q)^\top \in \mathbb{R}^4$

$$Q(p, q) = \frac{1}{2}(p_1^2 + p_2^2) - \frac{1}{\sqrt{q_1^2 + q_2^2}}$$



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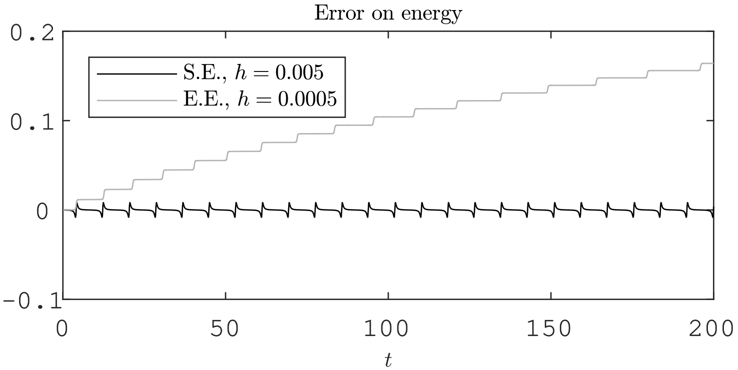

Geometric numerical integration

Given Hamiltonian $Q(p, q)$.

Symplectic Euler method – order 1

$$\begin{aligned} p_{n+1} &= p_n - hQ_q(p_{n+1}, q_n), \\ q_{n+1} &= q_n + hQ_p(p_{n+1}, q_n). \end{aligned}$$

Störmer-Verlet scheme – order 2

$$\begin{aligned} p_{n+1/2} &= p_n - \frac{h}{2} Q_q(p_{n+1/2}, q_n), \\ q_{n+1} &= q_n + \frac{h}{2}\big(Q_p(p_{n+1/2}, q_n) + Q_p(p_{n+1/2}, q_{n+1})\big), \\ p_{n+1} &= p_n - \frac{h}{2} Q_q(p_{n+1/2}, q_{n+1}). \end{aligned}$$

Geometric numerical integration

Given separable Hamiltonian $Q(p,q) = Q_1(p) + Q_2(q)$.

Symplectic Euler method – order 1, explicit

$$
\begin{aligned}
p_{n+1} &= p_n - hQ_2'(q_n), \\
q_{n+1} &= q_n + hQ_1'(p_{n+1}).
\end{aligned}
$$

Störmer-Verlet scheme – order 2, explicit

$$
\begin{aligned}
p_{n+1/2} &= p_n - \frac{h}{2}Q_2'(q_n), \\
q_{n+1} &= q_n + hQ_1'(p_{n+1/2}), \\
p_{n+1} &= p_n - \frac{h}{2}Q_2'(q_{n+1}).
\end{aligned}
$$

Several examples of separable Hamiltonians (Two-body problem, ...)

Outline

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); Kersting et al. (2018)
- Chkrebtii et al. (2016)
- Schober et al. (2014, 2018)
- ...

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

- Conrad et al. (2016)
- Lie et al. (2017)
- Abdulle and Garegnani (2018)
- ...

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: For $p > 1$ and $Q \in \mathbb{R}^{d \times d}$

$$\xi_n(h) \overset{\text{iid}}{\sim} \mathcal{N}(0, Qh^{2p+1}).$$

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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.

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 $p > 1$

$$H_n > 0 \text{ a.s.}, \quad \mathbb{E}\, H_n = h, \quad \operatorname{Var} H_n = Ch^{2p+1}.$$

Example: $H_n \overset{\text{iid}}{\sim} \mathcal{U}(h - h^{p+1/2}, h + h^{p+1/2})$.

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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.

Conservation of first integrals – Additive noise

Recall: $Y_{n+1} = \Psi_h(Y_n) + \xi_n(h)$, with $\mathbb{E}\,\xi_n(h)\xi_n(h)^\top = h^{2p+1}Q$

Linear first integrals: $I(y) = v^\top y$ such that $I(\Psi_h(Y_1)) = I(y_0)$. Then

$$I(Y_1) = v^\top(y_0 + \xi_0(h)) \implies \mathbb{E}\,I(Y_1) = I(y_0) \text{ iff } \mathbb{E}\,\xi_0(h) = 0.$$

Quadratic first integrals: $I(y) = y^\top Sy$ such that $I(\Psi_h(Y_1)) = I(y_0)$. Then

$$\begin{aligned} I(Y_1) &= I(y_0) + 2\xi_0(h)^T S\Psi_h(y_0) + \xi_0(h)^T S\xi_0(h), \\ \implies \mathbb{E}\,I(Y_1) &= I(y_0) + Q : Sh^{2p+1}, \quad (\text{with } \mathbb{E}\,\xi_0(h) = 0) \end{aligned}$$

Quadratic first integrals are not conserved on average!

Conservation of first integrals

Theorem (Conservation of invariants)

If the Runge-Kutta scheme defined by Ψ_h conserves an invariant $I(y)$ for an ODE, then the RTS-RK method conserves $I(y)$ for the same ODE.

Proof

If $I(\Psi_h(y)) = I(y)$ for any h, then $I(\Psi_{H_0}(y)) = I(y)$ for any value that H_0 can assume.

Symplecticity

Energy $Q\colon \mathbb{R}^{2d} \to \mathbb{R}$ and Hamiltonian system

$$y' = J^{-1}\nabla Q(y), \quad J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}.$$

Symplectic integrator Ψ_h of order q.

Theorem (Strong approximation of the Hamiltonian)

There exist positive constants κ, C_1, C_2, C_3, independent of h such that

$$\mathbb{E}|Q(Y_n) - Q(y_0)| \leq C_1 h^q,$$

for time intervals of length $\mathcal{O}(h^{1-2p})$.

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Idea of the proof

Use classical backward error analysis. Considering that $\mathbb{E}\, H_k = h$, we have at "first order" the same conservation as deterministic methods. The time interval reduction comes from the time steps' variance.

Numerical experiments – Geometric properties

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

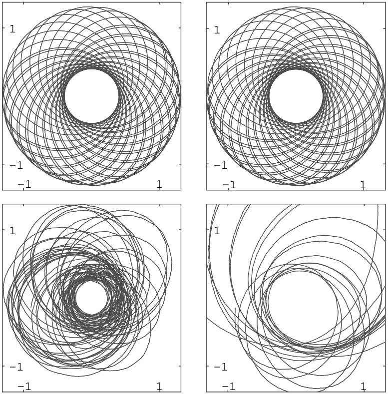
$$w_1' = v_1, \quad v_1' = -\frac{w_1}{\|w\|^3} - \frac{\delta w_1}{\|w\|^5},$$
$$w_2' = v_2, \quad v_2' = -\frac{w_2}{\|w\|^3} - \frac{\delta w_2}{\|w\|^5}.$$

The angular momentum is conserved (quadratic first integral)

$$I(v, w) = w_1 v_2 - w_2 v_1$$

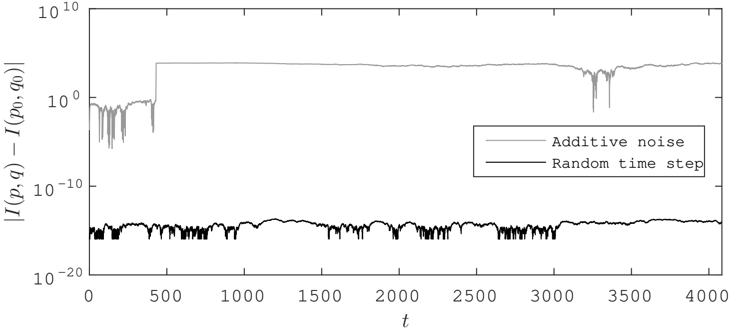
$\rightarrow$ employ a Gauss method (implicit midpoint rule).

Numerical experiments – 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 experiments – Geometric properties



Conservation of the angular momentum (quadratic first integral)

Numerical experiments – Geometric properties

Consider the pendulum system, Hamiltonian with energy

$$Q(v, w) = \frac{1}{2}v^2 - \cos(w).$$

Energy is separable: $Q(v, w) = Q_1(v) + Q_2(w)$.

Störmer-Verlet scheme – order 2

$$\begin{aligned} v_{n+1/2} &= v_n - \frac{h}{2} Q_w(v_{n+1/2}, w_n), \\ w_{n+1} &= w_n + \frac{h}{2}\big(Q_v(v_{n+1/2}, w_n) + Q_v(v_{n+1/2}, w_{n+1})\big), \\ v_{n+1} &= v_n - \frac{h}{2} Q_w(v_{n+1/2}, w_{n+1}). \end{aligned}$$

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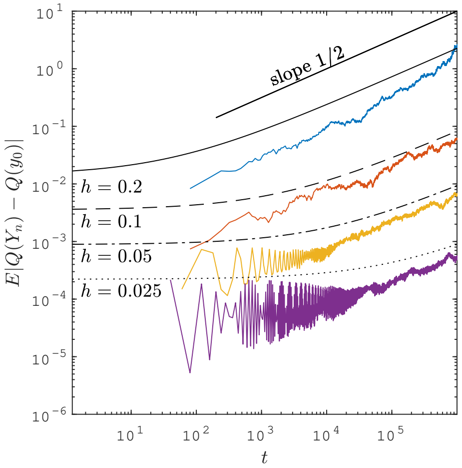
Störmer-Verlet scheme – order 2, explicit

$$\begin{aligned} v_{n+1/2} &= v_n - \frac{h}{2} Q_2'(w_n), \\ w_{n+1} &= w_n + h Q_1'(v_{n+1/2}), \\ v_{n+1} &= v_n - \frac{h}{2} Q_2'(w_{n+1}). \end{aligned}$$

Numerical experiments – Geometric properties



Mean error on the Hamiltonian for different values of the time step h.

Outline

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 $y(t)$, $t > 0$.

Bayesian inverse problems

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

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

Properties

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

Issue

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

Bayesian inverse problems

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

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

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

Bayesian inverse problems

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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

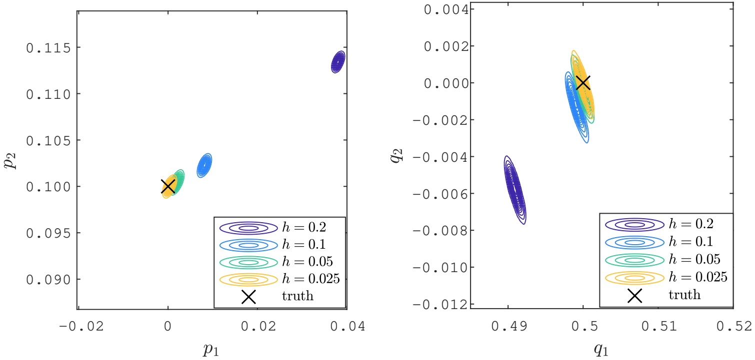
$$E(v, w) = \frac{1}{2}\|v\|^2 + \frac{1}{2}\|w\|^2 + w_1^2 w_2 - \frac{1}{3} w_2^3.$$

Chaotic problem for certain levels of energy.

Goal

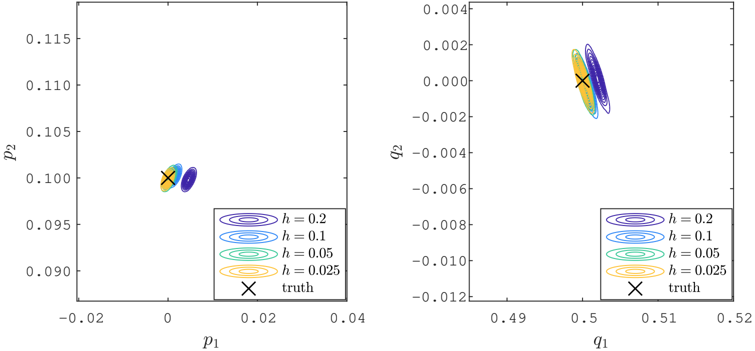
Find posterior $\pi((v_0, w_0) \mid \mathcal{Y})$ over the initial condition from a single observation of $(v(10), w(10))$

Numerical experiment – Bayesian inverse problems



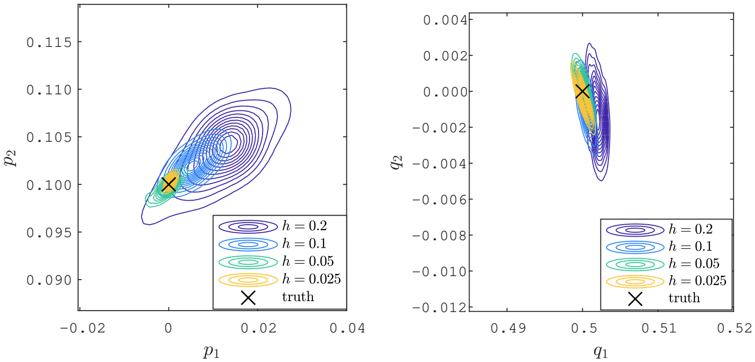
Posterior distributions given by deterministic Heun method.

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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