Principles of stochastic geometric numerical integration

Part I: nonlinear stability analysis

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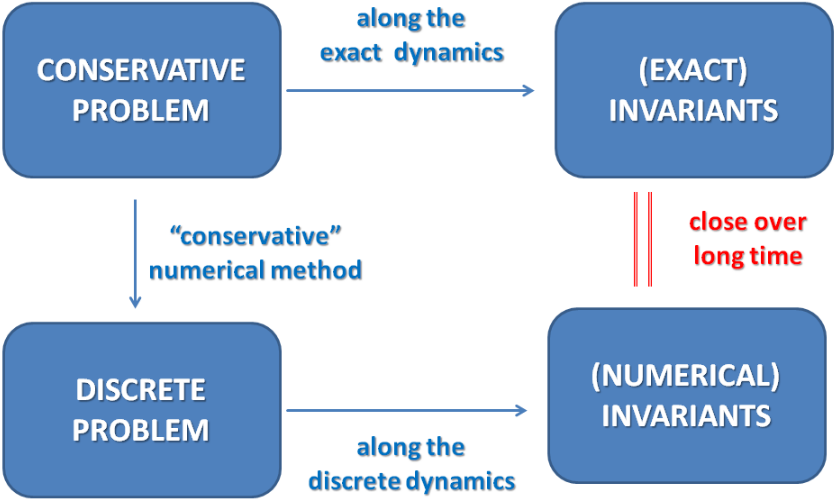
The numerics of preserving structures



Geometric numerical integration

- The denomination recalls the approach to geometry formulated by Felix Klein in his Erlangen program (1893);
- geometry = the study of invariants under certain transformations;
- geometric numerical methods launched to retain peculiar features of dynamical systems under discretizations;
- Arnold (2002), speech addressed to the participants of the International Congress of Mathematicians in Beijing:

  "*The design of stable discretizations of systems of PDEs often hinges on capturing subtle aspects of the structure of the system in the discretization. This new geometric viewpoint has provided a unifying understanding of a variety of innovative numerical methods developed over recent decades*";

Geometric numerical integration (ctd.)

- subtle connection with the so-called *geometric integration theory* by Hassler Whitney (1957);
- Arnold shows that the function spaces introduced by Whitney (the so-called Whitney elements) represent what is required for a geometric discretization of many PDEs.

Douglas N. Arnold, Differential complexes and numerical stability, Proceedings of the ICM, Beijing 2002, vol. 1, 137–157 (2002).

R. McLachlan, Featured Review: Geometric Numerical Integration: Structure-Preserving Algorithms for Ordinary Differential Equations. SIAM Review 45(4), 817–821 (2003).

E. Hairer, C. Lubich, G. Wanner, Geometric numerical integration. Structure-preserving algorithms for ordinary differential equations, Second edition, Springer Series in Computational Mathematics 31, Springer-Verlag, Berlin (2006).

E. Hairer, G. Wanner, Geometric numerical integration illustrated by the Störmer-Verlet method, Acta Numer. 12, 399–450 (2003).

Geometric numerical integration (ctd.)

A famous method: leapfrog method, also known as Störmer-Verlet method. This method, for the discretization of the second order problem

$$\ddot{q} = f(q),$$

is given by

$$q_{n+1} - 2q_n + q_{n-1} = h^2 f(q_n).$$

Extensively used in many fields, such as celestial mechanics and molecular dynamics.

- First due to Störmer (1907), a variant of this scheme to compute the motion of ionized particles in the Earth's magnetic field (aurora borealis);
- above formulation due to Verlet (1967) for the computer simulation of molecular dynamics models;
- interested in the history of science, he discovered that his scheme was previously used by several authors: for instance, by Newton in his Principia (1687), to prove Kepler's second law.

Geometric numerical integration (ctd.)

- Seminal contribution by De Vogelaere (1956), "*a marvellous paper, short, clear, elegant, written in one week, submitted for publication and never published*";
- examples of numerical methods (such as the symplectic Euler method) retaining the symplecticity of Hamiltonian problems;
- still regarding Hamiltonian problems, successive contributions by Ruth (1983) and Kang (1985);
- 1988 starting year for the establishment of a theory of conservative numerics for Hamiltonian problems: criterion for the numerical conservation of the symplecticity via Runge-Kutta methods independently by Lasagni, Sanz-Serna, Suris, depending on a similar condition discovered by Cooper (1987) for the numerical conservation of quadratic first integrals.

R. D'Ambrosio, *Numerical approximation of differential problems*, Springer, to appear.

Geometric numerical integration: applications

- Hamiltonian dynamics;
- Molecular dynamics is a rich source of applications for geometric integration;
- weather prediction;
- robotics;
- study of the Schrödinger equation and statistical mechanics.

N. Bou-Rabee, J. M. Sanz-Serna, *Geometric integrators and the Hamiltonian Monte Carlo method*, Acta Numerica 27, 113–206 (2018).

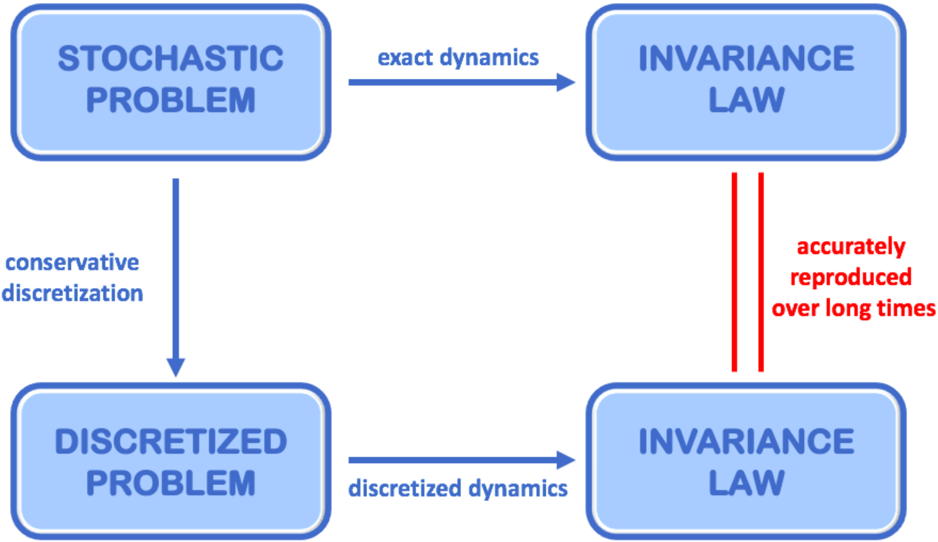
M. Fernandez-Pendas, E. Akhmatskaya, J. M. Sanz-Serna, *Adaptive multi-stage integrators for optimal energy conservation in molecular simulations*, J. Comp. Phys. 327, 434–449 (2016).

B.J. Leimkuhler, S. Reich, *Simulating Hamiltonian dynamics*, Cambridge University Press (2004).

R. McLachlan, *Symplectic integration of Hamiltonian wave equations*, Numer. Math. 66(1), 465–492 (1993).

M.Q. Zhang, *Explicit unitary schemes to solve quantum operator equations of motion*, J. Stat. Phys. 65(3), 793–799 (1991).

Stochastic geometric numerical integration



Nonlinear SDEs

Retaining dissipativity of stochastic differential equations

- E. Buckwar, R. D'Ambrosio, *Exponential mean-square stability properties of stochastic linear multistep methods*, submitted.
- R. D'Ambrosio, S. Di Giovacchino, *Mean-square contractivity of stochastic theta-methods*, Comm. Nonlin. Sci. Numer. Simul. 96, article number 105671 (2021).
- R. D'Ambrosio, S. Di Giovacchino, *Nonlinear stability issues for stochastic Runge-Kutta methods*, Comm. Nonlin. Sci. Numer. Simul. 94, article number 105549 (2021).
- R. D'Ambrosio, S. Di Giovacchino, *Optimal ϑ-methods for mean-square dissipative stochastic differential equations*, submitted.
- D.J. Higham, P.E. Kloeden, *Numerical methods for nonlinear stochastic differential equations with jumps*, Numer. Math. (2005).

Memorandum on nonlinear deterministic equations

Consider a nonlinear test problem

$$\begin{cases} y'(t) = \varphi\big(t, y(t)\big), & t \geq 0, \\ y(0) = y_0, \end{cases}$$

with $\varphi : \mathbb{R} \times \mathbb{R}^m \to \mathbb{R}^m$ satisfying a one-sided Lipschitz condition

$$\big(\varphi(t, y_1) - \varphi(t, y_2)\big)^{\mathsf{T}} (y_1 - y_2) \leq 0, \qquad (\star)$$

for all $t \geq 0$ and $y_1, y_2 \in \mathbb{R}^m$. Denote by $y(t)$ and $\tilde{y}(t)$ two solutions with initial conditions y_0 and $\tilde{y}_0$, respectively. Condition $(\star)$ implies the contractivity of the trajectories

$$\big\| y(t_2) - \tilde{y}(t_2) \big\| \leq \big\| y(t_1) - \tilde{y}(t_1) \big\|,$$

for $0 \leq t_1 \leq t_2$, where $\| \cdot \|$ is any norm in $\mathbb{R}^m$, and the corresponding problem is said to be dissipative.

Contractive numerical solutions for dissipative problems: AN-stability, G-stability, algebraic stability, … (pioneered by Dahlquist, 1975).

Stochastic contractivity

Nonlinear Itō problem:

$$dX(t) = f(X(t))dt + g(X(t))dW(t), \quad t \in [0, T]$$

Assumptions

(i) $\mathcal{C}^1$-**continuity** of drift and diffusion;

(ii) **one-sided Lipschitz condition** for the drift

$$< x - y, f(x) - f(y) > \leq \mu \|x - y\|^2, \quad \forall x, y \in \mathbb{R}^n;$$

(iii) **global Lipschitz** for the diffusion

$$\|g(x) - g(y)\|^2 \leq L \|x - y\|^2, \quad \forall x, y \in \mathbb{R}^n.$$

Stochastic contractivity (ctd.)

Theorem (Higham, Kloeden, 2005)

Assume (i) – (iii) hold. Then, two solutions $X(t)$ e $Y(t)$ of an Itō SDE with $\mathbb{E}\|X_0\|^2 < \infty$ and $\mathbb{E}\|Y_0\|^2 < \infty$ satisfy

$$\mathbb{E}\|X(t) - Y(t)\|^2 \leq \mathbb{E}\|X_0 - Y_0\|^2 e^{\alpha t},$$

where

$$\alpha = 2\mu + L.$$

$\boxed{\alpha < 0}$ provides mean-square contractivity.

- D.J. Higham, P.E. Kloeden, *Numerical methods for nonlinear stochastic differential equations with jumps*, Numer. Math. (2005).
- E. Buckwar, R. D'Ambrosio, *Exponential mean-square stability properties of stochastic linear multistep methods*, submitted.
- R. D'Ambrosio, S. Di Giovacchino *Mean-square contractivity of stochastic θ-methods*, Comm. Nonlinear Sci Numer. Simul. (2021).
- R. D'Ambrosio, S. Di Giovacchino *Nonlinear stability issues of stochastic Runge-Kutta methods*, Comm. Nonlinear Sci Numer. Simul. (2021).

Analysis of one-step methods

Theorem

Assume (i) − (iii) hold. Then, any one-step stochastic method

$$\alpha_2 X_{i+1} + \alpha_1 X_i = \Delta t(\beta_2 f(X_{i+1}) + \beta_1 f(X_i) + \gamma_1 g(X_i)\Delta W_i).$$

satisfies the following inequality

$$\mathbb{E}\|X_{i+1} - Y_{i+1}\|^2 \leq \mathbb{E}\|X_0 - Y_0\|^2 e^{\nu t_{i+1}},$$

with

$$\nu = \frac{1}{\Delta t}\log \beta_{\mathrm{OS}},$$

being

$$\beta_{\mathrm{OS}} = \frac{\alpha_1^2 - 2\alpha_1\beta_1\mu\Delta t + \beta_1^2 M\Delta t^2 + \gamma_1^2 L\Delta t^3}{\alpha_2 - 2\beta_2\mu\Delta t}$$

and $M = \sup_{t\in[0,T]} \mathbb{E}|f'(X(t))|^2.$

Contractivity of one-step methods

A one-step method is exponential mean-square contractive if $\nu < 0$, i.e. if

$$0 < \beta_{\text{OS}} < 1.$$

Example: Stochastic trapezoidal rule

$$X_{i+1} = X_i + \frac{1}{2}\Delta t f(X_i) + \frac{1}{2}\Delta t f(X_{i+1}) + g(X_i)\Delta W_i,$$

$$\beta_{\text{OS}} = \frac{4 - 4\mu\Delta t + (M + 4L)\Delta t^2}{4(1 - \mu\Delta t)}.$$

Hence, it is contractive if

$$\Delta t < \frac{8|\mu|}{M + 4L}.$$

Numerical test

Let
$$f(x) = -4x - x^3, \qquad g(x) = x.$$
Then, $\mu = -4$, $L = 1$.
$\alpha = 2\mu + L = -7 < 0 \;\Rightarrow\;$ exponential mean-square contractivity.

Stepsize restriction for the trapezoidal method:
$$\Delta t < \frac{8}{5}.$$

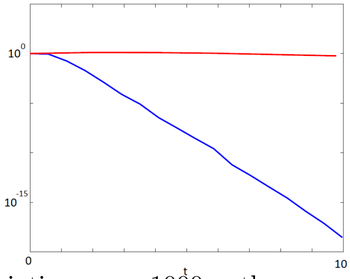


Figure: Mean-square deviations over 1000 paths computed by the trapezoidal method with stepsizes $\Delta t = 75/128 \approx 0.59$ and $\Delta t = 125/64 \approx 1.95$

Useful recursion for two-step methods

Stochastic two-step linear methods (Buckwar *et al.*, BIT 2006)

$$\alpha_2 X_{i+1} + \alpha_1 X_i + \alpha_0 X_{i-1} = \Delta t(\beta_2 f(X_{i+1}) + \beta_1 f(X_i) + \beta_0 f(X_{i-1}) \\ + \gamma_1 g(X_i)\Delta W_i + \gamma_0 g(X_{i-1})\Delta W_{i-1}).$$

Theorem

Assume (i) − (iii) hold. Then, any two numerical solutions $\{X_i\}_i$ *and* $\{Y_i\}_i$ *generated by a two-step method satisfy*

$$\mathbb{E}\|X_{i+1} - Y_{i+1}\|^2 \le \beta_{\mathrm{TS}}\mathbb{E}\|X_i - Y_i\|^2 + \gamma_{\mathrm{TS}}\mathbb{E}\|X_{i-1} - Y_{i-1}\|^2,$$

with

$$\beta_{\mathrm{TS}} = \frac{\alpha_1^2 + \alpha_0\alpha_1 + (-2\alpha_1\beta_1\mu - (\alpha_1\beta_0 + \alpha_0\beta_1 M))\,\Delta t + (\beta_1^2 + \beta_1\beta_0)M\Delta t^2 + \gamma_1^2 L\Delta t^3}{\alpha_2 - 2\beta_2\mu\Delta t},$$

$$\gamma_{\mathrm{TS}} = \frac{\alpha_0^2 + \alpha_0\alpha_1 + (-2\alpha_0\beta_0\mu - (\alpha_1\beta_0 M + \alpha_0\beta_1))\,\Delta t + (\beta_0^2 + \beta_1\beta_0)M\Delta t^2 + \gamma_0^2 L\Delta t^3}{\alpha_2 - 2\beta_2\mu\Delta t}.$$

Analysis of two-step methods

Theorem

Assume (i) − (iii) hold. Then, any two-step stochastic method satisfies

$$\mathbb{E}\|X_{n+1} - Y_{n+1}\|^2 \leq \mathbb{E}\|X_0 - Y_0\|^2 e^{\eta t_{n+1}},$$

with

$$\eta = \frac{1}{\Delta t} \log\left(\zeta_{n+1}\right),$$

where ζ_{n+1} is recursively defined by the three-term formula

$$\zeta_{n+1} = \beta_{\mathrm{TS}}\zeta_n + \gamma_{\mathrm{TS}}\zeta_{n-1},$$

with $\zeta_1 = \beta_{\mathrm{OS}}$ and $\zeta_2 = \beta_{\mathrm{TS}}\beta_{\mathrm{OS}} + \gamma_{\mathrm{TS}}$.

β_{TS} and γ_{TS} are given in the useful recursion; β_{OS} characterizes the one-step method employed to compute the missing starting values X_1 and Y_1.

Contractivity of two-step methods

A two-step method is exponential mean-square contractive if $\eta < 0$, i.e. if, after performing n steps,

$$0 < \zeta_n < 1,$$

Example: Adams-Moulton method

$$X_{n+1} - X_n = \Delta t \left(\frac{5}{12} f(X_{n+1}) + \frac{8}{12} f(X_n) - \frac{1}{12} f(X_{n-1}) + g(X_n)\Delta W_n \right).$$

It satisfies

$$\beta_{\mathrm{TS}} = \frac{36 - (3 - 48\mu)\Delta t + 14M\Delta t^2 + 36L\Delta t^3}{6(6 - 5\mu\Delta t)},$$

$$\gamma_{\mathrm{TS}} = \frac{(12 + 7\Delta t)M\Delta t}{24(5\mu\Delta t - 6)}.$$

In order to check $0 < \zeta_n < 1$, we compute the values of ζ_n for large enough values of n, assuming to employ the trapezoidal method as a starting method.

Numerical test

Let $$f(x) = -4x - x^3, \qquad g(x) = x.$$

Satisfies exponential mean-square contractivity.

Stepsize restriction for the Adams-Moulton method: for $n = 24$, we have

$$\Delta t \leq 0.6031007782344122.$$

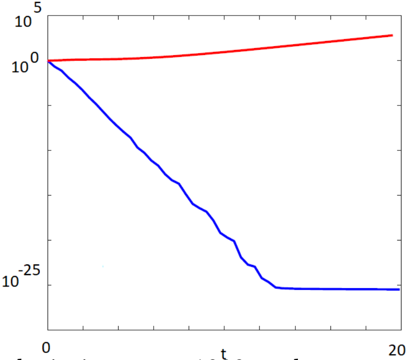


Figure: Mean-square deviations over 1000 paths computed by the Adams-Moulton method with stepsizes $\Delta t = 25/28 \approx 0.89$ and $\Delta t = 75/128 \approx 0.58$

Stochastic θ-methods

θ-Maruyama

$$X_{n+1} = X_n + (1-\theta)\Delta t f(X_n) + \theta \Delta t f(X_{n+1}) + g(X_n)\Delta W_n,$$

θ-Milstein

$$X_{n+1} = X_n + (1-\theta)\Delta t f(X_n) + \theta \Delta t f(X_{n+1}) + g(X_n)\Delta W_n \\ + \frac{1}{2} g'(X_n) g(X_n)(\Delta W_n^2 - \Delta t),$$

Nonlinear stability analysis:

R. D'Ambrosio, S. Di Giovacchino *Mean-square contractivity of stochastic θ-methods*, Commun. Nonlinear Sci. Numer. Simul. (2021).

θ-Maruyama

Theorem

Under the assumptions (i)–(iii), any two θ-Maruyama numerical solutions X_n and Y_n, $n \geq 0$, satisfy the inequality

$$\mathbb{E}\,|X_n - Y_n|^2 \leq \mathbb{E}\,|X_0 - Y_0|^2\, e^{\nu(\theta,\Delta t) t_n},$$

where

$$\nu(\theta,\Delta t) = \frac{1}{\Delta t}\ln\beta(\theta,\Delta t), \quad \beta(\theta,\Delta t) = 1 + \frac{\alpha + (1-\theta)^2 M\Delta t}{1 - 2\theta\mu\Delta t}\Delta t,$$

with

$$M = \sup_{t\in[0,T]} \mathbb{E}|f'(X(t))|^2.$$

Theorem

For any fixed value of $\theta \in [0,1]$, $|\nu(\theta,\Delta t) - \alpha| = \mathcal{O}(\Delta t)$.

θ-Milstein

Theorem

Under the assumptions (i)–(iii), any two θ-Maruyama numerical solutions X_n and Y_n, $n \geq 0$, satisfy the inequality

$$\mathbb{E}\left|X_n - Y_n\right|^2 \leq \mathbb{E}\left|X_0 - Y_0\right|^2 e^{\epsilon(\theta,\Delta t)t_n},$$

where

$$\epsilon(\theta, \Delta t) = \frac{1}{\Delta t}\ln\gamma(\theta, \Delta t), \quad \gamma(\theta, \Delta t) = \beta(\theta, \Delta t) + \frac{\widetilde{M}\Delta t^2}{2(1 - 2\theta\mu\Delta t)},$$

with $\quad \widetilde{M} = \sup_{t\in[0,T]} \mathbb{E}|h'(X(t))|^2, \quad h(X(t)) = g(X(t))g'(X(t)).$

Theorem

For any fixed value of $\theta \in [0,1]$, $|\epsilon(\theta, \Delta t) - \alpha| = \mathcal{O}(\Delta t)$.

Region of mean-square contractivity

Definition

For a nonlinear stochastic differential equation satisfying assumptions $(i) - (iii)$, a θ-method is said to generate mean-square contractive numerical solutions in a region $\mathcal{R} \subseteq \mathbb{R}^+$ if, for a fixed $\theta \in [0, 1]$,

$$\nu(\theta, \Delta t) < 0, \quad \forall \Delta t \in \mathcal{R}$$

for the θ-Maruyama,

$$\epsilon(\theta, \Delta t) < 0, \quad \forall \Delta t \in \mathcal{R}$$

for the θ-Milstein.

Definition

A stochastic θ-method is said unconditionally mean-square contractive if, for a given $\theta \in [0, 1]$, $\mathcal{R} = \mathbb{R}^+$.

Mean-square contractivity: θ-Maruyama

Mean-square contractivity holds true if

$$0 < \beta(\theta, \Delta t) < 1,$$

for any $\Delta t \in \mathcal{R}$, i.e.

$$\mathcal{R} = \begin{cases} \left(0, \dfrac{|\alpha|}{(1-\theta)^2 M}\right), & \theta < 1, \\ \mathbb{R}^+, & \theta = 1. \end{cases}$$

The θ-Maruyama method with $\theta = 1$ (implicit Euler-Maruyama) is unconditionally mean-square contractive.

Mean-square contractivity: θ-Milstein

Mean-square contractivity holds true if

$$0 < \gamma(\theta, \Delta t) < 1,$$

for any $\Delta t \in \mathcal{R}$, i.e.

$$\mathcal{R} = \begin{cases} \left(0, \dfrac{2|\alpha|}{2(1-\theta)^2 M + \widetilde{M}}\right), & \theta < 1, \\ \left(0, \dfrac{2|\alpha|}{\widetilde{M}}\right), & \theta = 1. \end{cases}$$

Parameter estimation as in global optimization algorithms.

Numerical experiments

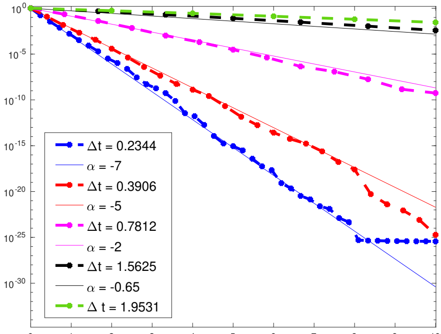
Problem 1: stochastic Ginzburg-Landau

M. Hutzenthaler, A. Jentzen, Numerical approximations of stochastic differential equations with non- globally Lipschitz continuous coefficients, Memoirs of the American Mathematical Society 236(1112), doi: 10.1090/memo/1112 (2015).

$$f(X(t)) = -4X(t) - X(t)^3, \qquad g(X(t)) = X(t)$$

$X_0 = 1$, $Y_0 = 0$. For this problem $L = 1$ and $\mu = -4$, so $\alpha = -7 < 0$.

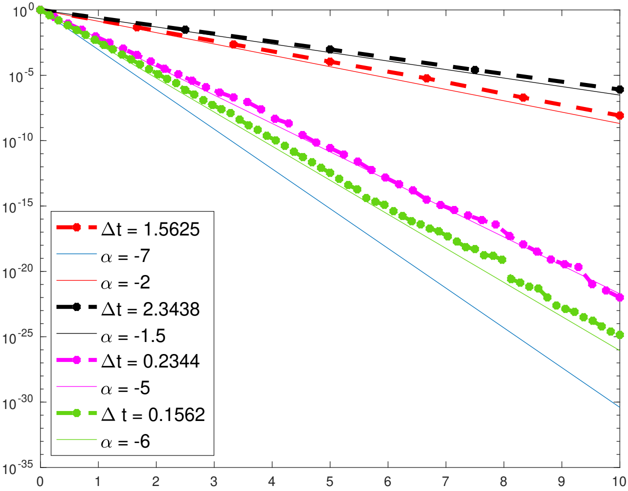
- stochastic trapezoidal methods ($\theta = 1/2$): $\mathcal{R} = \left(0,\ \frac{7}{4}\right)$;



Numerical experiments

Problem 1 (ctd.)

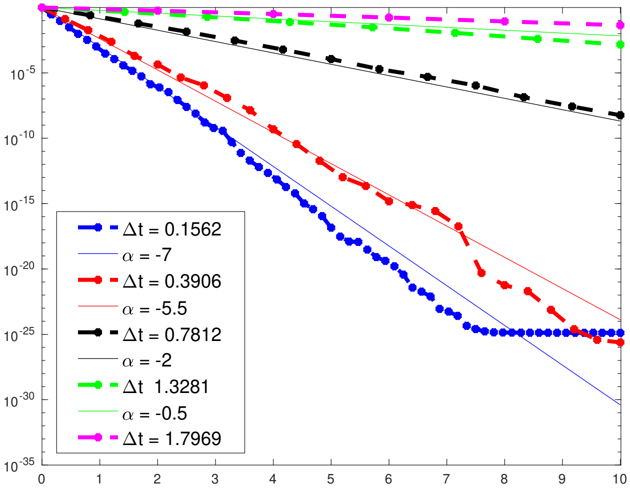
- stochastic implicit Euler, unconditionally mean-square contractive;



Numerical experiments

Problem 1 (ctd.)

- θ-Milstein method with $\theta = 1/2$: $\mathcal{R} = \left(0,\ \frac{14}{9}\right)$.



Numerical experiments

Problem 2

$$f(X(t)) = -4\begin{bmatrix} \sin(X_1(t)) \\ \sin(X_2(t)) \end{bmatrix}, \qquad g(X(t)) = \frac{1}{7}\begin{bmatrix} X_1(t) & \frac{3}{2}X_2(t) \\ \frac{5}{2}X_1(t) & -\frac{1}{2}X_2(t) \end{bmatrix}.$$

Initial data: $X_0 = [1 \quad 1]^\intercal$ and $Y_0 = [0 \quad 0]^\intercal$. For this problem the constants L and μ are estimated as $L = 0.148$ and $\mu = -3.56$, so $\alpha \approx -7.5 < 0$.

- Stochastic trapezoidal method: $\mathcal{R} = (0,\ 1.1875)$;
- stochastic implicit Euler method, unconditionally mean-square contractive.

Numerical experiments

Problem 2 (ctd.)

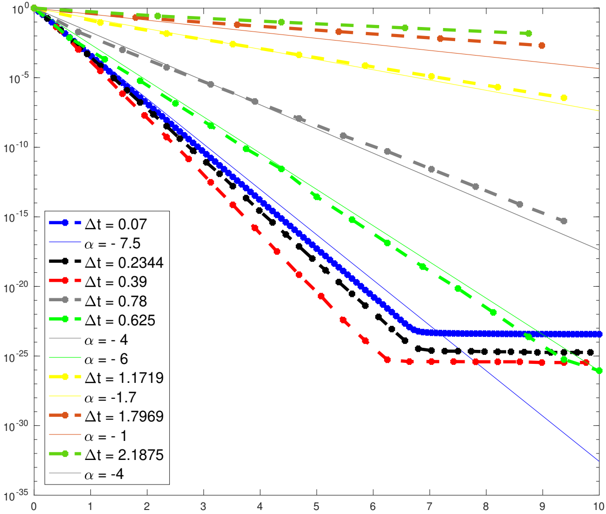


Figure: Mean-square deviations over 2000 paths for the trapezoidal method.

Numerical experiments

Problem 2 (ctd.)

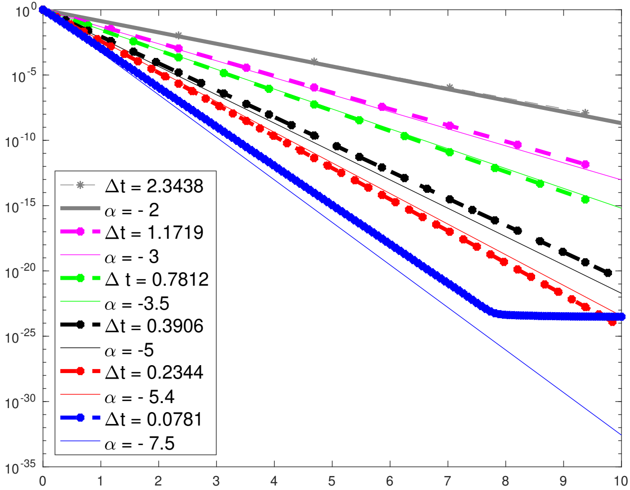


Figure: Mean-square deviations over 2000 paths for the implicit Euler method.