Modified equations, backward error analysis and numerical methods for stochastic differential equations.

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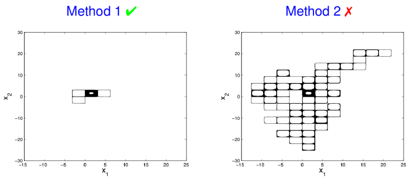
Outline

1. Introduction.
2. Main Idea.
3. Different Numerical Methods and Associated Modified Equations.
4. Applications:
   - SDEs Driven by Multiplicative Noise.
   - Linear SDEs, ∞-Modified Equations.
   - Long Time Behaviour and Homogenization.
5. Summary.

Motivating example



Interesting Question

- The two numerical methods have the same order of convergence but completely different qualitative behaviour.
- Is there a way to distinguish between these two methods?
- A very powerful tool for addressing this question is backward error analysis (modified equations).

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Modified equations for ODEs

$$\frac{dx}{dt} = f(x),$$

and let x_n be a numerical approximation of x of order p:

$$|x(n\Delta t) - x_n| = \mathcal{O}(\Delta t^p).$$

Can I find $X(t)$ satisfying another ODE (modified equation) such that:

$$|X(n\Delta t) - x_n| = \mathcal{O}(\Delta t^{p+q}).$$

Euler method-one dimension

$$\boxed{x_{n+1} = x_n + \Delta t f(x_n).}$$

Modified equation:

$$\frac{dX}{dt} = f(X) - \frac{\Delta t}{2} f'(X) f(X),$$

since

$$|X(n\Delta t) - x_n| = \mathcal{O}(\Delta t^2).$$

Sketch proof

$$\frac{dX}{dt} = f(X) + \Delta t g(X).$$

$$\begin{aligned} X(\Delta t) &= X(0) + \int_0^{\Delta t} \left(f(X(s)) + \Delta t g(X(s))\right) ds \\ &= X(0) + \Delta t f(X(0)) + \Delta t^2 g(X(0)) + \frac{\Delta t^2}{2} f(X(0)) f'(X(0)) + \mathcal{O}(\Delta t^3). \end{aligned}$$

Assume $x_0 = X(0)$ then

$$X(\Delta t) - x_1 = \Delta t^2 \left(g(X(0)) + \frac{1}{2} f(X(0)) f'(X(0)) \right) + \mathcal{O}(\Delta t^3),$$

and thus

$$\boxed{g(x) = -\frac{1}{2} f(x) f'(x).}$$

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Stochastic Differential Equations and Numerical Methods

$$dx = v(x)dt + \sigma(x)dW_t,$$

- Euler method:

$$x_{n+1} = x_n + \Delta t v(x_n) + \sqrt{\Delta t}\sigma(x_n)\xi_n,$$

- Milstein method:

$$x_{n+1} = x_n + \Delta t v(x_n) + \sqrt{\Delta t}\sigma(x_n)\xi_n + \frac{1}{2}\sigma(x_n)\sigma^{(1)}(x_n)(\Delta t\xi_n^2 - \Delta t),$$

where $\xi_n \sim \mathcal{N}(0,1)$.

Weak and Strong Convergence

- Weak convergence: We look at $|\mathbb{E}(\phi(x(n\Delta t))) - \mathbb{E}(\phi(x_n))|$.
- Strong convergence: We look at $\mathbb{E}|x(n\Delta t) - x_n|$.
- In general the weak and strong order of convergence of a numerical method NEEDS NOT to be the same!!!

Statement of the Problem

Let $x(t)$ satisfy the following SDE:

$$dx = v_1(x)dt + \sigma_1(x)dW_t,$$

and x_n be its numerical approximation at $T = n\Delta t$ by a weak p-order method i.e

$$|\mathbb{E}(\phi(x(T))) - \mathbb{E}(\phi(x_n))| = \mathcal{O}(\Delta t^p), \; \forall \phi \in C^\infty.$$

We want to develop a procedure that allows us to evaluate the properties of our weak numerical scheme.

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First Modified Equation

We want to find a modified SDE of the form (*i.e.*, find v_2 and σ_2)

$$d\tilde{x} = [v_1(\tilde{x}) + \Delta t v_2(\tilde{x})] + [\sigma_1(\tilde{x}) + \Delta t \sigma_2(\tilde{x})]\, dW_t,$$

for which

$$|\mathbb{E}(\phi(\tilde{x}(T))) - \mathbb{E}(\phi(x_n))| = \mathcal{O}(\Delta t^{p+1}),\ \forall \phi \in C^\infty.$$

For the rest of the talk we concentrate in the case where $p = 1$.

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Generators for ODEs and SDEs

- ODE:

$$\begin{aligned} dx &= h(x)dt, \\ \mathcal{L}u &:= h(x) \cdot \nabla_x u. \end{aligned}$$

- SDE:

$$\begin{aligned} dx &= h(x)dt + \sigma(x)dW_t, \\ \mathcal{L}u &:= h(x) \cdot \nabla_x u + \frac{1}{2}\sigma(x)\sigma^T(x) : \nabla_x \nabla_x u. \end{aligned}$$

Backward Kolmogorov Equation

$$\begin{aligned} \frac{\partial u}{\partial t} &= \mathcal{L}u, \\ u(x,0) &= \phi(x). \end{aligned}$$

Then

$$u(x,t) = \mathbb{E}(\phi(x(t))|x(0) = x).$$

Stochastic B-series

By integrating over time the backward Kolmogorov Equation and taking a Taylor expansion of $u(x,s)$ around $s=0$, we obtain, (assuming appropriate smoothness of the drift and diffusion terms)

$$u(x,\Delta t)-\phi(x)=\sum_{k=0}^{\infty}\frac{\Delta t^{k+1}}{(k+1)!}\mathcal{L}^{k+1}\phi(x).$$

Note that in the case where $\phi(x)=x$, $\sigma(x)=0$, this expansion correspond to the B-series expansion of the ODE

$$dx=v_1(x)dt.$$

Local Error/Global Error

A weak first order numerical method has the following expansion

$$u_{num}(x, \Delta t) - \phi(x) = \Delta t \mathcal{L}\phi(x) + \Delta t^2 \mathcal{L}_e \phi(x) + \mathcal{O}(\Delta t^3),$$

and so

$$u(x, \Delta t) - u_{num}(x, \Delta t) = \Delta t^2 \left(\frac{1}{2}\mathcal{L}^2\phi(x) - \mathcal{L}_e\phi(x) \right), \quad \text{Local Error}$$

which implies that

$$u(x, T) - u_{num}(x, T) = \mathcal{O}(\Delta t). \quad \text{Global Error}$$

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Generator of the Modified Equation

Remember that the 1-st modified equation is of the form

$$d\tilde{x} = [v_1(\tilde{x}) + \Delta t v_2(\tilde{x})] + [\sigma_1(\tilde{x}) + \Delta t \sigma_2(\tilde{x})]\, dW_t.$$

Its generator $\mathcal{L}$ can be written as

$$\mathcal{L} = \mathcal{L}_0 + \Delta t \mathcal{L}_1 + \Delta t^2 \mathcal{L}_2,$$

where $\mathcal{L}_0$ is the generator of the original SDE and

$$\mathcal{L}_1 \phi := v_2(x)\frac{d\phi}{dx} + \sigma_1(x)\sigma_2(x)\frac{d^2\phi}{dx^2}.$$

Main Equation

If we now subtract the Taylor expansion of the numerical method from the stochastic B-series of the modified equation we see that in order for the local error to be $\mathcal{O}(\Delta t^3)$ we need

$$\boxed{\mathcal{L}_1\phi = \mathcal{L}_e\phi - \frac{1}{2}\mathcal{L}_0^2\phi, \ \forall\phi \in C^\infty.}$$

Euler-Maryama Method

In the case of Euler-Maryama method in the case of multiplicative noise it turns out that a modified equation does not exist since

$$\mathcal{L}_1\phi \neq \cdots + \frac{\sigma_1^3(x)}{2}\sigma_1^{(1)}(x)\phi^{(3)}(x).$$

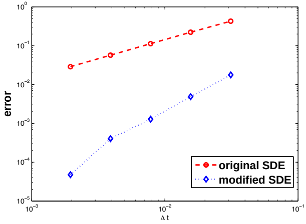
as $\mathcal{L}_1$ is a second order partial differential operator!!!

Milstein Method

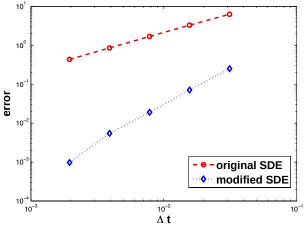
$$
\begin{aligned}
v_2(x) &= -\frac{1}{2}\left(v_1(x)v_1^{(1)}(x) + \frac{\sigma_1^2(x)}{2}v_1^{(2)}(x)\right),\\
\sigma_2(x) &= -\frac{1}{2}\left(\sigma_1(x)v_1^{(1)}(x) + v_1(x)\sigma_1^{(1)}(x) + \frac{\sigma_1^2(x)}{2}\sigma_1^{(2)}(x)\right).
\end{aligned}
$$

Geometric Brownian motion

$$
\begin{aligned}
dx &= \mu x dt + \sigma x dW_t, \\
d\tilde{X} &= \left[\left(\mu - \frac{\Delta t}{2}\mu^2\right)\tilde{X}\right] dt + \sigma \tilde{X}\left(1 - \Delta t \mu\right) dW_t.
\end{aligned}
$$



First moment



Second moment

Linear SDEs with additive noise

$$dx = Axdt + \Sigma dW_t.$$

Numerical Approximation:

$$x(\Delta t) = A(\Delta t)x + f(\Delta t, \omega).$$

Example (Euler-Maryama):

$$\begin{aligned} A(\Delta t) &= (I + \Delta t A), \\ f(\Delta t, \omega) &= \Sigma\sqrt{\Delta t}\xi. \end{aligned}$$

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∞ Modified Equation and its coefficients

$$dx = \tilde{A}xdt + \tilde{\Sigma}dW_t,$$

$$\begin{aligned} \tilde{A} &= \frac{\log(A(\Delta t))}{\Delta t}, \\ e^{\tilde{A}\Delta t}\tilde{\Sigma}\tilde{\Sigma}^T e^{\tilde{A}^T\Delta t} - \tilde{\Sigma}\tilde{\Sigma}^T &= \tilde{A}J + J\tilde{A}^T, \end{aligned}$$

where

$$J = \mathbb{E}(ff^T).$$

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Connection with ODEs

Let $M(t) = \mathbb{E}(x(t))$, then

$$\frac{dM}{dt} = AM.$$

The numerical method for SDE becomes this numerical method for the previous ODE

$$M_{n+1} = A(\Delta t)M_n,$$

which from ODE theory has this ∞-modified equation

$$\frac{d\tilde{M}}{dt} = \tilde{A}\tilde{M}.$$

Orstein Uhlenbeck Process

$$dx = -\gamma x dt + \sigma dW_t.$$

Forward Euler:

$$\begin{aligned} \tilde{A} &= \frac{\log(1-\gamma\Delta t)}{\Delta t}, \\ \tilde{\Sigma} &= \sigma\sqrt{\frac{2\log(1-\gamma\Delta t)}{(1-\gamma\Delta t)^2-1}}. \end{aligned}$$

Backward Euler:

$$\begin{aligned} \tilde{A} &= -\frac{\log(1+\gamma\Delta t)}{\Delta t}, \\ \tilde{\Sigma} &= \sigma\sqrt{\frac{2\log(1+\gamma\Delta t)}{1-(1+\gamma\Delta t)^{-2}}}. \end{aligned}$$

Invariant Measure

$$\lim_{t\to\infty} \mathbb{E}(x^2(t)) = \frac{\sigma^2}{2\gamma - \gamma^2\Delta t}, \quad \text{Forward Euler}$$

$$\lim_{t\to\infty} \mathbb{E}(x^2(t)) = \frac{\sigma^2(1+\gamma\Delta t)^2}{2\gamma + \gamma^2\Delta t}, \quad \text{Backward Euler.}$$

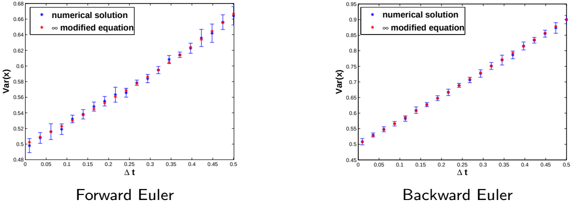

Figure: $\lim_{t\to\infty} \mathbb{E}(x^2(t))$ as a function of Δt.

Passive Tracers, Effective Diffusivity

$$dx = v(x)dt + \sigma dW_t,$$

where $v(x)$ is a periodic function. It is possible to show using homogenization that

$$\lim_{t\to\infty} \frac{\mathbb{E}(x(t)\otimes x(t))}{2t} = \mathcal{K}.$$

We will refer to $\mathcal{K}$ as the *effective diffusivity matrix*

Velocity Field of Interest

Example

We are interested in the following 2-dimensional incompressible velocity field

$$v(x) = \nabla^{\perp}\Psi(x), \text{ where } \Psi(x) = \sin x_1 \sin x_2$$

Result

In this case it is known that $\mathcal{K} = D(\sigma)I_2$*, where* $D(\sigma) \in \mathbb{R}$ *and that the following result is true*

$$D(\sigma) \sim \sigma, \quad \sigma \ll 1$$

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Key Property of the Velocity Field

Our velocity field $v(x)$ can be written as

$$\begin{aligned} v(x) &= \begin{pmatrix} -1/2 \\ +1/2 \end{pmatrix} \sin(x_1 + x_2) + \begin{pmatrix} -1/2 \\ -1/2 \end{pmatrix} \sin(x_1 - x_2), \\ &= \sum_{j=1}^{2} d_j v_j\big(\langle e_j, x \rangle \big), \end{aligned}$$

where $e_j, d_j \in \mathbb{R}^2$ with the property

$$\boxed{\langle e_j, d_j \rangle = 0.}$$

This is a key property for the construction of our method which is a stochastic extension of a **splitting** method proposed by Quispel 2003.

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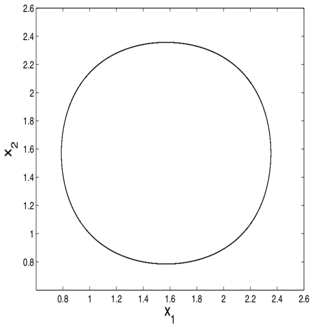
Description of the Method:

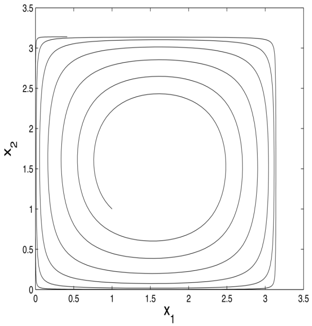
The method in the case of passive tracers involves these 3 steps:

- Step 1: Solve $\dot{x}_1 = d_1 v_1\big(\,\langle e_1, x_1\rangle\,\big)$,
- Step 2: Solve $\dot{x}_2 = d_2 v_2\big(\,\langle e_2, x_2\rangle\,\big)$,
- Step 3: Solve $\dot{x}_3 = \sigma\dot{\beta}_1$.

The Deterministic Case

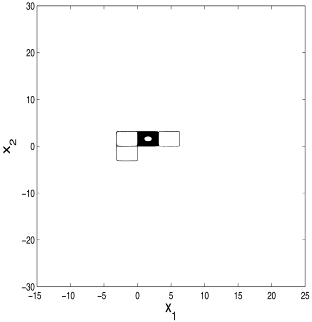


Splitting method for $\sigma = 0$.

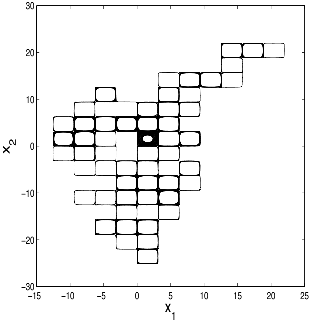


Euler method for $\sigma = 0$.

The Case $\sigma \ll 1$



Splitting method for $\sigma = 10^{-2}$.



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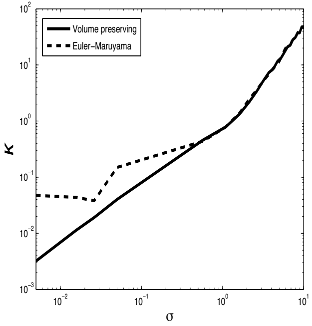
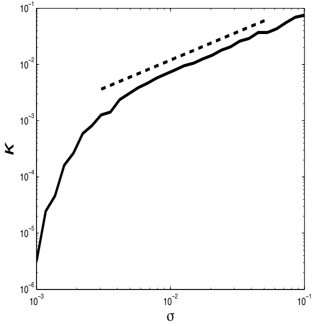
Calculating Effective Diffusivities



Comparison of the two methods.



Splitting Method.

Mean Hamiltonian

We apply Itô 's formula to $H = \Psi$ we obtain

$$\frac{d\Psi}{dt} = -\sigma^2 \Psi + \mathrm{M.T}$$

which implies that the mean Hamiltonian decays like $e^{-\sigma^2 t}$

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Numerical calculation of the mean Hamiltonian with the two methods

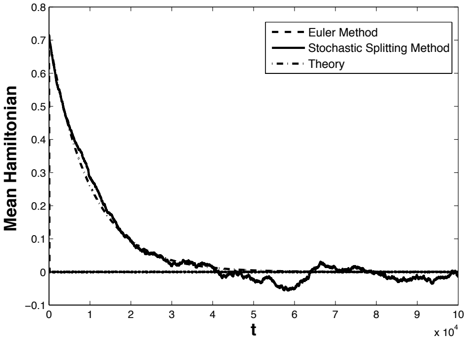

Figure: Mean value of the Hamiltonian as a function of time, for $\Delta t = 10^{-1}, \sigma = 10^{-2}$.

Modified Equations for the Euler Method

$$
\begin{aligned}
dx &= \left(v(x) - \frac{\Delta t}{2}(\nabla v(x))v(x) - \frac{\sigma^2 \Delta t}{4}\Delta v(x)\right) dt \\
&+ \sigma \left(1 - \frac{\Delta t}{2}\nabla v^T(x)\right) dW_t.
\end{aligned}
$$

$$
\begin{aligned}
\frac{d\Psi}{dt} &= -\frac{\Delta t}{2}(\cos^2 x_1 + \cos^2 x_2)\Psi - \sigma^2 \Psi(1 + \Delta t \cos x_1 \cos x_2) \\
&+ \frac{\sigma^2 \Delta t^2}{4}(\cos^2 x_1 \cos^2 x_2 \Psi - \Psi^3) + \mathrm{M}_{\Delta t}.
\end{aligned}
$$

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Conclusions

1. It is not always possible to write down a modified Itô SDE for a given numerical method.
2. In the case of linear SDEs with additive noise it is possible to write down an ∞-modified equation that the numerical method satisfies exactly in the weak sense.
3. It is possible to generalize ideas from the backward error analysis of ODEs to SDEs.

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Future work

1. Find modified equations for numerical methods with respect to strong convergence.
2. Give a rigorous explanation for failing to find a modified SDE for the Euler method in case of multiplicative noise.
3. Use modified equations to characterize the invariant measures approximated by different numerical schemes.
4. Use modified equations as a tool for constructing higher order methods.

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