A. DONEV

DEC-05-2011 15:42

Numerical Methods for Stochastic Differential Equations of the generic Langevin kind.

Recall the generic Langevin equation:

$$x_t = \underbrace{N(x)}_{\text{mobility matrix}} \cdot \underbrace{\frac{\partial H}{\partial x}}_{\text{thermodynamic driving force}} + \sqrt{2k_B T}\, \underbrace{K(x)}_{KK^* = \frac{N+N^*}{2}} \cdot \underbrace{\dot{B}}_{\text{independent Brownian motions (Wiener process}} + (k_B T)\frac{\partial}{\partial x} \cdot N^*$$

$$\boxed{dx = \left[N(x) \cdot \frac{\partial H}{\partial x} + (k_B T)\frac{\partial}{\partial x} \cdot N^*\right] dt + \sqrt{2k_B T}\, K \cdot dB}$$

DEC-05-2011 15:42

Generically, a stochastic differential equation in Ito form:

$$\boxed{dx = A(x)\,dt + K(x)\cdot dB} \quad \begin{cases} x \in \mathbb{R}^n \\ B \in \mathbb{R}^m \end{cases}$$

How do we integrate this in time?

Recall Euler–Maruyama method:

$$x^{n+1} = x^n + A(x^n)\,\Delta t + K(x^n)\,\underbrace{\Delta B(\Delta t)}_{\text{Wiener increment}}$$

x^{n+1}: Approx. $x(t+\Delta t)$

x^n: approx. $x(t)$

$$\boxed{x^{n+1} = x^n + A^n \Delta t + K^n \cdot W^n \cdot \Delta t^{1/2}}$$

$$W^n \equiv \mathcal{N}(0,1)$$ normal random variate

How do we quantify the order of accuracy?

We distinguish between:

1. **Strong order** of accuracy is p if:

$$\left\{ \begin{array}{l} E\left| X^{N=T/\Delta t} - X(t) \right| \leq C(\Delta t)^p \\ \forall \Delta t \leq \Delta t_{max} \end{array} \right.$$

This regards finite-time accuracy and pathwise convergence (approximation) for a fixed realization of the Brownian motion $B(t)$

Strong order is a very stringent criterion, especially when the noise term depends on x, $K(x) \neq$ const, called multiplicative noise. In fact, it is rather hard to construct efficient (and even less so simple) strong schemes of order ≥ 1! So

2. Weak order of accuracy is p if

$$\left\{ \begin{array}{l} \left| E\left[f(x^N)\right] - E\left[f(x(T))\right] \right| \leq C(\Delta t)^p \\ \forall f \in C^{2(p+1)} \text{ polynomial growth} \\ \text{and } \forall \Delta t \leq \Delta t_{max} \end{array} \right.$$

Weak order of accuracy is about convergence or approximation in distribution, for an ensemble of paths (realizations of $B(t)$), rather than individual paths.

Similar theorems as for ODEs hold: Stability + local order of convergence (truncation error) $(p+1)$ implies order p for global error

Note: Weak convergence is still finite-time

$$\boxed{\text{Euler-Maruyama: } \begin{cases} 1/2 & \text{strong} \\ 1 & \text{weak} \end{cases}}$$ order of convergence

$$dx = A(x)\,dt + K(x)\cdot dB$$

To get better strong convergence use Milstein's scheme:

$$\begin{cases} X^{n+1} = X^n + A^n \Delta t + K^n \cdot W^n \Delta t^{1/2} \\ + I^{(2)}_{\Delta t} : \left[(K^n)^* \cdot \frac{\partial}{\partial x} \right] (K^n)^* \end{cases}$$

$I_{jk} K_{ij} \partial_i K_{lk}$

$$\left[I^{(2)}_{\Delta t} \right]_{ij} = \int_t^{t+\Delta t} \left[B_j(t') - B_j(t) \right] dB_i(t')$$

twice-iterated stochastic integral

DEC-05-2011 15:42

The statistical properties of $I^{(2)}_{\Delta t}$ are much more complicated than that of the Wiener increment

$$\Delta B = I^{(1)}_{\Delta t} = \int_t^{t+\Delta t} dB \equiv W \, \Delta t^{1/2}$$

(Gaussian)

and so Milstein's scheme is rather impractical, <u>except</u> in one dimension, where

$$I^{(2)} = (\Delta B)^2 - \Delta t$$

Also, the scheme requires derivatives of $K(x)$, which is hard

So we focus on weak schemes instead. Turns out that even this is a lofty goal for multiplicative noise: getting second-order weak convergence requires $\underline{\underline{m^2}}$ normal random random numbers per time step!

Scope down even further to <u>additive-noise</u> equations

Additive: $$\boxed{dx = A(x)\,dt + K\cdot dB}$$

K: constant $[n \times m]$ matrix

Now we can construct higher-order methods, notably Euler is the same as Milstein!

The following is a <u>second-order weak stochastic Taylor series</u> that can be used to see the order of the local truncation error:

$$
\begin{cases}
x(t+\Delta t) = x(t) + A(X(t))\,\Delta t + K\cdot\Delta B \\
\quad + \frac{1}{2} A(t)\cdot\frac{\partial}{\partial x} A(x(t))\,(\Delta t)^2 \\
\quad + \frac{1}{2}\,\Delta B\cdot(K^*)\cdot\frac{\partial}{\partial x} A(x(t))\,\Delta t \\
\quad + \frac{1}{4}(KK^*) : \frac{\partial^2}{\partial x^2} A(x(t))\,\Delta t^2
\end{cases}
$$

$$+\ O(\Delta t^{5/2})$$

This in principle gives us a scheme directly:

$$\begin{cases} X^{n+1} = X^n + A^n \Delta t + K \cdot W^n \Delta t^{1/2} \\ \quad + \frac{1}{2} A^n \cdot \frac{\partial A^n}{\partial x} (\Delta t)^2 + \frac{1}{2} W^n \cdot K^* \cdot \frac{\partial A^n}{\partial x} \Delta t^{3/2} \\ \quad + \frac{1}{2} (KK^*) : \frac{\partial^2 A^n}{\partial x^2} \Delta t^2 \end{cases}$$

but this requires derivatives, which is not very practicable.

Instead, use <u>Runge-Kutta</u> like schemes to approximate derivatives

Consider the following trapezoidal method

$$\begin{cases} \tilde{X}^{n+1} = X^n + A(X^n)\,\Delta t + K W^n \Delta t^{1/2} \\ \text{(predictor)} \\ X^{n+1} = X^n + \frac{\Delta t}{2}\left[A(X^n) + A(\tilde{X}^{n+1})\right] + \Delta t^{1/2} K W^1 \\ \text{(corrector)} \end{cases}$$

Using Taylor series:

$$A(\tilde{X}^{n+1}) = A(X^n + \Delta X) \approx A^n + (\Delta X)\cdot \frac{\partial A^n}{\partial x}$$

$$+ \underbrace{\frac{1}{2}(\Delta X)^* \frac{\partial^2 A^n}{\partial x^2} \cdot \Delta X}_{} + O(\Delta X^3)$$

Also $\frac{1}{2}\left(\frac{\partial^2 A^n}{\partial x^2}\right) : \left[\Delta X\,(\Delta X)^*\right]$

A. DONEV Lecture 11 12

DEC-05-2011 15:43 P.012

For the trapezoidal PC method

$$\Delta x = K W^n \Delta t^{1/2} \Rightarrow$$

$$\langle (\Delta x)(\Delta x^*) \rangle = \left[K \langle W^n (W^n)^* \rangle K^* \right] \Delta t$$
$$= (K K^*) \Delta t$$

So we can approximate

$$\begin{cases} A(\tilde{x}^{n+1}) \simeq A^n + A^n \cdot \frac{\partial A^n}{\partial x} \Delta t + \\ \qquad + W^n \cdot K^* \cdot \frac{\partial A^n}{\partial x} \Delta t^{1/2} \\ \qquad + \frac{\Delta t}{2} (K K^*) : \frac{\partial^2 A^n}{\partial x^2} + O(\Delta t^{3/2}) \end{cases}$$

Plugging this into the corrector step we see that the trapezoidal PC (Runge-Kutta of second order) is consistent with the second-order weak Taylor series, so we conclude

$$\boxed{\text{Trapezoidal corrector} + \text{Euler-Maryama predictor} \Rightarrow 2^{nd} \text{ order weak accuracy}}$$

By contrast, if we do the same calculation for midpoint corrector:

$$\left[X^{n+1} = X^n + A\left(\frac{X^n + \tilde{X}^{n+1}}{2}\right)\Delta t + K W^n \Delta t^{1/2} \right.$$

we would get

$$x^{n+1} \approx x^n + \dots + \frac{1}{8}\left(KK^*\right) : \frac{\partial^2 A^n}{\partial x^2}\Delta t^2$$

should be 1/4 !

which is not consistent, unless $A(x)$ is linear in x so $\frac{\partial^2 A}{\partial x^2} = 0$.

Instead, we would do:

Midpoint method

$$\begin{cases} x^{n+1/2} = x^n + A^n \frac{\Delta t}{2} + K W_1^n \left(\frac{\Delta t}{2}\right)^{1/2} \\ x^{n+1} = x^n + A^{n+1/2}\Delta t + K\left(W_1^n + W_2^n\right)\left(\frac{\Delta t}{2}\right)^{1/2} \end{cases}$$

which is second-order accurate

One can similarly construct third-order weak Runge-Kutta schemes but in general more stages than a deterministic scheme will be required.

How about <u>(semi)-implicit schemes</u> for stiff systems (e.g., fluctuating hydro)?

Implicit midpoint works well (recall it is also symplectic)

$$\boxed{X^{n+1} = X^{n} + A\left(\frac{X^{n}+X^{n+1}}{2}\right) + KW^{n}\Delta t^{1/2}}$$

but requires nonlinear solvers.

As an alternative, consider <u>semi-implicit</u> schemes where we split:

$$A(x) = \underbrace{L}_{\text{linear part, e.g. diffusion}} x + B(x)$$

For example, we can do a semi-implicit (midpoint / trapezoidal) predictor-corrector:

$$\begin{cases} \tilde{x}^{n+1} = x^n + L\left(\frac{x^n + \tilde{x}^{n+1}}{2}\right)\Delta t + B^n \Delta t + K W^n \sqrt{\Delta t} \\ x^{n+1} = x^n + L\left(\frac{x^n + x^{n+1}}{2}\right)\Delta t + K W^n \sqrt{\Delta t} \\ \text{(trapezoidal)} \quad + \frac{1}{2}\left[B^n + B(\tilde{x}^{n+1})\right]\Delta t \end{cases}$$

For purely linear SDEs

$$\boxed{dx = Lx\,dt + K\,dB}$$

we can write the solution explicitly in the form of an exponential integrator

$$x(t) = e^{tL} \cdot x(0) + \int_0^t e^{(t-s)L} \, K \, dB(s)$$

Gaussian

which can be computed explicitly using only Gaussian (normal) random variables if we can compute the operator $\exp[Lt]$?

If we can diagonalize (e.g. Fourier basis)

$$L = \underbrace{U}_{\text{unitary}} \underbrace{\Lambda}_{\text{diagonal}} U^{*}$$

then $\exp[Lt] = U \exp[\Lambda]\, U^{*}$

and by changing coordinate systems so that L is diagonal we can also change the white noise (remains the same white noise in any orthonormal basis) to convert into a system of <u>scalar equations</u>, which we know how to solve (see lectures on Langevin equation).

Instead, we can try to approximate $\exp(L\Delta t)$ using a series of sorts, for example:

$$\exp(L\Delta t) \simeq I + L\Delta t + \frac{L^2}{2}\Delta t^2$$

or the 1-1 Pade approximant

$$\exp(L\Delta t) \simeq \left(I - L\frac{\Delta t}{2}\right)^{-1}\left(I + L\frac{\Delta t}{2}\right)$$

leading to the implicit midpoint:

$$\boxed{\left(I - L\frac{\Delta t}{2}\right)x^{n+1} = \left(I + L\frac{\Delta t}{2}\right)x^{n} + KW^{n}}$$

For linear equations, we can go beyond finite-time accuracy and explore the long-time weak accuracy by looking at the the equilibrium distribution of the numerical scheme.

The distribution is Gaussian so all we need to examine is the covariance

$$C = \lim_{n \to \infty} \langle X^n (X^n)^* \rangle \leftarrow \text{average over noise}$$

Any scheme can be written as

$$\boxed{X^{n+1} = M X^n + N W^n}$$

$$\langle (x^{n+1})(x^{n+1})^* \rangle = C^{n+1} =$$

$$\langle (Mx^n + Nw^n)(Mx^n + Nw^n)^* \rangle =$$

$$= M \langle x^n (x^n)^* \rangle M^* +$$

$$N \langle w^n (w^n)^* \rangle N^*$$

$$= M C^n M^* + N N^* = C^{n+1}$$

At steady state $C^n = C^{n+1} = C$

$$\Rightarrow \boxed{M C M^* - C = -N N^*}$$

Linear system for C

For example, Euler-Maruyama has:

$$X^{n+1} = X^n + L X^n \Delta t + K W^n \Delta t^{1/2} \Rightarrow$$

$$M = (I + L\Delta t) \text{ and } N = K\sqrt{\Delta t}$$

$$\Rightarrow (I + L\Delta t)\, C\, (I + L^* \Delta t) - C = -K K^* \Delta t$$

To leading order in Δt

$$(L C_0 + C_0 L^*)\Delta t = -(K K^*)\Delta t$$

$$\Rightarrow \boxed{K K^* = -(L C_0 + C_0 L^*)}$$

Fluctuation dissipation balance

"correct" or limiting covariance as $\Delta t \to 0$

For Euler we have:

$$(I+L\Delta t)\,C\,(I+L^{*}\Delta t)-C = (LC_0+C_0L^{*})\Delta t$$

which is an equation for the error

$$\Delta C = C - C_0 = O(\Delta t)$$

One can do the same calculation for predictor-corrector (no difference between midpoint and trapezoidal for linear equations) to see that

$$\Delta C = O(\Delta t^2)$$

One can also construct Runge-Kutta $O(\Delta t^3)$ methods ...

For implicit midpoint (Crank-Nicolson in the context of diffusion equations)

$$x^{n+1} = \underbrace{\left(I - L\frac{\Delta t}{2}\right)^{-1}\left(I + L\frac{\Delta t}{2}\right)}_{M} x^n + \underbrace{\left(I - L\frac{\Delta t}{2}\right)^{-1}}_{N} K W^n$$

$\boxed{MCM^* - C = -NN^*}$ becomes

$$\left(I - L\frac{\Delta t}{2}\right)^{-1}\left(I + L\frac{\Delta t}{2}\right) C \left(I + L^*\frac{\Delta t}{2}\right)\left(I - L^*\frac{\Delta t}{2}\right)^{-1} - C$$

$$= \Delta t \left(I - L\frac{\Delta t}{2}\right)^{-1}\left(L C_0 + C_0 L^*\right)\left(I - L^*\frac{\Delta t}{2}\right)^{-1}$$

Pre and post multiply by $\left(I - L\frac{\Delta t}{2}\right)$ to get

$$\left(I+\frac{L\Delta t}{2}\right) C \left(I+\frac{L^{*}\Delta t}{2}\right)-\left(I-\frac{L\Delta t}{2}\right) C \left(I-\frac{L^{*}\Delta t}{2}\right)$$

$$=\left(LC+CL^{*}\right)\Delta t=\left(LC_0+C_0L^{*}\right)\Delta t$$

Therefore $\boxed{C=C_0}$ for any Δt and the scheme is great in this weak sense. The implicit midpoint is also unconditionally stable.