SDE simulation without time discretization

Nawaf Bou-Rabee

in collaboration with Eric Vanden-Eijnden
Key Role of Hydrodynamic Interactions in Colloidal Gellation
Furukawa and Tanaka 2010 PRL

\[
\begin{align*}
    dY &= -M(Y) D\mathcal{E}(Y) \, dt + \beta^{-1} \text{div} \, M(Y) \, dt + \sqrt{2\beta^{-1}} \sigma(Y) \, dW \\
    M(x) &= \sigma(x) \sigma(x)^T
\end{align*}
\]

Initial condition:

Energy function:
\[
\mathcal{E}(x_1, \cdots, x_N) = \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} U(|x_i - x_j|)
\]

\[
\frac{1}{r^{24}}
\]

steep hard core with attractive tail
ODE solution using forward Euler, $t=0.05$, $R_g=7.33$
SDE solution using forward Euler with small time-step, $t=0.02$, $R_g=7.35$
SDE solution using forward Euler with large time-step
Cubic Oscillator

\[ dY = -Y^3 \, dt + \sqrt{2} \, dW \]

random global attractor

\[ dY = -Y^3 dt + \sqrt{2} dW \]

cubic oscillator

numerical drift is destabilizing
Stochastic simulations of DNA in flow: Dynamics & the effects of HI
Jendrejack, de Pablo, and Graham J Chem Phys 2002

\[
\begin{align*}
\dot{Y} &= \kappa Y dt - M(Y)D\varepsilon(Y)dt + \beta^{-1} \text{div} M(Y)dt + \sqrt{2\beta^{-1}}\sigma(Y)dW \\
M(x) &= \sigma(x)\sigma(x)^T
\end{align*}
\]

linear flow + spring force

heat bath

Extensional Flow

finitely extensible
springs (as in Giles’ talk)
forward Euler, $t=0.02$, $R_g=5.94$
forward Euler, $t=0.00$, $R_g=6.07$
forward Euler, $h=0.015625$

\[ dY = \beta (\alpha - Y) dt + \sigma \sqrt{Y} dW \]

boundary at zero is attainable

\[ X(t) \]

\[ Y \]

2\(\beta \alpha / \sigma^2 = 0.12\)
Lotka-Volterra Process
Issues with SDE simulation

- Exploding trajectories due to stiff coefficients
- Nonphysical moves in SDEs with boundaries
- Long duration simulation

Control of the approximation in space would solve these issues.
Kolmogorov equations with unbounded coefficients

\[
\begin{aligned}
    \frac{\partial u}{\partial t}(x, t) &= Lu(x, t) \quad \forall t > 0, x \in \Omega \subset \mathbb{R}^n \\
    u(x, 0) &= \varphi(x) \quad \varphi \in B_b(\Omega, \mathbb{R})
\end{aligned}
\]

\[L f(x) = \text{Trace} \left( \mu(x) D f(x)^T + D^2 f(x) \sigma(x) \sigma(x)^T \right)\]

Associated SDE:

\[dY = \mu(Y) dt + \sqrt{2} \sigma(Y) dW\]

Describes evolution of conditional expectation of an observable with respect to SDE solution:

\[u(x, t) = \mathbb{E}_x (\varphi(Y(t)))\]
semidiscrete Kolmogorov equations

\[
\begin{aligned}
\dot{u}_h(t) &= Q u_h(t) \quad \forall t \geq 0, \quad u_h(0) = \varphi|_S \\
\end{aligned}
\]

Q must satisfy

(a) \( Q f(x) = L f(x) + \mathcal{O}(h^p) \)

(b) \( Q f(x) = \sum_{y \in S} q(x, y)(f(y) - f(x)) \), \( q(x, y) \geq 0 \)

(a) implies accuracy on finite and infinite time intervals
(b) implies Q is infinitesimally stochastic
stochastic simulation algorithm (SSA)

Popularized by Dan Gillespie (1976)
due to “Joe” Doob (~1945)

Given current state and time: \(X(t_0) = x\)

**step 1** update time

\[
t_1 = t_0 + \delta t \ , \quad \delta t \sim \text{Exp}(\sum_{y \in S \setminus \{x\}} q(x, y))
\]

**step 2** update state with probability

\[
P(X(t_1) = y \mid X(t_0)) = \frac{q(x, y)}{\sum_{y \in S \setminus x} q(x, y)}
\]
Sample Paths

Cubic oscillator

Stationary Density Accuracy

Committor Function Accuracy

MFPT Accuracy

log PDF

relative error

spatial step size

error

x

Committor Function Accuracy

MFPT Accuracy

x

spatial step size

Cubic oscillator
Natural Boundary, $2\beta\alpha/\sigma^2 = 2$

- $\ell_1$ error
- $\text{CIR process}$

Spatial step size vs. $\ell_1$ error

- $Q_u$
- $Q_c$
- $O(\delta x)$
- $O(\delta x^2)$
Regular Boundary, $2\beta\alpha/\sigma^2 = 0.5$

$\ell_1$ error

$10^{-1}$
$10^{-2}$
$10^{-3}$
$10^{-4}$
$10^{-5}$
$10^{-6}$

spatial step size

$10^{-2}$
$10^{-1}$

$CIR$ process

coarsest grid

-log PDF

$10^{-4}$
$10^{-2}$
$10^{0}$
$10^{2}$

$O(\delta x)$

$O(\delta x^2)$
Spectrum of OU Operators in $L^p$ spaces with respect to invariant measures
Metafune, Pallara, and Priola 2002 J Funct Anal

\[ dY = AY \, dt + dW \]

\[ \sigma(A) = \{ \lambda_1, \lambda_2 \} \]

\[ \Re(\lambda_1), \Re(\lambda_2) < 0 \]

Twenty eigenvalues of largest real part of the operator $L$ used to benchmark spatial discretization $Q$

\[ \sigma(L) = \{ n_1 \lambda_1 + n_2 \lambda_2 : \ n_1, n_2 \in \mathbb{N} \} \]
Accuracy in $\sigma(L)$

$\ell_2$ relative error

$10^{-2}$

$10^{-3}$

$10^{-4}$

OU process

spatial grid size

$O(h)$

$O(h^2)$

$O(U)$ process
Stationary Density Accuracy

Asymmetric OU process

$\ell_1$ error vs. spatial grid size

$O(h^2)$
Population dynamics model of predator (y) and prey (x)

\[
\begin{align*}
\mu(x, y) &= \begin{bmatrix} k_1 x - xy - \gamma_1 x^2 \\ -k_2 y + xy - \gamma_2 y^2 \end{bmatrix} \\
(\sigma \sigma^T)(x, y) &= \text{diag}(x, y) \begin{bmatrix} M^{11} & M^{12} \\ M^{12} & M^{22} \end{bmatrix} \text{diag}(x, y)
\end{align*}
\]

Support of stationary distribution

\[\mathbb{R}^2 \times \{0\}\]

Support of finite-time probability distribution

\[\mathbb{R}^2_+\]
Stability Concept

Method is geometrically ergodic when underlying SDE is.

Assume dissipativity condition:

\[
\mu(x)^T x \leq \alpha - \beta |x|^2 \quad \forall x \in \mathbb{R}^n
\]

Markov process is irreducible because for any two grids points, it is possible to get from one to the other in a finite number of jumps.

Generator satisfies infinitesimal drift condition

\[
V(x) = \exp \left( a \frac{|x|^2}{2} \right)
\]

\[
\exists R^* : \frac{QV(x)}{V(x)} < 0 \quad \forall |x| > R^*
\]

By Harris Theorem the process is geometrically ergodic

\[
\|P_t f - \nu(f)\|_V \leq \|f - \nu(f)\|_V e^{-\lambda t}
\]
Accuracy Concepts

Define the global error of the numerical method:

\[ \epsilon(t) = u_S(t) - u_h(t) \]

Satisfies a non-homogeneous Cauchy problem on a Banach space

\[ \dot{\epsilon}(t) - Q\epsilon(t) = (L - Q)u \]

\[ \epsilon(0) = 0 \]

Since \( Q \) is a bounded linear operator and \( u \) is continuous, variation of constants formula gives unique solution

\[ \epsilon(t) = \int_0^t \exp(((t - s)Q)(L - Q)u(s))ds \]
For any \( f \in B_b(\Omega, \mathbb{R}) \) there exists positive constant s.t.

\[
\sup_{t \in [0,T]} \left| \mathbb{E}_x \{ f | S (X(t)) \} - \mathbb{E}_x \{ f (Y(t)) \} \right| \leq C_f(x) h^2
\]

for all \( x \in S \). Pass to the limit in global error to obtain

\[
|\nu_h (f | S) - \nu (f)| \leq C_f h^2
\]
In conclusion, in several SDE problems it is desirable to cap the size of the update in space (think BD, CIR, LV, CO, etc.)

This cap can be achieved by spatially discretizing the Kolmogorov equation in a way that induces a Markov process that can be simulated using SSA

The resulting method
1) eliminates nonphysical moves;
2) is geometrically ergodic when the underlying SDE is;
3) adjusts time-lag according to the stiffness of SDE coefficients;
4) possesses a transparent probabilistic structure; and,
5) scales quadratically with system size.

**SDE simulation without time discretization**

Nawaf Bou-Rabee & Eric Vanden-Eijnden

Preprint available via email.
New Perspectives in MCMC

What?
Summer school organized by Chus Sanz-Serna

Where?
Universidad de Valladolid, Spain

When?
June 8-12, 2015

Why?
To study current theory and practice of MCMC for simulating SDEs and sampling probability distributions

Who can apply?
Postdoctoral or graduate students, particularly those with research interests in MCMC methods

Where to register?
http://wmatem.eis.uva.es/npmcmc/