Structure-Preserving Algorithms for Self-Adjoint Diffusions

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General Context

There exists a stationary density, i.e.,

$$(L^*\nu)(x) = 0$$

Issues:
- density is irregular
- density is not integrable
- density is not known
- dimension is high
- $\sigma(x)\sigma(x)^T$ is not pdf

Aims:
- explicit method
- long-time stable
- finite-time accurate
- accurate in small noise limit
- scales with system size
Special case: Self-adjoint diffusion

\[ dY = -MDU \, dt + \beta^{-1} \, \text{div} \, M \, dt + \sqrt{2\beta^{-1}} \, B \, dW \]
\[ M(x) = B(x)B(x)^T \]

Proposition 1. Generator of \( Y \) is \textbf{self-adjoint} with respect to

\[ \nu(x) = \exp(-\beta U(x)) \]

\[ \langle Lf, g \rangle_\nu = \langle f, Lg \rangle_\nu \iff p_t(x, y)\nu(x) = p_t(y, x)\nu(y) \]

\textbf{Self-adjoint property}
Motivation: Brownian Dynamics

With application to simulate bead-spring models of polymers in solution.

Fixman Integrator

\[ dY = -MDU dt + \beta^{-1} \operatorname{div} M dt + \sqrt{2\beta^{-1}} B dW \]
\[ M(x) = B(x)B(x)^T \]

**Predictor step**

\[ \begin{align*}
\tilde{X}_1 &= X_0 - hM(X_0)DU(X_0) + \sqrt{2h}B(X_0)\xi \\
X_1 &= X_0 - \frac{h}{2} \left( M(X_0)DU(X_0) + M(\tilde{X}_1)DU(\tilde{X}_1) \right) \\
&\quad + \frac{\sqrt{2h}}{2} \left( M(X_0) + M(\tilde{X}_1) \right) B(X_0)^{-T} \xi
\end{align*} \]

**Corrector step**

Two-step discretization of ‘kinetic stochastic integral’
Aims & Scope

Present explicit structure-preserving methods for self-adjoint diffusions that are:

① Can handle irregularities in nu.
② Weakly accurate at constant temperature.
③ Second order accurate in small noise limit.
④ Avoid computing divergence of mobility matrix.
⑤ Algorithm is ergodic when

\[ Z = \int_{\mathbb{R}^n} \nu(x) dx < \infty \]

*First four properties do not require that density is integrable.*
Fixman integrator requires a very small time-step to resolve jumps in square well.

Self-adjoint diffusion, but density is not integrable.

\[
\begin{align*}
dX &= -(U'(x) - F)dt + \sqrt{2kT}dW, \quad X(0) \in \mathbb{R}, \\
U(x + L) &= U(x).
\end{align*}
\]
Formula for mean first passage time derived by Stratonovich, Radiotekh Electron (1958)
Application: bead-spring chain in a solvent

Solvent velocity satisfies: $\mu u''(x) = F_i(t)\delta(x - q_i(t))$, $u(0) = u(L) = 0$.

Bead dynamics satisfy: $dX = M \vec{F}_{spring} dt + kT \text{div}(M) dt + \sqrt{2kT} B dW$.
Zero $kT$
High $kT$

$\text{t=0}$

Solvent Velocity

Graph showing solvent velocity over time with high $kT$. The velocity decreases over time, indicating some form of relaxation or diffusion process.
Bead-spring chain in a solvent

Initial condition

Relative error

Time step size

$\beta = 10$

$\beta = 10^2$

$\beta = 10^3$

$\beta \to \infty$

$O(h^{1/2})$

$O(h^2)$
Cartoon Model of DNA

A collection of beads connected by springs. The spring forces represent entropic effects (an observed force that increases entropy of the system) and involve fudge factors that are used to fit to real experimental data.
Motivation: microfluidic devices that manipulate DNA

How to manipulate DNA?
Motivation: microfluidic devices that manipulate DNA
Griffis et al. (2013), Lab on a Chip
**Radius of Gyration**

DNA in a Solvent

\[ U_{WLC}(r) = \frac{\beta^{-1}}{2b_k} \left( \frac{\ell^2}{\ell - r} - r + \frac{2r^2}{\ell} \right) \]
Euler (h = 0.01)

\[ U(x, y) = 5(y^2 - 1)^2 + 1.25 \left(y - \frac{x}{2}\right)^2 \]

Small Noise Limit Issue

Structure-preserving integrator can get stuck if noise is small enough
Approach: *Infinitesimal FDT*

**Proposition 2.** If $Z$ satisfies:

$$dZ = b(Z) \, dt + \sqrt{2\beta^{-1}} B(Z) \, dW$$

and generator of $Z$ is self-adjoint, then $Z = Y$ a.s.

**Proof:**

$$\langle Lf, g \rangle_\nu = \langle f, Lg \rangle_\nu \implies b = -MDU + \beta^{-1} \text{div } M$$

*drift is uniquely determined*

*nu-symmetry & noise accuracy are sufficient for accuracy of numerical approximation*
Approach: use Metropolis-Hastings to design non-symmetric integrators

Technique to generate samples from a probability distribution.

Approach: Metropolis-Hastings

Samples from a known probability distribution P.
STEP 1: generate proposal move using Q;
STEP 2: accept/reject to enforce detailed balance.

Turns an explicit integrator into a scheme that preserves detailed balance.
Does not require normalization constant of target probability density.
Approach: *Optimize Proposal Move*

In small noise limit SDE reduces to ODE:

\[
\dot{X} = -M(X) DU(X)
\]

Introduce RK2 discretization of ODE:

\[
\begin{cases}
X_1 = X_0 - h(b_1 M(X_0) DU(X_0) + b_2 M(\tilde{X}_1) DU(\tilde{X}_1)) , \\
\tilde{X}_1 = X_0 - a_{21} h M(X_0) DU(X_0).
\end{cases}
\]

Second order accuracy requires that \(b_1 + b_2 = 1\) and \(b_1 a_{21} = 1/2\); leaving \(a_{21}\) a free parameter.

*Optimize over free parameter.*
Metropolized Integration Scheme

Given $X_0$ & $h$, compute $X_1$ via:

$$X_1 = \gamma X^*_1 + (1 - \gamma) X_0$$

$$X^*_1 = \tilde{X}_1 + h G_h(\tilde{X}_1) + (\tilde{X}_1 - X_0)$$

Proposal move:

$$\tilde{X}_1 = X_0 + \sqrt{\frac{h}{2}} B_h(X_0) \xi$$

Acceptance Probability:

$$\alpha_h(X_0, \xi) = \min\left(1, \frac{\det(B_h(X_0))}{\det(B_h(X^*_1))} \exp\left(-\beta \left[ \frac{|\eta|^2}{2} - \frac{|\xi|^2}{2} + U(X^*_1) - U(X_0) \right] \right)\right)$$

$$B_h(X^*_1) \eta = B_h(X_0) \xi + \sqrt{2h} G_h(\tilde{X}_1)$$

Proposal reduces to:

$$\lim_{\beta \to \infty} X^*_1 = X_0 + h G_h(X_0)$$

(can pick to be RK2 combination)
Two-step proposal move

\[
\begin{align*}
X_0 & \\
& \overset{\rightarrow}{\rightarrow} \\
& B_h(X_0) \xi \\
& \quad \quad \overset{\rightarrow}{\rightarrow} \\
& X_1^* = \tilde{X}_1 + \sqrt{\frac{h}{2}} B_h(X_1^*) \eta \\
& \quad \quad \quad \overset{\rightarrow}{\rightarrow} \\
& \tilde{X}_1 = X_0 + \sqrt{\frac{h}{2}} B_h(X_0) \xi \\
& X_1^* + X_0 = 2 \tilde{X}_1 + h G_h(\tilde{X}_1)
\end{align*}
\]

Acceptance probability does not involve derivatives of \( G_h \) or \( B_h \) because of step-reversal symmetry.
Property: ergodic if density is normalizable

Thm. (BoDoVa2013) For every sufficiently regular $G_h$ and $B_h$:

$$\frac{1}{T} \int_0^T f(X_{\lfloor t/h \rfloor}) dt \to \frac{1}{Z} \int_{\mathbb{R}^n} f(x) \nu(x) dx , \quad \text{as } T \to \infty , \quad \text{a.s.}$$

nu-symmetry property is enforced by using the correct acceptance probability

$$\alpha_h(X_0, \xi) = \min \left( 1, \frac{\det(B_h(X_0))}{\det(B_h(X_1^*))} \exp \left( -\beta \left[ \frac{|\eta|^2}{2} - \frac{|\xi|^2}{2} + U(X_1^*) - U(X_0) \right] \right) \right)$$

$$B_h(X_1^*) \eta = B_h(X_0) \xi + \sqrt{2h} G_h(\tilde{X}_1)$$
Property: $\frac{1}{2}$-weakly accurate at finite noise

Thm. (BoDoVa2013) For every sufficiently regular $G_h$ and $B_h$:

$$B_h(x)B_h(x)^T = M(x) + O(h)$$

Metropolis integrator is $\frac{1}{2}$-weakly accurate:

$$|\mathbb{E}_x(f(Y([t/h]h))) - \mathbb{E}_x(f(X_{[t/h]}))| \leq C(T)h^{1/2}$$

for every $t \in [0, T]$ and $x \in \mathbb{R}^n$

Holds for any $G_h$ including the trivial choice $G_h=0.$
Property: 3/2-weakly accurate if mobility constant

Thm. (BoDoVa2013) Let \( G_h \) be:

\[
G_h(x) = -b_1 MDU(x) - b_2 MDU(x_1)
\]

\[
x_1 = x - ha_{12} MDU(x)
\]

Assume parameters satisfy standard second-order conditions:

\[
b_1 + b_2 = 1, \quad b_2 a_{12} = 1/2
\]

**Metropolis integrator is 3/2-weakly accurate:**

\[
|\mathbb{E}_x(f(Y([t/h]h))) - \mathbb{E}_x(f(X_{[t/h]}))| \leq C(T)h^{3/2}
\]
\[ dY = -Y^3 \, dt + \sqrt{2} \, dW \]
Brownian Particle with Heavy-Tailed Stationary Density
M. Hairer (2009), How hot can a heat bath get?

\[ \eta = 1.5, h = 2^{-2} \]

\[ dY = -\eta Y^{-1} + \sqrt{2}dW \]
Property: 2\textsuperscript{nd}-order accurate in small noise limit

Thm. (BoDoVa2013) Using Ralston RK parameters:
\[
\begin{align*}
    b_1 &= 5/8, b_2 = b_3 = -3/8, b_4 = 9/8, \\
    d_1 &= 1/4, d_2 = 3/4, \\
    c_{21} &= a_{21} = 2/3
\end{align*}
\]

Metropolisized scheme is second-order accurate in small noise limit:
\[
\lim_{\beta \to \infty} \left( \mathbb{E}_x \left| Y \left( \left[ t/h \right] h \right) - X_{\left[ t/h \right]} \right|^2 \right)^{1/2} \leq C(T)h^2
\]

Staggered RK2 combination
\[
\begin{align*}
    G &= -b_1 M DU - b_2 M(x_1) DU \\
        & \quad - b_3 M DU(x_1) - b_4 M(x_1) DU(x_1), \\
    x_1 &= x - a_{21} h M DU
\end{align*}
\]

Approximation to covariance of noise
\[
\begin{align*}
    B_h B_h^T &= d_1 M + d_2 M(x_2) \\
    x_2 &= x + c_{21} h M DU
\end{align*}
\]
\[ \alpha_h(X_0, \xi) \sim 1 \land \exp(-\beta \mathcal{E}(X_0, h)) \text{ as } \beta \to \infty \]

**Dominant term argument is used to control sign of** \( E(x,h) \)

\[
\mathcal{E}(x, h) = -\frac{h^3}{4} \left( M - \frac{h}{2} MA(x)M \right) (A(x)MDU(x), A(x)MDU(x))
\]
\[+ \frac{h^3}{4} \left( a_{12} - \frac{2}{3} \right) D^3U(x)(MDU(x), MDU(x), MDU(x)) + O(h^4) \cdot \]

**where the following line integral of Hessian matrix has been introduced:**

\[
A(x) = \int_0^1 D^2U(x - sha_{12}MDU(x)) ds
\]
\[ a_{12} = \frac{1}{2} \]

\[ \alpha_h(X_0, \xi) \sim 1 \wedge \exp(-\beta \mathcal{E}(X_0, h)) \quad \text{as} \quad \beta \to \infty \]
\[ \alpha_h(X_0, \xi) \sim 1 \land \exp(-\beta \mathcal{E}(X_0, h)) \quad \text{as} \quad \beta \to \infty \]
Minimize $E(x,h)$ over $a_{12}$

Replace proposal move in Metropolis integrator with:

$$
\begin{align*}
\tilde{X}_1 &= X_0 + \sqrt{\frac{h}{2}} B_h(X_0) \xi \\
\{ a_{12} &= \arg\min_{\alpha \in [1/2,1]} \mathcal{E}(\tilde{X}_1, h) \} \bigg|_{a_{12}=\alpha} \\
X_1^* &= 2\tilde{X}_1 - X_0 + h G_h(\tilde{X}_1)
\end{align*}
$$
\[ \alpha_h(X_0, \xi) \sim 1 \wedge \exp \left( -\beta E(X_0, h) \right) \quad \text{as} \quad \beta \to \infty \]

\[ U(x) = \left( 1 - x^2 \right)^2 / 4 \]
Conclusion

Presented nu-symmetric integrators for self-adjoint diffusions

Properties:

① Explicit.
② Weakly accurate at finite noise.
③ Second order in small noise limit.
④ Avoids computing divergence of mobility matrix.
⑤ Algorithm is ergodic when density is normalizable.

*Metropolized Integration Schemes for Self-Adjoint Diffusions.*
Limitations

① does not apply to situations lots of problems of practical interest where nu-symmetry condition does not hold.
② relies on an explicit formula for nu.
③ acceptance probability may deteriorate in high dimension.
④ may be incompatible with fast solvers for evaluating $U(x)$.
⑤ does not apply to rare event simulation.

*Metropolized Integration Schemes for Self-Adjoint Diffusions.*