A. DONEV

Numerical methods

Recall the generalized Markovian description of Langevin dynamics:

$$\dot{x} = -M \cdot \frac{\partial H}{\partial x} + kT \frac{\partial}{\partial x} \cdot M + \sqrt{2kT} \cdot W(t)$$

$$\widetilde{M}\widetilde{M}^{*} = (M + M^{*})/2$$

where $M(x)$ is the mobility tensor

$$M = \Gamma^{-1} \leftarrow \text{friction tensor}$$

$$D = (kT)\, M \leftarrow \text{diffusion tensor}$$

Remember that the spurious drift depends on the stochastic integral convention.

As a particular (important) example, consider <u>Brownian dynamics</u> for a collection of <u>colloidal particles</u> suspended in a fluid.

Denote $q \equiv \{q_1, q_2, \dots, q_N\}$ the positions (configuration) of the particles, and $V(q)$ the interaction potential (<u>effective</u>).

Under additivity assumptions, mobility / friction is the <u>Oseen tensor</u> from hydrodynamics:

$$M_{ij} = \frac{1}{6\pi\eta a} \begin{cases} \frac{3}{4}\frac{a}{r_{ij}}\left(\mathbf{1} + \frac{\vec{r}_{ij} \otimes \vec{r}_{ij}}{r_{ij}^2}\right), & i \neq j \\ \mathbf{1} & \text{if } i = j \end{cases}$$

particle indexes

Our previous analysis of drift suggests that numerical methods can avoid the evaluation of $\nabla_q \cdot M(q)$ by using a Backward Euler method for the anti-Ito or "isothermal" SODE:

$$\dot{q} = -M \cdot \nabla_q V + \sqrt{2kT} \boxed{\cdot} \tilde{M} \cdot \mathcal{W}(t)$$

To avoid an implicit method, we can use an explicit predictor-corrector method

BAD IDEA!

Explicit "Backward" Euler NOT CONSISTENT

$$\begin{cases} \tilde{q} = q(t) + \left[M (\nabla_q V) \Delta t + \sqrt{2\Delta t (kT)}\, \tilde{M}\, \tilde{\mathcal{W}} \right]_t \\ \quad \uparrow \text{predictor} \\ q(t+\Delta t) = q(t) + \Delta t M (\nabla_q V) + \sqrt{2\Delta t (kT)}\, \tilde{M}(\tilde{q}) \cdot \tilde{\mathcal{W}} \end{cases}$$

In the Fixman algorithm one can evaluate the term $M \nabla_q V$ at midpoint to improve the deterministic order of accuracy to second-order, though the formal order of accuracy (weak sense) remains one.

$\boxed{\text{How to construct } \widetilde{M} \text{ from } M\text{ ?}}$

All that matters at this stage is that $\widetilde{M}\,\widetilde{M}^{*} = M$

1. $\widetilde{M} = \widetilde{M}^{*} = M^{1/2}$ (matrix square root)
2. $\widetilde{M}$ = lower triangular square (Cholesky factorization)
3. $\widetilde{M}$ = non-square (physics ?)

A. DONEV Lecture 6 5

OCT-19-2011 09:37

So far we proposed the algorithm based on "Backward Euler", which we can condense to leading order as:

$$q(t+\Delta t) = q^{n+1} = q^{n} + M(q^{n}) \cdot \frac{\partial V}{\partial q^{n}} \Delta t \; +$$

$$\sqrt{2\Delta t\,(kT)} \cdot \tilde{M}\left[q^{n} + \sqrt{2\Delta t(kT)}\, \tilde{M}(q^{n}) \cdot \tilde{W}^{n}\right] \cdot \tilde{W}'$$

We already checked that this is correct in one dimension, but how about the multivariable case?

Let's check the drift due to the <u>multiplicative noise</u> explicitly:

P.005

"Spurious" drift:

$$\Delta q_k = \sqrt{2\Delta t(kT)}\ \frac{\partial \widetilde{M}_{kl}}{\partial q_i}\ \sqrt{2\Delta t(kT)}\left(\widetilde{M}\,\widetilde{W}\right)_i \widetilde{W}_l$$

$$\Rightarrow \frac{\langle \Delta q_k \rangle}{2\Delta t\,(kT)} = \frac{\partial \widetilde{M}_{kl}}{\partial q_i}\ \widetilde{M}_{ij} \langle \widetilde{W}_j \widetilde{W}_l \rangle =$$

$$= \frac{\partial \widetilde{M}_{kl}}{\partial q_i}\ \widetilde{M}_{ij}\ \delta_{jl} = \frac{\partial \widetilde{M}_{kj}}{\partial q_i}\ \widetilde{M}_{ij}$$

What we want to get is

$$\frac{1}{2}\left(\frac{\partial}{\partial q}\cdot M\right)_k = \frac{1}{2}\ \frac{\partial}{\partial q_i} M_{ik}$$

A. DONEV

$$\frac{1}{2}\frac{\partial}{\partial q_i} M_{ik} = \frac{1}{2}\frac{\partial}{\partial q_i}\left(\widetilde{M}_{ij}\widetilde{M}_{kj}\right) =$$

$$= \frac{1}{2}\left[\frac{\partial \widetilde{M}_{ij}}{\partial q_i}\widetilde{M}_{kj} + \widetilde{M}_{ij}\frac{\partial \widetilde{M}_{kj}}{\partial q_i}\right]$$

?

Compare this to previous $\widetilde{M}_{ij}\dfrac{\partial \widetilde{M}_{kj}}{\partial q_i}$

Except for a single variable, this does not seem to match.

So our "backward explicit Euler" algorithm is actually <u>not consistent</u>.

Do <u>NOT</u> use it!

Instead, rewrite the Langevin equation

$$\dot{q} = -M \cdot \frac{\partial V}{\partial q} + \sqrt{2kT} \boxdot M \cdot N \cdot W(t)$$

where $$NN^* = M^{-1} = \Gamma \leftarrow \text{Symmetric}$$

This is equivalent to what we wrote before since all that matters is the noise covariance (think FPE):

$$(MN)(MN)^* = MNN^*M^* = M$$

At first glance this requires both M and M^{-1}, which complicates things..

Fixman proposed the following mid-point explicit predictor-corrector alg:

$$\tilde{q}^{n+1} = q^n + M(q^n) \cdot \frac{\partial V}{\partial q^n} \Delta t + \sqrt{2\Delta t (kT)}\, M^n \cdot N^n \cdot W^n$$

$$q^{n+1/2} = \left(q^n + \tilde{q}^{n+1}\right)/2 \qquad (\text{midpoint})$$

$$\left\{ \begin{array}{l} q^{n+1} = q^n + M(q^{n+1/2}) \cdot \dfrac{\partial V}{\partial q^{n+1/2}} \Delta t + \\[2ex] \sqrt{2\Delta t (kT)} \cdot M(q^{n+1/2}) \cdot \underbrace{N^n \cdot W^n}_{\text{same as predictor!}} \end{array} \right.$$

Is this algorithm now consistent?

To leading order, we are doing

$$q^{n+1} = q^n + M(q^n)\cdot\frac{\partial V}{\partial q^n}\Delta t + \sqrt{2\Delta t(kT)}\cdot M\left[q^n + \sqrt{\frac{\Delta t(kT)}{2}}\, M(q^n)\cdot N(q^n)\widetilde{W}^n\right]\cdot N(q^n)\cdot\widetilde{W}^n$$

Now the extra drift is

$$\Delta q_k = \sqrt{2\Delta t(kT)}\,\frac{\partial M_{kl}}{\partial q_i}\cdot\sqrt{\frac{\Delta t(kT)}{2}}\,(MN\widetilde{W})_i\,(N\widetilde{W})_l$$

$$= \Delta t\,(kT)\,\frac{\partial M_{kl}}{\partial q_i}\,M_{ij}\,N_{jm}\widetilde{W}_m\,N_{ln}\widetilde{W}_n$$

$$\frac{\langle \Delta q_k \rangle}{(kT)\,\Delta t} = \frac{\partial M_{kl}}{\partial q_i} M_{ij} \overbrace{\left(N_{jm} N_{lm} \right)}^{(NN^*)_{jl}} =$$

$$= \frac{\partial M_{kl}}{\partial q_i} M_{ij} \left(M^{-1} \right)_{jl} = \frac{\partial M_{kl}}{\partial q_i} \left(\delta_{il} \right)$$

$$= \frac{\partial M_{ki}}{\partial q_i} = \frac{\partial M_{ik}}{\partial q_i} = \left(\frac{\partial}{\partial q} \cdot M \right)_k$$

So indeed the extra drift is

$$kT \left(\frac{\partial}{\partial q} \cdot M \right)$$ as it should be.

but maybe there are other ways also...

Recall that for additive noise (no x dependence in stochastic term) or for Langevin dynamics there is no problem with extra drift terms, and the "mobility" matrix M is rather simple:

$$\mathcal{H} = \frac{m u^2}{2} + V(q) = \frac{p^2}{2m} + V(q)$$

$$\Rightarrow \quad \frac{\partial H}{\partial z} = \begin{bmatrix} \partial V / \partial q \\ \\ \frac{p}{m} = u \end{bmatrix} \quad \text{where } z = (q, p)$$

A. Donev Lecture 6

(13)

reversible
Hamiltonian

$\partial H / \partial z$

$$\dot{z} = \begin{bmatrix} \dot{q} \\ \dot{p} \end{bmatrix} = \begin{bmatrix} 0 & \underline{1} \\ -\underline{1} & 0 \end{bmatrix} \begin{bmatrix} \partial V / \partial q \\ u \end{bmatrix}$$

skew-adjoint Liouville operator

$$- \begin{bmatrix} 0 & 0 \\ 0 & \gamma \end{bmatrix} \begin{bmatrix} \partial V / \partial q \\ u \end{bmatrix} \leftarrow \frac{\partial H}{\partial z}$$

"irreversible" self-adjoint friction operator

$$+ \begin{bmatrix} 0 \\ \sqrt{2kT\gamma} \end{bmatrix} W(t)$$

fluctuations

$\tilde{M}$, with $\tilde{M} \tilde{M}^* = M$

Recall the FPE for Langevin dynamics:

$$\frac{\partial P}{\partial t} = -\mathcal{L} P = -(\mathcal{L}_1 + \mathcal{L}_2 + \mathcal{L}_3 + \mathcal{L}_4) P$$

$$\begin{cases} \mathcal{L}_1 = \frac{p}{m} \cdot \frac{\partial}{\partial q} & \text{(advection) or streaming} \\ \mathcal{L}_2 = -\frac{\partial V}{\partial q} \cdot \frac{\partial}{\partial p} & \text{(constant force acceleration} \\ \mathcal{L}_3 = -\frac{\gamma}{m} \frac{\partial}{\partial p} p & \text{(constant friction)} \\ \mathcal{L}_4 = -\gamma k T \frac{\partial^2}{\partial p^2} & \text{(noise)} \end{cases}$$

In general $\gamma = \gamma(q)$

Recall that for Hamiltonian dynamics (MD) we desired symplectic integrators and constructed them using operator splitting and the Trotter factorization

$$P(\Delta t) = e^{-\mathcal{L}\Delta t} P(0)$$

Strang splitting

$$\approx e^{-\mathcal{L}_\alpha \Delta t/2} e^{-\mathcal{L}_\beta \Delta t} e^{-\mathcal{L}_\alpha \Delta t/2} P(0)$$

most expensive in middle ?

where $\mathcal{L} = \mathcal{L}_\alpha + \mathcal{L}_\beta$

For this to work as written the two pieces $\mathcal{L}_\alpha$ and $\mathcal{L}_\beta$ should ideally be exactly solvable so that

$$e^{-\mathcal{L}_\alpha \Delta t} \text{ and } e^{-\mathcal{L}_\beta \Delta t} \text{ are exact.}$$

This suggests the splitting

$$\begin{cases} \mathcal{L}_\alpha = \mathcal{L}_1 & \text{(streaming advection)} \\ \mathcal{L}_\beta = \mathcal{L}_2 + \mathcal{L}_3 + \mathcal{L}_4 & \text{(Ornstein-Uhlenbeck momentum update)} \end{cases}$$

We already showed how to do this.

Explicitly:

$$\begin{cases} q^{n+1} = q^n + \dfrac{p^n}{m}\Delta t \quad (\text{this is } \chi_\alpha \Delta t) \\ p^{n+1} = p^n e^{-\alpha \Delta t} + \dfrac{m}{\gamma} F(q^n)\left(1 - e^{-\alpha\Delta t}\right) \\ \qquad + \sqrt{mkT\left(1 - e^{-2\alpha\Delta t}\right)} \cdot \underset{\uparrow \text{ random normal variate}}{\mathcal{N}(0,1)} \end{cases}$$

where $\alpha = \gamma / m$

This is the so-called <u>quasi-symplectic</u> <u>Stochastic Verlet</u> algorithm.

Another option is to do the splitting

$$\mathcal{L}_\alpha = \mathcal{L}_1 + \mathcal{L}_2$$ (Hamiltonian dynamics)

use any <u>second-order</u> symplectic integrator

$$\mathcal{L}_\beta = \mathcal{L}_3 + \mathcal{L}_4$$ (irreversible dynamics)

use previous formula with $F \equiv 0$

Both splittings give quasi-symplectic integrators (Jacobian not unity but constant), but it seems there is no common agreement on which one is "best".