Numerical Schemes for Overdamped Langevin Equations

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I. LANGEVIN EQUATION WITH POSITION-DEPENDENT FRICTION

Consider the simple system

$$\begin{aligned}
&\partial_t \boldsymbol{v} = \boldsymbol{F}(\boldsymbol{x}) - \epsilon^{-1}\boldsymbol{\gamma}(\boldsymbol{x})\,\boldsymbol{v} + \sqrt{2kT\epsilon^{-1}\boldsymbol{\gamma}(\boldsymbol{x})}\,\boldsymbol{\mathcal{W}}(t)\\
&\partial_t \boldsymbol{x} = \boldsymbol{v},
\end{aligned}$$

in the overdamped limit $\epsilon \to 0$. Taking this limit formally starts from rescaling time as $\tau = \epsilon^{-1} t$, to get a family of equations parameterized by ϵ,

$$\begin{aligned}
&\partial_\tau \boldsymbol{v} = \epsilon^{-1}\boldsymbol{F}(\boldsymbol{x}) - \epsilon^{-2}\boldsymbol{\gamma}(\boldsymbol{x})\,\boldsymbol{v} + \epsilon^{-1}\sqrt{2kT\boldsymbol{\gamma}(\boldsymbol{x})}\,\boldsymbol{\mathcal{W}}(t)\\
&\partial_\tau \boldsymbol{x} = \epsilon^{-1}\boldsymbol{v},
\end{aligned}$$

and then looking at the limit $\epsilon \to 0$. This is done by splitting the generator of this diffusion process and the solution of the Fokker-Planck equation into a part proportional to ϵ^{-1} and a part proportional to ϵ^{-2} and doing asymptotic analysis as $\epsilon \to 0$. This calculation gives the limiting dynamics as the **overdamped Langevin equation** (here we take $\epsilon = 1$ since in the limit the precise value does not matter so long as it is small enough) as the Ito equation

$$\partial_t \boldsymbol{x} = \left[\boldsymbol{\gamma}^{-1}(\boldsymbol{x})\right]\boldsymbol{F}(\boldsymbol{x}) + \sqrt{2kT\boldsymbol{\gamma}^{-1}(\boldsymbol{x})}\,\boldsymbol{\mathcal{W}}(t) + (kT)\,\partial_{\boldsymbol{x}}\cdot\boldsymbol{\gamma}^{-1}(\boldsymbol{x})\,. \tag{1}$$

A. Derivative-Free Methods

The well-known Fixman algorithm can be thought of as a predictor-corrector algorithm for solving (1) in the enlarged space,

$$\begin{aligned}
\boldsymbol{\gamma}^n\boldsymbol{v}^n =& \boldsymbol{F}^n + \sqrt{\frac{2kT}{\Delta t}}\;(\boldsymbol{\gamma}^n)^{\frac{1}{2}}\,\boldsymbol{W}^n\\
\boldsymbol{x}^{\star,n+1} =& \boldsymbol{x}^n + \boldsymbol{v}^n\Delta t\\
\boldsymbol{\gamma}^{\star,n+1}\boldsymbol{v}^{n+1} =& \boldsymbol{F}^{n+1} + \sqrt{\frac{2kT}{\Delta t}}\;(\boldsymbol{\gamma}^n)^{\frac{1}{2}}\,\boldsymbol{W}^n\\
\boldsymbol{x}^{n+1} =& \boldsymbol{x}^n + \left(\frac{\boldsymbol{v}^n + \boldsymbol{v}^{n+1}}{2}\right)\Delta t.
\end{aligned}$$

It is not hard to show that in the limit $\Delta t \to 0$ this converges to the solution of the Ito equation (1). The method is second-order deterministically but only first order weakly accurate and half-order strongly accurate in the stochastic setting.

An alternative way to get the correct thermal drift term $(kT)\,\partial_{\boldsymbol{x}} \cdot \boldsymbol{\gamma}^{-1}(\boldsymbol{x})$ is to handle it using a "random finite difference" approach and combine with Euler-Maruyama,

$$\begin{aligned}\boldsymbol{x}^{n+1} &= \boldsymbol{x}^{n} + (\boldsymbol{\gamma}^{n})^{-1}\,\boldsymbol{F}^{n}\Delta t + \sqrt{2kT\Delta t}\;\;(\boldsymbol{\gamma}^{n})^{-\frac{1}{2}}\,\boldsymbol{W}^{n} \\ &+ (kT)\,\Delta t\left\{\delta^{-1}\left[\boldsymbol{\gamma}^{-1}\left(\boldsymbol{x}+\frac{\delta}{2}\,\tilde{\boldsymbol{W}}^{n}\right)-\boldsymbol{\gamma}^{-1}\left(\boldsymbol{x}-\frac{\delta}{2}\,\tilde{\boldsymbol{W}}^{n}\right)\right]\tilde{\boldsymbol{W}}^{n}\right\},\end{aligned}$$

where $\tilde{\boldsymbol{W}}^{n}$ are auxiliary i.i.d. standard normal variates and δ is a small number (chosen based on roundoff considerations as with finite-difference methods).

B. Metropolization

Let us denote the mobility with $\boldsymbol{M}(\boldsymbol{x}) = \boldsymbol{\gamma}^{-1}(\boldsymbol{x})$. Assume that our trial (proposal) move is a step of the Euler-Maruyama method,

$$\tilde{\boldsymbol{x}} = \boldsymbol{x} + \boldsymbol{v}\,\Delta t + (2k_BT\Delta t)^{\frac{1}{2}}\,\boldsymbol{B}\Delta\boldsymbol{W} = \boldsymbol{x} + \boldsymbol{v}\,\Delta t + \Delta\boldsymbol{x}_{\text{rand}} = \boldsymbol{x} + \Delta\boldsymbol{x},$$

where $\boldsymbol{B}\boldsymbol{B}^{T} = \boldsymbol{M}$, $\Delta\boldsymbol{W}$ is a vector of i.i.d. standard normal variates, and $\boldsymbol{v} = -\boldsymbol{M}\boldsymbol{F}(\boldsymbol{x}) = \boldsymbol{M}\boldsymbol{\nabla}U(\boldsymbol{x})$ is the deterministic steady-state velocity. It is important to note, however, that one can also take $\boldsymbol{v} = \boldsymbol{0}$ and still get a consistent algorithm. From now on tilde will denote a quantity evaluated at $\tilde{\boldsymbol{x}}$.

The transition probability from $\boldsymbol{x}$ to $\tilde{\boldsymbol{x}}$ is trivial to calculate,

$$Q(\boldsymbol{x} \to \tilde{\boldsymbol{x}}) = (2\pi)^{-\frac{d}{2}}\,|\boldsymbol{M}|^{-\frac{1}{2}}\exp\left(-\frac{\Delta\boldsymbol{W}^{T}\Delta\boldsymbol{W}}{2}\right).$$

To write the reverse one, we need to calculate the noise that would take us back,

$$\boldsymbol{x} = \tilde{\boldsymbol{x}} + \tilde{\boldsymbol{v}}\,\Delta t + (2k_BT\Delta t)^{\frac{1}{2}}\,\tilde{\boldsymbol{B}}\Delta\tilde{\boldsymbol{W}},$$

and then set

$$Q(\tilde{\boldsymbol{x}} \to \boldsymbol{x}) = (2\pi)^{-\frac{d}{2}}\left|\tilde{\boldsymbol{M}}\right|^{-\frac{1}{2}}\exp\left(-\frac{\Delta\tilde{\boldsymbol{W}}^{T}\Delta\tilde{\boldsymbol{W}}}{2}\right).$$

The target distribution for the Metropolis-Hastings acceptance-rejection is the Gibbs-Boltzmann distribution $\sim \exp(-U(\boldsymbol{x})/k_BT)$.

After some algebra, we get that the acceptance probability for the trial move should be $\min(1,p)$ where

$$p=\left|\tilde{\boldsymbol{M}}^{-1}\boldsymbol{M}\right|^{\frac{1}{2}}\exp\left[\beta\left(U-\tilde{U}\right)-\beta\left(\bar{\boldsymbol{v}}\Delta t+\Delta\boldsymbol{x}_{\text{rand}}\right)^{T}\tilde{\boldsymbol{M}}^{-1}\bar{\boldsymbol{v}}-\frac{\beta}{4\Delta t}\Delta\boldsymbol{x}_{\text{rand}}^{T}\tilde{\boldsymbol{M}}^{-1}\Delta\boldsymbol{x}_{\text{rand}}+\frac{1}{2}\Delta\boldsymbol{W}^{T}\Delta\boldsymbol{W}\right],$$

which can alternatively be written as

$$\begin{aligned}
p &= \left|\tilde{\boldsymbol{B}}^{-1}\boldsymbol{B}\right|\exp\left[\beta\left(U-\tilde{U}\right)-\beta\left(\tilde{\boldsymbol{M}}^{-1}\bar{\boldsymbol{v}}\right)^{T}\Delta x\right.\\
&- \frac{\beta\Delta t}{4}\left(\tilde{\boldsymbol{v}}+\boldsymbol{v}\right)^{T}\tilde{\boldsymbol{M}}^{-1}\left(\tilde{\boldsymbol{v}}-\boldsymbol{v}\right)\\
&+ \left.\frac{1}{2}\Delta\boldsymbol{W}^{T}\left(\boldsymbol{I}-\boldsymbol{B}^{T}\tilde{\boldsymbol{M}}^{-1}\boldsymbol{B}\right)\Delta\boldsymbol{W}\right],
\end{aligned}\tag{2}$$

where $\bar{\boldsymbol{v}}=\left(\boldsymbol{v}+\tilde{\boldsymbol{v}}\right)/2$ is the average (midpoint estimate of the) drift, and recall that $\Delta\boldsymbol{x}=\boldsymbol{v}\,\Delta t+\Delta\boldsymbol{x}_{\text{rand}}$.

In the limit $\Delta t\to 0$ the resulting Metropolized Euler-Maruyama integrator converges to the solution of the Ito equation (1).