Langevin MC

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1 Motivation

2 Langevin Monte Carlo Algorithms

3 Langevin Equation

The Langevin equation is an SDE with the form

$$\mathrm{d}X_t = -\nabla U(X_t)\,\mathrm{d}t + \sqrt{2\gamma}\,\mathrm{d}W_t$$

We call U the potential function. It is the properties of this function that govern whether each scheme will converge? This equation has π as its invariant distribution, meaning that simply simulating the SDE for long enough will give an approximation of π. The obvious way to do this is using the Euler-Maruyama scheme, which gives the following approximation

$$X_{n+1} = X_n - \gamma\nabla U(X_n) + \sqrt{2\gamma}Z_{n+1}, \qquad X_0 = x_0$$

Here $Z_n \sim N(0,1)$ i.i.d. However, it is well known that this method does not always give the correct answer, and diverges whenever $\nabla U(x)$ is superlinear (See Roberts & Tweedie 1996). How can we solve this problem? We can look at either discretising the SDE in a different way (HOLA, LM); or we can modify the Euler scheme to mitigate the issues. Here we will focus on the latter, although our code has algorithms from both approaches.

4 Taming

Taming has been suggested for ULA by Brosse, Durmus, Moulines and Sabanis, as well as by Roberts & Tweedie for MALA (they called the result MALTA). The idea is to scale the gradient

5 ULA

$$X_{n+1} = X_n - \gamma\nabla U(X_n) + \sqrt{2\gamma}Z_{n+1}, \qquad X_0 = x_0$$

6 MALA

[2] Propose V_{n+1} using Langevin dynamics:

$$V_{n+1} = X_n - \gamma\nabla U(X_n) + \sqrt{2\gamma}Z_{n+1}$$

Calculate acceptance probability

$$\alpha(X_n, V_{n+1}) = 1 \wedge \frac{\pi(V_{n+1})q(V_{n+1}, X_n)}{\pi(X_n)q(X_n, V_{n+1})}$$

Here $q(x,y)$ is the transition probability, ¶$(X_{n+1} = y | X_n = x)$. If `rand`$\leq \alpha$,

$$X_{n+1} = V_{n+1}.$$

That is,

$$X_{n+1} = \mathbb{I}(u \leq \alpha)V_{n+1} + \mathbb{I}(u > \alpha)X_n$$

7 Taming the Gradient

7.1 tULA/c

$$X_{n+1} = X_n - \gamma T_\gamma(X_n) + \sqrt{2\gamma} Z_{n+1}, \qquad X_0 = x_0$$

where $T_\gamma(x) = \frac{\nabla U(x)}{1+\|\nabla U(x)\|}$ or $T_\gamma(x) = \left(\frac{\nabla U(x)}{1+|\partial_i U(x)|}\right)_{i=\{1,\dots,d\}}$

7.2 tHOLA

[3] Use an Itô-Taylor expansion

$$X_{n+1} - X_n + \mu_\gamma(X_n)\gamma + \sigma_\gamma(X_n)\sqrt{\gamma} Z_{n+1}$$

where

$$\mu_\gamma(x) = -\nabla U_\gamma(x) + \frac{\gamma}{2}\left(\left(\nabla^2 U \nabla U\right)_\gamma(x) - \vec{\Delta}(\nabla U)_\gamma(x)\right),$$

and $\sigma_\gamma(x) = \mathrm{diag}\left(\left(\sigma_\gamma^{(k)}(x)\right)_{k\in\{1,\dots,d\}}\right)$ with,

$$\sigma_\gamma^{(k)}(x) = \sqrt{2 + \frac{2\gamma^2}{3}\sum_{j=1}^{d} |\nabla^2 U_\gamma^{(k,j)}(x)|^2 - 2\gamma \nabla^2 U_\gamma^{(k,k)}(x)}$$

ALSO need to define the gamma subscript, i.e. the tamed variables. is gamma best subscript? Although fn depends on gamma it doesn't indicate that taming has occurred.

7.3 tMALA/c

Use the same taming T as in `tULA`. Is this sensible? Could compare with `MALTA`.

7.4 MALTA?

[?] Tame with

$$T = \frac{\nabla U(x)}{1 \vee \gamma|\nabla U(x)|}$$

for some constant $D > 0$

8 LM

[1] Non-Markovian scheme,

$$X_{n+1} = X_n + \gamma \nabla U(X_n) + \sqrt{\frac{\gamma}{2}}(Z_n + Z_{n+1})$$

9 RWM

Popular variant of the Metropolis-Hastings algorithm (CITE) with a normal proposal.

$$U_{n+1} = X_n + \sqrt{2\gamma} Z_{n+1}$$

Calculate acceptance probability

$$\alpha(X_n, U_{n+1}) = 1 \wedge \frac{\pi(U_{n+1}) q(U_{n+1}, X_n)}{\pi(X_n) q(X_n, U_{n+1})}$$

Here $q(x, y)$ is the transition probability, $\P(X_{n+1} = y | X_n = x)$. If `rand`$\leq \alpha$,

$$X_{n+1} = U_{n+1}.$$

That is,

$$X_{n+1} = \mathbb{I}(u \leq \alpha) U_{n+1} + \mathbb{I}(u > \alpha) X_n$$

10 Beyond Moments

References

[1] Charles Matthews and Benedict Leimkuhler. Rational Construction of Stochastic Numerical Methods for Molecular Sampling. *Applied Mathematics Research eXpress*, 2013(1):34–56, 06 2012.

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[3] Sotirios Sabanis and Ying Zhang. Higher order langevin monte carlo algorithm. Workingpaper, ArXiv, 8 2018.