Langevin Monte Carlo

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Metropolis-adjusted Langevin Algorithm or Langevin Monte Carlo is used to get samples from an intractable probability distribution function. It combines the equation of Langevin diffusion (which simulates a particle moving in a fluid with random fluctuations) with the Metropolis Hastings Algorithm. If we have a probability distribution function $\pi(\mathbf{X})$ where $\mathbf{X}$ is a d-dimensional vector, then we can define the Langevin distribution as

$$U(\mathbf{X}) = \log \pi(\mathbf{X})$$

The gradient of the Langevin distribution guides the random walk towards high probability areas. We start with an initial configuration $\mathbf{X}_0$. New states are proposed by the following formula

$$\mathbf{X}^*_{\mathbf{k+1}} = \mathbf{X}_{\mathbf{k}} + \epsilon \nabla U(\mathbf{X}_k) + \sqrt{2\epsilon}\xi_k$$

where $\xi_k \backsim \mathcal{N}_d(0, \mathbf{I})$, ϵ is the step size $(0 < \epsilon \ll 1)$. The acceptance criterion for each new state is given by

$$\gamma = \min\left(1, \frac{\pi(\mathbf{X}^*_{\mathbf{k+1}})q(\mathbf{X}_k|\mathbf{X}^*_{k+1})}{\pi(\mathbf{X}_k)q(\mathbf{X}^*_{k+1}|\mathbf{X}_k)}\right)$$

where

$$q(\mathbf{X}^*|\mathbf{X}) = \exp\left\{-\frac{1}{4\epsilon}\|\mathbf{X}^* - \mathbf{X} - \epsilon\nabla U(\mathbf{X})\|_2^2\right\}$$