

Langevin Monte Carlo for Ising Model Sampling

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Overdamped Langevin dynamics uses the following discrete update equation to generate new states -

$$X_{k+1} := X_k - \frac{1}{\gamma} \nabla U(X_k) + \frac{\sqrt{2}\sigma}{\gamma} \xi_k$$

where γ is the friction coefficient, σ is the noise strength, and $\xi_k \sim \mathcal{N}(0, I)$.

Since Langevin dynamics is guaranteed to sample from $\exp\{-\beta U(X)\}$ we can use it as a sampling algorithm by setting $U = -\log \pi$ where π is some probability distribution. Langevin Monte Carlo incorporates a Metropolis-Hastings accept-reject step. New steps are proposed by the following equation -

$$\tilde{X}_{k+1} := X_k + \tau \nabla \log(\pi(X_k)) + \sqrt{2\tau} \xi_k,$$

where τ is the step-size parameter, and accepted with probability

$$\alpha(X_k, \tilde{X}_{k+1}) = \min \left\{ 1, \frac{\pi(\tilde{X}_{k+1})q(\tilde{X}_{k+1} | X_k)}{\pi(X_k)q(X_k | \tilde{X}_{k+1})} \right\},$$

where $q(x | y)$ is the transition density from state x to y . This requires the target distribution π to be differentiable.

Suppose we want to sample from an Ising chain with N spins, coupling strength J , and external field h . I'm having trouble figuring out how to define a differentiable potential U such that the Langevin Monte Carlo samples from the Ising distribution. If we represent each $X_k = \{\sigma_i\}_{i=1}^N$ where $\sigma_i \in \{-1, 1\}$, and adjacent states differ by a single spin flip, then I don't understand how to compute the gradient. One idea I had was to relax each σ_i to take values in $[-1, 1]$ instead of $\{-1, 1\}$, but I'm confused on how to define the potential in that case.