Hamiltonian Monte Carlo on Ising Model

Yuze Zhou

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Ising Model Depiction

- Let $s = \{s_1, s_2 \cdots s_n\}$, $s_i \in \{0, 1\}^n$ be the binary random vector representing the spin configurations of the ferromagnet
- s is distributed as followed:

$$p(s) \propto \frac{1}{Z} exp(a^\tau s + \frac{1}{2} s^\tau W s)$$

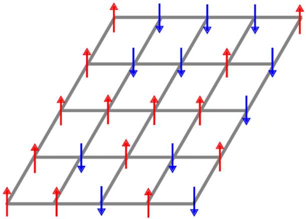

Figure 1: Ising Model on a Lattice

- W is a real-symmetric matrix representing the interactions between different electrons

Continuous Relaxation on Ising Model

- Conditioning on s, the continuous random vector $x \in \mathbb{R}^n$ is normally distributed as:

$$x|s \sim N(A(W+D)s, A^{\tau}(W+D)A)$$

- D is a diagonal matrix ensuring that $W + D$ is positive-definite
- A is an arbitrary non-singular matrix

Continuous Relaxation on Ising Model

- Let $a = diag(A)$, $d = diag(D)$ and $\alpha_X = A^{-1}x$
- The joint distribution of (x, s) is:
  $p(x,s) \propto exp(-\frac{1}{2}x^{\tau}(A^{-1})^{\tau}(W+D)^{-1}A^{-1}x + s^{\tau}A^{-1}x + (a-\frac{1}{2}d)^{\tau}s)$
- The marginal distribution for x is:
  $p(x) \propto exp(-\frac{1}{2}x^{\tau}(A^{-1})^{\tau}(W+D)^{-1}A^{-1}x)\prod_{i=1}^{n}(1+exp(\alpha_{X;i}+a_i-\frac{d_i}{2}))$
- The conditional distribution of s given x is Bernoulli whose parameter is given by:
  $$p(s_i|x) = \sigma(-\alpha_{X;i} - a_i + \frac{d_i}{2})^{1-s_i}\sigma(\alpha_{X;i} + a_i - \frac{d_i}{2})^{s_i}$$
  where $\sigma(z) = 1/(1+exp(-z))$

Continuous Relaxation on Ising Model

- s_i are conditionally independent given x
- If A is chosen as $(W + D)^{-1/2}$, x_i are also conditionally independent given s
- If $A = I$, s_i is conditionally dependent only on x_i

Hamiltonian Monte Carlo for Discrete Random Vector

- Sampling from s would be easy if we could sample the marginal distribution of x since the conditional distribution of s given x are independent Bernoullis.
- x has a continuous and differentiable probability density function, which guarantees that it could be sampled using Hamiltonian dynamics.
- Let the potential energy function $U(x)$ be:

$$
\begin{aligned}
U(x) &= -log(p(x)) \\
&= \frac{1}{2}x^{\tau}(A^{-1})^{\tau}(W+D)A^{-1}x - \sum_{i=1}^{n} log(1+exp(\alpha_{X;i}+a_i-\frac{d_i}{2}))
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$$

- The corresponding kinetic energy function $K(p)$ is:

$$K(p) = \sum_{i=1}^{n} \frac{p_i^2}{2m_i}$$

- The Hamiltonian is therefore:

$$H(x,p) = U(x) + K(p)$$

Hamiltonian Monte Carlo for Discrete Random Vector

- Let $l_X \in \mathbb{R}^n$ whose ith entry is:
$$l_{X;i} = \frac{exp(\alpha_{X;i}+a_i-\frac{d_i}{2})}{1+exp(\alpha_{X;i}+a_i-\frac{d_i}{2})}$$
- The gradient of the potential energy function would therefore be:
$$\frac{\partial U}{\partial x} = (A^{-1})^{\tau}(W+D)^{-1}A^{-1}x - A^{-1}l_X$$

Hamiltonian Monte Carlo for Discrete Random Vector

- The Hamoltonian Dynamics for sampling s is

Algorithm 1: Hamiltonian MCMC for Ising Model

Initialisation: Choose step-size ϵ, iteration times N and starting point (x^0, p^0);

for $0 \le n \le N-1$ **do**

$\tilde{p}_i^{n+1} = p_i^n - \frac{\epsilon}{2}\frac{\partial U}{\partial x_i}(x^n)$;

$x_i^{n+1} = x_i^n + \epsilon\frac{\tilde{p}_i^{n+1}}{m_i}$;

$p_i^{n+1} = \tilde{p}_i^{n+1} - \frac{\epsilon}{2}\frac{\partial U}{\partial x_i}(x^{n+1})$;

Accept the new state (x^{n+1}, p^{n+1}) with probability:

$$\min[1, exp(-U(x^{n+1}) + U(x^n) - K(p^{n+1}) + K(p^n))]$$

Otherwise set (x^{n+1}, p^{n+1}) as (x^n, p^n)

Compute $\alpha_X^{n+1} = A^{-1}x^{n+1}$

Sample $p(s_i^{n+1}|x) = \sigma(-\alpha_{X;i}^{n+1} - a_i + \frac{d_i}{2})^{1-s_i^{n+1}}\sigma(\alpha_{X;i}^{n+1} + a_i - \frac{d_i}{2})^{s_i^{n+1}}$

end

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