Non-reversible Monte Carlo simulations of spin models

Overview

In this discussion we will look at a non-reversible Monte Carlo simulation. Most Monte Carlo algorithms require the transition probabilities to satisfy the detailed balance equation. But especially for Markov chains on finite state space we can easily proof that we only need irreducibility and aperiodicity to achieve convergence to a unique invariant distribution. That is why we will relax the detailed balance condition and construct an algorithm with a non-reversible state update to speed up convergence.

Some Math

Define: $\Omega = \{1, ..., n\}$ finite state space, P stochastic matrix, π invariant distribution

Detailed balance equation: $\pi(x)P(x, y) = \pi(y)P(y, x)$ for all $x, y \in \Omega$.

Convergence Theorem:
Suppose that P is irreducible and aperiodic, with stationary distribution π. Then there exist constants $\alpha \in (0, 1)$ and $C > 0$ such that $\max_{x \in \Omega} \|P^t(x, \cdot) - \pi\|_{TV} \leq C\alpha^t$. See proof in [3], page 52.

Simple Random Walk

Transition probabilities:
$P(1, 1) = 0.5,\ P(n, n) = 0.5,$
$P(x, x + 1) = 0.5\ \forall x \in \{1, ..., n - 1\},\ P(x, x - 1) = 0.5\ \forall x \in \{2, ..., n\}$

Invariant Distribution: $\pi = [1/n\ \ ...\ \ 1/n]$

Directed Random Walk

Now we double the state space and introduce an extra label for up and down directions.

Transition probabilities:
$P((+, x), (+, x + 1)) = 1 - 1/n,\ P((+, x), (-, x + 1)) = 1/n$
$P((-, x), (-, x - 1)) = 1 - 1/n,\ P((-, x), (+, x - 1)) = 1/n$
$P((+, n), (-, n)) = 1 - 1/n,\ P((+, n), (+, n)) = 1/n$
$P((-, 1), (+, 1)) = 1 - 1/n,\ P((-, 1), (-, 1)) = 1/n$

Invariant distribution: $\pi(\pm, \cdot) = [1/2n\ \ ...\ \ 1/2n]$

Marginal invariant distribution: $\pi = [1/n\ \ ...\ \ 1/n]$, easily proven, because P is double-stochastic. See [2] Chapter 2.

Algorithm for non-uniform distributions

Step A: Metropolis update $(\pm, x) \rightarrow (\mp, x \pm 1)$ with acceptance probability:

$$p_{acc} = \min\left[1\,, \frac{\pi(\mp, x \pm 1)}{\pi(\pm, x)}\right]$$

Step B: Flip label to keep direction $(\pm, x) \rightarrow (\mp, x)$ with fixed probability $1 - \theta$.

See [1] Chapter 2 for more details.

Example:

One dimensional Mean-Field Ising Model over magnetization M with N spins.

$$p_{acc} = \min\left[1\,, \frac{N \mp M}{N \pm M + 2} \exp\left(\frac{2\beta J}{N}(\pm M + 1)\right)\right]$$

Fiber algorithm

Step A: Randomly select stepsize s from a given set.

Step B: Metropolis update $(\pm, x) \rightarrow (\mp, x \pm s)$ with acceptance probability:

$$p_{acc} = \min\left[1\,, \frac{\pi(\mp, x \pm s)}{\pi(\pm, x)}\right]$$

Step C: Flip label to keep direction $(\pm, x) \rightarrow (\mp, x)$ with fixed probability $1 - \theta$.

See [2] Chapter 5.2 for general approach.

References

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3. **Levin, Peres, Wilmer**
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   http://pages.uoregon.edu/dlevin/MARKOV/markovmixing.pdf

Material for this presentation: **http://tinyurl.com/kzmthcq**