

430.714

Estimation Theory

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Lecture outline

Metropolis updates

Symmetric proposals and the Boltzmann distribution

Gibbs sampling

Sequential updates from full conditional distributions

Markov blankets

Local information needed for each update

The Ising-model target

$$x \in \{-1, +1\}^N, \quad |\Omega| = 2^N$$

$$p(x) = \frac{e^{-\beta E(x)}}{Z}, \quad Z = \sum_{z \in \Omega} e^{-\beta E(z)}$$

β is inverse temperature. $E(x)$ is the configuration energy.

Enumerating all configurations grows exponentially with N .

The Metropolis algorithm

$$x' \sim q(\cdot \mid x), \quad q(x' \mid x) = q(x \mid x')$$

$$\alpha(x, x') = \min \left\{ 1, \frac{p(x')}{p(x)} \right\}$$

A proposal with higher target probability has acceptance 1.

The normalizing constant cancels

$$p(x) = \frac{\tilde{p}(x)}{Z}$$

$$\frac{p(x')}{p(x)} = \frac{\tilde{p}(x')/Z}{\tilde{p}(x)/Z} = \frac{\tilde{p}(x')}{\tilde{p}(x)}$$

Evaluate the unnormalized target at the current and proposed states.

Metropolis acceptance for an energy change

$$\Delta E = E(x') - E(x)$$

$$\alpha(x, x') = \min\{1, e^{-\beta \Delta E}\}$$

ΔE ($\beta = 1$)	Acceptance
-2	1
0	1
+2	0.1353

A Metropolis update

1. Propose x' from the symmetric distribution q .
2. Compute $\alpha(x, x')$ and draw U from $\text{Uniform}(0, 1)$.

$$X_{k+1} = \begin{cases} x', & U \leq \alpha(x, x'), \\ x, & U > \alpha(x, x'). \end{cases}$$

A rejection repeats the current state in the trajectory.

Metropolis–Hastings

An asymmetric proposal needs a reverse-proposal correction.

$$\alpha(x, x') = \min \left\{ 1, \frac{p(x')q(x \mid x')}{p(x)q(x' \mid x)} \right\}$$

Symmetric q recovers the Metropolis rule.

Detailed balance for Metropolis–Hastings

$$\begin{aligned} p(x)q(x' \mid x)\alpha(x, x') &= \min\{p(x)q(x' \mid x), \\ &\quad p(x')q(x \mid x')\} \\ &= p(x')q(x \mid x')\alpha(x', x) \end{aligned}$$

Equal flow in both directions makes p stationary.

Gibbs sampling

$$x = (x_1, \dots, x_d), \quad x_{-i} = (x_j)_{j \neq i}$$

$$x'_i \sim p(\cdot \mid x_{-i}), \quad x'_{-i} = x_{-i}$$

Update one coordinate while holding all others fixed.

The update uses the exact full conditional distribution.

A sequential Gibbs sweep

Choose an ordering and update each coordinate in turn.

$$x_i^{(k+1)} \sim p\left(x_i \mid x_1^{(k+1)}, \dots, x_{i-1}^{(k+1)}, x_{i+1}^{(k)}, \dots, x_d^{(k)}\right)$$

The newest values enter the next conditional

A sweep is one complete pass through the coordinates.

Keep observed variables fixed.

Gibbs as a Metropolis–Hastings proposal

$$x' = (x'_i, x_{-i})$$

$$q_i(x' \mid x) = p(x'_i \mid x_{-i})$$

$$q_i(x \mid x') = p(x_i \mid x_{-i})$$

Factorization for a Gibbs update

$$p(x) = p(x_i \mid x_{-i})p(x_{-i})$$

$$p(x') = p(x'_i \mid x_{-i})p(x_{-i})$$

Both states share the same unchanged coordinates x_{-i} .

The Gibbs acceptance ratio is one

$$\frac{p(x')q_i(x \mid x')}{p(x)q_i(x' \mid x)} = \frac{p(x'_i \mid x_{-i})p(x_{-i})p(x_i \mid x_{-i})}{p(x_i \mid x_{-i})p(x_{-i})p(x'_i \mid x_{-i})} = 1$$

$$\alpha_i(x, x') = \min\{1, 1\} = 1$$

Every exact full conditional proposal has acceptance one.

Comparison of MCMC algorithms

Method	Proposal	Acceptance
Metropolis	Symmetric q	Target ratio
Metropolis–Hastings	General q	Target and q ratios
Gibbs	Full conditional	1

All three generate dependent samples along a Markov chain.