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Reversibility & Metropolis-Hastings

Markov chain has state set X

transition matrix P

$$P_{xy} = \Pr(\text{transition } \underline{\text{from}} \ x \ \underline{\text{to}} \ y)$$

Stationary distrib $\pi^T P = \pi^T$.

Ergodic. $\exists$ finite t s.t. P^t is positive in every coord.

Theorem. Ergodic MC have unique stationary distrib and for any distrib of initial state x_0, say π_0, the distrib. of state after t transitions, x_t, converges to stationary distribution π.

Def. Trans. matrix P is reversible w.r.t. π if it satisfies

$$\forall x,y \quad \pi_x P_{xy} = \pi_y P_{yx}$$

Prop. P reversible wrt $\pi \implies \pi$ is stationary for P.

Proof. $(\pi^T P)_y = \sum_{x \in X} (\pi^T)_x P_{xy} = \sum_{x \in X} (\pi^T)_y P_{yx} = (\pi^T)_y$

Verifies $\pi^T P = \pi^T$.

The Metropolis-Hastings Procedure

Given unnormalized $w : X \to \mathbb{R}_{\geq 0}$,

and "proposal matrix" $K \in \mathbb{R}^{X \times X}$

which is symmetric and stochastic

$K_{xy} = K_{yx}$ $\qquad K_{xy} \geq 0, \quad K \cdot \vec{1} = \vec{1}.$

the Metropolis-Hastings transition probabilities are

$$P_{xy} = \begin{cases} K_{xy} \cdot \dfrac{\min\{w(x), w(y)\}}{w(x)} & x \neq y \\ 1 - \sum_{z \neq x} P_{xz} & x = y \end{cases}$$

To simulate one M-H transition starting from state x s.t. $w(x) > 0$:

(1) Draw y at random w. prob. K_{xy}.

(2) With prob $\frac{\min\{w(x), w(y)\}}{w(x)}$ move to y.

(3) With remaining probability remain at X.

Prop. M–H is reversible w.r.t. $\pi = \frac{w}{Z}$.

Proof. To prove $\forall x, y$

$$\left(\frac{w(x)}{Z}\right) P_{xy} = \left(\frac{w(y)}{Z}\right) P_{yx}$$

Assume $x \neq y$

K symmetric

min{·,·} symmetric

$$\frac{\cancel{w(x)}\, K_{xy} \min\{w(x), w(y)\}}{\cancel{Z} \cdot \cancel{w(x)}} \stackrel{?}{=} \frac{\cancel{w(y)}\, K_{yx} \min\{w(y), w(x)\}}{\cancel{Z} \cdot \cancel{w(y)}}$$

Metropolis-Hastings for q-colorings of G.

Recall.

$$X = \{\text{all functions } V(G) \to [q]\}$$

$$w(x) = \begin{cases} 1 & \text{if } x \text{ is proper coloring} \\ \phi & \text{if not.} \end{cases}$$

Use proposal distrib.

$$K_{xy} = \begin{cases} \frac{1}{|V(G)| \cdot q} & \text{if } \mathrm{HammDist}(x,y) = 1 \\ \frac{1}{q} & \text{if } x = y \\ 0 & \text{otherwise} \end{cases}$$

K_{xy} = Probability of getting y when you start with x, choose random v and color c, and define y as "x with v relabeled to c."

(1) Draw y at random w. prob. K_{xy}.

Pick random v and random c.
Propose to change v to color c.

(2) With prob $\frac{\min\{w(x), w(y)\}}{w(x)}$ move to y

Reject the move if the new color matches a neighbor.

(3) With remaining probability remain at x.

Else accept.

→ Glauber dynamics