

MCMC: Sampling from a state space using Markov Chains

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27 October

Spanning trees

Given $g = (V, E)$ with $|V| = n$, the number of spanning trees of $G = n^{n-2}$.

- a spanning tree has $|V| - 1$ edges.
- adding an edge creates a unique cycle

Every subgraph with $n - 1$ edges and no cycles is a spanning tree.

Aim: to sample uniformly from the set of spanning trees of G .

1. Let X_t be a spanning tree S_1 . Choose any edge e from $E(S_1)$ uniformly at random.
2. Let C be a unique cycle in $X_t \cup e$
3. Choose e' from $E(C)$ uniformly.
4. Set $X_{t+1} = (X_t \setminus \{e\}) \cup \{e'\}$

Exercise: Write the transition matrix of this chain and show that it is irreducible, aperiodic and symmetric.

Knapsack Problems

m items each with value v_i and weight w_i for $1 \leq i \leq n$. Find $S \subseteq \{1, \dots, n\}$ st $\sum_{i \in S} v_i = S$ and $\sum_{i \in S} w_i \leq C$.

Space of feasible solutions $S = \{z : \langle w, z \rangle \leq C\}$

- Start at some $z \in S$
- Choose $j \in \{1, \dots, n\}$ uniformly
- $y = (z_1, z_2, \dots, (1 - z_j) \dots, z_m)$.
- If $\langle w, y \rangle \leq C$,
 - $X_{t+1} = y$
 - otherwise $X_{t+1} = z$

However, the walk is more efficient if we instead sample $j \sim \pi(j) \propto e^{\beta \langle v, z \rangle}$ for some $\beta > 0$.

Metropolis algorithm

S is a discrete space. Q a symmetric transition matrix on S and π , the target distn.

Given X_t , X_{t+1} is chosen to follow MC,

1. Choose Y randomly according to Q , called the proposal. $P(Y = j | X_t = i) = q_{ij}$
2. Define the acceptance probability $\alpha = \min\{1, \pi_Y / \pi_i\}$
3. Let $U \sim \text{uniform}(0,1)$. If $U \leq \alpha$ then $X_{t+1} = Y$. Otherwise $X_{t+1} = X_t$

$$P_{ij} = q_{ij} * \alpha$$

Proposition: If Q is irreducible, symmetric and π a prob distn. st $\pi > 0 \forall i \in S$, then the Metropolis chain is also irr, and reversible wrt π .

Proof:

Q is irr $\implies P$ irr

$$\pi_i p_{ij} = \pi_i q_{ij} \alpha = q_{ij} \min\{\pi_i, \pi_j\} = \pi_j q_{ij} \min\{1, \pi_i/\pi_j\} = \pi_j p_{ji}$$