MCMC: Sampling from a state space using Markov Chains

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

   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 $1 < i < n$. Find $S = i$, st $\arg\max_{\{i,\}} \sum_i v_i = S$ and $\sum_i w_i < C$.

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

- Start at some $z \in S$
- Choose $j \in \{1, ..n\}$ uniformly
- $y = (z_1, z_2, \ldots (1 - z_j) \ldots, z_m)$.
- 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 $\pi(j) \propto e^{\beta \langle v,z \rangle}$ 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 ~ 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

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