Introduction to Markov Chains

Motivation from Chemistry

Basics

We assume a finite state space $[N]$. $P = (p_{ij})_{ij=1}^{N}$ is an $N \times N$ matrix representing transition probabilities, i.e., $p_{ij} = Pr(X_{t+1} = j | X_t = i)$, with this relation holding for all t. We can also obtain the s-step transition probabilities from P, $P^s = p_{ij}^{(s)} = Pr(X_{t+s} = j | X_t = i)$, independent of t. We denote the initial distribution of the Markov chain by the vector $\pi^{(0)}$, typically $\pi^{(0)} = (0, \ldots, 0, 1, 0, \ldots, 0)$. Also, $\pi^{(0)} P^s = \pi^s$ is the distribution after s steps if we started at $\pi^{(0)}$.

Definition : A Markov chain is *irreducible* if $\forall\, i, j \;\exists\, s$ s.t. $p_{ij}^{(s)} > 0$, i.e. you can reach i from j.

Definition : A Markov chain is *aperiodic* if $GCD(s | p_{ij}^{(s)} > 0) = 1 \;\forall\, i, j$.

Definition : A Markov chain is *ergodic* if $\exists$ a vector π (the *stationary distribution*) s.t. $\lim_{s \to \infty} p_{ij}^{(s)} = \pi_j, forall$i, j.

Theorem : Any finite chain which is aperiodic and irreducible is ergodic.

Definition : A Markov chain is *time reversible* if it satisfies "detail balance":

$$\pi_i p_{ij} = \pi_j p_{ji}$$

Using Markov chains to sample:

S is a set of combinatorial objects, e.g. $S =$ perfect matchings on a graph G of size n.

1) State Space Γ, s.t. $S \subset \Gamma$, with $|\Gamma| = N$.

2) Space is connected (low degree, i.e. polynomial).

3) The Markov chain is aperiodic, time-reversible, and irreducible, implying that $\exists!\, \pi$. We ensure aperiodicity by imposing a self-loop, i.e. $p_{ii} > 0$ (in fact we will want $p_{ii} \geq 1/2$, which we will explain later).

4) We want the stationary distribution π to be meaningful, genarally this means we would like π to be uniform on S and

$$\pi(s) = \sum_{s \in S} \pi(s) \geq \frac{1}{q(n)},$$

for some polynomial q.

5) The chain should be "rapidly mixing."

Tools for showing rapid mixing

1) Conductance - a measure of the structure of the Markov chain.

2) Coupling

Markov Chains for Matchings

We let $\Gamma = \{\text{all matchings}\}$ and start off at some state $M \in \Gamma$.

1) $M' = M$ with probability 1/2.

2) $Pick\ e \in_u E$

$$M' = \begin{cases} M \setminus \{e\} & \text{if } e \in M \\ M \cup \{e\} & \text{if } e \text{ can be added} \\ M \cup \{e\} \setminus \{e'\} & \text{if } e = (u, v) \text{ and only } u \text{ (or } v\text{) is matched in M (by the edge } e'\text{)} \\ soM & \text{otherwise} \end{cases}$$