Reversible Markov Chains

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1 Preliminaries

We will be working with a Markov chain $X(t)$ taking values in a countable state space E. We will assume the our time t is discrete, taking values in $\mathbb{Z}$. Our Markov chain is assumed to be time homogeneous, meaning that for any $k, j \in E$ and $t, \tau \in \mathbb{Z}$, $P(X(t+\tau) = k|X(t) = j)$ does not depend on t. Finally, we will assume that $X(t)$ is irreducible, meaning that every state E can be reached from every other state.

Recall that the transition probability $p(i, j)$ is defined by

$$p(i, j) = P(X(t+1) = i|X(t) = j)$$

where $i, j \in E$. We say that a process has an equilibrium distribution if there is a collection of positive numbers $\pi(j)$, all summing to one, such that they satisfy the equilibrium equations:

$$\pi(j) = \sum_{k \in E} \pi(k)p(k, j) \qquad j \in E$$

If an equilibrium distribution exists, it is unique and

$$\lim_{t \to \infty} P(X(t) = k|X(0) = j) = \pi(k) \qquad j, k \in E$$

2 Reversibility

Definition: A process is said to be *reversible* if $(X(t_1), X(t_2), ..., X(t_n))$ has the same distribution as $(X(\tau - t_1), X(\tau - t_2), ..., X(\tau - t_n))$ for all $t_1, ..., t_n, \tau \in \mathbb{Z}$.

This definition has an immediate consequence. Recall that a stochastic process is *stationary* if, for all $t_1, t_2, ..., t_n, \tau \in \mathbb{Z}$, $(X(t_1), X(t_2), ..., X(t_n))$ has the same distribution as $(X(t_1 + \tau), X(t_2 + \tau), ..., X(t_n + \tau))$.

Proposition: *A reversible process is stationary.*

Proof: Since $X(t)$ is reversible, $(X(t_1), ..., X(t_n))$ and $(X(t_1+\tau), ..., X(t_n+\tau))$ both have the same distribution as $(X(-t_1), X(-t_2), ..., X(-t_n))$. Hence $X(t)$ is stationary.

3 Major Theorems

Before we examine some examples of reversible processes, let us state some of the major theorems regarding reversible Markov chains.

Theorem: *A stationary process is reversible iff there exists a positive collection of numbers $\pi(j)$ summing to unity such that*

$$\pi(j)p(j,k) = \pi(k)p(k,j) \text{ for all } k, j \in E \tag{1}$$

When such a collection exists, it is the equilibrium distribution.

Remark: The equations given by (1) are known as the detailed balance equations.

Intuitively, $\pi(j)p(j,k)$ can be thought of as the probability flux from state j to state k. Thus the detailed balance equations say that the probability flux from state j to state k equals that from state k to state j. The equilibrium balance equations can be interpreted to say that the flux out of state j equals that into state j.

Notice that the detailed balance equations allow us to determine if a process is reversible based on the transition probabilities and the equilibrium distribution equations, while the equilibrium distribution equations are determined solely be the transition probabilities. Thus we are led to ask if it is possible to determine if a process is reversible from the transition probabilities alone. This turns out to be the case:

Theorem (Kolmogorov's Criterion): *A stationary Markov chain is reversible iff its transition probabilities satisfy*

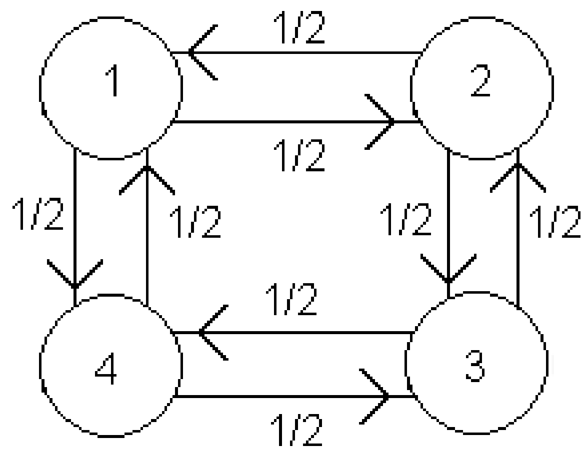
$$p(j_1, j_2)p(j_2, j_3)...p(j_{n-1}, j_n)p(j_n, j_1) = p(j_1, j_n)p(j_n, j_{n-1})...p(j_3, j_2)p(j_2, j_1)$$

for any sequence of states $j_1, j_2, ..., j_n \in E$.

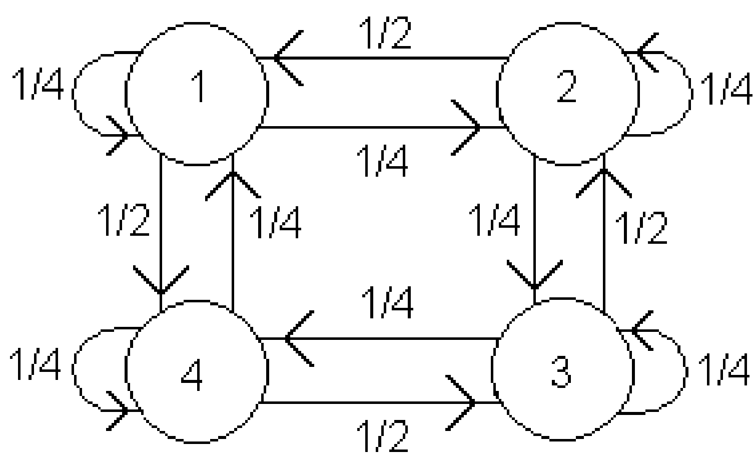
Intuitively, Kolmogorov's Criterion says that, given a starting point $j_1 \in E$, any path that ultimately returns to j_1 must have the same probability whether this path is traced in one direction or the other.

4 Examples

Examples of stochastic processes which are reversible include stationary birth-death processes, M/M/1 queues, and symmetric random walks. For instance, it is easy to see from Kolmogorov's Criterion that the Markov chain given below is reversible:



On the other hand, Kolmogorov's Criterion shows that the following process is not reversible, as a clockwise loop around the graph has probability $\frac{1}{256}$ while a counterclockwise loop has probability $\frac{1}{16}$:



5 Reversibility and Chemical Reaction Networks

Recall: A chemical reaction network is reversible if $\nu_k \to \nu_k^{'} \in \mathcal{R}$ implies $\nu_k^{'} \to \nu_k \in \mathcal{R}$. Note that this is different than the notion of reversibility for a Markov chain.

Consider a deterministically modeled system which is complex balanced with equilibrium c. For any closed, irreducible subset of the state space, Γ, the stochastically modeled system with intensities

$$\lambda_k(x) = \kappa_k \prod_{l=1}^{m} \frac{x_l!}{(x_l - v_{lk})}! \tag{2}$$

has stationary distribution of the form

$$\pi(x) = M \prod_{i=1}^{m} \frac{c_i^{x_i}}{x_i!}$$

where $x \in \Gamma$ and M is a normalizing constant.

A deterministically modeled chemical reaction network with equilibrium value c is said to be detailed balanced if for each pair of reversible reactions $\nu_k \rightleftharpoons \nu_k^{'}$, we have

$$\kappa_k c^{\nu_k} = \kappa_k^{'} c^{\nu_k^{'}}$$

where $\kappa_k, \kappa_k^{'}$ are the rate constants for the reactions $\nu_k \to \nu_k^{'}$, $\nu_k^{'} \to \nu_k$, respectively.

This brings us to the connection between reversible Markov chains and reversible reaction networks:

Theorem: Let $\{\mathcal{S}, \mathcal{C}, \mathcal{R}\}$ be a reversible chemical reaction network with rate constants $\{\kappa_k\}$. Then the deterministically modeled system has an equilibrium for which it is detailed balanced if and only if the stochastically modeled system with intensities (2) is reversible (in the sense of a Markov chain) when in its stationary distribution.

6 References

David F. Anderson, Gheorghe Craciun, and Thomas G. Kurtz, *Product-form stationary distributions for deficiency zero chemical reaction networks*, submitted, arXiv:0803.3042.

Frank P. Kelly, *Reversibility and Stochastic Networks*, Wiley, Chichester, 1979, reprinted 1987, 1994.