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Inference in Reversible Markov Chains

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Inference in Reversible Markov Chains

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Abstract

This dissertation describes the research that we have done concerning reversible Markov chains. We first present definitions for what it means for a Markov chain to be reversible. We then give applications of where reversible Markov chains are used and give a brief history of Markov chain inference. Finally, two journal articles are found in the paper, one that is already published and another which is currently being submitted.

The first article examines estimation of the one-step-ahead transition probabilities in a reversible Markov chain on a countable state space. A symmetrized moment estimator is proposed that exploits the reversible structure. Examples are given where the symmetrized estimator has superior asymptotic properties to those of a naive estimator, implying that knowledge of reversibility can sometimes improve estimation. The asymptotic mean and variance of the estimators are quantified. The results are proven using only elementary results such as the law of large numbers and the central limit theorem.

The second article introduces two statistics that assess whether (or not) a sequence sampled from a time-homogeneous Markov chain on a finite state space is reversible. The test statistics are based on observed deviations of transition sample counts between each pair of states in the chain. First, the joint asymptotic normality of these sample counts is established. This result is then used to construct two chi-squared-based tests for reversibility. Simulations assess the power and type one error of the proposed tests.

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Chapter 1

Introduction to Reversible Markov Chains

A Markov chain is a random process controlled by probability laws with many applications to finance, biology, statistics, queueing theory, chemistry, and more. Consider this simple example, start a knight at a random square, according to the initial distribution $\boldsymbol{\pi}^{(0)}$, on an otherwise empty 8×8 chessboard. Move the knight at random around the board according to valid moves that a knight can make, where each square is given a number 1 to 64. If the knight is currently in square i, the probability it moves next to square j is $p_{i,j}$ independent of all previous moves. The probability that the knight moves to the successive states $i_1, i_2, \ldots, i_k$ is $\pi_{i_1}^{(0)} p_{i_1,i_2} p_{i_2,i_3} \cdots p_{i_{k-1},i_k}$. Thus determining how the knight moves among the squares is determined by $\pi_i^{(0)}$ and the $p_{i,j}$'s. This dissertation considers statistical questions about the $p_{i,j}$'s. One such question is whether or not the knight moves randomly among the squares. In this case we would test whether or not the $p_{i,j}$'s are uniform in their rows for all distinct i. When the rows are uniform the process would be reversible. We note, for future reference of reversibility, the backwards movement of the knight among the squares would also be random.

A Markov chain is then a sequence of random variables $\{X_t\}_{t=0}^{\infty}$ taking values in the set $\{1, 2, \ldots, m\}$ with the property that

$$\mathrm{P}(X_{t+1} = j | X_0 = i_0, \ldots, X_t = i) = p_{i,j},$$

this is called the Markov property. When $X_t = j$, we say the Markov chain is in state j at time t. A Markov chain has the property that the probability of being in state j is conditionally independent of all previous states visited given the current state is i and the conditional probability is $p_{i,j}$. The finite dimensional distributions and hence the probability laws of the Markov chain are determined by the initial distribution, $\boldsymbol{\pi}^{(0)}$, and the $p_{i,j}$'s. Any probability statement about a Markov chain can be answered in terms of $\boldsymbol{\pi}^{(0)}$ and the $p_{i,j}$'s. Thus the $p_{i,j}$'s are the key parameters in a Markov chain and the dissertation considers statistical questions about them.

One important topic in Markov chain theory is determining when the stationary and limiting distributions exist. An irreducible Markov chain has stationary distribution $\boldsymbol{\pi}$, which satisfies

$$\boldsymbol{\pi} = \boldsymbol{\pi}\mathbf{P},$$

where $\mathbf{P}$ is the $m \times m$ matrix of the $p_{i,j}$'s. Note $\boldsymbol{\pi}$ is determined by the $p_{i,j}$'s. When the Markov chain is aperiodic $\boldsymbol{\pi}$ is also a limiting distribution in that

$$\pi_j = \lim_{t \to \infty} \mathrm{P}(X_t = j | X_0 = i).$$

A Markov chain is stationary when

$$(X_\tau, X_{\tau+1}, \ldots, X_{\tau+t}) \stackrel{\mathcal{D}}{=} (X_0, X_1, \ldots, X_t)$$

for all $\tau, t \in Z_+$, where $\stackrel{\mathcal{D}}{=}$ denotes equal in distribution. For an irreducible Markov chain a necessary and sufficient condition for stationarity is that the initial distribution is $\boldsymbol{\pi}$.

This dissertation considers statistical problems in reversible Markov chains. A Markov chain is reversible if the chain has the same distribution in forward and backward time, or

$$(X_0, X_1, \ldots, X_t) \stackrel{\mathcal{D}}{=} (X_t, X_{t-1}, \ldots, X_0)$$

for every t. Since a reversible Markov chain must be stationary, a necessary and sufficient condition for reversibility is the detailed balance equations;

$$\pi_i p_{i,j} = \pi_j p_{j,i}$$

for all states i and j. As will be seen in the next chapters, much of the statistical analysis developed in this dissertation is based upon the detailed balance equations. The next section will provide a survey of the relevant Markov chain literature.

1.1 History

There is an abundance of literature relating to the theory and applications of Markov chains. The literature relating to reversibility and statistical inference; however, is much smaller and references intersecting the two topics is nearly nonexistent. The book by Kelly (1979) is an exception, he does a wonderful job exploring reversibility in stochastic processes. One important topic in Markov chain theory is to determine the convergence rate of a Markov chain to its stationary distribution (Fill (1991)), this is an example where exploiting reversibility (as we aim to do) can give us a better result. If the Markov chain is known to be reversible, then we get a better convergence rate to stationarity (Desai and Rao (1993)). Other topics of interest include moments in stationary Markov chains (Tweedie (1983)), sensitivity of the stationary distribution (Meyer (1994)), maxima of stationary chains (Rootzén (1988)), etc.

Statistical inference on stochastic processes initiated in the 1950's with the dissertation of Grenander (1950) on inference in stochastic processes. The dissertation demonstrated that hypothesis testing and estimation apply to stochastic processes. The thrust of his work showed how the methods apply to time series. Bartlett (1950) sought to find a goodness of fit test for the frequency counts $N_{i,j}$, the number of times the chain makes a transition from state i to state j, for a Markov chain. In doing so, he used maximum likelihood principles to find

$$\hat{p}_{i,j} = \frac{N_{i,j}}{N_i}\mathbf{1}_{[N_i=0]} \tag{1.1}$$

and also established asymptotic normality of $N_{i,j}$. Whittle (1955) used a spectral representation of $p_{i,j}$ to derive the joint distribution of $(N_{i,j}, N_{k,l})$. Using results by Feller, Derman (1956) states that $N_{i,j} - L\pi_i p_{i,j}$ has the same asymptotic distribution as $N_{i,j} - \mathrm{E}(N_{i,j})$ and established joint asymptotic normality of the $N_{i,j}$'s. In the appendix, we provide a straightforward approach for calculating the covariances in this asymptotic normality. Anderson and Goodman (1957) view the $N_{i,j}$'s as multinomial random variables given $N_i = k_i$ for some constant k_i, $i \in S$. They also devised many hypothesis tests for Markov chains, which include testing if the transition probabilities are constant and the order of the Markov chain. Billingsley (1961) also discusses multinomial properties of the $N_{i,j}$'s and uses them to construct χ^2 hypothesis tests. Other authors (Basawa and Rao (1980), Bhat and Miller (2002)) used previous knowledge to construct new hypothesis tests for stationarity or testing for specified values in the one-step-ahead transition matrix. Part of this dissertation expands on the result by Greenwood and Wefelmeyer (1999), who show that there is a better symmetrized estimator for the one-step-ahead transition probabilities if it is known that the Markov chain is reversible. They show that

$$\hat{p}_{i,j}^{(R)} = \frac{N_{i,j} + N_{j,i}}{2N_i} \mathbf{1}_{[N_i=0]} \tag{1.2}$$

is a more efficient estimator than (1.1) for reversible chains.

We point out two things in particular that have been done previously and strive to do the same under reversibility; developing the estimator $\hat{p}_{i,j}$, and creating a hypothesis test for stationarity. In the next chapter, we show in some cases that $\hat{p}_{i,j}^{(R)}$ is twice as efficient as $\hat{p}_{i,j}$, and in others gives the same efficiency. The other part of our work devises statistical tests for reversibility.

1.2 Applications

Markov chains have many applications; any board game that is played with dice (Monopoly, Life, Candy Land), random walks, birth and death processes, Markov chain Monte Carlo methods, telephone exchanges, statistical mechanics (in particular the Ehrenfest model), migration processes, etc. Some of these form reversible Markov chains while others do not. To stick with our theme we will only present examples here were the Markov chain is reversible.

A simple application of our work arises in thermodynamics. Thermodynamics is the science of energy and its transformation; engineers are often interested in equilibrium processes. Classical thermodynamics deals with variables that can be measured in a laboratory; i.e. heat, pressure, etc. Statistical thermodynamics explains what happens to particles at a microscopic level; one such example is the Ehrenfest model of diffusion. In this model, N particles in total are floating around in a container with two compartments (0 and 1). The particles change compartments at rate λ, see figure 1.1 below. Let $X(t)$ be the number of particles in compartment 0 at time t. Then $X(t)$ is a birth-and-death process and the transition rates are known to be $q_{i,i-1} = i\lambda$ for $i = 1, 2, \ldots, N$, $q_{i,i+1} = (N - i)\lambda$ for $i = 0, 1, \ldots, N - 1$. This chain has equilibrium distribution $\pi_i = 2^{-N}\binom{N}{i}$.

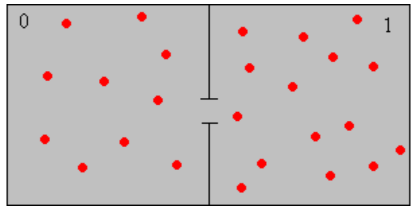

Figure 1.1: Ehrenfest Model of Diffusion

Using the detailed balance equations, we can easily confirm that this is a reversible process. This process is known to always be reversible. Hence, if we did not know the rate λ at which the particles change containers, we could estimate these transition probabilities efficiently by using the above proposed estimator $\hat{p}_{i,j}^{(R)}$.

Resnick (1992) presents a good example in exercise 2.22 of a case where a branching process with immigration is reversible. The process $\{Z_n\}$ obeying

$$Z_{n+1} = I_{n+1} + \sum_{j=1}^{Z_n} Z_{nj}$$

governs a branching process with immigration, where the random variables $\{I_n, n \geq 1\}$ count the number of immigrants per generation and $\{Z_{nj}, n \geq 1, j \geq 1\}$ are i.i.d. random variables that count the number of offspring that member j of generation n produces ($\{I_n\}$ and $\{Z_{nj}\}$ are assumed independent). It is easy to see that $\{Z_n\}$ is a Markov chain. Certain criteria guarantee that $\{Z_n\}$ has a stationary distribution and $\{Z_n\}$ can be found to be reversible. We could quickly do a test for reversibility to verify this claim.

Many communication systems are modeled as queueing networks; Jackson networks are one classic example. A Jackson network consists of J nodes. For $j = 1, 2, \ldots, J$, node j behaves like a M/M/s_j queue. Customers arrive to the network according to a Poisson process having rate λ, an arrival chooses node j with probability $p_{0,j}$, independent of all other events, where 0 corresponds to arrivals from outside of the network. A customer completing service at node j goes next to node k with probability $p_{j,k}$ and leaves the network with probability $p_{j,0}$ independent of all other transitions. Let $Q_j(t)$ be the number of customers at node j at time t and let $Q(t) = (Q_1(t), \ldots, Q_J(t))$. The process $\{Q(t); t \geq 0\}$ is a vector-valued continuous time Markov chain. Let $\mathbb{P}$ denote the $J+1 \times J+1$ matrix whose (i,j)th element is $p_{i,j}$, $i = 0, 1, \ldots, J$, $j = 0, 1, \ldots, J$. Assume $\mathbb{P}$ is irreducible and let γ be an invariant probability vector for $\mathbb{P}$. It is well known (Jackson (1963)), that if $\lambda\gamma_j < s_j\mu_j$ for all j, that $\{Q(t)\}$ has a limiting distribution which has a product form. It is also true, but slightly less known Melamed (1982) that $\{Q(t)\}$ is reversible as a Markov process if and only if $\mathbb{P}$ is the transition matrix for a reversible Markov chain, again we could use our test for reversibility on the transition matrix to determine if the process is reversible.

For more examples of reversible Markov chains, see the books by Kelly (1979), Kijima (1997), Ross (2007), and Stroock (2005).

1.3 Organization

This dissertation will proceed as follows. Our first paper compares one-step-ahead transition estimates to determine which one is better. We show in some instances that the estimator (1.2) is no more efficient than (1.1), but in some cases it is twice as efficient and prove that this is the best one can do. The next paper explores testing for the property of reversibility itself in a realization of a Markov chain. We present two test statistics, derive their asymptotic distributions, and present a simulation study.

Chapter 2

Estimation in Reversible Markov Chains

The following article is joint work with David H. Annis, Peter C. Kiessler and Robert Lund. It was published Annis et al. (2010) by *The American Statistician* in May 2010. Reprinted with permission from *The American Statistician.*

2.1 Introduction

This article studies estimation of the transition probabilities in a time-reversible Markov chain $\{X_t\}_{t=0}^{\infty}$. The chain's state space S is taken as a countable subset of $\{0, 1, \ldots\}$. The chain is assumed to be irreducible, aperiodic, and positive recurrent. Such chains have a unique limiting distribution with $\lim_{t\to\infty} \Pr[X_t = j | X_0 = i] = \pi_j$ for every $i \in S$, where $\pi_j > 0$ for $j \in S$. The one-step-ahead transition matrix $\mathbf{P} = (p_{i,j})_{i,j \in S}$ has (i, j)th entry $p_{i,j} = \Pr[X_{t+1} = j | X_t = i]$. The chain is assumed to be time-homogeneous in that $p_{i,j}$ does not depend on t. The data are assumed sampled from a stationary chain; sufficient for this is that $\Pr[X_0 = k] = \pi_k$ for all states $k \in S$.

The chain is said to be reversible if

$$\pi_i p_{i,j} = \pi_j p_{j,i}$$

for each pair of states i and j. Reversibility implies that the long-term flow rate from state i to j equals that from state j to i. Kolmogorov's criterion allows one to assess reversibility directly from the $p_{i,j}$'s; specifically, the chain is reversible if and only if

$$p_{i,i_1} p_{i_1,i_2} \dots p_{i_k,i} = p_{i,i_k} p_{i_k,i_{k-1}} \dots p_{i_1,i} \tag{2.1}$$

for each $k \geq 2$ and all states $i, i_1, \dots, i_k$ (Kijima 1997; Ross 2007). It is not clear whether one can statistically assess reversibility from a realization of a chain; however, the chain cannot be reversible if there exist i and j with $p_{i,j} > 0$ and $p_{j,i} = 0$. The works by Diaconis and Stroock (1991), Kijima (1997), Chen (2005), Stroock (2005), and Ross (2007) are good references for general properties of reversible chains.

Several broad classes of Markov chains, including random walks on graphs, birth and death chains, and many Markov chain Monte Carlo generated chains, are known to be reversible. For one example, a discrete-time birth and death chain on $S = \{0, 1, \dots\}$ is a chain that can only move one unit from its current position, either up or down, in any non-boundary transition. Specifically, the non-zero entries in the transition matrix have the form $p_{i,i+1} = \alpha_i$ and $p_{i,i-1} = 1 - \alpha_i$ when $i \geq 1$ (we take $p_{0,1} = \alpha_0$ and $p_{0,0} = 1 - \alpha_0$ where $\alpha_0 > 0$ so that the chain will be aperiodic). A second example of a reversible chain is a random walk on a graph. Here, S is a finite set and there is a collection of bivariate pairs of states called edges. The walk can transition from i to j only when the state pair (i, j) is an edge. It may be helpful to think of various U.S. cities as the states in the chain, with an edge existing between cities i and j when it is possible to fly directly from city i to j. The cost of traveling directly from city i to$j$ is $w_{i,j}$. Symmetry is assumed in that one can fly directly from j to i if it is possible to fly directly from i to j; we also take $w_{i,j} = w_{j,i}$. The probability of undergoing a transition from i to j is proportional to its cost in that

$$p_{i,j} = \frac{w_{i,j}}{\sum_{j \in S} w_{i,j}}.$$

See the books by Kijima (1997), Stroock (2005), and Ross (2007) for further examples of reversible chains.

Suppose we observe the data $X_0, \dots, X_t$ and wish to estimate the one-step-ahead transition probabilities $p_{i,j}$ for all states $i \neq j \in S$. The classical (naive) estimator of $p_{i,j}$ is

$$\hat{p}_{i,j}^{(N)}(t) = \frac{N_{i,j}(t)}{N_i(t)} 1_{[N_i(t)>0]}, \tag{2.2}$$

where $1_{[A]}$ is an indicator that is one when the event A occurs and zero otherwise, $N_{i,j}(t)$ is the number of one-step ahead transitions from i to j, and $N_i(t)$ is the number of times state i is visited up to time t. The indicator $1_{[N_i(t)>0]}$ in (2.2) is introduced to avoid division by zero. The counts $N_{i,j}(t)$ and $N_i(t)$ are

$$N_{i,j}(t) = \sum_{\ell=0}^{t-1} 1_{[X_\ell = i \cap X_{\ell+1} = j]}, \quad \text{and} \quad N_i(t) = \sum_{\ell=0}^{t} 1_{[X_\ell = i]}. \tag{2.3}$$

One may ask if a priori knowledge of a chain's reversibility aids transition probability estimation. In particular, is $\hat{p}_{i,j}^{(N)}(t)$ in (2.2) the best asymptotic estimator? This question is beautifully answered by Greenwood and Wefelmeyer (1999) and Greenwood, Schick, and Wefelmeyer (2001) who showed that the symmetrized (reversible) estimator

$$\hat{p}_{i,j}^{(R)}(t) = \frac{N_{i,j}(t) + N_{j,i}(t)}{2N_i(t)} 1_{[N_i(t)>0]} \tag{2.4}$$

is not only preferable, but also asymptotically most efficient. Since the joint distributions of $(X_0, \ldots, X_t)$ and $(X_t, \ldots, X_0)$ are identical in reversible chains, the estimator in (2.4) can be viewed as merely averaging forwards and backwards versions of (2.2).

The goal of this article is to further understand estimation for reversible chains. In Section 2, the reversible and naive estimators are reformulated from a renewal-based perspective. In Section 3, we show that both estimators are asymptotically unbiased and calculate their asymptotic variances in a straightforward manner, using only the classic limit theorems from probability. Our work will show that the asymptotic variance of the reversible estimator is never larger than that of the naive estimator, that

$$\lim_{t\to\infty} \frac{\mathrm{Var}(\hat{p}_{i,j}^{(R)}(t))}{\mathrm{Var}(\hat{p}_{i,j}^{(N)}(t))} \in \left[\frac{1}{2}, 1\right],$$

and that both bounds are tight (i.e., there are examples where the reversible estimator is, asymptotically, twice as efficient). Implications of our results are that the naive and reversible estimators have the same asymptotic performance for a birth and death chain, but that the reversible estimator is more efficient in the case of a random walk on a graph.

2.2 Reformulation of the estimators

This section uses renewal theory to express $\hat{p}_{i,j}^{(N)}(t)$ and $\hat{p}_{i,j}^{(R)}(t)$ in a form which facilitates their asymptotic analysis. Observe that the two estimators are identical when $i = j$; hence, we assume that $i \neq j$. The times at which the chain visits state i form a renewal sequence. Let $N_i(t)$ be the number of visits (renewals) to state i which have occurred up to time t. The renewal times partition the observed states into cycles, the ℓth cycle consisting of the succession of states visited between the ℓth and $(\ell+1)$st visits to state i. An initial sojourn of states prior to the beginning of the first cycle exists unless $X_0 = i$. Likewise, time t typically occurs during the interior times of a cycle; hence, the last cycle may be incomplete.

Let $C_\ell = 1$ if the ℓth cycle begins with a transition from state i to state j; otherwise, set $C_\ell = 0$. It follows that

$$N_{i,j}(t) = \sum_{\ell=1}^{N_i(t-1)} C_\ell,$$

and

$$\hat{p}_{i,j}^{(N)}(t) = \frac{\sum_{\ell=1}^{N_i(t-1)} C_\ell}{N_i(t)} 1_{[N_i(t)>0]}. \tag{2.5}$$

Set $D_\ell = 1$ if the ℓth cycle ends in state j; otherwise, set $D_\ell = 0$. For edge effects induced by the initial and possibly incomplete last cycle, set $E_1(t) = 1$ if the trajectory of states before the first cycle (before visiting state i for the first time) ends in state j; otherwise, take $E_1(t) = 0$. Take $E_2(t)$ as unity only when the observed data ends with a transition from j to i: $E_2(t) = 1_{[X_{t-1}=j, X_t=i]}$. Then

$$N_{j,i}(t) = E_1(t) + \sum_{\ell=1}^{N_i(t-1)-1} D_\ell + E_2(t).$$

It now follows that

$$\hat{p}_{i,j}^{(R)}(t) = \frac{\sum_{\ell=1}^{N_i(t-1)-1} \left(\frac{C_\ell + D_\ell}{2}\right) + E_1(t) + E_2(t) + E_3(t)}{N_i(t)} 1_{[N_i(t)>0]}, \tag{2.6}$$

where $E_3(t) = C_{N_i(t-1)}$ is a third edge effect. Other renewal representations are possible, but we have taken care to write all statistics as functions of $X_0, \ldots, X_t$ only.

We now collect a few limiting results needed to calculate the asymptotic bias and variance of the estimators. All convergences are as $t \to \infty$. Since the chain is aperiodic and positive recurrent, $N_i(t) \to \infty$ and $N_i(t)/t \to \pi_i$ with probability 1. The random vectors (C_ℓ, D_ℓ) are independent and identically distributed (iid). By the strong Markov property, the probability that a cycle begins with a transition from i to j is $p_{i,j}$; hence, $E[C_\ell] = p_{i,j}$. Since the chain is reversible, the probability that a cycle ends with a transition from j to i is the same that a cycle begins with a transition from i to j: $E[D_\ell] = p_{i,j}$. Using $C_\ell = C_\ell^2$ and $D_\ell = D_\ell^2$, we have

$$\mathrm{Var}(C_\ell) = \mathrm{Var}(D_\ell) = p_{i,j} - p_{i,j}^2.$$

We next compute $\mathrm{E}(C_\ell D_\ell)$. Observe that $C_\ell D_\ell$ is either zero or unity, with unity occurring if and only if $C_\ell = 1$ and $D_\ell = 1$. But $C_\ell = 1$ and $D_\ell = 1$ when the ℓth cycle begins with a transition from i to j and ends in state j. Since state i cannot be visited during the interior times of this cycle, $C_\ell D_\ell = 1$ with probability $p_{i,j} \sum_{k=0}^{\infty} {}_i p_{i,j}^{(k)} p_{j,i}$, where ${}_i p_{i,j}^{(k)}$ is the "taboo probability" that starting from state i, the chain is in state j at time k and the first return time to state i is greater than k. Here, the adjective "taboo" indicates that state i must be avoided during the interior times in the cycle. It follows that $\mathrm{E}(C_\ell D_\ell) = p_{i,j} \sum_{k=0}^{\infty} {}_i p_{i,j}^{(k)} p_{j,i}$ and the variance of $(C_\ell + D_\ell)/2$ is

$$\begin{aligned}
\mathrm{Var}\left(\frac{C_\ell + D_\ell}{2}\right) &= \frac{1}{4}\left[2p_{i,j} + 2p_{i,j}\sum_{k=0}^{\infty} {}_i p_{i,j}^{(k)} p_{j,i} - 4p_{i,j}^2\right] \\
&= \frac{1}{2}\left[(p_{i,j} - p_{i,j}^2) + \left(p_{i,j}\sum_{k=0}^{\infty} {}_i p_{i,j}^{(k)} p_{j,i} - p_{i,j}^2\right)\right].
\end{aligned}$$

Finally, note that $E_k(t)/N_i(t)^p \to 0$ with probability 1 for $k = 1, 2, 3$ and any $p > 0$.

2.3 Expectation and Variance

The three theorems to follow show that both estimators are consistent and asymptotically unbiased and determine their asymptotic variances. All convergences are as $t \to \infty$ unless otherwise noted.

Theorem 2.3.1. *The asymptotic mean of* $\hat{p}_{i,j}^{(N)}(t)$ *and* $\hat{p}_{i,j}^{(R)}(t)$ *is* $p_{i,j}$.

Proof. By the strong law of large numbers, as $m \to \infty$,

$$\frac{1}{m}\sum_{\ell=1}^{m} C_\ell \to p_{i,j} \qquad \text{and} \qquad \frac{1}{m}\sum_{\ell=1}^{m}\left(\frac{C_\ell + D_\ell}{2}\right) \to p_{i,j}$$

with probability 1. But since $N_i(t)$ is integer-valued and converges to infinity and $N_i(t-1)/N_i(t) \to 1$ with probability 1,

$$\frac{1}{N_i(t)}\sum_{\ell=1}^{N_i(t-1)} C_\ell \to p_{i,j} \qquad \text{and} \qquad \frac{1}{N_i(t)}\sum_{\ell=1}^{N_i(t-1)-1}\left(\frac{C_\ell + D_\ell}{2}\right) \to p_{i,j}$$

with probability 1. Also, $E_k(t)/N_i(t) \to 0$ for $k = 1, 2, 3$ and $1_{[N_i(t)>0]} \to 1$ with probability 1. Using these results and (2.5) and (2.6), we infer that $\hat{p}_{i,j}^{(N)}(t) \to p_{i,j}$ and $\hat{p}_{i,j}^{(R)} \to p_{i,j}$ with probability 1. Since both $\hat{p}_{i,j}^{(N)}(t)$ and $\hat{p}_{i,j}^{(R)}(t)$ are nonnegative and bounded above by unity, the convergence of $E[\hat{p}_{i,j}^{(N)}(t)]$ and $E[\hat{p}_{i,j}^{(R)}(t)]$ to $p_{i,j}$ follows from the dominated convergence theorem. □

Theorem 2.3.2. *As* $t \to \infty$, *we have the following distributional convergence:*

$$\sqrt{t}\left(\hat{p}_{i,j}^{(N)}(t) - p_{i,j}\right) \xrightarrow{\mathcal{D}} N\left(0, \frac{p_{i,j} - p_{i,j}^2}{\pi_i}\right) \overset{\mathcal{D}}{=} N\left(0, \frac{\mathrm{Var}(C_1)}{\pi_i}\right). \tag{2.7}$$

Proof. A careful analysis based on (2.5) and cases provides

$$\left(\hat{p}_{i,j}^{(N)}(t) - p_{i,j}\right) = \left[\frac{\sum_{\ell=1}^{N_i(t-1)}(C_\ell - p_{i,j})}{N_i(t-1)}\right]\frac{N_i(t-1)}{N_i(t)}1_{[N_i(t-1)>0]} - p_{i,j}1_{[N_i(t-1)=0]}. \tag{2.8}$$

To handle the edge-effect term in (2.8), note that

$$\sqrt{t}p_{i,j}1_{[N_i(t-1)=0]} \xrightarrow{\mathcal{P}} 0$$

due to $\Pr[N_i(t-1) = 0] = \Pr(\tau_1 > t-1) \le E[\tau_1]/(t-1)$, which is justified by Markov's inequality. Here, τ_1 is the first time the chain visits state i; $E[\tau_1]$ is finite by the assumed positive recurrence. Observe that $N_i(t-1)/N_i(t) \to 1$ and $1_{[N_i(t-1)>0]} \to 1$ (all with probability 1). An application of

Slutzky's theorem now shows that our work is done if we simply prove that

$$\frac{\sqrt{t}}{N_i(t-1)} \sum_{\ell=1}^{N_i(t-1)} (C_\ell - p_{i,j}) \xrightarrow{\mathcal{D}} N\left(0, \frac{\mathrm{Var}(C_1)}{\pi_i}\right). \tag{2.9}$$

To verify (2.9), apply the central limit theorem to the iid sequence $\{C_\ell\}$ to infer that as $m \to \infty$,

$$\frac{1}{\sqrt{m}} \sum_{\ell=1}^{m} (C_\ell - p_{i,j}) \xrightarrow{D} N(0, \mathrm{Var}(C_1)).$$

Since $N_i(t) \to \infty$, Theorem 17.1 in the book by Billingsley (1968) gives

$$\frac{1}{\sqrt{N_i(t-1)}} \sum_{\ell=1}^{N_i(t-1)} (C_\ell - p_{i,j}) \xrightarrow{D} N(0, \mathrm{Var}(C_1)),$$

which implies (2.7) and (2.9) when combined with $\sqrt{t/N_i(t-1)} \to \sqrt{1/\pi_i}$ and $\mathrm{Var}(C_1) = p_{i,j} - p_{i,j}^2$. □

A similar argument proves the following result, the essential change being that (2.6) is used in place of (2.5), and $\mathrm{Var}((C_1 + D_1)/2)$ replaces $\mathrm{Var}(C_1)$.

Theorem 2.3.3. *As $t \to \infty$*

$$\sqrt{t}\left(\hat{p}_{i,j}^{(R)}(t) - p_{i,j}\right) \xrightarrow{\mathcal{D}} N\left(0, \frac{(p_{i,j} - p_{i,j}^2) + (p_{i,j} \sum_{k=0}^{\infty} {}_i p_{i,j}^{(k)} p_{j,i} - p_{i,j}^2)}{2\pi_i}\right) \stackrel{\mathcal{D}}{=} N\left(0, \frac{\mathrm{Var}((C_1 + D_1)/2))}{\pi_i}\right). \tag{2.10}$$

In terms of asymptotic efficiencies, we have now shown that

$$\lim_{t\to\infty} \frac{\mathrm{Var}(\hat{p}_{i,j}^{(R)}(t))}{\mathrm{Var}(\hat{p}_{i,j}^{(N)}(t))} = \frac{\mathrm{Var}\left(\frac{C_1 + D_1}{2}\right)}{\mathrm{Var}(C_1)} = \frac{\sigma_R^2}{\sigma_N^2}, \tag{2.11}$$

where

$$\sigma_N^2 = \frac{p_{i,j} - p_{i,j}^2}{\pi_i} \quad \text{and} \quad \sigma_R^2 = \frac{(p_{i,j} - p_{i,j}^2) + (p_{i,j} \sum_{k=0}^{\infty} {}_i p_{i,j}^{(k)} p_{j,i} - p_{i,j}^2)}{2\pi_i}. \tag{2.12}$$

Observe that $\sum_{k=0}^{\infty} {}_i p_{i,j}^{(k)} p_{j,i} \leq \sum_{k=0}^{\infty} \mathrm{Pr}_i[\eta_i = k+1] \leq 1$, η_i denoting the time of first return to state i and Pr_i indicating the initial condition $X_0 = i$. Using this in (2.12) shows that $\sigma_R^2 \leq \sigma_N^2$. In the next section, we will show that $\sigma_R^2/\sigma_N^2 \geq 1/2$.

2.4 Lower bounds for σ_R^2/σ_N^2

We start with two examples. In the first, C_ℓ and D_ℓ are perfectly correlated and the asymptotic efficiency of the naive and reversible estimators is unity. In the second example, C_ℓ and D_ℓ are uncorrelated and the reversible estimator is twice as efficient as the naive estimator.

Consider a birth and death chain. This chain is skip-free in that from state $i \geq 1$, the only possible transitions are to states $i-1$ and $i+1$. The transition probabilities are $p_{i,i+1} = \alpha_i$ and $p_{i,i-1} = 1-\alpha_i$, where $\alpha_i \in [0,1]$ (at state 0, we take $p_{0,1} = \alpha_0$ and $p_{0,0} = 1-\alpha_0$). Assuming $\alpha_i > 0$ for all $i \geq 0$ and $\alpha_i < 1/2$ for all large i, the chain is irreducible, aperiodic, positive recurrent, and reversible and has a limiting distribution with form

$$\pi_j = \begin{cases} K & j = 0 \\ \frac{\alpha_1 \cdots \alpha_{j-1}}{(1-\alpha_1)\cdots(1-\alpha_j)} K & j > 0 \end{cases}.$$

Here, the constant K is such that the limiting distribution has unit mass.

The only nonzero $p_{i,j}$'s occur when $j = i-1$ or $j = i+1$. When $j = i+1$, then if $C_\ell = 1$, the ℓth cycle starts with a transition from i to $i+1$ and, by the skip free property, must end with a transition from $i+1$ to i. Hence, $D_\ell = 1$ for this cycle. If $C_\ell = 0$, then the ℓth cycle starts with a transition from i to $i-1$ and, by the skip-free property, must end with a transition from $i-1$ to i. Hence, $D_\ell = 0$ for this cycle. It now follows that $\text{Var}((C_\ell + D_\ell)/2) = \text{Var}(C_\ell)$. Thus, for skip-free chains, the reversible and naive estimators have the same asymptotic efficiency.

As a second example, consider an iid chain. Specifically, $X_0, X_1, \ldots$ are independent and have the common probability mass function $\Pr[X_i = j] = \pi_j$ with $\pi_j > 0$ for all j. Such a sequence can be regarded as a Markov chain with the transition probabilities $p_{i,j} = \pi_j$. The stationary distribution is $\{\pi_i\}_{i=0}^\infty$ and the chain is easily shown to be irreducible, aperiodic, positive recurrent, and reversible.

To calculate σ_R^2, note that the taboo probability is

$$\sum_{k=0}^\infty {}_i p_{i,j}^{(k)} = \sum_{k=0}^\infty (1-\pi_i)^k \pi_j = \pi_i^{-1}\pi_j.$$

It follows from (2.12) that

$$\sigma_R^2 = \frac{1}{2}\left(\pi_j - \pi_j^2 + \pi_j \pi_i^{-1} \pi_j \pi_i - \pi_j^2\right) = \frac{\pi_j - \pi_j^2}{2} = \frac{\sigma_N^2}{2}.$$

Hence, $\hat{p}_{i,j}^{(R)}(t)$ is asymptotically twice as efficient as $\hat{p}_{i,j}^{(N)}(t)$.

We close by showing that $\mathrm{Cov}(C_\ell, D_\ell) \geq 0$. With this and (2.11), we have $1/2 \leq \sigma_R^2/\sigma_N^2 \leq 1$ and the two examples above provide cases where the relative efficiencies of 1/2 and 1 are achieved.

Theorem 2.4.1. *C_ℓ and D_ℓ are non-negatively correlated; that is,* $\mathrm{Cov}(C_\ell, D_\ell) \geq 0$*.*

Proof. Because of the binary structure of C_ℓ and D_ℓ, it suffices to show that $\Pr(C_\ell = 1, D_\ell = 1) \geq \Pr(C_\ell = 1)\Pr(D_\ell = 1)$. To this end, we note that since

$$\begin{aligned} &\Pr(C_\ell = 1)\Pr(D_\ell = 1) \\ &= [\Pr(C_\ell = 1, D_\ell = 1) + \Pr(C_\ell = 1, D_\ell = 0)]\,[\Pr(C_\ell = 1, D_\ell = 1) + \Pr(C_\ell = 0, D_\ell = 1)] \\ &= \Pr(C_\ell = 1, D_\ell = 1)[1 - \Pr(C_\ell = 0, D_\ell = 0)] + \Pr(C_\ell = 1, D_\ell = 0)\Pr(C_\ell = 0, D_\ell = 1), \end{aligned}$$

it suffices to show that

$$\Pr(C_\ell = 1, D_\ell = 1)\Pr(C_\ell = 0, D_\ell = 0) \geq \Pr(C_\ell = 1, D_\ell = 0)\Pr(C_\ell = 0, D_\ell = 1). \tag{2.13}$$

Since $\Pr(C_\ell = 1, D_\ell = 0)$ is the probability that a cycle begins with a transition from i to j and ends with a transition from some state other than j to i, we have

$$\Pr(C_\ell = 1, D_\ell = 0) = \sum_A p_{i,j} p_{j,k_1} \cdots p_{k_n,i},$$

where $A = \cup_{n=1}^{\infty}\{(k_1, \ldots, k_n); k_h \neq i \text{ for } h = 1, \ldots, n \text{ and } k_n \neq j\}$. Similarly, since $\Pr(C_\ell = 0, D_\ell = 1)$ is the probability a cycle begins with a transition from i to some state other than j and ends with a transition from j to i,

$$\Pr(C_\ell = 0, D_\ell = 1) = \sum_B p_{i,l_1} \cdots p_{l_m,j} p_{j,i},$$

where $B = \cup_{m=1}^{\infty} \{(l_1, \ldots, l_m); l_h \neq i \text{ for } h = 1, \ldots, m \text{ and } l_1 \neq j\}$.

Thus,

$$\Pr(C_\ell = 1, D_\ell = 0)\Pr(C_\ell = 0, D_\ell = 1) = \sum_A \sum_B p_{i,j} p_{j,k_1} \cdots p_{k_n,i} p_{i,l_1} \cdots p_{l_m,j} p_{j,i}.$$

An application of Kolmogorov's criteria for reversibility in (2.1) gives

$$\Pr(C_\ell = 1, D_\ell = 0)\Pr(C_\ell = 0, D_\ell = 1) = p_{i,j} p_{j,i} \left(\sum_A \sum_B p_{i,k_n} \cdots p_{k_1,j} p_{j,l_m} \cdots p_{l_1,i} \right).$$

Since n and m are both at least 1 and l_1 and k_n do not equal j, each term in the double summation is the probability of some cycle that begins with a transition from i to some state other than j and ends with a transition from some state other than j to i. Thus, the term inside the parentheses is less than or equal to $\Pr(C_\ell = 0, D_\ell = 0)$ and

$$\Pr(C_\ell = 1, D_\ell = 0)\Pr(C_\ell = 0, D_\ell = 1) \leq p_{i,j} p_{j,i} \Pr(C_\ell = 0, D_\ell = 0). \tag{2.14}$$

Because one way for a cycle to have $C_\ell = 1$ and $D_\ell = 1$ is to make a transition from i to j and then immediately back to i, we have

$$p_{i,j} p_{j,i} \leq \Pr(C_\ell = 1, D_\ell = 1). \tag{2.15}$$

Combining (2.14) and (2.15) gives (2.13) and completes the proof. □

2.5 Conclusion and Comments

Reversibility is a structural property inherited by many Markov chains. Reversibility can be exploited in some cases to obtain transition probability estimates that have smaller asymptotic variances than naive estimators based on ratios of counts. The improvement in the asymptotic efficiency of a reversible estimate, relative to a naive estimate, is quantified in (2.11). In cases where the chain possesses the so-called skip-free property, such as the birth and death chain in Section 1, there is no improvement; in other cases, such as the random walk on a graph, some improvement may be possible. In any case, the reversible estimator's asymptotic variance can be no lower than half the naive estimator's asymptotic variance.

Chapter 3

Testing for Reversibility in Markov Chain Data

The following is joint work with Peter C. Kiessler and Robert Lund. It is being submitted to the *Annals of the Institute of Statistical Mathematics*.

3.1 Introduction

Let $\{X_t\}_{t=0}^{\infty}$ be a time-homogeneous Markov chain on the finite state space $S = \{1, 2, \ldots, m\}$ with one-step-ahead transition probability matrix $\mathbf{P} = (p_{i,j})_{i,j \in S}$ with entries $p_{i,j} = P[X_{n+1} = j | X_n = i]$. Without a priori information, it is natural to estimate $p_{i,j}$ by

$$\hat{p}_{i,j}^{(N)} = \frac{N_{i,j}}{N_i} 1_{[N_i > 0]},$$

where $N_{i,j}$ is the number of times the chain transitions from state i to state j in one step and N_i is the number of times the chain visits state i in a data realization of length L. Anderson and Goodman (1957), Basawa and Rao (1980), Billingsley (1961), and Derman (1956) explore properties of $\hat{p}_{i,j}^{(N)}$ in depth. Some of their results are reviewed/stated in the next section.

Suppose that the chain is aperiodic and irreducible. Due to the finite state space, the chain is positive recurrent and admits a unique stationary distribution $\pi = (\pi_1, \ldots, \pi_m)$ (this is also a limiting distribution). The chain is called reversible if it satisfies the so-called detailed balance equations

$$\pi_i p_{i,j} = \pi_j p_{j,i}, \quad \text{for all} \quad i, j \in S. \tag{3.1}$$

Markov chain Monte Carlo chains (MCMC), birth and death chains, and random walks on graphs are known to be reversible chains. In many settings, reversibility can be rationalized through physical reasoning without computation of π. More examples of reversible Markov chains can be found in Kijima (1997), Ross (2007), and Stroock (2005).

Knowing whether or not a chain is reversible is advantageous. A reversible chain contains fewer parameters than a non-reversible chain. Elaborating, there are $m(m-1)$ free parameters in the one-step-ahead transition matrix of a chain whose state space has cardinality m (one free parameter is lost in each row since all transition matrix row sums are unity). However, if a chain is known to be reversible, there are only $m(m-1)/2$ free parameters due to the restrictions in (3.1). Diagnostics are another application of the methods here. For example, any MCMC generated chain flunking a reversibility test would be suspect as these chains are reversible.

The rest of this paper proceeds as follows. The next section introduces two test statistics that assess chain reversibility. Section 3 establishes their asymptotic distributions under a null hypothesis of reversibility. Section 4 presents a simulation study showing the efficiency of the statistics in identifying reversibility. Section 5 presents coincluding remarks and an Appendix establishes two technical calculations.

3.2 Test Statistics

Suppose that state i is visited k times in the first $L-1$ time units; that is, suppose $N_i(L-1) = k$ (we work with time $L-1$ instead of time L because we do not have an observed transition from time L to $L+1$). Then $\mathbf{N}_i(L-1) = (N_{i,1}(L-1), ..., N_{i,M}(L-1))'$ is a multivariate multinomial random variable with k trials and success probability vector $\mathbf{p}_i = (p_{i,1}, \ldots, p_{i,M})'$. Using this and the central limit theorem for renewal sequences, Basawa and Rao (1980), Anderson and Goodman (1957), Billingsley (1961), and Derman (1956) argue that for each $i, j \in S$,

$$\sqrt{L}(\hat{p}_{i,j}^{(N)} - p_{i,j}) \xrightarrow{\mathcal{D}} N\left(0, \frac{p_{i,j}(1-p_{i,j})}{\pi_i}\right)$$

as $L \to \infty$. For joint inferences, they also show that

$$\sqrt{L}\begin{pmatrix} \hat{p}_{i,j}^{(N)} - p_{i,j} \\ \hat{p}_{i',j'}^{(N)} - p_{i',j'} \end{pmatrix} \xrightarrow{\mathcal{D}} N\left(\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \mathbf{\Sigma_P}\right), \tag{3.2}$$

where

$$\mathbf{\Sigma_P} = \begin{pmatrix} p_{i,j}(1-p_{i,j})/\pi_i & \delta_{i,i'}p_{i,j}(\delta_{j,j'} - p_{i,j'})/\pi_i \\ \delta_{i,i'}p_{i,j}(\delta_{j,j'} - p_{i,j'})/\pi_i & p_{i',j'}(1-p_{i',j'})/\pi_{i'} \end{pmatrix}$$

and $\delta_{i,j} = \mathbf{1}_{[i=j]}$ is the Kronecker delta indicator. For completeness, we argue (3.2) in Appendix A from elementary principles. Part of the reason we prove this is that most of the above cited authors state but do not prove the result, and the reader may be surprised that $\hat{p}_{i,j}^{(N)}$ and $\hat{p}_{i',j'}^{(N)}$ are asymptotically uncorrelated when $i \neq i'$. In fact, since the chain cannot be in state i' when it is in state i, one might erroneously rationalize negative dependence when $i \neq i'$.

When the chain is reversible, there are actually more efficient estimators of $p_{i,j}$ than $\hat{p}_{i,j}^{(N)}$. Annis et al. (2010) and Greenwood et al. (2001) show that the symmetrized estimator

$$\hat{p}_{i,j}^{(R)} = \frac{N_{i,j} + N_{j,i}}{2N_i} 1_{[N_i > 0]}$$

is asymptotically more efficient than $\hat{p}_{i,j}^{(N)}$ and quantify the efficiency gain. For example, $\hat{p}_{i,j}^{(N)}$ and $\hat{p}_{i,j}^{(R)}$ have unit efficiency when the chain is skip free. Skip free means that when the chain is in state i, the next transition must go to either state $i-1$ or $i+1$. We estimate π_i with

$$\hat{\pi}_i = \frac{N_i}{L}.$$

In view of (3.1), the deviations

$$\hat{\pi}_i \hat{p}_{i,j}^{(N)} - \hat{\pi}_j \hat{p}_{j,i}^{(N)} = \frac{N_{i,j} - N_{j,i}}{L} \tag{3.3}$$

should be small for each pair (i,j) with $i < j$ when the chain is reversible. Hence, the quadratic form

$$\sum\sum_{i<j} \left(\frac{N_{i,j} - N_{j,i}}{L}\right)^2 \tag{3.4}$$

should be statistically small under reversibility. The sum in (3.4) is inconvenient to quantify asymptotically. This is because the quantities $C_{i,j} := (N_{i,j} - N_{j,i})/L$ are correlated for varying pairs (i,j) with $j > i$.

To handle this issue, define the $m(m-1)/2$-dimensional discrepancy vector

$$\mathbf{C} = \frac{1}{L} \begin{bmatrix} N_{1,2} - N_{2,1} \\ \vdots \\ N_{1,m} - N_{m,1} \\ N_{2,3} - N_{3,2} \\ \vdots \\ N_{2,m} - N_{m,2} \\ \vdots \\ N_{m-1,m} - N_{m,m-1} \end{bmatrix}. \tag{3.5}$$

For notation, we denote the element of $\mathbf{C}$ corresponding to $L^{-1}(N_{i,j} - N_{j,i})$ as $C_{i,j}$. While this indexes a vector with bivariate subscripts, the notation is natural given the transition count components it involves.

Let $\mathbf{\Sigma_C} = \lim_{L\to\infty} L\text{Var}(\mathbf{C})$ denote the asymptotic information matrix of $\mathbf{C}$. If one can establish asymptotic normality of $\mathbf{C}$, then the quadratic form statistic

$$T_1 = L\mathbf{C}'\hat{\mathbf{\Sigma}}^+_{\mathbf{C}}\mathbf{C}. \tag{3.6}$$

will have an asymptotic χ^2 distribution. The degrees of freedom of T_1 will be the rank of $\mathbf{\Sigma_C}$, which is not necessarily $m(m-1)/2$. Specifically, $\mathbf{\Sigma_C}$ is not always invertible and the notation $\mathbf{\Sigma}^+_{\mathbf{C}}$ signifies the Moore-Penrose pseudoinverse in (3.6). These aspects are elaborated upon in detail below.

A second test statistic that could be used to assess reversibility is the maximum of the square of terms in (3.4); specifically,

$$T_2 = \max_{i<j} D^2_{i,j}, \tag{3.7}$$

where $D_{i,j}$ is the (i,j)th component in $\mathbf{D}$ defined by $\mathbf{D} = \sqrt{L}(\hat{\mathbf{\Sigma}}^+_{\mathbf{C}})^{1/2}\mathbf{C}$. Observe that $\mathbf{D}$ is an $m(m-1)/2$ dimensional vector and we have indexed its components akin to those in $\mathbf{C}$. We show below that T_2 converges asymptotically to the max of κ independent random variables, each of which has a chi-squared distribution with one degree of freedom. Here, κ is the rank of $\mathbf{\Sigma_C}$.

Small values of T_1 and T_2 suggest the null hypothesis of reversibility; that is, reversibility is rejected when T_1 and/or T_2 are statistically too big. To quantify how big the statistics need to be to warrant rejection of reversibility, we now derive the asymptotic distributions of T_1 and T_2 as $L \to \infty$ under the null hypothesis of reversibility. In the analysis below, we assume that the data sequence $X_1, \ldots, X_L$ is drawn from a time-homogeneous chain that is in its stationary state. As the initial state will not influence limiting behavior, one can apply the results below to any arbitrary initial state.

3.3 Asymptotic Distribution of the Test Statistics

This section derives the asymptotic distributions of T_1 and T_2 when the chain is reversible. We begin with the following lemma that quantifies the joint normality of the $N_{i,j}/L$'s. The result does not follow readily from the joint asymptotic normality of the $\hat{p}_{i,j}$'s in (3.2) because of the randomness in the $\hat{\pi}_i$'s. Although joint normality holds for any collection of the $N_{i,j}/L$'s, we state the result for two (i,j) pairs only for notational convenience. The proof of the result is presented in Appendix B.

Lemma 3.3.1. *Suppose that $\{X_t\}_{t=1}^{L}$ is a sample taken from a time-homogeneous aperiodic irreducible Markov chain on the finite state space S whose cardinality is $m < \infty$. Then*

$$\sqrt{L}\begin{pmatrix} \frac{N_{i,j}}{L} - \pi_i p_{i,j} \\ \frac{N_{i',j'}}{L} - \pi_{i'} p_{i',j'} \end{pmatrix} \xrightarrow{\mathcal{D}} N\left(\mathbf{0}, \mathbf{\Sigma_N}\right),$$

where

$$\mathbf{\Sigma_N} = \begin{pmatrix} \gamma_{i,j}^2 & \gamma_{ij,i'j'} \\ \gamma_{ij,i'j'} & \gamma_{i',j'}^2. \end{pmatrix}$$

Here,

$$
\begin{aligned}
\gamma_{i,j}^2 &= 2\pi_i p_{i,j} r_{j,i} p_{i,j} + \pi_i p_{i,j}(1 - \pi_i p_{i,j}); \\
\gamma_{ij,i'j'} &= \pi_i p_{i,j} r_{j,i'} p_{i',j'} + \pi_{i'} p_{i',j'} r_{j',i} p_{i,j} - \pi_i p_{i,j} \pi_{i'} p_{i',j'}; \\
\gamma_{i',j'} &= 2\pi_{i'} p_{i',j'} r_{j',i'} + 2\pi_{i'} p_{i',j'}(1 - \pi_{i'} p_{i',j'});
\end{aligned}
$$

and $r_{k,\ell}$ is the (k,ℓ)th entry in the matrix $\mathbf{R} = (\mathbf{I}_{m\times m} - \mathbf{P} + \mathbf{\Pi}_{m\times m})^{-1}$ with $\mathbf{\Pi}_{m\times m}$ being an $m \times m$ dimensional matrix with each row containing the limiting distribution π, and $\mathbf{I}_{m\times m}$ is the m-dimensional identity matrix.

Observe that on a chain whose state space has cardinality m, $\mathbf{\Sigma_N}$ is an $m^2 \times m^2$ dimensional matrix.

We will need to derive forms of $\mathbf{\Sigma_C}$ and $\mathbf{\Sigma_N}$ under a null hypothesis of reversibility. These quantities are denoted by $\mathbf{\Sigma_C}^{(R)}$ and $\mathbf{\Sigma_N}^{(R)}$, respectively. To compute these information matrices under reversibility, one simply replaces $\pi_j p_{j,i}$ with $\pi_i p_{i,j}$ when $j > i$; these expressions are left unaltered when $j \leq i$. For example, under reversibility, the limiting information for $N_{1,2}$ is written as $\pi_1 p_{1,2} r_{2,1} p_{1,2} + \pi_1 p_{1,2}(1 - \pi_1 p_{1,2})$; the limiting information for $N_{2,1}$ is written as $2\pi_2 p_{2,1} r_{1,2} p_{2,1} + \pi_2 p_{2,1}(1 - \pi_2 p_{2,1})$ in preference to $2\pi_1 p_{1,2} r_{1,2} p_{2,1} + \pi_1 p_{1,2}(1 - \pi_1 p_{1,2})$. The estimators $\hat{\mathbf{\Sigma}}_\mathbf{N}^{(R)}$ and $\hat{\mathbf{\Sigma}}_\mathbf{C}^{(R)}$ are computed by plugging in $\hat{\pi}_i$ for π_i and $\hat{p}_{i,j}^{(N)}$ for $p_{i,j}$ under the above "reflection scheme".

Theorem 3.3.2. *Under the assumptions of Lemma 1, $T_1 = L\mathbf{C}'(\hat{\mathbf{\Sigma}}_\mathbf{C}^{(R)})^+\mathbf{C} \xrightarrow{\mathcal{D}} \chi^2_\kappa$ as $L \to \infty$, where κ is the rank of $\mathbf{\Sigma_C}$. In the case where $\mathbf{P}$ has no zero elements or parameter restrictions, $\kappa = (m-1)(m-2)/2$.*

Proof. Throughout this proof, we assume that the null hypothesis of reversibility is in force. Then $\pi_i p_{i,j} = \pi_j p_{j,i}$ for all $(1, j) \in \{1, \ldots, m\}$. Let

$$
\mathbf{N} = L^{-1} \begin{bmatrix} N_{1,1} - L\pi_1 p_{1,1} \\ N_{1,2} - L\pi_1 p_{1,2} \\ \vdots \\ N_{m,m} - L\pi_m p_{m,m} \end{bmatrix}.
$$

Observe that $\mathbf{C}$ is a linear transformation of $\mathbf{N}$; hence, we write $\mathbf{C} = \mathbf{VN}$, where $\mathbf{V}$ is a $m(m-1)/2 \times m^2$ dimensional matrix whose only non-zero entries are positive or negative one. The form of $\mathbf{V}$ is messy to write down but the ones and minus ones lie in the following described locations.

$\mathbf{V}$ is written as $m-1$ blocks with block i containing $m-i$ rows, for $i=1,2,\ldots,m-1$. That is, $\mathbf{V}$ has the form

$$\begin{bmatrix} \mathbf{b}(1) \\ \mathbf{b}(2) \\ \vdots \\ \mathbf{b}(m-1) \end{bmatrix}.$$

Row r of the matrix $\mathbf{V}$ is in block i if $(i-1)(m-i/2)+1 \le r \le im - i(i+1)/2$. For block i, the entries in $\mathbf{b}(i)$ are

$$\mathbf{b}(i)_{k,\ell} = \begin{cases} 1, & \text{if } \ell = (i-1)m + i + k \\ -1, & \text{if } \ell = (i-1)m + i + km \\ 0, & \text{otherwise} \end{cases} .$$

When $m=3$, for example, we have

$$\mathbf{C} = L^{-1} \begin{bmatrix} 0 & 1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & -1 & 0 \end{bmatrix} \begin{pmatrix} N_{1,1} - L\pi_1 p_{1,1} \\ N_{1,2} - L\pi_1 p_{1,2} \\ N_{1,3} - L\pi_1 p_{1,3} \\ N_{2,1} - L\pi_2 p_{2,1} \\ N_{2,2} - L\pi_2 p_{2,2} \\ N_{2,3} - L\pi_2 p_{2,3} \\ N_{3,1} - L\pi_3 p_{3,1} \\ N_{3,2} - L\pi_3 p_{3,2} \\ N_{3,3} - L\pi_3 p_{3,3} \end{pmatrix}.$$

Under the reversible null, $\sqrt{L}\mathbf{N} \xrightarrow{\mathcal{D}} N(\mathbf{0}, \mathbf{\Sigma}_{\mathbf{N}}^{(R)})$ by Lemma 1 and hence $\sqrt{L}\mathbf{C} \xrightarrow{\mathcal{D}} N(\mathbf{0}, \mathbf{\Sigma}_{\mathbf{C}}^{(R)})$, where $\mathbf{\Sigma}_{\mathbf{C}}^{(R)} = \mathbf{V}\mathbf{\Sigma}_{\mathbf{N}}^{(R)}\mathbf{V}'$. Theorem 4.7.1 in Graybill (1976) and Slutzky's theorem give

$$(\sqrt{L}\mathbf{C}^T)(\hat{\mathbf{\Sigma}}_{\mathbf{C}}^{(R)})^{+}(\sqrt{L}\mathbf{C}) = L\mathbf{C}^T(\hat{\mathbf{\Sigma}}_{\mathbf{C}}^{(R)})^{+}\mathbf{C} \xrightarrow{\mathcal{D}} \chi^2_\kappa,$$

where κ is the rank of $\mathbf{\Sigma}_{\mathbf{C}}^{(\mathbf{R})}$.

To finish the proof, we need to determine the rank of $\mathbf{\Sigma}_{\mathbf{C}}^{(R)}$. This calculation caused the authors considerable consternation.

Since $\mathbf{\Sigma}_{\mathbf{C}}^{(R)}$ is an $m(m-1)/2 \times m(m-1)/2$ dimensional matrix, the rank of $\mathbf{\Sigma}_{\mathbf{C}}^{(R)}$ is $m(m-1)/2$ minus the rank of the null space of $\mathbf{\Sigma}_{\mathbf{C}}^{(R)}$. Perhaps surprisingly, the rank of the null space of $\mathbf{\Sigma}_{\mathbf{C}}^{(R)}$ is not zero. To see this, we must show that there exist non-zero vectors $\mathbf{u}$ such that

$$\mathbf{\Sigma_C}^{(R)}\mathbf{u} = \mathbf{0}$$

and identify how many linearly independent such $\mathbf{u}$ exist.

To do this, let $N_{i,\cdot} = \sum_{k=1}^{m} N_{i,k}$ and $N_{\cdot,j} = \sum_{k=1}^{m} N_{k,j}$. Then $N_{i,\cdot}$ is the total number of transitions out of state i in the data record and $N_{\cdot,i}$ is the total number of transitions into state i in the data record. Physical reasoning shows that $|N_{i,\cdot} - N_{\cdot,i}| \leq 1$ for each $i \in \{1, 2, \ldots, m\}$. As we show below, the lack of full rank for $\mathbf{\Sigma}_{\mathbf{C}}^{(R)}$ arises from these restrictions (and not reversibility).

For $i \in \{1, 2, \ldots, m\}$, define the $m(m-1)/2$ dimensional vector $\mathbf{u}^{(i)}$ componentwise via

$$u_{h,\ell}^{(i)} = \begin{cases} 1, & \text{if } h = i \text{ and } \ell \in \{i+1, i+1, \ldots, m\}, \\ -1, & \text{if } \ell = i \text{ and } h \in \{i-1, i-2, \ldots, 1\} \\ 0, & \text{otherwise} \end{cases} .$$

Here, we have indexed $\mathbf{u}^{(i)}$ with two components (h, ℓ) drawn over the set $\{1, 2, \ldots, m\}$ with $h < \ell$. For example, when $m = 3$,

$$\mathbf{u}^{(1)} = \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix}, \quad \mathbf{u}^{(2)} = \begin{bmatrix} -1 \\ 0 \\ 1 \end{bmatrix}, \quad \mathbf{u}^{(3)} = \begin{bmatrix} 0 \\ -1 \\ -1 \end{bmatrix}.$$

We now show that $\mathbf{u}^{(i)}$ belongs to the null space of $\mathbf{\Sigma}_{\mathbf{C}}^{(R)}$ for $i = 1, 2, \ldots, m$. To see this, observe that for $i = 1, 2, \ldots, m$,

$$N_{i,\cdot} - N_{\cdot,i} = \sum_{j>i} (N_{i,j} - N_{j,i}) - \sum_{j<i} (N_{j,i} - N_{i,j}). \tag{3.8}$$

The element of $\mathbf{\Sigma}_{\mathbf{C}}^{(R)}$ corresponding to $C_{h,\ell}$ and $C_{h',\ell'}$ is

$$\lim_{L\to\infty} L^{-1}\mathrm{E}[(N_{h,\ell} - N_{\ell,h})(N_{h',\ell'} - N_{\ell',h'})] = \lim_{L\to\infty} LE[C_{h,\ell}C_{h',\ell'}].$$

Thus, for $i = 1, 2, \ldots, m$, the (h, ℓ)th element of $\mathbf{\Sigma}_{\mathbf{C}}^{(R)}\mathbf{u}^{(i)}$ is

$$\lim_{L\to\infty} \left(\sum_{j>i} \mathrm{E}[(N_{h,\ell} - N_{\ell,h})(N_{i,j} - N_{j,i})] - \sum_{j>i} \mathrm{E}[(N_{h,\ell} - N_{\ell,h})(N_{j,i} - N_{i,j})] \right).$$

To show that this is zero, use Equation (3.8) to get that the (h, ℓ)th element of $\mathbf{\Sigma}_{\mathbf{C}}^{(R)}u^{(i)}$ is

$$\begin{aligned} &\lim_{L\to\infty} L^{-1} \sum_{j>i} \mathrm{E}\left[(N_{h,\ell} - N_{\ell,h}) \left(\sum_{j>i} (N_{i,j} - N_{j,i}) - \sum_{j<i} (N_{j,i} - N_{i,j}) \right) \right] \\ &= \lim_{L\to\infty} L^{-1}\mathrm{E}[(N_{h,\ell} - N_{\ell,h})(N_{i\cdot} - N_{\cdot i})]. \end{aligned}$$

Since $|N_{i,\cdot} - N_{\cdot,i}| \leq 1$ and $\mathrm{Var}(\frac{N_{h,\ell} - N_{\ell,h}}{\sqrt{L}}) < \infty$ (by Lemma 1), the Cauchy-Schwarz inequality gives

$$\begin{aligned} \lim_{L\to\infty} L^{-1}\mathrm{E}[(N_{h,\ell} - N_{\ell,h})(N_{i\cdot} - N_{\cdot i})] &= \lim_{L\to\infty} \mathrm{E}\left[\frac{(N_{h,\ell} - N_{\ell,h})}{\sqrt{L}} \frac{(N_{i\cdot} - N_{\cdot i})}{\sqrt{L}} \right] \\ &\leq \lim_{L\to\infty} \left(\mathrm{Var}\left(\frac{N_{h,\ell} - N_{\ell,h}}{\sqrt{L}} \right) \right)^{1/2} \frac{1}{\sqrt{L}} \\ &= 0. \end{aligned}$$

Hence, the (h, ℓ)th element of $\mathbf{\Sigma}_{\mathbf{C}}^{(R)}\mathbf{u}^{(i)}$ is zero and $\mathbf{u}^{(1)}, \ldots, \mathbf{u}^{(m)}$ are in the null space of $\mathbf{\Sigma}_{\mathbf{C}}^{(R)}$.

It is easy to see that there are $m - 1$ linearly independent vectors amongst $\mathbf{u}^{(1)}, \ldots, \mathbf{u}^{(m)}$. This can be seen by putting all $\mathbf{u}^{(i)}$ as rows in a matrix and row reducing. A rank of one is lost from m because

$$\sum_{i=1}^{m} \mathbf{u}^{(i)} = \mathbf{0},$$

which is a consequnce of

$$\sum_{i=1}^{m} (N_{i,\cdot} - N_{\cdot,i}) = 0.$$

It follows that the rank of the null space of $\boldsymbol{\Sigma}_{\mathbf{C}}^{(R)}$ is at least $m-1$. When there are no other parametric constraints on the entires of $\mathbf{P}$ (such as zeros), there are no other elements in the null space of $\boldsymbol{\Sigma}_{\mathbf{C}}^{(R)}$ besides linear combinations of those illuminated above. In this case, we obtain

$$\kappa = \frac{m(m-1)}{2} - (m-1) = \frac{(m-1)(m-2)}{2}$$

which completes our proof. □

Theorem 3.3.3. *As $L \to \infty$, $T_2 \xrightarrow{\mathcal{D}} \max_{1 \le \ell \le \kappa} \chi_\ell^2$, where $\{\chi_\ell^2\}_{\ell=1}^{\kappa}$ are independent and identically distributed chi-squared random variables each having one degree of freedom and κ is the rank of $\boldsymbol{\Sigma}_{\mathbf{C}}^{(R)}$. In the case where $\mathbf{P}$ has no zero elements or parameter restrictions, $\kappa = (m-1)(m-2)/2$.*

Proof. This result follows from the joint asymptotic normality of the $C_{i,j}$'s and the fact that the $D_{i,j}$'s are asymptotically uncorrelated. □

3.4 Simulation Examples

This section presents a simulation study assessing the performance of T_1 and T_2 as test statistics for reversibility. We consider a variety of transition matrices, some reversible, some non-reversible, and some non-reversible but close to reversible. In each case, ten thousand independent chains were generated from each transition matrix with the sample lengths $L = 250$, 1000 and 2500.

For reversible chains, one expects about 5% of the test statistics to exceed the 95% critical value. For non-reversible chains, one hopes for good power — that most of the test statistics exceed the 95% critical value.

We present five total examples. The first three examples have $m = 3$ with no zeros or other parameter restrictions in $\mathbf{P}$. In this case, the rank of $\boldsymbol{\Sigma}_{\mathbf{C}}^{(R)}$ is 1 and the 95% critical value for both T_1 and T_2 is 3.841. Example four takes $m = 5$ with no zeros or other parameter restrictions in $\mathbf{P}$. Here, the rank of $\boldsymbol{\Sigma}_{\mathbf{C}}^{(R)}$ is 6, the 95% critical value of T_1 is 12.592, and the 95% critical value of T_2 is 17.219. Example 5 considers a one-step-ahead transition matrix with several zero entries when $m = 4$. Here, the rank of $\boldsymbol{\Sigma}_{\mathbf{C}}^{(R)}$ is $\kappa = 2$, which gives 95% critical values for T_1 and T_2 as 5.991 and 7.352, respectively.

Our first example uses the transition matrix

$$\mathbf{P} = \begin{bmatrix} 1/5 & 2/5 & 2/5 \\ 2/5 & 1/5 & 2/5 \\ 2/5 & 2/5 & 1/5 \end{bmatrix}.$$

This chain is reversible, irreducible, and aperiodic with stationary distribution $\pi = (1/3, 1/3, 1/3)$. Figure 3.4 plots a kernel density estimate of the generated values of T_1 and T_2 against a chi-squared probability density function with one degree of freedom. Here, the Epanechnikov kernel function

$$K(x) = \frac{3(1-x^2)}{4}, \qquad -1 \leq x \leq 1,$$

was used with a smoothing bandwidth of 0.25 in all plots. Because the densities in question are supported on $[0, \infty)$, we have wrapped any probability mass that is assigned to $(-\infty, 0)$ back to the positive reals. As $L \to \infty$, it is seen that the test statistics match the χ^2 distribution with one degree of freedom reported in theorems 3.3.2 and 3.3.3, the fit improving with increasing L (the fit is so good in some cases that differences are hard to discern from the graphics).

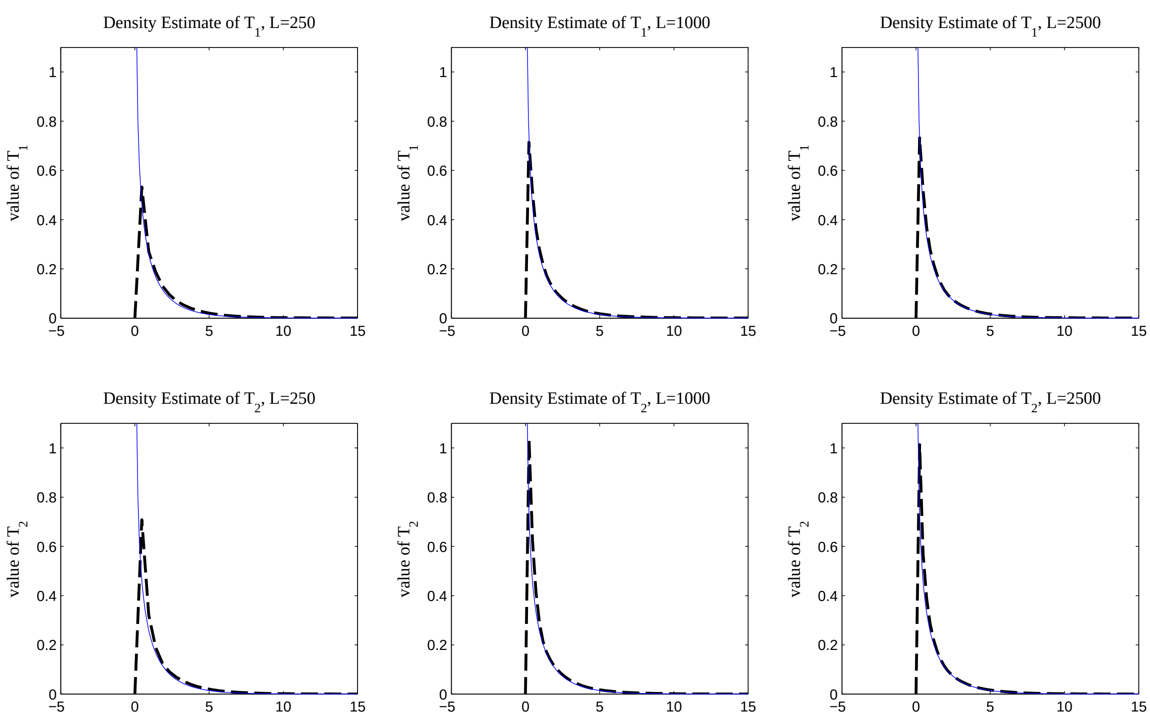

Figure 3.1: Sample Kernel Density Estimates Against the $\chi^2(1)$ Density.

For our second example, we consider

$$\mathbf{P} = \begin{bmatrix} 1/6 & 1/3 & 1/2 \\ 5/8 & 3/16 & 3/16 \\ 5/24 & 23/48 & 5/16 \end{bmatrix}.$$

This chain is not reversible, but is irreducible and aperiodic. In this case, the generated values of T_1 and T_2 are consistently above the 95% rejection threshold, even for the smaller values of L. Table 3.1 shows empirical powers of rejection for various L. These powers are reasonable, becoming perfect when $L = 1000$. In our first two examples, the test statistics are making good conclusions.

Table 3.1: Empirical Powers for Example 2

L	250	1000	2500
T_1	99.99%	100.00%	100.00%
T_2	99.99%	100.00%	100.00%

Our third example seeks to fool the methods by considering

$$\mathbf{P} = \begin{bmatrix} 8/15 & 1/3 & 2/15 \\ 9/33 & 20/33 & 4/33 \\ 1/3 & 1/3 & 1/3 \end{bmatrix}.$$

This chain is irreducible and aperiodic, but is not reversible. The chain's stationary distribution is $\pi = (55/144, 11/24, 23/144)$. While technically non-reversible, the equations in (3.1) are close to being satisfied. In particular, Table 3.3 shows values for both sides of the three reversible balance equations; two of these three equations "nearly hold".

Table 3.2 shows that the generated test statistics are close to zero and consistently below the 95% critical value. We attribute the slight non-monotonicity of the empirical powers (in L) to asymptotics not "kicking in". As expected, T_1 and T_2 have difficulty identifying non-reversibility with such small sample sizes.

Table 3.2: Empirical Powers for Example 3

L	250	1000	2500
T_1	7.88%	7.19%	9.45%
T_2	7.51%	7.14%	9.45%

To investigate this case more deeply, we ran additional simulations with much larger sample sizes, particularly $L = 10000$ and $L = 100000$. The empirical reversibility rejection powers reported in

Table 3.3: Detailed Balance Equations for Example 3

$\pi_1 p_{1,2} = \frac{55}{432} \approx 0.1273148148$	$\pi_2 p_{2,1} = \frac{1}{8} \approx 0.125$
$\pi_1 p_{1,3} = \frac{1}{72} \approx 0.152777777$	$\pi_3 p_{3,1} = \frac{23}{432} \approx 0.0532407407$
$\pi_2 p_{2,3} = \frac{1}{18} \approx 0.055555555$	$\pi_3 p_{3,2} = \frac{23}{432} \approx 0.0532407407$

Table 3.4 show that the methods do distinguish reversibility from non-reversibility asymptotically, but that it takes a large sample size L to do this effectively.

Table 3.4: Empirical Powers for Example 3 with Larger L

L	10000	100000
T_1	19.67%	94.08%
T_2	19.65%	94.07%

Our fourth example considers a larger state space — one where $m = 5$. Here, states one through five correspond to weather conditions of sunny, rainy, foggy, cloudy, and partly cloudy, respectively. We take the transition probabilities as

$$\mathbf{P} = \begin{bmatrix} 1/2 & 1/16 & 1/16 & 1/8 & 1/4 \\ 1/4 & 3/10 & 1/20 & 1/4 & 3/20 \\ 1/16 & 3/8 & 5/16 & 3/16 & 1/16 \\ 1/10 & 1/4 & 1/10 & 1/4 & 3/10 \\ 3/20 & 3/10 & 1/10 & 1/5 & 1/4 \end{bmatrix}.$$

This chain is not reversible, but is irreducible and aperiodic. Table 3.5 gives empirical powers of rejection at the 95% percentile. The numbers appear reasonable and the powers increase with increasing L. Here, T_2 performs much worse than T_1.

Table 3.5: Empirical Powers for Example 4

L	250	1000	2500
T_1	96.86%	100.00%	100.00%
T_2	61.14%	99.95%	100.00%

Our last example consider a case where the rank of $\mathbf{\Sigma}_{\mathbf{C}}^{(R)}$ is not the largest possible. We do this by taking $m = 4$ and imposing several elements of the transition matrix to be zero:

$$\mathbf{P} = \begin{bmatrix} 1/2 & 1/4 & 1/4 & 0 \\ 1/4 & 1/4 & 1/4 & 1/4 \\ 1/4 & 1/4 & 1/4 & 1/4 \\ 0 & 1/4 & 1/4 & 1/2 \end{bmatrix}.$$

This chain is reversible, aperiodic, and irreducible. The limiting distribution is $\pi = (1/4, 1/4, 1/4, 1/4)$. Suppose that physical reasoning dictates that $p_{1,4} = p_{4,1} = 0$ but that the other transition probabilities are non-zero. Here, the rank of null space of $\mathbf{\Sigma}_{\mathbf{C}}^{(R)}$ is $\kappa = 2$. This is seen by writing out the linear system for the asymptotic null space of $\mathbf{\Sigma}_{\mathbf{C}}^{(R)}$ as in the Proof of Theorem 1:

$$\begin{aligned} C_{1,2} + C_{1,3} + C_{1,4} &= 0 \\ -C_{1,2} + C_{2,3} + C_{2,4} &= 0 \\ -C_{1,2} - C_{2,3} + C_{3,4} &= 0 \\ -C_{1,4} - C_{2,4} - C_{3,4} &= 0 \end{aligned}$$

However, since we know that $p_{4,1} = 0$ and $p_{1,4} = 0$, $N_{1,4} = N_{4,1} = 0$ and the above linear system reduces to

$$\begin{aligned} C_{1,2} + C_{1,3} &= 0 \\ -C_{1,2} + C_{2,3} + C_{2,4} &= 0 \\ -C_{1,2} - C_{2,3} + C_{3,4} &= 0 \\ -C_{1,4} - C_{2,4} - C_{3,4} &= 0, \end{aligned}$$

which is easily verified to have rank 4. Hence, the rank of $\mathbf{\Sigma}_{\mathbf{C}}^{(R)}$ is $\kappa = 6 - 4 = 2$.

The Type I error probabilities in Table (3.6) are close to the designed 5% for the T_1 statistics, but smaller than 5% for T_2.

Table 3.6: Empirical Powers for Example 5

L	250	1000	2500
T_1	8.84%	7.41%	6.72%
T_2	5.01%	3.93%	3.56%

Overall, it seems that T_1 is superior to T_2, as can be seen by the slightly higher powers in the examples above when the chain is not reversible. However, the superiority is not not uniform (see Example 4 above). Overall, both statistics seem to function well.

3.5 Concluding Remarks

This paper considered the problem of detecting reversibility in a Markov chain data sequence. Two statistics were proposed and their asymptotic properties were derived. Both statistics performed reasonably well in a simulation study. The crux of the mathematical analysis lied with determining the asymptotic rank of an information matrix in a quadratic form.

Appendices

Appendix A Proof of Equation (3.2)

Proof. Write the counts up to time $L-1$ (the value of X_L does not affect the asymptotic analysis) as

$$N_i = \sum_{n=0}^{L-1} \mathbf{1}_{\{i\}}(X_n), \qquad N_{i,j} = \sum_{n=0}^{L-1} \mathbf{1}_{\{i,j\}}(X_n, X_{n+1}).$$

Then it is easy to see that $N_{i,j} - N_i p_{i,j} = \sum_{n=0}^{L-1} \mathbf{1}_{\{i\}}(X_n)(\mathbf{1}_{\{j\}}(X_{n+1}) - p_{i,j})$ has expectation 0. To handle the covariance term $\mathrm{E}[(N_{i,j} - N_i p_{i,j})(N_{i',j'} - N_{i'} p_{i',j'})]$, use

$$\begin{aligned}
&\sum_{n=0}^{L-1} \mathbf{1}_{\{i\}}(X_n)(\mathbf{1}_{\{j\}}(X_{n+1}) - p_{i,j}) \sum_{m=0}^{L-1} \mathbf{1}_{\{i'\}}(X_m)(\mathbf{1}_{\{j'\}}(X_{m+1}) - p_{i',j'}) \\
&= \sum_{n=0}^{L-1} \mathbf{1}_{\{i\}}(X_n)(\mathbf{1}_{\{j\}}(X_{n+1}) - p_{i,j})\mathbf{1}_{\{i'\}}(X_n)(\mathbf{1}_{\{j'\}}(X_{n+1}) - p_{i',j'}) \\
&+ \sum_{n=0}^{L-2} \sum_{m=n+1}^{L-1} \mathbf{1}_{\{i\}}(X_n)(\mathbf{1}_{\{j\}}(X_{n+1}) - p_{i,j})\mathbf{1}_{\{i'\}}(X_m)(\mathbf{1}_{\{j'\}}(X_{m+1}) - p_{i',j'}) \\
&+ \sum_{m=0}^{L-2} \sum_{n=m+1}^{L-1} \mathbf{1}_{\{i'\}}(X_m)(\mathbf{1}_{\{j'\}}(X_{m+1}) - p_{i',j'})\mathbf{1}_{\{i\}}(X_n)(\mathbf{1}_{\{j\}}(X_{n+1}) - p_{i,j}).
\end{aligned}$$

Consider the second piece in the expression above, for $m > n$, using the Markov property at time m,

$$\begin{aligned}
&\mathrm{E}[\mathbf{1}_{\{i\}}(X_n)(\mathbf{1}_{\{j\}}(X_{n+1}) - p_{i,j})\mathbf{1}_{\{i'\}}(X_m)(\mathbf{1}_{\{j'\}}(X_{m+1}) - p_{i',j'})] \\
&= \mathrm{E}[\mathbf{1}_{\{i\}}(X_n)(\mathbf{1}_{\{j\}}(X_{n+1}) - p_{i,j})\mathbf{1}_{\{i'\}}(X_m)\mathrm{E}[(\mathbf{1}_{\{j'\}}(X_{m+1}) - p_{i',j'})]|X_m = i'] \\
&= 0,
\end{aligned}$$

since $\mathrm{E}[(\mathbf{1}_{\{j'\}}(X_{m+1}) - p_{i',j'})]|X_m = i'] = p_{i',j'} - p_{i',j'} = 0$. A similar result holds when $n < m$. Hence, the crux lies with evaluating the first term in (9). When $i \neq i'$ this expectation is zero; however, when $i = i'$ we get

$$\sum_{n=0}^{L-1} \mathrm{E}[\mathbf{1}_{\{i\}}(X_n)(\mathbf{1}_{\{j\}}(X_{n+1}) - p_{i,j})(\mathbf{1}_{\{j'\}}(X_{n+1}) - p_{i',j'})]$$
$$= \sum_{n=0}^{L-1} \mathrm{E}[\mathbf{1}_{\{i\}}(X_n)\mathrm{E}[\mathbf{1}_{\{j\}}(X_{n+1})\mathbf{1}_{\{j'\}}(X_{n+1}) - p_{i,j}\mathbf{1}_{\{j'\}}(X_{n+1})$$
$$-p_{i,j'}\mathbf{1}_{\{j\}}(X_{n+1}) + p_{i,j}p_{i,j'}|X_n = i]].$$

From here we see that when $j = j'$, the inside conditional expectation equals $p_{i,j} - p_{i,j}^2 = p_{i,j}(1-p_{i,j})$ and when $j \neq j'$, it equals $-p_{i,j}p_{i,j'}$. Since the chain is assumed to be in stationarity, $\mathrm{E}[\mathbf{1}_{\{i\}}(X_n)] = \pi_i$ and we get

$$\mathrm{E}[(N_{i,j} - N_i p_{i,j})(N_{i',j'} - N_{i'} p_{i',j'})] = \begin{cases} L\pi_i p_{i,j}(1-p_{i,j}) & i = i' \quad j = j' \\ -L\pi_i p_{i,j} p_{i,j'} & i = i' \quad j \neq j' \\ 0 & i \neq i' \end{cases}$$

Applying Slutsky's Theorem, using the fact that $N_i/L \to \pi_i$ almost surely, and

$$\sqrt{L}(\hat{p}_{i,j} - p_{i,j}) = \sqrt{L}\left(\frac{L}{N_i}\left(\frac{N_{i,j} - N_i p_{i,j}}{L}\right)\right),$$

we get the central limit theorem presented by Anderson and Goodman (1957), Basawa and Rao (1980), Billingsley (1961) and Derman (1956)

$$\sqrt{L}\begin{pmatrix} \hat{p}_{i,j} - p_{i,j} \\ \hat{p}_{i',j'} - p_{i',j'} \end{pmatrix} \xrightarrow{\mathcal{D}} N\left(\mathbf{0}, \begin{pmatrix} p_{i,j}(1-p_{i,j})/\pi_i & \delta_{i,i'} p_{i,j}(\delta_{j,j'} - p_{i,j'})/\pi_i \\ \delta_{i,i'} p_{i,j}(\delta_{j,j'} - p_{i,j'})/\pi_i & p_{i',j'}(1-p_{i',j'})/\pi_{i'} \end{pmatrix}\right).$$

□

Appendix B Proof of Lemma 3.3.1

Proof. Derman (1956) establishes the asymptotic normality of the counts; however, he does not derive the asymptotic information matrix, which we now pursue. For this, express $N_{i,j}$ as the sum of indicator functions

$$N_{i,j} = \sum_{k=0}^{L-1} \mathbf{1}_{\{(i,j)\}}(X_k, X_{k+1})$$

and let $Y_k = (X_k, X_{k+1})$ for simplicity. Then

$$\begin{aligned}
\mathrm{E}[N_{i,j}] &= E\left[\sum_{k=0}^{L-1} \mathbf{1}_{\{(i,j)\}}(Y_k)\right] \\
&= \sum_{k=0}^{L-1} P(X_k = i, X_{k+1} = j) \\
&= \sum_{k=0}^{L-1} P(X_k = i, X_{k+1} = j | X_k = i) P(X_k = i) \\
&= \sum_{k=0}^{L-1} \pi_i p_{i,j} \\
&= L\pi_i p_{i,j}.
\end{aligned}$$

A similar tactic allows us to calculate the variance of $N_{i,j}$. Observe that

$$\begin{aligned}
(N_{i,j} - L\pi_i p_{i,j})^2 &= \sum_{k=0}^{L-1}\sum_{\ell=0}^{L-1} (\mathbf{1}_{\{(i,j)\}}(Y_k) - \pi_i p_{i,j})(\mathbf{1}_{\{(i,j)\}}(Y_\ell) - \pi_i p_{i,j}) \\
&= \sum_{k=0}^{L-1} (\mathbf{1}_{\{(i,j)\}}(Y_k) - \pi_i p_{i,j})^2 \\
&+ 2\sum_{k=0}^{L-2}\sum_{\ell=k+1}^{L-1} (\mathbf{1}_{\{(i,j)\}}(Y_k) - \pi_i p_{i,j})(\mathbf{1}_{\{(i,j)\}}(Y_\ell) - \pi_i p_{i,j}).
\end{aligned}$$

The expectation of the first term is simply a sum of variances of indicator functions:

$$\mathrm{E}\left[\sum_{k=0}^{L-1} (\mathbf{1}_{\{(i,j)\}}(Y_k) - \pi_i p_{i,j})^2\right] = \sum_{k=0}^{L-1} \mathrm{E}[(\mathbf{1}_{\{(i,j)\}}(Y_k) - \pi_i p_{i,j})^2] = L\pi_i p_{i,j}(1 - \pi_i p_{i,j}).$$

For the second term, we introduce some notation. For a one-step-ahead transition matrix $\mathbf{P}$ with invariant measure π, we define $\mathbf{\Pi}$ as a matrix whose all rows are $\boldsymbol{\pi}$. Define $\mathbf{Q} = \mathbf{P} - \mathbf{\Pi}$ and observe that by stationarity that $\mathbf{\Pi P} = \mathbf{\Pi}$, $\mathbf{P\Pi} = \mathbf{\Pi}$, and $\mathbf{\Pi}^n = \mathbf{\Pi}$. Hence, $\mathbf{Q}^n = \mathbf{P}^n - \mathbf{\Pi}$.

For $\ell > k$,

$$\begin{aligned} \mathrm{E}[(\mathbf{1}_{\{(i,j)\}}(Y_k) - \pi_i p_{i,j})(\mathbf{1}_{\{(i,j)\}}(Y_\ell) - \pi_i p_{i,j})] &= \mathrm{E}[\mathbf{1}_{\{(i,j)\}}(Y_k)\mathbf{1}_{\{(i,j)\}}(Y_\ell)] - (\pi_i p_{i,j})^2 \\ &= \pi_i p_{i,j} p_{j,i}^{(\ell-k-1)} p_{i,j} - (\pi_i p_{i,j})^2 \\ &= \pi_i p_{i,j}^2 (p_{j,i}^{(\ell-k-1)} - \pi_i) \\ &= \pi_i p_{i,j}^2 q_{j,i}^{(\ell-k-1)}, \end{aligned}$$

where the convention $q_{i,j^{(0)}} = \delta_{i,j}$ has been used. Summing the above equation over k and ℓ gives

$$\begin{aligned} \sum_{k=0}^{L-2} \sum_{\ell=k+1}^{L-1} q_{j,i}^{(\ell-k-1)} &= \sum_{k=0}^{L-2} \sum_{\ell'=0}^{L-k-1} q_{j,i}^{(\ell')} \\ &= \sum_{k=0}^{L-2} \sum_{\ell'=0}^{L-2} \mathbf{1}_{\{\ell' \le L-k-1\}} q_{j,i}^{(\ell')} \\ &= \sum_{\ell'=0}^{L-2} \sum_{k=0}^{L-2} \mathbf{1}_{\{k \le L-\ell'-1\}} q_{j,i}^{(\ell')} \\ &= \sum_{\ell'=0}^{L-2} (L - \ell' - 1) q_{j,i}^{(\ell')}. \end{aligned}$$

Combining the above and using that $E[N_{i,j}] = L\pi_i p_{i,j}$ gives

$$\mathrm{Var}(N_{i,j}) = 2\pi_i p_{i,j}^2 \sum_{\ell=0}^{L-2} (L - 1 - \ell) q_{j,i}^{(\ell)} + L\pi_i p_{i,j}(1 - \pi_i p_{i,j}).$$

To compute $\mathrm{Cov}(N_{i,j}, N_{i',j'})$, we assume that either $i \neq i'$ or $j \neq j'$ (else, one recalculates $\mathrm{Var}(N_{i,j})$). Then

$$
\begin{aligned}
(N_{i,j} - L\pi_i p_{i,j})(N_{i',j'} - L\pi_{i'} p_{i',j'}) &= \sum_{k=0}^{L-1}(\mathbf{1}_{\{(i,j)\}}(Y_k) - \pi_i p_{i,j}) \sum_{\ell=0}^{L-1}(\mathbf{1}_{\{(i',j')\}}(Y_\ell) - \pi_{i'} p_{i',j'}) \\
&= \sum_{k=0}^{L-2} \sum_{\ell=k+1}^{L-1} (\mathbf{1}_{\{(i,j)\}}(Y_k) - \pi_i p_{i,j})(\mathbf{1}_{\{(i',j')\}}(Y_\ell) - \pi_{i'} p_{i',j'}) \\
&+ \sum_{\ell=0}^{L-2} \sum_{k=\ell+1}^{L-1} (\mathbf{1}_{\{(i',j')\}}(Y_\ell) - \pi_{i'} p_{i',j'})(\mathbf{1}_{\{(i,j)\}}(Y_k) - \pi_i p_{i,j}) \\
&+ \sum_{k=0}^{L-1}(\mathbf{1}_{\{(i,j)\}}(Y_k) - \pi_i p_{i,j})(\mathbf{1}_{\{(i',j')\}}(Y_k) - \pi_{i'} p_{i',j'}).
\end{aligned}
\tag{9}
$$

Arguing as above, the expectation of the last term in (9) is $-L\pi_i p_{i,j}\pi_{i'} p_{i',j'}$. As evaluating the expectation of the first and second terms in (9) are similar, we only consider the first term. For $\ell > k$,

$$
\begin{aligned}
\mathrm{E}[(\mathbf{1}_{\{(i,j)\}}(Y_k) - \pi_i p_{i,j})(\mathbf{1}_{\{(i',j')\}}(Y_\ell) - \pi_{i'} p_{i',j'})] &= \mathrm{E}[\mathbf{1}_{\{(i,j)\}}(Y_k)\mathbf{1}_{\{(i',j')\}}(Y_\ell)] - \pi_i p_{i,j}\pi_{i'} p_{i',j'} \\
&= \pi_i p_{i,j} p_{j,i'}^{(\ell-k-1)} p_{i',j'} - \pi_i p_{i,j}\pi_{i'} p_{i',j'} \\
&= \pi_i p_{i,j} p_{i',j'} (p_{j,i'}^{(\ell-k-1)} - \pi_{i'}) \\
&= \pi_i p_{i,j} p_{i',j'} q_{j,i'}^{(\ell-k-1)}.
\end{aligned}
$$

Hence,

$$
\sum_{k=0}^{L-2} \sum_{\ell=k+1}^{L-1} \mathrm{E}[(\mathbf{1}_{\{(i,j)\}}(Y_k) - \pi_i p_{i,j})(\mathbf{1}_{\{(i',j')\}}(Y_\ell) - \pi_{i'} p_{i',j'})] = \pi_i p_{i,j} p_{i',j'} \sum_{\ell=0}^{L-2}(L-1-\ell) q_{j,i'}^{(\ell)}.
$$

When $\ell < k$, we have

$$
\sum_{k=0}^{L-2} \sum_{\ell=k+1}^{L-1} \mathrm{E}[(\mathbf{1}_{\{(i,j)\}}(Y_k) - \pi_i p_{i,j})(\mathbf{1}_{\{(i',j')\}}(Y_\ell) - \pi_{i'} p_{i',j'})] = \pi_{i'} p_{i',j'} p_{i,j} \sum_{\ell=0}^{L-2}(L-1-\ell) q_{j',i}^{(\ell)}.
$$

Combining the three expectations above gives

$$\mathrm{Cov}(N_{i,j}, N_{i',j'}) = \sum_{\ell=0}^{L-2} (L-1-\ell)[\pi_i p_{i,j} p_{i',j'} q_{j,i'}^{(\ell)} + \pi_{i'} p_{i',j'} p_{i,j} q_{j',i}^{(\ell)}] - L\pi_i p_{i,j} \pi_{i'} p_{i',j'}.$$

To get the asymptotic covariance matrix of the sample counts, we first note that $Q^n \to 0$ almost surely and $R := \sum_{n=0}^{\infty} Q^n = (I-Q)^{-1}$. By Kronecker's Lemma (see Theorem 6.1.3 in Ash and Dolèans-Dade), we have

$$\frac{1}{L}\sum_{\ell=0}^{L-2}(L-1-\ell)Q^\ell = \sum_{\ell=0}^{L-2} Q^\ell - \frac{1}{L}\sum_{\ell=0}^{L-2}(\ell+1)Q^\ell \to \sum_{\ell=0}^{\infty} Q^\ell = R.$$

Using the above expectations and taking limits gives

$$\begin{aligned} \lim_{L\to\infty} L\mathrm{Var}\left(\frac{N_{i,j}}{L}\right) &= \lim_{L\to\infty} \frac{1}{L}\mathrm{Var}(N_{i,j}) \\ &= 2\pi_i p_{i,j}^2 r_{j,i} + \pi_i p_{i,j}(1-\pi_i p_{i,j}) \end{aligned}$$

and

$$\begin{aligned} \lim_{L\to\infty} L\mathrm{Cov}\left(\frac{N_{i,j}}{L}, \frac{N_{i',j'}}{L}\right) &= \lim_{L\to\infty} \frac{1}{L}\mathrm{Cov}(N_{i,j}, N_{i',j'}) \\ &= \pi_i p_{i,j} p_{i',j'} r_{j,i'} + \pi_{i'} p_{i',j'} p_{i,j} r_{j',i} - \pi_i p_{i,j} \pi_{i'} p_{i',j'}. \end{aligned}$$

$\square$

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