PRACTICAL TESTS FOR SIGNIFICANCE IN MARKOV CHAINS

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Abstract. We give improvements to theorems which enable significance testing in Markov Chains.

1. Introduction

Consider a reversible Markov Chain $\mathcal{M}$ whose state-space $\Sigma$ is endowed with some labeling $\omega : \Sigma \to \mathbb{R}$, and for which $\pi$ is a stationary distribution. $\mathcal{M}$, $\pi$, $\omega$, and a fixed integer $k$ determine a vector

$$p_k^0, p_k^1, \ldots, p_k^k$$

where for each $i$, $p_k^i$ is the probability that for a $k$-step $\pi$-stationary trajectory $X_0, \ldots, X_k$, the minimum $\omega$ value occurs at $X_i$. In other words, $p_k^i$ is the probability that if we choose $X_0$ randomly from the stationary distribution $\pi$ and take $k$ steps in $\mathcal{M}$ to obtain the trajectory $X_0, X_1, \ldots, X_k$, that we observe that $\omega(X_i)$ is the minimum among $\omega(X_0), \ldots, \omega(X_k)$. Note that if we adopted the convention that we break ties among the values $\omega(X_0), \ldots, \omega(X_k)$ randomly, we would have that $p_k^0 + \cdots + p_k^k = 1$, for any $\mathcal{M}$, $\pi$, and $k$.

At first glance, it might be natural to assume that we must have something like $p_k^i \approx \frac{1}{k+1}$ for all $0 \leq i \leq k$. But this is actually quite far from the truth. In [CFP], we showed that for some $\mathcal{M}$, $\pi$, $k$, we can have $p_k^0$ as large as essentially $\frac{1}{\sqrt{2\pi k}}$.

As we proved in [CFP], this is essentially the worst possible behavior for $p_k^0$. In particular, we can generalize the vector $\{p_k^i\}$ defined above as possible: let us define, given $\mathcal{M}$, $\pi$, $k$, and $\varepsilon$, the vector

$$p_{0,\varepsilon}^k, p_{1,\varepsilon}^k, \ldots, p_{k,\varepsilon}^k$$

where each $p_{i,\varepsilon}^k$ is the probability that $\omega(X_i)$ is among the smallest $\varepsilon$ values in the list $\omega(X_0), \ldots, \omega(X_k)$. Then in [CFP] we proved:

**Theorem 1.1.** Given a reversible Markov chain $\mathcal{M}$ with stationary distribution $\pi$, an $\varepsilon > 0$, $k \geq 0$, and With $p_{i,\varepsilon}^k$ defined as above, we have that

$$p_{0,\varepsilon}^k \leq \sqrt{2\varepsilon}.$$
Note that the example from [CFP] realizing \( p_k^0 \approx \frac{1}{\sqrt{2\pi k}} \) shows that this theorem is best possible, up to constant factors.

One important application of Theorem 1.1 is that it characterizes the statistical significance associated to the result of a natural test for gerrymandering of political districtings. In particular, consider the following general procedure to evaluate a districting of a state:

**Local Outlier Test**

1. Beginning from the districting being evaluated,
2. Make a sequence of random changes to the districting, while preserving some set of constraints imposed on the districtings.
3. Evaluate the partisan properties of each districting encountered (e.g., by simulating elections using past voting data).
4. Call the original districting “carefully crafted” or “gerrymandered” if the overwhelming majority of districtings produced by making small random changes are less partisan than the original districting.

Naturally, the test described above can be implemented so that it precisely satisfies the hypotheses of Theorem 1.1. For this purpose, a (very large) set of comparison districtings are defined, to which the districting being evaluated belongs. For example, the comparison districtings may be the districtings built out of Census blocks (or some other unit) which are contiguous, equal in population up to some specified deviation, or include other constraints. A Markov chain \( \mathcal{M} \) is defined on this set of districtings, where transitions in the chain correspond to changes in districtings. (For example, a transition may correspond to randomly changing the district assignment of a randomly chosen Census block which currently borders more than one district, subject to the constraints imposed on the comparison set.) The “random changes” from Step 2 will then be precisely governed by the transition probabilities of the Markov chain \( \mathcal{M} \). By designing \( \mathcal{M} \) so that the uniform distribution \( \pi \) on the set of comparison districtings \( \Sigma \) is a stationary distribution for \( \mathcal{M} \), Theorem 1.1 gives an upper bound on the false-positive rate (in other words, global statistical significance) for the “gerrymandered” declaration when it is made in Step 4.

Apart from its application to gerrymandering, Theorem 1.1 has a simple informal interpretation for the general behavior of reversible Markov chains, namely: *typical (i.e., stationary) states are unlikely to change in a consistent way under a sequence of chain transitions*, with a best-possible quantification of this fact (up to constant factors).

Also, in the general setting of a reversible Markov chain, the theorem leads to a simple quantitative procedure for asserting rigorously that \( \sigma_0 \) is atypical with respect to \( \pi \) without knowing the mixing time of \( \mathcal{M} \): simply observe a random trajectory \( \sigma_0 = X_0, X_1, X_2, \ldots, X_k \) from \( \sigma_0 \) for any fixed \( k \). If \( \omega(\sigma_0) \) is an \( \varepsilon \)-outlier among \( \omega(X_0), \ldots, \omega(X_k) \), then this is statistically significant at \( \sqrt{2\varepsilon} \) against the null hypothesis that \( \sigma_0 \sim \pi \).
This quantitative test is potentially useful because $\sqrt{2\varepsilon}$ converges quickly enough to 0 as $\varepsilon \to 0$; in particular, it is possible to obtain good statistical significance from observations which can be made with reasonable computational resources. Of course, faster convergence to 0 would be even better, but, as already noted, $p \approx \sqrt{\varepsilon}$ is roughly a best possible upper bound.

Unknown to the authors at the time of the publication of [CFP], a 1989 paper of Besag and Clifford described a test related to that based on Theorem 1.1, which has essentially a one-line proof, which we discuss in Section 3:

**Theorem 1.2** (Besag and Clifford serial test). Fix any number $k$ and suppose that $\sigma_0$ is chosen from a stationary distribution $\pi$, and that $\xi$ is chosen uniformly in $\{0, \ldots, k\}$. Consider two independent trajectories $Y_0, Y_1, \ldots$ and $Z_0, Z_1, \ldots$ in the reversible Markov Chain $\mathcal{M}$ (whose states have real-valued labels) from $Y_0 = Z_0 = \sigma_0$. If we choose $\sigma_0$ from a stationary distribution $\pi$ of $\mathcal{M}$, then for any $k$ we have that

$$\Pr(\omega(\sigma_0) \text{ is an } \varepsilon\text{-outlier among } \omega(\sigma_0), \omega(Y_1), \ldots, \omega(Y_\xi), \omega(Z_1), \ldots, \omega(Z_{k-\xi})) \leq \varepsilon.$$ 

Here, a real number $a_0$ is an $\varepsilon$-outlier among $a_0, \ldots, a_k$ if

$$\# \{i \in \{0, \ldots, k\} \mid a_i \leq a_0\} \leq \varepsilon(k + 1).$$

In particular, the striking thing about Theorem 1.2 is that it achieves a best-possible dependence on the parameter $\varepsilon$. (Notice that $\varepsilon$ would be the correct value of the probability if, for example, the Markov chain is simply a collection of independent random samples.) The sacrifice is in Theorem 1.2’s slightly more complicated intuitive interpretation, which would be: typical (i.e., stationary) states are unlikely to change in a consistent way under two sequences of chain transitions of random complementary lengths. In particular, in applications of these statistical tests to aspects of public policy, it is desirable to have tests with simple, intuitive interpretations. To enable better significance testing in this sphere, one goal of the present note is to prove a theorem enabling Markov chain significance testing which is intuitively interpretable in the sense of Theorem 1.1, while having linear dependence on $\varepsilon$, as in Theorem 1.2.

One common feature of the tests based on Theorem 1.1 and 1.2 is the use of randomness. In particular, the probability space at play in these theorems includes both the random choice of $\sigma_0$ assumed by the null hypothesis and the random steps taken by the Markov chain from $\sigma_0$. Thus the measures of “how (globally) unusual” $\sigma_0$ is with respect to its performance in the local outlier test and “how sure” we are that $\sigma_0$ is unusual in this respect are intertwined in the final $p$-value. In particular, the effect size and the statistical significance are not explicitly separated.

To further the goal of simplifying the interpretation of the results of these tests, our approach in this note will also show that tests like these can be efficiently used in a way which separates the measure of statistical significance from the question of the magnitude of the effect. In particular, recalling the probabilities $p_{0, \varepsilon}^k, \ldots, p_{k, \varepsilon}^k$ defined previously, let us define the probability $p_{0, \varepsilon}(\sigma_0)$ to be the probability that
on a trajectory \( \sigma_0 = X_0, X_1, \ldots, X_k, \omega(\sigma_0) \) is among the smallest values in the list \( \omega(X_0, \ldots, X_k) \). Now we make the following definition:

**Definition 1.3.** For a fixed value of \( k \), the state \( \sigma_0 \) is an \((\varepsilon, \alpha)\)-outlier in \( M \) if, among all states in \( M \), \( p^k_{0,\varepsilon}(\sigma_0) \) is in the largest \( \alpha \) fraction of the values of \( p_{0,\varepsilon}(\sigma) \) over all states \( \sigma \in M \), weighted according to \( \pi \).

In particular, being an \((\varepsilon, \alpha)\)-outlier measures the likelihood of \( \sigma_0 \) to fail the local outlier test, ranked against all other states \( \sigma \sim \pi \) of the chain \( M \). For example, fix \( k = 10^9 \). If \( \sigma_0 \) is a \((10^{-6}, 10^{-5})\)-outlier in \( M \) and \( \pi \) is the uniform distribution, this means that among all states \( \sigma \in M \), \( \sigma_0 \) is more likely than all but a \( 10^{-5} \) fraction of states to have an \( \omega \)-value in the bottom \( 10^{-6} \) values \( \omega(X_0), \omega(X_1), \ldots, \omega(X_{10^9}) \).

Note that whether \( \sigma_0 \) is an \((\varepsilon, \alpha)\)-outlier is a deterministic question about the properties of \( \sigma_0, M, \) and \( \omega \). Thus it is a deterministic measure (defined in terms of certain probabilities) of the extent to which \( \sigma_0 \) is unusual (globally, in all of \( M \)) with respect to its local fragility in the chain.

The following theorem enables one to assert statistical significance for the property of being an \((\varepsilon, \alpha)\)-outlier. In particular, while tests based on Theorems 1.1 and 1.2 take as their null hypothesis that \( \sigma_0 \sim \pi \), the following theorem takes as its null hypothesis merely that \( \sigma_0 \) is not an \((\varepsilon, \alpha)\)-outlier.

**Theorem 1.4.** Consider \( m \) independent trajectories

\[ T^1 = (X^1_0, X^1_1, \ldots, X^1_k), \]

\[ \vdots \]

\[ T^m = (X^m_0, X^m_1, \ldots, X^m_k) \]

of length \( k \) in the reversible Markov Chain \( M \) (whose states have real-valued labels) from a common starting point \( X^1_0 = \cdots = X^m_0 = \sigma_0 \). Define the random variable \( \rho \) to be the number of trajectories \( T^i \) on which \( \sigma_0 \) is an \( \varepsilon \)-outlier.

If \( \sigma_0 \) is not an \((\varepsilon, \alpha)\)-outlier, then

\[ \Pr \left( \rho \geq m \sqrt{\frac{2\varepsilon}{\alpha}} + r \right) \leq e^{-\min(\varepsilon^2 \sqrt{\alpha/3m}, r/3)}. \]

In particular, apart from separating measures of statistical significance from the quantification of a local outlier, Theorem 1.4 connects the intuitive Local Outlier Test tied to Theorem 1.1 (which motivates the definition of a \((\varepsilon, \alpha)\)-outlier) to the better quantitative dependence on \( \varepsilon \) in Theorem 1.2.

To compare the quantitative performance of Theorem 1.4 to Theorems 1.1 and 1.2, consider the case of a state \( \sigma_0 \) for which a random trajectory \( \sigma_0 = X_0, X_1, \ldots, X_k \) is likely (say with some constant probability \( p' \)) to find \( \sigma_0 \) an \( \varepsilon' \)-outlier. For Theorem
1.1, significance at $p \approx \sqrt{2\varepsilon}$ would be obtained\(^1\), while using Theorem 1.2, one would hope to obtain significance of $\approx \varepsilon'$. Applying Theorem 1.4, we would expect to see $\rho$ around $m \cdot p'$. In particular, we could demonstrate that $\sigma_0$ is an $(\varepsilon', \alpha)$ outlier for $\alpha = \frac{3}{(p')^2}$ (a linear dependence on $\varepsilon$) at a $p$-value which can be made arbitrarily small (at an exponential rate) as we increase the number of observed trajectories $m$. As we will see in Section 4, the exponential tail in (1) can be replaced by a binomial tail. In particular, the following special case applies:

**Theorem 1.5.** With $T^1, \ldots, T^m$ as in Theorem 1.4, we have that if $\sigma_0$ is not an $(\varepsilon, \alpha)$ outlier, then

$$\Pr(\sigma_0 \text{ an } \varepsilon\text{-outlier on all of } T^1, \ldots, T^m) \leq \left(\frac{2\varepsilon}{\alpha}\right)^{m/2}.$$  

Theorem 1.5 also has advantages from the standpoint of avoiding the need to correct for multiple hypothesis testing, as we discuss in Section 2.

To prove Theorem 1.4, we will prove the following, which has a quantitative dependence on $\varepsilon$ which is nearly as strong as in Theorem 1.2, while eliminating the need for the random choice of $\xi$ there.

**Theorem 1.6.** Consider two independent trajectories $Y_0, \ldots, Y_k$ and $Z_0, \ldots, Z_k$ in the reversible Markov Chain $\mathcal{M}$ (whose states have real-valued labels) from a common starting point $Y_0 = Z_0 = \sigma_0$. If we choose $\sigma_0$ from a stationary distribution $\pi$ of $\mathcal{M}$, then for any $k$ we have that

$$\Pr(\omega(\sigma_0) \text{ is an } \varepsilon\text{-outlier among } \omega(\sigma_0), \omega(Y_1), \ldots, \omega(Y_k), \omega(Z_1), \ldots, \omega(Z_k)) < 2\varepsilon.$$  

Note that Theorem 1.6 is equivalent to the statement that the probabilities $p_{i,\varepsilon}^k$ always satisfy

$$p_{k,\varepsilon}^{2k} < 2\varepsilon.$$  

As in the case of Theorem 1.1, it seems like an interesting theoretical question to investigate the tightness of the constant 2. (What is the largest possible value of $p_{k,\varepsilon}^{2k}$ as a function of $\varepsilon$ and $k$?)

In their paper, Besag and Clifford also describe a parallel test, which we will discuss in Section 5. In particular, in Section 5 we will describe a test which generalizes Besag and Clifford’s serial and parallel tests in a way which could be useful in certain parallel regimes.

\(^1\)Multiple tests have limited utility here or with Theorem 1.2 since there is no independence (the null hypothesis $\sigma_0 \sim \pi$ is not being resampled). In particular, multiple runs might be done merely until a trajectory is seen on which $\sigma_0$ is indeed an $\varepsilon'$ outlier (requiring $1/p'$ runs, on average), in conjunction with multiple hypothesis testing.
When applying Theorem 1.4 directly, one cannot simply run \( m \) trajectories, observe the list \( \varepsilon_1, \varepsilon_2, \ldots, \varepsilon_m \) where each \( \varepsilon_i \) is the minimum \( \varepsilon_i \) for which \( \sigma_0 \) is an \( \varepsilon_i \)-outlier on \( T^i \), and then, post-hoc, freely choose the parameters \( \alpha \) and \( \varepsilon \) in Theorem 1.4 to achieve some desired tradeoff between \( \alpha \) and the significance \( p \).

The problem, of course, is that in this case one is testing multiple hypotheses (infinitely many in fact; one for each possible pair \( \varepsilon \) and \( \alpha \)) which would require a multiple hypothesis correction.

One way to avoid this problem is to essentially do a form of cross validation, where a few trajectories are run for the purposes of selecting suitable \( \varepsilon \) and \( \alpha \), and then discarded from the set of trajectories from which we obtain significance.

A simpler approach, however, is to simply set the parameter \( \varepsilon = \varepsilon(t) \) as the \( t \)-th smallest element of the list \( \varepsilon_1, \ldots, \varepsilon_m \) for some fixed value \( t \). The case \( t = m \), for example, corresponds to taking \( \varepsilon \) as the maximum value, leading to the application of Theorem 1.5.

The reasons this avoids the need for a multiple hypothesis correction is that we can order our hypothesis events by containment. In particular, when we apply this test with some value of \( t \), we will always have \( \rho = t \). Thus the significance obtained will depend just on the parameter \( \varepsilon(t) \) returned by taking the \( t \)-th smallest \( \varepsilon_i \) and on our choice of \( \alpha \) (as opposed to say, the particular values of the other \( \varepsilon_i \)'s which are not the \( t \)-th smallest). In particular, regardless of how we wish to tradeoff the values of \( \alpha \) and \( p \) we can assert from our test, our optimum choice of \( \alpha \) (for our fixed choice of \( t \)) will depend just on the value \( \varepsilon(t) \). In particular, we can view \( \alpha \) as a function \( \alpha(\varepsilon(t)) \), so that we when applying Theorem 1.4 with \( \varepsilon = \varepsilon(t) \), we are evaluating the single-parameter infinite family of hypotheses \( H_{\varepsilon(t), \alpha(\varepsilon(t))} \), and we do not require multiple hypothesis correction since the hypotheses are nested; i.e., since

\[
\varepsilon(t) \leq \varepsilon'(t) \implies H_{\varepsilon(t), \alpha(\varepsilon(t))} \subseteq H_{\varepsilon'(t), \alpha(\varepsilon'(t))}.
\]

Indeed, (2) implies that

\[
\Pr \left( \bigcup_{\varepsilon(t) \leq \beta} H_{\varepsilon(t), \alpha(\varepsilon(t))} \right) = \Pr(H_{\beta, \alpha(\beta)}),
\]

which ensures that when applying Theorem 1.4 in this scenario, the probability of returning a \( p \)-value \( \leq p_0 \) for any fixed value \( p_0 \) will indeed be at most \( p_0 \).

3. Proof background

We begin this section by giving the proof of Theorem 1.6. In doing so we will introduce some notation that will be useful throughout the rest of this note. To make things as accessible as possible, we give every detail of the proof.
In this manuscript, a Markov Chain $M$ on $\Sigma$ is specified by the transition probabilities $\{\pi_{\sigma_1, \sigma_2} | \sigma_1, \sigma_2 \in \Sigma\}$ of a chain. A trajectory of $M$ is a sequence of random variables $X_0, X_1, \ldots$ required to have the property that for each $i$ and $\sigma_0, \ldots, \sigma_i$, we have
\begin{equation}
\Pr(X_i = \sigma_i | X_{i-1} = \sigma_{i-1}, X_{i-2} = \sigma_{i-2} \ldots, X_0 = \sigma_0) = \pi_{\sigma_i, \sigma_{i-1}}.
\end{equation}

In particular, the Markov property of the trajectory is that the conditioning on variables $\{\sigma_1, \sigma_2 \mid \sigma_1, \sigma_2 \in \Sigma\}$ already gives the theorem, once we make the following trivial observation: $M$ is a stationary distribution if $\pi$ is a stationary distribution if $X_0 \sim \pi$ implies that $X_1 \sim \pi$ and thus also that $X_i \sim \pi$ for all $i \geq 0$; in this case we that the trajectory $X_0, X_1, \ldots$ is $\pi$-stationary. The Markov Chain $M$ is reversible if any $\pi$-stationary trajectory $X_0, \ldots, X_k$ is equivalent in distribution to its reverse $X_k, \ldots, X_0$.

We say that $a_j$ is $\ell$-small among $a_0, \ldots, a_s$ if there are at most $\ell$ indices $i \neq j$ among $0, \ldots, s$ such that $a_i \leq a_j$. The following simple definition is at the heart of the proofs of Theorems 1.1, 1.6, 1.2.

**Definition 3.1.** Given a Markov Chain $M$ with labels $\omega : \Sigma \rightarrow \mathbb{R}$ and stationary distribution $\pi$, we define for each $\ell, j \leq k$ a real number $\rho_{j, \ell}^k$, which is the probability that for a $\pi$-stationary trajectory $X_0, X_1, \ldots, X_k$, we have that $\omega(X_j)$ is $\ell$-small among $\omega(X_0), \ldots, \omega(X_k)$.

Observe that (3) implies that all $\pi$-stationary trajectories of a fixed length are all identical in distribution, and in particular, that the $\rho_{j, \ell}^k$’s are well-defined.

Next observe that if the sequence of random variables $X_0, X_1, \ldots$ is a $\pi$-stationary trajectory for $M$, then so is any interval of it. For example,
\[(X_{k-j}, \ldots, X_k, \ldots, X_{2k-j})\]
is another stationary trajectory, and thus the probability that $\omega(X_k)$ is $\ell$-small among $\omega(X_{k-j}), \ldots, \omega(X_{2k-j})$ is equal to $\rho_{j, \ell}^k$. In particular, since $\omega(X_k)$ is $\ell$-small among $\omega(X_{k-j}), \ldots, \omega(X_{2k-j})$ follows from
\[
(\omega(X_k) \text{ is } \ell\text{-small among } \omega(X_{k-j}), \ldots, \omega(X_{2k-j}))
\]
for all $j = 0, \ldots, k$, we have that
\begin{equation}
\rho_{k, \ell}^{2k} \leq \rho_{j, \ell}^k.
\end{equation}

We also have that $\sum_{j=0}^k \rho_{j, \ell}^k \leq \ell + 1$. Indeed, by linearity of expectation, this sum is the expected number of indices $j \in 0, \ldots, k$ such that $\omega(X_j)$ is $\ell$-small among $\omega(X_0), \ldots, \omega(X_k)$. Thus, averaging the left and right sides of (4) over $j$ from 0 to $k$, we obtain
\begin{equation}
\rho_{k, \ell}^{2k} \leq \frac{\ell + 1}{k + 1} < 2 \cdot \frac{\ell + 1}{2k + 1}.
\end{equation}

Line (5) already gives the theorem, once we make the following trivial observation:
Observation 3.2. Under the hypotheses of Theorem 1.6, we have that
\( Y_k, Y_{k-1}, \ldots, Y_1, \sigma_0, Z_1, Z_2, \ldots, Z_k \)
is a \( \pi \)-stationary trajectory.

This is an elementary consequence of the definitions, but since we will generalize this statement in Section 5, we give all the details here:

Proof of Observation 3.2. Our hypothesis is that \( Y_1, Y_2, \ldots, Y_k \) and \( Z_1, Z_2, \ldots, Z_k \) are independent trajectories from a common state \( Y_0 = Z_0 = \sigma_0 \) chosen from the stationary distribution \( \pi \). Stationarity implies that
\[
(Z_0, Z_1, \ldots, Z_k) \sim (X_k, X_{k+1}, \ldots, X_{2k}).
\]
Similarly, stationarity and reversibility imply that
\[
(Y_k, Y_{k-1}, \ldots, Y_0) \sim (X_0, X_1, \ldots, X_k).
\]
Finally, our assumption that \( Y_1, Y_2, \ldots, Y_k \) and \( Z_1, Z_2, \ldots, Z_k \) are independent trajectories from \( \sigma_0 \) is equivalent to the condition that, for any \( s_0, y_1, z_1, y_2, z_2, \ldots, y_k, z_k \in \Sigma \), we have for all \( j \geq 0 \) that
\[
\Pr(Z_j = z_j \mid Z_{j-1} = z_{j-1}, \ldots, Z_1 = z_1, Z_0 = Y_0 = s_0, Y_1 = y_1, \ldots, Y_k = y_k) = \Pr(Z_j = z_j \mid Z_{j-1} = z_{j-1}, \ldots, Z_1 = z_1, Z_0 = s_0)\]

Of course, since \( M \) is a Markov Chain, this second probability is simply
\[
\Pr(Z_j = z_j \mid Z_{j-1} = z_{j-1}) = \Pr(X_{k+j} = z_j \mid X_{k+j-1} = z_{j-1}).
\]
In particular, by induction on \( j \geq 1 \),
\[
(Y_k, Y_{k-1}, \ldots, Y_0 = Z_0, Z_1, \ldots, Z_j) \sim (X_0, X_1, \ldots, X_k, X_{k+1}, \ldots, X_{k+j}),
\]
and in particular
\[
(Y_k, \ldots, \sigma_0, \ldots, Z_k) \sim (X_0, \ldots, X_k, \ldots, X_{2k}).
\]

Pared down to its bare minimum, this proof of Theorem 1.6 works by using that \( \rho_{k,\ell}^2 \) is a lower bound on each \( \rho_{j,\ell}^k \), and then applying the simple inequality
\[
\sum_{j=0}^{k} \rho_{j,\ell}^k \leq \ell + 1.
\]

The proof of Theorem 1.2 of Besag and Clifford is in some sense even simpler, using only (8), despite the fact that Theorem 1.2 has better dependence on \( \varepsilon \) (on the other hand, it is not directly applicable to \( (\varepsilon, \alpha) \)-outliers in the way that we will use Theorem 1.6). Recall from Definition 3.1 that the \( \rho_{j,\ell}^k \)'s are fixed real numbers associated to a stationary Markov Chain. If \( \ell, k \) are fixed and \( \xi \) is chosen randomly from 0 to \( k \), then the resulting \( \rho_{\xi,\ell}^k \) is a random variable uniformly
distributed on the set of real numbers \{\rho_{0,\ell}^k, \rho_{1,\ell}^k, \ldots, \rho_{k,\ell}^k\}. In particular, Theorem 1.2 is proved by writing that the probability that \(\omega(\sigma_0)\) is \(\ell\)-small among \(\omega(\sigma_0), \omega(Y_1), \ldots, \omega(Y_\xi), \omega(Z_1), \ldots, \omega(Z_{k-\xi})\) is given by

\[
\frac{1}{k+1} (\rho_{0,\ell}^k + \rho_{1,\ell}^k + \cdots + \rho_{k,\ell}^k) \leq \frac{\ell + 1}{k+1},
\]

where the inequality is from (8). Note that we are using an analog of Observation 3.2 to know that for any \(j, Y_j, \ldots, Y_1, \sigma_0, Z_1, Z_{k-j}\) is a \(\pi\)-stationary trajectory.

4. Global significance for local outliers

Theorem 1.4 now follows easily from Theorem 1.6.

Proof of Theorem 1.4. For a \(\pi\)-stationary trajectory \(X_0, \ldots, X_k\), let us define \(p_{j,\varepsilon}^k(\sigma)\) to be the probability that \(\omega(X_j)\) is an \(\varepsilon\)-outlier among \(\omega(X_0, \ldots, X_k)\), conditioned on the event that \(X_j = \sigma\).

In particular, to prove Theorem 1.4, we will prove the following claim:

**Claim:** If \(\sigma_0\) is not an \((\varepsilon, \alpha)\)-outlier, then

\[
p_{0,\varepsilon}^k(\sigma_0) \leq \sqrt{\frac{2\varepsilon}{\alpha}}.
\]

Let us first see why the claim implies the theorem. Recall the random variable \(\rho\) is the number of trajectories \(T^i\) from \(\sigma_0\) on which \(\sigma_0\) is observed to be an \(\varepsilon\)-outlier with respect to the labeling \(\omega\). The random variable \(\rho\) is thus a sum of \(m\) independent Bernoulli random variables, which each take value 1 with probability \(\leq \sqrt{\frac{2\varepsilon}{\alpha}}\) by the claim. In particular, by Chernoff’s bound, we have

\[
\Pr \left( \rho \geq (1 + \delta)m\sqrt{\frac{2\varepsilon}{\alpha}} \right) \leq e^{-\min(\delta, \delta^2)m\sqrt{\frac{2\varepsilon}{\alpha}} / 3},
\]

giving the theorem. (Note the key point of the claim is that \(\alpha\) is inside the square root in (9), while a straightforward application of of Theorem 1.1 would give an expression with \(\alpha\) outside the square root.)

To prove (9), consider a \(\pi\)-stationary trajectory \(X_0, \ldots, X_k, \ldots, X_{2k}\) and condition on the event that \(X_k = \sigma\) for some arbitrary \(\sigma \in \Sigma\). Since \(\mathcal{M}\) is reversible, we can view this trajectory as two independent trajectories \(X_{k+1}, \ldots, X_{2k}\) and \(X_{k-1}, X_{k-2}, \ldots, X_0\) both beginning from \(\sigma\). In particular, letting \(A\) and \(B\) be the events that \(\omega(X_k)\) is an \(\varepsilon\)-outlier among the lists \(\omega(X_0), \ldots, \omega(X_k)\) and \(\omega(X_k), \ldots, \omega(X_{2k})\), respectively, we have that

\[
p_{0,\varepsilon}^k(\sigma)^2 = \Pr(A \cap B) \leq p_{k,\varepsilon}^k(\sigma).
\]

Now, the assumption that the given \(\sigma_0 \in \Sigma\) is not an \((\varepsilon, \alpha)\)-outlier gives that for a random \(\sigma \sim \pi\), we have that

\[
\Pr \left( p_{0,\varepsilon}^k(\sigma) \geq p_{0,\varepsilon}^k(\sigma_0) \right) \geq \alpha.
\]
Line 11 gives that $p^k_{0,\varepsilon}(\sigma)^2 \leq p^k_{k,\varepsilon}(\sigma)$, and Theorem 1.6 gives that $p^k_{k,\varepsilon} \leq 2\varepsilon$. Thus taking expectations with respect to a random $\sigma \sim \pi$, we obtain that

$$E_{\sigma \sim \pi} (p^k_{0,\varepsilon}(\sigma)^2) \leq E_{\sigma \sim \pi} (p^k_{k,\varepsilon}(\sigma)) = p^k_{k,\varepsilon} \leq 2\varepsilon.$$ 

On the other hand, we can use (12) to write

$$E_{\sigma \sim \pi} (p^k_{0,\varepsilon}(\sigma)^2) \geq \alpha \cdot p^k_{0,\varepsilon}(\sigma_0)^2,$$

so that we have

$$p^k_{0,\varepsilon}(\sigma_0)^2 \leq \frac{2\varepsilon}{\alpha}.$$ 

□

We close this section by noting that in implementations where $m$ is not enormous, it may be sensible to use the exact binomial tail in place of the Chernoff bound in (10). In particular, this gives the following version:

**Theorem 4.1.** With $\rho$ as in Theorem 1.4, we have that if $\sigma_0$ is not an $(\varepsilon, \alpha)$ outlier, then

$$\Pr(\rho \geq K) \leq \sum_{k=K}^{m} \binom{m}{k} \left( \frac{2\varepsilon}{\alpha} \right)^{k/2} \left( 1 - \sqrt{\frac{2\varepsilon}{\alpha}} \right)^{m-k}.$$ 

5. **Generalizing the Besag and Clifford tests**

Theorem 1.4 is attractive because it succeeds at separating statistical significance from effect size, and at demonstrating statistical significance for an intuitively-interpretable deterministic property of state in the Markov Chain.

In some cases, however, these may not be important goals. In particular, one may simply desire a statistical test which is as effective as possible at disproving the null hypothesis $\sigma \sim \pi$. This is a task at which Besag and Clifford’s Theorem 1.2 excels.

In their paper, Besag and Clifford also prove the following result, to enable a test designed to take efficient advantage of parallelism:

**Theorem 5.1** (Besag and Clifford parallel test). Fix numbers $k$ and $m$. Suppose that $\sigma_0$ is chosen from a stationary distribution $\pi$ of the reversible Markov Chain $M$, and suppose we sample a trajectory $X_1, X_2, \ldots, X_k$ from $X_0 = \sigma_0$, and then branch to sample $m-1$ trajectories $Z^*_1, Z^*_2, \ldots, Z^*_m$ ($2 \leq s \leq m$) all from the state $Z^*_0 = X_k$. Then we have that

$$\Pr(\omega(\sigma_0) \text{ is an } \varepsilon\text{-outlier among } \omega(\sigma_0), \omega(Z^*_1), \omega(Z^*_2), \ldots, \omega(Z^*_m)) \leq \varepsilon.$$ 

**Proof.** For this theorem it suffices to observe that $\sigma_0, Z^*_1, \ldots, Z^*_m$ are exchangeable random variables—that is, all permutations of the sequence $\sigma_0, Z^*_1, \ldots, Z^*_m$ are identical in distribution. This is because if $\sigma_0$ is chosen from $\pi$ and then the $Z^*_1$'s are chosen as above, the result is equivalent in distribution to the case where $X_k$ is chosen from $\pi$ and then each $Z^*_1$ is chosen (independently) as the end of a trajectory $X_k, Z^*_1, \ldots, Z^*_k$, and $\sigma_0 = Y_k$ is chosen (independently) as the end of a trajectory.
Here we are using that reversibility implies that \((X_k, Y_1, \ldots, Y_k)\) is identical in distribution to \((\sigma_0, X_1, \ldots, X_k)\). □

With an eye towards finding a common generalization of Besag and Clifford's serial and parallel tests, we define a **Markov outlier test** as a significance test with the following general features:

- The test begins from a state \(\sigma_0\) of the Markov Chain which, under the null hypothesis, is assumed to be stationary;
- random steps in the Markov chain are sampled from the initial state and/or from subsequent states exposed by the test;
- the ranking of the initial state’s label is compared among the labels of some (possibly all) of the visited states; it is an \(\varepsilon\)-outlier if its label is among the bottom \(\varepsilon\) of the comparison labels. Some function \(\rho(\varepsilon)\) assigns valid statistical significance to the test results, as in the above theorems.

In particular, such a test may consist of single or multiple trajectories, may branch once or multiple times, etc. In this section, we prove the validity of a parallelizable Markov outlier test with best possible function \(\rho(\varepsilon) = \varepsilon\), but for which it is natural to expect the \(\varepsilon\)-power of the test—that is, its tendency to return small values of \(\varepsilon\) when \(\sigma_0\) truly is an outlier—surpasses that of Theorems 1.2 and 5.1. In particular, we prove the following theorem:

**Theorem 5.2 (Star-split test).** Fix numbers \(m\) and \(k\). Suppose that \(\sigma_0\) is chosen from a stationary distribution \(\pi\) of the reversible Markov Chain \(M\), and suppose that \(\xi\) is chosen randomly in \(\{1, \ldots, k\}\). Now sample trajectories \(X_1, \ldots, X_\xi\) and \(Y_1, \ldots, Y_{k-\xi}\) from \(\sigma_0\), and then branch and sample \(m-1\) trajectories \(Z_s^1, Z_s^2, \ldots, Z_s^k\) (\(2 \leq s \leq m\)) all from the state \(Z_\xi^0 = X_\xi\). Then we have that

\[
\Pr\left( \omega(\sigma_0) \text{ is an } \varepsilon\text{-outlier among } \omega(\sigma_0), \omega(X_1), \ldots, \omega(X_{\xi-1}), \omega(Y_1), \ldots, (Y_{k-\xi}), \omega(Z_s^1), \ldots, \omega(Z_s^k) \right) \leq \varepsilon.
\]

In particular, note that the set of comparison random variables used consists of all random variables exposed by the test except \(X_\xi\).

To compare Theorem 5.2 with Theorems 5.1 and 1.2, let us note that it is natural to expect the \(\varepsilon\)-power of a Markov chain significance test to depend on:

(a) How many comparisons are generated by the test, and
(b) how far typical comparison states are from the state being tested, where we measure distance to a comparison state by the number of Markov chain transitions which the test used to generate the comparison.
If unlimited parallelism is available, then the Besag/Clifford parallel test is essentially optimal from these parameters, as it draws an unlimited number of samples, whose distance from the initial state is whatever serial running time is used. Conversely, in a purely serial setting, the Besag/Clifford test is essentially optimal with respect to these parameters.

But it is natural to expect that even when parallelism is available, the number \( n \) of samples we desire will often be be significantly greater than the parallelism factor \( \ell \) available. In this case, the Besag/Clifford parallel test will use \( n \) comparisons at distance \( d \approx \ell t/n \), where \( t \) is the serial time used by the test. In particular, the typical distance to a comparison can be considerably less than \( t \) when \( \ell \) compares unfavorably with \( n \).

On the other hand, Besag/Clifford serial test generates comparisons whose typical distance is roughly \( t/2 \), but cannot make use of parallelism beyond \( \ell = 2 \). For an apples-to-apples comparison, it is natural to consider the case of carrying out their serial test using only every \( d \)th state encountered as a comparison state for some \( d \). This is equivalent to applying the test to the \( d \)-th power of the Markov chain, instead of applying it directly. (In practical applications, this is a sensible choice when comparing the labels of states is expensive relative to the time required to carry out transitions of the chain.) Now if \( \ell \) is a small constant, we see that with \( t \cdot d \) steps, the BC parallel test can generate roughly \( n \) comparisons all at distance \( d \) from the state being tested, the serial test could generate comparisons at distances \( d, 2d, 3d, \ldots, kd \) (measured in terms of transitions in \( \mathcal{M} \)), where these distances occur with multiplicity at most 2, and \( k = \max(\xi, n - \xi) \geq n/2 \). In particular, the serial test generates a similar number of comparisons in this way but at much greater distances from the state we are evaluating, making it more likely that we are able to detect that the input state is an outlier.

Consider now the star-split test. Again, to facilitate comparison, we suppose the test is being applied to the \( d \)-th power of \( \mathcal{M} \). If serial time \( t \approx sd \) is to be used, then we will branch into \( \ell - 1 \) trajectories after \( \xi \cdot \mathcal{M}^d \) chain, where \( \xi \) is randomly chosen from \( \{0, \frac{s}{2}\} \). Thus comparisons used lie at a set of distances \( d, 2d, \ldots, (\xi + \frac{s}{2})d \) similar to the case of the Besag/Clifford serial test above. But now the distances \( d, 2d, \ldots, (\xi d - 1)d \) will have multiplicities at most 2 in the set of comparison distances, while the distances \( (\xi + 1)d, (\xi + 2)d, \ldots, (\xi + \frac{s}{2})d \) all have multiplicity at least \( \ell - 1 \). In particular, the test allows us to make more comparisons to more distance states, essentially by a factor of the parallelism factor being used. In particular, it is natural to expect performance to improve as \( \ell \) increases. Moreover, the star-split test is equivalent to the Besag/Clifford serial test for \( \ell \leq 2 \), and essentially equivalent to their parallel test in the large \( \ell \) limit. (To make this latter correspondence exact, once can apply Theorem 5.2 to the \( d \)-th power of a Markov chain \( \mathcal{M} \), and take \( k = 1 \).)

We now turn to the task of proving Theorem 5.2. Unlike Theorems 1.1, 1.6, and 1.2, the comparison states used in Theorems 5.1 and 5.2 cannot be viewed as a single trajectory in \( \mathcal{M} \). This motivates the natural generalization of the notion of a \( \pi \)-stationary trajectory as follows:
Definition 5.3. Given a reversible Markov Chain $\mathcal{M}$ with stationary distribution $\pi$ and an undirected tree $T$, a $\pi$-stationary $T$-projection is a collection of random variables $\{X_v\}_{v \in T}$ such that:

(i) for all $v \in T$, $X_v \sim \pi$;
(ii) for any edge $\{u,v\}$ in $T$, if we let $T_u$ denote the vertex-set of the connected component of $u$ in $T \setminus \{u,v\}$ and $\{\sigma_w\}_{w \in T}$ is an arbitrary collection of states, then

$$\Pr \left( X_v = \sigma_v \middle| \bigwedge_{w \in T_u} X_w = \sigma_w \right) = \pi_{\sigma_u,\sigma_v}. $$

In analogy to the case of $\pi$-stationary trajectories, Definition 5.3 easily gives the following, by induction:

Observation 5.4. For fixed $\pi$ and $T$, if $\{X_w\}_{w \in T}$ and $\{Y_w\}_{w \in T}$ are both $\pi$-stationary $T$-projections, then the two collections $\{X_w\}_{w \in T}$ and $\{Y_w\}_{w \in T}$ are equivalent in distribution. $\square$

This enables the following natural analog of Definition 3.1:

Definition 5.5. Given a Markov Chain $\mathcal{M}$ with labels $\omega : \Sigma \to \mathbb{R}$ and stationary distribution $\pi$, we define for each $\ell$, each undirected tree $T$, each vertex subset $S \subset T$ and each vertex $v \in S$ a real number $\rho_{T,S}^w,\ell$, which is the probability that for a $\pi$-stationary $T$-projection $\{X_w\}_{w \in T}$, we have that $\omega(X_v)$ is $\ell$-small among $\{\omega(X_w)\}_{w \in S}$.

Observe that as in (8) we have for any tree $T$ and any vertex subset $S$ of $T$, we have that

$$\sum_{w \in S} \rho_{T,S}^w \leq \ell + 1. $$

The following Observation, applied recursively, gives the natural analog of Observation 3.2. Again the proof is an easy exercise in the definitions.

Observation 5.6. Suppose that $T$ is an undirected tree, $v$ is a leaf of $T$, $T' = T \setminus v$, and $\{X_w\}_{w \in T'}$ is a $\pi$-stationary $T'$-projection. Suppose further that $X_v$ is a random variable such that for all $\{\sigma_w\}_{w \in T'}$ we have that

$$\Pr \left( X_v = \sigma_v \middle| \bigwedge_{w \in T'} (X_w = \sigma_w) \right) = \pi_{\sigma_u,\sigma_v}, $$

where $u$ is the neighbor of $v$ in $T$. Then $\{X_w\}_{w \in T}$ is a $\pi$-stationary $T$-projection. $\square$

We can rephrase the proof of Theorem 5.1 in this language. Let $T$ be the tree consisting of $m$ paths of length $k$ sharing a common endpoint and no other vertices, and let $S$ be the leaves of $T$. By symmetry, we have that $\rho_{T,S}^w,\ell$ is constant over $w \in S$. On the other hand, Observation 5.6 gives that under the hypotheses of Thoerem
5.1, $\sigma_0, X_1, \ldots, X_k$, and the $Z_s^*$’s are a $\pi$-stationary $T$-projection, with obvious assignments (e.g., $\sigma_0$ corresponds to a leaf of $T$; $X_k$ corresponds to the center). In particular, (14) implies that $\rho_{T,S}^{T,S} \leq \frac{k+1}{n}$, which gives the theorem.

On the other hand, the definitions make the following proof easy as well, using the same simple idea as Besag and Clifford’s Theorem 1.2.

**Proof of Theorem 5.2.** Define $T$ to be the undirected tree with vertex set $\{v_0\} \cup \{v_s^* \mid 1 \leq s \leq m, 1 \leq j \leq k\}$, with edges $\{v_0, v_s^*\}$ for each $1 \leq s \leq m$ and $\{v_j^*, v_{j+1}^*\}$ for each $1 \leq s \leq m, 1 \leq j \leq k - 1$. Now we let $S$ consist of all vertices of $T$ except the center $v_0$, and let $S_j$ denote the set of $m$ vertices in $S$ at distance $j$ from $v_0$. By symmetry, we have that $\rho_{T,S}^{T,S}$ is constant in each $S_j$; in particular, we have that

$$\rho_{v_s^*, T,S}^{T,S} = \frac{1}{n} \sum_{s=1}^{m} \rho_{v_s^*, j, T,S}^{T,S},$$

and together with (14) this gives that

$$\sum_{s=1}^{m} \rho_{v_s^*, j, T,S}^{T,S} \leq \frac{\ell + 1}{n}. \quad (16)$$

Now if we let

$$W_{v_0} = X_k,$$

$$W_{v_s^*} = \begin{cases} X_{\xi - j} & s = 1, 1 \leq j < \xi \\ \sigma_0 & s = 1, j = \xi \\ Y_{j-\xi} & s = 1, j > \xi \\ Z_s^* & 2 \leq s \leq m, 1 \leq j \leq k, \end{cases}$$

then $\{W_w\}_{w \in T}$ is a $\pi$-stationary $T$-projection under the hypotheses of Theorem 5.2, by recursively applying Observation 5.6. Moreover, as $\xi$ is chosen randomly among $\{1, \ldots, k\}$, the probability that $\omega(\sigma_0) = \omega(W_{v_1^*})$ is $\ell$-small among $\{\omega(W_w)\}_{w \in S}$ is given by

$$\frac{1}{k} \left( \rho_{v_1^*, 1, T,S}^{T,S} + \cdots + \rho_{v_k^*, 1, T,S}^{T,S} \right) \leq \frac{\ell + 1}{kn},$$

where the inequality is from (16), giving the Theorem. \hfill $\square$

**References**

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