We describe an exact test of the null hypothesis that a Markov chain is nth order versus the alternate hypothesis that it is (n+1)-th order. The procedure does not rely on asymptotic properties, but instead builds up the test statistic distribution via surrogate data and is valid for any sample size. Surrogate data are generated using a novel algorithm that guarantees, per shot, a uniform sampling from the set of sequences that exactly match the nth order properties of the observed data.
It often happens that it is useful to describe a process as a set of discrete states with probabilistic transitions. Examples abound in various fields such as the study of chemical processes [1], DNA sequences [2], finance [3], and nonlinear dynamics [4], among others. If a transition to a new state is conditioned only on the present state we call this model a Markov chain. An $n$-th order Markov chain is a generalization to include the past $n$ states in the transition probability. When the conditional probabilities are not otherwise given, they are estimated from a time series of observations.

If the order of the Markov chain is in question there are various tests and criteria available to narrow down the options. A classical approach is to formulate the question as a hypothesis test that a chain is $n$-th order versus $(n+1)$-th order [5]. When the test statistic has a known limiting distribution, such as $\chi^2$, a $p$-value can be calculated and a decision made based on a chosen significance level [6]. Another avenue are the information criteria tests such as AIC and BIC [7–9]. These produce rankings over multiple orders based on expected likelihood and have built-in corrections for over-fitting. Both of these approaches rely on approximations that are only valid in the limit of large samples. In small sample situations one cannot be sure of their efficacy.

It is possible to perform an exact hypothesis test that is valid for any sample size. Instead of relying on asymptotic properties, the test statistic distribution is discovered by generating samples (referred to here as surrogates) that exactly match the $n$-th order properties of the observed time series [10]. The challenge is in efficiently generating a large number of such samples, especially for higher orders. To our knowledge no solution to this problem has been reported in the literature. The contribution of this work is a surrogate data procedure that has ideal properties: one sample is generated per shot, samples are uniformly selected from the set of all possible surrogate sequences, computation time increases linearly with the length of the sequence, and any order can be accommodated. Armed with this new procedure it is now practical to perform exact hypothesis tests of Markov order.

We first describe how to do hypothesis testing of Markov order using the $\chi^2$ statistic, for which the distribution is known in the large sample limit. Next we describe the method of surrogate data generation based on Whittle’s formula. Then we compare the $\chi^2$ statistic in large and small sample cases using both the asymptotic distribution and the exact distribution obtained from the surrogates.

A sequence of observations $\{x_1 \ldots x_N\}$ form a Markov chain of order $n$ if the conditional probability satisfies
\begin{equation}
    p(x_{t+1}|x_t, x_{t-1} \ldots) = p(x_{t+1}|x_{t-1} \ldots x_{t-n+1}),
\end{equation}
for all $n < t \leq N$. For convenience we will label the states each measurement can take by positive integers up to $M$. A sequence of discrete measurements may come from a process that is naturally discrete, such as a DNA sequence, or from a continuous process that has been discretized by an analog-to-digital measuring device. Unless otherwise specified a Markov process is assumed to be first order ($n = 1$). This means that the transition probabilities to a future state depend only on the present state and not on prior states. An $n$th order process can always be cast as first order by grouping the present state with the relevant past states into a word, in which case the number of states can be up to $M^n$. A process that has no dependence on past or present (such as a random iid process) is said to be zeroth order.

To perform a hypothesis test of $n$-th order versus $(n+1)$-th order one begins with an assumption of $n$th order and then computes the distribution of a suitable $(n+1)$-th order statistic. If the observed $(n+1)$-th order statistic is highly unlikely then $n$-th order assumption is rejected. The initial assumption is called the null hypothesis and the probability of the observed statistic given the distribution implied by the null hypothesis is referred to as the $p$-value. Typically, a $p$-value less than or equal to 0.05 is taken as grounds to reject the null hypothesis.

Let us begin with the assumption that $\{x_t\}$ is first order ($n = 1$) and calculate the $p$-value of a second order statistic using a $\chi^2$ distribution. The null hypothesis is
\begin{equation}
    p(x_{t+1} = i|x_t = j, x_{t-1} = k) = p(x_{t+1} = i|x_t = j),
\end{equation}
or using Bayes’ rule
\begin{equation}
    p(x_{t+1} = i, x_t = j, x_{t-1} = k) = \frac{p(x_{t+1} = i, x_t = j)p(x_t = j, x_{t-1} = k)}{p(x_t = j)}.
\end{equation}
The l.h.s. of (3) multiplied by $N - 2$ is the expected number of times the word $(x_{t+1} = i, x_t = j, x_{t-1} = k)$ appears in the data given the null hypothesis. The quantities on the r.h.s. are not expected values; they are taken from the observed sequence. Let $E_w$ be the expected word count where $\sum E_w = N - 2$ and $w$ indexes the set of all words for which the expected count is greater than zero. Similarly, let $O_w$ be the corresponding count from the observed data. If the sequence $w'$ does not appear in the observed data, then $O_{w'} = 0$. We can now define the expected $\chi^2$ statistic
\begin{equation}
    \chi^2_{\text{exp}} = \sum_w \frac{(E_w - O_w)^2}{E_w}.
\end{equation}
Whittle’s formula [11]:

\[ M \text{ there are at most } n \text{ M } \]

block diagonal form with \( \sum (\text{F}) \) is the number of times word \( i \) transitions to word \( j \). Because words overlap and differ by only one observation, there are at most \( M \) nonzero entries in row \( i \) of \( F \). In the case that all words are present, \( F \) can be rearranged in block diagonal form with \( n M \times M \) blocks. In the case that some words are not present in the observed data, these blocks will be of differing size. If the size of the \( k \)th block is \( x_k \times c_k \), then the total number of degrees of freedom \( d \) is \( \sum (x_k - 1)(c_k - 1) \).

The hypothesis test as described above is not exact; it relies on the \( \chi^2 \) distribution in the asymptotic limit of infinite data. To discover the exact distribution for finite data one needs to know all possible sequences that satisfy the null hypothesis along with their likelihood. For the first order hypothesis these sequences must all have exactly the same zeroth and first order statistics. To discover the exact distribution for finite data one needs to know all possible sequences that satisfy the null hypothesis along with their likelihood. For the first order hypothesis these sequences must all have exactly the same zeroth and first order statistics. There is some freedom for the second order statistics; there is some freedom for the second order statistics.

The cardinality of the set \( S(x) \) is therefore 80. The transition count \( F \) determines the first order joint probabilities \( p(x_{n+1}, x_n) \) and, after fixing the first and the last symbol, the zeroth order probabilities \( p(x_n) \) as well. Therefore all 80 sequences in \( S \) have first order transition probabilities \( p(x_{n+1}|x_n) \) identical to the observed sequence \( x \).

For all but the shortest sequences the value of \( \sum (\text{F}) \) is so large that it cannot be computed using fixed precision arithmetic. In our algorithm we instead compute the natural logarithm of \( \sum (\text{F}) \) using a Stirling’s series for the factorial terms:

\[
\ln z! \sim z \ln z - z + \frac{1}{2} \ln(2\pi z) + \frac{1}{12z} - \frac{1}{360z^3} + \frac{1}{1260z^5} - \frac{1}{1680z^7}
\]

when \( z > 16 \).
To find the p-value we need to know the fraction of sequences have $\chi^2$ values less than or equal to $\chi^2_{\text{exp}}$. If $|S|$ is too large to enumerate all the sequences, the p-value can still be estimated to any desired accuracy provided one has a method of producing uniform random samples from the set $S$. Previously reported methods for generating samples from $S$ are impractical, especially for higher order testing [10]. Here we give an efficient procedure.

We construct a member $\{y_t\}$ of $S$ starting with $y_1 = u$, ending with $y_N = v$, and having the transition count matrix $F$. The candidates for the second element $y_2$ are the set $\{y_2 | F_{y_1 y_2} > 0\}$. For each candidate we compute $N_{y_2}(F')$, the number of sequences left, where $F'_{ij} = F_{ij} - \delta_{y_1 y_2}$. We choose a candidate randomly in proportion to the number of sequences left; a path that leads to a small number of possibilities is chosen less frequently than one that leads to a large number. Once $y_2$ is chosen $F$ is set equal to the appropriate $F'$ and the process is repeated for $y_3$ and so on until $y_{N-1}$ is reached.

Returning to our example case, we have $y_1 = 0$, $y_{12} = 1$, and $y_2 = \{0, 1\}$. The two choices for $y_2$ lead to the following number of sequences:

\[
N_{01} \begin{pmatrix} 0 & 4 \\ 3 & 3 \end{pmatrix} = 20, \\
N_{11} \begin{pmatrix} 1 & 3 \\ 3 & 3 \end{pmatrix} = 60. 
\]

Therefore $y_2 = 0$ is chosen with $20/80 = 1/4$ probability and $y_2 = 1$ with $3/4$ probability. By weighting our choice at each step by Whittle’s formula we guarantee paths that do not result in a valid sequence are not followed and that all valid paths are followed with uniform probability (Fig[1]). This method is suitable for the generation of very long surrogates, as the difficulty increases only linearly with $N$. For producing sequences of order $n > 1$ simply replace the elements of $y_i$ with length $n$ words. The matrix $F$ can be as large as $M^n \times M^n$, but has no more than $N - n$ nonzero elements and can be handled efficiently using sparse methods. Code is available for generating surrogates by this method [12].

Figure (2) shows the $\chi^2$ density computed in the asymptotic limit with the density estimated from 20000 surrogates of a random Markov process of 4 states. The degrees of freedom are calculated for 2nd order assuming fixed 1st order statistics. In the top panel ($N = 2500$) there is close agreement indicating that that the surrogate data statistics behave as expected in the asymptotic limit. The bottom panel uses the same time series, but only the first 200 data points. The significant disagreement between the two densities illustrates the need for an exact test when the sample is small.

The efficacy of a hypothesis test is quantified by its size and power. The size of a test is its probability of incorrectly rejecting the null hypothesis (Type I error). For an ideal test the size should be equal to the significance level (0.05). The power of a test is its probability of correctly rejecting the null hypothesis. The failure to do so is a Type II error. To estimate power we use data from Markov processes that are one order higher than the null hypothesis; other choices could yield different results.

Test cases are taken from a set of randomly generated $n$th order Markov processes with four states ($M = 4$). Recall that such a process is specified by the transition probabilities $p(x_{t+1} | x_t \ldots x_{t-n+1})$, which when expressed as a matrix...
is size $M \times n$. One way to create such a transition matrix is to populate it with $[0, 1]$ random numbers and normalize the rows. We have found, however, that this procedure tends to produce weakly $n$th order processes, particularly when either or both $M$ and $n$ are large. To produce strongly $n$th order processes we first scale the random numbers by adding one, raising them to the 10th power, and then row normalizing. This creates more variance in the transition probabilities.

We generated 2500 trials for each size and power estimate shown in the following tables. For each case we tabulate results using the asymptotic distribution (labeled $\chi^2$) and the exact $\chi^2$ distribution (labeled $\chi^2_{surg}$) obtained using 2500 surrogates. In addition we show $H_{surg}$, which relies on the same surrogate data, but instead of the $\chi^2$ statistic the $n$th order entropy rate is used:

$$H(x_{t+1}|x_t \ldots x_{t-n+1}) = H(x_{t+1}, x_t \ldots x_{t-n+1}) - H(x_t \ldots x_{t-n+1}).$$

As the surrogates have identical $n$th order block entropies, only $H(x_{t+1}, x_t \ldots x_{t-n+1})$ needs to be re-computed for each trial. The use of this statistic was suggested in [10].

| Data | Size $\pm 0.01$ | Power $\pm 0.01$ |
|------|----------------|------------------|
|      | $\chi^2$ $\chi^2_{surg}$ $H_{surg}$ | $\chi^2$ $\chi^2_{surg}$ $H_{surg}$ |
| 25   | 0.04 0.04 0.03 | 0.48 0.49 0.49   |
| 50   | 0.05 0.05 0.04 | 0.89 0.89 0.91   |
| 100  | 0.06 0.04 0.05 | 0.98 0.98 0.98   |
| 200  | 0.08 0.05 0.05 | 1.00 1.00 1.00   |
| 400  | 0.09 0.05 0.05 | 1.00 1.00 1.00   |

TABLE I. Estimated size of asymptotic and exact $\chi^2$ statistic for random 1st order Markov processes with 4 symbols, 2500 trials.

We break out each order in a separate table and list size and power versus data length. In the large sample limit both the exact and asymptotic methods should approach a power of 1 and a size equal to the significance level (0.05). The exact test is quite efficient; as little as 100 data points are needed for 1st and 2nd order tests, 200 for 3rd order, and 400 for 4th order. The asymptotic method is very slow to attain the ideal size even for the 1st order test ($10^6$ sample size, not shown). For higher order tests we do not recommend use of the $\chi^2$ distribution. There is no detectable difference between using the entropy rate as a test statistic and $\chi^2$. As entropy rate is a simpler quantity to calculate, we recommend its use over $\chi^2$.

Compared to the asymptotic $\chi^2$ test, the exact test is much slower; each step of Whittle’s algorithm requires the computation of the determinate of the transition matrix. Considering that the transition matrix changes in only one entry at each step there is potential to improve the efficiency over our naïve implementation. Even without such
TABLE II. Estimated size of asymptotic and exact $\chi^2$ statistic for random 2nd order Markov processes with 4 symbols, 2500 trials.

| Data | $\chi^2$ ± 0.01 | $\chi^2_{surg}$ | $H_{surg}$ | $\chi^2$ ± 0.01 | $\chi^2_{surg}$ | $H_{surg}$ |
|------|----------------|-----------------|-----------|----------------|----------------|-----------|
| 50   | 0.07           | 0.05            | 0.04      | 0.79           | 0.59           | 0.56      |
| 100  | 0.10           | 0.05            | 0.05      | 0.98           | 0.96           | 0.98      |
| 200  | 0.12           | 0.05            | 0.06      | 1.00           | 1.00           | 1.00      |
| 400  | 0.11           | 0.05            | 0.06      | 1.00           | 1.00           | 1.00      |

TABLE III. Estimated size of asymptotic and exact $\chi^2$ statistic for random 3rd order Markov processes with 4 symbols, 2500 trials.

| Data | $\chi^2$ ± 0.01 | $\chi^2_{surg}$ | $H_{surg}$ | $\chi^2$ ± 0.01 | $\chi^2_{surg}$ | $H_{surg}$ |
|------|----------------|-----------------|-----------|----------------|----------------|-----------|
| 50   | 0.07           | 0.05            | 0.01      | 0.44           | 0.04           | 0.03      |
| 100  | 0.18           | 0.05            | 0.05      | 0.97           | 0.56           | 0.52      |
| 200  | 0.22           | 0.05            | 0.05      | 1.00           | 0.99           | 0.99      |
| 400  | 0.22           | 0.05            | 0.05      | 1.00           | 1.00           | 1.00      |

optimizations, it is well within a desktop computer’s ability to generate many thousands of surrogate sequences in minutes. Because each surrogate is generated independently, parallelization is straightforward. For our tables, each case involving 2500 trials, we opted to use 2500 surrogates, requiring the generation of 6.25 million surrogates per table entry. The standard error of our $p$-value estimates as well as our size and power estimates is then $1/\sqrt{4 \times 2500}$ or ±0.01. If one doesn’t need to analyze so many data sets, we recommend using 10,000 or more surrogates.

In summary, we have described an exact test of the null hypothesis that a Markov chain is $n$th order versus the alternate hypothesis that it is $(n + 1)$-th order. At the heart of the test is an algorithm based on Whittle’s formula, which efficiently produces surrogate data sets that have identical word transition counts as the observed sequence. Whittle’s algorithm together with the entropy rate statistic make for a conceptually simple approach to Markov order hypothesis testing; no calculation of degrees of freedom or corrections for small sample size are necessary.

[1] Abraham Tamir, Applications of Markov chains in chemical engineering (Elsevier Science, Amsterdam, 1998).
[2] P. J. Avery and D. A. Henderson Fitting Markov chain models to discrete state series such as DNA sequences, Journal of the Royal Statistical Society: Series C, 48, 53-61 (1999).
[3] Robert A. Jarrow, David Lando, and Stuart M. Turnbull, A Markov model for the term structure of credit risk spreads, The Review of Financial Studies, 10, 481-523 (1997).
[4] Bai-Lin Hao and Wei-Mou Zheng, Applied Symbolic Dynamics and Chaos (World Scientific, Singapore, 1998).
[5] T. W. Anderson and Leo A. Goodman, Statistical inference about Markov chains, Ann. Math. Statist., 28, 89-110 (1957).
[6] Priscilla E. Greenwood and Michael S. Nikulin, A guide to chi-squared testing (Wiley-Interscience, New-York, 1996).
[7] H. Tong, Determination of the order of a Markov chain by Akaike’s information criteria, J. Appl. Prob. 12, 488-497 (1975).
[8] Richard W. Katz, On some criteria for estimating the order of a Markov chain, Technometrics, 23, 243-249 (1981).
[9] Kenneth P. Burnham and David R. Anderson, Multimodel Inference: Understanding AIC and BIC in Model Selection, Sociological Methods & Research, 33, 261-304 (2004).
[10] Marcel J. van der Heyden, Cees G. C. Diks, Bart P. T. Hooistra, and Jacob DeGoede, Testing the order of discrete Markov chains using surrogate data, Physica D 117 299-313 (1998).
[11] Patrick Billingsley, Statistical methods in Markov chains, The Annal of Mathematical Statistics, 32, 12-40 (1961).
[12] Shawn D. Pethel, Whittle Surrogate (http://www.mathworks.com/matlabcentral/fileexchange/40188-whittle-surrogate), MATLAB Central File Exchange.
| Data | Size ±0.01 | Power ±0.01 |
|------|------------|-------------|
|      | $\chi^2$   | $\chi_{surg}^2$ | $H_{surg}$ | $\chi^2$   | $\chi_{surg}^2$ | $H_{surg}$ |
| 50   | 0.01       | 0.00         | 0.00       | 0.02       | 0.00         | 0.00       |
| 100  | 0.12       | 0.01         | 0.01       | 0.61       | 0.03         | 0.02       |
| 200  | 0.49       | 0.04         | 0.03       | 1.00       | 0.44         | 0.42       |
| 400  | 0.74       | 0.05         | 0.05       | 1.00       | 0.99         | 0.99       |
| 800  | 0.77       | 0.05         | 0.05       | 1.00       | 1.00         | 1.00       |

TABLE IV. Estimated size of asymptotic and exact $\chi^2$ statistic for random 4th order Markov processes with 4 symbols, 2500 trials.