We generalize the method of surrogate data of testing for nonlinearity in time series to the case that the data are sampled with uneven time intervals. The null hypothesis will be that the data have been generated by a linear stochastic process, possibly rescaled, and sampled at times chosen independently from the generating process. The surrogate data are generated with their linear properties specified by the Lomb periodogram. The inversion problem is solved by combinatorial optimization.

The vast majority of methods of time series analysis deals with data measured at times which are an integer multiple of the fixed sampling interval $\Delta$. Unevenly sampled time series are often excluded although they are quite common in cases where measurements are restricted by practical conditions. For example, most astronomical observations cannot be made in the day time and must often be interrupted in the night due to cloudy weather; data from the stock exchange have gaps during the weekends and holidays, etc. The reason for excluding these is mainly technical: most methods cannot be easily generalized to this case. This is particularly true for nonlinear methods of time series analysis.

For the nonlinear approach to a given time series, we first have to ask for signatures of nonlinearity in the generating process. In this paper for the first time we present a method to test for nonlinearity in unevenly sampled time series. We will extend the common concept of surrogate data, where randomized data sets are used to obtain a Monte Carlo approximation to the probability distribution of a suitable test statistic.

For this approach, we have to be able to generate sequences that are random except for their linear correlations. Any additional structure can lead to spurious positive results. The null hypothesis in this paper is that the data have been generated by a linear stochastic process that is measured instantaneously and possibly rescaled. This excludes correlations or even a deterministic relationship between the sampling intervals and the observable. This method can however be generalized to that case.

Time series taken at varying time intervals are very difficult to handle and only few successful efforts have been made in this area. In certain situations, one can interpolate the data to equally spaced sampling times. However, in a test for nonlinearity, one could then not distinguish between genuine structure and nonlinearity introduced spuriously by the interpolation process.

If we want to generate surrogate data sets with the same linear properties as the original data, the autocorrelations have to be conserved. But even such simple things like autocorrelations are hard to maintain for unevenly sampled data. Any time interval can occur between successive points and it is possible to combine them to nearly arbitrary lags. One idea is to calculate autocorrelations by binning all possible intervals to the desired, discrete lags, a process that involves some nonlinearity. Using these autocorrelations for generating surrogates can lead to the spurious rejection of purely linear time series.

Besides the generation of surrogates, we have to be able to measure the degree of nonlinearity in the data. In contrast to the process of generating surrogates, interpolations are permitted here as part of the specification of a test statistic. A badly designed test statistic could in the worst case lower the discrimination power of the test, while still keeping it formally correct. In this paper we use a very simple test statistic that measures nonlinearity through deviations from time-reversibility. The main emphasis is laid on the generation algorithm for the surrogates.

Standard surrogate methods make use of the Fourier transformation to conserve the autocorrelations of the original data. The method of amplitude adjusted Fourier transformation (AAFT) rescales the original time series to a Gaussian distribution first. Then, the Fourier phases are randomized and the Fourier transformation is inverted. Finally, a rescaling to the original distribution is performed. A refined method has been suggested in Ref. where an iteration scheme is used to simultaneously conserve the spectrum and the distribution. It consists of alternating Fourier transformation and rescaling steps. Both methods cannot directly be applied to unevenly sampled data, because they utilize the Fourier transformation and its inverse.

In Ref., a general approach to the constrained randomization of time series is described. There, a desired property of the surrogate data is expressed through a cost function. The minimum of this cost function is reached if the surrogate fulfills the given property. In this paper, we will make use of this method with a cost function that can also be defined for unevenly sampled data. This will enable us to impose the desired linear correlation structure on the surrogate time series.

Let \( \{ y_n \} \) be a time series sampled at times \( \{ t_n \} \) that need not be equally spaced. The Power spectrum can then be estimated by the Lomb periodogram. This spectral estimator is discussed e.g. in Ref. Here we
give the final formula:

\[
P(\omega) = \frac{1}{2\sigma^2} \left\{ \frac{\sum_n (y_n - \bar{y}) \sin(\omega t_n - \tau)}{\sum_n \sin^2 \omega (t_n - \tau)} + \frac{\sum_n (y_n - \bar{y}) \cos(\omega t_n - \tau)}{\sum_n \cos^2 \omega (t_n - \tau)} \right\}^{1/2}
\]

where \( \tau \) is defined by

\[
\tan(2\omega\tau) = \frac{\sum_n \sin 2\omega t_n}{\sum_n \cos 2\omega t_n}
\]

and \( \bar{y}, \sigma^2 \) are the mean and the variance of the data, respectively. The result can be derived by fitting a least squares model \( y_n = a \cos \omega t_n + b \sin \omega t_n \) to the data for each given frequency \( \omega \). Therefore Lomb periodograms are often referred to as \textit{least squares periodograms}.

For time series sampled at constant time intervals, \( \Delta = t_n - t_{n-1} \) for all \( n \), the Lomb periodogram \( P(\omega) \) yields the standard squared Fourier transformation. Except for this particular case, there is no inverse transformation for the Lomb periodogram, which makes it impossible to use the standard surrogate data algorithms mentioned above. Therefore, we follow the general approach of Ref. [4], where constraints on the surrogate data are implemented by a cost function \( E(\{y_n\}) \) which has a global minimum when the constraint is fulfilled. As in Ref. [4] this cost function will be minimized by simulated annealing. Starting with a random permutation of the original time series, the surrogate is modified by exchanging two points chosen at random. The modification will be accepted if it yields a lower value for the cost function or else with a probability \( p = \exp(-\Delta E/T) \). The “system temperature” \( T \) will be lowered slowly to let the system settle down to a minimum. This idea goes back to Metropolis et al. [9]. See for example [10] for details.

In our case, we use the Lomb periodogram of the data as a constraint for the surrogates. It can be expressed as a cost function for example by:

\[
E = \left[ \frac{1}{N_f} \sum_{k=1}^{N_f} |P(k\omega_0) - P_{\text{data}}(k\omega_0)|^q \right]^{1/q}
\]

We use \( P \) at \( N_f \) equally spaced frequencies \( k\omega_0 \), other choices are possible. The parameter \( q \) specifies the distance measure between the two periodograms. For \( q = 2 \), the \( L^2 \)–distance is used. For the following examples we use \( q = 1 \). Higher “penalties” for large differences in single frequencies could be given by raising \( q \) above 1. Alternatively, one could use the differences between the square roots or logarithms of \( P \), which puts less stress on the peaks in the power spectrum than \( \left[ P(k\omega_0) - P_{\text{data}}(k\omega_0) \right]^q \). Another freedom lies in the choice of the minimum frequency \( \omega_0 \) and the number of frequencies \( N_f \) and one may have to consider different values for each individual application.

Recall that we are interchanging only the values of the time series \( y_n \), while fixing the times \( t_n \) where measurements are made. This excludes data like inter–beat intervals of electrocardiograms where we have the additional condition \( t_{n+1} = t_n + y_n \).

For the calculation of surrogates, simulated annealing is performed until \( E \) has fallen below a given value \( E_f \), the desired accuracy of the Lomb periodogram. In Monte Carlo simulations, new configurations are usually generated from “older” configurations. In order to avoid correlations between the different surrogates, we prefer to start with a completely random permutation of the original time series for each surrogate. The starting temperature can roughly be determined by calculating the cost function for some randomly shuffled data sets and choosing \( T_0 \) as a “typical” difference in cost between them. Once an adequate starting temperature is known, it can be used for further surrogates.

Two improvements that accelerate the annealing algorithm have been made. The first is to choose the two points that are candidates for an exchange with a probability that depends on their difference in magnitude. Exchanging two points with a big difference in their rank (eg. the smallest and the largest value) yields a larger change of the cost function than exchanging two points that do not differ much in their ranks. For good performance, it is desired to keep approximately the same acceptance rate through all temperatures. This can be achieved by choosing pairs of points \( \{y_i, y_j\} \) with \( i \neq j \) and probability \( p_{ij}(d, \mu) \) where \( d = |\text{rank}(y_i) - \text{rank}(y_j)| - 1 \). The probability \( p \) is chosen to have a maximum for \( d = 0 \) and to decrease for higher \( d \). The parameter \( \mu \) characterizes the “width” of the distribution \( p \) and should be varied proportional to \( N/T \). The exact shape of \( p \) does not seem to be of much importance. For example, we were not able to observe a significant difference in performance between exponential and Gaussian distributions. But in all cases we considered, a non–uniform \( p_{ij} \) substantially accelerated the annealing process, so that higher accuracy is reachable with the same computational effort.

Calculating \( E \) is very time consuming for long time series and many frequencies. With a typical value of \( N_f \propto N \) we have an algorithm of order \( N^2 \) for each annealing step. Additionally, the number of annealing steps grows at least linearly with \( N \). For our applications, it is not necessary to recalculate all sums in (3) for every exchange, because we only change the values \( y_n \) while fixing the times \( t_n \) and frequencies \( k\omega_0 \). In (3), \( \tau \) and the two denominators do not depend on \( y_n \) and can be stored in arrays for every frequency \( k\omega_0 \) at the beginning of the annealing process. The sums in the numerator do not change much either and only two terms have to be recalculated. This reduces the recalculation of the Lomb
FIG. 1. Delay–plot of an unevenly sampled Hénon map and one surrogate. The test finds a significant difference in time–asymmetry.

periodogram to order $N$.

But even with the described modifications to the algorithm the actual annealing is quite computer time intensive. Generating one surrogate for a time series with $N = 2000$ points while fixing $N_f = 1000$ frequencies takes about 5 hours CPU–time on a DEC alpha workstation at 166 MHz.

So far, we have described how to produce randomized versions of unevenly sampled time series with given linear correlations, which is the main point of this paper. Let us now demonstrate, how such surrogate sequences can be used in tests for nonlinearity. For this purpose, we have to be able to measure the degree of nonlinearity in a time series. Many statistics that have proven useful for evenly sampled time series (see e.g. [11]) cannot easily be generalized to unevenly spaced data. This generalization, in general, is a topic of future research.

Here, as a first simple statistic, we choose a measure for time–reversibility, which is a good indicator for nonlinearity. It is however not very enlightening about what source of nonlinearity there might be. For the data sorted in time order,

$$\gamma = \frac{1}{(\sigma^2)^2 (N-1)} \sum_{n=2}^{N} \left( \frac{y_n - y_{n-1}}{t_n - t_{n-1}} \right)^3 \tag{4}$$

is calculated, which is just the mean of the slopes, taken to the third power. For a time series generated by a linear process, and for the surrogates, we expect $\gamma \approx 0$. In contrast, time series with nonlinearities can be asymmetrical in time and may yield values of $\gamma \neq 0$. To pay regard to deviations in both directions ($\gamma > 0$ and $\gamma < 0$), a two sided test [12] has to be performed.

To test the functionality of the surrogate test, we use 10000 points of the Hénon map as a first example. From these, we pick $N = 1000$ points with their time indices chosen randomly. To generate surrogates, we calculate the Lomb periodogram for $N_f = 500$ frequencies in the interval $\nu \in [0, 0.5]$. A delay–plot of the data and one surrogate is shown in Fig. 1. A little trace of the Hénon attractor can be found in the left figure that is built by pairs of values with time delay one. For the original time series we get $\gamma = -0.58$, while 19 surrogates gave values $-0.30 < \gamma < 0.18$. This corresponds to a 90% level of significance for the time series not being time reversible and hence nonlinear in the sense of the null hypothesis.

In order to verify the new test method we also applied the test to linear time series based on an AR(1)–process

$$x_{n+1} = 0.95 x_n + \eta_n$$

which is however invertibly rescaled by $y_n = x_n \sqrt{x_n}$. Again we picked 1000 points randomly from the original 10000. A test performed with this data was unable to reject the null hypothesis, as expected since the null was true.

For a quantification of the power and the size [12] of the new method, many independent tests would be necessary. Such an extremely computer time–intensive study is beyond the scope of the present work.

Finally, the test is applied to experimental data. Data Set E of the Santa Fe time series contest is a set of measurements of the time–integrated intensity of light observed from a variable star. It consists of 17 parts with different numbers of points, the time range of which partly overlaps and partly shows gaps. Inside the blocks,
the data is evenly sampled with $\Delta = 10$ s. Special interest in low frequency components makes it desirable to consider the time series as a whole. The Lomb periodogram of the data set is shown in Fig. 2.

For the surrogate test we further down–sampled the data by integrating over 12 successive measurements. Therefore, surrogates could be generated in reasonable time. The resulting time series is $N = 2260$ points long with $\Delta = 120$ s except for 9 gaps taking up to 10000 s, as shown in Fig. 3. The Lomb periodogram is calculated at $N_f = 1130$ frequencies with up to $\nu_{\text{max}} = 1/240$ Hz. The value for the time–reversibility statistic $\gamma = -0.56 \times 10^{-7}$ s$^{-3}$ of the considered time series does not lie outside the interval $\gamma \in [-13 \times 10^{-7} \text{s}^{-3}, 29 \times 10^{-7} \text{s}^{-3}]$ spanned surrogates, and thus the null hypothesis cannot be rejected. One surrogate time series is also shown in Fig. 3.

Spurious high frequency components could be introduced by discrepancies in the overlapping parts of the recording. To deal with that problem we deleted points from one of the two parts and repeated the test. No significant differences in the surrogates and its values for the test statistics were observed.

Taking a closer look at the individual parts shows considerable differences in their autocorrelations, which makes it dangerous to consider the whole data set as stationary. In contrast, the generated surrogates are stationary by construction. If one could detect significant differences with a nonlinear statistic, non–stationarity would be an equally likely explanation as nonlinearity.

In this paper we presented a method for a test for nonlinearity for time series with uneven time intervals. Such a test consists of two main steps: generating surrogate data and calculating test statistics. The new method is able to achieve the first step using the constrained randomization scheme proposed in Ref. [4]. We offered only a first attempt on the second problem. More powerful test statistics are likely to be derivable from current nonlinear time series methods.

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