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SURROGATE-BASED HYPOTHESIS TEST WITHOUT SURROGATES

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Fourier surrogate data are artificially generated time series, that — based on a resampling scheme — share the linear properties with an observed time series. In this paper we study a statistical surrogate hypothesis test to detect deviations from a linear Gaussian process with respect to asymmetry in time (Q-statistic). We apply this test to a Fourier representable function and obtain a representation of the asymmetry in time of the sample data, a characteristic for nonlinear processes, and the significance in terms of the Fourier coefficients. The main outcome is that we calculate the expected value of the mean and the standard deviation of the asymmetries of the surrogate data analytically and hence, no surrogates have to be generated. To illustrate the results we apply our method to the saw tooth function, the Lorenz system and to measured X-ray data of Cygnus X-1.

Keywords: Fourier surrogates; nonlinear time series analysis.

1. Introduction

The theory of nonlinear dynamical systems offers notions to characterize processes beyond linearity. Different quantities are used therefore, among them the correlation dimension, Lyapunov exponent and nonlinear forecasting errors [Kantz & Schreiber, 1999]. To investigate the reliability of the estimates of these characteristics, the method of surrogate data has been invented [Theiler *et al.*, 1992; Theiler & Prichard, 1996, 1997; Kurths & Herzel, 1987; Schrieber & Schmitz, 2000]. The general idea is to simulate time series whose statistical properties are constrained to the null hypothesis one wants to test for [Schreiber, 1998]. The Fourier surrogates which were introduced to test for such a constraint null hypothesis have become very popular [Theiler *et al.*, 1992; Theiler & Prichard, 1996; Schreiber & Schmitz, 2000]. The basic idea of generating Fourier surrogates is that the linear properties of the time series are specified by the squared amplitudes of the (discrete) Fourier transform. Surrogate time series are readily created by multiplying the Fourier transform of the data by random phases and then transforming back to the time domain. So testing for a linear Gaussian process X_n one takes the Fourier transform of the data $\{x_n\}_{n=1}^{N}$

$$\tilde{x}_k = \frac{1}{\sqrt{N}} \sum_{n=1}^{N} x_n e^{-i2\pi nk/N} \tag{1}$$

Then the complex components $\tilde{x}_k$, $1 < k < N$ are multiplied by random independently and uniformly in $[0,\, 2\pi)$ distributed phases φ_k, $\tilde{x_k^s} = \tilde{x}_k e^{i\varphi_k}$, with the constraint $\varphi_{N-k} = -\varphi_k$. Then one computes the inverse Fourier transform

$$x_n^s = \frac{1}{\sqrt{N}} \sum_{k=1}^{N} \tilde{x}_k^s e^{i2\pi nk/N} \tag{2}$$

and takes x_n^s as a surrogate of the data. Different realizations of the phases φ_k generate new surrogates. This process of *phase randomization* preserves the periodogram and the Gaussian distribution (at least asymptotically for large N) [Schreiber & Schmitz, 2000].

If the time series $\{y_n\}$ is not Gaussian distributed one uses Amplitude Adjusted Fourier (AAFT) surrogates. One assumes that $\{y_n\}$ comes from a linear Gaussian process with a nonlinear, monotonic (invertible) observation function S (e.g. $y_n = s(x_n) = \exp(x_n)$ where $\{x_n\}$ comes from a linear Gaussian process). Transforming it to Gaussian marginal distribution the original linear Gaussian process (i.e. $s^{-1}(y_n) = \ln(\exp(x_n)) = x_n$) can be recovered. Then one generates surrogates x_n^s and transforms them using the function s, i.e. $y_n^s = s(x_n^s)$. One then yields surrogates that are constraint with the null hypothesis of the linear Gaussian process with a monotonic observation function. Alternatives to this approach are discussed in the literature [Schreiber & Schmitz, 1996; Kugiumtzis, 2000].

We are interested in the test and not in generating optimal surrogates. Hence, we can apply the test to the Gaussian marginal distribution transformed observed data, i.e. $x_n = s^{-1}(y_n)$. If this transformed data set is rejected by the hypothesis test, then the original data cannot be described sufficiently by a linear Gaussian process with a monotonic observation function. If it is not rejected, the test failed to recognize any significant deviation for the null hypothesis. Hence, it is sufficient to apply the test to the transformed time series (where the transformation is supposed to be monotonic). This approach can be used to apply the method presented in this paper to data that is not Gaussian distributed.

Note, that especially if the underlying process is the nonlinear process $x'_n = \exp(x_n)$ where $\{x_n\}$ again comes from a linear Gaussian process and the observation function is the identity $s(x'_n) = x'_n$, then the transform to Gaussian marginal distribution $\ln(x'_n) = x_n$ will remove the nonlinearity from $\{x'_n\}$. In this case the observed time series, though nonlinear, can be described by a linear Gaussian process with an nonlinear monotone observation function.

The test statistic we focus our attention on is the asymmetry $Q(m)$ in time — a characteristic of many nonlinear processes

$$Q(m) = \frac{\langle [x_n - x_{n+m}]^3 \rangle_n}{\langle [x_n - x_{n+m}]^2 \rangle_n} \tag{3}$$

where the time series is given by x_n. We call the hypothesis test based on the Fourier surrogates and the asymmetry as test statistic Q-statistic-test (QST). It results in a function $S(m)$ that is usually called "significance" and that is given by

$$S(m) = \frac{|Q(m) - \langle Q^s(m) \rangle_s|}{\sigma_{Q^s}(m)} \tag{4}$$

where s means "surrogates", and $\langle Q^s(m) \rangle$ is the ensemble mean of the asymmetries of the surrogates at lag m, and $\sigma_{Q^s}(m)$ is the corresponding standard deviation. $S(m)$ gives the significance of the asymmetry under the null hypothesis of a linear Gaussian process [Theiler *et al.*, 1992]. To calculate the quantile of the ensemble $\{Q^s(m)\}$, one usually assumes that it is Gaussian distributed for all times m. Simulations indicate that mixing processes fulfill this condition, though there is no proof for this assumption. Then one rejects the null hypothesis at an α-level of 1% if $S(\tau) > 2.6$ (the value 2.6 corresponds to the 1% quantile of the normal distribution). If the null hypothesis is not rejected it does not mean conclusively that the time series can be properly described by a linear Gaussian process. The test only failed to reject the null hypothesis then. If it is rejected on the other hand one cannot conclude that the time series is nonlinear (e.g. it could be nonstationary) [Timmer, 2000; Paluš, 1995].

This paper is structured as follows: in Sec. 2 we express the method of the QST in terms of the Fourier-coefficients of the measured time series. This enables us to calculate the expected value of the mean and the standard deviation of the asymmetries of the surrogates, and hence makes it unnecessary to generate surrogates which is the main result of this paper. To illustrate the results we apply the improved method in Sec. 3 to a saw tooth function, to the Lorenz system and to observed X-ray data of the black hole candidate Cygnus X-1.

2. Method

We start by applying the QST to a general function $f(t)$ with the Fourier representation

$$f(t) = \frac{a_0}{2} + \sum_{i=1}^{\infty} \{a_i \cos(i\omega t) + b_i \sin(i\omega t)\} \tag{5}$$

where t, a_i, b_i, ω are real numbers. Substituting a_i, b_i by the coefficients obtained from a Fourier transform, we can examine measured time series.

Analogously to the asymmetry $Q(m)$ given by Eq. (3) we compute

$$Q(\tau) = \frac{\langle [f(t) - f(t+\tau)]^3 \rangle_t}{\langle [f(t) - f(t+\tau)]^2 \rangle_t} \tag{6}$$

where t and τ now are continuous variables (whereas n and m are discrete variables). To evaluate the nominator of Eq. (6), we first calculate

$$\begin{aligned}&\langle [f(t) - f(t+\tau)]^3 \rangle \\ &= \frac{1}{T} \int_0^T \left\{ \sum_{i=1}^{\infty} \left[\tilde{a}_i \sin\left(i\omega \left(t + \frac{\tau}{2} \right) \right) \right.\right. \\ &\qquad \left.\left. + \tilde{b}_i \cos\left(i\omega \left(t + \frac{\tau}{2} \right) \right) \right] \right\}^3 dt \end{aligned} \tag{7}$$

where

$$\tilde{a}_i = 2a_i \sin\left(\frac{i\omega\tau}{2} \right)$$

$$\tilde{b}_i = -2b_i \sin\left(\frac{i\omega\tau}{2} \right)$$

and T is the length of the defining interval of $f(t)$. Evaluating the integrand of Eq. (7), we only obtain terms that contain products of three Fourier components. Using the orthogonality relations for the triple products of sine and cosine functions it is clear that only terms of the forms $\tilde{a}_i\tilde{a}_j\tilde{b}_{i+j}$, $\tilde{a}_i\tilde{b}_j\tilde{a}_{i+j}$ or $\tilde{b}_i\tilde{b}_j\tilde{b}_{i+j}$ contribute to the asymmetry (these relations can be derived based on the representation of the products as a sum of four sine and cosine functions). The denominator can be treated analogously. Assuming a uniform convergence of the Fourier-series,[1] so that we can change the order of the sum and the integral, we find

$$Q(\tau) = \frac{3 \displaystyle\sum_{i=1}^{\infty} \sum_{j=1}^{\infty} \{a_i a_j b_{i+j} - 2a_{i+j} a_i b_j - b_i b_j b_{i+j}\} \sin\left(\frac{i\omega\tau}{2} \right) \sin\left(\frac{j\omega\tau}{2} \right) \sin\left(\frac{(i+j)\omega\tau}{2} \right)}{\displaystyle\sum_{i=1}^{\infty} (a_i^2 + b_i^2) \sin^2\left(\frac{i\omega\tau}{2} \right)} \tag{8}$$

Hence, we can express the asymmetry only in terms of the Fourier coefficients. Next, we proceed analogously to calculate the significance $S(\tau)$

$$S(\tau) = \frac{|Q(\tau) - \langle Q^s(\tau) \rangle_s|}{\sqrt{\sigma^2_{Q^s}(\tau)}} \tag{9}$$

of the asymmetry $Q(\tau)$. Hereby, we generate surrogates $f^s(t)$ of $f(t)$, by adding random phases φ_i^s that are independently and identically distributed in $[0, 2\pi)$, i.e.

$$\begin{aligned} f^s(t) &= \frac{a_0}{2} + \sum_{i=1}^{\infty} \{a_i \cos(i\omega t + \varphi_i^s) \\ &\qquad + b_i \sin(i\omega t + \varphi_i^s)\} \\ &= \frac{a_0}{2} + \sum_{i=1}^{\infty} \{\alpha_i^s \cos(i\omega t) + \beta_i^s \sin(i\omega t)\} \end{aligned} \tag{10}$$

where

$$\alpha_i^s = a_i \cos(\varphi_i^s) + b_i \sin(\varphi_i^s) \tag{11}$$

$$\beta_i^s = -a_i \sin(\varphi_i^s) + b_i \cos(\varphi_i^s) \tag{12}$$

Here s is the index of the sth surrogate and φ_i^s are with respect to i uniformly distributed random numbers.

It is interesting to note that the surrogates can differ in the time domain very much from the original function. To illustrate this we apply this "phase randomization" to a saw tooth function (Fig. 1)

$$f(t) = \sum_{i=1}^{\infty} \frac{1}{i} \sin[i(\omega t - \pi)]$$

As we use only the first 50 coefficients of its Fourier representation we see small fluctuations, especially at the peaks of its graph. Note that by construction the periodogram of all these functions is the same.

To estimate $S(\tau)$ numerically, we have to use a finite number of surrogates. But here our approach enables also to calculate analytically the expected value for both $\langle Q^s(\tau) \rangle_s$ and $\sigma^2_{Q^s}(\tau)$, i.e. "**all** realizations of surrogates" are taken into account this way. Equation (10) allows to compute the asymmetry $Q^s(\tau)$ of a surrogate that is given by substitution of $a_i \to \alpha_i^s$ and $b_i \to \beta_i^s$ in Eq. (6). Then we

[1] For example, if $\exists\, L \geq 0$ so that $a_l, b_l = 0 \quad \forall\, l > L$ the series converges uniformly.

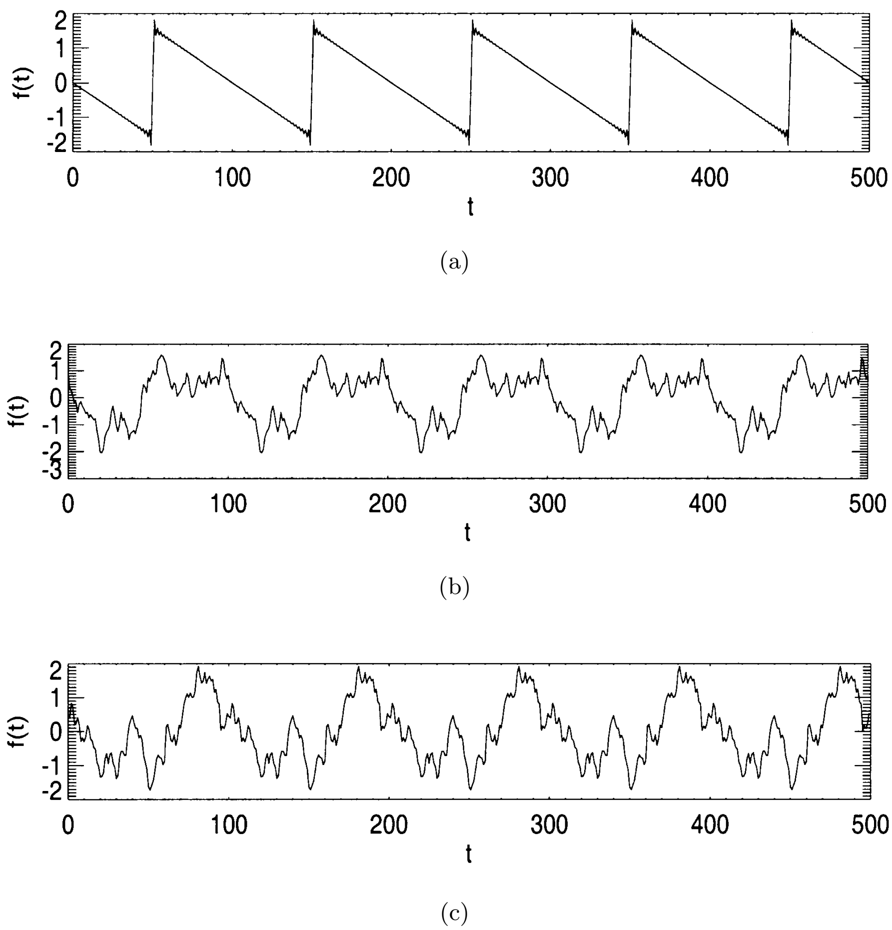


Fig. 1. The representation of the first 50 terms of the saw tooth function with $\omega = 2\pi/100$. (b) and (c) Two of its surrogates obtained by phase randomization. The surrogates differ rather much from the saw tooth function but show the same period.

can compute the expected value for the mean by the (infinite) integrations

$$\langle Q^s(\tau)\rangle_s = \int_0^{2\pi}\cdots\int_0^{2\pi} \frac{\sum_{i,j=1}^{\infty} 3\{\alpha_i^s\alpha_j^s\beta_{i+j}^s - 2\alpha_{i+j}^s\alpha_i^s\beta_j^s - \beta_i^s\beta_j^s\beta_{i+j}^s\}\sin\left(\frac{i\omega\tau}{2}\right)\sin\left(\frac{j\omega\tau}{2}\right)\sin\left(\frac{(i+j)\omega\tau}{2}\right)}{\sum_{i=1}^{\infty}((\alpha_i^s)^2+(\beta_i^s)^2)\sin^2\left(\frac{i\omega\tau}{2}\right)} \cdot \frac{d\varphi_1}{2\pi}\cdots\frac{d\varphi_\infty}{2\pi} \tag{13}$$

Note that α_i and β_i depend on φ_i. Substituting Eqs. (11) and (12) we find that the denominator is independent of φ_i. This integral can be solved due to the independence of the phases φ_i. This independence reflects the linearity of the surrogates. Then, we change the summation with the integration, which is possible due to the assumed uniform convergence of the sum, and find that

$$\langle Q^s(\tau)\rangle_s \equiv 0 \tag{14}$$

The standard deviation can be calculated analogously.

$$\sigma^2_{Q^s}(\tau) = \frac{\Sigma^I(\tau) + \Sigma^{II}(\tau)}{\{\Sigma^{III}(\tau)\}^2} \tag{15}$$

where

$$\Sigma^{I}(\tau) = \frac{27}{4}\sum_{i=1}^{\infty}\sum_{j=1}^{\infty}\{a_i^2 a_j^2 b_{i+j}^2 + a_i^2 a_j^2 a_{i+j}^2 + a_i^2 b_j^2 b_{i+j}^2 + a_j^2 b_i^2 b_{i+j}^2 + b_i^2 b_j^2 b_{i+j}^2 + b_i^2 b_j^2 a_{i+j}^2 + b_i^2 a_j^2 a_{i+j}^2 + a_i^2 b_j^2 a_{i+j}^2\} \cdot \sin^2\left(\frac{i\omega\tau}{2}\right)\sin^2\left(\frac{j\omega\tau}{2}\right) \cdot \sin^2\left(\frac{(i+j)\omega\tau}{2}\right) \tag{16}$$

$$\Sigma^{II}(\tau) = -\frac{9}{4}\sum_{i=1}^{\infty}\{2b_i^2 b_{2i}^2 a_i^2 + b_i^4 a_{2i}^2 + a_i^4 a_{2i}^2 + a_i^4 b_{2i}^2 + 2b_i^2 a_i^2 a_{2i}^2 + b_i^4 b_{2i}^2\} \cdot \sin^4\left(\frac{i\omega\tau}{2}\right)\sin^2(i\omega\tau) \tag{17}$$

$$\Sigma^{III}(\tau) = \sum_{i=1}^{\infty}(a_i^2 + b_i^2)\sin^2\left(\frac{i\omega\tau}{2}\right) \tag{18}$$

Using Eqs. (6), (14) and (15) we have an analytical representation of the significance $S(\tau)$, cf. Eq. (9), only in terms of the Fourier-coefficients.

Equations (6), (9) and (15) comprise the entire procedure of the QST. From now on we will call the method introduced by Theiler "Q-statistic-test" (QST) meaning the *recipe* to calculate the asymmetry Eq. (3) and the significance Eq. (4) including the generation of surrogates. On the other hand we will name the formulas Eqs. (6), (9), (15) — the distillate of the procedure of the Q-statistic-test — "Q-formula-test" (QFT).

3. Comparison of the Methods

We now compare the well-known QST and our QFT to three cases: the saw tooth function, the Lorenz system in a chaotic regime and observed X-ray data from the black hole candidate Cygnus X-1.

We consider the saw tooth function only to illustrate the behavior of the functions Q, σ_{Q_s} and S for an easily manageable set of Fourier coefficients. Hence, this example is not thought to be an hypothesis test.

Then, we apply both methods to the Lorenz system because it is a well-studied reference system. As it is a nonlinear system both are supposed to reject the null-hypothesis.

The last case concerns the observed X-ray flux of Cygnus X-1. It is still under debate whether the dynamics can be appropriately described by linear models [Timmer *et al.*, 2000; Viklinin *et al.*, 1994; Belloni & Hasinger, 1990].

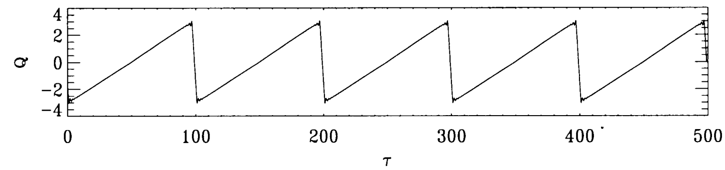
QST and so the QFT depend on the phases and hence make it possible to detect three point correlations (third order statistics) that the power spectrum cannot distinguish. Besides, we do not simply accept or reject the null hypothesis but we also consider the structure of $S(\tau)$. This structure yields a further criterion to model the process under consideration.

3.1. *Saw tooth function*

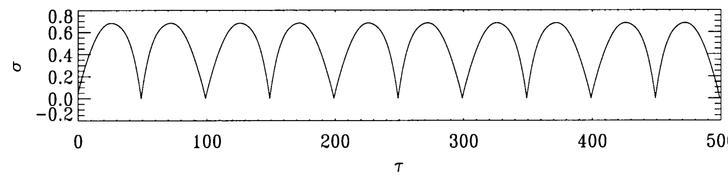
First we discuss is the truncated saw tooth function. "Truncated" means that we used in this example the first 50 coefficients of the Fourier series only [see Fig. 1(a)]. This time series can be considered as the Fourier decomposition of a time series of 100 data points.

The saw tooth function is asymmetric in time. The sum Eq. (5) converges uniformly due to the finiteness of the sum, and so the Q-formulas hold. Hence, Eqs. (8), (15) and (9) yield the asymmetry $Q(\tau)$, the standard deviation of the asymmetries of the surrogates $\sigma_{Q^s}(\tau)$ and the significance $S(\tau)$ respectively. The graphs of these functions are shown in Fig. 2. σ_{Q^s} has zeros at the same points as $Q(\tau)$ and also in the middle of the period of the saw function. $S(\tau)$ has peaks only at the beginning and end of the period [Fig. 2(c)]. This means that the division of the zeros of $Q(\tau)$ and σ_{Q^s} in the middle of the period, is in the limit finite.

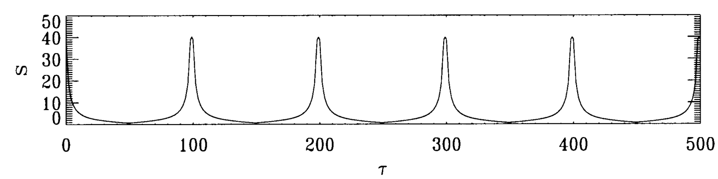
We compare the results of the QFT and QST using 100 surrogates. Due to the finite number of surrogate files the QST uses, the mean is now not equal to zero (Fig. 3). The significance [Fig. 3(c)] differs from the one calculated with the QFT. The peaks of the significance computed by QST are only about 65% as high as the peaks calculated by the QFT. Further we observe split peaks in the QST. This is mainly due to the nonvanishing mean of the asymmetries of the surrogates [see Fig. 3(b)] and numerical errors. At $m = 100$ one finds that $S(100) =$ "0"/"0" and hence small numerical errors yield large errors in the estimation of S. The smaller the number of surrogates one uses for the test the more pronounced is the effect.



(a)

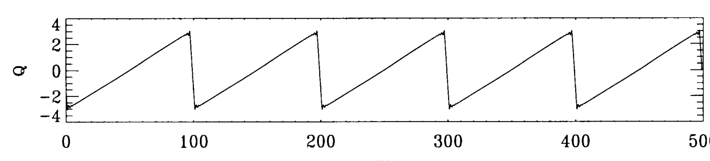


(b)

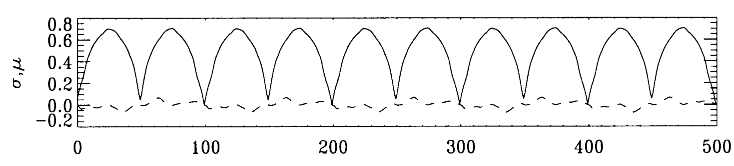


(c)

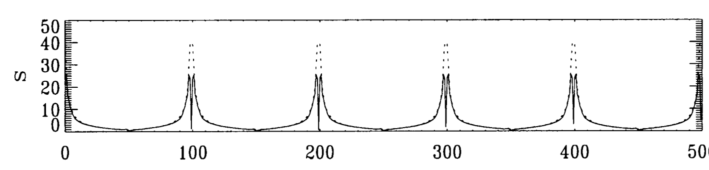
Fig. 2. Results of the QFT for the truncated saw tooth function. (a) Asymmetry $Q(\tau)$. (b) Standard deviation $\sigma_{Q^s}(\tau)$ of the asymmetries of the "surrogates". (c) Significance $S(\tau)$.



(a)



(b)



(c)

Fig. 3. Results of the QST for the truncated saw tooth function using 100 surrogates. (a) Asymmetry $Q(m)$. (b) Standard deviation $\sigma_{Q^s}(m)$ of the asymmetries (solid) and mean (dashed) of the "surrogates". (c) Significance $S(m)$ calculated with the QST (solid) and QFT (dashed).

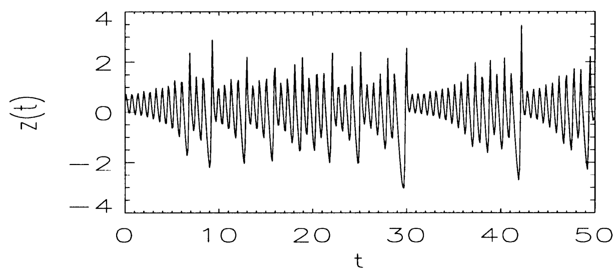


Fig. 4. z-component of the Lorenz system transformed to Gaussian distribution in absolute units of time.

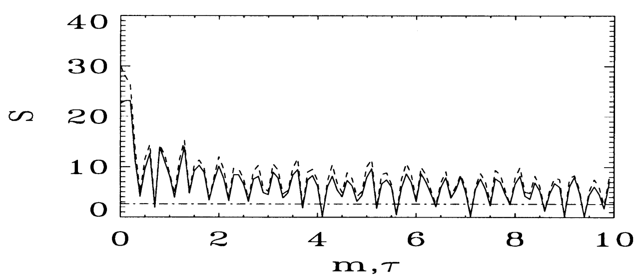


Fig. 5. Significance calculated by the QST (solid line) using 100 surrogates and calculated by the QFT (dashed line) for 5,000 data points of the z-component of the Lorenz system. (Dashed–dotted) Level of 1% significance.

QFT avoids these finite size problems. This is one important advantage to use QFT rather than QST.

3.2. *The Lorenz system*

Next we analyze the z-component of the Lorenz system in a chaotic regime [Lorenz, 1963]. We use the standard parameters $\sigma = 10$, $r = 28$ and $b = 8/3$ and integrate the equations with a Runge–Kutta algorithm of fourth order. The step-size for the integration is $h = 0.01$ and we use every tenth data point, i.e. $\Delta t = 0.1$. The absolute time of integration is 500 time units. Both methods are now applied to the z-component (Fig. 4). As expected both the QST and QFT clearly reject the null hypothesis of a linear Gaussian process (Fig. 5). Finite size effects and numerical errors cause — as in the case of the saw tooth function — slightly lower values of significance for the QST. The oscillating structure of $S(\tau)$ is due to the oscillations of sample time series.

3.3. *Results for Cygnus X-1*

Next we compare the QST and QFT for an observed time series. We apply them to Kalman filtered X-ray flux data of Cygnus X-1, one of the best investigated black hole candidates. Mass accretion from its primary HDE 226868 leads to X-ray emission which exhibits a variability in time scales from milliseconds up to months. The spectral features allow to distinguish five states that are called quiescent, low, intermediate, high and very high states. They are believed to correspond to increasing mass accretion rate. This data has been recently investigated by Timmer *et al.* [2000] by means of the QST. They have found a rejection of the null hypothesis of a linear Gaussian process for the X-ray flux. The nature of variability of the flux is still an open question in astrophysics [Belloni & Hasinger, 1990; Pottschmitt *et al.*, 1998]. Its analysis by the QST/QFT helps to learn whether a linear state space model is sufficient to describe the statistical properties of the data as suggested by Pottschmitt *et al.* [1998].

The data is recorded with the Proportional Counter Array (PCA) aboard the Rossi X-ray Timing Explorer (RXTE). The energy range is 2.0–14.1 keV and the sampling frequency is 256 Hz.

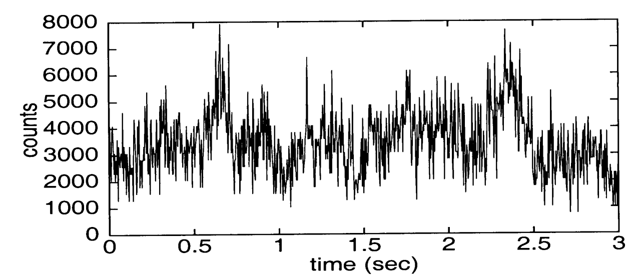


Fig. 6. Sample data of the X-ray flux of Cygnus X-1. The bin width is $\frac{1}{256}$ ms $\sim$ 4 ms.

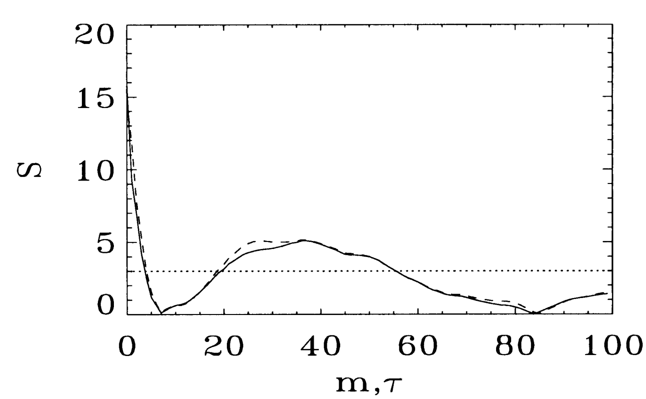


Fig. 7. Significance $S(\tau)$ calculated by the QST (solid) using 100 surrogates and calculated by the QFT (dashed) for 20,000 data points from the sample series. (Dashed–dotted) Level of 1% significance.

There are many data sets of the X-ray flux available that consist of 100,000–800,000 points.

We present an analysis of observations from 24 October, 1996 when Cygnus X-1 was in a low state. The measured X-ray flux looks rather erratic (Fig. 6). Applying the QST (using 100 surrogates) and QFT to the Kalman filtered X-ray flux, we find for both approaches a significant deviation of the observed time series from a typical realization of a linear Gaussian process (Fig. 7). The greatest deviation can be localized at lags of about $\tau = 30 \sim 30(1/256\text{ Hz}) \sim 120$ ms. Timmer *et al.* [2000] have found a similar deviation for an intermediate state of the black hole candidate. We now show the same behavior for a low state.

4. Conclusions and Outlook

We have shown in this paper, that the QST can be expressed in terms of the Fourier coefficients of the underlying time series. This representation allows to compute analytically the expected value of the mean and the standard deviation of the asymmetries without generating surrogates. Our approach eliminates effects that are due to the finite number of surrogates and hence reduces the errors of the second kind (false negatives).

The analytical solution for the asymmetry and the significance can reveal dependencies of higher than second order of the Fourier coefficients. The analytical expressions help to yield a deeper understanding of the difference between linear and nonlinear dynamics and how it is formed in terms of certain components of the time series.

One important point for the modeling of time series is that the structure of $S(\tau)$ gives a further piece of information about (nonlinear) dependencies. One way to reproduce these structures is to generate stochastic processes with nonlinearities [Tsay, 1973].

We also have extended the results of Timmer *et al.* [2000] but for a low state. Furthermore, the new representation of the QST, i.e. the QFT, will help to reveal the relations of the Fourier-coefficients that lead to the deviation from the linear process in the case of Cygnus X-1.

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