HIGH-PRECISION SURROGATE DATA BASED TESTS FOR GAUSSIANITY AND LINEARITY OF DISCRETE TIME RANDOM PROCESSES

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ABSTRACT

We have put Hinich's asymptotic tests for Gaussianity and linearity under scrutiny, and we show that these tests suffer from severe statistical problems. We propose the use of carefully designed surrogate data to ensure correct false alarm rate. Using theoretical considerations about estimation of higher order spectra, we propose new high-precision detections statistics for Gaussian and linear signals. Results from synthetic and experimental data demonstrate the applicability of the proposed tests.

1. INTRODUCTION

The power spectral density, or the power spectrum, is an indispensable quantity when describing the second-order statistics of stationary stochastic processes. If the process considered has a Gaussian amplitude distribution, it is well known that the mean value and the power spectrum characterize the process completely. If the process under study is non-Gaussian, or if it is the result of nonlinear dynamics, knowledge of the mean value and the power spectrum is not sufficient to fully characterize the process. Under such circumstances, one may have to consider higher order spectra (HOS) [5].

HOS based tests for Gaussianity and linearity of stationary processes are most often based on the complex valued skewness function [5]

$$\Gamma(f_1, f_2) = \frac{S_3(f_1, f_2)}{\sqrt{S_2(f_1)S_2(f_2)S_2(f_1 + f_2)}},\tag{1}$$

where $S_2(f)$ and $S_3(f_1, f_2)$ is the power- and bispectrum, respectively. Note that $\Gamma(f_1, f_2)$ in Eq. (1) has been referred to as bicoherence, although it is not a true coherence as the related and generalized quantities defined in [14, 9].

Theoretically, a Gaussian process has a zero valued skewness function (and bispectrum), and a linear non-Gaussian time series has a non-zero constant magnitude skewness function [5]. Rao and Gabr [17] proposed hypothesis tests for both Gaussianity and linearity, and Hinich [10] constructed asymptotic tests that are well established in time series analysis of economic data [1].

In this paper we present the following. In Section 2 we review HOS theory and estimation. In Section 3 we briefly review Hinich's asymptotic tests and we describe the theoretical problems with his approach. In Section 4 we propose and illustrate our proposed tests. The applicability of our tests are demonstrated in Section 5 using real data from a 1/f noise experiment. Finally, our conclusions are presented in Section 6.

2. HIGHER ORDER SPECTRA

The Cramér spectral representation of a zero-mean discrete time stochastic process x[n] is given by [3]

$$x[n] \triangleq \int_{1/2}^{1/2} e^{j2\pi f n} d\widetilde{X}(f), \tag{2}$$

where $d\widetilde{X}(f)$ is the corresponding stochastic increment process, f is the frequency and $j = \sqrt{-1}$.

As is well known, the Fourier transform does not in general exist for a stochastic process. In that sense, the spectral representation in Eq. (2) is a very powerful extension that allows the traditional frequency understanding for Fourier analysis to be valid also for stochastic processes. The randomness of the time process is represented through the increment process $d\widetilde{X}(f)$.

Given that the process' 2nd and 3rd order moments are absolutely summable, the integrated power- and bispectrum can be defined as [6]

$$S_2(f)df = \mathbb{E}\left[d\widetilde{X}(f)d\widetilde{X}^*(f)\right]$$
 (3)

$$S_3(f_1, f_2)df_1df_2 = \mathbb{E}\left[d\widetilde{X}(f_1)d\widetilde{X}(f_2)d\widetilde{X}^*(f_1 + f_2)\right],$$
 (4)

where * denotes complex conjugate operation.

Given a real valued finite length time series x[n], for n = $0, 1, \dots, N-1$, drawn from a stationary zero-mean stochastic process, the basic direct estimate of power and bispectrum is the periodogram and biperiodogram, respectively, defined as [6]

$$\widehat{S}_{2}^{per}[k] = \frac{1}{N}|X[k]|^2 ; k = 0, 1, \dots, N-1$$
 (5)

$$\widehat{S}_{3}^{per}[k,l] = \frac{1}{N}X[k]X[l]X^{*}[k+l] \; ; k,l = 0,1,\dots,N-1$$
 (6)

where $X[k] = \sum_{n=0}^{N-1} x[n] \exp(-j2\pi kn/N)$ is the discrete Fourier transform, and k corresponds to the discrete frequency $f_k = k/N$.

The statistical properties of $\widehat{S}_2^{per}[k]$ and $\widehat{S}_3^{per}[k,l]$ are well understood. Asymptotically $(N \to \infty)$ these estimators are unbiased, and, assuming a Gaussian time series, their variances can be approximated as [6]

$$\operatorname{Var}\left[\widehat{S}_{2}^{per}[k]\right] = (S_{2}[k])^{2} \tag{7}$$

$$\operatorname{Var}\left[\widehat{S}_{2}^{per}[k]\right] = (S_{2}[k])^{2}$$

$$\operatorname{Var}\left[\widehat{S}_{3}^{per}[k,l]\right] = NS_{2}[k]S_{2}[l]S_{2}[k+l],$$
(8)

for $k, l, k + l \neq 0, N/2$, where $S_2[k]$ is the true power spectrum of the process. Also, the (bi-) periodogram estimates for two distinct harmonic (pairs of) frequencies are asymptotically uncorrelated [6].

The inconsistency and anti-consistency of $\widehat{S}_2^{per}[k]$ and $\widehat{S}_3^{per}[k,l]$, shown in Eq. (7) and Eq. (8), respectively, clearly shows that these raw estimates should always be avoided. The variance of $\widehat{S}_2^{per}[k]$ and $\widehat{S}_{3}^{per}[k,l]$ can obviously be reduced by frequency smoothing as

$$\widehat{S}_{2}^{sm}[k] = \sum_{k'=k-a}^{k+a} W_{2}[k'] \widehat{S}_{2}^{per}[k']$$
 (9)

$$\widehat{S}_{3}^{sm}[k,l] = \sum_{k'=k-a}^{k+a} \sum_{l'=l-a}^{l+a} W_{3}[k',l'] \widehat{S}_{3}^{per}[k',l'], \quad (10)$$

where $W_2[k]$ and $W_3[k,l]$ is the second and third order smoothing window, respectively. Approximately unbiased estimates are obtained for normalized smoothing windows.

Theoretically, the highest variance reduction for a specified smoothing bandwidth corresponds to filtering the increment process $d\widetilde{X}(f)$ through a normalized ideal bandpass filter centered at f. For $\widehat{S}_2^{sm}[k]$ this can easily be approximated by using a uniform smoothing window, $W_2[k] = 1/(2a+1)$ for $|k| \leq a$. For $\widehat{S}_3^{sm}[k,l]$, the ideal bandpass filtering leads to the third order uniform smoothing window, which has a hexagonal region of support [16, 3],

$$W_3[k,l] = \begin{cases} 1/C & ; & k,l,k+l \le a \\ 0 & ; & \text{otherwise,} \end{cases}$$
 (11)

where C is the number of non-zero elements in $W_3[k, l]$. This hexagonal shape can easily be identified using the ideal bandpass filtered increment process in the definition of the bispectrum in Eq. (4).

Assuming a Gaussian process where the true HOS are approximately constant within the smoothing bandwidth, the variance reduction factor for uniform smoothing windows are identical to the number of frequency points averaged. The averaging clearly makes nearby frequency estimates correlated, reducing the frequency resolution of the HOS estimates.

It is well known that $\widehat{S}_2^{sm}[k]$ is asymptotically distributed as a chi-square random variable, where the number of degrees of freedom is proportional to the smoothing bandwidth. From [15] we have that $\widehat{S}_3^{sm}[k,l]$ is asymptotically distributed as a complex Gaussian random variable inside the principal domain (PD) [6] of the bispectrum.

A skewness function estimate $\widehat{\Gamma}^{sm}[k,l]$ can now easily be obtained by using $\widehat{S}_2^{sm}[k]$ and $\widehat{S}_3^{sm}[k,l]$ in the definition of $\Gamma[k,l]$ in Eq. (1). Theoretical analysis of the variance of skewness function estimates commonly ignores the variability of the power spectrum estimates [11, 14, 10], making $\widehat{\Gamma}^{sm}[k,l]$ asymptotically complex Gaussian distributed. The argument for this statistical reasoning is that the variability of the bispectrum estimate in the numerator is usually significantly larger than the power spectral estimates in the denominator.

3. CLASSICAL ASYMPTOTIC TESTS

Hinich's tests for Gaussianity and linearity [10] are based on the smoothed periodogram and biperiodogram. The standard uniform smoothing window $W_2[k]$, with a smoothing bandwidth such that $2a+1=N^c$ and c is slightly above 0.5, was recommended for the $\widehat{S}_2^{sm}[k]$ [10]. But, in contrast to the hexagonal shaped uniform window in Eq. (11), a quadratic smoothing window $W_3^{\Box}[k,l]=1/M^2$, for $|k|,|l|\leq a$, was applied for bispectrum estimation, $\widehat{S}_3^{\Box}[k,l]$.

Instead of using the skewness function directly for Gaussianity and linearity hypothesis tests, a related unity variance complex Gaussian distributed quantity $\widehat{\beta}[k,l]$ was defined as [10]

$$\widehat{\beta}[k,l] = \frac{1}{\sqrt{N(2a+1)^{-2}}} \frac{\widehat{S}_3^{\square}[k,l]}{\sqrt{\widehat{S}_2^{sm}[k]\widehat{S}_2^{sm}[l]\widehat{S}_2^{sm}[k+l]}}.$$
 (12)

Ignoring the variability of $\widehat{S}_2^{sm}[k]$, it is easy to verify the unity variance of Eq. (12) using Eq. (8) and $W_3^{\square}[k,l]$. For boundary points in PD, the normalization factor $1/\sqrt{N(2a+1)^{-2}}$ can be adjusted to ensure unity variance [10], but since all points outside the PD are ignored in $\widehat{S}_3^{\square}[k,l]$ a downward bias near the PD border is expected. Note that for non-white processes, modification of the denominator in Eq. (12) leads to a more precise variance expression [8].

The test statistic for the Gaussianity test is [10]

$$S = \sum_{[k,l] \in PD} 2 \left| \widehat{\beta}[k,l] \right|^2, \tag{13}$$

where the summation only includes uncorrelated bifrequency samples. For a Gaussian process we have that $2|\widehat{\beta}[k,l]|^2$ is approximately central chi-square distributed with two degrees of freedom.

The Gaussian hypothesis can thus be rejected if S > S', where S' is defined by the α significance level of the $\chi^2_{2P}(0)$ distribution.

If the process is non-Gaussian and linear, $2|\widehat{\beta}[k,l]|^2$ is non-central chi-square distributed with two degrees of freedom. The non-centrality parameter d can be estimated from the uncorrelated $\widehat{\beta}[k,l]$ in the PD given as [10]

$$\widehat{d} = \frac{1}{P} \sum_{[k,l] \in PD} 2\left(\left| \widehat{\beta}[k,l] \right|^2 - 1 \right), \tag{14}$$

which again has to be modified for points outside PD [10].

If the magnitude of the bicoherence varies within the PD, the non-central parameter d is not constant. The linearity test thus compares the interquartile range R of a $\chi^2_{2P}(\widehat{d})$ distribution with the sample interquartile range R_s of the uncorrelated $2|\widehat{\beta}[k,l]|^2$ where all points in the square averaging are inside PD. The sample interquartile range is assumed to be normal distributed with R as mean and σ_0 as variance, so that

$$Z = \frac{R_s - R}{\sqrt{\sigma_0^2}} \tag{15}$$

is standard normal distributed. Linearity is rejected if $R_s > R$, and the significance level is found using the upper α level of Z.

4. IMPROVING THE CLASSICAL TESTS

There are two important statistical problems connected with Hinich's tests: The estimation of $\hat{\beta}[k,l]$ in Eq. (12) and the estimation of the non-central parameter d in Eq. (14).

The square shaped region of support in $W_3^\square[k,l]$ is conceptually wrong and should never have been applied. This may lead to significant bias in the $\widehat{\beta}[k,l]$ for non-white processes, as we will illustrate later in this paper using Monte Carlo simulations and synthetic time series. The biased bispectrum estimate leads to an increased false alarm rate in both the Gaussianity and linearity test by Hinich. The downward bias introduced near the PD boundary, will furthermore reduce the power of the linearity test since only points of $\widehat{\beta}[k,l]$ where the full smoothing region are inside PD can be applied.

The variance of $\widehat{\beta}[k,l]$ is also a critical factor in Hinich's tests. For non-Gaussian processes, there exist no general approximation of the variance of HOS estimates. The use of approximations based on a Gaussian assumption when testing for linearity, which basically is done only when the process already is found to be non-Gaussian, is somewhat awkward. An increased variance can be expected for non-Gaussian processes, which clearly leads to a higher false alarm rate in the linearity test.

The estimation of the non-centrality parameter d in Eq. (14) clearly implies that the *theoretical* interquartile range R in Hinich's linearity test is a random variable. And since both R and R_s are based on the same $\widehat{\beta}[k,l]$, with some extra boundary points for R, these two random variables have to be correlated. This leads to Var[Z] < 1, which reduces the false alarm rate in the linearity test.

Although the estimation of $\widehat{\beta}[k,l]$ and d contribute in different directions for the false alarm rate, there is no reason to believe that they will counterbalance and provide the correct false alarm rate. Thus, the discussion of the power of Hinich's linearity test, as in e.g. [1], is clearly useless.

4.1 Skewness function estimation

To improve Hinich's tests we first apply the standard hexagonal shaped smoothing window $W_3[k,l]$ in Eq. (11) for the estimation of $\widehat{S}_3^{sm}[k,l]$. An unbiased estimate along the boundary of PD can be obtained by fully ignore the points outside the PD, and normalize $W_3[k,l]$ according to the number of bifrequency points averaged.

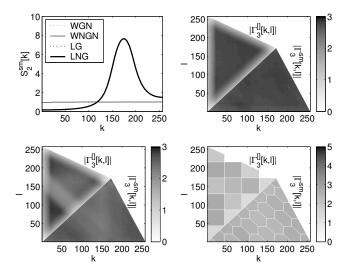


Figure 1: Upper left: $\widehat{S}_2^{sm}[k]$. Upper right: $|\widehat{\Gamma}[k,l]|$ for WNG. Lower left: $|\widehat{\Gamma}[k,l]|$ for LNG. Lower right: Uncorrelated $|\widehat{\Gamma}[k,l]|$ for LNG.

We have used synthetic data to illustrate our choice of $W_3[k,l]$. Based on zero-mean unity variance white Gaussian noise, $x_G[n]$ (WG), and convolution (*) through a second order linear autoregressive filter h[n], with parameters $a_1 = -0.8$ and $a_2 = 0.64$, we have generated the following test signals: White non-Gaussian noise $x_{NG}[n] = (x_G^2[n]-1)/\sqrt{2}$ (WNG), linear Gaussian process $x_{LG}[n] = x_G[n] \star h[n]$ (LG) and a linear non-Gaussian process $x_{LNG}[n] = x_{NG}[n] \star h[n]$ (LNG). Using N = 512 data samples for each test signals, we estimated the skewness function using both quadratic and hexagonal smoothing, with bandwidth from c = 0.6, and applied Hinich's tests for R = 1000 Monte Carlo repetitions.

In the upper left corner of Fig. 1, we have shown $\widehat{S}_2^{sm}[k]$ for the four signals averaged over the R=1000 repetitions. From these results, we can not distinguish between the WG and the WNG signals, nor between the LG and the LNG signals.

In the upper right plot of Fig. 1, we have shown $|\widehat{\Gamma}^{\square}[k,l]|$ and $|\widehat{\Gamma}^{sm}[k,l]|$, in the upper and lower triangular PD, respectively, for the WNG signal averaged over all repetitions. As expected, both estimators give a constant magnitude inside the PD, but the unbiasness of $|\widehat{\Gamma}^{sm}[k,l]|$ makes boundary points useful for linearity tests.

Turning to the LNG, shown in the lower left plot of Fig. 1, we find significant deviation from the expected constant magnitude inside the PD in the $|\widehat{\Gamma}^{\square}[k,l]|$ case. For the linearity test the quadratic smoothing in $|\widehat{\Gamma}^{\square}[k,l]|$ clearly contributes to false alarms. Since the variance contribute in a similar way to the Gaussianity test, the false alarm rate will also increase in this test. Introducing the hexagonal smoothing the bias is strongly reduced, as shown for $|\widehat{\Gamma}^{sm}[k,l]|$.

The optimal selection of uncorrelated samples in PD are shown in the lower right plot in Fig. 1, for $|\widehat{\Gamma}^{\square}[k,l]|$ and $|\widehat{\Gamma}^{sm}[k,l]|$ using the LNG signal. This clearly shows that there are more uncorrelated samples for hexagonal smoothing compared to the quadratic smoothing, using the same smoothing bandwidth. Note that the increased frequency resolution in $|\widehat{\Gamma}^{sm}[k,l]|$ is obtained with the classical tradeoff of an increased variance in the estimate.

4.2 Correct false alarm rate

To our knowledge, there exist no valid general variance expressions for HOS estimation for non-Gaussian processes. Without these expressions, there is no way to construct an asymptotic linearity test based on HOS.

To compensate for the lack of variance expressions, we propose to use the method of surrogate data [19]. The surrogate data should retain the dynamics of the original time series and, most im-

portantly, should also fulfill the null hypothesis under study. The classification method then goes as follows: Let Z_0 be the measured discrimination statistic for the original time series. Then calculate the discriminating statistic for the i-th set of the surrogate data Z_i , for $i=1,2,\ldots,N_Z$. For one-sided rejection tests, as will be applied in the Gaussianity and linearity test in this paper, we can reject the null hypothesis at the significance level $\alpha=1/(N_Z+1)$ if the value of Z_0 is above all the surrogate data Z_i .

The random phase (RPH) method [19] is a well known procedure the generates Gaussian (and linear) surrogate data. The RPH surrogate method is easy to implement, it has identical power spectrum as the original data and it works well in most cases [18]. Thus, we propose to use these surrogates to ensure the correct false alarm rate in HOS based Gaussianity tests.

The recently proposed iterative algorithm called the linearly filtered non-Gaussian (LFNG) surrogate method, generates satisfying data for HOS based linearity tests [2]. In contrast to other existing methods for generation of non-Gaussian surrogate data, this method provides surrogate data with almost identical power spectrum and skewness ($\mathbf{E}[x^3[n]]$) as the original time series, while also restricting the surrogate data to be linear. Due to the space considerations this method will not be explained further in this paper, and interested readers can obtain a copy of [2] from the leading author.

4.3 Simplified detection statistic

Since the method of surrogates effectively provides a measure of significance regardless of detection statistic, we instead propose to use the insample mean and variance of all uncorrelated points in PD of $|\widehat{\Gamma}^{sm}[k,l]|$ as our detection statistics for Gaussianity and linearity, respectively. Since $|\widehat{\Gamma}^{sm}[0,0]|$ generally has a significantly higher variance than other points in PD, we ignore this point in our calculation of the insample mean and variance.

These detection statistics mirrors the basic theoretical background of HOS based Gaussianity and linearity test [5, 17, 10], they are easy to implement, and the estimated $|\widehat{\Gamma}^{sm}[k,l]|$ can be used directly to visualize the detection results.

In Table 1, we present the rate of non-Gaussian and non-linear detections using Hinich original tests and our proposed tests on the four previously discussed syntectic time series. The emphasized results clearly show that Hinich's Gaussianity test fail to provide the correct false alarm rate for LG, and that his linearity test has extremely high false rates for both WNG and LNG. The proposed tests have correct false alarm rates in all cases, and they provide a complete non-Gaussian detection of all the WNG and LNG signals.

Time series	D_{NG}^{Hin}	D_{NL}^{Hin}	D_{NG}^{New}	D_{NL}^{New}
WG	4.4	3.6	5.7	5.7
WNG	100	59.0	100	5.6
LG	18.3	3.4	5.9	3.2
LNG	100	70.7	100	6.6

Table 1: Detection rate [%] of non-Gaussian and non-linear classifications using R=1000 synthetic test signals for $\alpha=5\%$. Significant deviation from 5% is expected for detection of non-Gaussianity in WNG and LNG, respectively.

5. EXPERIMENT

As an example application of our tests we have used voltage time series of low-frequency noise from silicon-germanium (SiGe) heterojunction bipolar transistors (HBT). Extensive research in this field (e.g [13, 12]) has been carried out using classical Fourier-based spectral analysis methods by means of specialized hardware, such as the HP-3561A dynamic signal analyzer.

A 0.18-µm SiGe HBT technology was used in this investigation. Details of this technology can be found in [7], and the measurement setup is described in [4]. We have concentrated on the

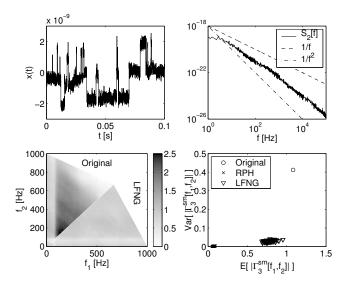


Figure 2: Upper left: First part of time series. Upper right: Power spectrum estimate from HP3561A Dynamic Signal Analyzer. Lower left: $|\widehat{\Gamma}^{sm}[k,l]|$ of original and LFNG surrogate data. Lower right: Detection statistics ($\alpha = 0.01\%$).

smallest HBTs from this technology generation with an emitter area of $0.256\mu\text{m}^2$, biased at $1\mu\text{A}$ base current and $V_{CB} = 0V$.

The first 0.1 seconds of the 30 seconds noise time series is shown in the upper left part of Fig. 2. A typical multilevel Random Telegraph Signal (RTS) is observed, which is characterized by sudden "jumps" between several discrete levels. The time spent at each level is characterized by time constants that can be found as *bumps* at corresponding frequencies (around 50 and 200 Hz) in the power spectrum estimates, as shown in the upper right part of Fig. 2. The spectrum shown here is the averaged periodogram estimate from the HP-3561A.

The physical mechanism behind the RTS noise is believed to be the trapping and de-trapping of carriers by defects. Controversy has been raised whether the traps are independent or not. The lower left part of Fig. 2 shows the skewness function estimate of original noise data, and LFNG surrogate data. We focus on frequencies below 1 kHz because the two main *bumbs* in the spectrum are contained in this frequency range. The surrogate data skewness function has a nearly constant amplitude, while the real data skewness function is clearly non-constant and has a peak below 200 Hz. This indicates coupling between the frequencies in the noise signal, and hence suggests that the traps causing the RTS noise could be coupled and not acting independently.

The lower right plot of Fig. 2 shows the Gaussian and linear detection statistics of the original, RPH and LFNG surrogate data. The strong separation between the original and RPH insample mean, clearly shows that the signal under study is non-Gaussian. Similarly, the distance between the original and the LFNG insample variance strongly indicates that the signal is non-linear.

6. CONCLUSION

Hinich's asymptotic tests for Gaussianity and linearity suffer from severe statistical problems. Thus, any discussion of the power of these tests is useless, and any classification of time series based on Hinich's tests have to be carefully reconsidered.

Using random phase and linearly filtered non-Gaussian surrogate data, the correct false alarm rates are obtained in Gaussianity and linearity tests, respectively.

Unbiased estimation of the skewness function, leads to intuitive and effective detection statistics for Gaussianity and linearity. Results from synthetic and experimental time series clearly demonstrate the applicability of our proposed tests.

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