Asymptotically pivotal statistic for surrogate testing with extended hypothesis

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The method of surrogate data provides a framework for testing observed data against a hierarchy of alternative hypotheses. The aim of applying this method is to exclude the possibility that the data are consistent with simple linear explanations before seeking complex nonlinear causes. However, in recent time the method has attracted considerable criticism, largely as a result of ambiguity about the formation of the underlying null hypotheses, or about the power of the chosen statistic. In this communication we show that by employing a special family of ranks statistics these problems can be avoided and the method of surrogate data placed of a firm statistical foundation.

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Since the framework of surrogate testing [18, 20] was proposed, it rapidly became a popular method to distinguish linear stochastic noise from nonlinear irregular time series, and was widely applied in many fields [11, 12, 15] albeit its intrinsic systematic problems, among which two of the most noticeable ones are: (1) “Wraparound artifact” [2, 14, 19], that is, adopting the Fourier transform to generate surrogates will result in artifact circular autocorrelation function; (2) Inconsistency for the surrogates to represent the null hypothesis [3, 4].

A few remedies were proposed to deal with the problems of (1) and (2). For example, for problem (1), to avoid the Wraparound artifact, the idea of limited phase randomization was suggested [2, 10]. A more elaborate solution (but more computation-intensive meanwhile) was to adopt the method of simulated annealing [17]. For problem (2), to decrease the inconsistency between the surrogates and the null hypothesis, the combination of linear and nonlinear discriminating statistics was recommended [3].

A closer examination on problem (1) and (2) reveals that, both problems are mainly ascribed to the adoption of the Fourier transform. Thus by discarding this technique one may circumvent those problems as well. As an example, a new algorithm was recently devised based on the linear superposition principle [6, 9].

This work is going to expose another important, yet less discussed problem. As pointed out in [20], a pivotal discriminating statistic could increase the accuracy of surrogate testing. Furthermore, with a pivotal statistic, the generated surrogates need not be constrained realizations, this therefore presents another possible strategy to relieve the problem of inconsistency between surrogates and the corresponding hypothesis. Here, a “pivotal statistic” refers to the statistical measure that has the same distribution for all of the processes consistent with a composite null hypothesis [2, 17, 20], where a composite null hypothesis means that the set of the relevant processes is not singleton. As an example, the correlation dimension was shown to be a pivotal test statistic for linear Gaussian noise [16].

Our focus is to derive a test statistic, namely the Wilcoxon signed rank statistic, which will be demonstrated to be pivotal for a family of linear stationary noise, including the linear stationary Gaussian noise considered in [18, 20], and asymptotically pivotal for the summation over realizations of linear stationary noise otherwise. Moreover, we will also show that, under our hypothesis (to be specified later), in general the Wilcoxon statistic will have a known asymptotical distribution (and even exact in certain situations), which is a considerable advantage for statistical inference in surrogate testing [3], in contrast to the popular statistics in the literature (including the correlation dimension), whose distributions are often analytically untraceable due to the complications in their computations.

In this work we confine our discussion to stationary time series as well [18, 19, 20]. Our null hypothesis is to assume that the time series \( \{ x_i \} \) under study is from a general \( p \)-th order linear autoregressive process, i.e.,

\[
x_i = a_0 + \sum_{j=1}^{p} a_j x_{i-j} + \epsilon_i,
\]

with unknown coefficients \( \{ a_i \}_{i=0}^{p} \), regressive order \( p \) and innovation term \( \epsilon_i \). In general, based on the Wold’s decomposition [13] of a stationary stochastic time series, the innovation term in Eq. (11) is shown to be white. In particular, if \( \epsilon_i \) is assumed to follow a Gaussian distribution, then it returns to the scenario considered in [18, 19, 20].

To derive our test statistic, let us first consider a specific family of the innovation terms. We call innovation terms \{ \epsilon_i \} jointly symmetric if there exists a constant \( \mu \) such that \( \{ \epsilon_i - \mu \} \) and \( \{ \mu - \epsilon_i \} \) follow the same joint distribution, i.e., their probability density functions satisfy that \( f(\epsilon_1 - \mu, \epsilon_2 - \mu, ...) = f(\mu - \epsilon_1, \mu - \epsilon_2, ...) \) [1].

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For instance, innovation terms with normal or uniform distributions are jointly symmetric.

For a linear stochastic process \( \{x_t\} \) with jointly symmetric innovation terms, we use an ordinary least square (OLS) predictor

\[
\hat{x}_i^k = a_{i,0} + \sum_{j=1}^{p'} a_{i,j} \hat{x}_i^{k-j} \tag{2}
\]

to obtain the \( k \)-step ahead prediction value \( \hat{x}_i^k \) given the historical record \( \{x_i, x_{i-1}, x_{i-2}, \ldots\} \) up to time index \( i \), where \( \{a_{i,j} : j = 0, 1, \ldots, p'\} \) are the coefficients estimated based on the history (up to time index \( i \)) with the fitting order \( p' \). Consequently, we have the corresponding prediction error \( \hat{e}_i^k = x_{i+k} - \hat{x}_i^k \). And it was proved that the prediction error \( \hat{e}_i^k \) is symmetric about zero, which is independent of the choice of fitting order \( p' \). With this fact, \( \hat{e}_i^k \) and \( -\hat{e}_i^k \) shall share the same distribution so that their probability \( \Pr(\hat{e}_i^k > 0) = \Pr(-\hat{e}_i^k > 0) = \Pr(\hat{e}_i^k < 0) = 1/2 \) (with the assumption that \( \Pr(\hat{e}_i^k = 0) = 0 \) in the sense of Lebesgue measure). Furthermore, let \( I(e_i^k) \) denote the indicator of \( e_i^k \) satisfying that \( I(e_i^k) = 1 \) if \( e_i^k > 0 \) and \( I(e_i^k) = -1 \) otherwise, then it can be shown that \( \{I(e_i^k)\} \) is an independent series.

The signed rank statistic \( SR_m \) can be derived from a set of \( m \) prediction errors \( \{e_i^k \colon i = i_s, \ldots, i_m\} \), where \( \{i_s : j = 1, 2, \ldots, m\} \) are admissible indices for a given time series. Without loss of generality, let us suppose the time indices \( i = 1, 2, \ldots, m \), then a test statistic can be constructed as follows

\[
SR_m = \sum_{i=1}^{m} I(e_i^k) \times S_i(\text{rank}(|e_i^k|)), \tag{3}
\]

where \( \{S_i(\text{rank}(|e_i^k|))\}_{i=1}^{m} \) is the set of scores of \( \{|e_i^k|\}_{i=1}^{m} \) with \( \text{rank}(|e_i^k|) \) denoting the rank of the absolute value \( |e_i^k| \) among the set \( \{|e_i^k|\}_{i=1}^{m} \). In this work we choose \( S_i(\text{rank}(|e_i^k|)) = \text{rank}(|e_i^k|) \) so that the test statistic is reduced to the Wilcoxon signed rank statistic

\[
W_m = \sum_{i=1}^{m} i \times I(e_i^k). \tag{4}
\]

For more detail about the signed rank statistic, the readers are referred to, for example, [3].

In Eq. (3) \( W_m \) is discretely distributed. Theoretically one can enumerate all of its possible values and thus obtain the full knowledge of its distribution. But in practice enumeration will be inefficient for large \( m \). Thus for the sake of convenience, it is suggested to use the Gaussian distribution \( N(0, m(m+1)(2m+1)/6) \) for approximation based on the central limit theorem, as adopted in our work. It was shown that, even for a small integer, say \( m = 6 \), one can still approximate the discrete distribution quite well [3].

The above deduction means that the Wilcoxon signed rank statistic \( W_m \) is a pivotal test statistic for the linear stochastic processes with jointly symmetric innovations. But for a general linear stochastic process, the foregoing conclusion does not necessarily hold because of the possible asymmetry of innovation terms. Nevertheless, we may apply the linear superposition principle, as will be described below, to reduce the asymmetry based on the central limit theorem. Through numerical experiments we will also show that, for nonlinear processes, the summation over its realizations might exhibit different characters from those of linear stochastic ones.

Without lost of generality, let us consider, for example, two linear stochastic time series \( \{x_i\}_{j=0}^{n-1} \) and \( \{x_i\}_{j=k}^{n-1} \) produced by the same process described in Eq. (4), then their summation \( \{y_i\}_{h=0}^{n-1} \equiv \{y_i : y_i = c_1 x_{i+k} + c_2 x_{i+k+h}\}_{h=0}^{n-1} \) for any coefficients \( c_1 \) and \( c_2 \), also follows a linear stochastic process

\[
y_h = (c_1 + c_2)a_0 + \sum_{j=1}^{p} a_j y_{h-j} + (c_1 \epsilon_{s+h} + c_2 \epsilon_{t+h}) \tag{5}
\]

with the innovation terms being \( (c_1 \epsilon_{s+h} + c_2 \epsilon_{t+h}) \). This conclusion can be extended to general situations with, say, \( n \) time series. And then the drift and the innovation term become \( \sum_{i=1}^{n} c_i \epsilon_i \) and \( \sum_{i=1}^{n} \epsilon_i \), where \( c_i \) and \( t_i \) are the coefficient and time index associated with the \( i \)-th time series respectively.

Since the white noise \( \{\epsilon_i\} \) under consideration is considered as an independent [21] sequence with finite variance (because of the stationarity), the central limit theorem is applicable to the summation \( \sum_{i=1}^{n} c_i \epsilon_i \), i.e., one may expect that the distribution of \( \sum_{i=1}^{n} \epsilon_i \) can be approximated by a normal distribution for large \( n \). Therefore, even if originally \( \epsilon_i \) does not have a jointly symmetric distribution, the asymmetry would be reduced by summing over a number of independent variables. Thus the Wilcoxon statistic \( W_m \) is an asymptotically pivotal measure for the summation of a number of linear stochastic time series. In general, depending on the choice of scores in Eq. (3), one may derive a family of asymptotically pivotal test statistics.

In the following we will verify the above idea through few numerical examples, which are: (a) \( ARMA(1,1) \) process \( x_i = 0.1 + 0.5 x_{i-1} + \epsilon_i - 0.5 \epsilon_{i-1} \), where \( \epsilon_i \) follows the normal distribution \( N(0,1) \); (b) \( AR(2) \) process \( x_i = 0.9x_{i-1} - 0.3x_{i-2} + \eta_i \) with \( \eta_i \) following the (asymmetric) beta distribution \( f(x) = (x(1-x))/B(2,5) \), where \( B(2,5) \) denotes the beta function. For comparison of the performance, we also include two nonlinear cases: (c) Henon map \( H(x,y) = (y+1-1.4x^2, 0.3x) \); and (d) Rössler system \( (\dot{x}, \dot{y}, \dot{z}) = (-y-z, x+0.15y, 0.2+z-10x) \), where for both the cases the \( x \) components will be singled out for calculation.

As the first step, we apply the Wilcoxon statistic \( W_m \) to directly examine the above data generation processes (DGP). At this stage, let us test the null hypothesis which assumes that the time series under examination is linear stochastic with jointly symmetric innovations, while later we will extend the hypothesis to a broader range as aforementioned.

For each DGP, the hypothesis testing is conducted 1000 times. Each time a different realization of the same DGP is produced by varying the initial condition(s). Each realization contains 2000 data points, among which
the last 200 points are taken out for out-of-sample one-step ahead prediction based on the OLS predictor in Eq. (2), thus the number of prediction errors \( m = 200 \). Recall that, for a linear stochastic process with symmetric innovation terms, theoretically the fitting order \( p' \) in Eq. (2) does not affect the symmetry of the prediction errors, so in our calculations we do not choose any particular fitting orders, instead we simply set \( p' = 6, 7, 8, 9, 10 \) for all cases. For demonstration, one example of such prediction errors is plotted in Fig. 1 for each DGP \( (p' = 8) \).

Since the distribution of \( W_m \) is known \( (N(0, m(m + 1)(2m + 1)/6)) \), we can specify the false rejection rate \( \alpha \) (i.e., the rate that one falsely rejects the null hypothesis), which is associated with two critical points \( C_{\alpha/2} \) and \( C_{1-\alpha/2} \) for two-sided tests, where in general notation \( C_{\delta} \) denotes the critical point at which the probability function \( Pr(x) \) of a random variable \( x \) satisfies that \( Pr(x \leq C_{\delta}) = \delta \). Therefore if the value of \( W_m \) in a test falls on the interval \( [C_{\alpha/2}, C_{1-\alpha/2}] \), we do not reject the hypothesis, otherwise we reject.

In our calculations, we set \( \alpha = 5\% \) for all cases. Therefore one would expect that, for a process consistent with the null hypothesis, e.g., the ARMA(1,1) process, the actual rejection rate shall be the same as the nominal one 5\% (with slight statistical fluctuations in practice).

But for the processes not consistent with the null, this conclusion is not necessarily true. In fact, as indicated in Table I, the actual rejection rates of the AR(2) process, the Henon map and the Rössler system deviate from the nominal in all cases, therefore we could reject the null hypothesis, which means that those three DGPs cannot be linear stochastic processes with jointly symmetric innovation terms.

Next let us extend the tests to a broader range, i.e., we consider the null hypothesis assuming that the time series is linear stochastic governed by Eq. (1), but now let us remove the assumption of joint symmetry previously imposed on the innovation term \( \epsilon_i \). In general, the prediction errors are not necessarily symmetric, consequently the Wilcoxon statistic might not really follow the expected distribution, thus the actual rejection rates would deviate from the specified one. For example, see the AR(2) process (with the innovation term following the asymmetric beta distribution) demonstrated in Table II.

The above problem could be tackled by instead testing the summations over a number of different realizations of the same underlying process, as discussed previously. In our calculations, 20 realizations are summed over for each test (As before, there are 1000 tests in total). Before the summation each of them is multiplied by a random coefficient uniformly distributed on \([1, 2]\), therefore all of the realizations are nearly equally weighted to prevent over-
dominance of any particular sequence. For comparison, all the other computation settings are simply the same as those adopted at the first step, and the test results are reported in Table I from which we could see that, statistically the tests on the summations do not affect the rejection rate of the ARMA(1, 1) process. However, for the AR(2) process its rejection rates now become very close to the nominal one (with possible statistical fluctuations), which supports our argument. In contrast, the rejection rates of the Henon map and the Rossler system still deviate from the expected one, therefore one could reject the null hypothesis, which means that their realizations are not generated by linear stochastic processes. Again, for demonstration we plot in Fig. 2 the prediction errors of the summations for each DGP ($p' = 8$).

Up to now, we have presented two folds of advantages of the Wilcoxon signed rank statistic derived in this work. One is that, this measure has an explicitly enumerable distribution, therefore one could specify the exact false rejection rate for surrogate testing, which is an unreachable property for many test statistics adopted in the relevant literature. The other is that, this statistic is pivotal for a special family of linear stochastic processes, including the widely studied linear Gaussian noise. Moreover, it also exhibits to be asymptotically pivotal for the summations of realizations of general linear stochastic processes. Because of this property it becomes possible now to extend the null hypothesis of surrogate testing to more general situations.

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