

## Constrained Randomization of Time Series Data

Thomas Schreiber

*Physics Department, University of Wuppertal, D-42097 Wuppertal, Germany*

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A new method is introduced to create artificial time sequences that fulfil given constraints but are random otherwise. Constraints are usually derived from a measured signal for which surrogate data are to be generated. They are fulfilled by minimizing a suitable cost function using simulated annealing. A wide variety of structures can be imposed on the surrogate series, including multivariate, nonlinear, and nonstationary properties. When the linear correlation structure is to be preserved, the new approach avoids certain artifacts generated by Fourier-based randomization schemes. [S0031-9007(98)05488-X]

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Randomization of data and Monte Carlo resampling of probability distributions is a common technique in statistics [1]. In the context of nonlinear time series analysis it has been discussed by several authors and is usually referred to as the *method of surrogate data* [2]. A null hypothesis for the nature of a time series can be tested by comparing the value of an observable  $\gamma$  obtained using the data with values obtained using a collection of *surrogate* time series representing the null hypothesis. All but the simplest null assumptions allow for certain structures, for example, linear serial correlations. There are two distinct ways to implement such structures when creating surrogate series. Traditional bootstrap methods use explicit model equations that have to be extracted from the data. This *typical realizations* approach can be very powerful for the computation of confidence intervals, provided the model equations can be extracted successfully. As discussed in Ref. [3], the alternative approach of *constrained realizations* is more suitable for the purpose of hypothesis testing. It avoids the fitting of model equations by directly imposing the desired structures onto the randomized time series. However, the choice of possible null hypothesis has so far been limited by the difficulty of imposing arbitrary structures on otherwise random sequences. Algorithms exist mainly for the following cases. (1) The null hypothesis of independent random numbers from a fixed but unknown distribution can be tested against permutations without repetition of the data since these conserve the sample distribution exactly. (2) The case of Gaussian noise with arbitrary linear correlations leads to the Fourier transform method. The Fourier transform of the data is multiplied by random phases and then transformed back, conserving the sample periodogram. (See Ref. [4] for the multivariate case.) (3) Surrogates with a given distribution and given linear correlations are needed for the null hypothesis of a monotonically rescaled Gaussian linear stochastic process. This is approximately achieved by the amplitude adjusted Fourier transform (AAFT) algorithm [2] and the more accurate iterative method proposed in Ref. [5].

This paper will introduce a general method for generating random time sequences subject to quite general constraints. Any null hypothesis that leads to a complete set of observables can thus be tested for. All of the above cases can be dealt with (often with higher accuracy), but also multivariate, nonstationary, nonlinear, or other constraints can be implemented. In all of the applications in this paper, the single time probability distribution will be one of the constraints, leading to the requirement that the randomized sequence is a permutation of a fixed collection of values. All other constraints, for example part or all of the lags of the autocorrelation function, will be formulated in terms of a cost function which is then minimized among all possible permutations by the method of simulated annealing.

After giving the actual randomization scheme we will discuss some major applications. We will show that the algorithm yields a more accurate nonlinearity test and avoids known artifacts that are introduced by end effects with ordinary, Fourier-based surrogates [6,7]. We will also give examples with a more general null hypothesis than that of a rescaled stationary linear stochastic process. For these examples, previous methods could not provide appropriate surrogates.

The algorithm is conceptually very simple: (1) Specify constraints  $C_i(\{\tilde{x}_n\}) = 0$  in terms of a *cost function*  $E(\{\tilde{x}_n\})$ , constructed to have a global minimum when the constraint is fulfilled. (2) Minimize  $E(\{\tilde{x}_n\})$  among all permutations  $\{\tilde{x}_n\}$  of a time series  $\{x_n\}$  by simulated annealing. Configurations are updated by exchanging pairs in  $\{\tilde{x}_n\}$ . Examples of its use will be given below.

The simulated annealing method is particularly useful for combinatorial minimization with false minima. It goes back to Metropolis *et al.* [8], and is thoroughly discussed in the literature [9]. Essentially, the cost function is interpreted as an energy in a thermodynamic system. At some finite "temperature"  $T$ , system configurations are visited consecutively with a probability according to the Boltzmann distribution  $e^{-E/T}$  of the canonical ensemble. This is achieved by accepting changes of the configuration with a probability  $p = 1$  if the energy is decreased, ( $\Delta E < 0$ )

and  $p = e^{-\Delta E/T}$  if the energy is increased ( $\Delta E \geq 0$ ). The temperature is decreased slowly, thereby “annealing” the system to the ground state of minimal “energy,” that is, the minimum of the cost function. In the limit  $T \rightarrow 0$ , all ground state configurations can be reached with equal probability. Although some general rigorous convergence results are available, in practical applications of simulated annealing some problem-specific choices have to be made. In particular, apart from the cost function itself, one has to specify a method of updating the configurations and a schedule for lowering the temperature. A way to efficiently reach all permutations by small individual changes is by exchanging randomly chosen (not necessarily close-by) pairs. In many cases, an exchange of two points is reflected in a rather simple update of the cost function. This is important for speed of computation. Many cooling schemes have been discussed in the literature [9]. In this work, the temperature is multiplied by  $\alpha$  at each cooling step. Cooling is done if either the number of successful updates since the last cooling exceeds  $N_{\text{succ}}$ , or the total number of configurations visited during this cooling step exceeds  $N_{\text{total}}$ . It is difficult to give general rules on how to choose  $\alpha$ ,  $N_{\text{succ}}$ , and  $N_{\text{total}}$ . Slow cooling is necessary if the desired accuracy of the constraint is high. It seems reasonable to increase  $N_{\text{succ}}$  and  $N_{\text{total}}$  with the system size, but also with the number of constraints incorporated in the cost function. Generally, one can choose a tolerance for the constraints, start with rather fast cooling, and repeat the analysis with a slower cooling rate if the accuracy has not been met. Other more sophisticated cooling schemes may be suitable depending on the specific situation. The reader is referred to the standard literature [9].

Let us first demonstrate that the algorithm yields more accurate results than previous methods for the most prominent application of surrogate data, which is statistical testing for nonlinearity in a time series. Consider the null hypothesis that there is a sequence  $\{y_n\}$  that has been generated by a Gaussian linear stochastic process. As the only allowed kind of nonlinearity, the actual data  $\{x_n\}$  consists of observations of  $\{y_n\}$  made through a monotone instantaneous measurement function:  $x_n = f(y_n)$ . As discussed, e.g., in Ref. [5], the corresponding Monte Carlo sample has to be constrained to have (i) the same single time probability distribution and (ii) the same sample auto-covariance function [10]

$$C(\tau) = \frac{1}{N - \tau} \sum_{n=\tau}^{N-1} x_n x_{n-\tau} \quad (1)$$

for all lags  $\tau = 0, \dots, N - 1$ . (Zero mean has been imposed for simplicity of notation.)

In the actual test, a nonlinear observable  $\gamma$  is computed for the data and a collection of surrogate data sets. (See Ref. [11] for a comparison of the performance of different statistics  $\gamma$ .) The null hypothesis will be rejected if the result  $\gamma_0$  obtained for the data is incompatible with the probability distribution of  $\gamma$  estimated from the

surrogates. Note that although even different realizations of the same process will have the same sample auto-covariance function only up to statistical fluctuations, it is essential that the surrogates are constrained to  $C(\tau)^{(\text{data})}$  as accurately as possible—since almost every discriminating statistic  $\gamma$  will depend on  $C(\tau)$ , we are otherwise likely to introduce a bias and possibly spurious rejections of the null hypothesis. See also the discussion in Ref. [3].

Previous attempts to implement the above constraints have been only partially successful. In the scheme introduced here, property (i) is easily implemented by considering as candidates for randomized series all permutations of the measured time sequence  $\{y_n\}$ . Requirement (ii) can be achieved by finding a permutation of  $\{y_n\}$  which, within the desired accuracy, minimizes a cost function like the following [12]:

$$E^{(q)} = \left[ \sum_{\tau=0}^{N-1} |C(\tau) - C^{(\text{data})}(\tau)|^q \right]^{1/q}. \quad (2)$$

Provided the annealing scheme is brought to convergence with high accuracy, the known artifacts that remain with previous approaches can be avoided.

As discussed in [5], the original (AAFT) algorithm [2] can show a bias towards a flat spectrum for short sequences. The iterative scheme proposed in [5] removes this bias to a satisfactory approximation for practical work. Let us, however, compare the accuracy of the previously proposed schemes to the present algorithm. For comparability, a cost function is chosen with respect to the time periodic sample auto-covariance function

$$C_p(\tau) = \frac{1}{N} \sum_{n=0}^{N-1} x_n x_{(n-\tau) \bmod N}, \quad (3)$$

which corresponds to the Fourier spectrum through the Wiener-Khinchin theorem. Minimizing  $E_p^{(\infty)} = \max_{\tau=0}^{N/2} |C_p(\tau) - C_p^{(\text{data})}(\tau)|$  will reproduce the auto-covariance  $C_p^{(\text{data})}$  measured on the data. Time series of length  $N = 1000$  are generated by an autoregressive model, but measured using a nonlinear measurement function:  $x_n = y_n^3, y_n = 0.9y_{n-1} + \eta_n$ . The residual maximal deviations of the auto-covariances of the time series and surrogate sets were determined for (i) random permutations of the data, (ii) usual AAFT surrogates [2], (iii) surrogates created with the iterative scheme given in Ref. [5], and (iv) outcomes of the annealing procedure for different cooling protocols. Note that with slower cooling, arbitrarily high accuracy can be reached in principle. Averages over 20 realizations were determined for cases (i) to (iii). The iterative scheme (iii) was repeated until a fixed point was reached which was the case after about 200 iterations. Table I summarizes the results. Computation time on a DEC alpha workstation at 400 MHz clock rate is given only for relative comparison. The price for the superior accuracy of the annealing scheme is its much higher computational cost.

TABLE I. Residual deviation from the desired auto-covariance function for different methods of randomizing time series.

Algorithm	$\alpha$	CPU time	$(N/2)^{-1}E_p^{(\infty)}$
Scramble		...	$0.82 \pm 0.02$
AAFT		0.01 s	$0.08 \pm 0.02$
Iterative		2 s	$0.03 \pm 0.01$
Annealing	0.8	2 m	0.0055
	0.9	25 m	0.0009
	0.98	10 h	0.0003

As mentioned earlier, all previous randomization schemes [2,5] make use of the Fourier transform in order to achieve the desired linear correlation structure. Note, however, that two sequences with the same Fourier amplitudes do not quite have the same auto-covariance function  $C(\tau)$ , Eq. (1). The Wiener-Khinchin theorem says only that the *periodic* sample auto-covariance function  $C_p(\tau)$ , Eq. (3), will be the same. This amounts to assuming that the measured time series is exactly one period of an infinite periodic signal, which is, of course, not what we believe to be the case. The artifact generated by this flaw of previous algorithms has been discussed, e.g., in Ref. [7]. The periodically extended sequence may undergo a phase slip or even a finite jump at  $n = N$ . The surrogate series will have the power contained in that slip spread out over the whole observation time, leading to additional high frequency content. Although spurious results can be partially suppressed by selecting a segment of the data that approximately returns to the initial value, it is desirable to preserve the auto-covariance function  $C(\tau)$  in Eq. (1) rather than  $C_p(\tau)$  in Eq. (3). With the annealing scheme proposed in this paper, this can be easily done by choosing an appropriate cost function.

As an illustration, consider a particular autoregressive process of order two,  $x_n = 1.3x_{n-1} - 0.31x_{n-2} + \eta_n$ . Since it is almost unstable, short realizations often show a large difference between the first and the last point. Periodic continuation turns this difference into a large step with broad frequency content. For a realization of 160 points we found that for a Fourier-based surrogate [method in Ref. [5], same *periodic* auto-covariance function  $C_p(\tau)$ ], the sample autocorrelation  $C(1)/C(0)$  was reduced from 0.92 to 0.85. Consequently, the power in the first differences is increased by a factor of 2 and short term predictability is strongly reduced. This can lead to spurious rejections of the null hypothesis of a linear process. A sequence obtained by minimizing  $E^{(\infty)} = \max_{\tau=0}^{N-1} |C(\tau) - C^{(\text{data})}(\tau)|/\tau$  yielded the correct value of  $C(1)$  within  $2 \times 10^{-4}$ .

Apart from its potential for greater accuracy, the most striking feature of the new scheme is its generality and flexibility. This point will be demonstrated in the following examples which are by no means exhaustive. Note that none of the examples below could be studied with previ-

ous surrogate data schemes. Let us first study a multivariate example, a simultaneous recording of the breath rate and the instantaneous heart rate of a human subject during sleep. (Data set B of the Santa Fe Institute time series contest in 1991 [13], samples 1800–4350.) Regarding the heart rate recording on its own, one easily detects nonlinearity, in particular, an asymmetry under time reversal. An interesting question, however, is how much of this structure can be explained by linear dependence on the breath rate, the breath rate also being non-time-reversible. In order to answer this question, one has to make surrogates that have the same autocorrelation structure, but also the same cross-correlation with respect to the fixed input signal, the breath rate. (Here the breath rate data is not randomized, which is, of course, also possible within this framework.) Accordingly, a constraint is formulated involving all lags up to 500 of the auto-covariance and the cross-covariance ( $C_{xy}$ ) functions. The cost function is taken to be

$$\max_{\tau=0}^{500} \left( \frac{|C(\tau) - C^{(\text{data})}(\tau)|}{\tau} \right) + \max_{\tau=-500}^{500} \left( \frac{|C_{xy}(\tau) - C_{xy}^{(\text{data})}(\tau)|}{|\tau| + 1} \right),$$

other choices are possible. Further suppose that during one minute the equipment spuriously recorded a constant value. In order not to interpret this artifact as structure, the same artifact is generated in the surrogates, simply by excluding these data points from the permutation scheme.

Figure 1 shows the measured breath rate (upper trace) and instantaneous heart rate (middle trace). The lower trace shows a surrogate conserving both, auto- and cross-correlations. The cooling rate was  $\alpha = 0.95$ ,  $N_{\text{succ}} = 10\,000$ ,  $N_{\text{total}} = 3 \times 10^5$ . None of the auto- and cross-covariances differed from the goal by more than  $5 \times 10^{-4}$  in units of the variance of the data after 3 h of annealing.

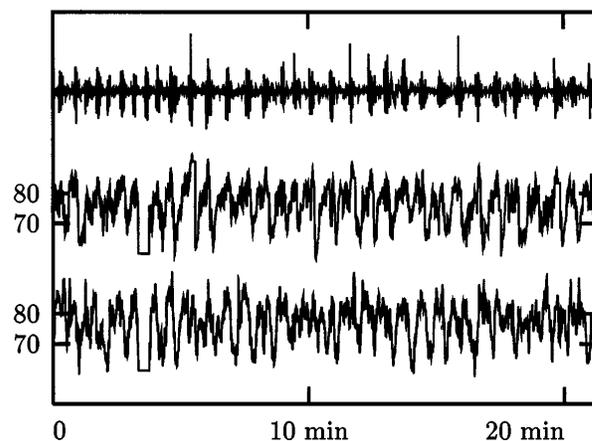


FIG. 1. Simultaneous measurements of breath and heart rates [3], upper and middle traces. Lower trace: a surrogate heart rate series preserving the autocorrelation structure and the cross-correlation to the fixed breath rate series, as well as a gap in the data. Auto- and cross-correlation together seems to explain some, but not all of the structure present in the heart rate series.

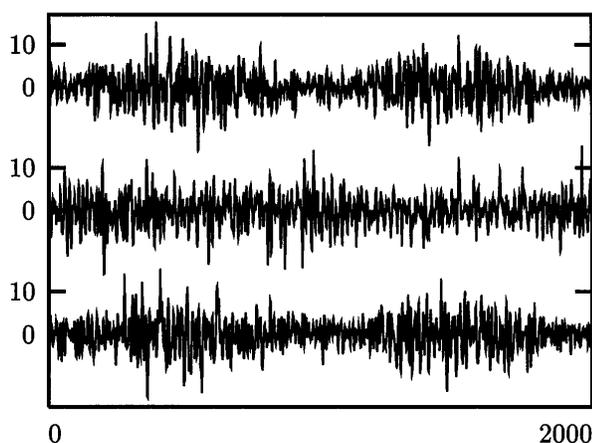


FIG. 2. A realization of a linear process with time dependent variance (upper), a usual AAFT surrogate (middle), and a surrogate with the same autocorrelations and the same running variance as the original series.

(DEC alpha workstation at 400 MHz clock rate.) The visual impression from Fig. 1 is that while the linear cross-correlation with the breath rate explains the cyclic structure of the heart rate data, other features remain unexplained. In particular, the surrogates don't show the asymmetry under time seen in the data. Possible explanations of the remaining structure include artifacts due to the peculiar way of deriving heart rate from interbeat intervals, nonlinear coupling to the breath activity, nonlinearity in the cardiac system, and others.

Let us finally give a nonstationary example, an AR(2) process with periodically modulated variance:  $x_n = 1.6x_{n-1} - 0.8x_{n-2} + b_n\eta_n$  with  $b_n = 1 + \sin^2 2\pi n/1000$ . In Fig. 2 a realization ( $N = 2000$ ) is shown together with two surrogate series. The first (middle trace) has been generated by the AAFT algorithm, the second (lower trace) has been generated by the annealing scheme to preserve the first 100 lags of  $C(\tau)$ , but also the running variance in blocks of length 200, overlapping by 100.

In this paper it has been demonstrated that randomization under a wide variety of constraints can be achieved with a permutation scheme that minimizes a suitable cost function using simulated annealing. The approach is very general. Constraints are not restricted to linear correlations. Multivariate, nonlinear, but also time dependent, nonstationary properties can be easily implemented.

Resampling with constraints is the method of choice for hypothesis testing, where it is preferable to parametric bootstrap methods. Although a general, nonparametric resampling scheme has been introduced in this paper, care has to be taken when similar ideas are to be exploited for the determination of error bounds. The variance of statistical estimators usually depends on the constraints

imposed. To which extent reliable error distributions can be obtained by selecting a minimal set of constraints and using resampling with replacement will be a subject of future work.

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  - [10] Strictly speaking, the two constraints overspecify the problem. There are at most finitely many solutions  $\{x'_n\}$ , including the original sequence and the time reversed sequence  $\{x_{N-n-1}\}$ . However, we will not usually find the absolute minimum, or otherwise we could penalize similarity to the original sequence.
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  - [12] In principle, any function that has a global minimum at  $C(\tau) \equiv C^{(\text{data})}(\tau)$  can be used. In most cases we found good convergence using  $E^{(q)}$  at  $q = 1$ ,  $q = 2$ , or  $q = \infty$ . ( $E^{(\infty)}$  simply picks the maximal deviation.) For highly correlated sequences we found it advantageous to enhance the convergence at small lags by weighting the terms in the cost function by  $1/\tau$ . Some structures are rather difficult to build up by interchanging arbitrary pairs. Different weights in the cost function can help, but also alternative updating schemes are possible.
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