Surrogate for nonlinear time series analysis

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We present a surrogate for use in nonlinear time series analysis. This surrogate algorithm has significant advantages over the most commonly used surrogates, in that it provides a more robust statistical test by producing an entire population of surrogates that are consistent with the null hypothesis. We will show that for the currently used surrogate algorithms, although individual surrogate files are consistent with the null hypothesis the population of surrogates generated is not. The surrogate is tested on a linear stochastic process and a continuous nonlinear system.

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I. INTRODUCTION

Performing statistical analysis on experimental data from nonlinear systems often involves testing a null hypothesis based on some nonlinear measure. Whether the measure in question is a traditional nonlinear measure such as the correlation dimension [1,2] or the Lyapunov exponent [3,4] or is an experimentally motivated measure like the frequency of encounters with unstable periodic orbits [5,6], surrogate data is usually required to perform the test. The probability distributions of the statistical measures are typically not known *a priori* and often depend in very complex ways on various statistical properties of the data. By using surrogate data we can determine these distributions empirically.

The most commonly used techniques for generating surrogate data for the statistical analysis of nonlinear processes include random shuffling of the original time series, Fourier-transformed surrogates [7], amplitude adjusted Fourier-transformed (AAFT) surrogates [8], and iterated AAFT surrogates [9]. Each of these methods has strengths and weaknesses with respect to the power of the null hypothesis that can be rejected, the computational complexity of the algorithm and the accuracy with which the method models the statistical properties of the data being analyzed.

In this paper we will discuss the difficulties and limitations of the simplest of these methods, the shuffled and AAFT surrogates, and how the iterated AAFT surrogate attempts to resolve these issues. We will then discuss some difficulties that have not been resolved with the implementation of these surrogates. Finally, we present a surrogate that addresses these problems.

A. Shuffled surrogates

The simplest algorithm for generating surrogate data is random shuffling. A random permutation of the original data file is made. All of the original data are included in a completely random order. This method guarantees that the surrogate data will be consistent with the null hypothesis of a δ-correlated random process, while exactly preserving the distribution of the original data. This algorithm is of limited usefulness because the only statistical property of the original data that is preserved is the distribution. For example, Theiler *et al.* showed that shuffled surrogates are unsuitable for a nonlinearity test based on calculations of the correlation dimension [7].

B. Fourier-transformed surrogates

Theiler *et al.* went on to describe an algorithm for testing the null hypothesis of a linear stochastic process that can be applied to data that is normally distributed. This method takes the discrete Fourier transform of the original data and then assigns a random phase to each positive frequency component. The negative frequency components are assigned corresponding phases to assure that the inverse Fourier transform will be real. The result is a time series with the same power spectrum as the original data, but which is in every other respect randomized.

C. Amplitude adjusted Fourier-transformed surrogates

The preceding method is not suitable when the original data is not normally distributed, since the Fourier-transformed surrogate will then have a different distribution from the original data. The AAFT surrogate was developed to resolve this limitation [9]. These surrogates attempt to test the null hypothesis that the original data is from a linear stochastic process that has undergone a static nonlinear transformation. The algorithm for generating this type of surrogate data is described as follows:

(1) The original data is rescaled to a normal distribution. This is done by generating a time series of Gaussian white noise and sorting it according to the ranking of the original data.

(2) A Fourier-transformed surrogate of the rescaled data is constructed.

(3) The final surrogate is scaled to the distribution of the original data by sorting the original data according to the ranking of the Fourier-transformed surrogate.

This algorithm guarantees that the distribution will be preserved and approximately preserves the power spectrum as well. The ability of this algorithm to properly preserve the

power spectrum depends on the existence of a continuous static transformation from the original distribution to a normal distribution. In theory this is a requirement on the data itself, i.e., the data distribution must be continuous. If the data distribution includes singularities or sharp transitions, then the algorithm could produce unpredictable results. In practice an additional limitation is noted. Since the underlying distribution of the original data is, in general, unknown, the transformation must be determined empirically. The rescaling in step 1 constitutes an empirical transformation from the distribution of the original data to that of a specific finite realization of a Gaussian distributed process. The rescaling in step 3 then transforms from an independent realization of a different Gaussian distributed process back to the original data distribution. The forward and backward transformations are not exact inverses of each other, and this results in changes to the power spectrum of the final surrogate. The result of this alteration is to whiten the power spectrum of the original data [9]. Of course the amount of whitening that occurs depends on both the length of the time series (for long time series the distribution will be very nearly continuous, reducing the effect) and on the degree to which the original distribution is non-Gaussian.

D. Iterated AAFT surrogates

A method was developed by Schreiber and Schmitz [9] that addresses the issue of power spectrum whitening by performing a series of iterations in which the power spectrum of an AAFT surrogate is adjusted back to that of the original data before the distribution is rescaled back to that of the original data. The process can be described as follows:

(1) An AAFT surrogate is generated using the procedure above. The Fourier amplitudes calculated in step 2 are recorded for later use.

(2) The surrogate is Fourier transformed, and its Fourier amplitudes are adjusted back to the amplitudes recorded in step 1.

(3) The result of step 2 is inverse Fourier transformed and rescaled back to the original data distribution as in step 3 of the AAFT algorithm.

(4) Steps 2 and 3 are repeated until the whitening of the power spectrum is sufficiently small.

The basic assumptions of this method are that, with each iteration, the change to the distribution that occurs when the Fourier amplitudes are adjusted will be smaller than in the previous iteration, and that the alteration of the power spectrum when the rescaling is performed will therefore also be smaller than in the previous iteration. In fact, Schreiber showed that, for a nonlinearly transformed autoregression process, the iteration procedure will converge towards the power spectrum of the original data until a saturation point is reached, where the Fourier amplitude adjustment is so small that the rescaling puts the data into the exact order it had before the amplitude adjustment [9].

II. DIFFICULTIES WITH CURRENT ALGORITHMS

As mentioned previously, for surrogate data to be used to properly test a null hypothesis, it is necessary that the surrogate data be consistent with the null hypothesis. It is clear that by preserving the distribution and power spectrum of the original data while randomizing the data in all other respects, a surrogate file generated by the iterated AAFT algorithm will be consistent with the null hypothesis that the data were drawn from a nonlinear static transformation of a linear stochastic process. But in order to reject a null hypothesis, it is not sufficient for each surrogate file to individually satisfy the null hypothesis. The entire population of surrogates must satisfy the null hypothesis. In this case, this means that all the surrogates must be statistically independent realizations of a nonlinear static transformation of a linear stochastic process.

The iterated AAFT surrogates do not satisfy this requirement. A set of statistically independent realizations of a nonlinear static transformation of a linear stochastic process will all have slightly different power spectra. Given a power spectrum estimate P_k where k is the frequency bin, the variance of P_k over the set of surrogates is given by

$$\sigma_k^2 = P_k^2 . \tag{1}$$

That is, the variation in the power from one file to the next in any given frequency bin is equal to the square of the amount of power in that frequency bin [10]. It is because of this high variance that power spectra are typically averaged over several frequency bins, sacrificing frequency resolution for a more accurate power spectrum estimate. Equation (1) becomes

$$\sigma_i^2 = \frac{1}{N} P_i^2 , \tag{2}$$

where N is the number of frequency bins averaged and i denotes the new larger frequency bins.

The iterated AAFT surrogates will produce populations that, by construction, all have exactly the same power spectrum estimates. These populations of surrogates are therefore not consistent with the null hypothesis. It is clear that this issue can result in erroneous results for statistical tests. If the measured statistic being analyzed is sensitive to variations in the power spectrum of the data, then it is likely that the variance of the statistic will be much smaller for the population of surrogates than it would be if the null hypothesis were actually true, resulting in a false-positive statistic. This effect has been demonstrated in a recent paper by Kugiumtzis [11], where the very small variance in power spectra for the AAFT and iterated AAFT surrogates results in false rejections using a nonlinear predictor statistic. This difficulty with spectral variance of surrogate data has also been discussed by Schreiber and Schmitz in a recent review article [12].

A. Digitally filtered shuffled surrogates

We will now present a surrogate algorithm that resolves the issues described above. This algorithm, which we will refer to as the digitally filtered, shuffled (DFS) surrogate algorithm, convolves a random permutation of the data with a response function based on the estimated power spectrum of the data. Since each surrogate is made from a different ran-

dom permutation, each is by construction a statistically independent realization of the process. The procedure for generating DFS surrogates is as follows:

(1) Estimate the power spectrum of the data using overlapping windowed Fourier transforms. The data should be demeaned for this calculation.

(2) Calculate a response function by taking the square root of the power spectrum estimate and taking its inverse Fourier transform.

(3) Make a random permutation of the data (a shuffled surrogate as described in Sec. I A above).

(4) Digitally filter the shuffled surrogate by convolving it with the response function. The shuffled surrogate should be demeaned before filtering.

(5) Rescale the filtered surrogate back to the original data distribution. The rescaling can be done as for the AAFT surrogates.

By using an overlapping windowed Fourier transform to estimate the power spectrum, the accuracy of the estimate can be greatly improved. This is done by calculating the Fourier transform of N samples of length L, each overlapping by 50% [13]. These samples are multiplied by a windowing function such as the Welch window [14]. Any other favorite windowing function may be substituted for the Welch function.

$$w_i = 1 - \left(\frac{2i - (L-1)}{(L+1)} \right)^2, \tag{3}$$

where i ranges from 0 to $L-1$. This windowing function goes to zero at both ends, reducing any high-frequency artifacts due to lack of periodicity. The power spectrum estimate made with this technique will thus have a variance given by

$$\sigma_i^2 = \frac{11}{9N} P_i^2 . \tag{4}$$

Because a demeaned, shuffled surrogate has a white power spectrum, the convolution with the response function will result in a time series with the appropriate power spectrum. This also allows variations in the power spectrum from one surrogate to the next, since each surrogate is made from a statistically independent shuffled surrogate.

B. Rescaling and power spectrum whitening

As with the AAFT surrogates, the process of rescaling to the original data distribution alters the power spectrum. An iterated method, similar to what is used for the iterated AAFT surrogates, can be used to reduce the whitening. The procedure for this is to adjust repeatedly the Fourier amplitudes and subsequently to rescale the result. The amplitudes to which we should adjust are not the Fourier amplitudes of the original data, but instead of the surrogate just before the first rescaling (step 4).

III. COMPARISON OF METHODS

To demonstrate that the DFS algorithm is properly preserving the linear properties of the data we will initially look

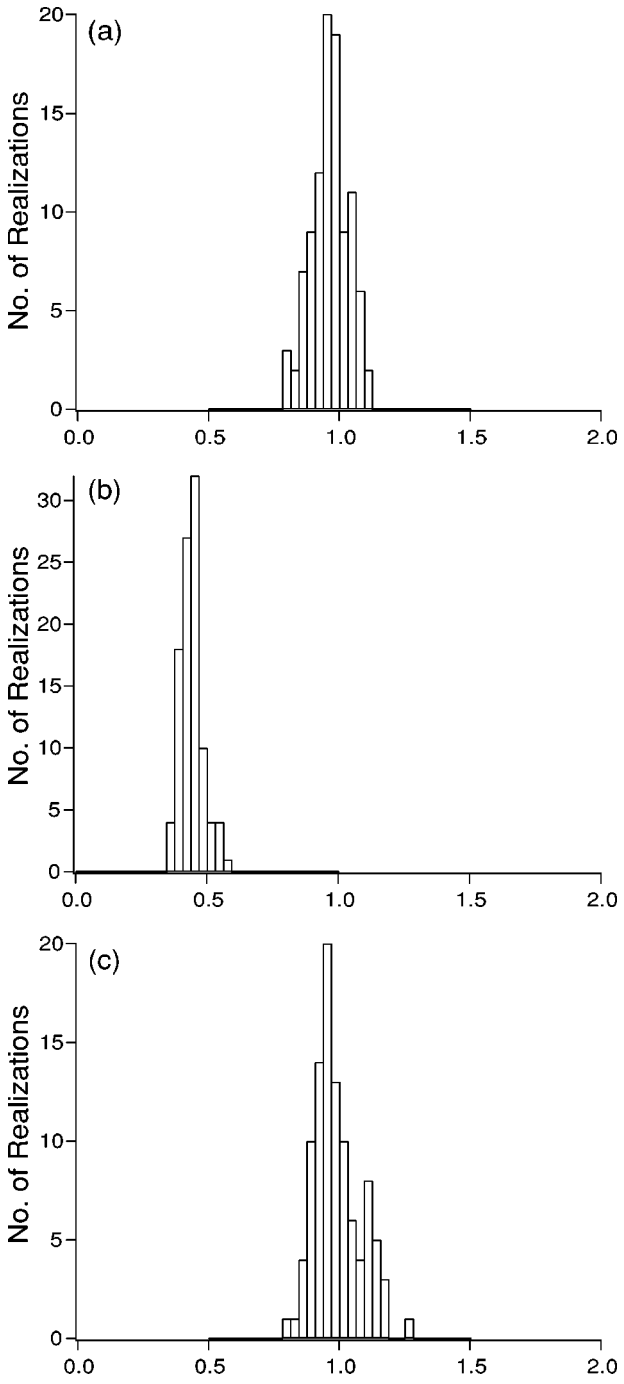

FIG. 1. Histograms of the measure α for the DFS surrogates (a), AAFT surrogates (b), and 100 realizations of the actual AR process (c).

at a simple nonlinearly transformed autoregression (AR) process,

$$x_{n+1} = 0.7 x_n + \xi_n ,$$

$$y_n = x_n^3 , \tag{5}$$

where ξ_n is Gaussian white noise.

First we will establish that the DFS algorithm is producing the proper degree of variability from one surrogate file to

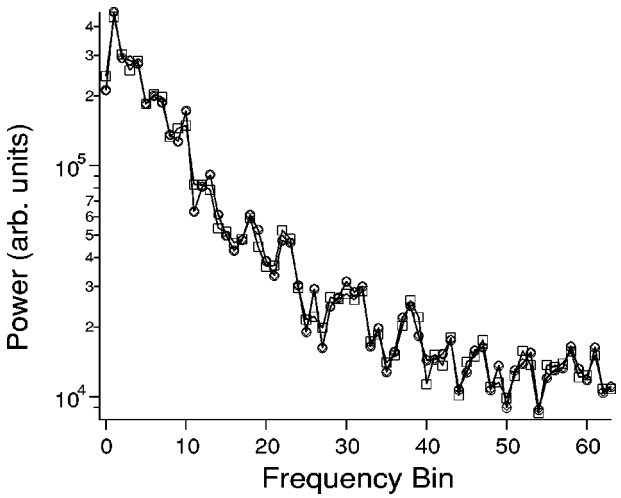

FIG. 2. Power spectrum estimate of the AR process (circles), DFS surrogates (squares), and AAFT surrogates (diamonds). A log scale was used to show variations more precisely. Sixty-four frequency bins were used to average out statistical fluctuations.

the next. To do this we generate a time series from the above AR process of length 2048 points. We then generate a population of 100 DFS surrogates. Next we introduce the following measure of spectral variability:

$$\alpha = \frac{1}{N} \sum_{i=1}^{N} \frac{(P_i - \overline{P}_i)^2}{\overline{P}_i^2}, \tag{6}$$

where N is the number of frequency bins (in this case 1025), P_i is the power in the ith frequency bin of the surrogate, and $\overline{P}_i$ is the average power in the ith frequency bin, averaged over the other 99 surrogate files. This yields a value of α for each surrogate.

If our hypothesis that each surrogate is an independent realization of the same process is true, then we can predict the following:

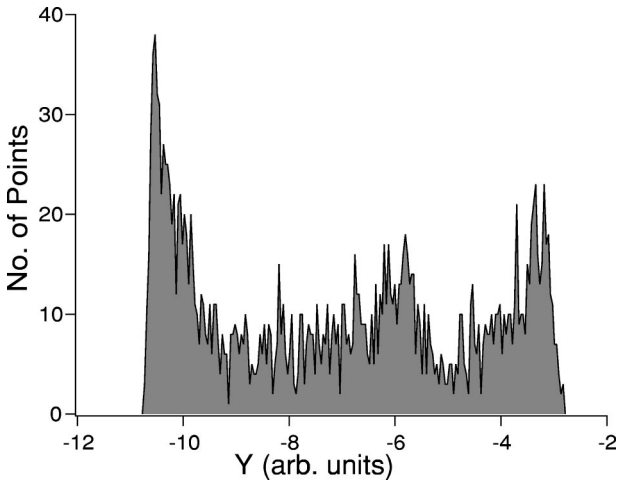

FIG. 3. Distribution of Rössler section data: Note the highly non-Gaussian, multimodal distribution.

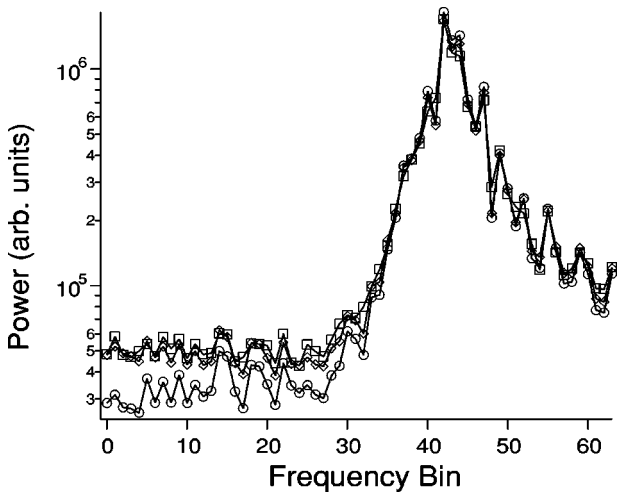

FIG. 4. Power spectra of the original Rössler section data (circles), DFS surrogates (squares), and AAFT surrogates (diamonds). Note the significant systematic increase in power at the lower frequencies due to the power spectrum whitening effect.

$$\langle (P_i - \overline{P}_i)^2 \rangle = \overline{P}_i^2, \tag{7}$$

which implies that the expectation value of α should be 1. Figure 1(a) shows the distribution of α for the 100 DFS surrogates. Figure 1(b) shows the distribution for 100 AAFT surrogates, and Fig. 1(c) shows the measure α for 100 independent realizations of the actual AR process as a control example.

We can see from Fig. 1 that the DFS surrogates preserve the appropriate degree of variability between surrogates whereas the AAFT surrogates show a much lower degree of variability. In fact, it is clear from the description of the AAFT algorithm that the only reason α is not zero for all of the AAFT files is that the whitening effect described above introduces a small amount of variability.

This suggests the question, how well have the AAFT and DFS surrogate algorithms preserved the power spectrum of the data? We have calculated the power spectrum of the original AR data, as well as the spectra of the AAFT and DFS surrogates. The results are shown in Fig. 2.

We see that both surrogates properly preserve the power spectrum of this data. Although the power spectrum whitening effect due to the rescaling is nonzero for this data, it is insignificant. This is not always the case though, particularly when the data is strongly non-Gaussian.

To demonstrate the iterated version of the DFS algorithm, we look at a classic nonlinear system, the Rössler system [15].

$$\dot{x} = -(y+z),$$

$$\dot{y} = x + ay,$$

$$\dot{z} = b + z(x-c) + \sqrt{2D}\xi(t), \tag{8}$$

where $a = b = 0.2$, $c = 5.7$. Dynamical noise was also added, where $\xi(t)$ is Gaussian white noise with zero mean and unit

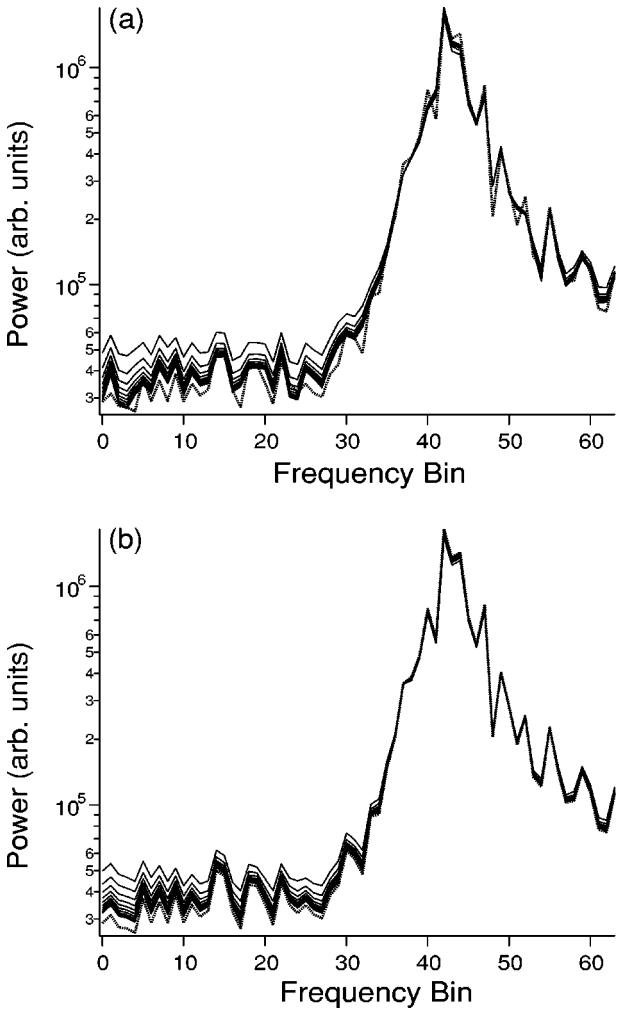

FIG. 5. Power spectra for iterated DFS surrogates (a) and iterated AAFT surrogates (b). The dotted line represents the power of the actual data, and the solid lines show consecutive iterations of the surrogate algorithms.

variance, and the intensity $D=0.01$. The Rössler system is chaotic for these parameter values. A Poincaré section of this data was made by measuring y at every positive zero crossing of x. Such, 2048 crossings were recorded. Figure 3 shows the distribution of this data.

Once again 100 surrogates of both the DFS and AAFT-type were made. Figure 4 shows the power spectrum of the surrogates compared to that of the original data. In this case the whitening due to the rescaling is not negligible. We therefore apply the iterated technique described above. Figure 5 shows the spectra of ten iterations of the DFS and AAFT algorithms. Note that both surrogates converge towards the proper spectrum at approximately the same rate.

This demonstrates that the iterated version of the DFS algorithm can compensate for the power spectrum whitening caused by the rescaling. But what effect has this iterated process had on the variability of the surrogates? We now apply the measure defined in Eq. (6) to each iteration of the surrogate process. Figure 6 shows the results of this analysis.

The iterated DFS algorithm preserves the proper variability throughout the iteration process. As we would expect, the variability of the AAFT surrogates goes to zero as we iterate, since the variability is entirely due to the whitening in this case.

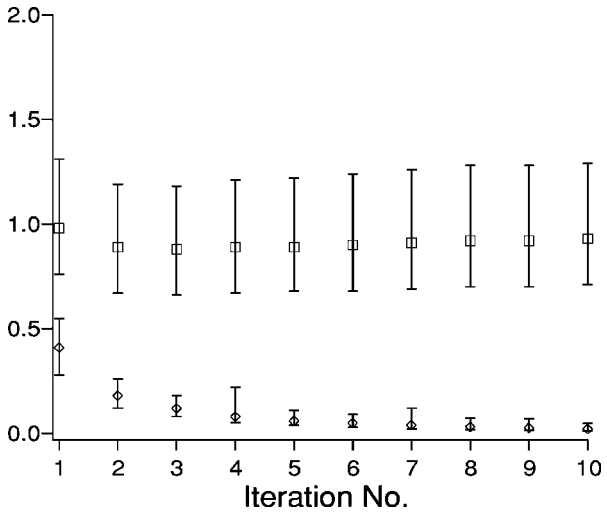

FIG. 6. The variability measure α for each iteration of the DFS (squares) and AAFT (diamonds) algorithms. The error bars represent the 99% confidence interval given by the smallest and largest values of α for each iteration.

IV. DISCUSSION

We have clearly shown that the AAFT and iterated AAFT algorithms do not properly test the null hypothesis of a nonlinear static transformation of a linear stochastic process. The DFS surrogate algorithm described herein has been demonstrated not only to preserve the power spectrum of the original data as well as the AAFT algorithm, but also to produce the appropriate intersurrogate variability. Likewise the iterated DFS algorithm converges to the proper spectrum just as quickly as the iterated AAFT algorithms, but without sacrificing its variability properties. For statistical tests in which the variability of the power spectra estimates is not a significant factor, the AAFT methods can still produce statistically meaningful results. But in general, to formally reject the null hypothesis described above, the AAFT surrogates are not sufficient.

It should further be noted that the computational complexity of the DFS and the iterated DFS algorithms are about the same as that of the AAFT and iterated AAFT algorithms. This algorithm can also be modified to operate in the time domain, which may be more efficient for data streams that are much longer than the required frequency resolution.

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