

Reduction of noise of large amplitude through adaptive neighborhoods

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We propose a noise reduction algorithm based on adaptive neighborhood selection that is able to obtain high levels of noise reduction for chaotic vector time series corrupted by observational noises with a noise-to-signal ratio of up to 300%.

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I. INTRODUCTION

This research treats the noise reduction of vector chaotic time series corrupted by observational noise of large amplitude. The aim is to isolate the deterministic component of the signal. The goal is more than merely detecting chaos. A totally or partially cleaned signal can be used for accurate short-term forecasting of its deterministic component and to improve the forecasting of its probable long-term behavior.

Early research on noise reduction [1–8] was based on local linear estimations of the unknown dynamics using least-squares methods. The algorithms proposed in these papers showed the possibility of separating the signal from the noise for time series of large lengths and low or moderate noise amplitudes. These algorithms have two intrinsic limitations that can be insubstantial for noises of small amplitude but which may be crucial for the analysis of chaotic time series corrupted by noises of moderate or large amplitudes:

(i) The inaccuracy of the least-squares method in the local estimation of the dynamics was recognized already in the early literature on noise reduction [7,9]. All the nonparametric algorithms were, however, based on this method.

(ii) All noise reduction algorithms use an iterative procedure that takes the output of the algorithm as the input in the next iteration. If the method is to be efficient, there must be a significant difference between the noise levels of the outputs of the first and the final iterations. For time series corrupted by noises of large amplitude, the neighborhoods used in estimating the local dynamics in the early iterations must contain a significant fraction of the data points, whereas in the final iterations the use of big neighborhoods is clearly inappropriate due to the errors caused by nonlinearities. In order to design an efficient algorithm, it is crucial to have efficient criteria for determining the optimal sizes of the neighborhoods to be used in the local estimations of the dynamics at each iteration.

Issue (i) above was addressed in our previous paper [10] using the theory of *measurement error models* [11]. This theory gives unbiased and consistent estimators which, for Gaussian errors, are those of maximum likelihood. Such estimators can be regarded as a local linear projection onto an optimal linear subspace, with respect to a metric that incorporates the information contained in the error covariance matrix. Judd [12] pointed out the failure of the maximum like-

lihood methods to identify the true trajectory of a chaotic dynamical system specially in the case of large noise. Judd also observed that the residuals present too many outliers and in general their distribution is not consistent with the original distribution of the noise. Our results confirm such observation; the kurtosis of the residuals are considerably higher than the given by the Gaussian distribution. We overcome this difficulty through an smoothing device based on averaging multiple estimations of the value of each clean data point.

In this paper we address the issue of overcoming the basic limitation (ii) pointed out above. Our adaptive neighborhoods technique is based on a statistical test with null computational cost. At a given iteration, it determines from the properties and level of the remaining noise a single uniform size and shape for the neighborhoods of all data points. The criterion used for determining the neighborhoods is to keep their sizes as small as possible while guaranteeing, with a given confidence level, that the relevant information is contained in the neighborhoods. As the number of iterations increases, the noise level decreases and the sizes of the neighborhoods reduce accordingly, thus minimizing the errors due to nonlinearity. Another issue addressed when constructing the neighborhoods is that of determining their optimal shapes. Our algorithm is designed for vector time series and if the degree of uncertainty in the observed state variables is different then the appropriate neighborhoods will be non-spherical. They should be instead ellipsoids for which the semiaxial lengths are related to the uncertainties in the corresponding coordinates.

The results that we obtain with our algorithm are good for noises of small and medium amplitudes. Furthermore they are remarkable for short length time series corrupted by noises of large amplitude: we obtain a noise reduction of up to 84% for a Henon time series of only 500 data points with a 300% noise-to-signal ratio. Such a result is achieved because the algorithm takes full advantage of the heteroskedasticity of the noise (the noise-to-signal ratio is 10% in the first component and 300% in the second component of the time series). The lower level of uncertainty in the first coordinate allows noise reduction in the second coordinate out of reach for existing algorithms, which have until now not been used to analyze chaotic noisy time series with noise-to-signal ratios in such a large range.

Kern *et al.* [13] also proposed an adaptive neighborhood criterion. At each iteration and for each point, they take neighborhoods of different sizes and choose that which optimizes the quality of the best linear fit to the local dynamics. They showed their method to be advantageous only in the

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case of noises of medium amplitudes, but for noises of small or large amplitudes, they do not find justified the high computational cost required.

Efficient noise reduction algorithms based also on local linear projections into optimal linear subspaces are those developed for speech enhancement. The method consists of minimizing the signal distortion while the residual noise energy is maintained below some given threshold [14–16]. For this type of time series, almost periodic, a method for the automatic detection of the best neighborhood size, based on recurrence plots, is the given in [17].

The paper is organized as follows. In Sec. II we describe our algorithm, focusing attention on the local linear estimation of the dynamics using the theory of measurement error models and on the adaptive neighborhoods method. Section III presents some results obtained by our algorithm for Henon and Lorenz time series corrupted by noises of large noise-to-signal ratio.

II. ALGORITHM

We assume that the observed time series $\{\mathbf{X}_i, i=1, \dots, N\} \subset \mathbb{R}^d$ is the sum of an unknown deterministic time series $\{\mathbf{s}_i, i=1, \dots, N\}$ and an unknown stochastic time series $\{\mathbf{e}_i, i=1, \dots, N\}$, where \mathbf{e}_i are independent and identically distributed (i.i.d.) random variables with null mean. Then $\mathbf{X}_i = \mathbf{s}_i + \mathbf{e}_i$, $1 \leq i \leq N$, and $\mathbf{s}_{i+1} = f(\mathbf{s}_i)$, where $f: M \subset \mathbb{R}^d \rightarrow M$ is an unknown smooth chaotic dynamics. The aim of noise reduction algorithms is the separation of the deterministic component of the time series from the observational noise.

The noise level in the j th component of the observed time series is given by the noise-to-signal ratio

$$(R_{NS})_j := \sqrt{\frac{\sum_{i=1}^N [(\mathbf{e}_i)_j]^2}{\sum_{i=1}^N [(\mathbf{s}_i)_j]^2}}, \quad j = 1, \dots, d, \quad (1)$$

where $(\mathbf{s}_i)_j$ and $(\mathbf{e}_i)_j$ denote the j th components of \mathbf{s}_i and \mathbf{e}_i respectively. We denote by \mathbf{R}_{NS} the vector whose components are $(R_{NS})_j, j=1, \dots, d$.

The algorithm we design takes as input data the vector time series $\{\mathbf{X}_i, i=1, \dots, N\}$ instead of a scalar time series as do most existing noise reduction algorithms.

A. Local estimations of the dynamics and noise reduction

The principal technique used in noise reduction algorithms is local orthogonal projection of the data on optimal linear subspaces, which is equivalent to finding the best local linear estimations of the unknown dynamics. This technique is also used in the forecasting problem, for the estimation of the Lyapunov spectrum [18,19], and for the estimation from a time series of the degrees of freedom of a dynamical system [20].

Let \mathbf{s}_i be any point of the clean time series and let U_i be a small neighborhood of \mathbf{s}_i . Since f is a differentiable dynamics,

$$f(\mathbf{s}) - f(\mathbf{s}_i) \approx Df(\mathbf{s}_i)(\mathbf{s} - \mathbf{s}_i), \quad \text{for } \mathbf{s} \in U_i,$$

where $Df(\mathbf{s}_i)$ is the tangent map of f at \mathbf{s}_i . The tangent space $\mathbf{y} = f(\mathbf{s}_i) + Df(\mathbf{s}_i)(\mathbf{s} - \mathbf{s}_i)$ is the best d -dimensional linear sub-

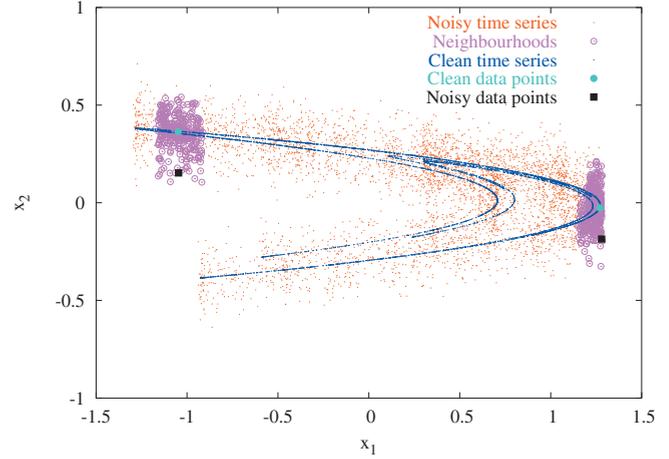


FIG. 1. (Color) Confidence ellipsoids for $\alpha_0=0.1$ at two points of a Henon time series with $N=5000$ data points corrupted by Gaussian noise with noise level $\mathbf{R}_{NS}=(1\%, 40\%)$. Observe the difference between the clean (blue circles) and the noisy data (black squares) at which the neighborhood is constructed and the convenience of taking the best linear subspaces through the mean points of the neighborhoods instead of taking them through the observed noisy points.

space of \mathbb{R}^{2d} through $(\mathbf{s}_i, f(\mathbf{s}_i))$ for the data points $\{(\mathbf{s}, f(\mathbf{s})), \text{for } \mathbf{s} \in U_i\}$. Such data points are arbitrarily close to this tangent space when the size of U_i is sufficiently small. In [21], it is shown how to estimate $Df(\mathbf{s}_i)$ from a time series and what are the conditions guaranteeing that such estimations converge to the tangent map.

The effect of the noise is to separate the observed data points from the tangent spaces. Then the noise can be partially removed by projecting the observed data points on the best d -dimensional linear subspaces through $(\langle \mathbf{X}_i \rangle, \langle \mathbf{X}_{i+1} \rangle)$, where $\langle \mathbf{X}_i \rangle = \frac{1}{\#U_i} \sum_{\mathbf{X}_j \in U_i} \mathbf{X}_j$, $\#U_i$ denotes the number of points within U_i , and U_i is now a small neighborhood of \mathbf{X}_i . Since the errors have null mean, the point $(\langle \mathbf{X}_i \rangle, \langle \mathbf{X}_{i+1} \rangle)$ is likely to be closer to $(\mathbf{s}_i, \mathbf{s}_{i+1})$ than the point $(\mathbf{X}_i, \mathbf{X}_{i+1})$ is and it is better to seek the best linear subspace through $(\langle \mathbf{X}_i \rangle, \langle \mathbf{X}_{i+1} \rangle)$ rather than that through $(\mathbf{X}_i, \mathbf{X}_{i+1})$ (see Fig. 1).

A fact to be considered is that the unknown dynamics is chaotic. Then a small ball B_i centered at \mathbf{s}_i is mapped by f onto an ellipsoid centered at \mathbf{s}_{i+1} with the principal axes oriented in the directions of the unstable manifold at \mathbf{s}_i . Therefore a local estimation of f based on the data points $(\mathbf{X}_j - \langle \mathbf{X}_i \rangle, \mathbf{X}_{j+1} - \langle \mathbf{X}_{i+1} \rangle)$, for $\mathbf{X}_j \in U_i$, is likely to be good on the unstable manifold and poor on the stable manifold. Reciprocally the ball B_i is mapped by f^{-1} onto an ellipsoid centered at \mathbf{s}_{i-1} and with the principal axes oriented in the directions of the stable manifold at \mathbf{s}_i . This indicates that in order to obtain good estimations of the clean values of the time series using local estimations of the dynamics, we should incorporate information about the past, the present, and the future as was already pointed out by Grassberger *et al.* [3].

This is done by taking the best d -dimensional linear subspace \mathbf{T}_i (according to a criterion described below) for the data points $\{\mathbf{Z}_j - \langle \mathbf{Z}_i \rangle : \mathbf{Z}_j := (\mathbf{X}_{j-1}, \mathbf{X}_j, \mathbf{X}_{j+1}), \mathbf{X}_j \in U_i\}$ and then projecting the points $\mathbf{Z}_j - \langle \mathbf{Z}_i \rangle$ onto \mathbf{T}_i . Then the estimation of

TABLE I. Sample mean $\langle(R_p)_2\rangle$ and sample standard deviation $s_{(R_p)_2}$ (in parentheses) of $(R_p)_2$ for Henon time series corrupted by Gaussian noise with the noise-to-signal levels in each component given in the first row of the table by \mathbf{R}_{NS} .

| | $\mathbf{R}_{NS}=(2\%, 100\%)$ | $\mathbf{R}_{NS}=(5\%, 200\%)$ | $\mathbf{R}_{NS}=(10\%, 300\%)$ | $\mathbf{R}_{NS}=(50\%, 300\%)$ |
|----------|--------------------------------|--------------------------------|---------------------------------|---------------------------------|
| $N=500$ | 83.28 (2.38) | 85.00 (3.14) | 84.21 (3.96) | 80.66 (2.96) |
| $N=1000$ | 87.34 (2.06) | 87.83 (2.35) | 86.68 (2.91) | 81.82 (2.57) |
| $N=5000$ | 92.46 (1.22) | 90.73 (1.04) | 88.31 (1.50) | 82.92 (1.51) |

$$\mathbf{z}_j := (\mathbf{s}_{j-1}, \mathbf{s}_j, \mathbf{s}_{j+1}) \quad (2)$$

obtained from the neighborhood U_i is

$$\hat{\mathbf{z}}_j^i = \langle \mathbf{Z}_i \rangle + \mathbf{P}_{\mathbf{T}_i}(\mathbf{Z}_j - \langle \mathbf{Z}_i \rangle), \quad (3)$$

where $\mathbf{P}_{\mathbf{T}}\mathbf{Z}$ denotes the orthogonal projection, with respect to the metric used to obtain \mathbf{T}_i , of the vector \mathbf{Z} onto \mathbf{T}_i . The optimization criterion is the minimization of the mean-square distance of the points $\mathbf{Z}_j - \langle \mathbf{Z}_i \rangle$ to the subspace, taking as the metric that induced by $\hat{\Sigma}_3^{-1}$, where $\hat{\Sigma}_3^{-1}$ is the empirical covariance matrix of the errors $(\mathbf{e}_{j-1}, \mathbf{e}_j, \mathbf{e}_{j+1})$ contained in \mathbf{Z}_j and then

$$\mathbf{T}_i := \arg \min_{\mathbf{T}} \sum_{j: \mathbf{x}_j \in U_i} \mathbf{v}_j^t \hat{\Sigma}_3^{-1} \mathbf{v}_j, \quad (4)$$

where $\mathbf{v}_j := \mathbf{Z}_j - \langle \mathbf{Z}_i \rangle - \mathbf{P}_{\mathbf{T}}(\mathbf{Z}_j - \langle \mathbf{Z}_i \rangle)$ and $\mathbf{P}_{\mathbf{T}}\mathbf{Z} := \arg \min_{\mathbf{u} \in \mathbf{T}} (\mathbf{u} - \mathbf{Z})^t \hat{\Sigma}_3^{-1} (\mathbf{u} - \mathbf{Z})$ (see Appendix A). The distance induced by $\hat{\Sigma}_3^{-1}$, called the Mahalanobis distance in the statistical literature, takes into account that the independent variables \mathbf{s}_j in the underlying linear model in the variables $(\mathbf{s}_{j-1}, \mathbf{s}_j, \mathbf{s}_{j+1})$ are also measured with error, and exploits in the optimal way the information about the structure of the error, in particular the degree of uncertainty in each of the coordinates of the time series. The solution of Eq. (4) gives unbiased and consistent estimators of the parameters of the model [11], which are also those of maximum likelihood if the errors are Gaussian.

If $\hat{\Sigma}_3$ is a multiple of the identity matrix, the solution of Eq. (4) is called the orthogonal least-squares solution and the Mahalanobis distance coincides with the Euclidean distance. Hegger and Schreiber [4] also proposed a noise reduction algorithm for vector time series based on local orthogonal projections onto optimal linear subspaces, but taking as the metric on \mathbb{R}^{3d} one that gives almost all the weight to the d -central coordinates of the data points. This weight is the same for the d -coordinates, so all the individual coordinates are treated as they have the same degree of uncertainty. In the case of scalar time series, Grassberger *et al.* [3] proposed a metric which is designed to exploit the characteristics of the embedded time series and Cawley and Hsu [1] used the Euclidean metric.

B. Adaptive neighborhood construction

In the case of a clean time series, \mathbf{T}_i is obtained as in Eq. (4) using the neighborhood $\{\mathbf{s}_j: (\mathbf{s}_j - \mathbf{s}_i)^t (\mathbf{s}_j - \mathbf{s}_i) \leq r_0^2\}$, where r_0 is fixed (and should tend to zero as N tends to infinity). For the estimation of a d -dimensional linear subspace, there are needed at least $d+1$ points \mathbf{s}_j such that the corresponding vectors $\mathbf{z}_j - \langle \mathbf{z}_i \rangle$ [see Eq. (2)] are linearly independent. The value of r_0 must guarantee this condition. Furthermore, since f is not a linear function, the clean data do not belong to the tangent spaces and the estimates of \mathbf{T}_i have more statistical robustness if the number of points used is greater than $d+1$.

For noisy time series, the optimal subspace obtained using the neighborhood $\{\mathbf{X}_j: (\mathbf{X}_j - \mathbf{X}_i)^t (\mathbf{X}_j - \mathbf{X}_i) \leq r_0^2\}$ may be far from the optimal linear subspace for the clean data. This is due to the noise, which introduces false neighbors in the neighborhoods and it separates points which are close in the clean time series. The neighborhoods must be sufficiently large as to guarantee that a significant portion of the data within them corresponds to close neighbors for the clean time series. It is desirable to eliminate from the neighborhoods as many false neighbors as possible. Furthermore, the sizes of such neighborhoods should be reduced in accordance with the noise reduction occurring as the iterative process progresses.

On the other hand, since the uncertainties of the individual coordinates of the time series may be different, the Euclidean distance is not the most appropriate for the construction of the neighborhoods. We use the distance induced by $\hat{\Sigma}_1^{-1}$, where $\hat{\Sigma}_1$ is the estimate of the $d \times d$ covariance matrix of the error in the time series \mathbf{X} . This gives a neighborhood of the form $\{\mathbf{X}: (\mathbf{X} - \mathbf{X}_i)^t \hat{\Sigma}_1^{-1} (\mathbf{X} - \mathbf{X}_i) \leq r\}$, where r is a value which depends on the noise level and on the value r_0 we consider suitable in the case of N noise-free data points. The value of r is fixed as small as possible while guaranteeing, with a given confidence level $1 - \alpha_0$, that the relevant information is contained in the neighborhoods (see Appendix B for details). Figure 1 shows these neighborhoods at two points of a noisy Henon time series.

C. Further details of the algorithm

1. Estimation of Σ_1 and Σ_3

An estimate $\hat{\Sigma}_3$ of the sample covariance matrix of the errors in $\{\mathbf{Z}_j, j=2, \dots, N-1\}$ is needed for the estimation of

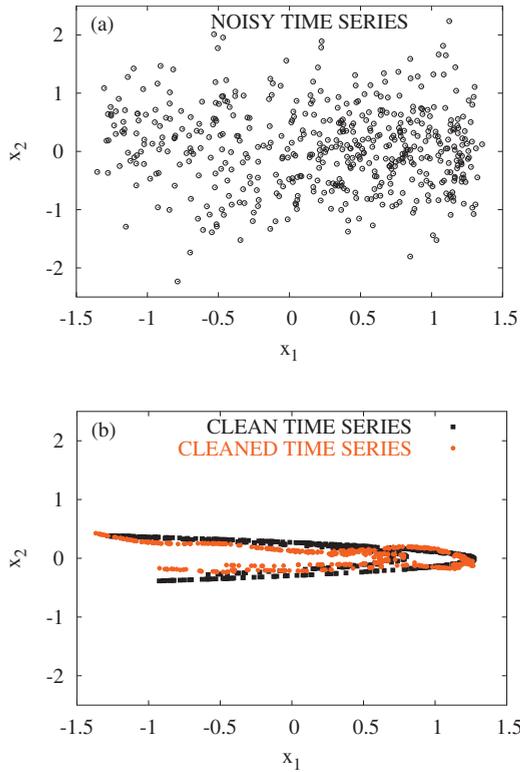


FIG. 2. (Color) (a) Noisy and (b) clean and cleaned time series of a Henon time series with $N=500$ corrupted by Gaussian noise with noise level $\mathbf{R}_{NS}=(10\%, 300\%)$.

the subspaces \mathbf{T}_i . An estimate $\hat{\Sigma}_1^k$ of the sample covariance matrix of the errors in $\{\mathbf{X}_j, j=1, \dots, N\}$ is needed in constructing the neighborhoods U_i . We estimate the errors at iteration $k > 1$ from the corrections made by the algorithm at such iteration.

Let $\{\hat{\mathbf{s}}_i^k, i=1, \dots, N\}$ be the cleaned time series at iteration k , which is also the input time series at iteration $k+1$, and let $\hat{\mathbf{s}}_i^0 = \mathbf{X}_i$, $i=1, \dots, N$. At the first iteration, we take $\hat{\Sigma}_1^0 = \mathbf{I}$, where \mathbf{I} is the $d \times d$ identity matrix and as U_i the neighborhoods which contain a fixed percentage N_{points} of the data points, corresponding to the points closest to \mathbf{X}_i in the Euclidean distance. The value of N_{points} we choose depends on an *a priori* estimation of the noise level. At iteration $k+1$, $k > 1$, we take as $\hat{\Sigma}_1^k$ the sample covariance matrix of the estimated errors

$$\hat{\mathbf{e}}_j^k := \hat{\mathbf{s}}_j^k - \hat{\mathbf{s}}_j^{k-1}, \quad j = 1, \dots, N \quad (5)$$

at iteration k and as $\hat{\Sigma}_3^k$ the sample covariance matrix of its three embedding.

2. Minimum and maximum numbers of neighbors

We check that all the neighborhoods U_i contain at least a given number $N_{\min} \geq d+1$ of neighbors, where N_{\min} is a parameter of the algorithm. It applies to the final iterations mainly to compensate the reduced sizes of the confidence ellipsoids that for large noise amplitudes and large k result from the underestimation of the real errors by the estimated errors given by Eq. (5). This is because expression (5) re-

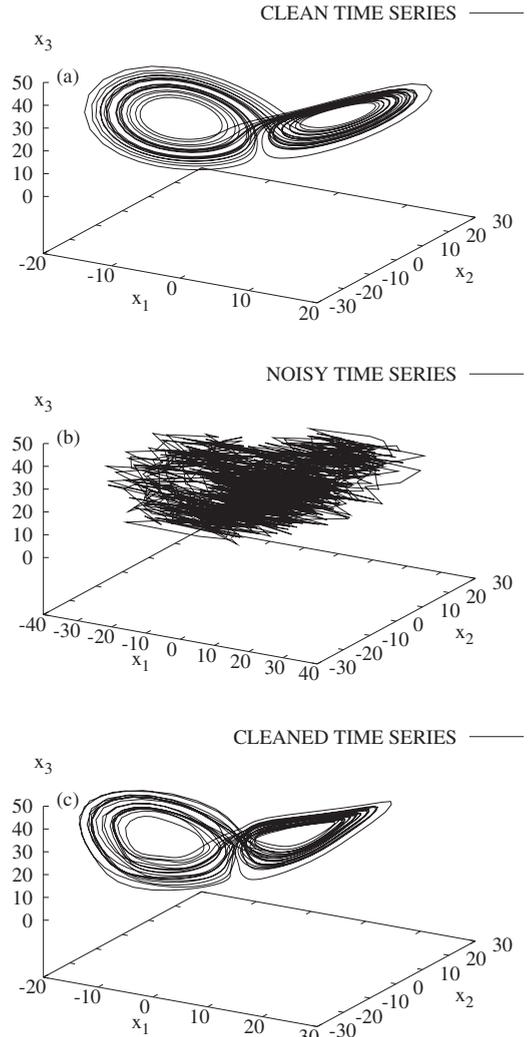


FIG. 3. (a) Clean, (b) noisy, and (c) cleaned time series of 1500 data points generated by Lorenz dynamics ($\sigma=10$, $R=28$, $b=8/3$, and sampling time $\tau=0.02$) corrupted by Gaussian noise with noise level $\mathbf{R}_{NS}=(100\%, 10\%, 5\%)$.

flects the convergence of the outputs of the algorithm, but does not incorporate the remaining errors contained in such outputs.

In the results of the next section, the value of N_{\min} taken at a given iteration is $N_{\min} := \max\{0.014N, N_{mean} - s_N\}$, where N_{mean} and s_N are the sample mean and the sample standard deviation of the distribution of the number of points within each U_i at that iteration.

Another parameter of the algorithm is the maximum N_{\max} of the number of points permitted to be contained in a neighborhood U_i . It serves to ensure that at initial iterations and for noise levels larger than 100%, the neighborhoods do not contain too large a fraction of the data points. In the results of Sec. III, we take $N_{\max}=0.25N$.

3. Embedding space

We have assumed that the dimension D of the space in which the unknown dynamics f is defined coincides with the number d of coordinates of the observed noisy time series

(see in [20,22] how to estimate D when it is unknown). However our algorithm can be adapted to the case $D \neq d$. Assume that the observed time series $\{\mathbf{X}_i, i=1, \dots, N\} \subset \mathbb{R}^d$ satisfies $\mathbf{X}_i = g(\mathbf{s}_i) + \mathbf{e}_i$, where $\{\mathbf{e}_i, i=1, \dots, N\} \subset \mathbb{R}^d$ is an unknown i.i.d. stochastic time series, $\mathbf{s}_{i+1} = f(\mathbf{s}_i)$, $i=1, \dots, N-1$, where $f: M \subset \mathbb{R}^D \rightarrow M$ is the unknown smooth dynamics, and $g: M \subset \mathbb{R}^D \rightarrow \mathbb{R}^d$ is an unknown smooth vector function or observable. Then \mathbf{T}_i will be the best D -dimensional subspace instead of the best d -dimensional subspace [i.e., the matrix \mathbf{B} in expression (A1) in Appendix A has as columns the vectors $\{\mathbf{w}_{3d-D+1}, \dots, \mathbf{w}_{3d}\}$]. Furthermore, if $D > d$ and $3d < 2D + 1$ then the working space \mathbb{R}^{3d} (i.e., the three-embedding of the time series) must be replaced by $\mathbb{R}^{(2m+1)d}$ with m such that $(2m+1)d > 2D + 1$ in order to guarantee we have a good reconstruction [23] of the unknown dynamics.

III. NUMERICAL RESULTS

In this section, we show the results obtained applying our algorithm to time series generated by Hénon and Lorenz dynamics corrupted by noise. The Hénon map is given by the equations

$$x_1(k+1) = 1 - ax_1(k)^2 + x_2(k), \quad x_2(k+1) = bx_1(k), \quad (6)$$

and we take the parameter values $a=1.4$ and $b=0.3$. The Lorenz dynamics is defined by

$$x'_1 = \sigma(x_2 - x_1), \quad x'_2 = x_1(R - x_3) - x_2, \quad x'_3 = x_1x_2 - bx_3.$$

The equations were integrated using a fourth order Runge-Kutta algorithm with an integration step of $\Delta t = 0.001$. The values used for the sampling time τ and the parameters σ, R , and b are given in Table II.

In all the examples below, we use uncorrelated and heteroskedastic errors with Gaussian distributions. For the construction of the neighborhoods, we take $\alpha_0 = 0.01$ (see Appendix B).

We quantify the noise removed by the algorithm using the pointwise distance between the clean \mathbf{s} and the cleaned $\hat{\mathbf{s}}$ time series

$$d_p(\mathbf{s}, \hat{\mathbf{s}}) := \left[\frac{1}{N} \sum_{i=1}^N (\|\hat{\mathbf{s}}_i - \mathbf{s}_i\|_2)^2 \right]^{1/2}.$$

If $d_p(\mathbf{s}, \hat{\mathbf{s}}) < d_p(\mathbf{s}, \mathbf{X})$, then the noise level in $\hat{\mathbf{s}}$ is less than the noise level in the input time series \mathbf{X} . The percentage of global pointwise noise reduction is $R_p := 100(1 - \frac{d_p(\mathbf{s}, \hat{\mathbf{s}})}{d_p(\mathbf{s}, \mathbf{X})})$ and that corresponding to the j th coordinate is $(R_p)_j := 100(1 - \frac{d_p((\mathbf{s})_j, (\hat{\mathbf{s}})_j)}{d_p((\mathbf{s})_j, (\mathbf{X})_j)})$, where

$$d_p((\mathbf{s})_j, (\hat{\mathbf{s}})_j) := \left\{ \frac{1}{N} \sum_{i=1}^N ((\hat{\mathbf{s}}_i)_j - (\mathbf{s}_i)_j)^2 \right\}^{1/2}, \quad j = 1, \dots, d.$$

Notice that these measures require knowledge of the clean time series. We use such knowledge only to quantify the noise level reduction. This information is used neither in the noise reduction scheme nor in deciding when the algorithm must stop. Thus the algorithm may work on data generated by an unknown process. The stopping criterion we use is

related to our adaptive neighborhood construction. As the iterations increase, the remaining noise level and the size of the neighborhood U_i must decrease. A clear indication that further iterations of the algorithm will not reduce the remaining noise is the stabilization of the mean number of points in the neighborhoods.

We focus our attention on time series of short lengths corrupted by noises with large amplitudes. We intend to show through numerical experiments that the combination of the measurement error theory and the adaptive neighborhood construction allows us to reduce noises having large amplitudes in one of the components especially if the other components of the time series are corrupted by noises of smaller amplitudes.

The results for a Henon time series corrupted by noise of large amplitude (up to 300%) in the second component and by noise of small or moderate amplitude in the first component are shown in Table I. For short length time series and high noise levels, the results of the algorithm depend strongly on the realization of the error term and also on the clean time series considered. Thus the noise level reduction achieved by any noise reduction algorithm must be understood in terms of the distribution of the output of the algorithm. For this reason, we give as results the sample mean $\langle (R_p)_2 \rangle$ and the sample standard deviation $s_{(R_p)_2}$ of $(R_p)_2$ obtained from 50 noisy time series.

The results show values of $\langle (R_p)_2 \rangle$ higher than 80% in all the cases. These values increase with N whereas $s_{(R_p)_2}$ decreases with N . For noise levels $(R_{NS})_2$ up to 200%, the average global pointwise noise reduction in the second component $\langle (R_p)_2 \rangle$ achieves values greater than 90% for time series with $N=5000$. The results are very good even for time series of only 500 data points, although they present greater variability. For instance, for $N=500$ and a noise level $\mathbf{R}_{NS} = (5\%, 200\%)$, we obtain $\langle (R_p)_2 \rangle = 85.00\%$ and $s_{(R_p)_2} = 3.14$ and the 50 values of $(R_p)_2$ belong to the interval (72.2%, 89.62%).

Figure 2 shows the output of the algorithm for one of the 50 noisy time series corresponding to a noise level $\mathbf{R}_{NS} = (10\%, 300\%)$ and $N=500$. The figure shows that even for a time series having such a large noise level and such a short length, the algorithm is able to recover a significant part of the geometric structure of the clean time series.

The use of adaptive neighborhoods is more relevant for noises of large amplitude. Then the mean number of neighbors in the initial iterations may be close to N_{\max} whereas in the final iterations it is stabilized and close to N_{\min} . For instance, for a Henon time series with $N=1000$ and a noise level $\mathbf{R}_{NS} = (10\%, 300\%)$, the mean number of neighbors in U_i at the first iteration is $N_{\max} = 250$ and at iteration 20, this mean number is only 25.

Another measure of noise reduction standard in the noise reduction literature is based on the deviation of the time series from the deterministic behavior. It assumes that the dynamics f is known and is defined through

$$d_{dyn}(\hat{\mathbf{s}}) := \left\{ \frac{1}{N-1} \sum_{i=1}^{N-1} [\|\hat{\mathbf{s}}_{i+1} - f(\hat{\mathbf{s}}_i)\|_2]^2 \right\}^{1/2}. \quad (7)$$

If $d_{dyn}(\hat{\mathbf{s}}) < d_{dyn}(\mathbf{X})$, then the cleaned time series emulates better the dynamics than does the input time series. The per-

TABLE II. Sample means and sample standard deviations (in parentheses) of $\langle R_p \rangle_1$, $\langle R_{dyn} \rangle_1$, $\langle R_p \rangle$, and $\langle R_{dyn} \rangle$ in Lorenz time series corrupted by Gaussian noises with the noise-to-signal levels in each component given in the first row of the table by \mathbf{R}_{NS} .

| N | $\mathbf{R}_{NS}=(100\%, 10\%, 5\%)$ $\sigma=16, R=45.92, b=4, \tau=0.03$ | | | | $\mathbf{R}_{NS}=(100\%, 10\%, 5\%)$ $\sigma=10, R=28, b=8/3, \tau=0.02$ | | | |
|------|--|---|-----------------------|---------------------------|---|---|-----------------------|---------------------------|
| | $\langle\langle R_p \rangle_1\rangle$ | $\langle\langle R_{dyn} \rangle_1\rangle$ | $\langle R_p \rangle$ | $\langle R_{dyn} \rangle$ | $\langle\langle R_p \rangle_1\rangle$ | $\langle\langle R_{dyn} \rangle_1\rangle$ | $\langle R_p \rangle$ | $\langle R_{dyn} \rangle$ |
| 1500 | 76.73 (7.54) | 86.65 (7.43) | 69.70 (13.9) | 83.94 (8.13) | 79.80 (3.05) | 94.03 (1.15) | 73.79 (4.3) | 86.47 (1.32) |
| 3000 | 78.83 (5.49) | 88.21 (3.63) | 71.86 (11.78) | 74.47 (2.77) | 81.79 (2.34) | 94.74 (0.53) | 76.23 (3.85) | 87.13 (0.75) |
| 5000 | 81.10 (1.08) | 89.79 (0.70) | 74.78 (1.12) | 86.91 (0.72) | 82.32 (1.73) | 94.90 (0.81) | 77.01 (1.99) | 87.27 (0.74) |

centage of global dynamical noise reduction is $R_{dyn} := 100(1 - \frac{d_{dyn}(\hat{\mathbf{s}})}{d_{dyn}(\mathbf{X})})$ and that corresponding to the j th coordinate is $(R_{dyn})_j := 100(1 - \frac{(d_{dyn}(\hat{\mathbf{s}}))_j}{(d_{dyn}(\mathbf{X}))_j})$, where

$$(d_{dyn}(\hat{\mathbf{s}}))_j := \left(\frac{1}{N-1} \sum_{i=1}^{N-1} \{(\hat{s}_{i+1})_j - (f(\hat{\mathbf{s}}_i))_j\}^2 \right)^{1/2}, \quad j = 1, \dots, d.$$

If f is unknown, a measure \hat{R}_{dyn} of the dynamical noise reduction is obtained by replacing f in Eq. (7) by its local linear estimations.

The values of $\langle R_p \rangle$, $\langle R_{dyn} \rangle$, and $\langle\langle R_{dyn} \rangle_2\rangle$ for the time series of Table I differ slightly from $\langle\langle R_p \rangle_2\rangle$ and are omitted for the sake of clarity. The only significant difference is for a noise level $\mathbf{R}_{NS}=(50\%, 300\%)$, where the values of $\langle R_p \rangle$ and $\langle R_{dyn} \rangle$ are around 60% and 70% respectively, which are values significantly smaller than the values of $\langle\langle R_p \rangle_2\rangle$ in Table I.

We have tested in all these examples that the stopping criterion based on the stabilization of the mean number of points within the neighborhoods gives results analogous to those obtained using as the stopping criterion the stabilization of R_p or R_{dyn} , which criteria require knowledge of the clean time series or f . A stopping criterion based on the stabilization of \hat{R}_{dyn} , which does not require additional information, gives poorer results because \hat{R}_{dyn} stabilizes at high values even when R_p and R_{dyn} indicate that the algorithm is still able to reduce a significant part of the remaining noise.

Our algorithm estimates very effectively the initial noise levels in each of the components of a noisy time series. Such estimations are given by $(\hat{R}_{NS})_j := \sqrt{\frac{\sum_{i=1}^N [(X_i - \hat{s}_i)_j]^2}{\sum_{i=1}^N [(\hat{s}_i)_j]^2}}$, $j = 1, \dots, d$. For instance, the mean of the values of $\hat{\mathbf{R}}_{NS} := [(\hat{R}_{NS})_1, (\hat{R}_{NS})_2]$ obtained from 50 Henon time series of 1000 data points corrupted by Gaussian noise with noise level $\mathbf{R}_{NS}=(2\%, 100\%)$ is $\hat{\mathbf{R}}_{NS}=(2.012\%, 100.803\%)$ and the corresponding vector of standard deviations is (0.074, 2.89).

Some results obtained for Lorenz time series are shown in Table II. These two examples differ in the values of the parameters in the Lorenz dynamics and in the sampling times. In both cases $\mathbf{R}_{NS}=(100\%, 10\%, 5\%)$ so the noise level is large in the first component and moderate in the other two

components. In fact, since the mean value of the z component of the clean time series is not zero, $(R_{NS})_3=5\%$ is equivalent to 15% noise level in terms of the standard deviation of z in the clean time series. In this case, f is unknown and the values of $\langle R_{dyn} \rangle$ and $\langle\langle R_{dyn} \rangle_1\rangle$ of the table are obtained by approximating f using the fourth-order Runge-Kutta method used to generate the clean time series. The values of the dynamical noise reduction are significantly greater than the values of pointwise noise reduction, achieving values of $\langle\langle R_{dyn} \rangle_1\rangle$ close to 95% for the second set of parameters, for all the lengths considered. Figure 3 shows the output of one of the noisy time series of Table II. It can be seen that the algorithm is able to recover a significant part of the geometric structure and the dynamics of the clean time series.

IV. CONCLUSIONS

We have proposed a noise-reduction algorithm that combines the measurement error models theory with an adaptive neighborhoods selection based on a statistical test. The algorithm works efficiently for short-time series corrupted by noises of large amplitude. The results could be improved by the consideration of nonlinearity effects added to our adaptive neighborhood method. The size of the neighborhoods should be fixed as a compromise between the effects of nonlinearity (see [3]) and the amount of information in the neighborhoods.

Our results show the possibility of detection and forecasting of deterministic scalar time series of small amplitudes buried in observational noises of amplitudes much larger than that of the signal if they are coupled through a smooth dynamical system to other state variables which can be observed with lower uncertainties. The high performance of our algorithm for short length time series gives hope that the scope of application of this method might extend to research in the social sciences.

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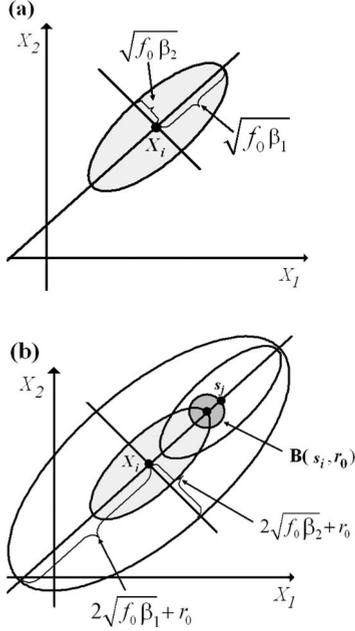


FIG. 4. (a) Confidence ellipsoid for s_i and (b) confidence ellipsoid for $B(s_i, r_0)$.

APPENDIX A: TECHNICAL DETAILS

1. Estimation of the best subspaces and the projection matrix

The solution of Eq. (4) is (see Appendix in Ref. [10]) $\mathbf{T}_i := \text{span}\{\hat{\Sigma}_3 \mathbf{w}_1, \dots, \hat{\Sigma}_3 \mathbf{w}_{3d}\}$, where $\{\mathbf{w}_1, \dots, \mathbf{w}_{3d}\}$ is an orthonormal basis of eigenvectors of the matrix $M_{ZZ} := \frac{1}{\#U_i} \sum_{j: X_j \in U_i} (\mathbf{Z}_j - \langle \mathbf{Z}_i \rangle) (\mathbf{Z}_j - \langle \mathbf{Z}_i \rangle)^t$ in the metric of $\hat{\Sigma}_3$, i.e.,

$$M_{ZZ} \mathbf{w}_j = \lambda_j \hat{\Sigma}_3 \mathbf{w}_j, \quad j = 1, \dots, 3d$$

and

$$\mathbf{w}_j \hat{\Sigma}_3 \mathbf{w}_k = \delta_{jk}, \quad j, k = 1, \dots, 3d,$$

where $\lambda_1 \geq \dots \geq \lambda_{3d}$ are the corresponding eigenvalues. Such a basis of eigenvectors is given by the columns of the matrix $Q\Lambda^{-1/2}H$, where Q is a matrix whose columns are an orthonormal basis of eigenvectors of $\hat{\Sigma}_3$ (in the Euclidean metric), Λ is the diagonal matrix of eigenvalues of $\hat{\Sigma}_3$, and the columns of H are an orthonormal basis of eigenvectors of the matrix $\Lambda^{-1/2}Q^t M_{ZZ} Q \Lambda^{-1/2}$.

The matrix of the projection onto the subspace \mathbf{T}_i is $\mathbf{I} - \hat{\Sigma}_3 \mathbf{B} \mathbf{B}^t$, where \mathbf{I} is the $3d \times 3d$ identity matrix and \mathbf{B} is the matrix whose columns are $\{\mathbf{w}_{2d+1}, \dots, \mathbf{w}_{3d}\}$. Then Eq. (3) can be written as

$$\hat{\mathbf{z}}_j^i = \mathbf{Z}_j - \hat{\Sigma}_3 \mathbf{B} \mathbf{B}^t (\mathbf{Z}_j - \langle \mathbf{Z}_i \rangle) \quad \text{for } \mathbf{X}_j \in U_i. \quad (\text{A1})$$

2. Problem of multiple 3d-dimensional estimations

Since any point \mathbf{X}_j belongs to many neighborhoods U_i , we take the average of all the values $\{\hat{\mathbf{z}}_j^i: \mathbf{X}_j \in U_i\}$ [see Eq. (3)] as the final estimation of \mathbf{z}_j , i.e.,

$$\hat{\mathbf{z}}_j := \frac{1}{\#\{i: \mathbf{X}_j \in U_i\}} \sum_{\{i: \mathbf{X}_j \in U_i\}} \hat{\mathbf{z}}_j^i, \quad j = 2, \dots, N-1. \quad (\text{A2})$$

This is a $3d$ -dimensional time series that is not the three-embedding of a d -dimensional time series so there remains the problem of estimating the deterministic part of the observed time series.

3. Estimation of the deterministic component

Let $(\hat{\mathbf{z}}_j)_i$ denote the i th coordinate of $\hat{\mathbf{z}}_j$, $j = 2, \dots, N-1$. Since $\hat{\mathbf{z}}_j = (\hat{s}_{j-1}, \hat{s}_j, \hat{s}_{j+1})$, this time series gives as estimations of $(s_j)_i$, $j = 3, \dots, N-2$, the three values $(\hat{\mathbf{z}}_{j-1})_{2d+i}$, $(\hat{\mathbf{z}}_j)_{d+i}$, and $(\hat{\mathbf{z}}_{j+1})_i$. These are the estimations of s_j obtained from the past, the present, and the future. We take a weighted average of these three values as the estimation of $(\hat{s}_j)_i$, $i = 1, \dots, d$, with weights w_l^i , $l = 1, \dots, 3$ related with the sample variances of the coordinates of the corrections $\epsilon := \mathbf{Z} - \hat{\mathbf{z}}$ and then

$$(\hat{s}_j)_i = \sum_{l=1}^3 w_l^i (\hat{\mathbf{z}}_{j-1+(l-1)})_{(3-l)d+i} \quad \text{for } j = 3, \dots, N-2; \quad i = 1, \dots, d. \quad (\text{A3})$$

This cleaned time series $\{\hat{s}_j, j = 1, \dots, N\}$ will be the input time series in the next iteration of the algorithm.

The combination of the averages (A2) and (A3) increases the statistical robustness of the estimations without requiring controls for avoiding large corrections as do many noise reduction algorithms. These smoothing devices partially overcome the problems of the maximum likelihood estimates pointed out by Judd [12].

APPENDIX B: THE ADAPTIVE NEIGHBORHOOD CONSTRUCTION

If we assume that the errors $\{e_i\}$ have a $N(0, \Sigma_1)$ distribution, then $(\mathbf{X}_i - s_i)' \Sigma_1^{-1} (\mathbf{X}_i - s_i)$ has a χ^2 distribution with d degrees of freedom and

$$\{\mathbf{X}: (\mathbf{X} - \mathbf{X}_i)' \Sigma_1^{-1} (\mathbf{X} - \mathbf{X}_i) \leq \chi_d^2(\alpha_0)\}$$

provides a $100(1 - \alpha_0)\%$ confidence ellipsoid for s_i , where $\chi_d^2(\alpha_0)$ is the number such that $\Pr\{\chi_d^2 > \chi_d^2(\alpha_0)\} = \alpha_0$.

Since in general Σ_1 is unknown, it is replaced by the sample covariance matrix $\hat{\Sigma}_1$. Let $T^2 := (\mathbf{X}_i - s_i)' \hat{\Sigma}_1^{-1} (\mathbf{X}_i - s_i)$.

Then $\frac{(N-d)}{d(N-1)}T^2$ is distributed (see [24]) as an F distribution with degrees of freedom d and $N-d$.

A $100(1-\alpha_0)\%$ confidence ellipsoid for \mathbf{s}_i is given by

$$\left\{ \mathbf{X}: (\mathbf{X} - \mathbf{X}_i)^t \hat{\Sigma}_1^{-1} (\mathbf{X} - \mathbf{X}_i) \leq \frac{d(N-1)}{N-d} F_{d;N-d}(\alpha_0) \right\} \\ = \left\{ \mathbf{X}: \sum_{j=1}^d \left(\frac{(\mathbf{Y} - \mathbf{Y}_i)_j}{\sqrt{f_0 \beta_j}} \right)^2 \leq 1 \right\}$$

where $\mathbf{Y} := \mathbf{M}'\mathbf{X}$, $(\mathbf{Y})_j$ is the j th coordinate of \mathbf{Y} , \mathbf{M} is a matrix whose columns are an orthonormal basis of eigenvectors of $\hat{\Sigma}_1$, $\{\beta_j, j=1, \dots, d\}$, are the eigenvalues of $\hat{\Sigma}_1$ and $f_0 := \frac{d(N-1)}{N-d} F_{d;N-d}(\alpha_0)$. It is an ellipsoid centered at \mathbf{X}_i whose axes are the eigenvectors of $\hat{\Sigma}_1$ and with j th semiaxis of length $\sqrt{f_0 \beta_j}$ [see Fig. 4(a)]. Since we want a confidence ellipsoid for the points $\{\mathbf{s}_j: (\mathbf{s}_j - \mathbf{s}_i)^t (\mathbf{s}_j - \mathbf{s}_i) \leq r_0^2\}$, we take $2\sqrt{f_0 \beta_j} + r_0$ as the length of the j th semiaxis instead of $\sqrt{f_0 \beta_j}$ [see Fig. 4(b)] and therefore

$$U_i := \left\{ \mathbf{X}: \sum_{j=1}^d \left(\frac{(\mathbf{Y} - \mathbf{Y}_i)_j}{2\sqrt{f_0 \beta_j} + r_0} \right)^2 \leq 1 \right\} \subset \mathbb{R}^d \quad (\text{B1})$$

is the neighborhood of \mathbf{X}_i that we consider.

We refine this neighborhood slightly by removing from U_i those points which are neighbors only due to the noise. We construct a neighborhood $V_i \subset \mathbb{R}^{3d}$ of \mathbf{Z}_i using the same procedure we use to build the neighborhood U_i of \mathbf{X}_i , and we remove from U_i the points \mathbf{X}_j for which $\mathbf{Z}_j = (\mathbf{X}_{j-1}, \mathbf{X}_j, \mathbf{X}_{j+1}) \notin V_i$.

A parameter needed for the construction of the neighborhoods U_i at each iteration is r_0 . In the results of Sec. III, we take $r_0 = r_{mean} + s_r$, where r_{mean} and s_r are the sample mean and the sample standard deviation of the distribution of radii corresponding to the minimum radius r needed to get $0.014N$ neighbors in the balls centered at \mathbf{X}_i , $i=1, \dots, N$, and with radius r with respect to the Euclidean metric. Since the noise is reduced as the iterations increase, the value of r_0 decreases.

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