

Optimal embedding parameters: A modeling paradigm

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Abstract

Reconstruction of a dynamical system from a time series requires the selection of two parameters, the embedding dimension d_e and the embedding lag τ . Many competing criteria to select these parameters exist, and all are heuristic. Within the context of modeling the evolution operator of the underlying dynamical system, we show that one only need be concerned with the product $d_e\tau$. We introduce an information theoretic criteria for the optimal selection of the embedding window $d_w = d_e\tau$. For infinitely long time series this method is equivalent to selecting the embedding lag that minimises the nonlinear model prediction error. For short and noisy time series we find that the results of this new algorithm are data dependent and superior to estimation of embedding parameters with the standard techniques.

Key words: Embedding dimension, lag, window, minimum description length

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1 Reconstruction

The celebrated theorem of Takens [1] guarantees that, for a sufficiently long time series of scalar observations of an n -dimensional dynamical system with a C^2 measurement function, one may recreate the underlying dynamics (up to homeomorphism) with a time delay embedding². Unfortunately the theorem

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² Takens' theorem has many extensions and is described in various forms by several contemporary authors. We do not intend to dwell on the evolution of these fundamental results here.

is silent on exactly how to proceed when the data is limited and contaminated by noise. In practice, time delay embedding is routinely employed as a first step in the analysis of experimentally observed nonlinear dynamical systems (see [2,3]). Typically, one identifies some characteristic embedding lag τ (usually related to the sampling rate and time scale of the time series under consideration) and utilises d_e lagged version of the scalar observable for sufficiently large d_e . In general, τ is determined by identifying linear or nonlinear temporal correlations in the data and one will progressively increase d_e until the results obtained are self consistent.

In this paper we consider the problem of reconstructing the underlying dynamics from a finite scalar time series in the presence of noise. We recognise that in general the quality of the reconstruction will depend on the length of the time series and the amount of noise present in the system. Employing the minimum description length model selection criteria we show that the optimal model of the dynamics does not depend on the choice of the embedding lag, only on the maximum lag ($d_e\tau$ in the above scheme). We call that maximum embedding lag $d_w := d_e\tau$, the embedding window, and show that for long noise-free time series the optimal d_w minimises the one-step model prediction error. For short or noisy data, the optimal value of d_w is data dependent. To estimate the one-step model prediction error and d_w we apply a generic local constant modeling scheme to several computational examples. We show that this method proves to be consistent and robust, and the results that we obtain capture the salient features of the underlying dynamics. Finally, we also find that in general there is no single characteristic time lag τ . Generically, the optimal reconstruction may be obtained by considering the lag vector

$$(\tau_1, \tau_2, \dots, \tau_k) \tag{1}$$

where $0 < \tau_i < \tau_{i+1} \leq d_w$ ³.

The textbooks [2,3] contain copious detail on the estimation of d_e and τ . We briefly review only the most relevant developments here.

Often, the primary aim of time delay embedding is the estimation of dynamic invariants. In these instances, one may estimate τ with a variety of heuristic techniques: usually autocorrelation, pseudo-period or mutual information. One then computes the dynamic invariant for increasing values of d_e until some sort of plateau onset occurs (see [5] and the references therein). For estimation of correlation dimension, d_c , it has been shown that $d_e > d_c$ is sufficient [6]. However, for reconstruction of the underlying dynamics this is not the case. Alternatively, the method of false nearest neighbours [7] and its various extensions apply a topological reasoning: one increases d_e until the geometry

³ This is the so called “variable embedding” described in [4] and elsewhere.

of the time series does not change.

We note that several authors have speculated on whether the individual parameters d_e and τ , or only their product $d_e\tau$, is significant. For example, Lai and Lerner [8] provide an overview of selection of embedding parameters to estimate dynamic invariants (in their case, correlation dimension). They impose some fairly generous constraints on the correlation integral and use these to estimate the optimal value of d_e and τ . Their numerical results from long clean data imply that correct selection of τ is crucial, selection of d_w (and therefore d_e) is not. Conversely, utilising the BDS statistic [9], Kim and co-workers [5] concluded that the crucial parameter for estimating correlation dimension is d_w .

Unlike these previous methods, the question we consider is: “What is the optimal choice of embedding parameters to reconstruct the underlying dynamic evolution from a time series?” In answering this question we conclude that only the embedding window d_w is significant, selection of optimal embedding lags is, essentially, a modeling problem [4]. Clearly, successful reconstruction of the underlying dynamics will depend on ones’ ability to identify any underlying periodicity (and therefore τ). The results of this paper shows that it is possible to estimate the optimal value of d_w , and subsequently use this optimal value to derive a suitable embedding lag τ . However, as previous authors have observed in many examples, estimation of τ for nonlinear systems is model dependent [4] (and may even be *state* dependent).

In the following section we introduce our main result and the rational for the calculations that follow. Section 3 demonstrates the application of this method to several test systems, and section 4 studies the problem of modelling several experimental time series. In section 5 we conclude.

2 A modeling paradigm

Let $\phi : \mathcal{M} \longrightarrow \mathcal{M}$ be the evolution operator of a dynamical system, and $h : \mathcal{M} \longrightarrow \mathbf{R}$ a C^2 differentiable observation function. Through some experiment we obtain the time series $\{h(X_1), h(X_2), \dots, h(X_N)\}$. Denote $x_i \equiv h(X_i)$. Takens’ theorem [1] states that for some $m > 0$ the mapping g

$$x_i \xrightarrow{g} (x_i, x_{i-1}, x_{i-2}, \dots, x_{i-m-1}) \quad (2)$$

is such that the evolution of $g(x_i) = (x_i, x_{i-1}, \dots, x_{i-m-1})$ ⁴ is homeomorphic to ϕ

We will generalise the embedding map (2) and consider \hat{g} as

$$x_i \xrightarrow{\hat{g}} (a_1 x_i, a_2 x_{i-1}, a_3 x_{i-2}, \dots, a_d x_{i-d-1}). \quad (3)$$

The objective of a successful embedding is to find $a = [a_1, a_2, \dots, a_d]$ where $a_i \in \{0, 1\}$. Note that $\hat{g}(x_i)$ is simply the subspace projection of $g(x_i)$ onto a ,

$$\hat{g}(x_i) = \text{Proj}_a g(x_i).$$

The embedding is completely defined by $a \in \{0, 1\}^d$ and we wish to make the best choice of a and d , which we write (a, d) . Note that, in general one could consider $a \in \mathbf{R}^{d_e \tau}$. We restrict ourselves to $\{0, 1\}^d$ as the more general case is concerned with the optimal model of the dynamics rather than the necessary information. For a uniform embedding with embedding parameters d_e and τ we have that $a \in \{0, 1\}^d$ and $(a)_i \neq 0$ if and only if τ divides i .

Let $z_i = \hat{g}(x_i) \in \mathbf{R}^d$ and let

$$f(z) = \sum_{i=1}^m \lambda_i \theta(z; w_i) \quad (4)$$

where θ is some basis and $\lambda_i \in \mathbf{R}$ and $w_i \in \mathbf{R}^k$ are linear and nonlinear model parameters. The selection of this particular model architecture is arbitrary, but does not alter the results. We assume that there exists some algorithm to select $\mathcal{P} = (m, \lambda_1, \lambda_2, \dots, \lambda_m, w_1, w_2, \dots, w_k)$ such that $e_i = f(z_{i-1}) - z_i \sim N(0, \sigma)$ (or at the very least, $\sum (f(z_{i-1}) - z_i)^2 = \sigma^2$ is minimised). We do not consider the model selection problem here, rather we seek to find out what is the best choice of (a, d) . Our own model selection work is summarised in [10].

The most obvious approach to this problem is to look for the maximum likelihood solution:

$$\max_{(a,d)} \max_{\mathcal{P}} P(x|x_0, a, d, \mathcal{P})$$

where x is the vector of all the time series observations and $x_0 \in \mathbf{R}^d$ is a vector of model initial conditions. Unfortunately this leads to the redundant solution $d = N$. To solve this problem one could either resort to Bayesian

⁴ In writing $g(x_i) = (x_i, x_{i-1}, \dots, x_{i-m-1})$ we take a slight liberty with the notation, but the meaning remains clear.

regularisation [11] or the minimum description length model selection criteria [12]. We choose the later approach.

The description length of a time series is the length of the shortest (most compact) description of that time series. The description length of a time series with respect to a given model is the length of the description of that model, the initial conditions of that model and the model prediction error. We intend to optimise the description length of the observed time series $\{x_i\}_{i=1}^N = x$ with respect to (a, d) . At this point we make the fairly cavalier assumption that for a given (a, d) one can obtain the optimal model \mathcal{P} . We will address this assumption in more detail later in this section.

The description length of the data $DL(x)$ is given by

$$DL(x) = DL(x|x_0, a, d, \mathcal{P}) + DL(x_0) + DL(a, d) + DL(\mathcal{P}) \quad (5)$$

where $x_0 = (x_1, x_2, \dots, x_d)$ are the model initial conditions. Notice that the description length of the model prediction errors $DL(x|x_0, a, d, \mathcal{P})$, is equal to the negative log likelihood of the errors under the assumed distributed. Similarly x_0 is a sequence of d real numbers which for small d we approximate by d realisations of a random variable. Therefore $DL(x_0)$ can also be computed as a negative log-likelihood of some probability distribution. If we assume that x and x_0 are approximated by Gaussian random variables with variance σ^2 and σ_D^2 respectively, then (5) becomes

$$DL(x) \approx -\ln P(x|N(0, \sigma^2)) - \ln P(x_0|N(0, \sigma_X^2)) + d + DL(d) + DL(\mathcal{P}). \quad (6)$$

Since a is a sequence of d independent zeros or ones $DL(a) = d$, furthermore the description length of an integer d is given by $DL(d) = \lceil \log(d) \rceil + \lceil \log \lceil \log(d) \rceil \rceil + \dots$ where the last term in this expansion is 0[12]. Compared to the term d , $DL(d)$ is very slowly varying and has little effect on the results. The final term $DL(\mathcal{P})$ is the description length of the optimal model for the given (a, d) .

Substituting for the probability distributions $P(x|N(0, \sigma^2))$ and $P(x_0|N(0, \sigma_X^2))$ and estimating σ^2 and σ_X^2 directly from the data, one finally obtains

$$DL(x) \approx \frac{d}{2} (1 + \ln 2\pi\sigma_X^2) + \frac{N-d}{2} (1 + \ln 2\pi\sigma^2) + DL(\bar{x}) + d + DL(d) + DL(\mathcal{P}) \quad (7)$$

$$\begin{aligned} &\approx \frac{d}{2} \ln \left[\frac{1}{d} \sum_{i=1}^d (x_i - \bar{x})^2 \right] + \frac{N-d}{2} \ln \left[\frac{1}{N-d} \sum_{i=d+1}^N e_i^2 \right] \\ &\quad + \frac{N}{2} (1 + \ln 2\pi) + d + DL(d) + DL(\bar{x}) + DL(\mathcal{P}). \end{aligned} \quad (8)$$

In this form, equation (8) provides the first suggestion of what the optimal embedding strategy should be. We see that a does not feature in this calculation. Hence, if we adopt the modeling paradigm suggested here, the embedding lag (or more generally the embedding strategy) is not crucial: one should only be concerned with the maximum embedding dimension d . Of course, this does not mean that to reconstruct the dynamics the embedding lag is unimportant. When one applies numerical modeling to reconstruct the dynamics, embedding strategies are of very great significance, however selection of the optimal embedding co-ordinates (or rather those that are most significant in predicting the dynamics) is inherently part of the modeling process [4]. Furthermore, the modelling algorithm should be allowed to choose from all possible embedding lags within the embedding window. Indeed, one often finds that the “optimal” embedding strategy is not fixed within a single model [4]. This result shows that it is preferable to identify the embedding window d_w and let the model building process determine which of the d_w co-ordinates are most useful.

The description length of the mean of the data $DL(\bar{x})$ is a fixed constant and we drop it from the calculation. Optimising (8) over all (a, d) requires selection of the optimal model for a given (a, d) and computation of the model prediction error of that model. For a given model, $DL(\mathcal{P})$ can be calculated precisely [13]. However, selection of the optimal model is a more difficult problem.

Instead, we restrict our attention to a particular *class* of model, and choose the optimal model from that class. To simplify the computation of (8) we restrict our attention to the class of local constant models on the attractor. We have two good reasons for choosing this particular class. Firstly, because the models are simple, estimates of the error as a function of (a, d) are relatively well behaved. Secondly, these models rely on no additional parameters and therefore $DL(\mathcal{P}) = 0$, simplifying our calculation considerably⁵.

In trials, we tested many alternative model classes. We found radial basis functions [13] and neural networks [10] to be excessively nonlinear and difficult to optimise for the purpose of determining embedding windows. Complex local modeling regimes such as triangulation and tessellation [14] or parameter dependent local linear schemes [15] we found to be overly sensitive to small changes in the data. In comparison the local constant scheme we employ here appears remarkably robust.

⁵ Alternatively, one could argue that the data are the parameters, in either case the description length of the model is constant.

As local constant models have no explicit parameters (other than the embedding strategy (a, d)), $DL(\mathcal{P}) = 0$. Therefore, for a given (a, d) computation of (8) only requires estimation of $\sum e_i^2$. We employ an in-sample local constant prediction strategy. Let z_s be the nearest neighbour to z_t (excluding z_t), then

$$x_{t+1} = x_{s+1} \tag{9}$$

and therefore $e_{t+1} = x_{t+1} - x_{s+1}$. In other words, for each point in the time series we determine the prediction error based on the difference between the successor to that point and the successor to its nearest neighbour⁶. Since this is a form of interpolation rather than extrapolation, this strategy does not provide a *predictive* model, likewise (as with all local techniques) it does not describe the underlying dynamics. However, the strength of this particular approach is that it is simple and it provides a realistic estimate of the size of the optimal model’s prediction error as a function of (a, d) .

The proposed algorithm may be summarised as follows. We seek to minimise (8) over d . To achieve this we need to estimate the model prediction error as a function of d . Hence, for increasing values of d we employ the local constant “modelling” scheme suggested by (9) to compute the model prediction error and substitute this into (8). The optimal embedding window d_w is the value of d that minimises (8).

3 Examples

In this section we describe the application of the above method to several numerical time series. First, we examine the performance of the algorithm and importance of the choice of modelling algorithm (9).

The example we consider is 2000 points of the x component of a numerically integrated (sampling rate of 0.2) trajectory of the Rössler system, contaminated by additive Gaussian noise with a standard deviation of 5% of the standard deviation of the data. The Rössler equations are given by

$$\begin{pmatrix} \dot{x} \\ \dot{y} \\ \dot{z} \end{pmatrix} = \begin{pmatrix} -y - z \\ x + ay \\ b + z(x - c) \end{pmatrix} \tag{10}$$

⁶ This is a technique sometimes referred to as “drop-one-out” interpolation.

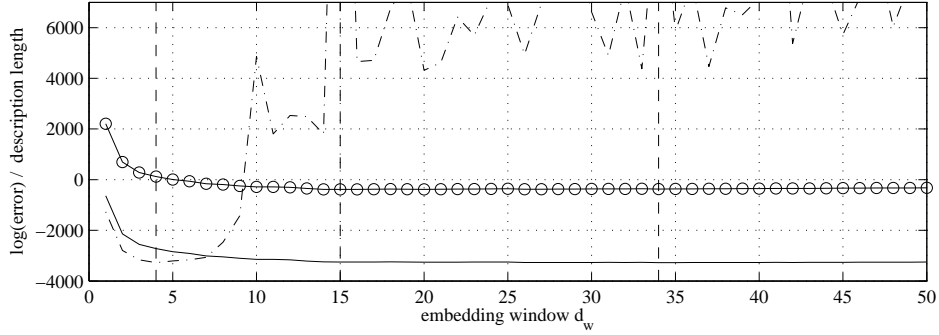


Fig. 1. **Computation of description length as a function of embedding window for Rössler time series data.** The solid line and dot-dashed line are proportional to the logarithm of the sum of the squares of the model prediction error using a local constant and local linear method respectively. The local constant model utilised is described in section 2, the local linear scheme is that described in [15]. For the second modelling scheme a clear minimum occurs at 4. The local constant modelling scheme employs only lags that provide an improvement to model prediction error and its error as a function of embedding window is therefore monotonic (plateau onset occurs at 34). For small values of embedding window the linear scheme performs best, but for large values, behaviour is poor and extremely erratic. Computation of description length utilising the local constant scheme (solid line with circles) yields an optimal embedding window of 15. For clarity, the values $d_w = 4, 15, 34$ are marked as vertical dashed lines.

where $a = 0.398$, $b = 2$ and $c = 4$. For these parameter values the data exhibits broad band chaos. Figure 1 demonstrates the computation of (8) as a function of embedding window. To estimate model prediction error we employ the rather simple interpolative scheme described in the previous section. For comparison, the performance of alternative (more complex) modelling schemes is also shown in figure 1. We find that alternative, more parametric, modelling methods produce results which are sensitively dependent on “correct” choice of modelling algorithm parameters⁷.

The first zero of the autocorrelation function occurs at a lag of 8 and the data exhibits a pseudo period of about 31 samples. With the embedding lag set at 8, false nearest neighbours indicates a minimum embedding dimension of 4. Standard methods, therefore, suggest an embedding window of roughly 32.

By coincidence⁸, the minimum of the model prediction error for a constant model occurs at this value. Conversely, the minimum of the error of the local

⁷ By modelling algorithm parameters we mean parameters associated with the model selection scheme itself rather than only the parameters optimised by that scheme.

⁸ In other examples, and for other amounts of noise or with other lengths of data this proved not to be the case.

linear model occurs at a value of 4. This comparatively low value of embedding window is due to the relative complexity of the local linear modelling scheme [16]. Although this scheme performs best for small embedding windows, the additional information introduced with larger embedding windows is not recognised by this scheme. The main reason for this is that the parameters of the scheme (neighbourhood size, neighbourhood weights and so on) are also dependent on the embedding dimension and embedding lag. For example, values of neighbourhood size which work well for a small dimension embedding may not work well for larger embedding dimension. Moreover, as embedding dimension becomes larger it becomes difficult to find good values for these parameters.. This general behaviour is observed in every example we consider. Therefore, although the local linear scheme often provides a good estimate of the optimal embedding *dimension* (as would false nearest neighbours), the description length estimated from a local constant model provides a much better estimate of the optimal embedding *window*.

We have already mentioned that the local constant modelling scheme selects only lags that provide some improvement in model prediction error. Clearly, as d_w increases there is a combinatorial explosion. To address this combinatorial explosion is both difficult and beyond the requirements of this algorithm. We consider only whether the addition of *successive* lags offers an improvement. Suppose for a d_e dimensional embedding the chosen model includes the lags $\{\ell_1, \ell_2, \dots, \ell_k\}$ (where $0 \leq \ell_1 \leq \ell_i < \ell_{i+1} \leq \ell_k < d_e$). To determine the set of model lags for the (d_e+1) -dimensional embedding we consider the performance of the local constant model with lags $\{\ell_1, \ell_2, \dots, \ell_k, d_e\}$. If this model performs better than the model with lags $\{\ell_1, \ell_2, \dots, \ell_k\}$ then it is accepted, otherwise we retain only the lags $\{\ell_1, \ell_2, \dots, \ell_k\}$.

Therefore, the selected lags may be used as an estimate of the optimal lags for a generalised variable embedding (1). In the case of the Rössler system data analysed in figure 1, the optimal lags were 1 to 15 and 19, 20, 24, 26, 29, 32 and 34. Altogether, 22 different lags. Clearly, a 22 dimensional embedding is excessive, and some subset of these lags would probably prove sufficient. Moreover, the minimum description length optimal embedding window is 15, limiting the selection to the first 15 lags. It is reasonable to suppose that each of these large number of lags may contribute some significant novel information to the modelling scheme. However, the expression we hope to optimise (8) is independent of which lags are included (indeed, in this example, they are *all* included⁹), and therefore we do not consider this issue more closely here. We defer the selection of optimal lags from this set for the modelling phase of dynamic reconstruction.

In figure 2 we examine the effect of various noise levels and different length

⁹ This is not the case in general.

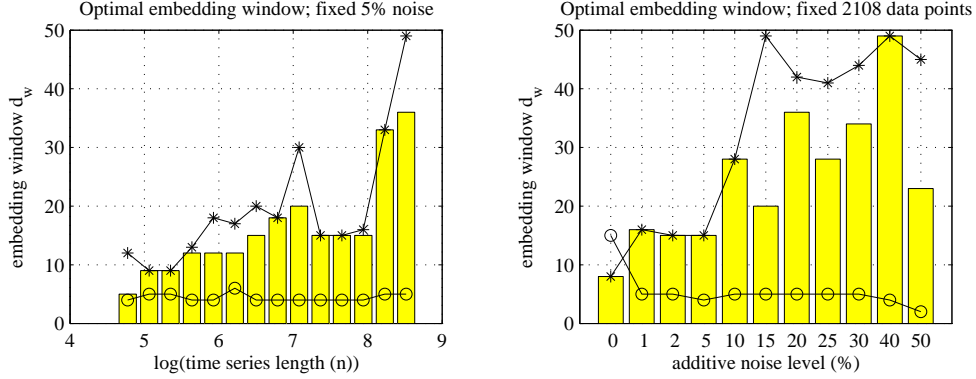


Fig. 2. Optimal embedding dimension as a function of data length and noise level The solid bars depict the optimal model size utilising the methods described in this paper for a single realisation of Rössler time series data. The panel on the left is for a fixed noise level of 5% and time series length between 118 and 5000 data. The panel on the right is for fixed data length of 2108 data and various noise levels (expressed as percentage of the standard deviation of the data). For the cases where noise was added to the time series, the results depicted here are for a single realisation of that noise (not an average). This is the likely cause of the moderate variation in the results observed for larger noise levels. For comparison, the embedding window that yielded minimum error for the local constant (asterisks) and local linear (circles) models is also shown.

time series on the selection of embedding window. We observe that for longer time series, the optimal embedding window is larger. This is consistent with what one might expect. For short time series the optimal model can only capture the short term dynamics and therefore only recent past history (a small embedding window) is required. For larger quantities of data one is able to characterise the more sensitive long term dynamics and a larger embedding window provides significant advantage. Initially, an embedding window of about 10 is sufficient, while for the longest time series an embedding window of 35 is optimal. Significantly, these two values correspond to approximately the first zero of the autocorrelation function (or one-quarter of the pseudo-period) and the pseudo-period of the observed time series.

We note in passing, that, the optimal embedding window for the local constant window is an upper bound on the minimum description length best window. This is as we would expect. The description length is the sum of a term proportional to the model prediction error and a function which increase monotonically with embedding dimension (the description length of the local constant model). Therefore the minimum of the model prediction error must be no less than the minimum of the description length.

Conversely, we find that the optimal embedding window for the local linear method remains about 4 or 5 (roughly corresponding to the optimal embedding

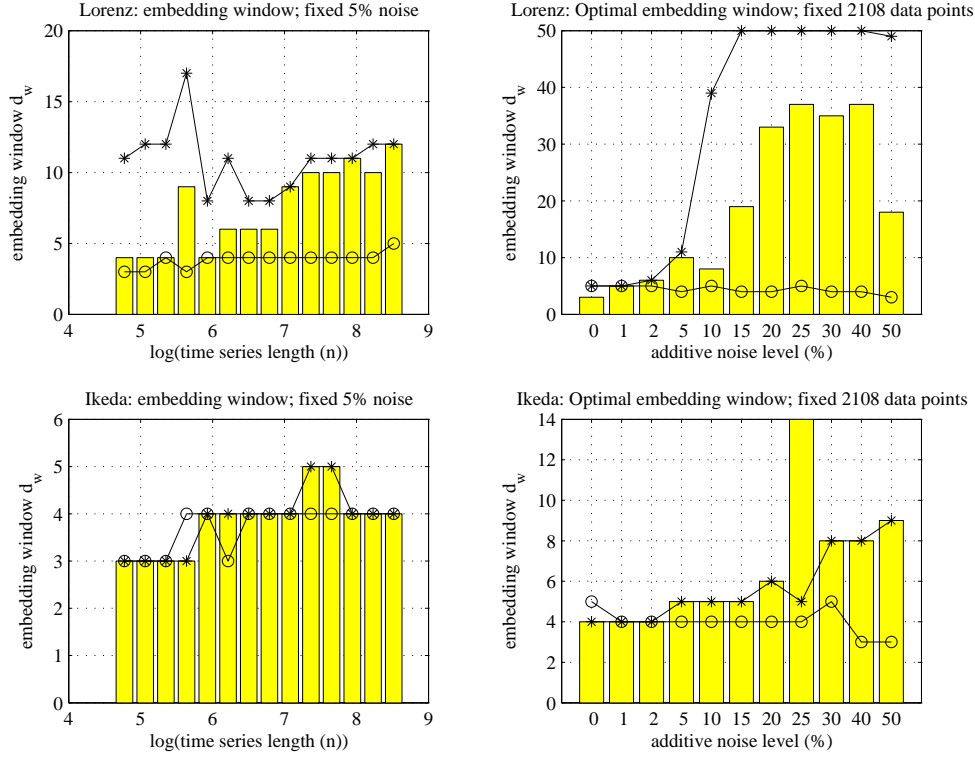


Fig. 3. Optimal embedding windows for Lorenz and Ikeda time series. The calculations depicted in figure 2 are repeated for time series of two standard systems. The top two panels are for a single realisation of the chaotic Lorenz system, the bottom two panels are for a single realisation of the chaotic Ikeda map. The solid bars depict the optimal model size utilising the methods described in this paper. The leftmost panels are for a fixed noise level of 5% and time series length between 118 and 5000 data. The panels on the right are for fixed data length of 2108 data and various noise levels (expressed as percentage of the standard deviation of the data). This is the likely cause of the moderate variation in the results observed for larger noise levels. For comparison, the embedding window that yielded minimum error for the local constant (asterisks) and local linear (circles) models is also shown.

dimension).

Variation in the noise level for a fixed length time series demonstrates similar behaviour. For noisier time series a larger embedding window is required, as increasing the noise on each observation decreases the useful information provided. As the information provided to the optimal model by each observation decreases, more observations (a larger embedding window) is required to provide all the available information. For noise levels of up to 30% this method provides consistent, repeatable, results. Noisier time series tend to yield a larger variation in the optimal estimates of embedding window. Note that in contrast, the local linear scheme performs progressively worse, utilising a diminishing window as the noise level is increased. We believe that this is due

model	MDL	RMS	size
Standard ($d_e = 4, \tau = 8$)	-655 ± 23	0.158 ± 0.003	15.6 ± 2.9
Windowed ($d_w = 15$)	-716 ± 17	0.151 ± 0.004	21.1 ± 5.5

Table 1

Comparison of model performance with standard constant lag embedding (a *Standard Embedding*) and embedding over the embedding window suggested in figure 2 (a *Windowed Embedding*). Figures quoted are the mean of 60 nonlinear models, fitted with a stochastic optimisation routine to the same data set, and standard deviations. Figures quoted here are for 2000 data points with 5% noise, other values of these parameters gave similar, consistent, results. The three indicators are minimum description length (MDL) of the optimal model, root-mean-square model prediction error (RMS) and the model size (number of nonlinear terms in the optimal model). For each indicator, the new embedding strategy shows clear improvement. MDL and RMS have decreased, indicating a more compact description of the data and a smaller prediction error, respectively. Conversely, the mean model size has increased indicating that more structure is extracted from the data. Several other measures were also considered: mean amplitude of oscillation, correlation dimension, entropy and estimated noise level [18]. However, for each of these measures the variance between simulations of models built using the same embedding strategy was as large as that between the different embedding strategies. The results of these calculations are therefore omitted.

to the additional parametric complexity of this modelling method. As more noise is added to the data, the (relatively) complex rules used to determine near neighbours and derive a weighted linear prediction from these, becomes more prone to the system noise, and actually performs worse.

In figure 3 we repeat the above calculations for time series generated from the standard chaotic Lorenz system and the Ikeda map [17]. Variation of optimal embedding window as a function of noise and data length for the Lorenz data is very similar to the results depicted in figure 2 for the Rössler system. Increasing noise level or time series length yields a larger optimal model. Furthermore, optimal embedding window values tend to coincide with the pseudo-period of the time series, or one-quarter, or one-half of this value.

Results for the Ikeda map are substantially different. In this case the optimal embedding window estimated coincides with the value that minimises the error of the local constant and linear models. In general, an embedding dimension of 3 or 4 is suggested, and this is what one would expect for this system¹⁰.

We now return to the main purpose of estimating the embedding window, namely the reconstruction of the dynamics. For the Rössler system analysed

¹⁰ Although the fractal dimension of the Ikeda map is less than two, a delay reconstruction of this map is highly “twisted” and requires an embedding dimension of 3 or 4 to successfully remove all intersecting trajectories.

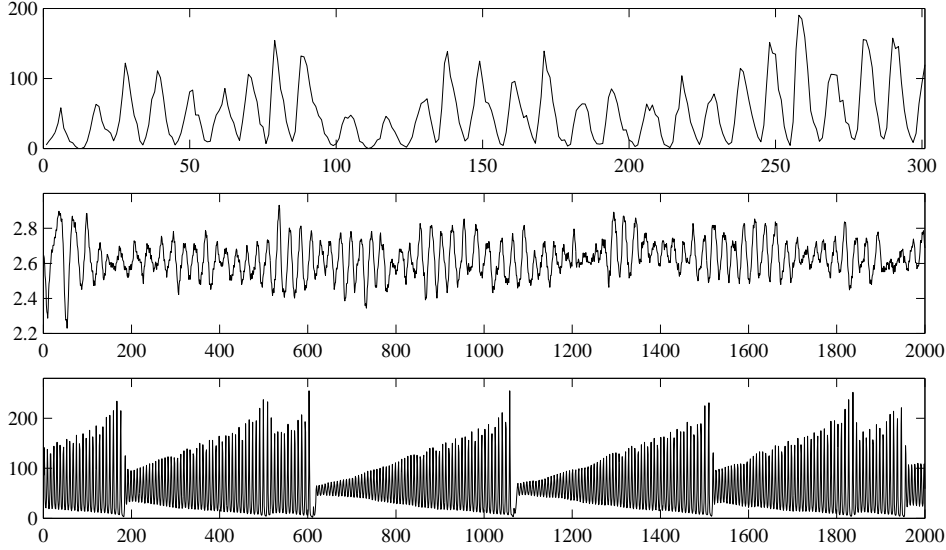


Fig. 4. **Experimental time series data** The three experimental time series examined in this paper are depicted (from top to bottom): annual sunspot numbers for the period 1700 to 2000, a recording of human electrocardiogram rhythm during ventricular fibrillation, and the chaotic “Santa-Fe” laser times series. For the lower two panels only the first 2000 points are utilised for time series modelling.

in figures 1 and 2 we build nonlinear models following the methods described in [4] with embedding suggest by either autocorrelation and false nearest neighbours (namely $d_e = 4$ and $\tau = 8$), hereafter referred to as a *Standard Embedding*, or with the embedding window (of 34), hereafter a *Windowed Embedding*. Table 1 compares the average model size (number of nonlinear basis functions in the optimal model) and model prediction error for 60 models of this time series (2000 observations and 5% noise) with each of these two embedding strategies. These models are built to minimise the description length of the data given the model, and therefore a comparison of the optimal model description length is also given. These qualitative measures show a consistent improvement in the model performance for the model built from the windowed embedding.

4 Applications

We now consider the application of this method to three experimental time series: the annual sunspots times series [19], human electrocardiogram (ECG) recordings of ventricular fibrillation (VF) [20,21], and experimental laser intensity data [22,23]. The raw time series data are depicted in figure 4.

Since the main motivation for selection of embedding window with the method

data	MDL	RMS	size	CD
sunspots				
$(d_e = 6, \tau = 3)$	1267.9 ± 12.1	13.16 ± 1.116	7.32 ± 1.818	0.938 ± 0.456
$(d_w = 6)$	1230.1 ± 11.6	12.31 ± 0.6886	6.96 ± 1.50	0.7836 ± 0.4145
VF ECG				
$(d_e = 5, \tau = 8)$	-14333 ± 28	0.02468 ± 0.0003846	31.47 ± 7.326	1.003 ± 0.099
$(d_w = 2)$	-14163 ± 14	0.02751 ± 0.0001500	15.38 ± 2.66	1.124 ± 0.107
laser				
$(d_e = 5, \tau = 2)$	5753.6 ± 153.9	2.405 ± 0.2954	100.8 ± 12.3	n/a
$(d_w = 10)$	5239.8 ± 159.0	1.767 ± 0.1992	109.5 ± 12.3	0.8637 ± 0.7999

Table 2

Comparison of model performance with standard constant lag embedding and embedding over the embedding window suggested in figure 2. Figures quoted are the mean of 60 nonlinear models, fitted with a stochastic optimisation routine to the same data set, and standard deviations. Figures quoted here are for 2000 data points, where more data is available, longer time series samples gave similar, consistent, results. The four indicators are minimum description length (MDL) of the optimal model, root-mean-square model prediction error (RMS), the model size (number of nonlinear terms in the optimal model), and the correlation dimension (CD) of the free run dynamics. For the laser time series, none of the models built using the standard embedding produced stable dynamics and it was therefore not possible to estimate correlation dimension. The correlation dimension estimated directly from these three data sets was 0.396, 1.090, 1.182 (note that the low value for the first data set is an artifact of the short time series).

described in this paper is to improve modelling results we concentrate exclusively on the comparison of the performance of nonlinear models of this data with standard embedding techniques and the windowed embedding suggested by the algorithm proposed here. By construction, the local constant modelling scheme performs best with the windowed embedding. Therefore, we consider a more complicated nonlinear radial basis modelling algorithm, first proposed in [13] and most recently described in [10]. Like the windowed embedding strategy, this modelling scheme is designed to optimise the description length of the time series [10].

We are interested in two types of measures of performance: short term behaviour (for example mean square prediction error) and dynamic behaviour (invariant measures of the dynamical systems). Results equivalent to those depicted in table 1 have also been computed and are summarised in table 2.

Table 2 shows that for the sunspot time series and the experimental laser intensity recording, the windowed embedding improved model performance.

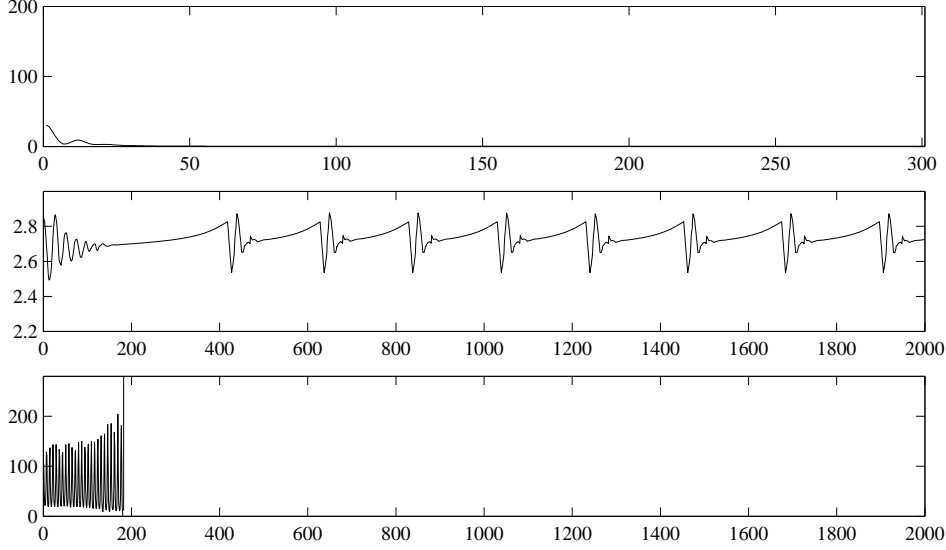


Fig. 5. **Typical model behaviour using the standard embedding strategy** (d_e, τ): Three simulated time series from models of the experimental data examined in this paper are depicted. The panels correspond to those of figure 4 and the horizontal and vertical axes in these figures are fixed to be the same values as the corresponding panels of figure 4.

That is, the description length was lower, the one-step model prediction error was less and the models were larger. However, with the exception of one step model prediction error the difference in these measures was not statistically significant. For the recording of human VF the new method did not improve model performance and, in fact, the optimal embedding window was $d_w = 2$: substantially smaller than one would reasonably expect from such a complex biological system. It seems plausible, that in this case, the time series under consideration is too short, noisy or non-stationary (this conclusion is supported by figure 4). Finally, we note that the result for the sunspot time series is particularly encouraging because this improvement in short term predictability is achieved with a much smaller embedding ($d_w = 6$ compared to $d_e \tau = 18$).

However, as has been observed elsewhere [10], short term predictability is not the best criteria with which to compare models of nonlinear dynamical systems. Therefore, for each model we estimated correlation dimension, noise level and entropy, using a method described in [18]. Furthermore, under the premise that these models should exhibit pseudo-periodic dynamics we also computed mean limit cycle diameter (i.e. the amplitude of the limit cycle oscillations). In every case we found that the dynamics exhibited by models built from the traditional (i.e. uniform) embedding strategy was more likely to either be a stable fixed point or divergent.

Finally, figures 5 and 6 show typical noise free dynamics in models of each of these three systems. No effort was made to ensure that the models performed

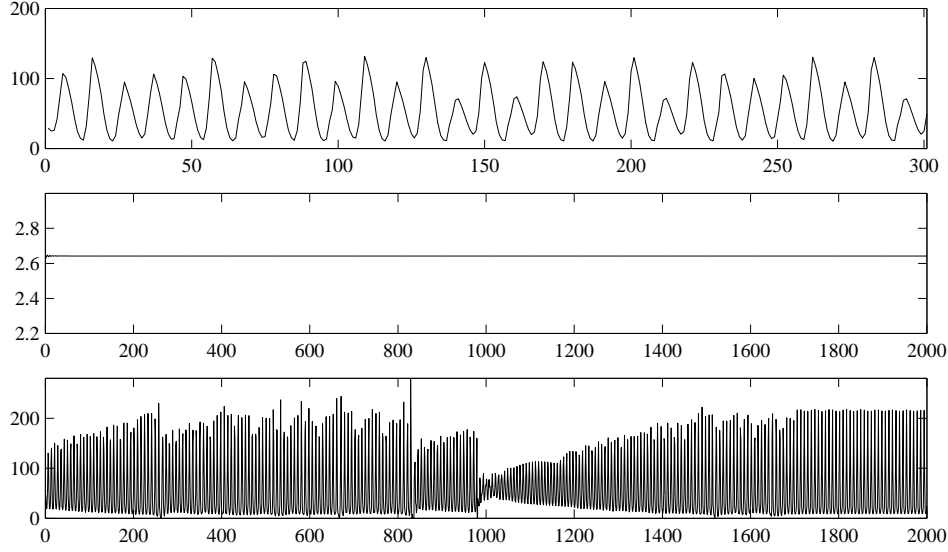


Fig. 6. **Typical model behaviour using the windowed embedding strategy (d_w):** Three simulated time series from the experimental data examined in this paper are depicted. The panels correspond to those of figure 4 and the horizontal and vertical axes in these figures are fixed to be the same values as the corresponding panels of figure 4.

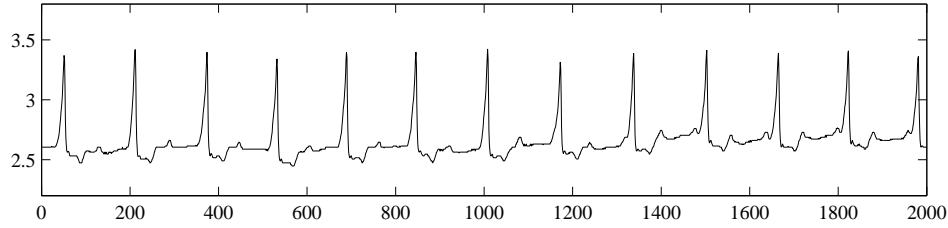


Fig. 7. **Observed electrocardiogram trace after resuscitation:** Following the episode of VF depicted in figure 4, electrical resuscitation was successfully applied. The waveform depicted in this figure was observed 120 seconds after application of defibrillation. Notice that the waveform observed here is similar to the asymptotic behaviour of the model depicted in figure 5. Both the period and the shape of these time series are similar.

well and the models and simulations presented in these figures were selected at random. For the sunspots and laser dynamics (top and bottom panels) the new method clearly performs better. Typically, the original method produced laser dynamics and sunspots simulations that were divergent and a stable fixed point (respectively). These results are typical. In contrast the windowed method yields models which exhibit bounded (almost) aperiodic dynamics¹¹.

¹¹ Closer examination of the laser dynamics indicates that it eventually settles to a stable periodic orbit (this phenomenon can be observed toward the end of the time series depicted in figure 6).

Using the windowed embedding we found that the long term dynamics for models of the VF data performed badly. However, this is to be expected as the optimal embedding window was 2. For this data none of the models produced with either method performed well. Hence, with this short, noisy and non-stationary data the models (built with either embedding strategy) failed to capture the underlying dynamics. Significantly, the estimate of d_w provided by our algorithm indicated that this would be the case. We found that the optimal embedding is only two dimensional and this suggests that the best thing to do is to not build a model of the dynamics at all. Hence, even this negative result is encouraging: we have established the limitations of this algorithm and found that even in this situation the results are consistent. We note with some curiosity that the dynamics exhibited in the second panel of figure 5 closely resembles the human electrocardiogram during regular rhythm (see figure 7 for a representative recording), despite the data being recorded during VF — we have no explanation for this. This behaviour, although exhibited by this one model was not present in simulations from all similar models. It is suggestive that the VF waveform includes information concerning the underlying (slower) sinus rhythm dynamics. But the evidence for this is definitely not conclusive.

5 Conclusions

We have approached the problem of optimal embedding from a modelling perspective. In contrast to previous studies (which focused on estimating dynamic invariants) our primary concern was selection of embedding parameters that provide the optimal reconstruction of the underlying dynamics for an observed time series. To achieve this we assumed that the optimal model is that which minimises the description length the data. From this foundation we showed that the best embedding has a constant lag ($\tau = 1$) and a relatively large embedding window d_w . In general the optimal d_w will be determined by the amount of noise and the length of the time series. From an information theoretic perspective this is what one would expect: $\tau > 1$ implies some information is missing from the embedding. The optimal value of d_w reflects a balance between a small embedding with too little information to reconstruct the dynamics and a large embedding where the model ceases to describe the dynamics.

To compute the quantity d_w we introduced an extremely simple *non-predictive* local constant model of the data and select the value of d_w for which this model performs best. One can see that this offers a new and intuitive method for selection of embedding parameters. In essence, one could neglect description length and simply choose the embedding such that this model performs best. However, the addition of description length makes the optimal d_w dependent not only on the noise but also on the length of the time series. We see that

for short time series one shouldn't be confident of a large embedding window.

The similarity between this new method of embedding window selection and the well established false nearest neighbour technique [24] is more than superficial¹². In section 3 and 4 we provided an explicit comparison to between our technique and the “standard” false nearest neighbour method. However, there are various improvements to this algorithm (such as [24]) which are worthy of further consideration. Nonetheless, there are several important distinctions between our method, and these false nearest neighbour techniques. As we have already emphasised, the aim of this method (to achieve the best model of the dynamics) differs from that of false nearest neighbours (topological unfolding). Furthermore, the incorporation of minimum description length means that our method explicitly penalises for short or noisy time series.

At a functional level, the two algorithms are similar because both methods seek to avoid data points which are close, but which quickly diverge. Such points are (respectively) either false nearest neighbour or bad nonlinear predictors of one another. However, where as false nearest neighbour methods seek only to avoid this situation (i.e. spreading out the data is sufficient), the windowed embedding method insists that the neighbours which are the best predictors be found.

Consider the situation where a systems' dynamics are either stochastic or extremely high dimensional. Using false nearest neighbour methods, one may simply embed the data in a high enough dimension so that the data are sufficiently sparse. However, doing so does not improve the nonlinear prediction error, consequently, the windowed embedding method would prefer a small embedding window.

Conversely, consider the situation at a separatrix. Points which are close do rapidly diverge from one another and so they will appear as false near neighbours for large embedding dimension, until (at a time scale similar to that of the underlying system) the points are eventually, sufficiently spread). But from a nonlinear prediction view-point, these points are equally difficult to predict for all embedding dimension, and again the windowed embedding method will indicate a much smaller embedding dimension than that suggested by a strict application of false nearest neighbours¹³.

¹² The comparison of this method to that described in [24] is particularly apt. Cao introduces a modified false nearest neighbour approach which, like our method, avoids many of the subjective parameters of alternative techniques.

¹³ We acknowledge that this problem is actually related to the “plateau” observed in plots of the fraction of false nearest neighbours against embedding dimension. In many cases, prudent selection of “plateau-onset” can minimise the problem. However, this remains somewhat subjective.

Finally, we note that the examples of section 3 showed that this method performed consistently and the applications in section 4 showed that selecting embedding parameters in this way improved the model one-step prediction error. In effect, this is a demonstration that the method is working as expected. More significantly, we found that the dynamics produced by models built from windowed embedding also behaved more like the experimental dynamics than for models built from a standard embedding. This is a very positive results, however, we are now faced with a more substantial problem. The problem of building the best nonlinear model for the data once the embedding window has been determined [10]. Information theory has shown us that the optimal embedding should fix $\tau = 1$, we now need to consider the practice of nonlinear modelling to determine which lags $\ell = 1, 2, 3, \dots, d_w$ are significant for practical reconstruction from specific experimental systems.

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