Optimal Neural Network Feature Selection for Forecasting of Spatial-Temporal Series

Eurico Covas, Emmanouil Benetos

***Abstract*—We show empirical evidence on how to construct the optimal feature selection or architecture for the input layer of a feedforward neural network for the propose of forecasting spatial-temporal signals. The approach is based on results from dynamical systems theory, namely the non-linear embedding theorems. We demonstrate it for a variety of two-dimensional signals with one spatial dimension and one time dimension, and show that the optimal input layer seems to consist of a two dimensional grid, with spatial/temporal lags determined by the minimum of the mutual information of the spatial/temporal signals and the number of points taken in space/time decided by the embedding dimension of the signal. We present evidence of this conjecture by running a Monte Carlo simulation of several combinations of input layer architectures and show that the one predicted by the non-linear embedding theorems seems to be optimal or close of optimal. In total we show evidence in four unrelated systems: a series of coupled Hénon maps; a series of couple Ordinary Differential Equations (Lorenz-96) phenomenologically modelling atmospheric dynamics; the Kuramoto-Sivashinsky equation and finally real data from sunspot areas in the Sun (in latitude and time) from 1870 to today.**

***Index Terms*—IEEE, IEEEtran, journal, LaTeX, paper.**

I. Introduction

GIVEN a physical data set one of the most important questions one can pose is:"Can we predict the future?" This question can be put forward irrespectively of the fact that we may already have some insight or even be certain on what the exact model behind some or all the observed variables is. For example, for chaotic dynamical systems [1], [2], we may even have the underlying dynamics but still find it hard to predict the future, given that chaotic systems have exponential sensitivity to initial conditions. The more chaotic a system is (as measured by the positiveness of their largest Lyapunov exponents [3], [4]) the harder it gets to predict the future, even within very short time horizons. In the limit case of a random system, it is not possible to predict the future at all, although one can opine on certain future statistics [5]. For the case of weakly chaotic systems, there is an extensive literature on forecasting methods ranging from linear approximations [6]; truncated functional expansion series [7], [8]; non-linear embeddings [9]; auto-regression methods [10]; hidden Markov models [11] to state-of-the-art neural networks and deep learning methodologies [12].

Most literature on forecasting chaotic signals is dedicated to a single time series, or treat a collection of related time series as a non-extended set, i.e. a multivariate set of discrete as opposed to continuous time series. For forecasting spatial-temporal chaos we refer the reader to [13]–[21] and references therein. Even rarer are attempts to forecast spatial-temporal chaos using neural networks and deep learning methodologies [22]–[29], although this field of research is clearly growing at the moment. Nonetheless, this area of research is of importance, as most physical systems are spatially extended, e.g. the atmospheric system driving the weather [30]; the solar dynamo driving the Sun's sunspots [31]; and the influence of sunspots on the Earth's magnetic field via the solar wind, coronal mass ejections and solar flares – the so-called space weather [32]–[46].

The reasons why spatial-temporal chaos is so difficult to forecast are: first the Hausdorff dimension of the attractor [47] – usually quite large, the so-called curse of dimensionality; and second how to choose the variables to use for forecasting, i.e., is there enough information on the same point back in time to derive the future of that particular point, or do spatial correlations and spatial propagation affect it in a way that one must take into account some spatial and temporal neighbours set to forecast the future, and if so, can that set be defined and how can it be constructed? It is this last question that we investigate in this article, in the particular context of spatial-temporal forecasting using neural networks. Feature extraction and the design of the architecture of the input layer for a neural network is considered to be an art form, relying mostly on trial and error and domain knowledge. For forecasting of time series, a simple approach consists of designing the input layer as a vector of previous data using a time delay, the time delay neural network method [48]–[53]. For spatial-temporal series, one can generalize it to include temporal and spatial delays [20], [22]. This is where the connection to dynamical systems can be useful. In 1981, Takens established the theoretical background [54] in the Takens embedding theorem for a mathematical method to reconstruct the dynamics of the underlying attractor of a chaotic dynamical system from a time ordered sequence of data observations. Notice the reconstruction conserves the properties of the original dynamical system up to a diffeomorphism. Further developments established a series of theorems by [55], [54], [56] and [57]. These theorems serve the basis for a non-linear embedding and forecasting on the original variables. The theorems and related articles propose to use a time delay based on the first minima of the *mutual information* - see [58]–[60]) and to use the number of points using the method of *method of false nearest neighbours* detection suggested by [61] and reported in detail in [59], [62]–[64]. Using this theoretical framework, we propose that this non-linear embedding method can be used to indicate what

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the best way is to construct the input layer for a neural network in both space and time.

In this paper we show empirical evidence for an optimal architecture of the input layer of a neural network which tries to forecast or predict a spatial-temporal signal. Here we show the empirical evidence for fours particular cases of two-dimensional data series s_m^n, where byy two-dimensional we mean a scalar field which can be defined by a $N \times M$ matrix with components $s_m^n \in \mathbb{R}$.

A. Neural networks for time-series forecasting

Describe the use of feedforward artificial neural networks, then recurrent networks and other methods (put all references). Put all references to pure time only forecasts [65]. DO WE REALLY NEED THIS SECTION?

B. Neural networks for spatial-temporal forecasting

There has been several attempts to forecast spatial-temporal data series in the literature using neural networks (ADD MORE REFERENCES [23], [24], [66], [67]). The references above confine themselves to attempts to forecast the actual full scalar field s_m^n, as opposed to the ongoing research on pattern recognition in moving images (2D and 3D), which attempt to pick particular features in images (e.g. car, pedestrian, bicycle, person) and to forecast where those features will be in subsequent images within the particular moving sequence (ADD REFERENCES) or research on word sequences (ADD REFERENCES).

C. Input layer architecture for neural networks for spatial-temporal forecasting

Some authors discuss the use of either mutual information and/or embedding dimension as a constraint on the input layer, i.e. the feature selection [50], [52], [53], [68]–[86] used the mutual information and/or the false nearest neighbours' methods to estimate the suitable embedding parameters. [69], [70], [74], [84], [85], [87], [88] attempted to forecast the solar sunspot number using neural networks and they used the embedding dimension of the sunspot time series as way to define the architecture of the input layer. [89] generalize the mutual information approach to higher dimensions but does not connect it to the problem of the neural network input layer architecture optimization. There are also authors [90] that try to use neural networks to determine the optimal embedding and time delay for the purposes of local reconstruction of states with a view to forecast (the opposite of what we try to empirically demonstrate here). Other authors [18] try to use Support Vector Machines (SVMs) to forecast in space and time and use time delays and embedding approaches to define the states vectors. In fact, Parlitz and Merkwirth [16] in the ESANN 2000 meeting proceedings paper mentioned that local reconstruction of states "... may also serve as a starting point for deriving local mathematical models in terms of polynomials, radial basis functions or neural networks.". Here we attempt to show empirical evidence that this is not just a starting point, but the optimal neural network input architecture.

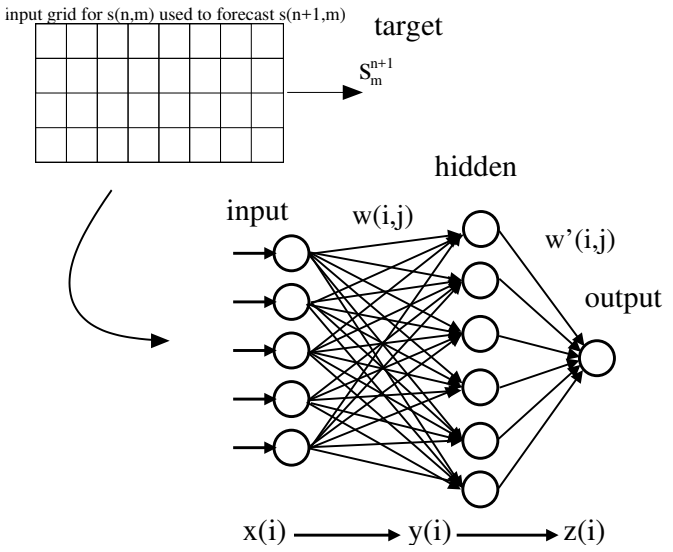

Fig. 1. Forecasting method illustration. The neural network is made of an input layer, one or more hidden layer(s) and one output layer. In this article, we use only one hidden layer and the output layer is made of a single neuron. Each input pattern $x(i)$ is sent to the input layer, then each of the hidden neurons values is calculated from the sum of the product of the weights by the inputs $\sum w(i,j)x(i)$ and passed via the activation function. Then the output is made by the product of the second set of weights times the hidden node values $\sum w'(i,j)y(i)$ again passed to another (or the same) activation function. Each input pattern $x(i)$ is actually a matrix constructed using an embedding space of spatial and temporal delays, calculated from the actual physical spatial-temporal data values $s(n,m)$. After many randomly chosen input patterns are passed via the neural network, the weights hopefully converge to an optimal training value.

All of the references above on neural network forecasting of spatial-temporal data series either use a simple delay based architecture for the input layer, or use a time delay based on the first minima of the *mutual information* as proposed in [58]–[60]) and/or use the number of points dictated by the embedding theorems by [55], [54], [56] and [57] using the method of *method of false nearest neighbours* detection suggested by [61] and reported in detail in [59], [62]–[64]. However, as far as we are aware, all the references to using the embedding theorems and the related mutual information method and the false nearest neighbours method seems to be not justified, i.e., the approach is explained but not proven either theoretically or empirically.

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II. Neural Network architecture

The neural network architecture we choose to demonstrate our possible conjecture is a form of the basic feedforward neural network, sometimes called the time-delayed neural network [48], trained using the so-called back-propagation algorithm [91]–[93]. We focus on spatial-temporal series, so we have extended the usual time-delayed neural network to be a time and space delayed network. The overall architecture of the network is depicted in detail in Fig. 1.

Under this architecture, we use the ideas proposed in [16] to construct a grid of input values which are then fed to the neural network to produce a single output, the future state.

Formally, let $n = 1, ..., N$ and $m = 1, ..., M$. Consider a spatial-temporal data series $\mathbf{s}$ which can be defined by a $N \times M$ matrix with components $s_m^n \in \mathbb{R}$. To these components, we will call *states* of the spatial-temporal series. Consider a number $2I \in \mathbb{N}$ of neighbours in space of a given s_m^n and a number $J \in \mathbb{N}$ of temporal past neighbours relative to s_m^n (see Fig. 2 for details). For each s_m^n, we define the input (feature) vector $\mathbf{x}(s_m^n)$ with components given by s_m^n, its $2I$ spatial neighbours and its J past temporal neighbours, and with K and L being the spatial and temporal lags:

$$\mathbf{x}(s_m^n) = \{s_{m-IK}^n, ..., s_m^n, ..., s_{m+IK}^n, s_{m-IK}^{n-L}, ..., s_m^{n-L}, ..., s_{m+IK}^{n-L}, \cdots \cap s_{m-IK}^{n-JL}, ..., s_m^{n-JL}, ..., s_{m+IK}^{n-JL}\} \quad (1)$$

So, the input is a $(2I + 1)(J + 1)$ vector $\mathbf{x}(s_m^n)$ and the target (output) to train the network is the value s_m^{n+1}. In Fig. 2 we show the details of this method. We train the network using stochastic gradient back-propagation (using momentum and weigh decay for regularization) by running a stochastic batch where we randomly sample pairs of inputs and outputs from the training set: $\mathbf{x}(s_m^n)$ and s_m^{n+1}, respectively. Then at test time we choose inputs $\mathbf{x}(s_m^n)$, such that $n = N_{train}$, N_{train} being the number of temporal slices on the training set.

As for the back-propagation hyperparameters, we included an adaptive learning rate $\eta_n = \eta/(1 + n/10000)$, where the parameter η is the initial learning rate and η_n is the learning rate used at time step n, we included a momentum α and a weight decay ρ. In addition, we use one hidden layer with N_h nodes. A further hyperparameter is the choice of the activation function, we use either ReLu or a sigmoid function depending on the test case we are working with. We also normalize the data before passing it through the neural network, in most cases we scale it in linear fashion $x \to \alpha_{nor} + x/\beta_{nor}$, and in the case of real physical data as we will see later, we scale it in logarithmic fashion it by $x \to \alpha_{nor} + \frac{\ln(1+x)}{\beta_{nor}}$, where x is the initial data, and α_{nor} and β_{nor} are the arbitrary shift and scaling constants, respectively. For the weight (and bias) initialization we choose random numbers with a constant distribution between $[0, 1]$ and shifted by α_{rng} and scaled by β_{rng}. The final hyperparameter is the number of steps taken on the stochastic gradient descent (equivalent to a mini-batch approach of $N_{\text{batch}} = 1$) which we denote by N_{steps}. All of these hyperparameters are calibrated and fixed before we do any simulations with respect to the parameters I, J, K, L, which are auto-calibrated by the below mentioned methods derived from dynamical systems theory. In this sense these are not hyperparameters of the neural network.

We then compare the goodness of fit by first visual inspection and second by numerically calculating the so-called structural similarity SSIM(x, y) which has been proposed by [94] and used already in the context of spatial-temporal forecasting in [20], [22]. It has also been used in the context of deep learning used for enhancing resolution on two dimensional images [95] and restoring missing data in images [96]. For details on the SSIM measure see [94], [97], [98]. The SSIM index is a metric quantity used to calculate the perceived quality of digital images and videos. It allows two images to be compared and provides a value of their similarity - a value of SSIM = 1 corresponds to the case of two perfectly identical images. We use it by calculating the SSIM(x, y) between the entire test set and the predicted set.

Although most papers using neural networks for forecasting in time, or in space and time (ADD REFERENCES) may use implicitly (convolutional ones?) or explicitly (TDNNs) (ADD REFERENCES), as far as the authors are aware there has been no firm evidence, either theoretical or empirical on how to generically choose the inputs for a neural network for spatial-temporal forecasting (see however Fig. 6 in [99] who show how the forecasting error for a pure time series prediction changes with the delay and the number of time delay points used as an input – they use a reinforcement learning based dimension and delay estimator to derive the best dimension and delay, but do not seem to show that it is the dynamical systems derived values that are indeed optimal for forecasting neither they show any extension to spatial-temporal signals as we show in this paper). Also notice [50] do show in their Fig. 2 that for forecasting pure time series the window size (dimension) heuristics correspond well to the the optimal one indicated by the relative error of the forecast. Nonetheless, this example is for pure time series only and was not generalized to all the architecture parameters in that work.

Here we propose that the optimal time delay/spatial delays (L and K, respectively) must be the ones based on the first minima of the *mutual information* [58]–[60] and that the optimal number of temporal/spatial points to use (J and I, respectively) must be the ones based on the the method of *method of false nearest neighbours* detection [59], [61]–[64]. We conjecture that as any set of architectures "approach" this optimal architecture, then the SSIM $\to$ 1. In the case of finite training sets and/or noisy training sets $SSIM \to x < 1$, where x is the best forecast possible given the data set. Visually we believe that the SSIM versus some reasonable metric constructed to represent the distance between any architecture and the optimal architecture will show a skewed bell shape as depicted in Fig. 3. In this conjecture we use the most obvious candidate to represent the distance between any architecture and the optimal architecture, the Euclidian distance between the architecture four parameters $d_e = \sqrt{(I - I^*)^2 + (J - J^*)^2 + (K - K^*)^2 + (L - L^*)^2}$.

III. Monte Carlo results

In order to empirically substantiate our conjecture, we take four examples of spatial-temporal series and attempt to forecast using our feedforward neural network. First, we calculate the optimal time delay/spatial delays (L^* and K^*, respectively) using the first minima of the mutual information optimal number of temporal/spatial points to use (J^* and I^*, respectively) using the method of method of false nearest neighbours. We then use a Monte Carlo simulation on each one of our four examples, sampling randomly values of I, J, K, L and calculating the values $d_e(I, J, K, L)$ and SSIM(I, J, K, L).

We first take a physical system example, a real data example, and then we progress from "simpler" systems (maps) capable of generating spatial-temporal chaos to more "complex" systems (Ordinary Differential Equations - ODEs) to really

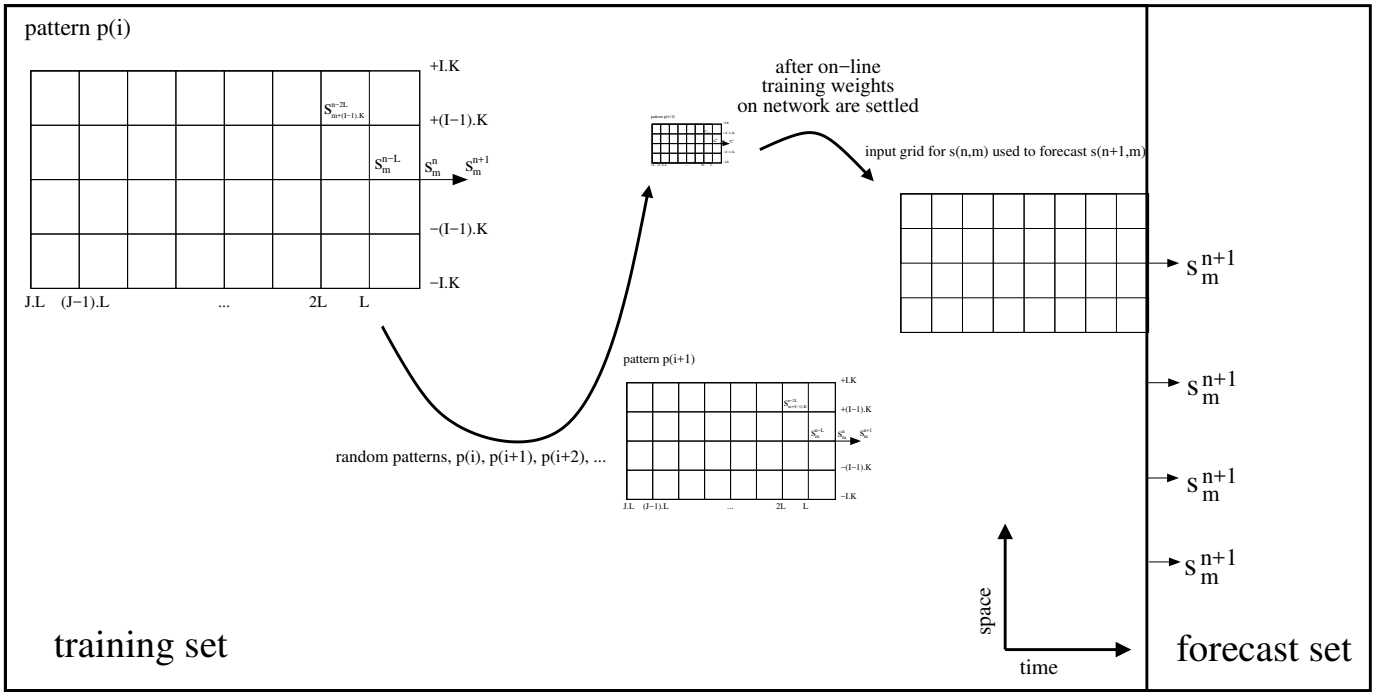

Fig. 2. Forecasting method illustration. One constructs an embedding space using space and time delays, then assemble randomly positioned grid input patterns within the training set to pass to the neural network (in this figure we show 3 randomly selected input patterns). The input is a $(2I+1)(J+1)$ vector $\mathbf{x}(s_m^n)$ and the target (output) to train the network is the value s_m^{n+1}. After training with a sequence of patterns $p(i)$, $p(i+1)$, $p(i+2)$, ... then the patterns adjacent to the forecast set are used to calculate the outputs to compare against the forecast. To forecast the $n+2$ slice we concatenate the previously predicted $n+1$ and progress accordingly.

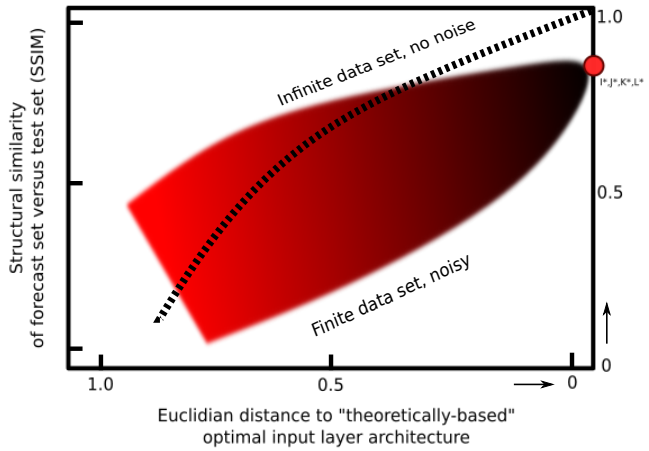

Fig. 3. Our main conjecture. For a infinite noiseless training set, the SSIM approaches SSIM $\rightarrow 1$. For real data sets, there is a dispersion of the SSIM versus some reasonable metric constructed to represent the distance between any architecture (e.g. $d_e\sqrt{(I-I^*)^2+(J-J^*)^2+(K-K^*)^2+(L-L^*)^2}$).

"complex" systems (Partial Differential Equations - PDEs). This is partially motivated by results in the literature that show that general universalities are present in different levels of simplification of physical models [100], from the original PDEs to truncated ODE expansions (e.g. spectral method expansions [101]) to the most extreme simplification or discretization such as maps which capture the essence of the problem. In all cases we take examples with one spatial and one temporal dimension. However, we believe that our conjecture will extend to multiple spatial and one temporal dimensional systems. Notice that here we are not trying to demonstrate that neural networks, and in particular feedforward neural networks can perform well in predicting spatial-temporal chaos, but rather to show that the optimal choice of the input layer features is given by dynamical systems theory and does not need to be another neural network hyperparameter calculated by the "dark art" of trial and error.

A. *Sunspot data - a physical system example*

The first example we take is a physical real data example based on a previous paper of one of us [22], where a neural network using this type of architecture above (Fig. 1) was used to forecast sunspot areas $A(t,\theta)$ in our Sun in both space (θ latitude) and time (Carrington Rotation index).

Several authors [69], [74], [79], [81], [82], [84], [85], [87], [88], [102]–[144] have already attempted to use neural networks to forecast aspects of the sunspot cycle, although none in both space and time, having restricted themselves to using these neural networks to forecast mostly either the sunspot number or the sunspot areas as a function of time. There are a few examples ([22]) of actual spatial-temporal forecasts using neural networks (SEE MINE AND THE ONE ON MDI/HDI DATA).

We take as a "training set" the data from the year 1874 to approximately 1997 (i.e. the first 1646 Carrington Rotations). We then attempt to reproduce or forecast the sunspot area

butterfly diagram from Carrington Rotation 1921 to 2162 (the last one corresponding approximately to the year 2015); that is, we use 1646 time slices (~122.92 years) to reproduce the next 242 time slices (~18.07 years). The training set corresponds to around 12 solar cycles (cycle 11 to 22), while the "forecasting set" (or validation set) equates to around 1.5 cycles (cycle 23 and half of cycle 24). The entire dataset, including the training and forecasting sets, is a grid $x_j^i = x(i, j)$, with $i = 1888$ and $j = 50$. The training set is a grid $x(1646, 50)$. For this case the optimal values were $I^* = 2$, $J^* = 6$, $K^* = 9$ and $L^* = 70$. The hyperparameters of the neural network were: $N_h = 70$, $\eta = 0.3$, $\alpha = 0.01$, $\rho = 0$, a logarithmic normalization of the inputs scaled with $\alpha_{nor} = 10$ and $\beta_{nor} = 0$, weight initialization with $\alpha_{rng} = 10^{-2}$ and $\beta_{rng} = -0.5$ and N_{steps} =1,000,000 We used the logistic sigmoid function as the activation on both the hidden and output layers. The results are depicted in Fig. 4. It shows a dispersion as conjectured and a convergence to the highest SSIM value we could obtain for this particular slicing of the training and test sets SSIM = 0.836876152.

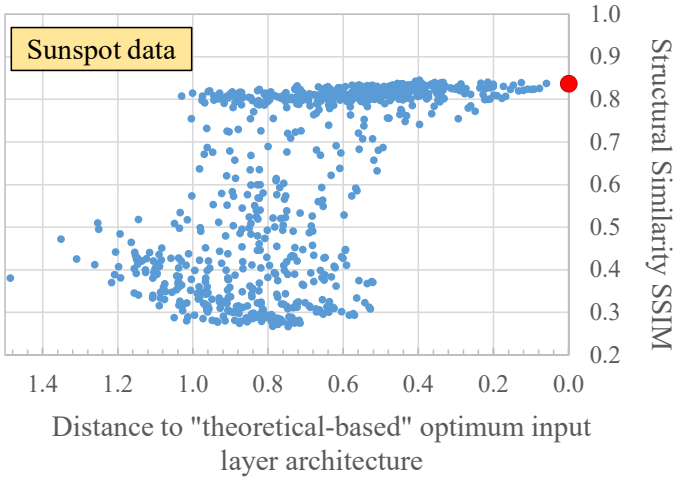

Fig. 4. Monte Carlo simulation of different architectures of the input layer for the neural network forecast for the sunspot data. It shows the structural similarity (SSIM) against how far (in an Euclidean space metric) the particular parameters of a particular run were from the supposely optimal architecture parameters (red dot).

B. Coupled Hénon maps - a discrete-time dynamical system

Motivated by having a real case from a physical system, we then tried to investigate if this same conjecture holds in a very simplified example of a spatial-temporal model. Coupled maps are widely used as models of spatial-temporal chaos and pattern/structure formation [145]–[147].

Following [16], [17] we then take a lattice of $M = 100$ coupled Hénon maps:

$$u_m^{n+1} = 1 - 1.45\left[\frac{1}{2}u_m^n + \frac{u_{m-1}^n + u_{m+1}^n}{4}\right]^2 + 0.3v_m^n, \qquad (2)$$
$$v_m^{n+1} = u_m^n.$$

with fixed boundary conditions $u_1^n = u_M^n = \frac{1}{2}$ and $v_1^n = v_M^n = 0$.

We run the simulation for $N = 531$ time steps, and divided the set into $N_{\text{train}} = 500$ time steps for the training set and $N_{\text{test}} = 31$ time steps for the test set. The other parameters of the neural network were: $N_h = 10$, $\eta = 0.1$, $\alpha = 0$, $\rho = 0$, a linear input normalization scaling with $\alpha_{nor} = 2.947992$, $\beta_{nor} = 0.515$, $\alpha_{rng} = 10^{-3}$, $\beta_{rng} = -0.5$ and $N_{\text{steps}} = 1,000,000$. We used the ReLu function as the activation on both the hidden and output layers.

For this case the optimal values were $I^* = 1$, $J^* = 3$, $K^* = 2$ and $L^* = 3$. The results are depicted in Fig. 4. It shows a dispersion as conjectured and a convergence to the highest SSIM value we could obtain for this particular slicing of the training and test sets SSIM = 0.71139101.

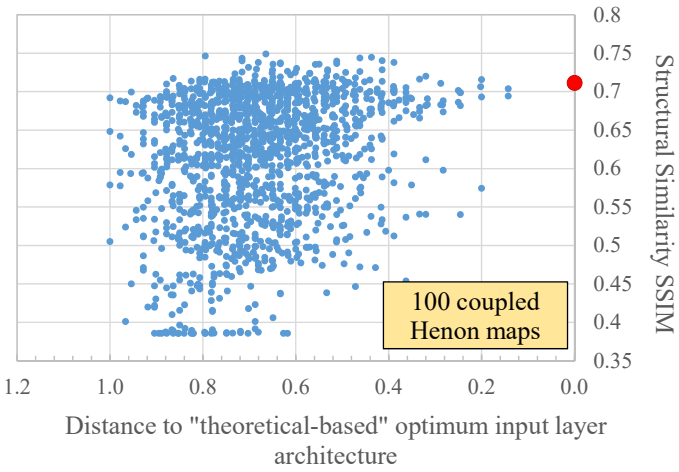

Fig. 5. Monte Carlo simulation of different architectures of the input layer for the neural network forecast for a series of 100 coupled Hénon maps. It shows the structural similarity (SSIM) against how far (in a Euclidean space metric) the particular parameters of a particular run was from the supposedly optimal architecture parameters (red dot). The green line (trendline) seems to show that as the parameters of a randomly chosen architecture get close to the supposedly optimal architecture ones, the SSIM converges to what seems to be the best possible forecast value given the limited dataset.

Results seems to suggest the same structure as depicted in our conjecture diagram and in the previous results for sunspots.

C. Coupled Ordinary Differential Equations - Lorenz-96 model

For the spatially extended ODEs model we used a well-known 40 couple ODE dynamical system proposed by Edward Lorenz in 1996 [148]

$$lCr\frac{d\,x_j}{d\,t} = \left(x_{j+1} - x_{j-2}\right)x_{j-1} - x_j + F, j = 1, \ldots, N = 40, \quad (3)$$

where $x_{-1} = x_{N-1}$, $x_0 = x_N$ and $x_{N+1} = x_1$. We use the forcing $F = 5$ to get some interesting behaviour in space and time. We used a time step $\Delta t = 0.05$ and we have integrated this equation using Matlab (ADD REFERENCE).

We run the simulation for $N = 531$ time steps, and divided the set into $N_{\text{train}} = 500$ time steps for the training set and $N_{\text{test}} = 31$ time steps for the test set. The other parameters of the neural network were: $N_h = 10$, $\eta = 0.05$, $\alpha = 0.001$, $\rho = 0$, a linear normalization input scaling with $\alpha_{nor} = 10$ and $\beta_{nor} = 0.430$, weight initialization with $\alpha_{rng} = 10^{-3}$ and $\beta_{rng} = -0.5$ and $N_{\text{steps}} = 100,000$. We used the ReLU function as the activation on both the hidden and output layers.

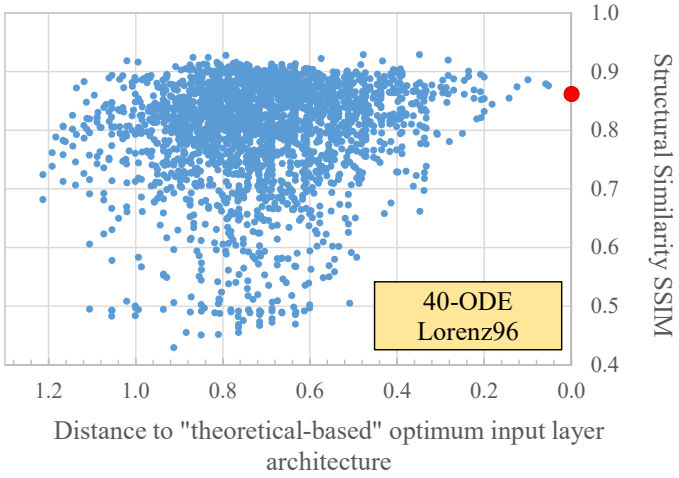

Fig. 6. Monte Carlo simulation of different architectures of the input layer for the neural network forecast for the 40-ODE Lorenz 96 system. It shows the structural similarity (SSIM) against how far (in a Euclidean space metric) the particular parameters of a particular run was from the supposedly optimal architecture parameters (red dot). The green line (trendline) seems to show that as the parameters of a randomly chosen architecture get close to the supposedly optimal architecture ones, the SSIM converges to what seems to be the best possible forecast value given the limited (and noisy) dataset.

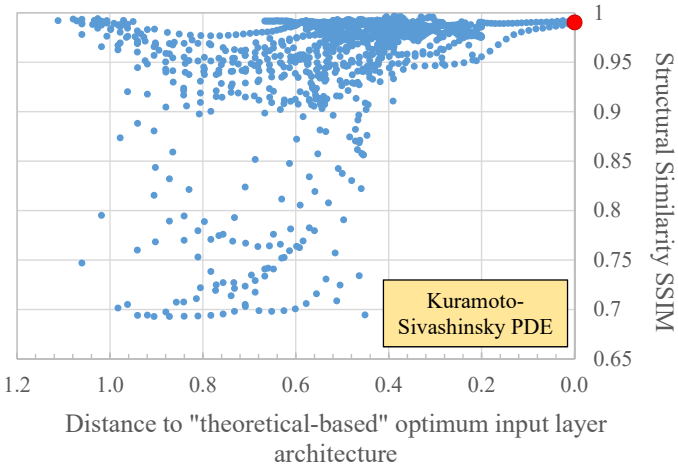

Fig. 7. Monte Carlo simulation of different architectures of the input layer for the neural network forecast for Kuramoto-Sivashinsky with $L = 22$ system. It shows the structural similarity (SSIM) against how far (in a Euclidean space metric) the particular parameters of a particular run was from the supposedly optimal architecture parameters (red dot). The green line (trendline) seems to show that as the parameters of a randomly chosen architecture get close to the supposedly optimal architecture ones, the SSIM converges to what seems to be the best possible forecast value given the limited (and noisy) dataset.

For this case the optimal values obtained before the Monte Carlo simulation were $I^* = 2$, $J^* = 2$, $K^* = 1$ and $L^* = 9$. The results are depicted in Fig. 6. It shows a dispersion as conjectured and a convergence to the highest SSIM value we could obtain for this particular slicing of the training and test sets SSIM = 0.861844038. Results seems to suggest the same structure as depicted in our conjecture diagram and in the previous results for sunspots and the coupled Hénon maps.

D. Partial Differential Equations - Kuramoto-Sivashinsky model

Finally we take a full PDE system, the Kuramoto-Sivashinsky model [149], [150], a very well-known system capable of spatiatemporal chaos and complex spatial-temporal dynamics. It is a fourth-order nonlinear PDE introduced in the 1970s by Yoshiki Kuramoto and Gregory Sivashinsky to model the diffusive instabilities in a laminar flame front.

The model is described by the following equation:

$$\frac{\partial u(x,t)}{\partial t} = -\frac{\partial^4 u(x,t)}{\partial x^4} - \frac{\partial^2 u(x,t)}{\partial x^2} - u(x,t)\frac{\partial u(x,t)}{\partial x}, \quad (4)$$

where $x \in [-\frac{L}{2}, +\frac{L}{2}]$ with a period boundary condition $u(x + L, t) = u(x, t)$. The nature of solutions depends on the system size L and on the initial $u(x, t = 0)$. We have integrated this equation using Matlab (ADD REFERENCE) using a time step of$\Delta t = 0.5$ and $L = 22$ fourier modes which is know to be "turbulent" or chaotic.

We run the simulation for $N = 531$ time steps, and divided the set into $N_{\text{train}} = 500$ time steps for the training set and $N_{\text{test}} = 31$ time steps for the test set. The other parameters of the neural network were: $N_h = 50$, $\eta = 0.1$, $\alpha = 0$, $\rho = 0$, a linear normalization input scaling with $\alpha_{nor} = 5.8472$ and $\beta_{nor} = 0.5$, weight initialization with $\alpha_{rng} = 10^{-3}$ and $\beta_{rng} = -0.5$ and $N_{\text{steps}} = 1,000,000$. We used the ReLU function as the activation on both the hidden and output layers.

The results of the Monte Carlo simulation can be see below in Fig. 7. For this case the optimal values obtained before the Monte Carlo simulation were $I^* = 1$, $J^* = 2$, $K^* = 2$ and $L^* = 39$. It shows a dispersion as conjectured and a convergence to the highest SSIM value we could obtain for this particular slicing of the training and test sets a surprising high value of SSIM = 0.990264382. Results seems to suggest the same structure as depicted in our conjecture diagram and in the previous results for sunspots, the coupled Hénon maps.

IV. Conclusion

We have shown empirical evidence for the existence of an optimal architecture of the input layer of feedforward neural networks used for forecasting spatial-temporal series. We believe that the selection of the features of the input layer can be uniquely determined by the data itself, using two techniques from dynamical systems embedding theory: the mutual information and the false neighbours methods. The former procedure determines the temporal and spatial delays to take when selecting features, while the latter procedure determines the number of data points in space and time to take as inputs. We conjecture that this optimal architecture gives the best forecast, as measured by a standard image similarity index and imply that the shape of the dispersion of points on a Monte Carlo simulation across all possible architectures in the forecast similarity versus distance to optimal architecture was a skewed bell shape with the highest value being the optimal architecture/maximum similarity index.

In order to substantiate our conjecture, we choose four independently related systems, in order of complexity: a set of spatially extended coupled maps; a set of spatially extended ODEs; a one-dimensional spatial PDE and a real spatial-temporal data set from sunspots areas in our Sun. In all four

cases, we were able to first use the mutual information and the false neighbours methods to determine the four parameters defining the input layer architecture[1]. After calibration of the hyperparameters we then were able to forecast reasonably the test. We then show that for a Monte Carlo simulation across all possible architectures, the neural network did not, as expected, forecast as well as for the specific set of four parameters defining the input layer architecture. The Monte Carlo simulations show that the shape of the distribution of points in the forecast similarity versus distance to optimal architecture was a skewed bell shape with the highest value being the optimal architecture/maximum similarity index (subject to noise), as conjectured.

Given how important spatial-temporal systems are [151] and how we want to forecast the future as accurately as possible, it is quite important to attempt to reduce the number of hyperparameters in neural network prediction, and try to constraint the architecture from the data properties only. If indeed our conjecture turns out to be true, it would remove the input layer architecture as another free variable in the already complex process of choosing the details of the neural network to use for forecasting.

In this paper we have focused first and foremost in establishing empirical evidence for our conjecture, within a simple framework of feedforward neural networks with one hidden layer for the purpose of prediction in one spatial and one temporal dimensions. Naturally, there are many clear extensions to our research. First to include more complex architectures, with deeper networks with more hidden layers, to possible tackle systems which are hyperchaotic. Second, to attempt to extend the conjecture with empirical evidence in high dimensions, e.g. 3+1 dimensional weather systems. Third, to extend the conjecture to more complex and fashionable neural networks models, such as recurrent neural networks, particularly echo state networks and long short-term memory networks. Fourth and last but not least, to prove the conjecture would show how dynamical systems theory can clarify the so call "dark artsŠŠ in neural network architecture construction. (HOW? MARKOV CHAINS?).

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[1]We have four parameters for the input layer architecture in these cases, with one temporal and one spatial dimension. For higher dimensional systems, there will be more parameters, the exact number being double the number of dimensions of the system.

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