ABSTRACT

A two-module, feedforward neural network architecture called mapper-coach network has been introduced to reconstruct an unobserved, continuous latent variable input, driving two observed dynamical systems. The method has been demonstrated on time series generated by two chaotic logistic maps driven by a hidden third one. The network has been trained to predict one of the observed time series based on its own past and on the other observed time series by error-backpropagation. It was shown, that after this prediction have been learned successfully, the activity of the bottleneck neuron, connecting the mapper and the coach module, correlates strongly with the latent common input variable. The method has the potential to reveal hidden components of dynamical systems, where experimental intervention is not possible.

Keywords dynamical systems, artificial neural networks, latent variables, common cause, intrinsic dimension

1 Introduction & Background

Theory of nonlinear dynamical systems has plenty to offer for neural architecture design. Here we take a dualistic approach, incorporating the principles of nonlinear time series techniques and the application of simple feedforward learning algorithms to achieve the reconstruction an unobserved common input of two observed chaotic dynamical systems.

A dynamical system has a state and an update rule. It can have a discrete time dynamics or it can be a continuous time flow. In the former, the current state ($s_t$) is updated according to the update rule ($f$) thus gives rise to the future states of the system.

$$s_{t+1} = f(s_t)$$

Here the state is a $p$-dimensional continuous variable.

If we have an observation ($g$) of the system state producing a time series ($x_t$), we can still reconstruct the state up to a continuous transformation.

$$x_t = g(s_t)$$

Takens theorem [1] ensures that this topological equivalence has high probability, and shows that time delay embedding – shown in (3) – is such a reconstruction procedure.

$$X_t = [x_t, x_{t-1}, \ldots, x_{t-(2p-1)}]$$

Where $X_t$ is the reconstructed state at time $t$. 

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In the case of coupled systems, one can reconstruct the cause from the effect \[2, 3, 4\], because the directed causal connection leaves the fingerprint of the former on the latter. So the full coupled system’s state can be reconstructed or decoded form the observation of the effect.

When two subsystem share a common input, then the dynamics of the latent variable is encoded in both systems and appears as some kind of redundancy. This can be leveraged to identify the existence common input between subsystems \[5, 6\]. Hirata et al. applied the technique of recurrence maps to identify the existence of the hidden common cause. Benko et al. measured the intrinsic dimensionality of reconstructed statespaces, thus identified the existence of the latent common cause by determining the number of the redundant degrees of freedom between the two reconstructed dynamics.

There are only a few methods to reconstruct hidden common input from multivariate time series observations and the use of these is restricted to specific types of hidden common inputs \[7, 8\]. Sauer demonstrated, that reconstruction of common input from time series is possible if the hidden variable is discrete \[7\]. Wiskott and Sejnowski introduced slow feature analysis, which can reconstruct slow latent common input \[9\].

However, no method existed yet, which can reconstruct a continuous hidden common input with general dynamics. Here we introduce a new method to reconstruct continuous hidden common input from time series by a feedforward neural network.

2 Example: Coupled logistic maps

We use logistic maps as simple example systems, to simulate coupled dynamical systems with hidden common inputs and to generate the observed data series for the analysis, where the hidden common input is known. The logistic map is a discrete time dynamical system exhibiting chaotic behaviour if the parameter of the system is properly selected \[10\]. Let’s take three logistic maps, which are connected in a way that \(z\) is a common cause of \(x\) and \(y\) (Fig. 1):

\[
\begin{align*}
  f &: x_t = rx_{t-1}(1 - x_{t-1} - \beta_{xz}z_{t-1}) \\
  g &: y_t = ry_{t-1}(1 - y_{t-1} - \beta_{yz}z_{t-1}) \\
  h &: z_t = rz_{t-1}(1 - z_{t-1})
\end{align*}
\]

where \(x, y\) and \(z\) are the state variables, \(r\) is the parameter of the logistic map and \(\beta_{ij}\) are the coupling parameters. Furthermore, \(x\) and \(y\) are observed, however \(z\) is hidden.

In the followings, we show an actual mapping that reconstructs the hidden common cause from one of the observed time series. We know from the theory \[2\] that we can represent the \((z_t, y_t)\) state of the subsystem solely based on the observed variable \(y\). We can obtain such representation by time delay embedding:

\[
Y_t = [y_t, y_{t-1}]
\]

where \(y_t\) is the scalar value of \(y\) at time \(t\), and \(Y_t\) is a 2D vector representing the reconstructed state of the system according to the Takens’ theorem \[1\].
Figure 2: The architecture of the mapper-coach network. The feedforward neural network predicts present values of $x$. One cannot predict accurately $x(t)$ values based on solely $x(t-1)$, because the lack of information about $z(t-1)$. This missing information is sipped out from $Y(t)$ through the red bottleneck. At the training phase the full mapper-coach network can be trained with backpropagation algorithm and – after successful training – the activity of the red hidden unit has a one-to-one correspondence with values of the latent $z$ variable. At this reconstruction stage, the coach can be detached from the mapper, which latter estimates the mapping ($\phi$) from the reconstructed state space of the effect ($Y$) to the state space of the hidden variable ($z$).

To see that $Y_t$ truly described the state of the system, we show how one can express $z$ from $Y$. First, we reorder the equation, which realizes the $g$ mapping in (4) thus we get the expression for $z_{t-1}$:

$$
\phi : z_{t-1} = \frac{1 - y_{t-1} - \frac{y_t}{\beta y_{t-1}}}{\beta y_z}
$$

(6)

and second, we compose $\phi$ with $h$ to get $z_t$:

$$
z_t = (h \circ \phi)(y_t, y_{t-1})
$$

(7)

thus we have a mapping from $Y$ to $z$. By this, we demonstrated that there exists a one-to-one mapping between $Y_t$ and $(z_t, y_t)$, thus $Y$ is a state space reconstruction of the subsystem.

On the other side, to predict the value of $x_t$, one needs the previous value of $x_{t-1}$ and $z_{t-1}$ according to the update rule $f$ in (4). Since $Y$ contains all information about $z$, we can use $Y_t$ instead of $z_{t-1}$, and predict $x_t$ given $x_{t-1}, Y_t$ and the mappings.

When blindly analyzing the observed $x_t$ and $y_t$ time series from this coupled system, the reconstruction and update mappings are unknown, and one has to estimate them from data. For this purpose, it is practical to use feedforward neural networks as these are general function approximators.

3 Results

3.1 Proposed architecture: the mapper-coach network

We reconstruct the hidden common input for a dataset generated from the logistic map system in (4). To estimate the hidden $z$ input we had to approximate the $\phi$ mapping, we implemented this function by a feedforward neural network: the mapper (Fig. 2). The input space is the reconstructed state space of $Y$ (composed by two successive values of $y$) and the intended output is the value of $z$.

But how to find the exact mapping from $Y$ to $z$, when $z$ is unobserved? To asses this challenge, we attached a coach network (coach) to the output of the mapper. The coach takes input from the mapper and also directly from $x$, the other variable influenced by $z$. The output of the coach is a prediction on the current value of $x$, therefore the subnetwork intends to implement the $f$ function from (4).

The fusion of the two parts is the mapper-coach network, which predicts $x(t)$ values based on the observation of $x(t-1), y(t-1)$ and $y(t)$. 

3
Figure 3: Learning and prediction performance of the network. A Learning curves. The learning-process of twenty mapper-coach networks is shown on the left. 7 instances could not learn, 6 instances are lost in local minima and 7 instances converged to smaller mean squared loss values. B Prediction performance of the best model on the test set. The correlogram shows the actual values against the predicted ones. The point-cloud nicely lies around the diagonal, the coefficient of determination is very high ($r^2 = 0.99$).

3.2 Performance on the logistic map system

According to the previous arguments, we trained the mapper-coach network with the backpropagation algorithm to reconstruct $x$ at the output of the coach module, and found that the output of the mapper network was equivalent to the hidden variable.

The network produced very accurate predictions on the present values of $x$ after the learning procedure ($r^2 = 0.99$, Fig. [3]). We split the data into training and test sets ($n = 10000$ each), trained the network on the former and evaluated the results on the latter. We reinitialized the training twenty times with random weights, and selected the best-performing model for evaluation. According to the learning characteristics, we identified three clusters of the models. For seven case out of the twenty, the learning was not successful (cluster 1), for further six cases the system were stuck in local minima (cluster 2) and in the third type the learning was successful (cluster 3, 7/20 cases).

We found that the mapper part of the network reconstructed the past values of the hidden common input quiet accurately: the correlation between the mapper output and the actual hidden common input was $r^2 = 0.97$, (Fig.4). We detached the coach and investigated the output of the mapper by providing $Y(t)$ test inputs ($n = 10000$). The output reflected the values of $z(t - 1)$, so the mapper network approximately implemented the $\phi$ mapping in (6).

We showed that the prediction- and the reconstruction performance were related: the better the model predicted $x$ the better it reconstructed $z$ (Fig.5). The trained network instances achieved different prediction performance on the test set, 13 of the 20 networks had estimable output. We plotted the prediction performance against the reconstruction performance for each model. We saw that better quality predictions implied better quality reconstructions (Fig.5).

4 Discussion

However we demonstrated, that reconstruction of a continuous latent variable was possible with the backpropagation algorithm, several challenges remain to be assessed.

We reconstructed the latent common input from example time series, leveraging the theoretical properties of the underlying coupled chaotic logistic maps. We implemented the method by the mapper-coach network, where the mapper part realized the mapping $z(t - 1) = \phi(Y)$ and the coach implemented $x(t) = f(x(t - 1), z(t - 1))$.

The architecture of the network is asymmetric: the role of the $Y$ and $x$ input is not equivalent. The reconstructed space of $Y$ contains all information about the hidden variable $z$, but the $x(t - 1)$ value lacks this information. The vital point is that the coach sips out the required information about $z$ from the $Y$ input through the mapper, and this information is only available in the $Y$, not in the $x$ input pathway.
To ensure that the mapper outputs information about the hidden variable, the dimensionality of the coach-input has to be minimal. In more complex systems, it could be more difficult to obtain this minimality. The number of input units from the mapper should equal to dimensionality of the common hidden dynamics. Also, the number of direct input units (from $x$ in the example) has to equal to the remaining degrees of freedom in $X$ which is independent from $Y$. Therefore, to determine the proper number of units for mapper output and $x$-input, one has to investigate the intrinsic dimensionality and the mutual dimension between the embedded $X, Y$ variables [11,12,6].

We demonstrated, that the proposed architecture works for a discrete time, deterministic noise-free dynamical system, but whether this approach is applicable to continuous flows and how robust is to noise is yet to be investigated. Theoretically there are no obstacles for the former and – since state-space reconstruction can be robust up to moderate noise levels [13] – the latter can be handled in some cases.

Figure 4: The output and performance of the mapper in reconstruction-mode on the test set. A Traces of original unobserved time series (black) and reconstructed values (red). After reversing and rescaling the amplitudes, the values are almost identical. B Reconstruction performance on the test set. The subplot shows the original values against the reconstructed ones. The points lie around the negative slope diagonal, thus reconstruction has high quality ($r^2 = 0.97$). The negative slope shows, that the reconstructed space is inverted compared with the original $z$ space.

Figure 5: Prediction performance against the quality of reconstruction. The figure shows the coefficient of variation metrics for different model-instances from the learning procedure ($n = 13$). Reconstruction quality of $z$ is correlated with prediction performance on $x$. 
Finally, we analyzed the example from a dynamical systems aspect, and clearly, there are connections e.g. to autoencoders, representation learning and hidden Markov models which await to be worked out in details.

5 Methods

5.1 Data handling

We generated $N = 20000$ data points according to (4) and split the set: the first half became training and second half become test data ($r = 3.99, \beta = 0.2$). We embedded the $y$ variable, thus produced $Y(t) = [y(t), y(t-1)]$, and aligned the time-scale of $x(t)$ and $z(t)$ time series according to the time-shift produced by the embedding procedure.

5.2 Model implementation

We implemented the mapper-coach network in python[14] with the Keras[15] framework using the Tensorflow[16] backend. For the sake of simplicity we chose the number of hidden units to be the same for each hidden layers ($n = 20$).

5.3 Training and evaluation

We randomly initialized the weights and started training with 2000 batch size and for 4000 epochs. We used the ADAM optimizer and mean squared loss function. We repeated this procedure twenty times and selected the best model for evaluation on the test set.

We used the coefficient of determination ($r^2$) to evaluate model test performance. We measured the performance linearly, so the coefficient is the square of the Pearson correlation coefficient ($r$):

$$ r_{xy} = \frac{\sum_{i=1}^{N}(x_i - \mu_x)(y_i - \mu_y)}{\sigma_x \sigma_y} $$

where $x_i$ and $y_i$ are the sample points, $\mu_{x_{i}}$ are the sample means and the $\sigma_{x_{i}}$-s are the sample standard deviations. This coefficient describes the linear dependence between the two variables.

We computed $r^2$ between $x(t)$ and the predicted values $\hat{x}(t)$, and also between $z(t-1)$ and the output of the mapper network ($\hat{z}(t-1)$). We displayed these results on correlograms and on a time series plot (Fig. 3–4).

We also computed the reconstructed $z(t-1)$ values and the $r^2$ values for the not optimal models, and plotted the prediction performance against the reconstruction performance of the models (Fig 5).

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