Reservoir Computing and its Sensitivity to Symmetry in the Activation Function

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Reservoir computing has repeatedly been shown to be extremely successful in the prediction of nonlinear time-series. However, there is no complete understanding of the proper design of a reservoir yet. We find that the simplest popular setup has a harmful symmetry, which leads to the prediction of what we call mirror-attractor. We prove this analytically. Similar problems can arise in a general context, and we use them to explain the success or failure of some designs. The symmetry is a direct consequence of the hyperbolic tangent activation function. Further, four ways to break the symmetry are compared numerically: A bias in the output, a shift in the input, a quadratic term in the readout, and a mixture of even and odd activation functions. Firstly, we test their susceptibility to the mirror-attractor. Secondly, we evaluate their performance on the task of predicting Lorenz data with the mean shifted to zero. The short-time prediction is measured with the forecast horizon while the largest Lyapunov exponent and the correlation dimension are used to represent the climate. Finally, the same analysis is repeated on a combined dataset of the Lorenz attractor and the Halvorsen attractor, which we designed to reveal potential problems with symmetry. We find that all methods except the output bias are able to fully break the symmetry with input shift and quadratic readout performing the best overall.

I. INTRODUCTION

Machine Learning (ML) has shown to be tremendously successful in categorization and recognition tasks and the use of ML algorithms has become common in technical devices of daily living. But the application of ML also pervades more and more areas of science including research on complex systems. For a very recent collection see\textsuperscript{2,3} and references therein.

In nonlinear dynamics ML-based methods have recently attracted a lot of attention, because it was demonstrated that the exact short term prediction of nonlinear system can be significantly improved. Furthermore, it was shown that ML techniques also allow for a very accurate reproduction of the long term properties (“the climate”) of complex systems.\textsuperscript{4} Several ML methods like deep feed-forward artificial neural network (ANN), recurrent neural network (RNN) with long short-term memory (LSTM) and reservoir computing (RC) fulfill the prediction tasks.\textsuperscript{5} RC has attracted most attention. It is a machine learning method that has been independently discovered as Liquid State Machines (LSM) by Maass\textsuperscript{6} and as echo state networks (ESN) by Jaeger.\textsuperscript{7} We focus here on the ESN approach, which falls under the category of Recurrent Neural Networks (RNN). The main difference to other RNNs such as LSTMs is that in RC only the last layer is explicitly trained via linear regression. Instead of hidden layers it uses a so-called reservoir, which in the case of the ESN is typically a network with recurrent connections. The popularity of RC has several reasons. First, RC often shows superior performance. Second, ESNs offer conceptual advantages. As only the output layer is explicitly trained, the number of weights to be adjusted is very small. Thus, the training of ESNs is comparably transparent, extremely CPU-efficient (orders of magnitude faster than for ANNs) and the vanishing-gradient-problem is circumvented. Furthermore, small, smart and energy-efficient hardware implementations us-

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ing photonic systems\cite{8} spintronic systems\cite{9} and many more are conceivable and being develop\cite{10} (and references therein).

Ongoing research is focused on identifying the necessary conditions for a good reservoir. Recent studies focused mainly on the influence of the size and topology of the reservoir on the prediction capabilities.\cite{11,12} Less attention has so far been paid on the role of activation and onto the overall performance of RC.

In this paper we study in detail the sensitivity of RC to symmetries in the activation function. We reveal that previously reported shortcomings for simple ESNs can unambiguously be attributed to symmetry properties of the activation function (and not of the input signal). We propose and assess four different methods to break the symmetries that were developed for obtaining more reliable prediction results.

The paper is organized as follows: Sec.\,\,I first discusses the different measures used and the two test systems: the Lorenz and the Halvorsen equations. Afterwards the different ESN designs used in this study are introduced and the symmetry of the simple ESN is proven. In Sec.\,\,III the three numerical experiments we conducted and their results are presented. Finally we discuss our findings in Sec.\,\,IV

II. METHODS

A. Measures and System Characteristics

1. Forecast Horizon

As in\,\,\cite{13,14} we use the forecast horizon to measure the quality of short-time predictions. It is defined as the time between the start of a prediction and the point where it deviates from the test data more than a fixed threshold. The exact condition reads

$$|\mathbf{v}(t) - \mathbf{v}_R(t)| > \delta .$$  \hspace{1cm} (1)

Due to the chaotic nature of our training data, any small perturbation will usually grow exponentially with time. Thus, this indicates the end of a reliable prediction of the actual trajectory. The measure is not very sensitive to the exact value of the threshold for the same reason.

The norm is taken elementwise and we use $\delta = (5.8, 8.0, 6.9)^T$ for the Lorenz system without preprocessing. In general the values of $\delta$ are chosen to be approximately 15\% of the spatial extent of the respective attractor in the given direction. This is useful if the dynamics of a system takes place on different lengthscales.

2. Correlation Dimension

To evaluate the climate of a prediction we use two measures. To understand the structural complexity of the attractor it is interesting to look at the correlation dimension. This is a way to quantify the dimensionality of the space populated by the trajectory.\cite{15} The correlation dimension is based on the discrete form of the correlation integral

$$C(r) = \lim_{N \to \infty} \frac{1}{N^2} \sum_{i,j=1}^{N} \theta(r - |\mathbf{x}_i - \mathbf{x}_j|) ,$$  \hspace{1cm} (2)

which returns the fraction of pairs of points that are closer than the threshold distance $r$. $\theta$ represents the Heaviside function. The correlation dimension is then defined by the relation

$$C(r) \propto r^\nu ,$$  \hspace{1cm} (3)

as the scaling exponent $\nu$. For a self-similar strange attractor this relation holds in some range of $r$, which needs to be properly calibrated. Here we adjusted it for every given problem beforehand on simulated data, which is not used for training or testing. We note that precision is not essential here, since we are only interested in comparisons and not in absolute values.

To get the correlation dimension for a given dataset we use the Grassberger Procaccia algorithm.\cite{14}

3. Largest Lyapunov Exponent

The second measure we use to evaluate the climate is the largest Lyapunov exponent. In contrast to the correlation dimension it is indicative of the development of the system in time. A $d$-dimensional chaotic system is characterized by $d$ Lyapunov exponents of which at least one is positive. They describe the average rate of exponential growth of a small perturbation in each direction in phase space. The largest Lyapunov exponent $\lambda$ is the one associated with the direction of the fastest divergence.

$$d(t) = C e^{\lambda t} .$$  \hspace{1cm} (4)

Since it dominates the dynamics it has a special significance. It can be calculated from data with relative ease by using the Rosenstein algorithm.\cite{15} It is also possible to determine the complete Lyapunov spectrum from the equations, which we have access to for our testdata as well as for our ESNs.\cite{13,14} However, we found that the comparison is clearer in our case with the data-driven approach, because it is completely independent of details of the system, e.g. the question if it is discrete or continuous. This method is also computationally less costly. We can further define the Lyapunov time $\tau_\lambda = \frac{1}{\lambda}$ as characteristic timescale of a system.

B. Lorenz and Halvorsen system

A standard example of a chaotic attractor is provided by the Lorenz system.\cite{16} It is widely used as a test case
for prediction of such systems with RC. It is defined by the equations
\[
\begin{align*}
\dot{x} &= \sigma(y - x) \\
\dot{y} &= x(\rho - z) - y \\
\dot{z} &= xy - \beta z + x,
\end{align*}
\] where we use the standard parameters \( \sigma = 10, \beta = 8/3 \) and \( \rho = 28 \). We simulate the dynamics by integrating these equations using the Runge-Kutta method with timesteps of \( \Delta t = 0.02 \). We use varying starting points on the attractor.

The equations are symmetric under the transformation \((x, y, z) \rightarrow (-x, y, z)\). Thus the mirror-attractor differs only in the z-coordinate. Furthermore, the mean of the attractor in z-direction is far away from the origin at \( \bar{z} \approx 23.5 \). This makes it an especially useful example for breaking the symmetry in the reservoir.

As a secondary test case we use the Halvorsen equations:
\[
\begin{align*}
\dot{x} &= -\sigma x - 4y - 4z - y^2 \\
\dot{y} &= -\sigma y - 4z - 4x - z^2 \\
\dot{z} &= -\sigma z - 4x - 4y - x^2,
\end{align*}
\] with \( \sigma = 1.3 \). We simulate the dynamics in the same way as for the Lorenz equations. This system also exhibits chaotic behavior but does not have any symmetries under inversion of its coordinates. It has a cyclic symmetry, which should however not be relevant in this context. Both Lorenz and Halvorsen system are 3-dimensional autonomous dissipative flows.

C. Reservoir Computing and Simple ESN

There is a multitude of ways to design an ESN. In this paper we use several different variants, which will be introduced in the following sections. In general the input is fed into the reservoir and influences its dynamics. A usually linear readout is trained to translate the state of the reservoir into the desired output. The reservoir state is then a random, high-dimensional, nonlinear transformation of all previous input data. This naturally gives it a kind of memory.

In an ESN the dynamics of the reservoir are generally governed by an update equation for the reservoir state \( r_t \in \mathbb{R}^N \) of the form
\[
r_{t+1} = f(A r_t, W_{in} x_t)
\] Here \( f \) is called activation function, the adjacency matrix \( A \in \mathbb{R}^{N \times N} \) represents the network, \( x_t \in \mathbb{R}^{d_x} \) is the input fed into the reservoir and \( W_{in} \in \mathbb{R}^{d_x \times N} \) is the input matrix. There are many possible choices for \( f \) and ways to construct \( A \) and \( W_{in} \). Here we always create \( A \) as an Erdős-Renyi random network. Sparse networks have been found to be advantageous. The weights of the network are then drawn uniformly from \([-1, 1]\) and afterwards rescaled to fix the spectral radius \( \rho \) to some fixed value. \( \rho \) is a free hyperparameter. We chose \( W_{in} \) to be also sparse, in the sense that every row has only one nonzero element. This means every reservoir node is only connected to one degree of freedom of the input.\[2\] We fixed the number of nodes per dimension to be the same plus or minus one. The nonzero elements are drawn uniformly from the interval \([-1, 1]\) and then rescaled with a factor \( s_{input} \), which is another free hyperparameter.

From this we can then compute the output \( y_t = t \in \mathbb{R}^{d_y} \).

Here we are interested in the prediction case, where we train the ESN to approximate \( y_t \approx x_{t+1} \). Thus, the dimension of input and output are the same, so we use \( d_x = d_y = d \). The readout is characterized by
\[
y_t = W_{out} r_t
\]
where typically \( r_t = r_t \), but \( r_t \in \mathbb{R}^N \) can also be some nonlinear transformation or extension of \( r_t \). The readout matrix \( W_{out} \in \mathbb{R}^{d_x \times N} \) is the only part of the ESN that is trained. This is typically done via simple Ridge Regression.\[22\]

To train the reservoir the training data \( x^{\text{train}} = \{x_0, ..., x_{T_{\text{train}}} \} \) is fed into the reservoir to get the sequence \( r^{\text{train}} = \{r_0, ..., r_{T_{\text{train}}} + 1 \} \). The first \( T_{\text{sync}} \) timesteps of \( r \) are then discarded. This transient period is only used to synchronize the reservoir with the training data. This frees the ESN of any influence of the reservoir’s initial condition thanks to the fading memory property. The state of a properly designed reservoir continuously loses its dependence on past states over time. For a detailed description see e.g. \[6, 23, 24\]

Now the readout matrix can be calculated by minimizing
\[
\sum_{T_{\text{sync}} \leq t \leq T_{\text{train}}} \| W_{out} r_t - v_t \|^2 - \beta \| W_{out} \|^2,
\]
where we get another hyperparameter \( \beta \) from the regularization. The target output \( v_t \) is in the case of prediction just \( x_{t+1} \). We thus get
\[
W_{out} = (r^T r + \beta I)^{-1} r^T v,
\] where \( r \) is \( r^{\text{train}} \) in matrix form after discarding the synchronization steps and \( v \) is analogous.

In the following we always use a network with \( N = 200 \), \( T_{\text{train}} = 10500 \) and \( T_{\text{sync}} = 500 \) and average degree \( k = 4 \) unless otherwise stated. The spectral radius \( \rho \), the regularization parameter \( \beta \) and the input scaling \( s_{input} \) are optimized for specific problems.

Our basic setup is close to what Jaeger\[27\] originally proposed and it is one of the most widely used variants. We
FIG. 1. Failed prediction of the Lorenz system with a simple ESN. The trajectory jumps down to the mirror-attractor.

FIG. 2. Failed prediction of zero-mean, normalized Lorenz data. The trajectory jumps frequently between the original and the mirror-attractor.

call it simple ESN because all other designs we use are extensions of it. It is defined by the following equations:

\[ r_{t+1} = \tanh(Ar_t + W_{in}x_t) \] (11)

\[ y_t = W_{out}r_t \] (12)

The activation function is a sigmoidal function, specifically a hyperbolic tangent, which is the typical choice. The reservoir states are not transformed before the readout. With this setup successful predictions of different datasets have been made in many cases. However, we can sometimes see very specific ways in which they fail as illustrated in figure 1 and figure 2. When predicting the Lorenz attractor (see 1B), the prediction sometimes jumps to an inverted version of the training dataset, which we call mirror-attractor. For non-preprocessed data, we found that in 98.5% of cases where the prediction crossed the zero in the z-direction it made a jump to the other attractor. The first jump happened on average after 31000 timesteps, where the 18% of realizations, where no jump happened in 500000 timesteps, were excluded from the statistic.

FIG. 3. Prediction of the z-coordinate after synchronization with original data (upper) and inverted data (lower) for the simple ESN.

This still allows for decent short-time predictions. We were able to reach average forecast horizons of ca 400 timesteps after hyperparameter optimization. However, when the data is brought to zero-mean the ability to make accurate predictions largely breaks down. After hyperparameter optimization we get a forecast horizon of ca.90 timesteps. Since the two attractors overlap, the prediction jumps between them very frequently as we can see in figure 2. Sometimes it even travels outside of both for a short time. Since this kind of preprocessing is considered good practice in machine learning and usually leads to better results, this shows a severe failure of the method. Difficulties in predicting the Lorenz system, which is a widespread test case for ESNs, when using this kind of setup have been noted by previous studies. They were linked to the symmetry of the Lorenz equation under the transformation \((x, y, z) \rightarrow (-x, -y, z)\). However, we observe these problems with other datasets as well. We can largely explain this phenomenon by mathematical analysis independent of the input data.

To prove this we do the following: Assume \( r_0 = 0 \) w.l.o.g. because of the fading memory property. Let us now analyze what happens, when instead of the original training sequence \( x_{\text{train}} = \{x_0, ..., x_{T_{\text{train}}}\} \) we use its inverted version \( -x_{\text{train}} = \{-x_0, ..., -x_{T_{\text{train}}}\} \) to train the readout matrix:
\[ r_0(-x^{\text{train}}) = 0 = -r_0(x^{\text{train}}) \] (13)

\[ r_1(-x^{\text{train}}) = \tanh(-W_{in}x_n) \]
\[ = -\tanh(W_{in}x_n) \] (14)

\[ = -r_1(x^{\text{train}}) \] (16)

This serves as the base case for our mathematical induction. We follow up with the induction step. Assume

\[ r_i(-x^{\text{train}}) = -r_i(x^{\text{train}}) \] (17)

Then

\[ r_{i+1}(-x^{\text{train}}) = \tanh(Ar_i(-x^{\text{train}}) - W_{in}x_i) \] (18)

\[ = -\tanh(Ar_i(x^{\text{train}}) + W_{in}x_i) \] (19)

\[ = -r_{i+1}(x^{\text{train}}) \] (20)

Overall we get \( r^{\text{train}}(-x^{\text{train}}) = -r^{\text{train}}(x^{\text{train}}) \). So the dynamics of the reservoir only changed sign and are otherwise unaffected. This is a consequence of the antisymmetry of the hyperbolic tangent.

Obviously, because of the linearity of the readout, we also get

\[ y_i(-x^{\text{train}}) = -W_{out}r_i(x^{\text{train}}) = -y_i(x^{\text{train}}) \] (21)

And finally

\[ W_{out}(-x) = (r^T(-x)r(-x) + \beta I)^{-1}r^T(-x)(-x) \] (22)

\[ = (r^T(x)r(x) + \beta I)^{-1}r^T(x)x \] (23)

\[ = W_{out}(x) \] (24)

So training the simple ESN with inverted data is equivalent to training on the original data and both lead to learning the exact same parameters. Thus, it can never map these sequences to either the same output or any output that differs by anything other than the sign. It is therefore not universal. It can only fully learn the dynamics of systems that are themselves point symmetric at the origin.

Furthermore, when we use a simple ESN for prediction it is now obvious that it learns to replicate the inverted mirror-attractor as well as the real attractor. In cases where they overlap they are however incompatible. When they do not overlap, but are close enough to each other this makes jumps possible.

In figure 3 this is demonstrated by comparing the predictions of an already trained simple ESN after being synchronized with additional Lorenz data either unchanged or inverted. We can see that the prediction of inverted data is simply the inversion of the prediction of the original data, just as expected from theory.

For a jump to happen, the reservoir has to arrive at a state that matches better with the mirror-attractor than with the real one. Since the reservoir has memory it is not obvious how fast input data from the phase-space region of the mirror-attractor can actually make that happen. Empirically we found that crossing the zero in the z-direction leads to a jump in 98.5% of cases. We further observed that inverting the input in a single timestep was reliably enough to push the prediction on the mirror-attractor. This implies a strong sensitivity to the input data with regards to inducing jumps.

It is clear that this kind of symmetry creates a significant limitation for the simple ESN. We can therefore easily explain the previous problems with this kind of approach as well as the so far mostly empirical success of some methods combating them. In many recent publications the readout was extended with a some kind of nonlinear transformation. The empirical advantage of this has been explored without theoretical explanation by Chattopadhyay et al. 5

Typically quadratic terms are included in the readout (see section II D 2). This was to our knowledge originally introduced by Lu et al in order to specifically solve a problem relating to the symmetry of the Lorenz equations, when using the ESN as an observer. It has since been used successfully in many more general cases without theoretical explanation. From our analysis it is now clear that this readout breaks the antisymmetry of the ESN as a whole, which is completely independent of any symmetries of the input data.

A similar analysis can be fruitful on many different designs of ESN. For example in a recent Paper by Carroll and Pecora the following update equation was used:

\[ r_i(t + 1) = \alpha r_i(t) + (1 - \alpha) \tanh \left( \sum_{j=1}^{M} A_{ij} r_j(t) + w_i x(t) + 1 \right) \] (25)

Where \( w_i \) are the elements of what they call input vector. Empirically they found that the performance suffered for \( w_i = 1 \) \( \forall i \) compared to \( w_i \in \{+1, -1\} \). We can explain this with a symmetry under the transformation \( s(t) \rightarrow -s(t) - \frac{2}{w} \) for any constant \( w_i = w \) \( \forall i \) similar to what we found for the simple ESN. As soon as \( w_i \) takes on different values for different \( i \) this symmetry is broken.

D. Breaking Symmetry

To better understand what is the best way to break the harmful antisymmetry in the simple ESN, we test four different designs. There are two main ways of approaching the problem. We can either break the symmetry in the reservoir, e.g. by changing the activation function, or in the readout. When choosing the latter option, equation 17 still holds. The dynamics of the reservoir still do not change meaningfully with the sign of the training data. Only during prediction does the influence of the readout actually come into play.

We use two designs following each approach.
FIG. 4. Prediction of the $z$-coordinate after synchronization with original data (upper) and inverted data (lower) for the ESN with output bias. The prediction of inverted data is perturbed but still in the mirror-attractor.

1. Output Bias

This is one of the simplest ways to break the symmetry. The readout is changed by using $\tilde{r} = \{r_1, r_2, \ldots, r_N, 1\}$. Effectively this leads to

$$y_t = W_{out} \tilde{r}_t = \tilde{W}_{out} r_t + b$$  \hspace{1cm} (27)

where $b \in \mathbb{R}^d$ is called bias-term and is fixed in the Linear Regression. This very basic extension of Linear Regression is often already seen as good practice. Formally this breaks the symmetry.

$$y_t(-r_t) = -W_{out} r_t + b = -y_t(r_t) + 2b$$  \hspace{1cm} (28)

we note however that this way there are only $d$ parameters to represent the difference under sign-change.

2. Lu Readout

As previously mentioned, a quadratic extension of the readout has recently become popular after its introduction by Lu et al. In its most powerful version it consists of using $\tilde{r} = \{r_1, r_2, \ldots, r_N, r_1^2, r_2^2, \ldots, r_N^2\}$ in the readout. Weaker, but more efficient variants are also possible. We focus here on the former for simplicity and in order to test the full potential of this approach. Effectively we get

$$y_t = W_{out} \tilde{r}_t = W_{out}^1 r_t + W_{out}^2 r_t^2$$  \hspace{1cm} (29)

where $W_{out} \in \mathbb{R}^{d \times 2N}$ can be divided in $W_{out}^1$ and $W_{out}^2 \in \mathbb{R}^{d \times N}$. And

$$y_t(-r_t) = -W_{out}^1 r_t + W_{out}^2 r_t^2 = -y_t(r_t) + 2W_{out}^2 r_t^2$$  \hspace{1cm} (30)

The number of parameters that represent the difference under sign-change is $d \times N$.

3. Input Shift

This design for an ESN has been proven to be universal by Grigoryeva and Ortega. Specifically this means it can approximate any causal and time-invariant filter with the fading-memory property, which naturally excludes any problems with symmetry. This is also recommended in “A practical guide to Applying Echo State Networks” by Lukoševičius.

For this design the activation function of the simple ESN is extended by including a random bias term in every node of the reservoir. It can be written as a random vector $\gamma \in \mathbb{R}^N$ and gives the following new update equation:

$$r_{t+1} = \tanh(\mathbf{A} r_t + W_{in} x_t + \gamma) \hspace{1cm} (32)$$

The readout is unchanged from the simple ESN. Unlike the first two methods this breaks the symmetry in the reservoir itself.

We draw the elements of $\gamma$ uniformly from $[-s_{\gamma}, s_{\gamma}]$ where $s_{\gamma}$ is a new hyperparameter to be optimized. This was a somewhat arbitrary choice for simplicity. In principle we could instead use a normal distribution, the distribution of the training data, etc.
4. Mixed Activation Functions

Another way of breaking the symmetry directly in the reservoir is to replace some of the odd tanh activation functions with even functions. This was inspired by a different framing of the problem: Every node in the network can be understood as a function of the concatenation of input datum and reservoir state \( \mathbf{x} = \{r_1, ..., r_N, x_1, ..., x_d\} \). The readout is then simply a linear combination of these functions, where the weights are optimized to approximate the output. The nodes differ by the random parameters introduced through the elements of \( \mathbf{W}_{in}, \mathbf{A} \) and \( \gamma \), if input shift is included. In general we want this set of functions to approximate a basis in the corresponding function space to be as powerful as possible. In the case of the simple ESN these functions are all odd and any linear combination of them will still be odd. Mixing in even functions gives us access to the whole function space as any function can be divided in an even and an odd part.

As even function we simply used \( \tanh^2 \). We assigned half of the nodes connected to each input dimension to be even nodes, where this activation functions is used.

| ESN design       | F.H. in \( \Delta t \) (\( \tau_y \)) | \( \lambda \pm \sigma \) | \( \nu \pm \sigma \) |
|------------------|---------------------------------|-----------------|-----------------|
| Simple ESN       | 90.9(1.6)                       | 0.2 ± 0.2       | 1.6 ± 0.5       |
| Output Bias      | 149.7(2.6)                      | 0.3 ± 0.2       | 2.0 ± 0.5       |
| Mixed Activations| 538.2(9.4)                      | 0.87 ± 0.03     | 1.97 ± 0.13     |
| Input Shift      | 629.3(10.9)                     | 0.87 ± 0.02     | 1.978 ± 0.008   |
| Lu Readout       | 631.3(11.0)                     | 0.87 ± 0.02     | 1.978 ± 0.008   |
| Test Data        | \( \infty \)                   | 0.87 ± 0.02     | 1.978 ± 0.008   |

TABLE I. Performance of the different ESN designs on zero-mean Lorenz data. Comparison to the original Lorenz data in last row.

III. RESULTS

A. Predicting The Mirror-Attractor

To test the ability of the four methods to break the symmetry of the simple ESN, we tried to force them to predict the mirror-attractor of the Lorenz equations after being trained with regular data. If the symmetry is truly broken, we expect this prediction to fail completely, indicating that the ESN did not learn anything about the mirror-attractor.

To accomplish this we trained our ESNs with regular Lorenz data and then synchronized it with the inverted next 500 timesteps of the simulation. We then measured the forecast horizon of the prediction in regards to the (also inverted) test data. For comparison, we also looked at the prediction after synchronization with the same data without inversion.

In figure 4 we see the behavior of the ESN with output bias. It differs from before in that the prediction of the mirror-attractor is not simply the inversion of the regular prediction as for the simple ESN in figure 3. However, even though it is generally a worse prediction, it clearly follows the inverted trajectory. The ESN has still learned a slightly perturbed version of the mirror-attractor. When using input shift, Lu readout or mixed activations, we never observed a prediction staying in the vicinity of the mirror-attractor. Most of them instead leave it immediately and quickly converge to the real Lorenz attractor as in figure 5. In some cases the trajectory finds some other fixed point instead, but it never stays in the mirror-attractor. Qualitatively we get the same behavior when using mixed activations or input shift instead.

Furthermore, we made 1000 predictions of the mirror-attractor with all four designs while varying the network and the starting point of the training data. The distribution of forecast horizons is shown in figure 6. The output bias clearly sticks out as the only method showing the ability to predict the mirror-attractor. Many realizations reach forecast horizons of the order \( O(10) \) while the other three methods never go beyond \( O(1) \). Again there is no significant difference detectable between input shift, Lu readout and mixed activation functions.

We also tested the rate of jumps between the attractors for the ESN with output bias analogously to the simple ESN in section II.C by making 1000 predictions with 500000 timesteps. Network and training data were varied for every realizations. 30.5% of them did not show any jump. For the others the average time of the first jump was after about 33000 timesteps. 95.2% of times the \( z \)-coordinate crossed zero it lead to a jump. Thus, we observed an improvement, but the basic problem has not been solved by the output bias.
We did not observe any jumps when we used the other three methods.

B. Zero-mean Lorenz

![Distribution of forecast horizons for normalized, zero-mean Lorenz data with all five variants of ESN. Based on 1000 realizations (varying training data, network and starting point of prediction) for each.]

To further compare the performance of the different ESNs, we test the ability to learn and predict Lorenz data where the mean has been shifted to the origin. As already discussed, this leads to overlap between real and mirror-attractor. So even though this preprocessing is usually preferred, it makes the simple ESN’s problems with antisymmetry especially severe. We also rescaled all data to have a standard deviation of 1.

To get reliable quantitative results, we first carried out a hyperparameter optimization on this task for every design used. We used a grid search with 100 realizations for each point in parameter space. The best parameters are chosen on the basis of the highest average forecast horizon. Further details and results can be found in the appendix.

With the optimized hyperparameters we created 1000 realizations for each design and measured forecast horizon, largest Lyapunov exponent and correlation dimension. To accurately represent the climate we used predictions with a length of 20000 timesteps. The results are compiled in table I and figure 7 and 8. The simple ESN’s forecast horizon consistently lies in a region below 200 timesteps with a mean of 90.9 and similarly to the first task the output bias offers a noticeable but small improvement with a mean of 149.7 timesteps. The other three methods to break the symmetry all seem to work in principle. Their forecast horizons mostly lie between 400 and 800 timesteps. Lu readout and input shift show no significant difference with an average forecast horizon of ≈ 630, while mixed activation functions shows a lower average forecast horizon of 538.2.

In agreement with the results for the forecast horizon, the simple ESN’s climate produces values of largest Lyapunov exponent and correlation dimension far away from the desired region. Again the output bias is only a small improvement. All results for Lu readout and input shift lie in the direct vicinity of the target and the mean values and standard deviations match those of the test data within uncertainty. The mixed activation functions also reproduce the correct mean values but with much higher standard deviation. This can be attributed to the clear outliers visible in the plot. We note that the results for the climate are less reliable than those for the forecast horizon since we did not optimize the hyperparameters for this task.

Overall this implies that the mixed activation functions do not perform quite as well on this standard task as input shift and Lu readout.

C. Halvorsen and Lorenz

Finally, we compare the five different ESNs on a task that is specifically designed to test their symmetry breaking abilities. For this goal we create a dataset by simulating both the Lorenz and the Halvorsen system. The mean of the Lorenz data is shifted to (1, 1, 1) and the mean of the Halvorsen data is shifted to (−1, −1, −1). Both are rescaled so that no datapoint has a distance higher than 1 from the mean in any dimension. This ensures that the two attractors do not overlap while lying completely in the region of each others mirror-attractor. To train the ESN to simultaneously be able to predict both systems we use the following trick. Firstly, we synchronize it with the Lorenz data and record \( r_{\text{train}}^{\text{Lorenz}} \) after the initial transient period. We do however not calculate \( W_{\text{out}} \) yet. Instead we repeat the process with the Halvorsen data. Now the transient period has the additional use of letting the reservoir forget about the Lorenz system. To train the ESN to simultaneously be able to predict both systems we use the following trick. Firstly, we synchronize it with the Lorenz data and record \( r_{\text{train}}^{\text{Lorenz}} \) after the initial transient period. We do however not calculate \( W_{\text{out}} \) yet. Instead we repeat the process with the Halvorsen data. Now the transient period has the additional use of letting the reservoir forget about the Lorenz system. This way we get \( r_{\text{train}}^{\text{Lorenz}} \) and \( r_{\text{train}}^{\text{Halvorsen}} \). We simply concatenate them to get a single dataset \( r_{\text{train}} \), from which we finally compute the readout matrix. As desired output we use an analogous concatenation of the Lorenz data and the Halvorsen data. We note that, since the linear readout is in no way sensitive to the causal relationship between the reservoir states and the transient period at the second training stage was discarded, the transition between the two systems in itself does not influence training.

This way the ESN has to learn dynamics that are governed by a completely different set of equations instead of the mirror-attractor. In the end it should be able to predict both attractors depending on the starting point of the reservoir states. Since this is a more difficult task and to make sure that possible failures are not just due to
a lack of nodes we use $N = 500$ in this experiment. However, we made similar qualitative observations for smaller and larger networks. To be able to do a quantitative analysis, we first performed a hyperparameter optimization as described in the appendix. We used the product of forecast horizons on both systems as a measure of performance. Afterwards we carried out the same experiment as in section with this combined dataset. We always made a prediction on both attractors with the same network. The results are compiled in table. Unsurprisingly we observe that the simple ESN is not able to master this task (see figure). Most predictions completely diverge from both attractors. In the handful of cases where one of the predictions actually reproduced
the climate of one attractor, the other one was always a complete failure. Qualitatively we see the same results when including an output bias.

Since all predictions with the simple ESN and almost all with the ESN with output bias either diverged or converged to some fixed point, we could not provide meaningful results for the climate. We note however that the short-term prediction of the Lorenz system was actually significantly better for both than in section III. We attribute this to the higher number of nodes. Still the inability to reproduce long-term behavior indicates that this kind of problem can only be solved with a properly broken symmetry as we assumed.

Again all three other methods to break the symmetry are successful (see as an example figure 10). The results are qualitatively the same for input shift and mixed activation functions. All three are able to predict both attractors with the same training quite well.

It is notable that the Lu readout performed significantly better than the others in terms of the forecast horizon on both systems. In contrast there was also a small number (26) of predictions that completely diverged or got stuck in a fixed point with this design. These made a proper calculation of the largest Lyapunov exponent impossible and are thus not included in that statistic. The same did not happen when using input shift or mixed activation functions. This might be due to the fact that the Lu readout does not break the symmetry in the reservoir itself. For this more complicated task the additional parameters in the readout might not always be sufficient to encode the difference in the dynamics for a sign change. It could be related to the fact that those dynamics are completely independent of each other.

| ESN design       | F.H. in Δt (τₐ) | λ ± σ | μ ± σ |
|------------------|-----------------|-------|-------|
| Simple ESN       | 183.2(3.2)      | -     | -     |
|                  | 54.2(0.8)       | -     | -     |
| Output Bias      | 226.3(3.9)      | -     | -     |
|                  | 57.7(0.9)       | -     | -     |
| Mixed Activations| 563.4(9.8)      | 0.87 ± 0.03| 1.99 ± 0.02 |
|                  | 709.4(10.5)     | 0.74 ± 0.03| 1.88 ± 0.04 |
| Input Shift      | 570.5(9.9)      | 0.87 ± 0.02| 1.992 ± 0.007 |
|                  | 721.4(10.7)     | 0.74 ± 0.03| 1.88 ± 0.04 |
| Lu Readout       | 610.9(10.6)     | 0.87 ± 0.05| 1.9 ± 0.3 |
|                  | 784.1(11.6)     | 0.74 ± 0.03| 1.87 ± 0.03 |
| Test Data        | ∞               | 0.87 ± 0.02| 1.993 ± 0.007 |
|                  | ∞               | 0.74 ± 0.03| 1.87 ± 0.04 |

TABLE II. Performance of the different ESN designs on combined Lorenz and Halvorsen data. Upper value is always Lorenz and lower Halvorsen. Comparison to the original data in last row.

IV. DISCUSSION

In the present work we showed a mathematical proof for the antisymmetry of the simple ESN with regards to changing the sign of the input. This is a consequence of the antisymmetry of the activation function. It makes it impossible to fully learn the dynamics of any attractor that is not point symmetric around the origin. In practice we observed that the prediction jumps to an inverted version of the real attractor we call mirror-attractor. This is especially disastrous if the two overlap. From this we conclude that this setup is not suitable for general tasks and should not be used.

Furthermore, we note that the sensitivity to this kind of symmetries with regards to the input is a universal property of ESNs and Reservoir Computers in general. This is in no way limited to the specifics of the simple ESN. It must be kept in mind in every reservoir design and can explain the empirical success or failure of some of them. In our experiments with the output bias we found that formally breaking the symmetry alone is not enough to solve the problems associated with it. It was only able to improve the performance marginally and we still observed the appearance of an only slightly perturbed mirror-attractor. This might be due to the fact that the number of parameters representing the symmetry break in this approach is too low to accurately model the difference.

We were however able to successfully break the symmetry and solve the problem with three other approaches: Introducing an input shift in the activation function, using a mixture of even and odd activation functions and including the squared reservoir states in the readout. All of them were able to eliminate the mirror-attractor and make qualitatively good predictions even for zero-mean Lorenz data, where the overlap with the mirror-attractor is a severe problem for the simple ESN. They were further all able to master the task of predicting a dataset made of Lorenz and Halvorsen data, where it was necessary to learn completely different dynamics in the regime of the mirror-attractor.

The mixed activations approach consistently showed the worst ability for short-time prediction of these three and some outliers in the climate. At least for our implementation we also found it to have a higher time cost. Thus, we do not recommend its use in the given form. However, the usage of different functions, different ratios, etc. could lead to better performance. Further research is needed.

In some cases the Lu readout completely failed at the more complicated task of predicting the combined Halvorsen-Lorenz system. This might imply that breaking the symmetry in the reservoir itself is necessary for reliable prediction. However, it also showed the best results in terms of forecast horizon for this task. In addition, it was generally on par with the input shift for the zero-mean Lorenz data, where both reproduced the climate with the same variance as the simulated data. Thus, it
proved to be particularly good at short-time prediction even though long-term prediction was less reliable in the last case. It also requires one less hyperparameter to be optimized and is very easy to implement, even for a physical reservoir, where the dynamics might be inaccessible. It is worth noting that to our knowledge universality is only proven for ESNs with input shift. Together with the fact that we never observed any prediction of this design to really fail, this makes it a particularly reliable tool. Additionally, one might consider making the dynamics of the reservoir more complex, while keeping the simple linear readout, to be more in line with the philosophy of RC.

In light of these results we recommend both the input shift and the Lu readout as methods to break the symmetry.

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**DATA AVAILABILITY**

The data that support the findings of this study are available from the corresponding author upon reasonable request.

**APPENDIX HYPERPARAMETER OPTIMIZATION**

The Hyperparameter Optimization was carried out as a simple grid search with the aim to maximize the forecast horizon. For the simple ESN we searched over \( a \) and \( \epsilon \), with

\[
s_{\text{input}} = a(1 - \epsilon) \\
\rho = a\epsilon
\]

The same was done for the ESN with output bias and the ESN with Lu readout. For the ESN with input shift we additionally varied the scale \( s_\gamma \) and for the mixed activations we replaced \( a \) with \( a_1 \) and \( a_2 \), which were optimized for the tanh-nodes and the tanh\(^2\)-nodes separately.

**A. Predicting the mirror-attractor**

Since we were less interested in quantitative results in this case we did not perform a real hyperparameter optimization procedure. Instead we used the parameters from our previous work \(^{11}\) for the simple ESN and manually searched the parameters for the others to reproduce the Lorenz attractor reasonably well. This left us with the parameters in table \(^{11}\).

| Simple ESN | Output Bias | Lu readout | Mixed | Input Shift |
|------------|-------------|------------|-------|-------------|
| \( a \)   | 0.32        | 0.32       | -     | 0.32        |
| \( \epsilon \) | 0.5         | 0.5        | 0.5   | 0.5         |
| \( \beta \) | \( 1.9 \times 10^{-11} \) | \( 1.9 \times 10^{-11} \) | \( 1.9 \times 10^{-11} \) | \( 1.9 \times 10^{-11} \) |
| \( s_\gamma \) | -           | -          | -     | 13.         |
| \( a_1 \) | -           | -          | -     | 0.32        |
| \( a_2 \) | -           | -          | -     | 0.32        |

**TABLE III. Hyperparameter choices for the Prediction of the mirror-attractor.**

**B. Zero-mean Lorenz**

In the case of the zero-mean Lorenz data we simulated 100 trajectories of training data and 100 trajectories of test data. At every point in hyperparameter space we generate a new network and a new \( W_{\text{in}} \) for each trajectory. We then choose the hyperparameters with the highest average forecast horizon. Since it did not seem to depend strongly on the other hyperparameters, the problem or the specific design, we simply set \( \beta = 1.9 \times 10^{-11} \) as in the first task to save time with the already very costly grid search.

| Hyperparameter | Min | Max | Step Size | Optimal |
|----------------|-----|-----|-----------|---------|
| \( a \)       | 0.1 | 3.0 | 0.1       | 1.0     |
| \( \epsilon \) | 0.0 | 1.0 | 0.05      | 0.7     |

**TABLE IV. Hyperparameter range and results for the simple ESN on zero-mean Lorenz data.**

**TABLE V. Hyperparameter range and results for the ESN with output bias on zero-mean Lorenz data.**

| Hyperparameter | Min | Max | Step Size | Optimal |
|----------------|-----|-----|-----------|---------|
| \( a \)       | 0.1 | 3.0 | 0.1       | 1.0     |
| \( \epsilon \) | 0.0 | 1.0 | 0.05      | 0.7     |

**TABLE VI. Hyperparameter range and results for the ESN with Lu readout on zero-mean Lorenz data.**
TABLE VII. Hyperparameter range and results for the ESN with input shift on zero-mean Lorenz data.

| Hyperparameter | Min | Max | Step Size | Optimal |
|----------------|-----|-----|-----------|---------|
| $\alpha$       | 0.2 | 3.0 | 0.2       | 1.2     |
| $\epsilon$     | 0.0 | 1.0 | 0.1       | 0.6     |
| $s_\gamma$     | 0.3 | 3.0 | 0.3       | 1.5     |

TABLE VIII. Hyperparameter range and results for the ESN with mixed activation functions on zero-mean Lorenz data.

| Hyperparameter | Min | Max | Step Size | Optimal |
|----------------|-----|-----|-----------|---------|
| $\alpha_1$     | 0.2 | 3.0 | 0.2       | 0.6     |
| $\alpha_2$     | 0.2 | 3.0 | 0.2       | 0.8     |
| $\epsilon$     | 0.1 | 1.0 | 0.1       | 0.6     |

TABLE IX. Hyperparameter range and results for the simple ESN on combined Lorenz and Halvorsen data.

| Hyperparameter | Min | Max | Step Size | Optimal |
|----------------|-----|-----|-----------|---------|
| $\alpha$       | 1.1 | 4.0 | 0.1       | 2.0     |
| $\epsilon$     | 0.0 | 1.0 | 0.05      | 0.4     |

TABLE X. Hyperparameter range and results for the ESN with output bias on combined Lorenz and Halvorsen data.

| Hyperparameter | Min | Max | Step Size | Optimal |
|----------------|-----|-----|-----------|---------|
| $\alpha$       | 1.1 | 4.0 | 0.1       | 1.9     |
| $\epsilon$     | 0.0 | 1.0 | 0.05      | 0.4     |

TABLE XI. Hyperparameter range and results for the ESN with Lu readout on combined Lorenz and Halvorsen data.

| Hyperparameter | Min | Max | Step Size | Optimal |
|----------------|-----|-----|-----------|---------|
| $\alpha$       | 1.1 | 4.0 | 0.1       | 2.3     |
| $\epsilon$     | 0.0 | 1.0 | 0.05      | 0.45    |

TABLE XII. Hyperparameter range and results for the ESN with input shift on combined Lorenz and Halvorsen data.

| Hyperparameter | Min | Max | Step Size | Optimal |
|----------------|-----|-----|-----------|---------|
| $\alpha_1$     | 1.2 | 4.0 | 0.2       | 3.0     |
| $\alpha_2$     | 1.2 | 4.0 | 0.2       | 2.8     |
| $\epsilon$     | 0.1 | 1.0 | 0.1       | 0.2     |

TABLE XIII. Hyperparameter range and results for the ESN with mixed activation functions on combined Lorenz and Halvorsen data.

C. Halvorsen and Lorenz

For the combined dataset of Halvorsen and Lorenz attractor we simulate 100 training and test trajectories of each system and use them as described in Sec. III C. As before we train a completely new reservoir on each trajectory for every point in parameter space. For every realization the product of the two forecast horizons is calculated. The optimal hyperparameters are chosen as those were this product averaged over the trajectories is maximal.

For this task we did include the regularization parameter $\beta$ in the search with a logarithmic scale from $10^{-13}$ to 0.001 in 11 steps. We consistently found $\beta = 10^{-10}$ to be the best choice for all five designs.

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