Forecasting Using Reservoir Computing:
The Role of Generalized Synchronization

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Abstract

Reservoir computers are a form of recurrent neural network (RNN) that may be used for forecasting from time series data. These can be multivariate or multidimensional data. As with all RNNs, selecting the hyperparameters for the reservoir network presents a challenge when training on a new input system. We present a systematic method that gives direction in designing and evaluating the architecture and hyperparameters of a reservoir computer—with the goal of achieving accurate prediction/forecasting after training—based on generalized synchronization (GS) and tools from dynamical systems theory. The ‘auxiliary method’ for GS provides a pre-training test that guides hyperparameter selection. Furthermore, we provide a metric for a “well trained” network using the geometry of the phase space dynamics and the reproduction of the input system’s Lyapunov Exponent spectrum. The traditional ML approach of using a test dataset is not sufficient for dynamical systems forecasting.

1 Introduction

Machine learning (ML) is a computing paradigm for data-driven prediction in which a ML “device” accepts input data in a training phase. Then this is used in a predict/forecast phase that is used to extrapolate a learned process to data that has not been seen before. When the data is in the form of a time series, such a device is denoted a “recurrent neural network” (RNN) [1]. This is in contrast to other ML network architectures, such as feed forward neural networks (also known as multilayer perceptrons), that assume the statistical independence of inputs [2, 3].

RNNs have feedback in the connection topology of the network, enabling self excitation as a dynamical system and distinguishing them from feed forward networks that only represent functions [4]. This feature identifies RNNs as an attractive choice for data driven forecasting [5].

These networks tend to be trained with some version of the backpropagation algorithm [6, 7] which can lead to training instabilities [8] and issues with vanishing and exploding gradients [9–11].

A kind of RNN architecture that has been successful for time series prediction is reservoir computing (RC) [12], where a large random network is constructed and only the final layer is trained. This method is much simpler to train due to the fixed weights in the reservoir layer.

1.1 Reservoir Computing

Reservoir Computing [4, 12–20] is a type of RNN framework with demonstrated capability for forecasting dynamical systems output. The training input signal to the network, denoted \( u(t) \), may be generated from a known dynamical system [21, 22], or from observations where the underlying dynamical rules are undetermined. The RC approach has a clear advantage over its RNN counterparts due to its simplicity and the ease of training. This characteristic makes RC ideal for constructing simple networks which nevertheless accurately reproduce the system dynamics of \( u(t) \).
Figure 1: Flow of operations for utilizing a Reservoir Computation (RC) to perform forecasting/prediction of a D-dimensional input $u(t)$ presented to an RC with N-dimensional dynamical degrees-of-freedom $r(t)$. When the input and the reservoir exhibit generalized synchronization, $u_a = \varphi_a(r)$; $a = 1, 2, \ldots D$, training consists of estimating any parameters in a representation of $\varphi(r)$.
Given the many years of investment in training internal connections in RNNs such as LSTMs [23], the success of using a randomly generated RC to forecast system dynamics is remarkable. It is natural to ask how it might be that a random network could accurately reproduce the dynamical properties associated with \( u(t) \). In probing this question, the idea arose [21, 24, 25] that the explanation might be a form of synchronization known as ‘generalized synchronization’ (GS) [26–28]. In the physical sciences, one is familiar with encountering GS in many places. GS has been found experimentally with coupled laser systems, electronic circuits, [29–34] and found to hold in a geophysical setting, connecting the El Niño-Southern Oscillation and monthly hydrological anomalies of rainfall and streamflows in Colombia. [35]. It also plays a role in cryptography [36].

The ability to develop a data-driven model using a method such as RC is attractive for a number of practical reasons.

- RC allows us to construct predictive models of unknown or poorly understood dynamics given well curated data \( u(t) \). Should the input signal \( u(t) \) arise from measurements of high dimensional geophysical or laboratory flows [37, 38], the speedup in computing with a reservoir network realized in hardware [34, 39] may permit the exploration of detailed statistical questions about the observations that might be difficult or impossible otherwise.

- RC has the potential to provide significant computational cost savings in prediction applications, since the RC dynamics typically comprises a network with computationally simple active dynamics at its nodes.

- RC can be understood through analyzing two dynamical properties of the combined input-reservoir system: generalized synchronization and their Conditional Lyapunov exponents (CLE).

1.2 Goals of This Paper

The success of RNNs and their increased adoption in research applications has rapidly outpaced the understanding of these data driven processes. Generally, it is not known how best to design a network for a particular problem, nor how much or what kind of data is most useful for training. General guidelines are well established, [14] but tend to be justified with empirical rather than theoretical considerations.

We move from this ad hoc approach to a systematic strategy where we ensure that the input \( u_\alpha(t) ; \alpha = 1, 2, ..., D \) and the reservoir degrees-of freedom \( r_\alpha(t); \alpha = 1, 2, ..., N \) show generalized synchronization \( u_\alpha(t) = \varphi_\alpha(r(t)), \) and point out that it is parameters in the function \( \varphi(r) \) that we need to estimate. We also give a systematic way to choose a region of hyperparameters of the adjacency matrix \( A_{\alpha,\beta} \), including its spectral radius (SR) and the probability of non-zero connections among the \( N \) active units (pnz), where generalized synchronization occurs and skillful forecasting of the training input data \( u(t) \) is expected to be possible. We argue that the vague references in the literature to the “edge of chaos” are not particularly informative.

A glimpse of the insight we will discuss is illustrated in Fig. (2). We include two operations in the training phase: (1) estimation of parameters in an approximation of \( \varphi(r) \), and (2)
Figure 2: Examples of dynamical system forecasting using a tanh RC for the D=5 Lorenz96 system Top Panels and the Colpitts Oscillator Bottom Panels. The input dynamical systems are described in the supplementary material. For the Lorenz96 data the reservoir has dimension N = 2000, SR = 0.9, Probability of Nonzero Connections (pnz) = 0.02, and $\lambda_1 = .55$ The Lorenz96 driver has dimension D = 5. For the Colpitts Oscillator data the reservoir has dimension N = 500, SR = 0.85, Probability of Nonzero Connections (pnz) = 0.02, and $\lambda_1 = 0.09$. The Colpitts driver has dimension D = 3.
use of the input $u(t)$ to “synchronize” the model before forecasting. The second may be quite brief, often only a few steps in time may be required.

A related issue is that the traditional method of evaluating the effectiveness of a RNN, with training and testing data sets, is not sufficient when performing dynamical systems forecasting, as that method gives no indication of the stability of the forecast. A simple approach to evaluation, showing a prediction of a single time series, also gives no indication of the stability of the predictions over the entire range of inputs. In this paper we attempt to rectify these deficiencies by using dynamical properties of the reservoir itself to design and evaluate a trained network.

The goals of this paper are as follows:

1. Introduce a numerical test, based on GS and using the ‘auxiliary method’, that can guide hyperparameter selection in RNNs.

2. Provide a metric for a “well trained” network using the geometry of the phase space dynamics and the reproduction of the input system’s Lyapunov exponent spectrum.

### 2 Forecasting with RC

#### 2.1 RC Definition

RCs are applied to forecasting problems where the task is to predict a $D$-dimensional input sequence $u(t)$ generated from a dynamical system

$$\frac{du(t)}{dt} = F_u(u(t)), \quad (1)$$

$F_u(u(t))$ is the vector field of the $u$ dynamics.

An RC consists of three layers: an input layer, the reservoir itself, and an output layer. The reservoir, described as a dynamical system $F_r$, is composed of $N$ nodes at which we locate nonlinear models, in ML called ‘activation functions’, [19, 40–44]. The nodes in the network are connected through an $N \times N$ adjacency matrix $A_{\alpha\beta}$, chosen randomly to have a connection density $pnz$ and non-zero elements uniformly chosen from a uniform distribution in $[-1, 1]$. This is then normalized by the largest eigenvalue of $A_{\alpha\beta}$: the spectral radius (SR).

The input layer maps the input signal $u(t)$ from $D$ dimensions into the $N$ dimensional reservoir space.

The output layer $\varphi(r(t))$ is a function such that $\varphi_a(r) = u_a(t)$, chosen during the training phase during which we estimate any parameters in $\varphi(r)$.

This is the only part of the reservoir computer that is trained. It is common practice to choose $\varphi(r)$ as a linear function of $r$, but this is by no means the only choice of output function. The structure of a RC is shown in Fig.(1).

$r(t)$ can be viewed as representing the information in the input time series $\{u(0), u(1), \ldots, u(t_{\text{final}})\}$ in $N > D$ dimensional space consistent with Takens embedding theorem [45].
Figure 3: **Top Left and Top Right** Synchronization between an \( N = 2000 \) tanh reservoir output (red) and the Lorenz63 input (black). In \( A_{\alpha \beta} : \text{SR} = 0.9 \) and \( \text{pnz} = 0.02 \). The black vertical line at \( t = 0 \) is the end of the “training period.” **Bottom Left** The average forecast time of the reservoir depends strongly on the RC hyperparameters. Here we show the forecast time variation (in units of \( \lambda_1 t \)) as a function of SR and pnz. **Bottom Right** 3-D display of **Bottom Left**.

The reservoir dynamics acts at the nodes of the network \( r(t) \). The dynamics of \( r(t) \) can be posed as either a discrete time mapping or differential equation in continuous time. In this paper differential equations are used. In what we call the “training phase” the equation governing the evolution of the reservoir is

\[
\frac{dr(t)}{dt} = F_r[r(t), u(t)].
\] (2)

In the prediction phase the reservoir dynamics becomes

\[
\frac{dr(t)}{dt} = F_r[r(t), \varphi(r(t))].
\] (3)

### 2.2 Synchronization and Training

What advantage does GS give us in the analysis of reservoir computing networks?

GS assures us that the dynamical properties of the stimulus \( u(t) \) and the reservoir \( r(t) \) are now essentially the same. They share global Lyapunov exponents [46], attractor dimensions, and other classifying nonlinear system quantities [26].
Figure 4: **Left Panel** Gaussian fit to the prediction times for 10 N=2000 tanh RCs trained on Lorenz63 data with the same hyperparameters but different random seeds and training data. Each reservoir predicts 4000 randomly selected training points. These points are different for each reservoir. The 10 RC’s prediction times overlap closely; the (mean(10 reservoirs)) = 5.92 and the (RMS deviation(10 reservoirs)) = 0.24. This shows the robustness of this set of hyperparameters to training data and randomization of the reservoir layers. **Right Panel** A histogram and the Gaussian fit to it from the **Left Panel** better displays the variation shown in one hyperparameter setting of the reservoir computer.

| Parameter | Description |
|-----------|-------------|
| SR        | Largest eigenvalue of the adjacency matrix $A_{\alpha \beta}$ |
| pnz       | Density of the adjacency matrix $A_{\alpha \beta}$ |
| N         | Degrees-of-Freedom of the reservoir |
| $\mu$     | Time constant of the reservoir computer |
| $\sigma$  | Strength of input signal |

Table 1: Hyperparameters of the tanh reservoir computer that need to be selected for individual problems. Other reservoirs also have various hyperparameters that depend on the active units at their nodes.
The principal power of GS in RC is that we may replace the initial non-autonomous reservoir dynamical system
\[
\frac{d\mathbf{r}_\alpha(t)}{dt} = \mathbf{F}_\alpha[\mathbf{r}(t), \mathbf{u}(t)],
\]
with an autonomous system operating on the synchronization manifold \[47\]
\[
\frac{d\mathbf{r}_\alpha(t)}{dt} = \mathbf{F}_\alpha[\mathbf{r}(t), \varphi(\mathbf{r}(t))].
\]

In practice, the function \(\mathbf{u} = \varphi(\mathbf{r})\) is approximated in some manner, through training, and then this is substituted for \(\mathbf{u}\) in the reservoir dynamics. In previous work on this \[21, 22, 24\] the authors approximated \(\varphi(\mathbf{r})\) via a polynomial expansion in the components \(r_\alpha; \alpha = 1, 2, ..., N\), and used a regression method to find the coefficients of the powers of \(r_\alpha\).

This means we write \(u_a(t) = \varphi_a(\mathbf{r}(t)) = \sum_{\alpha,\beta=1}^N J_{a\alpha} r_\alpha(t) + Z_{a\alpha\beta} r_\alpha(t) r_\beta(t) + \ldots\), and we evaluate the coefficients \(\{J, Z, \ldots\}\) by minimizing with respect to the constant matrices \(J_{a\alpha}\) and \(Z_{a\alpha\beta}\)
\[
\sum_t \left[ u_a(t) - \left\{ \sum_{\alpha,\beta=1}^N J_{a\alpha} r_\alpha(t) + Z_{a\alpha\beta} r_\alpha(t) r_\beta(t) + \ldots \right\} \right]^2 + \text{regularization term, if required}
\]
\[6\]. The dimension of \(J_{a\alpha}\) is \(D\) by \(N\). The dimension of \(Z_{a\alpha\beta}\) is \(D\) by \(N(N+1)/2\) as it is symmetric in \(\{\alpha, \beta\}\). If one simplifies to keeping only ‘diagonal’ terms in \(\{\alpha, \beta\}\), then the second term in Eq. \(6\) is \(Z_{a\alpha}[r_\alpha]^2\) and this has dimension \(D\) by \(N\).

We use this polynomial representation for \(\varphi(\mathbf{r})\), noting there are many ways of approximating multivariate functions of \(\mathbf{r}\).

Another, perhaps useful, expression is this:
\[
\frac{du_a(t)}{dt} = \frac{\partial \varphi_a(\mathbf{r}(t))}{\partial r_\beta(t)} \frac{dr_\beta(t)}{dt}.
\]

We have expressions for \(\frac{du_a(t)}{dt}\) and \(\frac{dr_\beta(t)}{dt}\) from the vector fields of the equations of motion for the driver and the reservoir, respectively.

### 2.3 The Auxiliary Method for GS

There are a variety of approaches for determining whether \(\mathbf{r}(t)\) and \(\mathbf{u}(t)\) exhibit GS. Perhaps the easiest approach is to establish two identical reservoirs \[27\] driven by the same \(\mathbf{u}(t)\),
\[
\frac{d\mathbf{r}_A(t)}{dt} = \mathbf{F}_r(\mathbf{r}_A(t), \mathbf{u}(t)),
\]
and
\[
\frac{d\mathbf{r}_B(t)}{dt} = \mathbf{F}_r(\mathbf{r}_B(t), \mathbf{u}(t)).
\]

Then we compare some function, say \(\chi(\mathbf{r}) = \mathbf{r} \cdot \mathbf{r}\), of \(\mathbf{r}_A(t)\) against the same function of \(\mathbf{r}_B(t)\). This should yield a straight line at \(\pi/4\) in the \(\{\chi(\mathbf{r}_A), \chi(\mathbf{r}_B)\}\) plane. (See Fig.
Figure 5: When one selects the hyperparameters outside the region of GS, for example using \( N = 2000, \ SR = 1.6 \) and \( \text{puz} = 0.02 \) for the \textit{tanh} reservoir, the function \( \varphi(\mathbf{r}) \) does not exist. We may expect the reservoir to operate poorly in producing a replica of the input \( \mathbf{u}(t) \). This feature is displayed in the \textbf{Left Panel} of Figure for \( z(t) \) and in the \textbf{Right Panel} for \( x(t) \) from time series taken from the Lorenz63 dynamics. This result is in sharp contrast to Fig.(3). The vertical black line at \( t = 0 \) separates the training and prediction phases.

1 in [26]), for an example. In other words, the two states \( \mathbf{r}_A(t) \) and \( \mathbf{r}_B(t) \) should be identical after a short transient period, even though the initial conditions of the reservoirs are typically different.

In the situation where one does not have a replica RC network, one can follow [29] in comparing \( \chi(\mathbf{r}(t)) \) versus \( \chi(\mathbf{r}(t+\tau)) \) for a long enough time delay \( \tau \) so that \( t \) and \( t+\tau \) are ‘independent of each other’. A straight line at \( \pi/4 \) should appear when \( \tau \) is of appropriate magnitude. In the experiments of [29] \( \tau \approx 150 \text{ ms} \).

This does not tell us what the function \( \varphi(\mathbf{r}) \) is or what any of its properties may be. It only gives us confidence that \( \varphi(\mathbf{r}) \) exists.

2.4 Synchronization Test

GS provides us with a test of whether a particular reservoir, with choice of architecture, dynamics and hyperparameters, has the capability to learn the dynamics implied by the data. Following the previous section, \textbf{without training}, one can simply evolve \( \mathbf{F}_r(\mathbf{r}(t), \mathbf{u}(t)) \) with the input \( \mathbf{u}(t) \) present for two different initial conditions, and then test if GS occurs. If GS does not occur between the reservoir and the data then the reservoir is almost certainly untrainable and the choice of hyperparameters needs to be changed.

This is what happens in Fig.(5) when the hyperparameters are chosen outside the region of GS—here with a \( SR > 1 \). The reservoir ceases to synchronize with the data and the reservoir prediction rapidly decreases to 0. This statement matches one of the rules of thumb given for reservoir computers [14].

One does not need to train the reservoir in order to check if GS occurs. We were able to test reservoirs with Fitzhugh-Nagumo neurons at the reservoir nodes as well as with
Hodgkin Huxley neurons at the reservoir nodes (not shown). Even though not much is known about training these kinds of reservoirs, we were still able to find large regions of parameter space where it would be impossible to train the network to learn the input data.

We found large regions of parameter space where learning is a possibility. When searching for a reservoir that will give good predictions, one should stick to the parameters where GS is shown to occur. Looking for GS greatly reduces the number of hyperparameters that must be searched in a traditional grid search in RC. GS can be tested by either the auxiliary method or by directly calculating the conditional Lyapunov exponents of the driven reservoir. These approaches yield quite similar results.

The advantage of searching first for GS comes from the fact that the auxiliary test is fast and efficient. The CLEs being negative mean that, by definition, the two reservoir states \(r_A\) and \(r_B\) should converge exponentially towards each other. In practice this property means that one can look at a much smaller segment of time than is required for accurate training. In addition, the training step does not need to be completed, so searching for GS is computationally much more efficient than training a reservoir and then evaluating it by predicting at multiple points.

3 A Geophysical Example: The Shallow Water Equations

The shallow water equations (SWE) describe fluid dynamics in a domain in which the horizontal length scales greatly exceed the vertical length scales. The SWEs often serve as a basic model for geophysical fluid dynamics due to the thickness of the atmosphere or ocean in relation to the size of the Earth. The troposphere, where most weather phenomena occur, varies from 6-20 km, while the ocean has an average depth of 3.7 km. These fluids constitute a thin film in relation to the size of flows over the surface of the Earth, which has a radius between 6357 km to 6378 km, depending on latitude.

Accurate numerical solutions to the SWEs on a grid have been investigated in detail by Sadourny [52] who concluded that a potential-enstrophy conserving scheme is effective. The details of this scheme can be found in Section 2 of [52]. We use a form of the SWEs with three dynamical variables: surface height \(h(x, y, t)\), and the \(u(x, y, t)\) and \(v(x, y, t)\) components of velocity. We solve the SWEs numerically on a discretized grid of size \(N_\Delta = 8\) in two horizontal directions, resulting in an \(8 \times 8\) grid. Including the three dynamical variables, this yields a \(D = 192\)-dimensional dynamical system.

Inspired by the scheme used in [20] on a 1 dimensional grid, we use this discretized numerical integration of the SWEs to drive a set of localized reservoirs arranged in 16 overlapping local “patches” on a 2 dimensional grid. Each patch receives input from a subset of 48 local variables of the total 192-dimensional input vector. The 48 variables input to each local reservoir consist of 16 \(u(t)\), 16 \(v(t)\) and 16 \(h(t)\) that are located at the 16 points on a local patch of the grid. Each local reservoir is used to predict 12 (4 \(u(t)\), 4 \(v(t)\), 4 \(h(t)\)) of these after training, thus creating the overlapping scheme.

From the dynamical variables \(\{u(x, y, t), v(x, y, t), h(x, y, t)\}\) we compare the reservoir output for normalized height and for the normalized vorticity \(\omega_z(x, y, t)\) with their coun-
Figure 6: We display two ways of computing regions of GS for a reservoir (N = 100) with Fitzhugh-Nagumo neurons at the nodes. Both methods give approximately the same result. **Left** The largest CLE calculated for Lorenz63 input and a Fitzhugh-Nagumo based ML device for variation in hyperparameters. Here **Blue** shows regions with positive CLEs. This means the hyperparameters in this region do not show GS. **Red** shows regions of negative CLE. This means GS exists in this region. **Right** The error between the response system and the auxiliary response system. A cutoff was picked for the error, determined by the criterion: $\|r_A - r_B\|/T < $ Threshold. $r_A/r_B$ are the two systems and $T$ is the number of time points, and tell us that the two systems do not show GS with one another. Choices for hyperparameters in the **Blue** regions indicate the absence of GS, while choices in the **Red** regions show GS.
Figure 7: **Top Left Panel** 3D Image of GS and NoGS regions Blue/Purple indicates a region of parameters, SR (0.9) and $\sigma$ (0.1), in the compound tanh reservoir model ($N = 5000$) which shows GS with a driving signal from the $8 \times 8$ SWE as $u(t)$. The red region shows no GS. **Top Right Panel** Contour Plot from **Top Left Panel. Bottom Panels** Forecast for the variables normalized height and vorticity in the 192 dimensional $8 \times 8 \times 3$ Shallow Water Equations SWE.
terparts in the data. We recall

\[ \omega_z(x, y, t) = \frac{\partial v(x, y, t)}{\partial x} - \frac{\partial u(x, y, t)}{\partial y}. \]

Even in this complicated set of overlapping localized RCs, it is straightforward and computationally efficient to apply our GS test to the data. Applying the auxiliary test we see—Fig. (7)—that there is a broad region where our 16 reservoir scheme synchronizes with the data. This test is much more computationally efficient than evaluating the reservoir by training, thus giving us guidance as to where to focus our search. Then, after a traditional search over this smaller grid of hyperparameters, a set of hyperparameters were found that produce reasonable and robust predictions over a short time scale. The test enables us to significantly reduce the number of hyperparameters searched.

4 Evaluations of the Reservoir

After running the test for generalized synchronization and performing a hyperparameter search, the question arises of how to guarantee stable forecasting? Many times in RC one encounters one of two situations:

- The forecast starts out close to the data but then quickly diverges and becomes non-physical
- The forecast is “good” for certain initial starting conditions not for others.

The typical approach for evaluating machine learning predictions with the mean squared error over a test set does not capture a key feature of RC. A well trained RC should be able to give good short term predictions for all initial starting points and be stable in the medium to long term. This feature is called attractor reconstruction in [24]. Instead of a test set, we propose an additional criteria for RC evaluation; a well trained RC reproduces the spectrum of Lyapunov exponents of the input system \( F_u \).

We show this calculation for the Lorenz63 and Lorenz96 systems. Our results show that the more of the spectrum of Lyapunov exponents are matched by the RC, the better the predictions. If the Lyapunov spectrum of the RC does not match that of the input then the two situations above are most likely to occur. In situations where it is difficult to exhaustively test the RC, perhaps because the model is expensive to run or there is limited data, evaluating the Lyapunov exponents of the reservoir will guarantee that the global error growth of the RC is the same as the data. A similar calculation is performed in [24] but without systematically tying the results to the average prediction time.

The results presented in Fig. (8) and in Fig. (9) again show the suggestion that the reservoir operates best at “the edge of chaos” [13, 55, 56], that is, the maximal prediction time of the reservoir corresponds to a SR just less than 1. We make the case that the “edge” corresponds to the state where the reservoir Lyapunov exponents approximately match all the non-negative exponents of the input system. In the case of the Colpitt’s oscillator (not shown) all three Lyapunov exponents are matched: positive, zero and negative.
Figure 8: **Top Left** Average prediction time of a N=2000 tanh reservoir as a function of SR for Lorenz63 Driver. The time units are in $\lambda_1 t$. The error bars indicate variation in prediction depending on the stability of the input stimulus. **Top Right** Largest Lyapunov exponent of the forecasting reservoir and the Lorenz63 input system as a function of the spectral radius. **Bottom** $\lambda_2, \lambda_3, \lambda_4$ Lyapunov exponents for the predicting reservoir. The method for computing the Lyapunov Exponents of an RC is discussed in [13, 24, 53, 54].
Figure 9: **Top Left** Average prediction time of a N=2000 tanh reservoir as a function of SR for $D = 5$ Lorenz96 Driver. The time units are in $\lambda_1 t$. The error bars indicate variation in prediction depending on the stability of the input stimulus. **Top Right** Largest Lyapunov exponent of the forecast reservoir and the input system (black line) as a function of the spectral radius. **Bottom** $\lambda_1, ..., \lambda_5$ Smaller Lyapunov exponents for the predicting reservoir. The method for computing the Lyapunov Exponents of an RC is discussed in [13, 24, 53, 54].
4.1 Discussion

The forecast reservoir LEs are estimated while the reservoir is on the synchronization manifold. Thus the LEs can be split into those transverse to the manifold—the conditional Lyapunov exponents (CLE)—and those longitudinal to it. The reservoir produces the best predictions when the longitudinal LEs are the same as the LEs of the input system and the transverse exponents are negative. When the longitudinal exponents don’t match then the polynomial approximation Eq. (6) is not a good approximation of $\varphi$, generating motions in extraneous dimensions and adding noise to the system. When the CLEs are positive then the systems are not coupled through GS.

Figure 10: The KY dimension (Olive Green), Eq.(25), of the forecasting reservoir (tanh, $N=2000$) driven by a Lorenz63 Left and Lorenz96 Right systems as a function of the SR plotted along with the prediction time (Red). The predicting reservoir KY dimension is an estimate of the dimensionality of the synchronization manifold where the RC resides. As the SR crosses $\approx 1.1$, corresponding to the largest CLE of the reservoir crossing 0 (Fig. 8), the dimension of the reservoir increases rapidly. This corresponds to the reservoir moving off the low dimensional generalized synchronization manifold.

One can see this more clearly and gain additional insight by plotting the forecast against the fractal dimension of the synchronization manifold in Fig.(10). The interpretation is that the lower the dimension of the synchronization manifold, the better are the predictions. This could be because even though the reservoir acts to “unfold” the attractor in a high dimensional space, if there are too many degrees of freedom there is movement in directions that do not correspond to physically meaningful signals. Thus the effect of the extra dimensions is to add the equivalent of noise into the reservoir.

A similar situation occurs when attempting to embed a chaotic signal in time delay coordinates [53]. There is a minimum embedding dimension for the signal given by the false nearest neighbors calculation [53, 57]. If one attempts to embed the signal in a higher dimension than the minimum embedding dimension then noise is introduced into the system and the calculation of quantities such as the Lyapunov exponents may be incorrect. If the dimension is too low, this will not unfold the attractor.
5 Conclusions

Recurrent neural networks are a powerful tool for time series prediction tasks. While much intuition and knowledge for practical applications have been built up for specific tasks over the years, understanding the tradeoffs when designing a particular network is of the utmost importance. In this paper we

1. Introduced a test based on the property of GS that helps narrow down the hyperparameter search space when designing an RNN for a specific problem
2. Explained the connection between generalized synchronization and RCs, which led us to be able to gain insight into how the properties (LEs, dimension) of the synchronization manifold affect the ability of the RC to predict forward in time, thus enabling us to set new evaluation criteria for RC

We have explored the role of generalized synchronization, where the input \( u(t) \) driving the reservoir and the reservoir coordinates \( r(t) \) satisfy \( u_a(t) = \varphi_a(r(t)) \). We have elaborated on the notion that the only training required to provide accurate estimations/forecasts by the trained reservoir involves the estimation of parameters in representations of \( \varphi(r) \).

Finally, we repeat our suggested strategy for achieving practical RC:

- given the dynamics of an RNN reservoir
  \[
  \frac{dr(t)}{dt} = F_r[r(t), u(t)], \tag{10}
  \]
  determine, perhaps by the ‘auxiliary’ method, if regions, dependent on the hyperparameters of \( A_{\alpha\beta} \), the reservoir adjacency matrix, have generalized synchronization (GS) between the drive signal \( u(t) \) and the reservoir coordinates \( r(t) \)
  \[
  u_a(t) = \varphi_a(r(t)) \quad a = 1, 2, ..., D \tag{11}
  \]
- Choose hyperparameters in those regions with GS.
- Select a representation for the function \( \varphi(r) \).
- Determine the parameters in the representation of \( \varphi(r) \) by whatever convenient means you may chose.
- Solve the autonomous differential equation for the evolution of
  \[
  \frac{dr(t)}{dt} = F_r[r(t), \varphi(r(t))], \tag{12}
  \]
  on the GS manifold.
- Evaluate the expected forecasting capability of parts in the GS regions by an examination of the Lyapunov Exponents.

As a final comment, let us recall that for the use of these methods in a practical use of forecasting with RC, it seems likely we will need to implement the reservoir in hardware for computational efficiency. [39]
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Supplementary Materials

A Dynamical Systems Used at the Nodes of the Reservoir Network

Any nonlinear dynamical system can be used for the reservoir dynamics. We use a uniform notation to include the adjacency/connectivity matrix \(A_{\alpha\beta}\), \(\alpha, \beta = 1, 2, ..., N\) and a reservoir vector \(R_{\alpha}(N, D, t)\) which specifies the connections within the reservoir \(A_{\alpha\beta}\) and the manner in which the driving data stream \(\zeta_{\alpha,b} u_b; \ b = 1, 2, ..., D\) is distributed among the active elements at the nodes of the reservoir network:

\[
R_{\alpha}(N, D, t) = \sum_{\beta=1}^{N} A_{\alpha\beta} r_{\beta}(t) + \sum_{b=1}^{D} \zeta_{\alpha,b} u_b(t)
\]  

(13)

A.1 Hodgkin-Huxley Model

The connection \(R_{\gamma}(N, D, t)\) for this input model uses

\[
\zeta_{\alpha,b} = \chi_{\alpha,b} I_0(V_{\alpha}(t))
\]  

(14)

The Hodgkin-Huxley equations [58–60] for the neurons with Na, K, and Leak Channels operating at reservoir sites \(\alpha = 1, 2, ..., N\) are given by:

\[
C_m \frac{dV_{\gamma}(t)}{dt} = g_{Na} m(V_{\gamma}(t))^3 h(V_{\gamma}(t))(E_{Na} - V_{\gamma}(t)) + g_{K} (n(V_{\gamma}(t))^4 (E_{K} - V_{\gamma}(t)) + g_{L} (E_{L} - V_{\gamma}(t)) + R_{\gamma}(N, 4, t)
\]

\[
\frac{dm_{\gamma}(t)}{dt} = \alpha_m(V_{\gamma}(t))(1 - m_{\gamma}(V_{\gamma}(t)) - \beta_m(V_{\gamma}(t)) m_{\gamma}(V_{\gamma}(t))
\]

\[
\frac{dh_{\gamma}(t)}{dt} = \alpha_h(V_{\gamma}(t))(1 - h_{\gamma}(V_{\gamma}(t)) - \beta_h(V_{\gamma}(t)) h_{\gamma}(V_{\gamma}(t))
\]

\[
\frac{dn_{\gamma}(t)}{dt} = \alpha_n(V_{\gamma}(t))(1 - n_{\gamma}(V_{\gamma}(t)) - \beta_n(V_{\gamma}(t)) n_{\gamma}(V_{\gamma}(t))
\]  

(15)

in which:

\[
\alpha_m(V) = \frac{0.1(V + 40)}{1 - \exp[-(V + 40)/10]}; \ \beta_m(V) = 4 \exp[-(V + 65)/18]
\]

\[
\alpha_h(V) = 0.07 \exp[-(V + 65)/20]; \ \beta_h(V) = \frac{1}{1 + \exp[-(V + 35)/10]}
\]

\[
\alpha_n(V) = \frac{0.01(V + 55)}{1 - \exp[-(V + 55)/10]}; \ \beta_n(V) = 1.125 \exp[-(V + 65)/80]
\]  

(16)
and

\[ I_0(V) = \frac{1}{2}[1 + \tanh(K(V - V_p)/2)]. \tag{17} \]

The values of the constants are chosen as: \( C_m = 1 \mu F/cm^2 \); \( g_{Na} = 120 mS/cm^2 \); \( E_{Na} = 50mV \); \( g_K = 36 mS/cm^2 \); \( E_K = -77 mV \); \( g_L = 0.3 mS/cm^2 \); \( E_L = -54 mV \); \( K = 10/mV \); \( V_p = 0 mV \).

**A.2 Fitzhugh-Nagumo Model**

The connection \( R_\gamma(N, D, t) \) for this input model uses

\[ \zeta_{\alpha, b} = \chi_{\alpha, b} I_0(V_\alpha(t)) \] \tag{18} \]

The equations for the Fitzhugh-Nagumo Model (FHN) \cite{61, 62} operating at reservoir sites \( \gamma = 1, 2, ..., N \) are

\[
\frac{dV_\gamma(t)}{dt} = \frac{1}{\tau} \left[ V_\gamma(t) - \frac{1}{3} V_\gamma(t)^3 - w_\gamma(t) \right] + R_\gamma(N, 2, t) \\
\frac{dw_\gamma(t)}{dt} = V_\gamma(t) - \eta w_\gamma(t) + \xi
\]

The constants here are \( \xi = 0.7 \), \( \eta = 0.8 \), \( \tau = 0.08 \) ms, and we choose \( I_0(V) = \frac{1}{2}[1 + \tanh(K(V - V_p))] \). \( K = 3/2 \), \( V_p = 1 \).

\( A \) is the \( N \times N \) adjacency matrix, \( A_{\alpha, \beta} \), where entries are selected with (probability of non-zero connections (\( pnz \))) in the range from \( \{-1, 1\} \) and then rescaled by the largest singular value of \( A \), namely the spectral radius (\( SR \)).

**A.3 The Hyperbolic Tangent Model**

Here the input to reservoir connection \( R_\alpha(N, D, t) \)

\[ \zeta_{\alpha, b} = \sigma W_{in-\alpha, b} u_b \] \tag{19} \]

We use the differential equation version of the combined linear operator in \( R_\alpha(N, D, t) \). We also use a scaling constant \( \mu \) to adjust the timescale of the reservoir dynamics.

\[
\frac{d\mathbf{r}(t)}{dt} = \mu \left[ -\mathbf{r}(t) + \tanh \left( \sum_{b=1}^{D} R_{\alpha b}(N, D, t) u_b(t) \right) \right]. \tag{20}
\]
B Data used for Driving Signals

Data are generated from a variety of simple dynamical systems to act as a nonlinear driving signal for the RC. Each model is described in detail below.

B.1 Lorenz 1963 Model

The Lorenz63 [63] equations form a deterministic nonlinear dynamical system that exhibits chaos for certain ranges of parameters. It was originally found as a three dimensional, reduced, approximation to the partial differential equations for the heating of the lower atmosphere of the earth by sunlight. The dynamical equations of motion are

\[
\begin{align*}
\frac{dx(t)}{dt} &= \sigma[y(t) - x(t)] \\
\frac{dy(t)}{dt} &= x(t)[\rho - z(t)] - y(t) \\
\frac{dz(t)}{dt} &= x(t)y(t) - \beta z(t)
\end{align*}
\]

with time independent parameters \(\sigma = 10, \rho = 28, \beta = 8/3\).

The Lyapunov exponents are \(\{\lambda_1, \lambda_2, \lambda_3\} = \begin{bmatrix} 0.9, 0, -14.7 \end{bmatrix}\) calculated via the QR decomposition algorithm given by Eckmann and Ruelle [54].

B.2 Colpitts Oscillator

The Colpitts Oscillator is a three dimensional nonlinear dynamical system describing chaos in a nonlinear circuit used widely in practice when it oscillates in a periodic limit cycle. The equations of the system are given

\[
\begin{align*}
\frac{dx(t)}{dt} &= \alpha y(t) \\
\frac{dy(t)}{dt} &= -\gamma(x(t) + z(t)) - qy(t) \\
\frac{dz(t)}{dt} &= \eta(y(t) + 1 - \exp(-x(t)))
\end{align*}
\]

with \(\alpha = 5, \gamma = 0.0797, q = 0.6898\) and \(\eta = 6.2723\). For \(\alpha < 5\) this circuit has limit cycle oscillations.

The Lyapunov exponents are \(\{\lambda_1, \lambda_2, \lambda_3\} = \begin{bmatrix} 0.09, 0, -0.8 \end{bmatrix}\) calculated via the QR decomposition algorithm given by Eckmann and Ruelle [54].
B.3 Lorenz96 Model

The dynamical equations introduced by [64]:

\[
\frac{dx_a(t)}{dt} = x_{a-1}(t)(x_{a+1}(t) - x_{a-2}(t)) - x_a(t) + f
\]  

and \( a = 1, 2, \ldots, D; \) \( x_{-1}(t) = x_{D-1}(t); \) \( x_0(t) = x_D(t); \) \( x_{D+1}(t) = x_1(t). \) \( f \) is a fixed parameter which we take to be in the range 8.0 to 8.2 where the solutions to these dynamical equations are chaotic [65]. The equations for the states \( x_a(t); \) \( a = 1, 2, \ldots, D \) are meant to describe ‘stations’ on a periodic spatial lattice. We use \( D = 5. \)

The Lyapunov exponents are \( \{\lambda_1, \ldots, \lambda_5\} = [0.6, \ 0, \ -0.4, \ -1.4, \ -3.8] \) calculated via the QR decomposition algorithm given by Eckmann and Ruelle [54].

C Details of Reservoir Implementation

C.1 Kaplan-Yorke Dimension

The Kaplan-Yorke (KY) dimension [66, 67] or Lyapunov dimension gives an upper bound on the dimension of a dynamical system through the Lyapunov exponents of that system. By definition, to calculate the KY dimension, arrange the Lyapunov exponents from largest to smallest \( \lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n, \) where \( n \) here is the dimension of the system or reservoir.

Let \( \alpha \) be the index for which

\[
\sum_{i=1}^{\alpha} \lambda_i \geq 0
\]

and

\[
\sum_{i=1}^{\alpha+1} \lambda_i < 0
\]

Thus the Lyapunov/KY or information dimension, \( D, \) of the system is [53]

\[
D = \alpha + \frac{\sum_{i=1}^{\alpha} \lambda_i}{|\lambda_{\alpha+1}|}.
\]  

C.2 Definition of Lyapunov Exponents

\( \mathbf{F}(x(t), u(t)) \) is the vector field for a dynamical system with external forcing. The LEs calculated for a nonautonomous system are called Conditional Lyapunov Exponents (CLE), conditioned on \( u(t) \) [68] If \( \mathbf{F}(x(t)) \) does not depend explicitly on time, then it is an autonomous system, and we are calculating LEs.

\[
\frac{dx(t)}{dt} = \mathbf{F}(x(t), u(t))
\]

\[
\frac{dx_a(t)}{dt} = F_a(x(t), u(t)); \ a = 1, 2, \ldots, N
\]
with $x(t)$ the state of the system and $F(x, u)$ the vector field of the dynamics.

The spectrum of LEs, one for each dimension of the state $x(t)$: $[\lambda_1, \lambda_2, \ldots, \lambda_N]$ can be evaluated using the variational equation of Eq.(26). This is formed by taking the derivative of Eq.(26)

$$\frac{\partial}{\partial x_b(t')} \frac{dx_a(t)}{dt} = \frac{d\phi_{ab}(t, t')}{dt}$$

$$= DF_{ac}(x(t))\phi_{cb}(t, t').$$

$$\phi_{ab}(t, t') = \frac{\partial x_a(t)}{\partial x_b(t')}; \quad DF_{ab}(x(t)) = \frac{\partial F_a(x(t))}{\partial x_b(t)} \quad (27)$$

The solution to this, arrived at by iteration of Eq.(27) involves the time ordering operator $[69] T_+$ for two operators (here matrices) $A(t)$ and $B(t')$ which do not commute.

$$T_+ A(t) B(t') = \begin{cases} A(t)B(t') & \text{if } t > t' \\ B(t')A(t) & \text{if } t < t'. \end{cases} \quad (28)$$

The variational equation is much easier to work with in discrete time $t = t_0 + n\Delta t$; $t' = t_0 + n'\Delta t$ where it appears as

$$\phi(n, n') = DF(n)\phi(n, n'), \quad (29)$$

and $\phi(n, n) = I$.

Then the solution for $\phi(n + L, n)$ is

$$\phi(n + L, n) = DF(n + L) \cdot \phi(n + L - 1, n)$$

$$= DF(n + L) \cdot DF(n + L - 1)\phi(n + L - 2)$$

$$\phi(n + L, n) = DF(n + L) \cdot DF(n + L - 1) \cdot \ldots \cdot DF(n) \quad (30)$$

The matrix $\phi(t, t')$ describes how small perturbations to a state $x(t)$ propagate to the state at $x(t')$. Given equations (26) and (27) one can solve them concurrently to find the Oseledec matrix $OSE(t, t') = \phi(t, t')\phi(t, t')^T$.

$$\lim_{t' \to \infty} \frac{1}{2t'} \log \phi(t, t')\phi(t, t')^T \quad (31)$$

The eigenvalues of the log of $OSE(t, t')$ for large times are the global Lyapunov Exponents; the $N$ eigenvalues are by definition real and the eigenvectors orthogonal since $OSE$ is a symmetric $N \times N$ matrix. We order the LEs $\lambda_1, \lambda_2, \ldots, \lambda_N$ with $\lambda_1 > \lambda_2 > \ldots > \lambda_N$.

Oseledec’s multiplicative ergodic theorem $[46]$ ensures that all $N$ LEs of a dynamical system (a) exist, (b) are independent of the initial starting point $x(t)$, and (c) are invariant under smooth coordinate transformations.

For a continuous time dynamical system one of the LEs must be 0, and $\sum_{a=1}^{N} \lambda_a \leq 0$.

OSE is an ill-conditioned matrix, so accurately evaluating all of its eigenvalues takes a quite stable algorithm. This is found in $[53, 54]$.

These definitions carry over to the nonautonomus dynamics with vector field $F(x(t), u(t))$ which we find in driven RNNs which include the RC systems we have considered. Then they are called CLEs as they are conditioned on the driving forces $u(t)$. $[68]$