Echo State Networks trained by Tikhonov least squares are $L^2$ approximators of ergodic dynamical systems

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Abstract

Echo State Networks (ESNs) are a class of single-layer recurrent neural networks with randomly generated internal weights, and a single layer of tuneable outer weights, which are usually trained by regularised linear least squares regression. Remarkably, ESNs still enjoy the universal approximation property despite the training procedure being entirely linear. In this paper, we prove that an ESN trained on a sequence of scalar observations from an ergodic dynamical system (with invariant measure $\mu$) using Tikhonov least squares will approximate future observations of the dynamical system in the $L^2(\mu)$ norm. We call this the ESN Training Theorem.

We demonstrate the theory numerically by training an ESN using Tikhonov least squares on a sequence of scalar observations of the Lorenz system, and compare the invariant measure of these observations with the invariant measure of the future predictions of the autonomous ESN.

Keywords: Reservoir computing; liquid state machine; time series analysis; Lorenz equations; dynamical system; delay embedding; Ergodic theory; recurrent neural networks.

1. Introduction

Echo state networks (ESNs) are a class of single layer recurrent neural networks introduced at the turn of the millennium, independently by Jaeger (2001) and Maass et al. (2002). These simple networks have been used to solve a range of machine problems where the input data is a time-series, including speech recognition (Skowronski and Harris, 2007), learning the rules of grammar (Tong et al, 2007), financial time series prediction (Ilie et al, 2007), Lin et al. (2008), short term traffic forecasting (Ser et al, 2020), placing UAV base stations (Peng et al, 2019) and learning about the behaviour of seals (Ser et al. 2018). ESNs are also a plausible model for the information processing of biological neurons (Girel and Egert, 2010). In this paper, we will present just enough definitions and theory to make sense of our results, but encourage the interested reader to read the recent review paper by Tanaka et al. (2019) who cover recent developments and open questions in the field of reservoir computing, a field encompassing ESNs. The ESN is effectively defined by the recursion relation

$$r_{k+1} = \tanh(Ar_k + W^{in}u_k + b)$$

where $r_k$ are $n$ dimensional state vectors, $A$ is the $n \times n$ reservoir matrix, representing the connection weights between neurons, $W^{in}$ is the $n \times 1$ input matrix connecting the scalar inputs $u_k$ to the reservoir matrix $A$, and $b$ is a bias vector. The reservoir matrix $A$, input matrix $W^{in}$ and bias vector $b$ are initialised randomly and remain unchanged. The ESN can be trained to approximate a sequence of scalars $a_k$ by solving the regularised linear squares problem

$$\min_{W^{out}} \sum_{k=1}^{K} ||W^{out}r_k - a_k||^2 + \lambda ||W^{out}||^2$$

where $\lambda > 0$ is the Tikhonov regularisation parameter. If the target scalars $a_k$ are equal to the observations $u_k$, then the ESN is being trained to predict the future. To see this,
we can set up a sequence of scalars $v_k$ like so

$$v_{k+1} = W^{\text{out}} s_k$$

$$s_{k+1} = \tanh(As_k + W^{\text{in}}v_{k+1} + b)$$

and we hope that $v_k \approx u_k$ for sufficiently many future values of $k$. We can view $s_k$ as the state of a discrete time autonomous dynamical system which we will call the ESN autonomous phase. In this paper, we will suppose $u_k$ are a sequence of sequential, scalar observations from an ergodic dynamical system, with invariant measure $\mu$. We will go on to prove that the system \[1\] will approximate the future observations of the ergodic dynamical system in the $L^2(\mu)$ norm. Our first step toward this result is to present some theory and notations for Echo State Networks trained on a sequence of scalar observations from a dynamical system. These definitions are presented in greater detail by [Hart et al. (2019)].

**Definition 1.1.** (Echo State Network) Let the activation function $\sigma$ be a function $\sigma \in C^1(\mathbb{R}, (-1,1))$ that has its derivative take values in the range $(0,1)$. Let $n \in \mathbb{N}$, $A$ be a real $n \times n$ matrix, and $W^{\text{in}}$ a real $n \times 1$ matrix. Let $h_i \in \mathbb{R}$ $\forall i \in \{1, ..., n\}$. Let $I_n := [-1,1]^n$ and define the function $\varphi : \mathbb{R}^n \to I_n$ component-wise by

$$\varphi_i(r) = \sigma(r_i + h_i) \quad \forall i \in \{1, ..., n\}.$$ 

We then define an Echo State Network (ESN) of size $n$ to be the triple $(\varphi, A, W^{\text{in}})$.

**Definition 1.2.** (ESN autonomous phase) The ESN autonomous phase with parameters $(A, W^{\text{in}}, W^{\text{out}}, \varphi)$ is a discrete time autonomous dynamical system $\psi \in C^1(\mathbb{R}^n)$ defined by

$$\psi(s) = \varphi((A + W^{\text{in}}W^{\text{out}})s).$$

**Definition 1.3.** (Echo State Family) Let $M$ be a compact $m$-manifold and $n \in \mathbb{N}$. Let $A$ be an $n \times n$ matrix; suppose that $\|A\|_2 < 1$, and $W^{\text{in}}$ an $n \times 1$ matrix: let the triple $(\varphi, A, W^{\text{in}})$ be an ESN. Let the discrete dynamical system be $\phi \in \text{Diff}^2(M)$ and let the observation function $\omega$ in $C^1(M, \mathbb{R})$. Let the family of functions $F = \{f^s_k : M \to I_n : r_0 \in I_n, k \in \mathbb{N}_0\}$ be defined as follows:

$$f^0_k(x) = r_0$$

$$f^0_k(x) = \varphi(Af^0_k \circ \phi^{-1}(x) + W^{\text{in}}\omega(x)).$$

We call the set of functions $F$ the Echo State Family according to [Hart et al. (2019)].

**Theorem 1.4.** (Echo State Mapping Theorem) With the notation and hypotheses of Definition 1.3 and the further assumption that $\|A\|_2 < \min(1,1/\|D\phi^{-1}\|_\infty)$, there exists a unique solution $f \in C^1(M, \mathbb{R}^n)$ of the equation

$$f = \varphi(Af \circ \phi^{-1} + W^{\text{in}}\omega)$$

such that for all $r_0 \in I_n$ the sequence $f^0_k$ converges in the $C^1$ topology to $f$ as $k \to \infty$. We call $f$ the Echo State Map.

**Proof.** [Hart et al. (2019)].

One can interpret the Echo State Map $f$ evaluated at $x \in M$ as the reservoir state $r$ of an Echo State Network trained on the input sequence $(\omega \circ \phi^{-2}(x), \omega \circ \phi^{-1}(x), \omega(x))$ extending forever into the past. Hart et al. (2019) have shown that if $A, W^{\text{in}}, b$ are drawn from appropriate distributions, then $f \in C^1(M, \mathbb{R}^n)$ is an embedding with positive probability. This theorem is stated below.

**Theorem 1.5.** (Weak ESN Embedding Theorem) Let $M$ be a compact $m$-manifold and $n \geq 2m + 1$. Let $A$ be a random variable with a distribution that has full support on the space of $n \times n$ matrices for which $\|A\|_2 < \min(1/\|D\phi^{-1}\|_\infty, 1)$, and let $W^{\text{in}}$ be a random variable with a distribution that has full support on the space of $m \times 1$ matrices, and let the triple $(\varphi, A, W^{\text{in}})$ be an ESN. Suppose $\phi \in \text{Diff}^2(M)$ has the following two properties:

1. $\phi$ has only finitely many periodic points with periods less than or equal to $2m$.

2. If $x \in M$ is any periodic point with period $k < 2m$ then the eigenvalues of the derivative $D\phi^k$ at $x$ are distinct.

Then for a generic observation function $\omega \in C^2(M, \mathbb{R})$ the Echo State Map $f$ is a $C^1$ embedding with probability $\alpha > 0$.

**Proof.** [Hart et al. (2019)].

The remainder of the paper is organised as follows. In section 2 we motivate the ESN Training Theorem. In section 3 we define an ergodic dynamical system and present Birkhoff’s Ergodic Theorem. We then introduce the major result of this paper we have called the ESN Training Theorem, stating that an ESN trained on a sequence of scalar observations from an ergodic dynamical system using Tikhonov least squares will $L^2(\mu)$ approximate the future observations of the system. In section 4 we present the work of [Luzzatto et al. (2005)] culminating in a proof that the Lorenz attractor is mixing, hence ergodic. This suggests the conditions of the ESN Training Theorem hold on the Lorenz attractor. We then demonstrate this numerically, by training an ESN using Tikhonov least squares on a sequence of scalar observations of the Lorenz system, then comparing the invariant measure of these observations with the invariant measure of the future predictions of the autonomous ESN.

2. Motivation for the ESN Training Theorem

Before we introduce the ESN Training Theorem, we will present a related theorem by [Hart et al. (2019)] stating that, given a structurally stable dynamical system, then for a sufficiently large ESN, there exists a linear readout layer $W^{\text{out}}$ for which the autonomous ESN has dynamics that are topologically conjugate to a structurally stable
dynamical system. One of the theorem’s assumptions is that the Echo State Map $f$ is an embedding, which holds with positive probability if $A, W^\text{in}, b$ are drawn randomly from appropriate distributions.

**Theorem 2.1. (ESN Approximation Theorem)** Let $M$ be a compact $n$-manifold and $n \in \mathbb{N}$ such that $n > 2m$. Let $A$ be an $n \times n$ matrix such that $\|A\|_2 < \min(1/\|D\phi^{-1}\|_\infty, 1)$, and $W^\text{in}$ an $n \times 1$ matrix, and let the triple $(\varphi, A, W^\text{in})$ be an ESN. Let $\phi \in \text{Diff}^1(M, \mathbb{R})$ be structurally stable, and let $\omega \in C^1(M, \mathbb{R})$. Suppose the Echo State Map $f \in C^1(M, \mathbb{R}^d)$ is a $C^1$ embedding.

Let $(x_j)_{j \in \mathbb{N}}, (y_j)_{j \in \mathbb{N}}$, and $(b_j)_{j \in \mathbb{N}}$ be sequences of i.i.d. $\mathbb{R}^n$, $\mathbb{R}$, and $\mathbb{R}$-valued random variables, respectively, with full support. Let $\alpha \in (0, 1)$. Then, with probability $\alpha$, there exists $d \in \mathbb{N}$ with $d > n$, an $d \times 1$ matrix $W^\text{out}$, an $n \times d$ matrix $A$, and a $d \times 1$ matrix $W^\text{in}$ assembled from the $n \times n$ matrix $A$, the $(d-n) \times n$ matrix $X$ with $j$th row $x_j$, and the $(d-n) \times 1$ matrix $Y$ with $j$th row $y_j$, like so:

$$
\tilde{A} = \begin{bmatrix} A & 0 \\ X & 0 \end{bmatrix} \quad \text{and} \quad \tilde{W}^\text{in} = \begin{bmatrix} W^\text{in} \\ Y \end{bmatrix},
$$

and an activation function

$$
\tilde{\phi}_i(r) = \sigma(r_i + b_i) \quad \forall \ i \in \{1, \ldots, d\},
$$

such that the autonomous ESN $\psi \in C^1(\mathbb{R}^d)$ with parameters $(\tilde{A}, \tilde{W}^\text{in}, \tilde{W}^\text{out}, \tilde{\phi})$ has a normally hyperbolic attracting submanifold on which $\psi$ is topologically conjugate to $\phi$.

**Proof.** Hart et al. (2019).

The ESN approximation theorem is an existence result, and we are motivated to develop a constructive result for $W^\text{out}$ obtained by Tikhonov regularised least squares. This is because, in practice, the readout layer $W^\text{out}$ of the autonomous ESN is found by solving the Tikhonov regularised least squares problem. For examples of ESNs trained by least squares on the trajectory of a dynamical system see Jæger (2001), Xi et al. (2003), Schrauwen et al. (2007), Shi and Han (2007), Yong Song et al. (2010), Pathak et al. (2017), Løkse et al. (2017), Ye (2019), Chattopadhyay et al. (2019), Vlachas et al. (2019), and Hart et al. (2019).

3. The ESN Training Theorem

In this section, we will prove that, for an ergodic dynamical system, an ESN trained on a 1D observation of almost any sufficiently long orbit using least squares will yield an autonomous phase that approximates the embedded dynamical system in the $L^2(\mu)$ norm.

We require that the underlying dynamical system is ergodic so that minimising the mean square differences between observations and predictions does not create a bias toward areas with lots of training data. The ergodicity ensures that that training data generated from a 1D observation of a trajectory initialised at almost any point $x_0 \in M$ will fairly represent the dynamics on $M$. To make this formal, we will introduce the definition of ergodicity and the celebrated Ergodic Theorem.

**Definition 3.1. (Generic Point)** Suppose $\phi : X \to X$ is a measure preserving map with respect to the measure space $(X, \Sigma, \mu)$. Then $x_0 \in X$ is called a generic point if the orbit of $x_0$ is uniformly distributed over $X$ according to the measure $\mu$.

**Proposition 3.2.** Suppose $\phi : X \to X$ is a measure preserving map with respect to the probability space $(X, \Sigma, \mu)$ and $s \in L^1(\mu)$. Suppose $x_0$ is a generic point in $X$ then

$$
\lim_{j \to \infty} \frac{1}{j} \sum_{k=0}^{j-1} s \circ \phi^k(x_0) = \int_X s \, d\mu.
$$

**Definition 3.3.** (Ergodic) Let $\phi : X \to X$ be a measure preserving transformation on the probability space $(X, \Sigma, \mu)$. Then $\phi$ is ergodic if for every $\sigma \in \Sigma$ with $\phi^{-1}(\sigma) = \sigma$ either $\mu(\sigma) = 0$ or $\mu(\sigma) = 1$.

**Theorem 3.4.** (Birkhoff’s Ergodic Theorem) Suppose $\phi : X \to X$ is ergodic with respect to the probability space $(X, \Sigma, \mu)$ and $s \in L^1(\mu)$. Then $\mu$-almost all $x \in X$ are generic hence for $\mu$-almost all $x \in X$

$$
\lim_{j \to \infty} \frac{1}{j} \sum_{k=0}^{j-1} s \circ \phi^k(x) = \int_X s \, d\mu.
$$

**Proof.** Birkhoff (1931).

The left hand side of (2) is called the *time average* taken from initial point point $x \in M$, and the right hand side called the *space average*. The Ergodic Theorem then states that the time average taken from almost all initial points equals the space average. Now we can state a preliminary result relating Tikhonov least squares to Ergodic theory, which we will prove in two different ways.

**Theorem 3.5.** Let $\phi : X \to X$ be ergodic with respect to the probability space $(X, \Sigma, \mu)$, with $X \subset \mathbb{R}^d$ and let $x_0$ be a generic point of $\phi$. Let $g : X \to \mathbb{R}$ be integrable with respect to $\mu$ and $\lambda > 0$. Then

$$
\lim_{j \to \infty} \arg \min_{W} \left( \frac{1}{j} \sum_{k=0}^{j-1} (W \phi^k(x_0) - g \circ \phi^k(x_0))^2 + \lambda \|W\|_2^2 \right)
$$

$$
= \int_X g(x) x^\top d\mu \left( \int_X x x^\top d\mu + I \lambda \right)^{-1}
$$

$$
= \arg \min_{W} \left( \int_X (W - g(x))^2 d\mu + \lambda \|W\|_2^2 \right)
$$

$$
= \arg \min_{W} \|W - g\|_{L^2(\mu)} + \lambda \|W\|_2^2
$$

where $W : \mathbb{R}^d \to \mathbb{R}$ is the map $x \mapsto Wx$.  


Proof. (Using linear algebra) Consider that
\[
\arg\min_W \left( \int_X (Wx - g(x))^2 d\mu + \lambda \|W\|^2 \right)
\]
satisfies
\[
0 = D \left( \int_X (Wx - g(x))^2 d\mu + \lambda \|W\|^2 \right)
\]
where \(D\) is the derivative operator with respect to \(W\). Now
\[
0 = \int_X D(Wx - g(x))^2 d\mu + \lambda D\|W\|^2
\]
\[
= \int_X 2(Wx - g(x))x^\top d\mu + 2\lambda W
\]
\[
= \int_X (Wx - g(x))x^\top d\mu + \lambda W
\]
\[
= W \int_X x^\top d\mu - \int_X g(x)x^\top d\mu + \lambda W
\]
\[
W \left( \int_X x x^\top d\mu + I\lambda \right) = \int_X g(x)x^\top d\mu.
\]
Now, we observe that the matrix on the left hand side
\[
\left( \int_X x x^\top d\mu + I\lambda \right)
\]
is symmetric positive definite for any \(\lambda > 0\) and is therefore invertible. We can now write down a closed form expression for the unique critical point \(W\)
\[
W = \int_X g(x)x^\top d\mu \left( \int_X x x^\top d\mu + I\lambda \right)^{-1}.
\]
Next, we observe that
\[
\int_X g(x)x^\top d\mu = \lim_{j \to \infty} \frac{1}{j} \sum_{k=0}^{j-1} g \circ \phi^k(x_0)\phi^k(x_0)^\top
\]
\[
\int_X x x^\top d\mu = \lim_{j \to \infty} \frac{1}{j} \sum_{k=0}^{j-1} \phi^k(x_0)\phi^k(x_0)^\top
\]
by the Ergodic Theorem, so
\[
W = \lim_{j \to \infty} \frac{1}{j} \sum_{k=0}^{j-1} g \circ \phi^k(x_0)\phi^k(x_0)^\top
\]
\[
\times \left( \lim_{j \to \infty} \frac{1}{j} \sum_{k=0}^{j-1} \phi^k(x_0)\phi^k(x_0)^\top + I\lambda \right)^{-1}
\]
\[
= \lim_{j \to \infty} \left( \frac{1}{j} \sum_{k=0}^{j-1} g \circ \phi^k(x_0)\phi^k(x_0)^\top \right)
\]
\[
\times \left( \frac{1}{j} \sum_{k=0}^{j-1} \phi^k(x_0)\phi^k(x_0)^\top + I\lambda \right)^{-1}
\]
by continuity of the inverse map
\[
= \lim_{j \to \infty} \left( \frac{1}{j} \sum_{k=0}^{j-1} g \circ \phi^k(x_0)\phi^k(x_0)^\top \right)
\]
\[
\times \left( \frac{1}{j} \sum_{k=0}^{j-1} \phi^k(x_0)\phi^k(x_0)^\top + I\lambda \right)^{-1}
\]
by the algebra of limits
\[
= \lim_{j \to \infty} Y_j^\top X_j(X_j^\top X_j + I\lambda)^{-1}.
\]
where \(X_j\) is a \(j\times d\) matrix with \(k+1\)th row equal to \(\phi^k(x_0)\), and \(Y_j\) is a \(j\)-vector with \(k+1\)th entry equal to \(g \circ \phi^k(x_0)\). Now we recognise the regularised least squares solution
\[
Y_j^\top X_j(X_j^\top X_j + I\lambda)^{-1}
\]
\[
= \arg\min_W \left( \frac{1}{j} \sum_{k=0}^{j-1} (W \phi^k(x_0) - g \circ \phi^k(x_0))^2 + \lambda \|W\|^2 \right)
\]
so
\[
W = \lim_{j \to \infty} Y_j^\top X_j(X_j^\top X_j + I\lambda)^{-1}
\]
\[
= \lim_{j \to \infty} \arg\min_W \left( \frac{1}{j} \sum_{k=0}^{j-1} (W \phi^k(x_0) - g \circ \phi^k(x_0))^2 + \lambda \|W\|^2 \right)
\]
and the proof is complete. \(\Box\)

Before we prove Theorem 3.5 again, we will prove that the map \(\arg\min\) defined on strictly convex functions is continuous when viewed as a map from \(C^0(\mathbb{R}^n, \mathbb{R})\) to the space \(\mathbb{R}^n\) with topologies induced by the supremum norm and euclidean norm respectively.

**Lemma 3.6.** Let
\[
\arg\min : \{ s \in C^0(\mathbb{R}^d, \mathbb{R}) \mid s \text{ is strictly convex} \} \to \mathbb{R}^d
\]
return the unique minimum of a convex strictly function \(s \in C^0(\mathbb{R}^d, \mathbb{R})\). Then \(\arg\min\) is continuous.
Proof.

\[ \| \arg \min(s_n) - \arg \min(s) \|_2 \leq 2 \| s_n - s \|_\infty \]

so \( \arg \min \) is Lipschitz continuous and therefore continuous.

We are now ready to prove Theorem 3.5 again.

\textbf{Proof.} (Using topology) First, we realise \( \arg \min \) is a map

\[ \arg \min : \{ s \in C^0(\mathbb{R}^d, \mathbb{R}) \mid s \text{ is strictly convex} \} \to \mathbb{R}^d \]

returning the unique minimum of a strictly convex function. Consequently

\[ \arg \min \frac{1}{j} \sum_{k=0}^{j-1} (W \phi^k(x_0) - g \circ \phi^k(x_0))^2 + \lambda \| W \|_2^2 \]

is well defined because the Tikhonov least squares problem is strictly convex. Now,

\[ \lim_{j \to \infty} \arg \min \frac{1}{j} \sum_{k=0}^{j-1} (W \phi^k(x_0) - g \circ \phi^k(x_0))^2 + \lambda \| W \|_2^2 \]

\[ = \arg \min \frac{1}{j} \sum_{k=0}^{j-1} (W \phi^k(x_0) - g \circ \phi^k(x_0))^2 + \lambda \| W \|_2^2 \]

\[ = \arg \min \int_X (W x - g(x))^2 d\mu + \lambda \| W \|_2^2 \]

by the Ergodic Theorem

\[ = \arg \min \| W \cdot g \|_{L^2(\mu)} + \lambda \| W \|_2^2 \]

and the proof is complete.

With these results about Ergodicity, we are ready to state and prove the ESN training theorem. We will assume \( \phi \) has at least 1 generic point, and note that if \( \phi \) is ergodic almost all points in \( M \) are generic. The statement of the ESN training theorem is quite verbose, so we will summarise it in words first. Suppose we have a function \( u \in C^1(M, \mathbb{R}) \) that we wish to approximate to a tolerance \( \epsilon > 0 \), with probability of success \( \alpha \in (0, 1) \). If our objective is to predict the future observations then we can set \( u := \omega \circ \phi \). Then there exists a finite number of training points \( \ell \in \mathbb{N} \) and an interval of admissible regularisation values \((0, \lambda^*)\), and a reservoir size \( d \), such that, an ESN trained by Tikhonov least squares with regularisation parameter \( \lambda \in (0, \lambda^*) \) on a scalar training trajectory of length \( \ell \), originating from a generic point \( x_0 \), will \( L^2(\mu) \) approximate \( u \) to a tolerance \( \epsilon \) with probability \( \alpha \).

\textbf{Theorem 3.7.} (ESN Training Theorem) Let \( M \) be a compact \( m \)-manifold and \( n \in \mathbb{N} \) such that \( n > 2m \). Let \( A \) be an \( n \times n \) matrix where \( \| A \|_2 < \min(1/\|D \phi^{-1}\|_\infty, 1) \), and \( W^{\text{in}} \) an \( n \times n \) matrix, and let the triple \((\phi, A, W^{\text{in}})\) be an ESN. Suppose \( \phi \in \text{Diff}(M) \) has a generic point \( x_0 \in M \) and let \( \omega \in C^1(M, \mathbb{R}) \). Suppose the Echo State

Map \( f \in C^1(M, \mathbb{R}^n) \) is a \( C^1 \) embedding. Let \((x_j)_{j \in \mathbb{N}}, (y_j)_{j \in \mathbb{N}}, \) and \((b_j)_{j \in \mathbb{N}}\) be sequences of i.i.d. \( \mathbb{R}^n \), \( \mathbb{R} \), and \( \mathbb{R} \)-valued random variables, respectively, with full support. Let \( u \in C^1(M, \mathbb{R}) \), and \( \alpha \in (0, 1) \) and \( \epsilon > 0 \). Then, with probability \( \alpha \), there exists an open interval \((0, \lambda^*)\), a \( d \in \mathbb{N} \), and \( \ell \in \mathbb{N} \), such that, for any \( \alpha \in (0, \lambda^*) \)

\[ \| W^{\text{out}} f - u \|_{L^2(\mu)} < \epsilon \]

where

\[ W^{\text{out}} := \arg \min_{W} \sum_{k=0}^{\ell-1} \| W \circ \phi^{-k}(x_0) - u \circ \phi^{-k}(x_0) \|^2 + \lambda \| W \|_2^2, \]

and \( f \) is the Echo State Map for the \( d \)-dimensional ESN \((\varphi, A, W^{\text{in}})\) comprised of a \( d \times d \) matrix \( A \), and a \( d \times 1 \) matrix \( W^{\text{in}} \), which are assembled from the \( n \times n \) matrix \( A \), the \((d-n) \times n \) matrix \( X \), with \( j \)th row \( x_j \), and the \((d-n) \times n \) matrix \( X \) with \( j \)th row \( x_j \), like so:

\[ \bar{A} = \begin{bmatrix} A & 0 \\ X & 0 \end{bmatrix} \quad \text{and} \quad \bar{W}^{\text{in}} = \begin{bmatrix} W^{\text{in}} \\ Y \end{bmatrix}, \]

and an activation function

\[ \bar{\varphi}_i(r) = \sigma(r_i + b_i) \quad \forall \ i \in \{1, ..., d\}. \]

Proof. By assumption, the Echo State Map \( f \) defined for the ESN \((\varphi, A, W^{\text{in}})\) with respect to \((\phi, \omega)\) is an embedding, so the Echo State Map \( f \) defined for \((\bar{\varphi}, \bar{A}, \bar{W}^{\text{in}})\) with respect to \((\bar{\phi}, \bar{\omega})\) is also an embedding. For the remainder of the proof we will restrict the codomain of \( f \) to its image in order to yield a \( C^1 \) diffeomorphism. Before we proceed, we establish some preliminary results. First we define \( y : M \to y(M) \subset \mathbb{R}^{n+1} \) by

\[ y_1(x) = \omega(x) \quad \text{and} \quad \begin{bmatrix} y_2(x) \\ y_3(x) \\ \vdots \\ y_{n+1}(x) \end{bmatrix} = f \circ \phi^{-1}(x). \]

Now, for any given value \( \alpha \in (0, 1) \) and \( \epsilon > 0 \), by the Random Universal Approximation Theorem \cite{Hart2013}, there exists a \( d \in \mathbb{N} \) and a \( d \times 1 \) matrix \( W^{\text{out}} \) such that \( g \in C^1(\mathbb{R}^{n+1}, \mathbb{R}) \) defined by

\[ g(z) = \sum_{i=1}^{d} W_i^{\text{out}} \sigma(\begin{bmatrix} [\bar{W}^{\text{in}} \bar{A}]_i & z & b_i \end{bmatrix}) \quad \text{(3)} \]

satisfies

\[ \| g - u \circ y^{-1} \|_{\infty} < \frac{\epsilon}{3C} \quad \text{(4)} \]
where $[\hat{W}^\text{in}, \hat{A}]$ is a $1 \times (n + 1)$ matrix with 1st entry $\hat{W}^\text{in}$ and $(j + 1)$th entry $\hat{A}_j$, and $C$ is a constant that satisfies $\|s\|_{L^2(\mu)} \leq C\|s\|_\infty \forall s \in C^0(\mathbb{R}^{n+1}, \mathbb{R})$. Now let
\[
\lambda^* = \frac{\epsilon}{3\|W^\text{out}\|_2^2}
\]
so that for any $\lambda \in (0, \lambda^*)$ we have
\[
\lambda\|W^\text{out}\|_2^2 < \frac{\epsilon}{3}.
\]
Now define a sequence of vectors
\[
W^\text{out}_j := \arg\min W \left\{ \sum_{k=0}^{j-1} \|W \hat{f} \circ \phi^{-k}(x_0) - u \circ \phi^{-k}(x_0)\|^2 + \lambda\|W\|_2^2 \right\}
\]
where
\[
\arg\min : \{ s \in C^0(\mathbb{R}^d, \mathbb{R}) \mid s \text{ is strictly convex} \} \rightarrow \mathbb{R}^d
\]
is the map returning the unique minimum of a strictly convex function $s \in C^1(\mathbb{R}^d, \mathbb{R})$. Note that argmin is continuous with respect to the $C^0$ topology. Now define the limit
\[
W^\text{out} := \lim_{j \to \infty} W^\text{out}_j
\]
\[
= \arg\min_W \left( \lim_{j \to \infty} \sum_{k=0}^{j-1} \|W \hat{f} \circ \phi^{-k}(x_0) - u \circ \phi^{-k}(x_0)\|^2 + \lambda\|W\|_2^2 \right)
\]
by continuity of argmin
\[
= \arg\min_W \int_M \|W \hat{f} - u\|^2 + \lambda\|W\|_2^2 \ d\mu
\]
by the Ergodic Theorem
\[
= \arg\min_W \|W \hat{f} - u\|_{L^2(\mu)} + \lambda\|W\|_2^2
\]
so we can see by minimality that
\[
\|W^\text{out}_\infty \hat{f} - u\|_{L^2(\mu)} + \lambda\|W^\text{out}_\infty\|_2^2 \leq \|W^\text{out} \hat{f} - u\|_{L^2(\mu)} + \lambda\|W^\text{out}\|_2^2
\]
so
\[
\|W^\text{out} \hat{f} - u\|_{L^2(\mu)} \leq \|W^\text{out} \hat{f} - u\|_{L^2(\mu)} + \lambda\|W^\text{out}\|_2^2.
\]
Now choose $\ell \in \mathbb{N}$ sufficiently large that
\[
\|W^\text{out}_\ell - W^\text{out}\|_2 < \frac{\epsilon}{3\|f\|_{L^2(\mu)}}.
\]
We are now ready to prove the result.
\[
\|W^\text{out}_\ell \hat{f} - u\|_{L^2(\mu)} = \|W^\text{out}_\ell \hat{f} - W^\text{out}_\ell \hat{f} + W^\text{out}_\ell \hat{f} - u\|_{L^2(\mu)}
\]
\[
\leq \|W^\text{out}_\ell \hat{f} - W^\text{out}_\ell \hat{f}\|_{L^2(\mu)} + \|W^\text{out}_\ell \hat{f} - u\|_{L^2(\mu)}
\]
\[
\leq \|\hat{f}\|_{L^2(\mu)} \|W^\text{out}_\ell - W^\text{out}\|_{L^2(\mu)} + \|W^\text{out}_\ell \hat{f} - u\|_{L^2(\mu)}
\]
\[
< \epsilon + \|W^\text{out}_\ell \hat{f} - u\|_{L^2(\mu)} \text{ by } (3)
\]
\[
< \epsilon + \|W^\text{out}_\ell \hat{f} - u\|_{L^2(\mu)} + \lambda\|W^\text{out}\|_2^2 \text{ by } (4)
\]
\[
< \epsilon + \frac{\epsilon}{3} \frac{C}{3C} + \lambda\|W^\text{out}\|_2^2 \text{ by } (5).
\]

The ESN Training theorem guarantees an approximation in the $L^2(\mu)$ norm, which is sadly weaker than the $C^1$ norm. That is to say, a sequence which converges in $C^1$ also converges in $L^2(\mu)$, but the converse does not hold in general. In fact, one can imagine an autonomous phase trained by least squares regression that is close to an embedded dynamical system on average, yielding a good $L^2(\mu)$ approximation, but with a single small region of $\mathbb{R}^d$ on which the approximation is very far from the embedded dynamics. Alternatively, one could imagine an autonomous phase that is very close the embedded dynamics everywhere, but rapidly oscillates as a consequence of having very high derivatives. These would yield poor $C^1$ approximations, which are necessary to ensure that an autonomous trajectory remains near the embedded dynamical system for all future time, and replicates the system's topology. To increase the chance of obtaining a good $C^1$ approximation, we might introduce Tikhonov regularisation, in the hope that this will tame the derivatives of the autonomous ESN, leading to a sufficiently strong $C^1$ approximation for a topologically conjugate autonomous phase.

We must conclude that least squares regression does not guarantee a topologically conjugate autonomous phase, but we note that real data sets are contaminated by noise and finite precision arithmetic where an $L^2(\mu)$ approximation may be most suitable. Moreover, computing the
(regularised) least squares solution using the SVD decomposition, or some other algorithm, is much faster than minimising the maximal pointwise distance, which may be necessary to yield a good $C^1$ approximation. Despite the theoretical limitations of the regularised least squares approach - it seems to work well in practice. In fact we can interpret bad $C^1$ approximations in the parlance of machine learning as overfitted solutions, as they fit the training data well, in exactly the terms that we define a good fit, but fail to make good predictions about the unseen future.

3.1. Convergence rate of the time average to the space average

The ESN training theorem guarantees, under appropriate conditions, that, with probability $\alpha$, a sufficiently large amount of training data $\ell$ will yield an arbitrarily good $L^2(\mu)$ approximation. The question remains as to how much training data is required for a given $L^2(\mu)$ approximation. To answer this, we turn our attention to the convergence rate of the time average to the space average

$$
\lim_{j \to \infty} \frac{1}{j} \sum_{k=0}^{j-1} s \circ \phi^k(x) = \int_M s \, d\mu \tag{2}
$$

as the timespan over which training data is collected grows. We know the function $s \in L^1(\mu)$ is given by

$$
s(x) = \|W \tilde{f}(x) - \omega \circ \phi(x)\|^2 + \lambda \|W\|^2_2
$$

but the underlying ergodic operator $\phi$ is unknown, so we seek a uniform estimate for the rate of convergence for $s$ (which we note depends on $\phi$) over all ergodic maps $\phi$. Unfortunately, no such estimate can possibly exist. Kachurovskii (1996) presents negative results that (in the author’s words) leave no hope that estimates of the rate of convergence depending only on the averaged function $s$ can be obtained in ergodic theorems. The negative results presented by Kachurovskii (1996) prove that the amount of training data required is strictly dependent on the dynamical system.

Though we cannot say exactly how many data points we need for a good $L^2(\mu)$ approximation, the central limit theorem for ergodic dynamical systems suggests that for an initial point chosen uniformly over the invariant measure of $\phi$, the difference between the finite time average and space average converges to normal distribution with standard deviation converging to 0 with order $1/\sqrt{k}$. We will make this precise in the following theorem.

**Theorem 3.8.** (Central Limit Theorem for Ergodic Dynamical Systems) Let $\phi : X \to X$ be ergodic with respect to the probability space $(X, \Sigma, \mu)$. Let $s \in L^1$ be $\Sigma$-measurable. Then the random variables $X_k = s \circ \phi^k(X_0)$ whose sum is denoted $S_k$ satisfy the central limit theorem:

$$
\lim_{k \to \infty} \mu \left\{ \left. \frac{S_k - kE[f]}{\sqrt{k}} \right| \leq z \right\} = \frac{1}{2\pi \sigma_f} \int_{-\infty}^{z} e^{-\frac{\tau^2}{2\sigma_f^2}} \, d\tau
$$

almost surely, or in other words, $\frac{S_k - kE[f]}{\sqrt{k}}$ converges in law to $N(0, 1)$.

**Proof.** Cami (2010).

4. The Lorenz attractor is stably mixing

We showed in the previous section that we can $L^2(\mu)$ approximate an ergodic dynamical system using an ESN and Tikhonov least squares. Many authors have used ESNs trained by Tikhonov least squares to reconstruct dynamical systems including Jaeger (2001), Xi et al. (2007), Schrauwen et al. (2007), Shi and Harl (2007), Yong Song et al. (2010), Pattak et al. (2017), Lokse et al. (2017), Yeo (2019), Chattopadhyay et al. (2019), Vlachas et al. (2019), and Hart et al. (2019) and had remarkable success. Many authors including Chattopadhyay et al. (2019) successfully predict the future observations of the Lorenz system, while Pattak et al. (2017), Vlachas et al. (2019), and Hart et al. (2019) additionally recover topological invariants including Lyapunov exponents, fixed point eigenvalues and homology groups. In this section, we will offer a possible explanation for this success. It turns out, the Lorenz attractor is mixing which implies it is ergodic, suggesting the conditions of the ESN Training Theorem hold and we can $L^2(\mu)$ approximate the Lorenz attractor. To make this formal, we will present some theory, starting with the definition of a mixing dynamical system.

**Definition 4.1.** (Mixing) Let $\phi : X \to X$ be a measure preserving transformation on the measure space $(X, \Sigma, \mu)$ with $\mu(X) = 1$. Then $\phi$ is mixing if for any $A, B \in \Sigma$

$$\lim_{j \to \infty} \mu(A \cap \phi^j(B)) = \mu(A)\mu(B).$$

**Lemma 4.2.** (Mixing implies ergodic) Let $\phi : X \to X$ be a measure preserving transformation on the measure space $(X, \Sigma, \mu)$ with $\mu(X) = 1$. Suppose $\phi$ is mixing, then $\phi$ is ergodic.

**Proof.** Suppose $\phi$ is mixing and $A, B \in \Sigma$. Then

$$\lim_{j \to \infty} \mu(A \cap \phi^{-j}(B)) = \mu(A)\mu(B)$$

$$\implies \lim_{j \to \infty} \frac{1}{j} \sum_{k=0}^{j-1} \mu(A \cap \phi^{-k}(B)) = \mu(A)\mu(B)$$

$$\implies \lim_{j \to \infty} \frac{1}{j} \sum_{k=0}^{j-1} \mu(A \cap \phi^{-k}(A)) = \mu(A)^2. \tag{7}$$

Now suppose $\mu(A) = \mu(\phi^{-1}(A))$. Then (7) reduces to $\mu(A) = \mu(A)^2$ hence $\mu(A) = 1$ or $\mu(A) = 0$, so $\phi$ is ergodic.

**Definition 4.3.** (Stable Mixing) Let $\phi : X \to X$ be a measure preserving transformation on the measure space $(X, \Sigma, \mu)$ with $\mu(X) = 1$. Then $\phi$ is stably mixing if sufficiently small $C^1$ perturbations of $\phi$ are mixing.
Theorem 4.4. The Lorenz (1963) system

\[\begin{align*}
\dot{x} &= \sigma(y - x) \\
\dot{y} &= x(p - z) - y \\
\dot{z} &= xy - \beta z
\end{align*}\]  

with parameters \(\sigma = 10, \beta = 8/3, \rho = 28\) admits a robust attractor that is stably mixing.

Proof. Luzzatto et al. (2005) \(\Box\)

Now, the Lorenz attractor is stably mixing, so any sufficiently good \(C^1\) approximation to the evolution operator \(\phi\), obtained by numerical methods, is also stably mixing. Consequently, a numerically approximated Lorenz system is ergodic, by Lemma 4.2. Thus, we expect that an ESN, trained using Tikhonov least squares, on a sequence of scalar observations of a numerically integrated trajectory of the Lorenz attractor will \(L^2(\mu)\) approximate the attractor.

5. Replicating an invariant measure of the Lorenz system

To demonstrate the theory presented so far, we numerically integrated a trajectory of the Lorenz system, shown in Figure 1, using the MATLAB ODE45 Runge-Kutta integrator. We then created a sequence of equally spaced scalar observations by taking \(\omega(x, y, z) = x\). We trained an ESN on this time series using Tikhonov least squares, then let the autonomous ESN produce a sequence of future predictions. We have shown the scalar observations and future predictions consecutively in Figure 2. We then binned the scalar observations and the future predictions into separate histograms, both of which we expect to converge to the invariant measure of the \(x\) component of the Lorenz system. The histograms are illustrated in Figure 3 while the convergence of the time average to the space average is shown in Figure 4.

The ESN was initialised with the following parameters: spectral radius \(\rho = 1\), reservoir size \(n = 300\), and activation function \(\varphi = \tanh\). The reservoir matrix \(A\) is an Erdős-Rényi matrix with mean 6 and connection weights (where they are non-zero) i.i.d Gaussian, re-scaled such that \(\rho = 1\). The matrix \(W_{\text{out}}\) is populated with i.i.d Gaussian weights \(\sim N(0, 1)\) which are then scaled by a 'strength parameter' \(p = 0.1\). We choose a regularisation parameter \(\lambda = 10^{-6}\) to solve the regularised least square problem

\[\min_{W_{\text{out}}} \sum_{k=1}^{K} \|W_{\text{out}} r_k - u_k\|^2 + \lambda \|W_{\text{out}}\|^2\]

using the SVD decomposition method presented by Hansen et al. (2006).

Figure 1: A picture of the famous Lorenz attractor. Here the trajectory was initialised at \((1, 1, 1)\) and quickly converges to the attractor.

Figure 2: Here the 1D observations are shown in blue (up to time 100 for those of you reading in black and white) and future predictions shown in red (onwards from time 100).

6. Conclusions and future work

The main result of this paper is the ESN Training Theorem, which states that an ESN trained on a sequence of scalar observations from an ergodic dynamical system (with invariant measure \(\mu\)) using Tikhonov least squares will \(L^2(\mu)\) approximate the dynamical system. We then presented the work of Luzzatto et al. (2005) building on the work of Afraimovich et al. (1977), Guckenheimer and Williams (1979), Pesin (1992), Williams (1979), and Tucker (1999) culminating with the seminal work of Tucker (2002) which resolved Smale’s 14th problem (Do the properties of the Lorenz attractor exhibit that of a strange attractor?). This result implies the Lorenz attractor exists and is mixing, hence ergodic. This allowed us to conclude that an ESN trained on a sequence of scalar observations taken from the Lorenz system using Tikhonov Least Squares should \(L^2(\mu)\) approximate the dynamics in the attractor. We believe this explains the success many authors including Pathak et al. (2017), Vlachas et al. (2018), and Hart et al. (2019) have had reconstructing the Lorenz attractor using an ESN trained with Tikhonov least squares.

We discussed in section 3 that the \(L^2(\mu)\) norm is weaker than the \(C^1\) norm, in the sense that convergence in \(C^1\) implies convergence in \(L^2(\mu)\), while the converse does not hold. This is somewhat unsatisfying, because we need the autonomous phase of the ESN to be a \(C^1\) approximator of the embedded (structurally stable) dynamics for the autonomous dynamics to be topologically conjugate to the
Lorenz system. is compared to invariant measure of the scalar observations of the Lorenz system that were trained on a sequence of scalar observations of the Lorenz system. Figure 3: The invariant measure of the future predictions of an ESN trained on a sequence of scalar observations of the Lorenz system.

(b) Numerically computed invariant measure of the future predictions of the Lorenz system.

Figure 3: The invariant measure of the future predictions of an ESN trained on a sequence of scalar observations of the Lorenz system is compared to the invariant measure of the scalar observations of the Lorenz system.

(a) Numerically computed invariant measure of the x-component of the Lorenz system.

Figure 4: Here we can see the time average of the x-component of the Lorenz system (blue) and the future predictions of the ESN (red) converge toward the space average of the x-component.

Figure 4: Here we can see the time average of the x-component of the Lorenz system.

It may be a fruitful to try to develop a training method beyond Tikhonov least squares that guarantees a $C^1$ approximation. Alternatively, it may be intriguing to explore under what conditions Tikhonov least squares does provide a sufficiently good $C^1$ approximation, which appears to happen frequently in simulations. Authors including Pathak et al. (2017), Vlachas et al. (2019), and Hart et al. (2019) have demonstrated that an ESNs trained with Tikhonov least squares can replicate topological invariants of dynamical systems like Lyapunov exponents, fixed point eigenvalues, and homology groups, suggesting a sufficiently good $C^1$ approximation was achieved.

Though the $L^2(\mu)$ approximation may not be sufficient for topological results, it may be powerful enough to prove interesting results about ESNs applied to control problems. We can view a control system as a dynamical system, for which we have at every state $x \in M$ a set of actions $a \in A$ available to us, and we seek a map $\pi : M \to A$, called an optimal controller in the language of control theory, and an optimal policy in the language of reinforcement learning, which maximises some reward function. To determine the optimal policy $\pi$ it suffices to determine the so-called value function $u : M \to \mathbb{R}$ which, we can in principal approximate with an ESN from only partial observations of the control system. Developing algorithms to find the optimal controller/policy may be a rewarding direction of future work.

We also believe much of the theory presented here could be generalised or modified for other recurrent neural networks like long short term memory networks (LSTMs). LSTMs are used extensively in industry and perform very well at context dependant time series problems. These are problems where events that happened a long time in the past may suddenly become important in the present. The ESN is not well suited to such problems, because the importance of events necessarily decays (at least) exponentially quickly as we move further into the past, while the structure of an LSTM sidesteps this problem. A detailed explanation of the architecture is provided by Gers (1999).

Equations for a peephole LSTM are listed below:

\[
\begin{align*}
    f_k &= \phi_g(A_f c_k + W_f^{i_k} u_k) \\
    i_k &= \phi_g(A_i c_k + W_i^{i_k} u_k) \\
    o_k &= \phi_g(A_o c_k + W_o^{i_k} u_k) \\
    c_k &= f_k \odot c_{k-1} + i_k \odot \varphi_c(W_c^{i_k} u_k) \\
    h_k &= \varphi_h(o_k \odot c_k)
\end{align*}
\]

where $f_k, i_k, o_k, c_k, h_k \in \mathbb{R}^n$ are the vectors of the forget gate, input gate, output gate, cell state, and hidden state (also known as the output state) associated to the LSTM at time $k$. Next, $u_k \in \mathbb{R}$ is the scalar input of the LSTM at time $k$ and $\varphi_g : \mathbb{R}^n : \mathbb{R}^n$ is a componentwise sigmoid function, $\varphi_c : \mathbb{R}^n : \mathbb{R}^n$ is the componentwise tanh function, and $\varphi_h : \mathbb{R}^n : \mathbb{R}^n$ is some function that is usually the identity map. $A_f, A_i, A_o, A_c$ are $n \times n$ matrices and the
$W^i, W^f, W^o, W^c$ are $1 \times n$ matrices. Finally, the symbol $\odot$ here represents the Hadamard product (taking componentwise product of 2 vectors).

We can see that LSTMs admit ESNs as a special case by fixing $A_f = 0, W^f = 0, b_f = 0, b_i = 0, b_c = \arctanh(1/2), W^c = 0$, so we can view LSTMs as a curious generalisation of ESNs. It may therefore interest the academic community studying LSTMs, as well as those with industrial applications in mind, to generalise the theory of ESNs presented here and elsewhere to LSTMs.

Another theoretical direction of future work may be to expand on the results of [Grigoryeva and Ortega (2018)] and [Gonon et al. (2020)] who have shown that ESNs (with free and randomly generated weights $A, W^i$ respectively) are universal filters. Roughly speaking, a filter is a map from a space of $n$-vector valued sequences to a space of $n$-vector valued sequences. The authors prove under mild conditions that an arbitrary filter can be approximated arbitrarily well by an ESN. These results could be generalised by proving an analogous result for LSTMs. Furthermore, one could assume the filter obeys some *ergodic-like* property for which we can guarantee a $W^\text{out}$ produced by Tikhonov least squares results in an ESN that $L^2$ approximates the filter.

One shortcoming of Echo State Networks (that is typical in a *machine learning* paradigm) is that physical information about the underlying dynamical system is typically ignored. The question of how one might integrate some basic knowledge of the underlying dynamical system into the ESN architecture was recently explored numerically by Huhn and Magri (2020) and Doan et al. (2020). Developing ideas further may be an intriguing direction of future work.

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