Initialization and Self-Organized Optimization of Recurrent Neural Network Connectivity

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Reservoir computing (RC) is a recent paradigm in the field of recurrent neural networks. Networks in RC have a sparsely and randomly connected fixed hidden layer, and only output connections are trained. RC Networks have recently received increased attention as a mathematical model for generic neural microcircuits, to investigate and explain computations in neocortical columns. Applied to specific tasks, their fixed random connectivity, however, leads to significant variation in performance. Few problem specific optimization procedures are known, which would be important for engineering applications, but also in order to understand how networks in biology are shaped to be optimally adapted to requirements of their environment. We study a general network initialization method using permutation matrices and derive a new unsupervised learning rule based on intrinsic plasticity (IP). The IP based learning uses only local learning, and its aim is to improve network performance in a self-organized way. Using three different benchmarks, we show that networks with permutation matrices for the reservoir connectivity have much more persistent memory than the other methods, but are also able to perform highly non-linear mappings. We also show that IP based on sigmoid transfer functions is limited concerning the output distributions that can be achieved.

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INTRODUCTION

Recurrent loops are abundant in the neural circuits of the mammalian cortex. Massive reciprocal connections exist on different scales, linking different brain areas as well as connecting individual neurons in cortical columns. In these columns as many as 80% of the synapses of neocortical interneurons form a dense local network (Maass and Markram, 2006) using very specific connectivity patterns for different neuron types (Douglas et al., 2004). These recurrent microcircuits are very stereotypical and repeated over the entire neocortex (Silberberg et al., 2002).

Two challenges for computational models of the neocortex are (a) explaining how these stereotypical microcircuits enable an animal to process a continuous stream of rapidly changing information from its environment (Maass et al., 2002), and (b) how these circuits contribute to the prediction of future events, one of the critical requirements for higher cognitive function (Maass and Markram, 2006).

To address these challenges, a mathematical model for generic neural microcircuits, namely the *liquid state machine* (LSM), was proposed by Maass et al. (2002). The framework for this model is based on real-time computation without stable attractors. The neural microcircuits are considered as dynamical systems, and the time-varying input is seen as a perturbation to the state of the high-dimensional excitable medium implemented by the microcircuit. The neurons act as a series of non-linear filters, which transform the input stream into a high-dimensional space. These transient internal states are then transformed into stable target outputs by readout neurons, which are easy to train (e.g. in order to do prediction or classification of input signals) and avoid many of the problems of more traditional methods of recurrent neural network training like slow convergence and vanishing gradients (first described in Hochreiter (1991), see also Bengio et al. (1994) and Hochreiter et al. (2001)). This approach to neural modeling has become known as *reservoir computing* (see Verstraeten et al. (2007) and Lukosevicius and Jaeger (2007) for reviews), and the LSM is one particular kind of model following this paradigm.

Echo state networks (ESN) (Jaeger, 2001a; Jaeger and Haas, 2004) are another reservoir computing model similar to LSM. They implement the same concept of keeping a fixed high-dimensional *reservoir* of neurons, usually with random connection weights between reservoir neurons small enough to guarantee stability. Learning procedures train only the output weights of the network to generate target outputs, but while LSM use spiking neuron models, ESN are usually implemented with sigmoidal nodes, which are updated in discrete time steps. We use ESN in all the experiments of this study for their better analytical tractability. An illustration of the architecture of ESN is given in Fig. 1. Please refer to the *Materials and Methods* section for a more detailed introduction to the mathematical model.

One problem of the reservoir computing approach is that there is considerable variation when different random reservoir initializations are used with all other network parameters remaining fixed (Ozturk et al., 2007). There has been early work on unsupervised optimization of recurrent neural networks by Hochreiter and Schmidhuber (1997a) and Klapper-Rybicka et al. (2001), and several reservoir specific optimization methods have been presented (e.g. Rad et al. (2008); Schmidhuber et al. (2007, 2005); Schrauwen et al.

TABLE I: Glossary

Recurrent Neural Network:	A special type of artificial neural network model, which allows loops and recurrent connections among its nodes.
Echo State Network:	A discrete-time recurrent neural network with a hidden layer having fixed (non-adaptive) random connectivity between its nodes. The only trainable connections are the output connections. This significantly reduces the learning problem to basically doing linear regression. An important part of the echo state network idea is the echo state property. Its definition gives a prerequisite for the global asymptotic stability of the network for any input it might encounter.
Liquid State Machine:	A continuous-time recurrent neural network, which implements the same basic ideas as echo state networks: to use a hidden layer neurons with fixed random connectivity and only train the output connections. Liquid state machines were created in order to model biologically relevant computations (while echo state networks were conceived as an engineering tool) and as such they are usually implemented with spiking neuron models (while echo state networks use analog sigmoid type neurons).
Reservoir Computing:	A unified name for different computational approaches using recurrent neural networks with a fixed random hidden layer and only train a linear output connections. This encompasses Echo State Networks, Liquid State Machines, and, as a special learning rule, backpropagation-decorrelation (BPDC) learning (Steil, 2004).
Reservoir:	Usually denotes the hidden layer of a recurrent neural network following the reservoir computing approach.
Reservoir Matrix:	A matrix whose individual entries are the connection strength values for the connections between each of the nodes in the reservoir. Sometimes also called reservoir connectivity matrix.
Spectral Radius:	The absolute value of the largest eigenvalue of a matrix. In discrete-time dynamical systems such as ESN, the spectral radius will give an indication of the longest time constant of the network, i.e., how long information will persist in the network before it decays. A larger spectral radius means longer time constants. It is also an important measure to determine stability criteria of the network, see for instance the *echo state property* in the Materials and Methods section.
Central Limit Theorem:	A mathematical theorem in probability theory attributed to Laplace, which states that the sum of a sufficiently large number of independent and identically distributed random variables, each with finite mean and variance, will approximate a Gaussian distribution.

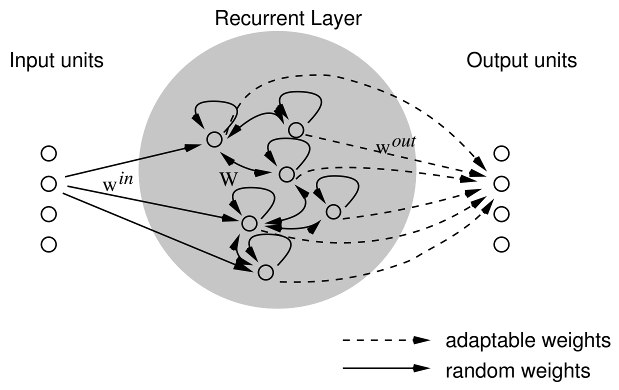

FIG. 1: Architecture of an echo state network. In echo state networks, usually only the connections represented by the dashed lines are trained, all other connections are setup randomly and remain fixed. The recurrent layer is also called a *reservoir*, analogously to a liquid, which has fading memory properties. As an example, consider throwing a rock into a pond; the ripples caused by the rock will persist for a certain amount of time and thus information about the event can be extracted from the liquid as long as it has not returned to its single attractor state — the flat surface.

(2008); Steil (2007); Wierstra et al. (2005); however, as of yet there is no universally accepted standard method. We study the effect of approaches aiming to reduce this dependency on a random initialization. In order to do this, we investigate two different approaches: the first one is based on a very specific initialization of the reservoirs of ESNs (Hajnal and Lőrincz, 2006; White et al., 2004), and the second one implements a pre-training phase for the reservoirs using a local adaptation mechanism. This mechanism models changes in a neurons intrinsic excitability in response to stimulation. Specifically, it models the phenomenon that biological neurons lower their firing threshold over time when they receive a lot of stimulation, and raise it when stimulation is lacking (see e.g. Zhang and Linden (2003) and Daoudal and Debanne (2003) for more details). A learning rule based on this phenomenon was introduced by Triesch (2005), further studied in (Triesch, 2007), and has been termed *intrinsic plasticity* (IP). The reservoir initialization method is based on the idea of optimally exploiting the high dimensionality of the reservoir. The methods based on IP, while also using high-dimensional reservoirs, aim to adapt the reservoir for a high entropy of codes. Moreover, we investigate an IP based learning rule for high sparsity of codes as these have been shown to improve information processing Field (1994).

We evaluate the different reservoir shaping and initialization methods using three different standard benchmarks. We find that reservoirs initialized with orthogonal column vectors in their connectivity matrix exhibit superior short-term memory capacity, and are also able to perform well in tasks requiring highly non-linear mappings. Furthermore, we identify a problem with an existing IP based rule and point out limitations of the approach if traditional neuron models are used. We discuss our contributions in the wider context of recurrent neural network research, and review possible solutions to the limitations that are identified as consequences of our results in this study.

RESULTS

We first present an IP based learning rule that changes a neurons output distribution to approximate a Laplace distribution. Consequently, we present results for the evaluation of ESN with random reservoirs, reservoirs using permutation matrices, and reservoirs pre-trained with IP for Gaussian and Laplace distributions, respectively.

IP Learning and a Rule for a Laplace Output Distribution

IP learning was introduced in (Triesch, 2005) as a way to improve information transmission in neurons while adhering to homeostatic constraints like limited energy usage. For a fixed energy expenditure (represented by a fixed mean of the neurons output distribution), the distribution that maximizes the entropy (and therefore the information transmission) is the exponential distribution. This was used for single neurons in (Triesch, 2005) and for neurons in a reservoir in (Steil, 2007) where it lead to a performance improvement over standard random reservoirs. In (Schrauwen et al., 2008), IP learning for a Gaussian output distribution of reservoir neurons was investigated, which is the maximum entropy distribution if, in addition to the mean, the variance of the output distribution is fixed. Again, an overall increase in performance was noted for several benchmark problems.

A Laplace distribution would lead to sparser codes than the Gaussian, and our hypothesis is that enough entropy would be preserved for a good input signal approximation. Researching Laplace output distributions was also suggested in Schrauwen et al. (2008) for similar reasons. Here, analogous to the calculations in (Schrauwen et al., 2008; Triesch, 2005), we derive an IP learning rule for this distribution to test our hypothesis.

In order to model the changes in intrinsic excitability of the neurons, the transfer function of our neurons is generalized with a gain parameter a and a bias parameter b:

$$y = f(x) = \tanh(ax + b).$$

The Laplace distribution, which we desire as the reservoir neurons' output distribution, is defined as

$$f(x \mid \mu, c) = \frac{1}{2c} \exp(-\frac{|x - \mu|}{c}), \quad c \neq 0.$$

Let $\tilde{p}_y(y)$ denote the sampled output distribution of a reservoir neuron and let the desired output distribution be $p(y)$, thus $p(y) = f(y \mid \mu, c)$. In the learning process, we try to minimize the difference between $\tilde{p}_y(y)$ and $p(y)$, which can be measured with the Kullback-Leibler divergence D_{KL}. Thus, we try to minimize:

$$D_{KL} = \int \tilde{p}_y(y) \log \left(\frac{\tilde{p}_y(y)}{\frac{1}{2c} \exp(-\frac{|y-\mu|}{c})} \right) dy$$

Taking derivatives of this function with respect to the gain and bias parameters of the neurons' transfer function (see Materials and Methods section for details), we arrive at the following learning rules for

TABLE II: Average memory capacity and normalized root mean squared error (NRMSE) for the NARMA modeling and the Mackey-Glass prediction tasks in the four different conditions (averaged over 50 simulation runs), standard dev. in parenthesis. Note that the errors for Mackey-Glass are scaled by a factor of 10^{-4}. For the memory capacity (first row) higher values are better, while lower values in the errors are better for the prediction tasks (second and third row).

	PMT	**RND**	**IPGAUSS**	**IPLAP**
Memory Capacity	**62.501** (5.086)	31.884 (2.147)	33.019 (2.464)	32.175 (3.127)
$\text{NRMSE}_{\text{NARMA}}$	**0.385** (0.022)	0.473 (0.035)	0.465 (0.053)	0.482 (0.041)
$\text{NRMSE}_{\text{Mackey-Glass}}$	3.373 (0.292)	2.411 (0.242)	2.802 (0.416)	**2.375** (0.416)

stochastic gradient descent with learning rate η:

$$\Delta b = -\eta \left(2y + \frac{y(1-y^2+\mu y)-\mu}{c|y-\mu|} \right).$$

$$\begin{aligned}\Delta a &= -\eta(-\frac{1}{a}) - \eta \left(2xy + \frac{yx(1-y^2+\mu y)-\mu x}{c|y-\mu|} \right) \\ &= \frac{\eta}{a} + \Delta b x.\end{aligned}$$

Effects of Reservoir Shape on Memory Capacity and Prediction Accuracy

In order to compare the different reservoir shaping and initialization methods, we tested them on three different standard benchmarks (cf. Materials and Methods section for details). The first set of experiments evaluated the short-term memory capacity (MC) of the different networks. In addition, we evaluated the networks on the task of modeling a 30th order NARMA (nonlinear auto regressive moving average) system, and with respect to their one-step prediction performance on the Mackey-Glass time-series. These tasks cover a reasonably wide spectrum of tests for different useful properties of reservoirs and are widely used in the literature, e.g. in Jaeger (2001a,b); Rad et al. (2008); Schrauwen et al. (2008); Steil (2007).

We tested ESN with four different conditions for the connectivity matrix of the reservoir. In condition **RND**, the reservoir matrix was initialized with uniform random values between $[-1; 1]$. Condition **PMT** tested a permutation matrix for the reservoir connectivity. Finally, we used IP optimization with a Gaussian distribution (cf. Schrauwen et al. (2008)) in **IPGAUSS** and a Laplace distribution (as described in the *Materials and Methods* section) in **IPLAP**. In all conditions, the reservoirs were scaled to have a spectral radius of 0.95. In the case of the IP methods, this scaling was done once before the IP training was started.

The results of the experiments are given in Table II, averaged over 50 simulation runs for each of the four conditions. The networks in the **PMT** condition essentially show double the memory capacity of networks in the other conditions, while networks pre-trained with **IPGAUSS** and **IPLAP** have very similar values

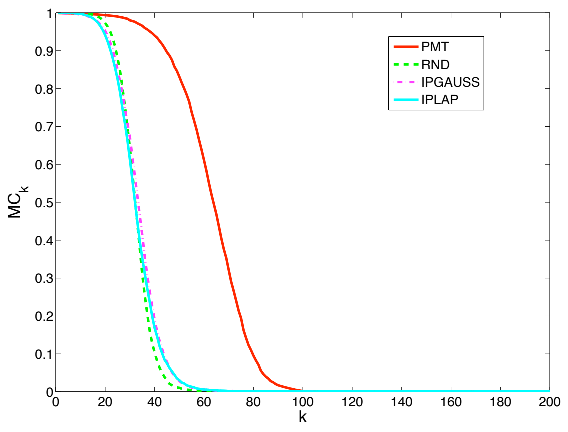

FIG. 2: The $\mathrm{MC_k}$ curves for the uniform random input data. The plot indicates how well the input signal can be reconstructed ($\mathrm{MC_k}$) for increasing delay times k

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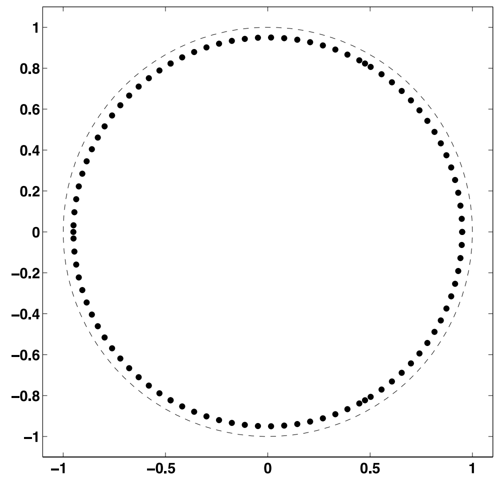
and show a slight increase compared to condition **RND**. Fig. 2 shows plots of the individual MC_k curves (see *Materials and Methods* for their definition) for all conditions in the MC task, with the curve for **PMT** showing much longer correlations than all the others. The results for the NARMA modeling task are less pronounced, but look similar in that the **PMT** networks perform better than the other tested conditions. The normalized root mean squared error (NRMSE) for **IPLAP** and **IPGAUSS** is very similar again, however, only **IPGAUSS** has a slight advantage over **RND**. For the Mackey-Glass one-step prediction, the performance of the **IPLAP** networks is better than the other ones, slightly ahead of **RND** (difference well within the standard deviation of the error, however). The **PMT** networks perform worst on this task.

The superior performance of networks in **PMT** on the short-term memory task could be expected: networks with a connectivity based on permutation matrices form are a particular instance of orthogonal networks, which, in turn, can be seen as a multidimensional version of a delay line (for details, see the *Materials and Methods* section). From a system theory perspective, the eigenvalues (poles) of the linearized system implemented by the network correspond to bandpass filters with center frequencies according to their angle in the complex plane (Ozturk et al., 2007). Larger eigenvalues will lead to longer time constants for the filters, preserving information for longer time in the network. Figure 3 (a) shows that the eigenvalues of the connectivity matrix of a 100 node ESN in the **PMT** condition are all of the same magnitude, and are spaced relatively uniformly just below the unit circle (the reservoir matrix was scaled to have a maxiumum absolute eigenvalue of 0.95 in this case, i.e., the matrix elements were either 0 or 0.95). The filters implemented by this network will thus have long time constants and provide support for many different frequencies in order to reconstruct the input signal. Compare this to the distribution of the eigenvalues of a connectivity matrix of an equally sized **RND** network in Figure 3 (b): they are much less uniformly distributed and have very different magnitudes, resulting in a mixture of both longer and shorter time constants for the network.

The **PMT** networks also outperform the other methods on the highly non-linear NARMA task, which

(a)



(b)

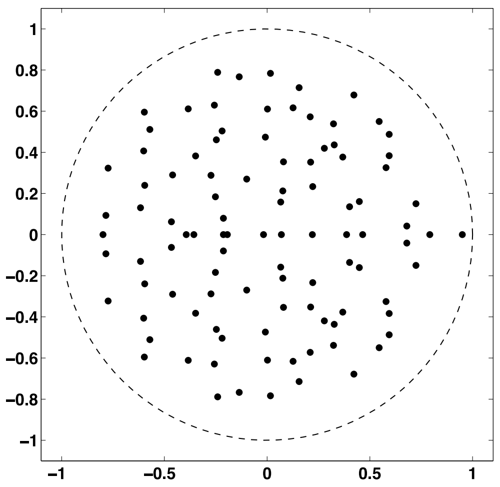


FIG. 3: Plot of the reservoir matrix eigenvalues in the complex plane for a 100 node network (a) in the PMT condition, and (b) in the RND condition. Both matrices have been scaled to have a spectral radius of 0.95

is less obvious. The NARMA task needs long memory, which the orthogonal reservoirs in **PMT** are able to provide; but one might suspect that the specific, rather sparse connectivity would not be able to perform the kind of non-linear mappings that the task requires (since there is less interaction between neurons in the reservoir than in networks which are more densely connected). The results show that this is not the case.

The Mackey-Glass prediction task requires shorter time constants and less memory than the other two tasks. In this case, the **IPLAP** networks perform best, slightly ahead of the **RND** condition. The **PMT** networks have the same spectral radius as the ones in **RND**, however, all eigenvalues in **PMT** have the same (large) magnitude. Therefore, the network is missing elements implementing shorter time constants, which would let it react to fast changes in the input. The best results we got on this task were actually achieved using ESN with fermi neurons and IP learning with an exponential output distribution (results not shown). In this case, the results were significantly better than the ones in **RND** (cf. also (Steil, 2007)).

IP Revisited

A closer investigation of the almost identical performance of both IP methods revealed that **IPLAP** also generated normally distributed output, very similar to **IPGAUSS**. To better understand the effect of the different IP rules, we used IP to approximate the Laplace, the Gaussian (both with a tanh activation function), and the exponential distribution (fermi activation function), respectively, with a single feedforward unit and uniformly distributed input on the interval $[-1; 1]$. As expected, the IP learning rule can successfully generate exponentially distributed output values (Fig. 5 a). IP fails, however, to generate output distributions that resemble the Gaussian or the Laplace (Fig. 5, b and c). This seems surprising in particular for the Gaussian, as IP has successfully been used to shape the output distribution of a reservoir (Schrauwen et al., 2008). A possible explanation for this phenomenon is discussed in the next section.

DISCUSSION

Recurrent neural network models are attractive because they hold the promise of explaining information processing in biological systems like the human neocortex, as well as being able to serve as tools for engineering applications. Moreover, they are computationally more powerful than simple feedforward architectures since they can exploit long-term dependencies in the input when calculating the output. Their theoretical analysis is complex, yet they are increasingly popular — mainly due to new, efficient architectures and training methods published in recent years (see (Hammer et al., 2009) for an excellent recent overview). These include, for instance, self-organizing maps for time series (Hammer et al., 2005), long short-term memory (LSTM) networks (Hochreiter and Schmidhuber, 1997b), Evolino (Schmidhuber et al., 2007, 2005), and also the reservoir computing approach as mentioned earlier in the article.

One of the obstacles to the initial applicability of recurrent neural networks was the problem of slow convergence and instabilities of training algorithms like backpropagation-through-time (BPTT) (Werbos, 1990) or real-time recurrent learning (RTRL) (Williams and Zipser, 1989). One of the important insights of the reservoir computing approach to overcome these limitations was that it often suffices to choose a fixed recurrent layer connectivity at random and only train the output connections. Compared to BPTT or RTRL, this simplifies the training process to a linear regression problem, resulting in significant speed improvements. It also enabled the use of much larger networks than possible with BPTT or RTRL. Results on standard benchmarks using reservoir methods were better than any previous of these methods and practical applications were also shown (Jaeger, 2003).

Compared to "traditional" recurrent neural network learning methods such as BPTT or RTRL, the reservoir computing paradigm represents a significant step forward for recurrent neural network technologies. On the other hand, it is clear that the approach gives up many of the degrees of freedom the networks would normally have by fixing the recurrent layer connectivity. Advanced methods such as LSTM networks (Hochreiter and Schmidhuber, 1997b) share the advantage of fast learning with ESN, but without restricting the networks to a fixed connectivity, using a more involved architecture and training method. For ESN, it has been shown that fixing the connectivity has the effect that different random initializations of a reservoir will lead to rather large variations in performance if all other parameters of the network setup remain the same (Ozturk et al., 2007). There have been proposals on how to manually design ESN in order to give performance that will consistently be better than random initializations (Ozturk et al., 2007), but there are no universally accepted standard training algorithms to adapt the connectivity in a problem specific and automatic way, before the output connections are trained.

This article makes two contributions with regard to this problem. As a first contribution, we investigate permutation matrices for the reservoir connectivity. Their benefit lies in the simple and inexpensive way in which they can be constructed, and we show that they implement a very effective connectivity for problems involving a long input history as well as non-linear mappings. For problems requiring fast responses of the network (or a mixture of slow and fast responses), their usefulness is limited. Furthermore, the method is general and not problem-specific. The IP based approaches we present and reference throughout the paper represent a problem-specific training method. They make use of the input signal in order to shape the output of the reservoir neurons according to a desired probability distribution. The second contribution in the article is a variation of the IP based approach by deriving a new learning rule to shape the reservoir node outputs according to a Laplace distribution, and to point out limitations of this method when standard sigmoidal neuron types are used in the network.

Concerning this last point, the illustration in Fig. 4 sheds light on the reason why an approximation of some distributions with IP is more difficult than others: given a uniform input distribution and a sigmoid transfer function, IP learning selects a slice from an output distribution that peaks towards either end of the input range, but never in the center. The output of an IP trained self-recurrent unit gives an insight why it is possible to achieve a Gaussian output distribution in a reservoir (Fig. 5, d). From the *central limit theorem* it follows that the sum of several i.i.d. random variables approximates a Gaussian. Even though in case of a recurrent reservoir not all inputs to a unit will be i.i.d., IP has to make input distributions only similar to each other to approximate a normal distribution in the output. This also explains why the output of an IP Laplace trained reservoir is normally distributed (several inputs with equal or at least very similar distributions are summed up). For uniform input and a single unit without recurrence, the best IP can do is to choose the linear part of the activation function, so that the output is also uniformly distributed (a slice more in the middle of Fig. 4). With self-recurrent connections, this leads to initially uniform distributions, which sum up. The resulting output, and eventually the whole reservoir output distribution become more and more Gaussian. A consequence of this effect is that IP with sigmoid transfer functions cannot be generalized to arbitrary distributions.

Our results confirm two important points that have been suggested for versatile networks, i.e., networks which should perform well even when faced with several different input signals or which might be used

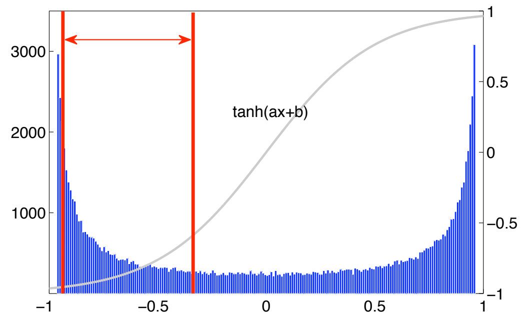


FIG. 4: Uniform input on the interval $[-1;1]$ and a $\tanh(\cdot)$ transfer function lead to the output distribution in the histogram. IP selects a slice of this distribution, as illustrated by the vertical lines. Adapting gain and bias changes width and position of the slice.

for tasks with different requirements. Ozturk et al. (2007) proposed that the eigenvalue distribution of reservoir matrices should be as uniform as possible, and that it would be needed to scale the effective spectral radius of the network up or down. For this scaling, they suggested an adaptable bias to the inputs of each reservoir node. With regard to this proposed requirement, we observed another limitation of purely IP-based reservoir pre-training: in our experiments (also reported in (Steil, 2007)), the IP learning rule always increased the spectral radius of the reservoir matrix (dependent on the setting of the IP parameters, cf. (Schrauwen et al., 2008)), and never decreased it (this is only true for reservoirs which are initialized with spectral radius < 1). This leads to longer memory, making it harder for the network to react quickly to new input, and causing interference of slowly fading older inputs with more recent ones. To alleviate this problem, a combination of instrinsic and synaptic plasticity as studied by Lazar et al. (2007) could enable scaling of the reservoir matrix depending on the current requirements of the task. The efficiency of synergy effects that result from a combination of intrinsic and synaptic plasticity was also shown by Triesch (2007), who additionaly suggested that this combination might be useful in driving networks to the region of best computational performance (*edge of chaos*, cf. (Bertschinger and Natschläger, 2004)) while keeping a fixed energy expenditure for the neurons. In (Lazar et al., 2007), this hypothesis was confirmed to the extent that networks with a combination of intrinsic and extrinsic plasticity were generally closer to this region than networks trained with only one form of plasticity.

MATERIALS AND METHODS

Echo State Networks

Learning algorithms for recurrent neural networks have been widely studied (e.g. see Doya (1995) for an overview). They have, however, not been widely used (Jaeger, 2003) because these learning algorithms, when applied to arbitrary network architectures, suffer from problems of slow convergence. ESN provide a

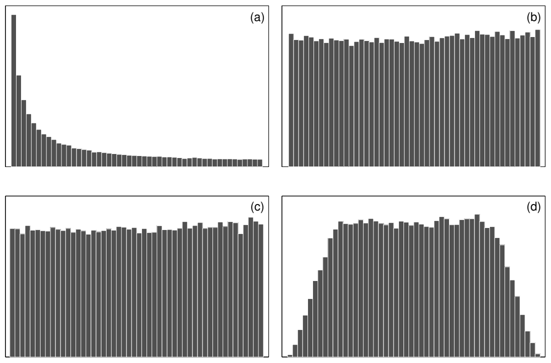


FIG. 5: Panels (a–c) show the effect of IP learning on a single feedforward neuron. Panel (a) shows the result of IP learning with a single fermi neuron without self-recurrence and a learning rule for the exponential output distribution. IP successfully produces the desired output distribution. In panels (b) and (c), we see the effect of IP learning on a single *tanh* neuron without self-recurrence, trained with a learning rule for a Gaussian, and a Laplace output distribution, respectively. In both cases, IP learning fails to achieve the desired result: the best it can do is to drive the neuron to a uniform output distribution, which has the smallest distance (for the given transfer function) to the desired distributions. Panel (d) shows the effect of **IPGAUSS** for a single self-recurrent *tanh* unit. The achieved output distribution is significantly more Gaussian-shaped than without the self-recurrence. The effect is amplified in a network where the neurons receive additional inputs with similar distributions. All units were trained using 100000 training steps and uniformly distributed input data on the interval $[-1; 1]$.

specific architecture and a training procedure that aims to solve the problem of slow convergence (Jaeger, 2001a; Jaeger and Haas, 2004). ESN are normally used with a discrete-time model, i.e. the network dynamics are defined for discrete time-steps t, and they consist of inputs, a recurrently connected hidden layer (also called *reservoir*) and an output layer (see Fig. 1).

We denote the activations of units in the individual layers at time t by $\mathbf{u}_t$, $\mathbf{x}_t$, and $\mathbf{o}_t$ for the inputs, the hidden layer and the output layer, respectively. We use $\mathbf{w}^{in}$, $\mathbf{W}$, $\mathbf{w}^{out}$ as matrices of the respective synaptic connection weights. Using $f(x) = \tanh x$ as output nonlinearity for all hidden layer units, the network dynamics is defined as:

$$\begin{aligned}\mathbf{x}_t &= \tanh(\mathbf{W}\mathbf{x}_{t-1} + I_t)\\ I_t &= \mathbf{w}^{in}\mathbf{u}_t\\ \mathbf{o}_t &= \mathbf{w}^{out}\mathbf{x}_t\end{aligned}$$

The main differences of ESN to traditional recurrent network approaches are the setup of the connection weights and the training procedure. To construct an ESN, units in the input layer and the hidden layer are connected randomly. Connections between the hidden layer and the output units are the only connections that are trained, usually with a supervised, offline learning approach: Training data are used to drive the network, and at each time step t, activations of all hidden units $\mathbf{x}(t)$ are saved as a new column to a state matrix. At the same time, the desired activations of output units $\mathbf{o}_{\text{teach}}(t)$ are collected in a second matrix. Training in this approach then means to determine the weights $\mathbf{w}^{out}$ so that the error $\epsilon_{\text{train}}(t) = (\mathbf{o}_{\text{teach}}(t) - \mathbf{o}(t))^2$ is minimized. This can be achieved using a simple linear regression (see Jaeger (2001a) for details on the learning procedure).

For the approach to work successfully, however, connections in the reservoir cannot be completely random; ESN reservoirs are typically designed to have the *echo state property*. The definition of the echo state property has been outlined in Jaeger (2001a). The following section describes this property in a slightly more compact form.

The Echo State Property

Consider a time-discrete recursive function $\mathbf{x}_{t+1} = F(\mathbf{x}_t, \mathbf{u}_t)$ that is defined at least on a compact sub-area of the vector-space $\mathbf{x} \in R^n$, with n the number of internal units. The $\mathbf{x}_t$ are to be interpreted as internal states and $\mathbf{u}_t$ is some external input sequence, i.e. the stimulus.

The definition of the echo state property is as follows: Assume an infinite stimulus sequence: $\bar{\mathbf{u}}^\infty = \mathbf{u}_0, \mathbf{u}_1, \ldots$ and two random initial internal states of the system $\mathbf{x}_0$ and $\mathbf{y}_0$. To both initial states $\mathbf{x}_0$ and $\mathbf{y}_0$ the sequences $\bar{\mathbf{x}}^\infty = \mathbf{x}_0, \mathbf{x}_1, \ldots$ and $\bar{\mathbf{y}}^\infty = \mathbf{y}_0, \mathbf{y}_1, \ldots$ can be assigned. The update equations for $\mathbf{x}_{t+1}$ and $\mathbf{y}_{t+1}$ are then:

$$\mathbf{x}_{t+1} = F(\mathbf{x}_t, \mathbf{u}_t)$$
$$\mathbf{y}_{t+1} = F(\mathbf{y}_t, \mathbf{u}_t)$$

The system $F(\cdot)$ will have the echo states if it is independent from the set $\mathbf{u}_t$, and if for any $(\mathbf{x}_0,\mathbf{y}_0)$ and all real values $\epsilon > 0$, there exists a $\delta(\epsilon)$ for which

$$d(\mathbf{x}_t, \mathbf{y}_t) \leq \epsilon$$

for all $t \geq \delta(\epsilon)$, where d is a square Euclidean metric.

Network Setup

For all of the experiments, we used ESNs with 1 input and 100 reservoir nodes. The number of output nodes was 1 for the NARMA and Mackey-Glass tasks, and 200 for the MC evaluation. In the latter, the 200 output nodes were trained on the input signal delayed by k steps ($k = 1 \ldots 200$). The input weights were always initialized with values from a uniform random distribution in the range $[-0.1; 0.1]$.

The output weights were computed offline using the pseudoinverse of a matrix $\mathbf{X}$ composed of the reservoir node activations over the last 1000 of a total of 2000 steps as columns, and the input signal. In the case of the MC task, the delayed input was used as follows: $\mathbf{w}^{out,k} = (\mathbf{u}_{1001-k \ldots 2000-k} * \mathbf{X}^\dagger)^T$ with $\mathbf{X}^\dagger$ denoting the pseudoinverse, and $k = 1 \ldots 200$.

For all three benchmark tasks, the parameter μ of the IP learning rule (both for **IPGAUSS** and **IPLAP**) was set to 0. The other IP related parameters were set according to table III. For both IP methods the reservoir was pre-trained for 100000 steps in order to ensure convergence to the desired probability distribution, with a learning rate of 0.0005. In all conditions, the spectral radius of the reservoir connectivity matrix was scaled to 0.95 (prior to pre-training in case of IP).

TABLE III: Settings of IP parameters σ (for IPGAUSS) and c (for IPLAP) for the different benchmark tasks. These settings were determined empirically through systematic search of the parameter space for the optimal values.

	σ	c
MC	0.09	0.08
NARMA	0.05	0.06
Mackey-Glass	0.07	0.05

Different input time-series were used for training the output weights and for testing in all cases. The input length for testing was always 2000 steps. The first 1000 steps of the reservoir node activations were discarded to get rid of transient states due to initialization with zeros before calculating the output weights and the test error.

Benchmark Description

To evaluate the short-term memory capacity of the different networks, we computed the k-delay memory capacity (MC_k) defined in Jaeger (2001b) as

$$MC_k = \frac{cov^2(\mathbf{u}_{t-k}, \mathbf{o}_t)}{\sigma^2(\mathbf{u}_{t-k})\sigma^2(\mathbf{o}_t)}$$

This is essentially a squared correlation coefficient between the desired signal delayed by k steps and the reconstruction by the kth output node of the network. The actual short-term memory capacity of the network is defined as $MC = \sum_{k=1}^{\infty} MC_k$, but since we can only use a finite number of output nodes, we limited their number to 200, which is sufficient to see a significant drop-off in performance for the networks in all of the tested conditions. The input for the MC task was random values sampled from a uniform random distribution in the range $[-0.8; 0.8]$.

The evaluation for the NARMA modeling and the Mackey-Glass prediction tasks was done using the normalized root mean squared error measure, defined as:

$$NRMSE = \sqrt{\frac{\langle(\tilde{y}(t) - y(t))^2\rangle_t}{\langle(y(t) - \langle y(t)\rangle_t)^2\rangle_t}},$$

where $\tilde{y}(t)$ is the sampled output and $y(t)$ is the desired output. For the NARMA task, the input time series $x(t)$ was sampled from a uniform random distribution between $[0, 0.5]$. The desired output at time $t + 1$ was calculated as:

$$y(t+1) = 0.2y(t) + 0.004y(t)\sum_{i=0}^{29} y(t-i) \\ + 1.5x(t-29)x(t) + 0.001,$$

The Mackey-Glass time-series for the last experiment was computed by integrating the system

$$\dot{y} = \frac{0.2y(t-\tau)}{1+y(t-\tau)^{10}} - 0.1y(t),$$

from time step t to $t+1$. The τ parameter was set to 17 in order to yield a mildly chaotic behavior.

Reservoirs Based on Permutation Matrices

Orthogonal networks (White et al., 2004) have an orthogonal reservoir matrix $\mathbf{W}$ (i.e. $\mathbf{W}\mathbf{W}^{\mathbf{T}} = 1$) and linear activation functions. These networks are inspired by a distributed version of a delay line, where input values are embedded in distinct orthogonal directions, leading to high memory capacity (White et al., 2004). Permutation matrices, as used by Hajnal and Lőrincz (2006), consist of randomly permuted diagonal matrices and are a special case of orthogonal networks. Here, and in Hajnal and Lőrincz (2006), the hyperbolic tangent (tanh) activation function was used, in order to facilitate non-linear tasks beyond memorization.

Derivation of the IP Learning Rule for a Laplace Output Distribution

Using the initial form presented in the Results section, we get:

$$\begin{aligned} D_{KL} &= \int \tilde{p}_y(y) \log\left(\frac{\tilde{p}_y(y)}{\frac{1}{2c}\exp(-\frac{|y-\mu|}{c})}\right) dy \\ &= \int \tilde{p}_y(y)\log\tilde{p}_y(y)dy - \int \tilde{p}_y(y)\log(\frac{1}{2c})dy \\ &\quad - \int \tilde{p}_y(y)\log\left(\exp(-\frac{|y-\mu|}{c})\right) dy \\ &= \int \tilde{p}_y(y)\log\tilde{p}_y(y)dy + \int \tilde{p}_y(y)\frac{|y-\mu|}{c}dy + C \\ &= \int \tilde{p}_y(y)\log\left(\frac{\tilde{p}_x(x)}{\frac{dy}{dx}}\right) dy + \int \tilde{p}_y(y)\frac{|y-\mu|}{c}dy + C \\ &= \int \tilde{p}_y(y)\log\tilde{p}_x(x)dy - \int \tilde{p}_y(y)\log(\frac{dy}{dx})dy \\ &\quad + \int \tilde{p}_y(y)\frac{|y-\mu|}{c}dy + C \\ &= \log\tilde{p}_x(x) + E\left(-\log(\frac{dy}{dx}) + \frac{|y-\mu|}{c}\right) + C \end{aligned}$$

where we have made use of the relation $\tilde{p}_y(y)dy = \tilde{p}_x(x)dx$ where $\tilde{p}_x(x)$ is the sampled distribution of the input. Writing this as $\tilde{p}_y(y) = \frac{\tilde{p}_x(x)}{\frac{dy}{dx}}$ and substituting it for $\tilde{p}_y(y)$ in the first term of the above equation. In order to minimize the function D_{KL}, we first derive it with respect to the bias parameter b:

$$\begin{aligned}\frac{\partial D_{KL}}{\partial b} &= \frac{\partial}{\partial b} E\left(-\log(\frac{dy}{dx}) + \frac{|y-\mu|}{c}\right)\\ &= E\left(-\frac{\frac{\partial^2 y}{\partial b \partial x}}{\frac{dy}{dx}} + \frac{(y-\mu)(1-y^2)}{c|y-\mu|}\right)\end{aligned}$$

The first term in the above equation is

$$\frac{\partial^2 y}{\partial b \partial x}\left(\frac{dy}{dx}\right)^{-1} = \frac{-2ay(1-y^2)}{a(1-y^2)} = -2y$$

so we have:

$$\frac{\partial D_{KL}}{\partial b} = E\left(2y + \frac{y(1-y^2+\mu y)-\mu}{c|y-\mu|}\right) \quad y \neq \mu.$$

The derivation with respect to the gain parameter a is analogous and yields:

$$\frac{\partial D_{KL}}{\partial a} = E\left(2xy + \frac{yx(1-y^2+\mu y)-\mu x}{c|y-\mu|} - \frac{1}{a}\right) \quad y \neq \mu.$$

From these derivatives, we identify the following learning rules for stochastic gradient descent with learning rate η:

$$\Delta b = -\eta\left(2y + \frac{y(1-y^2+\mu y)-\mu}{c|y-\mu|}\right).$$

$$\begin{aligned}\Delta a &= -\eta(-\frac{1}{a}) - \eta\left(2xy + \frac{yx(1-y^2+\mu y)-\mu x}{c|y-\mu|}\right)\\ &= \frac{\eta}{a} + \Delta b x.\end{aligned}$$

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