UnICORNN: A recurrent model for learning *very* long time dependencies

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Abstract

The design of recurrent neural networks (RNNs) to accurately process sequential inputs with long-time dependencies is very challenging on account of the exploding and vanishing gradient problem. To overcome this, we propose a novel RNN architecture which is based on a structure preserving discretization of a Hamiltonian system of second-order ordinary differential equations that models networks of oscillators. The resulting RNN is fast, invertible (in time), memory efficient and we derive rigorous bounds on the hidden state gradients to prove the mitigation of the exploding and vanishing gradient problem. A suite of experiments are presented to demonstrate that the proposed RNN provides state of the art performance on a variety of learning tasks with (very) long-time dependencies.

1. Introduction

Recurrent Neural Networks (RNNs) have been very successful in solving a diverse set of learning tasks involving sequential inputs (LeCun et al., 2015). These include text and speech recognition, time-series analysis and natural language processing. However, the well-known *Exploding and Vanishing Gradient Problem* (EVGP) (Pascanu et al., 2013) and references therein, impedes the efficiency of RNNs on tasks that require processing (very) long sequential inputs. The EVGP arises from the fact that the backpropagation through time (BPTT) algorithm for training RNNs entails computing products of hidden state gradients over a large number of steps and this product can either be exponentially small or large as the number of recurrent interactions increases.

Different approaches to solve the EVGP has been suggested in recent years. These include the use of gating mechanisms, such as in LSTMs (Hochreiter & Schmidhuber, 1997) and GRUs (Cho et al., 2014), where the additive structure of the gates mitigates the vanishing gradient problem. However, gradients might still explode, impeding the efficiency of LSTMs and GRUs on problems with very long time dependencies (LTDs) (Li et al., 2018). The EVGP can also be mitigated by constraining the structure of the recurrent weight matrices, for instance requiring them to be orthogonal or unitary (Henaff et al., 2016; Arjovsky et al., 2016; Wisdom et al., 2016; Kerg et al., 2019). Constraining recurrent weight matrices may lead to a loss of expressivity of the resulting RNN, reducing its efficiency in handling realistic learning tasks (Kerg et al., 2019). Finally, restricting weights of the RNN to lie within some prespecified bounds might lead to control over the norms of the recurrent weight matrices and alleviate the EVGP. Such an approach has been suggested in the context of *independent neurons* in each layer in (Li et al., 2018), and using a coupled system of damped oscillators in (Rusch & Mishra, 2021), among others. However, ensuring that weights remain within a pre-defined range during training might be difficult. Furthermore, *weight clipping* could also reduce expressivity of the resulting RNN.

In addition to EVGP, the learning of sequential tasks with very long time dependencies can require significant computational resources, for training and evaluating the RNN. Moreover, as the BPTT training algorithms entail storing all hidden states at every time step, the overall memory requirements can be prohibitive. Thus, *the design of a fast and memory efficient RNN architecture that can mitigate the EVGP is highly desirable for the effective use of RNNs in realistic learning tasks with very long time dependencies.* The main objective of this article is to propose, analyze and test such an architecture.

The basis of our proposed RNN is the observation that a large class of dynamical systems in physics and engineering, the so-called *Hamiltonian systems* (Arnold, 1989), allow for very precise control on the underlying states. Moreover, the fact that the phase space volume is preserved by the trajectories of a Hamiltonian system, makes such systems *invertible* and allows one to significantly reduce the storage requirements. Furthermore, if the resulting hidden state gradients also evolve according to a Hamiltonian dynamical system, one can obtain precise bounds on the hidden state

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Proceedings of the 38^{th} International Conference on Machine Learning, PMLR 139, 2021.

gradients and alleviate the EVGP. We combine and extend these ideas into an RNN architecture that will allow us to prove rigorous bounds on the hidden states and their gradients, mitigating the EVGP. Moreover, our RNN architecture results in a fast implementation that attains state of the art performance on a variety of learning tasks with very long time dependencies.

2. The proposed RNN

Our proposed RNN is based on the time-discretization of the following system of *second-order ordinary differential equations* (ODEs),

$$\mathbf{y}'' = -[\sigma\left(\mathbf{w} \odot \mathbf{y} + \mathbf{V}\mathbf{u} + \mathbf{b}\right) + \alpha \mathbf{y}]. \tag{1}$$

Here, $t \in [0,1]$ is the (continuous) time variable, $\mathbf{u} = \mathbf{u}(t) \in \mathbb{R}^d$ is the time-dependent *input signal*, $\mathbf{y} = \mathbf{y}(t) \in \mathbb{R}^m$ is the *hidden state* of the RNN with $\mathbf{w} \in \mathbb{R}^m$ is a weight vector, $\mathbf{V} \in \mathbb{R}^{m \times d}$ a weight matrix, $\mathbf{b} \in \mathbb{R}^m$ is the bias vector and $\alpha \geq 0$ is a control parameter. The operation $\odot$ is the Hadamard product and the function $\sigma : \mathbb{R} \mapsto \mathbb{R}$ is the *activation function* and is applied component wise. For the rest of this paper, we set $\sigma(u) = \tanh(u)$.

By introducing the auxiliary variable $\mathbf{z} = \mathbf{y}'$, we can rewrite the second order ODE (1) as a first order ODE system:

$$\mathbf{y}' = \mathbf{z}, \quad \mathbf{z}' = -[\sigma\left(\mathbf{w} \odot \mathbf{y} + \mathbf{V}\mathbf{u} + \mathbf{b}\right) + \alpha \mathbf{y}]. \tag{2}$$

Assuming that $\mathbf{w}_i \neq 0$, for all $1 \leq i \leq m$, it is easy to see that the ODE system (2) is a *Hamiltonian system*,

$$\mathbf{y}' = \frac{\partial H}{\partial \mathbf{z}}, \quad \mathbf{z}' = -\frac{\partial H}{\partial \mathbf{y}}, \tag{3}$$

with the *time-dependent Hamiltonian*,

$$H(\mathbf{y}, \mathbf{z}, t) = \frac{\alpha}{2}\|\mathbf{y}\|^2 + \frac{1}{2}\|\mathbf{z}\|^2 + \sum_{i=1}^{m} \frac{1}{\mathbf{w}_i} \log(\cosh(\mathbf{w}_i \mathbf{y}_i + (\mathbf{V}\mathbf{u}(t))_i + \mathbf{b}_i)), \tag{4}$$

with $\|\mathbf{x}\|^2 = \langle \mathbf{x}, \mathbf{x} \rangle$ denoting the Euclidean norm of the vector $\mathbf{x} \in \mathbb{R}^m$ and $\langle \cdot, \cdot \rangle$ the corresponding inner product.

The next step is to find a discretization of the ODE system (2). Given that it is highly desirable to ensure that the discretization respects the Hamiltonian structure of the underlying continuous ODE, the simplest such *structure preserving discretization* is the *symplectic Euler* method (Sanz Serna & Calvo, 1994; Hairer et al., 2003). Applying the symplectic Euler method to the ODE (2) results in the following discrete dynamical system,

$$\begin{aligned} \mathbf{y}_n &= \mathbf{y}_{n-1} + \Delta t \mathbf{z}_n, \\ \mathbf{z}_n &= \mathbf{z}_{n-1} - \Delta t[\sigma\left(\mathbf{w} \odot \mathbf{y}_{n-1} + \mathbf{V}\mathbf{u}_n + \mathbf{b}\right) + \alpha \mathbf{y}_{n-1}], \end{aligned} \tag{5}$$

for $1 \leq n \leq N$. Here, $0 < \Delta t < 1$ is the time-step and $\mathbf{u}_n \approx \mathbf{u}(t_n)$, with $t_n = n\Delta t$, is the input signal. It is common to initialize with $\mathbf{y}_0 = \mathbf{z}_0 = \mathbf{0}$.

We see from the structure of the discrete dynamical system (5) that there is *no interaction* between the neurons in the hidden layer of (5). Such an RNN will have very limited expressivity. Hence, we *stack* more hidden layers to propose the following deep or *multi-layer* RNN,

$$\begin{aligned} \mathbf{y}_n^\ell &= \mathbf{y}_{n-1}^\ell + \Delta t \hat{\sigma}(\mathbf{c}^\ell) \odot \mathbf{z}_n^\ell, \\ \mathbf{z}_n^\ell &= \mathbf{z}_{n-1}^\ell - \Delta t \hat{\sigma}(\mathbf{c}^\ell) \odot [\sigma(\mathbf{w}^\ell \odot \mathbf{y}_{n-1}^\ell + \mathbf{V}^\ell \mathbf{y}_n^{\ell-1} + \mathbf{b}^l) \\ &\quad + \alpha \mathbf{y}_{n-1}^\ell]. \end{aligned} \tag{6}$$

Here $\mathbf{y}_n^l, \mathbf{z}_n^l \in \mathbb{R}^m$ are hidden states and $\mathbf{w}^\ell, \mathbf{V}^\ell, \mathbf{b}^\ell$ are weights and biases, corresponding to layer $\ell = 1, \ldots, L$. We set $\mathbf{y}_n^0 = \mathbf{u}_n$ in the multilayer RNN (6).

In Fig. 1, we present a schematic diagram of the proposed multi-layer recurrent model UnICORNN.

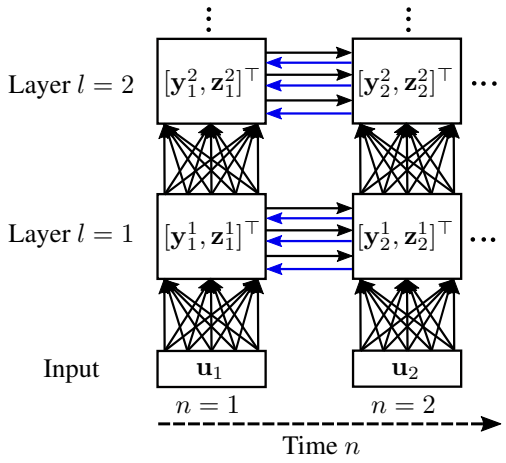

Figure 1. Schematic diagram of the multi-layer UnICORNN architecture, where the layers (respectively the input) are densely connected and the hidden states evolve independently in time. The invertibility of UnICORNN is visualized with blue arrows, emphasizing that the hidden states can be reconstructed during the backward pass and do not need to be stored.

Observe that we use the same step-size Δt for every layer, while multiplying a trainable parameter vector $\mathbf{c} \in \mathbb{R}^m$ to the time step. The action of $\mathbf{c}$ is modulated with the sigmoidal activation function $\hat{\sigma}(u) = 0.5 + 0.5 \tanh(u/2)$, which ensures that the time-step Δt is multiplied by a value between 0 and 1. We remark that the presence of this trainable vector $\mathbf{c}$ allows us to incorporate *multi-scale behavior* in the proposed RNN, as the effective time-step is learned during training and can be significantly different from the nominal time-step Δt. It is essential to point out that including this multi-scale time stepping is only possible, as each

neuron (within the same hidden layer) is independent of the others and can be integrated with a different effective time step. Finally, we also share the control hyperparameter α across the different layers, which results in a memory unit of L layers with a total of only 2 hyperparameters.

2.1. Motivation and background

The ODE system (2) is a model for a nonlinear system of uncoupled driven oscillators (Guckenheimer & Holmes, 1990). To see this, we denote $\mathbf{y}_i(t)$ as the displacement and $\mathbf{z}_i(t)$ as the velocity. Then, the dynamics of the i-th oscillator is determined by the frequency α and also by the *forcing* or *driving* term in the second equation of (2), where the forcing acts through the input signal $\mathbf{u}$ and is modulated by the weight $\mathbf{V}$ and bias $\mathbf{b}$. Finally, the weight $\mathbf{w}$ modulates the frequency α and allows each neuron to oscillate with its own frequency, rather than the common frequency α of the system. The structure of $\mathbf{w}$ implies that each neuron is independent of the others. A key element of the oscillator system (2) is the absence of any damping or friction term. This allows the system to possess a Hamiltonian structure, with desirable long time behavior. Thus, we term the resulting RNN (6), based on the ODE system (2) as **Un**damped **I**ndependent **C**ontrolled **O**scillatory **RNN** or **UnICORNN**. We remark that networks of oscillators are very common in science and engineering (Guckenheimer & Holmes, 1990; Strogatz, 2015) with prominent examples being pendulums in mechanics, electrical circuits in engineering, business cycles in economics and functional brain circuits such as cortical columns in neurobiology.

2.2. Comparison with related work.

UnICORNN lies firmly in the class of ODE-based or ODE-inspired RNNs, which have received considerable amount of attention in the machine learning literature in recent years. Neural ODEs, first proposed in (Chen et al., 2018), are a prominent example of using ODEs to construct neural networks. In this architecture, the continuous ODE serves as the learning model and gradients are computed from a sensitivity equation, which allows one to trade accuracy with computing time. Moreover, it is argued that these neural ODEs are invertible and hence, memory efficient. However, it is unclear if a general neural ODE, without any additional structure, can be invertible. Other RNN architectures that are based on discretized ODEs include those proposed in (E, 2017) and (Chang et al., 2018), where the authors proposed an *anti-symmetric* RNN, based on the discretization of a stable ODE resulting from a skew-symmetric hidden weight matrix, thus constraining the gradient dynamics.

Our proposed RNN (6) is inspired by two recent RNN architectures. The first one is *coRNN*, proposed recently in (Rusch & Mishra, 2021), where the underlying RNN architecture was also based on the use of a network of oscillators. As long as a constraint on the underlying weights was satisfied, coRNN was shown to mitigate the EVGP. In contrast to coRNN, our proposed RNN does not use a *damping* term. Moreover, each neuron, for any hidden layer, in UnICORNN (6) is independent. This is very different from coRNN where all the neurons were coupled together. Finally, UnICORNN is a multi-layer architecture whereas coRNN used a single hidden layer. These innovations allow us to admit a Hamiltonian structure for UnICORNN and facilitate a fast and memory efficient implementation.

Our proposed architecture was also partly inspired by *IndRNN*, proposed in (Li et al., 2018; 2019), where the neurons in each hidden layers were independent of each other and interactions between neurons were mediated by stacking multiple RNN layers, with output of each hidden layer passed on to the next hidden layer, leading to a deep RNN. We clearly use this construction of independent neurons in each layer and stacking multiple layers in UnICORNN (6). However in contrast to IndRNN, our proposed RNN is based on a discretized Hamiltonian system and we will not require any constraints on the weights to mitigate the EVGP.

Finally, we would like to point out that discrete Hamiltonian systems have already been used to design RNNs, for instance in (Greydanus et al., 2019) and also in (Chen et al.), where a symplectic time-integrator for a Hamiltonian system was proposed as the RNN architecture. However, these approaches are based on underlying time-independent Hamiltonians and are only relevant for mechanical systems as they cannot process time-dependent inputs, which arise in most realistic learning tasks. Moreover, as these methods enforce exact conservation of the Hamiltonian in time, they are not suitable for learning long-time dependencies, see (MacKay et al., 2018) for a discussion and experiment on that issue. Although we use a Hamiltonian system as the basis of our proposed RNN (6), our underlying Hamiltonian (4) is time-dependent and the resulting RNN can readily process any time-dependent input signal.

2.3. On the Memory Efficiency of UnICORNN

As mentioned in the introduction, the standard BPTT training algorithm for RNNs requires one to store all the hidden states at every time step. To see this, we observe that for a standard multi-layer RNN with L layers and a mini-batch size of b (for any mini-batch stochastic gradient descent algorithm), the storage (in terms of floats) scales as $\mathcal{O}(Nbd + LbmN)$, with input and hidden sequences of length N. This memory requirement can be very high. Note that we have ignored the storage of trainable weights and biases for the RNN in the above calculation.

On the other hand, as argued before, our proposed RNN is

a symplectic Euler discretization for a Hamiltonian system. Hence, it is invertible. In fact, one can explicitly write the *inverse* of UnICORNN (6) as,

$$\begin{aligned}\mathbf{y}_{n-1}^l &= \mathbf{y}_n^l - \Delta t\hat{\sigma}(\mathbf{c}^l)\odot\mathbf{z}_n^l,\\ \mathbf{z}_{n-1}^l &= \mathbf{z}_n^l + \Delta t\hat{\sigma}(\mathbf{c}^l)\odot[\sigma(\mathbf{w}^l\odot\mathbf{y}_{n-1}^l + \mathbf{V}^\ell\mathbf{y}_n^{\ell-1}+\mathbf{b}^l)\\ &\quad + \alpha\mathbf{y}_{n-1}^l].\end{aligned} \tag{7}$$

Thus, one can recover all the hidden states in a given hidden layer, only from the *stored* hidden state at the final time step, for that layer. Moreover, only the input signal needs to be stored as the other hidden states can be reconstructed from the formula (7). Hence, a straightforward calculation shows that the storage for UnICORNN scales as $\mathcal{O}(Nbd + Lbm)$. As $L << N$, we conclude that UnICORNN allows for a significant saving in terms of storage, when compared to a standard RNN.

3. Rigorous Analysis of UnICORNN

On the dynamics of the hidden state gradients for ODE (2). In order to investigate the EVGP for the proposed RNN (6), we will first explore the dynamics of the gradients of hidden states $\mathbf{y}, \mathbf{z}$ (solutions of the ODE (2)) with respect to the trainable parameters $\mathbf{w}, \mathbf{V}$ and $\mathbf{b}$. Denote any scalar parameter as θ and $f_\theta = \frac{\partial f}{\partial \theta}$, then differentiating the ODE (2) with respect to θ results in the ODE,

$$\begin{aligned}\mathbf{y}_\theta' &= \mathbf{z}_\theta,\\ \mathbf{z}_\theta' &= -\sigma'(\mathbf{A})\odot(\mathbf{w}\odot\mathbf{y}_\theta) - \alpha\mathbf{y}_\theta - \sigma'(\mathbf{A})\odot\mathbf{C}(t),\end{aligned} \tag{8}$$

where $\mathbf{A} = \mathbf{w}\odot\mathbf{y} + \mathbf{V}\mathbf{u} + \mathbf{b}$ is the pre-activation and the coefficient $\mathbf{C}\in\mathbb{R}^m$ is given by $\mathbf{C}_i = \mathbf{y}_i$ if $\theta = \mathbf{w}_i$, $\mathbf{C}_i = \mathbf{u}_j$ if $\theta = \mathbf{V}_{ij}$ and $\mathbf{C}_i = 1$ if $\theta = \mathbf{b}_i$, with all other entries of the vector $\mathbf{C}$ being zero.

It is easy to check that the ODE system (8) is a *Hamiltonian system* of form (3), with the following time-dependent Hamiltonian;

$$\begin{aligned}\mathbf{H}(\mathbf{y}_\theta,\mathbf{z}_\theta,t) &:= \frac{\alpha}{2}\|\mathbf{y}_\theta\|^2 + \frac{1}{2}\|\mathbf{z}_\theta\|^2\\ &+ \frac{1}{2}\sum_{i=1}^m \sigma'(\mathbf{A}_i)\mathbf{w}_i((\mathbf{y}_\theta)_i)^2 + \sum_{i=1}^m \sigma'(\mathbf{A}_i)\mathbf{C}_i(t)(\mathbf{y}_\theta)_i.\end{aligned} \tag{9}$$

Thus, by the well-known Liouville's theorem (Sanz Serna & Calvo, 1994), we know that the phase space volume of (8) is preserved. Hence, this system cannot have any asymptotically stable fixed points. This implies that $\{\mathbf{0},\mathbf{0}\}$ cannot be a stable fixed point for the hidden state gradients $(\mathbf{y}_\theta,\mathbf{z}_\theta)$. Thus, we can expect that the hidden state gradients with respect to the system of oscillators (2) do not remain near zero and suggest a possible mechanism for the mitigation of the vanishing gradient problem for UnICORNN (6), which is a structure preserving discretization of the ODE (2).

On the Exploding Gradient Problem for UnICORNN. We train the RNN (6) to minimize the loss function,

$$\mathcal{E} := \frac{1}{N}\sum_{n=1}^N \mathcal{E}_n, \quad \mathcal{E}_n = \frac{1}{2}\|\mathbf{y}_n^L - \bar{\mathbf{y}}_n\|_2^2, \tag{10}$$

with $\bar{\mathbf{y}}$ being the underlying ground truth (training data). Note that the loss function (10) only involves the output at the last hidden layer (we set the affine output layer to identity for the sake of simplicity). During training, we compute gradients of the loss function (10) with respect to the trainable weights and biases $\mathbf{\Theta} = [\mathbf{w}^\ell, \mathbf{V}^\ell, \mathbf{b}^\ell, \mathbf{c}^\ell]$, for all $1\le\ell\le L$, i.e.,

$$\frac{\partial\mathcal{E}}{\partial\theta} = \frac{1}{N}\sum_{n=1}^N \frac{\partial\mathcal{E}_n}{\partial\theta}, \quad \forall\,\theta\in\mathbf{\Theta}. \tag{11}$$

We have the following upper bound on the hidden state gradient,

Proposition 3.1. *Let the time step $\Delta t << 1$ be sufficiently small in the RNN (6) and let $\mathbf{y}_n^\ell, \mathbf{z}_n^\ell$, for $1\le\ell\le L$, and $1\le n\le N$ be the hidden states generated by the RNN (6). Then, the gradient of the loss function $\mathcal{E}$ (10) with respect to any parameter $\theta\in\mathbf{\Theta}$ is bounded as,*

$$\left|\frac{\partial\mathcal{E}}{\partial\theta}\right| \le \frac{1-(\Delta t)^L}{1-\Delta t} T(1+2\gamma T)\overline{\mathbf{V}}(\bar{Y}+\mathbf{F})\mathbf{\Delta}, \tag{12}$$

with $\bar{Y} = \max_{1\le n\le N}\|\bar{\mathbf{y}}_n\|_\infty$, be a bound on the underlying training data and other quantities in (12) defined as,

$$\gamma = \max\left(2, \|\mathbf{w}^L\|_\infty + \alpha\right) + \frac{\left(\max\left(2, \|\mathbf{w}^L\|_\infty + \alpha\right)\right)^2}{2},$$

$$\overline{\mathbf{V}} = \prod_{q=1}^L \max\{1, \|\mathbf{V}^q\|_\infty\}, \quad \beta = \max\{1+2\alpha, 4\alpha^2\}$$

$$\mathbf{F} = \sqrt{\frac{2}{\alpha}(1+2\beta T)}, \quad T = N\Delta t,$$

$$\mathbf{\Delta} = 2 + \sqrt{2(1+2\beta T)} + (2+\alpha)\sqrt{\frac{2}{\alpha}(1+2\beta T)}.$$

This proposition, proved in Appendix **C.2**, demonstrates that as long as the weights $\mathbf{w}^L, \mathbf{V}^q$ are bounded, there is a uniform bound on the hidden state gradients. This bound grows at most as $(N\Delta t)^3$, with N being the total number of time steps. Thus, there is no exponential growth of the gradient with respect to the number of time steps and the *exploding gradient problem* is mitigated for UnICORNN.

On the Vanishing Gradient Problem for UnICORNN. By applying the chain rule repeatedly to each term on the

right-hand-side of (11), we obtain

$$\frac{\partial \mathcal{E}_n}{\partial \theta} = \sum_{\ell=1}^{L} \sum_{k=1}^{n} \frac{\partial \mathcal{E}_{k,\ell}^{(n,L)}}{\partial \theta}, \quad \frac{\partial \mathcal{E}_{k,\ell}^{(n,L)}}{\partial \theta} := \frac{\partial \mathcal{E}_n}{\partial \mathbf{X}_n^L} \frac{\partial \mathbf{X}_n^L}{\partial \mathbf{X}_k^\ell} \frac{\partial^+ \mathbf{X}_k^\ell}{\partial \theta},$$
$$\mathbf{X}_n^\ell = \left[\mathbf{y}_n^{\ell,1}, \mathbf{z}_n^{\ell,1}, \ldots, \mathbf{y}_n^{\ell,j}, \mathbf{z}_n^{\ell,j}, \ldots, \mathbf{y}_n^{\ell,m}, \mathbf{z}_n^{\ell,m}\right]. \tag{13}$$

Here, the notation $\frac{\partial^+ \mathbf{X}_k^\ell}{\partial \theta}$ refers to taking the partial derivative of $\mathbf{X}_k^\ell$ with respect to the parameter θ, while keeping the other arguments constant. The quantity $\frac{\partial \mathcal{E}_{k,\ell}^{(n,L)}}{\partial \theta}$ denotes the contribution from the k-recurrent step at the l-th hidden layer of the deep RNN (6) to the overall hidden state gradient at the step n. The vanishing gradient problem (Pascanu et al., 2013) arises if $\left|\frac{\partial \mathcal{E}_{k,\ell}^{(n,L)}}{\partial \theta}\right|$, defined in (13), $\to 0$ exponentially fast in k, for $k << n$ (long-term dependencies). In that case, the RNN does not have long-term memory, as the contribution of the k-th hidden state at the ℓ-th layer to error at time step t_n is infinitesimally small.

We have established that the hidden state gradients for the underlying continuous ODE (2) do not vanish. As we use a symplectic Euler discretization, the phase space volume for the discrete dynamical system (5) is also conserved (Sanz Serna & Calvo, 1994; Hairer et al., 2003). Hence, one can expect that the gradients of the multilayer RNN (6) do not vanish. However, these heuristic considerations need to be formalized. Observe that the vanishing gradient problem for RNNs focuses on the possible smallness of contributions of the gradient over a large number of recurrent steps. As this behavior of the gradient is independent of the number of layers, we focus on the vanishing gradient problem for a single hidden layer here, while presenting the multilayer results in Appendix **C.4**. Also, for the sake of definiteness, we set the scalar parameter $\theta = \mathbf{w}^{1,p}$ for some $1 \leq p \leq m$. Similar results also hold for any other $\theta \in \mathbf{\Theta}$.

We have the following representation formula (proved in Appendix **C.3**) for the hidden state gradients,

Proposition 3.2. *Let $\mathbf{y}_n$ be the hidden states generated by the RNN (6). Then the gradient for long-term dependencies, i.e. $k << n$, satisfies the representation formula,*

$$\frac{\partial \mathcal{E}_{k,1}^{(n,1)}}{\partial \mathbf{w}^{1,p}} = -\Delta t \hat{\sigma}(\mathbf{c}^{1,p})^2 t_n \sigma'(\mathbf{A}_{k-1}^{1,p}) \mathbf{y}_{k-1}^{1,p} \left(\mathbf{y}_n^{1,p} - \overline{\mathbf{y}}_n^p\right) + \mathcal{O}(\Delta t^2). \tag{14}$$

It is clear from the representation formula (14) that there is no k-dependence for the gradient. In particular, as long as all the weights are of $\mathcal{O}(1)$, the leading-order term in (14) is $\mathcal{O}(\Delta t)$. Hence, the gradient can be small but is independent of the recurrent step k. Thus, we claim that the *vanishing gradient problem*, with respect to recurrent connections, is mitigated for UnICORNN (6).

4. Experiments

The details of the training procedure for each experiment can be found in Appendix **A**. Code to replicate the experiments can be found at **https://github.com/tk-rusch/unicornn**.

Implementation The structure of UnICORNN (6) enables us to achieve a very fast implementation. First, the transformation of the input (i.e. $\mathbf{V}^\ell \mathbf{y}_n^{\ell-1}$ for all $l = 1, \ldots, L$), which is the most computationally expensive part of UnICORNN, does not have a sequential structure and can thus be computed in parallel over time. Second, as the underlying ODEs of the UnICORNN are uncoupled for each neuron, the remaining recurrent part of UnICORNN is solved independently for each component. Hence, inspired by the implementation of Simple Recurrent Units (SRU) (Lei et al., 2018) and IndRNN, we present in Appendix **B**, the details of an efficient CUDA implementation, where the input transformation is computed in parallel and the dynamical system corresponding to each component of (6) is an independent CUDA thread.

We benchmark the training speed of UnICORNN with $L = 2$ layers, against the fastest available RNN implementations, namely the cuDNN implementation (Appleyard et al., 2016) of LSTM (with 1 hidden layer), SRU and IndRNN (both with $L = 2$ layers and with batch normalization). Fig. 2 shows the computational time (measured on a GeForce RTX 2080 Ti GPU) of the combined forward and backward pass for each network, averaged over 100 batches with each of size 128, for two different sequence lengths, i.e. $N = 1000, 2000$. We can see that while the cuDNN LSTM is relatively slow, the SRU, IndRNN and the UnICORNN perform similarly fast. Moreover, we also observe that UnICORNN is about $30 - 40$ times faster per combined forward and backward pass, when compared to recently developed RNNs such as expRNN (Casado & Martínez-Rubio, 2019) and coRNN (Rusch & Mishra, 2021). We thus conclude that the UnICORNN is among the fastest available RNN architectures.

Permuted sequential MNIST A well-established benchmark for testing RNNs on input sequences with long-time dependencies is the permuted sequential MNIST (psMNIST) task (Le et al., 2015). Based on the classical MNIST data set (LeCun et al., 1998), the flattened grey-scale matrices are randomly permuted (based on a fixed random permutation) and processed sequentially by the RNN. This makes the learning task more challenging than sequential MNIST, where one only flattens the MNIST matrices without permuting them. In order to make different methods comparable, we use the same fixed seed for the random permutation, as in (Casado & Martínez-Rubio, 2019; Casado, 2019; Helfrich et al., 2018). Table 1 shows the results for UnICORNN with 3 layers, together with other recently pro-

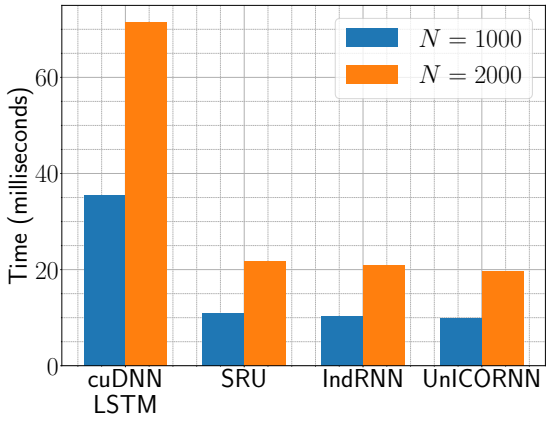

Figure 2. Measured computing time for the combined forward and backward pass for the UnICORNN as well as for three of the fastest available RNN implementations.

posed RNNs, which were explicitly designed to learn LTDs as well as two gated baselines. We see that UnICORNN clearly outperforms the other methods.

Table 1. Test accuracies on permuted sequential MNIST together with number of hidden units as well as total number of parameters M for each network. All other results are taken from the corresponding original publication, cited in the main text, except that we are using the results of (Chang et al., 2017) for GRU and of (Helfrich et al., 2018) for LSTM.

MODEL	TEST ACC.	#UNITS	M
LSTM	92.9%	256	270K
GRU	94.1%	256	200K
EXPRNN	96.6%	512	127K
CORNN	97.3%	256	134K
INDRNN (L=6)	96.0%	128	86K
DENSE-INDRNN (L=6)	97.2%	128	257K
UNICORNN (L=3)	97.8%	128	35K
UNICORNN (L=3)	**98.4%**	256	135K

Noise padded CIFAR-10 A more challenging test for the ability of RNNs to learn LTDs is provided by the recently proposed noise padded CIFAR-10 experiment (Chang et al., 2018). In it, the CIFAR-10 data points (Krizhevsky et al., 2009) are fed to the RNN row-wise and flattened along the channels resulting in sequences of length 32. To test long term memory, entries of uniform random numbers are added such that the resulting sequences have a length of 1000, i.e. the last 968 entries of each sequences are only noise to distract the RNNs. Table 2 shows the result of the UnICORNN with 3 layers together with the results of other recently proposed RNNs, namely for the LSTM, anti.sym. RNN and gated anti.sym. RNN (Chang et al., 2018), Lipschitz RNN (Erichson et al., 2021), Incremental RNN (Kag et al.), FastRNN (Kusupati et al., 2018) and coRNN (Rusch & Mishra, 2021). We conclude that the proposed RNN readily outperforms all other methods on this experiment.

Table 2. Test accuracies on noise padded CIFAR-10 together with number of hidden units as well as total number of parameters M for each network. All other results are taken from literature, specified in the main text.

MODEL	TEST ACC.	#UNITS	M
LSTM	11.6%	128	64K
INCREMENTAL RNN	54.5%	128	12K
LIPSCHITZ RNN	55.8%	256	158K
FASTRNN	45.8%	128	16K
ANTI.SYM. RNN	48.3%	256	36K
GATED ANTI.SYM. RNN	54.7%	256	37K
CORNN	59.0%	128	46K
UNICORNN (L=3)	**62.4%**	128	47K

EigenWorms The EigenWorms data set (Bagnall et al., 2018) is a collecting of 259 very long sequences, i.e. length of 17984, describing the motion of a worm. The task is, based on the 6-dimensional motion sequences, to classify a worm as either wild-type or one of four mutant types. We use the same train/valid/test split as in (Morrill et al., 2020), i.e. 70%/15%/15%. As the length of the input sequences is extremely long for this test case, we benchmark UnICORNN against three sub-sampling based baselines. These include the results of (Morrill et al., 2020), which is based on signature sub-sampling routine for neural controlled differential equations. Additionally after a hyperparameter fine-tuning procedure, we perform a random sub-sampling as well as truncated back-propagation through time (BPTT) routine using LSTMs, where the random sub-sampling is based on 200 randomly selected time points of the sequences as well as the BPTT is truncated after the last 500 time points of the sequences. Furthermore, we compare UnICORNN with three leading RNN architectures for solving LTD tasks, namely expRNN, IndRNN and coRNN, which are all applied to the full-length sequences. The results, presented in Table 3, show that while sub-sampling approaches yield moderate test accuracies, expRNN as well as the IndRNN yield very poor accuracies. In contrast, coRNN performs very well. However, the best results are obtained for UnICORNN as it reaches a test accuracy of more than 90%, while at the same time yielding a relatively low standard deviation, further underlining the robustness of the proposed RNN.

As this data set has only recently been proposed as a test for RNNs in learning LTDs, it is unclear if the input sequences

Table 3. Test accuracies on EigenWorms using 5 re-trainings of each best performing network (based on the validation set) together with number of hidden units as well as total number of parameters M for each network.

MODEL	TEST ACC.	#UNITS	M
T-BPTT LSTM	57.9% ± 7.0%	32	5.3K
SUB-SAMP. LSTM	69.2% ± 8.3%	32	5.3K
SIGN.-NCDE	77.8% ± 5.9%	32	35K
EXPRNN	40.0% ± 10.1%	64	2.8K
INDRNN (L=2)	49.7% ± 4.8%	32	1.6K
CORNN	86.7% ± 3.0%	32	2.4K
UNICORNN (L=2)	**90.3%** ± **3.0%**	32	1.5K

truly exhibit very long-time dependencies. To investigate this further, we train UnICORNN on a subset of the entries of the sequences. To this end, we consider using only the last entries as well as using a random subset of the entries. Fig. 3 shows the distributional results (10 re-trainings of the best performing UnICORNN) for the number of entries used in each sub-sampling routine, ranging from only using 1000 entries to using the full sequences for training. We can see that in order to reach a test accuracy of 80% when training on the last entries of the sequences, at least the last 10k entries are needed. Moreover, for both sub-sampling methods the test accuracy increases monotonically as the number of entries for training is increased. On the other hand, using a random subset of the entries increases the test accuracy significantly when compared to using only the last entries of the sequences. This indicates that the important entries of the sequences, i.e. information needed in order to classify them correctly, are uniformly distributed throughout the full sequence. We thus conclude that the EigenWorms data set indeed exhibits *very* long-time dependencies.

Healthcare application: Vital signs prediction We apply UnICORNN on two real-world data sets in health care, aiming to predict the vital signs of a patient, based on PPG and ECG signals. The data sets are part of the TSR archive (Tan et al., 2020) and are based on clinical data from the Beth Israel Deaconess Medical Center. The PPG and ECG signals are sampled with a frequency of 125Hz for 8 minutes each. The resulting two-dimensional sequences have a length of 4000. The goal is to predict a patient's respiratory rate (RR) and heart rate (HR) based on these signals. We compare UnICORNN to 3 leading RNN architectures for solving LTDs, i.e. expRNN, IndRNN and coRNN. Additionally, we present two baselines using the LSTM as well as the recently proposed sub-sampling method of computing signatures for neural controlled differential equations (NCDE) (Morrill et al., 2020). Following (Morrill et al., 2020), we split the 7949 sequences in a training set, validation set and testing set, using a 70%/15%/15% split. Table 4 shows the distributional results of all networks using 5 re-trainings of the best performing RNN. We observe that while the LSTM does not reach a low L^2 testing error in both experiments, the other RNNs approximate the vital signs reasonably well. However, UnICORNN clearly outperforms all other methods on both benchmarks. We emphasize that UnICORNN significantly outperforms all other state-of-the-art methods on estimating the RR, which is of major importance in modern healthcare applications for monitoring hospital inpatients as well as for mobile health applications, as special invasive equipment (for instance capnometry or measurement of gas flow) is normally needed to do so (Pimentel et al., 2016).

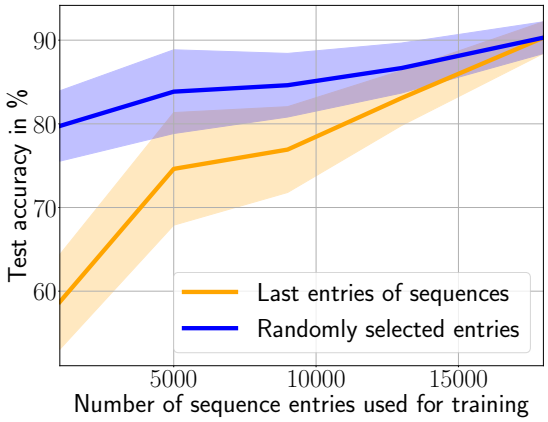

Figure 3. Test accuracy (mean and standard deviation) for the UnICORNN on EigenWorms for two types of sub-sampling approaches, i.e. using the last entries of the sequences as well as using a random subset of the entries. Both are shown for increasing number of entries used in each corresponding sub-sampling routine.

Table 4. L^2 test error on vital sign prediction using 5 re-trainings of each best performing network (based on the validation set), where the respiratory rate (RR) and heart rate (HR) is estimated based on PPG and ECG data.

MODEL	RR	HR
SIGN.-NCDE	1.51 ± 0.08	2.97 ± 0.45
LSTM	2.28 ± 0.25	10.7 ± 2.0
EXPRNN	1.57 ± 0.16	1.87 ± 0.19
INDRNN (L=3)	1.47 ± 0.09	2.10 ± 0.2
CORNN	1.45 ± 0.23	1.71 ± 0.1
UNICORNN (L=3)	**1.06** ± **0.03**	**1.39** ± **0.09**

Table 5. Test accuracies on IMDB together with number of hidden units as well as total number of parameters M (without embedding) for each network. All other results are taken from literature, specified in the main text.

MODEL	TEST ACC.	#UNITS	M
LSTM	86.8%	128	220K
SKIP LSTM	86.6%	128	220K
GRU	85.2%	128	99K
RELU GRU	84.8%	128	99K
SKIP GRU	86.6%	128	165K
CORNN	87.4 %	128	46K
UNICORNN (L=2)	**88.4**%	128	30K

Sentiment analysis: IMDB As a final experiment, we test the proposed UnICORNN on the widely used NLP benchmark data set IMDB (Maas et al., 2011), which consists of 50k online movie reviews with 25k reviews used for training and 25k reviews used for testing. This denotes a classical sentiment analysis task, where the model has to decide whether a movie review is positive or negative. We use 30% of the training set (i.e. 7.5k reviews) as the validation set and restrict the dictionary to 25k words. We choose an embedding size of 100 and initialize it with the pretrained 100d GloVe (Pennington et al., 2014) vectors. Table 5 shows the results for UnICORNN with 2 layers together with other recently proposed RNN architectures and gated baselines (which are known to perform very well on these tasks). The result of ReLU GRU is taken from (Dey & Salemt, 2017), of coRNN from (Rusch & Mishra, 2021) and all other results are taken from (Campos et al., 2018). We can see that UnICORNN outperforms the other methods while requiring significantly less parameters. We thus conclude, that the UnICORNN can also be successfully applied to problems, which do not necessarily exhibit long-term dependencies.

Further experimental results As stated before, UnICORNN has two hyperparameters, i.e. the maximum allowed time-step Δt and the damping parameter α. It is of interest to examine how sensitive the performance of UnICORNN is with respect to variations of these hyperparameters. To this end, we consider the noise padded CIFAR-10 experiment and perform an ablation study of the test accuracy with respect to variations of both α and Δt. Both hyperparameters are varied by an order of magnitude and the results of this study are plotted in Fig. 4. We observe from this figure, that the results are indeed somewhat sensitive to the maximum allowed time-step Δt and show a variation of approximately 15% with respect to to this hyperparameter. On the other hand, there is very little noticeable variation with respect to the damping parameter α. Thus, it can be set to a default value, for instance $\alpha = 1$, without impeding the performance of the underlying RNN.

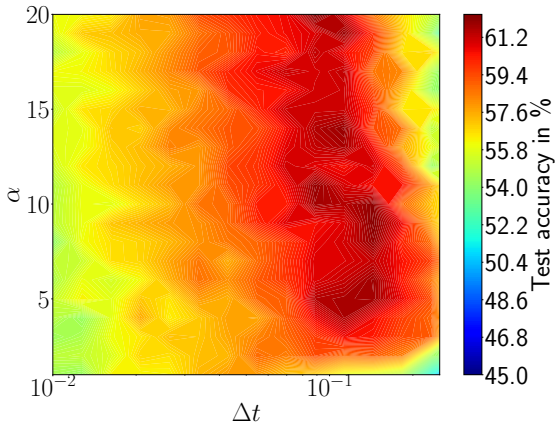

Figure 4. Ablation study on the hyperparameters Δt and α of UnICORNN (6) using the noise padded CIFAR-10 experiment.

Next, we recall that the design of UnICORNN (6) enables it to learn the effective time step (with a possible maximum of Δt) from data. It is instructive to investigate if this ability to express *multi-scale* behavior is realized in practice or not. To this end, we consider the trained UnICORNN of the psMNIST task with 3 layers and 256 neurons. Here, a maximum time step of $\Delta t = 0.19$ was identified by the hyperparameter tuning. In Fig. 5, we plot the effective time step $\Delta t \hat{\sigma}(\mathbf{c}_i^l)$, for each hidden neuron $i = 1, \ldots, 256$ and each layer $l = 1, 2, 3$. We observe from this figure that a significant variation of the effective time step is observed, both within the neurons in each layer, as well as between layers. In particular, the minimum effective time step is about 28 times smaller than the maximum allowed time step. Thus, we conclude from this figure, that UnICORNN exploits its design features to learn multi-scale behavior that is latent in the data. This perhaps explains the superior performance of UnICORNN on many learning tasks.

5. Discussion

The design of RNNs that can accurately handle sequential inputs with long-time dependencies is very challenging. This is largely on account of the exploding and vanishing gradient problem (EVGP). Moreover, there is a significant increase in both computational time as well as memory requirements when LTD tasks have to be processed. Our main aim in this article was to present a novel RNN architecture which is fast, memory efficient, *invertible* and mitigates the EVGP. To this end, we proposed UnICORNN (6), an RNN based on the symplectic Euler discretization of a Hamiltonian system of second-order ODEs (2) modeling a network of independent, undamped, controlled and driven oscillators.

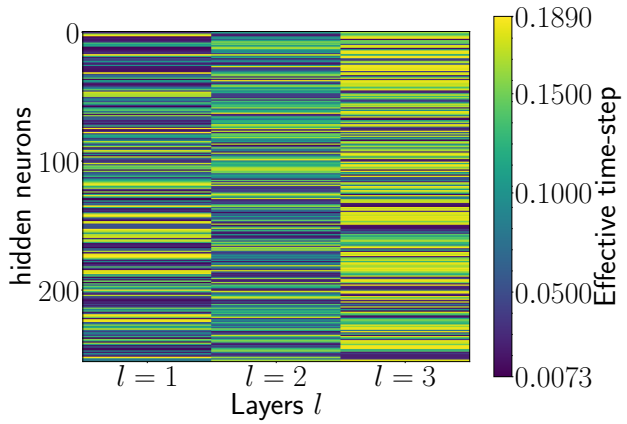

Figure 5. Effective time-step $\Delta t\hat{\sigma}(\mathbf{c}_i^l)$ for each hidden neuron $i = 1, \ldots, m$ and each layer $l = 1, \ldots, L$ of UnICORNN, after training on the psMNIST task using $m = 256$ hidden units and $L = 3$ layers.

In order to gain expressivity, we stack layers of RNNs and also endow this construction with a multi-scale feature by training the effective time step in (6).

Given the Hamiltonian structure of our continuous and discrete dynamical system, invertibility and volume preservation in phase space are guaranteed. Invertibility enables the proposed RNN to be memory efficient. The independence of neurons within each hidden layer allows us to build a highly efficient CUDA implementation of UnICORNN that is as fast as the fastest available RNN architectures. Under suitable smallness constraints on the maximum allowed time step Δt, we prove rigorous upper bounds (12) on the gradients and show that the exploding gradient problem is mitigated for UnICORNN. Moreover, we derive an explicit representation formula (14) for the gradients of (6), which shows that the vanishing gradient problem is also mitigated. Finally, we have tested UnICORNN on a suite of benchmarks that includes both synthetic as well as realistic learning tasks, designed to test the ability of an RNN to deal with long-time dependencies. In all the experiments, UnICORNN was able to show state of the art performance.

It is instructive to compare UnICORNN with two recently proposed RNN architectures, with which it shares some essential features. First, the use of coupled oscillators to design RNNs was already explored in the case of coRNN (Rusch & Mishra, 2021). In contrast to coRNN, neurons in UnICORNN are independent (uncoupled) and as there is no damping, UnICORNN possesses a Hamiltonian structure. This paves the way for invertibility as well as for mitigating the EVGP without any assumptions on the weights whereas the mitigation of EVGP with coRNN was conditional on restrictions on weights. Finally, UnICORNN provides even better performance on benchmarks than coRNN, while being significantly faster. While we also use independent neurons in each hidden layer and stack RNN layers together as in IndRNN (Li et al., 2018), our design principle is completely different as it is based on Hamiltonian ODEs. Consequently, we do not impose weight restrictions, which are necessary for IndRNN to mitigate the EVGP. Moreover, in contrast to IndRNNs, our architecture is invertible and hence, memory efficient.

This work can be extended in different directions. First, UnICORNN is a very flexible architecture in terms of stacking layers of RNNs together. We have used a fully connected stacking in (6) but other possibilities can be readily explored. See Appendix **C.5** for a discussion on the use of residual connections in stacking layers of UnICORNN. Second, the invertibility of UnICORNN can be leveraged in the context of normalizing flows (Papamakarios et al., 2019), where the objective is to parametrize a flow such that the resulting Jacobian is readily computable. Finally, our focus in this article was on testing UnICORNN on learning tasks with long-time dependencies. Given that the underlying ODE (2) models oscillators, one can envisage that UnICORNN will be very competitive with respect to processing different time series data that arise in healthcare AI such as EEG and EMG data, as well as seismic time series from the geosciences.

Acknowledgements

The research of TKR and SM was performed under a project that has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (grant agreement No. 770880).

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