Analyzing and Exploiting NARX Recurrent Neural Networks for Long-Term Dependencies

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Abstract

Recurrent neural networks (RNNs) have achieved state-of-the-art performance on many diverse tasks, from machine translation to surgical activity recognition, yet training RNNs to capture long-term dependencies remains difficult. To date, the vast majority of successful RNN architectures alleviate this problem by facilitating long-term gradient flow using nearly-additive connections between adjacent states, as originally introduced in long short-term memory (LSTM). In this paper, we investigate a different approach for encouraging gradient flow that is based on NARX RNNs, which generalize typical RNNs by allowing direct connections from the distant past. Analytically, we 1) generalize previous gradient decompositions for typical RNNs to general NARX RNNs and 2) formally connect gradient flow to edges along paths. We then introduce an example architecture that is based on these ideas, and we demonstrate that this architecture matches or exceeds LSTM performance on 5 diverse tasks. Finally we describe many avenues for future work, including the exploration of other NARX RNN architectures, the possible combination of mechanisms from LSTM and NARX RNNs, and the adoption of recent LSTM-based advances to NARX RNN architectures.

1 Introduction

Recurrent neural networks [34] [36] [40] are a powerful class of neural networks that are naturally suited to modeling time series data and other sequential data. For example, in recent years alone, RNNs have achieved state-of-the-art performance on tasks as diverse as machine translation [41], speech recognition [30], generative image modeling [31], and surgical activity recognition [8].

These successes, and the majority of other RNN successes, rely on a specific mechanism that was introduced by long short-term memory [21] [15], which was designed to mitigate the so called vanishing gradient problem [20] [4] [32]. The vanishing gradient problem is illustrated in Figure 1. As shown in Section 3 every path from \( t - \tau \) to \( t \) yields a gradient component that can be expressed as a product of factors, one factor per edge. If we denote the maximum spectral norm of any such factor as \( \lambda \), then the norm of the product is upper bounded by \( \lambda^{n_e} \), where \( n_e \) is the number of edges along the path. When \( \lambda < 1 \), events at \( t - \tau \) for large \( \tau \) have nearly no effect on gradients, thus making it extremely difficult to learn from these events.
2 Background and Related Work

Recurrent neural networks, as commonly described in literature, take on the general form

\[ h_t = f(h_{t-1}, x_t, \theta) \]  

which compute a new state \( h_t \) in terms of the previous state \( h_{t-1} \), the current input \( x_t \), and some parameters \( \theta \) (which are shared over time).

One of the earliest variants, now known to be especially vulnerable to the vanishing gradient problem, is that of simple RNNs [10], described by

\[ h_t = \tanh(W_h h_{t-1} + W_x x_t + b) \]  

\footnote{The acronym NARX stems from Nonlinear AutoRegressive models with eXogeneous inputs.}

\footnote{In this paper, we use \( h_t \) for consistency, but to avoid confusion, we note that the term 'hidden state' does not always refer to \( h_t \). LSTM and RNNs with multiple layers are notable examples.}
In this equation and elsewhere in this paper, all weight matrices $W$ and biases $b$ collectively form the parameters $\theta$ to be learned, and $\tanh$ is always written explicitly\(^3\).

Long short-term memory \cite{4,21}, the most widely-used RNN architecture to date, was introduced specifically to address the vanishing gradient problem. In LSTM, the vanishing gradient problem is mitigated through a nearly-additive path among adjacent memory cells. The term LSTM is often overloaded; in this paper we specifically refer to the variant with forget gates and without peephole connections, which performs similarly to more complex variants \cite{17}. This variant is described by

\begin{align}
    \ell_t &= \sigma(\mathbf{W}_{\ell_h}h_{t-1} + \mathbf{W}_{\ell_x}x_t + b_{\ell}) \\
    i_t &= \sigma(\mathbf{W}_{ih}h_{t-1} + \mathbf{W}_{ix}x_t + b_i) \\
    o_t &= \sigma(\mathbf{W}_{oh}h_{t-1} + \mathbf{W}_{ox}x_t + b_o) \\
    c_t &= \tanh(\mathbf{W}_{ch}h_{t-1} + \mathbf{W}_{cx}x_t + b_c) \\
    h_t &= o_t \odot \tanh(c_t)
\end{align}

where $\sigma(\cdot)$ denotes the element-wise sigmoid function and where $\odot$ denotes element-wise multiplication. Here, $\ell_t$, $i_t$, and $o_t$ are referred as the forget, input, and output gates, which can be interpreted as controlling how much we reset, write to, and read from the memory cell $c_t$. LSTM has better gradient properties than simple RNNs because of the mechanism in Equation\(^3\) which introduces a path between $c_{t-1}$ and $c_t$, which is modulated only by the forget gate. We also remark that gated recurrent units (GRUs) \cite{4} mitigate the vanishing gradient problem using this exact same idea.

NARX RNNs \cite{28} also address the vanishing gradient problem, but using a mechanism that is different from (and possibly complementary to) that of LSTM. This is done by allowing delays, or direct connections from the past. NARX RNNs in their general form are described by

\begin{equation}
    h_t = f(h_{t-1}, h_{t-2}, \ldots, x_t, x_{t-1}, \ldots, \theta)
\end{equation}

but literature usually describes the specific variant explored in \cite{28},

\begin{equation}
    h_t = \tanh \left( \sum_{d=1}^{n_d} \mathbf{W}_d h_{t-d} + \mathbf{W}_x x_t + b \right)
\end{equation}

which we refer to as simple NARX RNNs. From an efficiency perspective, notice that if the dimensionality of $h_t$ is similar to or greater than that of $x_t$, as is often the case in practice, then a simple NARX RNN has approximately $n_d$ times as many parameters and requires approximately $n_d$ times as much computation as its corresponding simple RNN (with $n_d = 1$).

Finally, we remark that other approaches have also been proposed to capture long-term dependencies. Notable approaches include Hessian-free optimization \cite{29}, operating explicitly at multiple time scales \cite{9,22}, using associative or explicit memory \cite{33,7,16,39,35}, and initializing or restricting weight matrices to be orthogonal \cite{11,19}.

### 3 The Vanishing Gradient Problem in the Context of General NARX RNNs

In this section we generalize the gradient decomposition in \cite{4,32} to NARX RNNs and formally connect gradient components with paths and edges. We begin with the chain rule for ordered derivatives \cite{38}. This chain rule is quickly obtained from the standard chain rule \cite{37} and solidifies intuitions that are based on the backpropagation-through-time algorithm. Finally we remark that we avoid being overly formal here, relying on slightly overloaded notation for clarity. Otherwise notation quickly becomes cumbersome (see \cite{37}).

### 4 Disambiguating Notation

We begin by disambiguating the symbol $\frac{\partial f}{\partial x}$, as it is routinely overloaded in literature. We illustrate this by example. Consider the Jacobian of $f(u(x), v(x))$ with respect to $x$; from the ordinary chain rule, we have $\frac{\partial f}{\partial x} = \frac{\partial f}{\partial u} \frac{\partial u}{\partial x} + \frac{\partial f}{\partial v} \frac{\partial v}{\partial x}$. Next, consider the Jacobian of $f(x, u(x))$; from a naive

\(^3\)tanh is a common choice, but it is of course also possible to use other activation functions.
We remark that the simpler case of simple RNNs is included in the supplementary material for clarity. This simple decomposition extends the result from [32] to general NARX RNNs. This decomposition expresses the full derivatives \( \frac{\partial f}{\partial x} \), a collection of full derivatives, whereas on the right \( \frac{\partial f}{\partial x} \) denotes \( \frac{\partial f(x, u)}{\partial x} \), a collection of partial derivatives. In this paper we denote full derivatives with \( \frac{\partial f}{\partial x} \) and partial derivatives with \( \frac{\partial f}{\partial x} \). This notation is consistent with [37, 38], but is the exact opposite of the convention in [32].

4.1 The Chain Rule for Ordered Derivatives

Consider an ordered system of \( n \) vectors \( v_1, v_2, \ldots, v_n \), where each is a function of all previous:

\[
v_i \equiv v_i(v_{i-1}, v_{i-2}, \ldots, v_1), \quad 1 \leq i \leq n
\]  

The chain rule for ordered derivatives expresses the full derivatives \( \frac{\partial^+ v_i}{\partial v_j} \) for any \( j < i \) in terms of the full derivatives that relate \( v_i \) to all previous \( v_k \):

\[
\frac{\partial^+ v_i}{\partial v_j} = \sum_{i > k > j} \frac{\partial^+ v_i}{\partial v_k} \frac{\partial v_k}{\partial v_j}, \quad j < i
\]  

4.2 Gradient Decomposition

Consider NARX RNNs in their general form (Equation 9), and for simplicity consider the situation that is most often encountered in practice, where the loss at time \( t \) is defined in terms of the current state \( h_t \) and its own parameters \( \theta_t \) (which are independent of \( \theta \)):

\[
l_t = f_i(h_t, \theta_i)
\]

Then the Jacobian (or transposed gradient) with respect to \( \theta \) can be written as

\[
\frac{\partial^+ l_t}{\partial \theta} = \frac{\partial^+ f_i}{\partial h_t} \frac{\partial h_t}{\partial \theta}
\]

because the additional term \( \frac{\partial f_i}{\partial \theta} \frac{\partial^+ h_t}{\partial \theta} \) is 0. Now, by letting \( v_1 = \theta \), \( v_2 = x_1 \), \( v_3 = x_2 \), and so on in Equations 11 and 12 we obtain

\[
\frac{\partial^+ h_t}{\partial \theta} = \sum_{\tau = 0}^{t-1} \frac{\partial^+ h_t}{\partial h_{t-\tau}} \frac{\partial h_{t-\tau}}{\partial \theta}
\]  

because all partials \( \frac{\partial h_{t-\tau}}{\partial \theta} \) are 0.

This simple decomposition extends the result from [32] to general NARX RNNs. This decomposition breaks \( \frac{\partial^+ h_t}{\partial \theta} \) into its temporal components, making it clear that the spectral norm of \( \frac{\partial^+ h_t}{\partial h_{t-\tau}} \) plays a major role in how \( h_{t-\tau} \) affects the final gradient \( \frac{\partial^+ l_t}{\partial \theta} \). In particular, if the norm of \( \frac{\partial^+ h_t}{\partial h_{t-\tau}} \) is extremely small, then \( h_{t-\tau} \) has only a negligible effect on the final gradient, which in turn makes it extremely difficult to learn from events that occurred at \( t - \tau \).

4.3 Gradient Components as Paths

Here we will apply Equation 12 repeatedly to associate gradient components with paths connecting \( t - \tau \) to \( t \), beginning with Equation 15. First, by applying Equation 12 to expand \( \frac{\partial^+ h_t}{\partial h_{t-\tau}} \), we obtain

\[
\frac{\partial^+ h_t}{\partial h_{t-\tau}} = \sum_{t \geq t' > t-\tau} \frac{\partial^+ h_t}{\partial h_{t'}} \frac{\partial h_{t'}}{\partial h_{t-\tau}}
\]  

We remark that the simpler case of simple RNNs is included in the supplementary material for clarity, but here we move directly to simple NARX RNNs and general NARX RNNs.
We will now expand Equation 16. From Equation 10, we can see that up to $n$ gradient components as paths, with each component being a product with one factor per edge along the path, gives us useful insight into various RNN architectures. When relating a loss between $t$ and $t' = t - \tau$ and $t'$ and $t - \tau$ share an edge. Collecting these $t'$ as the set $V_{t - \tau} = \{t' : t' > t - \tau \text{ and } (t - \tau, t') \in E\}$, we can write

$$\frac{\partial^+ h_t}{\partial h_{t - \tau}} = \sum_{t' \in V_{t - \tau}} \frac{\partial^+ h_{t'}}{\partial h_{t'}} \frac{\partial h_{t'}}{\partial h_{t - \tau}}$$  \hspace{1cm} (17)$$

By applying this same process to each $\frac{\partial^+ h_{t'}}{\partial h_{t'}}$ and defining $V_{t'} = \{t'' : t'' > t' \text{ and } (t', t'') \in E\}$ for all $t'$, we can write

$$\frac{\partial^+ h_{t'}}{\partial h_{t - \tau}} = \sum_{t'' \in V_{t'}} \sum_{t''' \in V_{t''}} \frac{\partial^+ h_{t''}}{\partial h_{t''}} \frac{\partial h_{t''}}{\partial h_{t'}} \frac{\partial h_{t'}}{\partial h_{t - \tau}}$$ \hspace{1cm} (18)$$

By simply repeating this process until only partials remain, we finally obtain a summation over all possible paths from $t - \tau$ to $t$. Each term in the sum is a product over factors, one per edge:

$$\frac{\partial h_t}{\partial h_{t - \tau}} \cdots \frac{\partial h_{t''}}{\partial h_{t'}} \frac{\partial h_{t'}}{\partial h_{t - \tau}}$$ \hspace{1cm} (19)$$

The situation for general NARX RNNs is the same, with each term corresponding to a product over factors, one per edge. The only difference from simple NARX RNNs is the specific sets of edges that are considered.

4.3.2 Discussion

In all cases, we can bound the spectral norm of each term in the summation, one term per path:

$$\left\| \frac{\partial h_t}{\partial h_{t - \tau}} \cdots \frac{\partial h_{t''}}{\partial h_{t'}} \frac{\partial h_{t'}}{\partial h_{t - \tau}} \right\| \leq \left\| \frac{\partial h_t}{\partial h_{t - \tau}} \right\| \cdots \left\| \frac{\partial h_{t''}}{\partial h_{t'}} \right\| \leq \lambda^{n_e}$$ \hspace{1cm} (20)$$

where $\lambda$ is the maximum spectral norm of any factor and $n_e$ is the number of edges on the path. All terms with $\lambda < 1$ vanish exponentially fast, and in this paper we focus on worst-case behavior, where all terms have $\lambda < 1$. In this case, because $\lambda^{n_e}$ tends to 0 quickly as the number of edges $n_e$ increases, shortest paths dominate the sum. Thus by introducing architectures with short paths between $t - \tau$ and $t$, we obtain gradient components with few multiplicative factors, which in turn are more capable of carrying long-term gradient information.

5 Example Architecture: Mixed History Recurrent Neural Networks

Viewing gradient components as paths, with each component being a product with one factor per edge along the path, gives us useful insight into various RNN architectures. When relating a loss at time $t$ to events at time $t - \tau$, simple RNNs and LSTM contain shortest paths of length $\tau$, while simple NARX RNNs contain shortest paths of length $\frac{\tau}{n_d}$, where $n_d$ is the number of delays.

One can envision many NARX RNN architectures which reduce these shortest paths further. In this section we introduce one such architecture using base-2 exponential delays. In this case, for all

| Table 1: Parameter counts ($n_p$), hidden unit counts ($n_h$), and optimal learning rates ($\alpha^*$) |
|---|---|---|
| Copy ($D = 100$) | TIMIT | Sequential pMNIST |
| $n_p$ | $n_h$ | log$_{10} \alpha^*$ | $n_p$ | $n_h$ | log$_{10} \alpha^*$ | $n_p$ | $n_h$ | log$_{10} \alpha^*$ |
| Simple RNNs | 203 | -2.12 ± 0.11 | 197 | -1.09 ± 0.25 | 198 | -2.27 ± 0.10 |
| LSTM | 100 | -1.55 ± 0.32 | 100 | -0.63 ± 0.06 | 100 | -1.11 ± 0.11 |
| MIST RNNs | 141 | -1.47 ± 0.66 | 139 | -0.91 ± 0.16 | 139 | -1.35 ± 0.08 |
$\tau \leq 2^{n_d-1}$, shortest paths exist with only $\log_2 \tau$ edges, leading to a drastic reduction for large $\tau$ with even moderately large $n_d$.

We also remark that, as mentioned in Section 2, simple NARX RNNs increase computation linearly with $n_d$, which is unacceptable for even moderately large $n_d$. Here we avoid this computational growth by instead sharing weight matrices over delays and combining an attention-like mechanism [3] over delayed states and a reset mechanism from gated recurrent units [5]. As long as $n_d$ is less than the number of hidden units $n_h$, as is the case in practice, then the proposed architecture requires even fewer operations than LSTM.

The proposed architecture, which we call mixed history RNNs (MIST RNNs), is described by

\begin{align*}
a_t &= \text{softmax}(W_{ah}h_{t-1} + W_{ax}x_t + b_a) \\
r_t &= \sigma(W_{rh}h_{t-1} + W_{rx}x_t + b_r) \\
h_t &= \tanh \left( W_h \left[ r_t \odot \sum_{i=0}^{n_d-1} a_i h_{t-2i} \right] + W_x x_t + b \right)
\end{align*}

Here, $a_t$ is a learned vector of coefficients which sum to 1, and $r_t$ is a reset gate [5]. At each time step, a convex combination of delayed states is formed according to $a_t$; components of this combination are reset according to $r_t$; and finally the typical linear layer and nonlinearity are applied.

6 Experiments

In this section we empirically compare MIST RNNs to simple RNNs and LSTM. First we consider three real datasets in the domains of surgical activity recognition and phoneme recognition, and then we consider the copy problem and the sequential permuted MNIST task, as they have been used extensively to test RNN architectures for their ability to capture long-term dependencies [21, 29, 24, 1, 19, 7].

6.1 Surgical Activity Recognition

Here we consider the tasks of online surgical gesture recognition using the JIGSAWS dataset [13, 25, 8] and online surgical maneuver recognition using the MISTIC-SL dataset [12, 8]. Gestures are short, low-level activities, such as reaching for needle or pushing needle through tissue, while maneuvers are longer, higher-level activities, such as suture throw or knot tying. Both datasets were collected using a da Vinci, and the goal is to map robot kinematics over time (e.g., $x$, $y$, $z$) to activities over time (which are densely labeled on a per-frame basis). We follow [8] (which achieves state-of-the-art performance on these tasks) as closely as possible, using the same kinematic inputs, test setup, and hyperparameters; details can be found in the original work or in the supplementary material. The primary difference is that we replace their LSTM layer with our simple RNN, LSTM, or MIST RNN layer.

Results are shown in Table 2. We can see that simple RNNs, LSTM, and MIST RNNs perform nearly identically for gesture recognition. This suggests that long-term dependencies do not play a key role for gesture recognition, which is reasonable because they are short in duration. Also in Table 2 we can see that LSTM and MIST RNNs perform similarly in the case of maneuver recognition, and that both significantly outperforming simple RNNs. Again this result is not surprising, as maneuvers are long in duration and thus depend on long-term behavior. Finally we remark that the small differences between the LSTM results reported in [8] and this paper are likely due to small differences in implementation, such as their use of peephole connections in the LSTM architecture.

6.2 Phoneme Recognition

Here we consider the task of online framewise phoneme recognition using the TIMIT corpus [14]. Each frame is originally labeled as 1 of 61 phonemes. We follow common practice and collapse these into a smaller set of 39 phonemes [22], and we include glottal stops to yield 40 classes in total. We follow [17] for data preprocessing and [18] for training, validation, and test splits. LSTM with 100 hidden units is used as a baseline, with hidden unit counts for other architectures chosen to match the number of parameters, as summarized in Table 1. Means and standard deviations are computed...
Table 2: Error rates for surgical gesture recognition (left) and surgical maneuver recognition (right).

|                     | Error Rate (%) |                      |                      |
|---------------------|----------------|----------------------|----------------------|
|                     | LSTM [8]       | Simple RNNs (ours)   | LSTM (ours)          |
|                     | 19.5 ± 6.2     | 20.2 ± 8.0           | 20.5 ± 7.0           |
|                     | MIST RNNs (ours) | 20.1 ± 7.9          |                      |
|                     | LSTM [8]       | Simple RNNs (ours)   | LSTM (ours)          |
|                     | 12.2 ± 2.7     | 38.0 ± 6.2           | 13.9 ± 3.0           |
|                     | MIST RNNs (ours) | 14.1 ± 3.9          |                      |

Figure 2: Validation curves for the copy problem. At each point, the error rate is computed using the entire validation set.

using the top 5 randomized trials out of 50 (ranked according to performance on the validation set), with random learning rates and initializations. Other experimental details can be found in the supplementary material.

Table 3 shows that LSTM and MIST RNNs perform nearly identically, again both outperforming simple RNNs, as we might expect since phonemes often span many frames. We remark that our results are somewhat similar to those in [17], but that these numbers cannot be compared: their results are for offline predictions rather than online predictions (using bidirectional RNNs), and they use the full set of 61 phonemes.

6.3 The Copy Problem

The copy problem is a synthetic task that explicitly challenges a network to store and reproduce information from the past. Our setup follows [1], which is in turn based on [21]. An input sequence begins with $L$ relevant symbols to be copied, is followed by a delay of $D - 1$ special blank symbols and 1 special go symbol, and ends with $L$ additional blank symbols. The corresponding target sequence begins with $L + D$ blank symbols and ends with a copy of the relevant symbols from the inputs (in the same order). We run experiments with copy delays of $D = 50, 100, 200,$ and $400$. LSTM with 100 hidden units is used as a baseline, with hidden unit counts for other architectures chosen to match the number of parameters, as summarized in Table 1. Additional experimental details can be found in the supplementary material.

Results are shown in Figure 2 showing validation curves of the top 5 randomized trials out of 50, with random learning rates and initializations. With a short copy delay of $D = 50$, we can see that all methods, even simple RNNs, can solve the task in a reasonable amount of time. However, as the copy delay $D$ is increased, we can see that simple RNNs and LSTM become unable to learn a solution, whereas MIST RNNs are relatively unaffected. We also note that our LSTM results are consistent with [1][19]. Finally we note that it is known that orthogonal-weight-matrix based approaches are
Table 3: Test-set error rates for TIMIT phoneme recognition.

|                      | Error Rate (%) |
|----------------------|----------------|
| Simple RNNs          | 34.1 ± 0.3     |
| LSTM                 | 32.1 ± 0.2     |
| MIST RNNs            | 32.0 ± 0.3     |

Table 4: Test-set error rates for sequential pMNIST classification.

|                      | Error Rate (%) |
|----------------------|----------------|
| Simple RNNs          | 12.9 ± 0.8     |
| LSTM                 | 10.4 ± 0.7     |
| MIST RNNs            | 5.5 ± 0.2      |

particularly well suited to this problem [19]. MIST RNNs, without using such initializations, perform similarly to such approaches [1, 19].

6.4 Sequential pMNIST Classification

The sequential MNIST task [24] consists of classifying 28x28 MNIST images [26] as one of 10 digits, by scanning pixel by pixel – left to right, top to bottom – and emitting a label upon completion. Sequential pMNIST [24] is a challenging variant where a random permutation of pixels is chosen and applied to all images before classification. Data preprocessing is kept minimal, with each input image individually shifted and scaled to have mean 0 and variance 1. We split the official training set into two parts, the first 58,000 used for training and the last 2,000 used for validation. Our test set is the same as the official test set, consisting of 10,000 images. Training is carried out by minimizing cross-entropy loss. LSTM with 100 hidden units is used as a baseline, with hidden unit counts for other architectures chosen to match the number of parameters, as summarized in Table 1. Means and standard deviations are computed using the top 5 randomized trials out of 50 (ranked according to performance on the validation set), with random learning rates and initializations.

Test error rates are shown in Table 4. Here, MIST RNNs significantly outperform both simple RNNs and LSTM. We remark that our LSTM error rates are consistent with best previously-reported values, such as the error rates of 9.8% in [6] and 12% in [1], which also use 100 hidden units. Finally one may wonder if the difference in performance is due to hidden-unit counts. To test this we also increased the LSTM hidden unit count to 139 (to match MIST RNNs). This decreases the error rate by 2% but is still significantly outperformed by MIST RNNs (now with fewer parameters).

7 Conclusions and Future Work

We analyzed general NARX RNNs in detail and introduced NARX RNNs with noncontiguous delays as a useful mechanism for overcoming the vanishing gradient problem. In particular, we extended previous gradient-decomposition results from simple RNNs to general NARX RNNs, formally related gradient components to edges, introduced an example NARX RNN architecture based on these ideas (with exponential delays), and showed that this example architecture matches or exceeds LSTM performance across a wide range of tasks.

We are also excited by many directions for future work, which come somewhat naturally since the mechanism introduced in this paper is orthogonal to that of LSTM. In particular, one can envision many architectures other than MIST RNNs, with various types of noncontiguous delays, various ways of combining delayed states, and so on. In addition it will be interesting to see if performance benefits result from combining the mechanisms of these two orthogonal approaches, for example by letting the cell update of the LSTM depend directly on multiple states from the distant past. Finally we note that there are many recent techniques that have focused on LSTM that are immediately transferable to NARX RNNs, for example variational dropout [11], batch normalization [6], layer normalization [2], and zoneout [23].
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References

[1] Martin Arjovsky, Shah Amar, and Yoshua Bengio. Unitary evolution recurrent neural networks. *International Conference on Machine Learning (ICML)*, 2016.

[2] Jimmy Lei Ba, Jamie Ryan Kiros, and Geoffrey E Hinton. Layer normalization. *arXiv preprint arXiv:1607.06450*, 2016.

[3] Dzmitry Bahdanau, KyungHyun Cho, and Yoshua Bengio. Neural machine translation by jointly learning to align and translate. *International Conference on Learning Representations (ICLR)*, 2015.

[4] Yoshua Bengio, Patrice Simard, and Paolo Frasconi. Learning long-term dependencies with gradient descent is difficult. *IEEE Transactions on Neural Networks*, 5(2):157–166, 1994.

[5] Kyunghyun Cho, Bart van Merriënboer, Çağlar Gülçehre, Dzmitry Bahdanau, Fethi Bougares, Holger Schwenk, and Yoshua Bengio. Learning phrase representations using rnn encoder-decoder for statistical machine translation. *Proceedings of the 2014 Conference on Empirical Methods in Natural Language Processing (EMNLP)*, 2014.

[6] Tim Cooijmans, Nicolas Ballas, César Laurent, and Aaron Courville. Recurrent batch normalization. *arXiv preprint arXiv:1603.09025*, 2016.

[7] Ivo Danihelka, Greg Wayne, Benigno Uria, Nal Kalchbrenner, and Alex Graves. Associative long short-term memory. *International Conference on Machine Learning (ICML)*, 2016.

[8] Robert DiPietro, Colin Lea, Anand Malpani, Narges Ahmidi, S Swaroop Vedula, Gyusung I Lee, Mija R Lee, and Gregory D Hager. Recognizing surgical activities with recurrent neural networks. *International Conference on Medical Image Computing and Computer-Assisted Intervention*, pages 551–558, 2016.

[9] Salah El Hihi and Yoshua Bengio. Hierarchical recurrent neural networks for long-term dependencies. *Advances in neural information processing systems (NIPS)*, 1995.

[10] Jeffrey L Elman. Finding structure in time. *Cognitive science*, 14(2):179–211, 1990.

[11] Yarin Gal and Zoubin Ghahramani. A theoretically grounded application of dropout in recurrent neural networks. In *Advances in Neural Information Processing Systems*, pages 1019–1027, 2016.

[12] Yixin Gao, S Swaroop Vedula, Gyusung I Lee, Mija R Lee, Sanjeev Khudanpur, and Gregory D Hager. Unsupervised surgical data alignment with application to automatic activity notation. *Robotics and Automation (ICRA), 2016 IEEE International Conference on*, 2016.

[13] Yixin Gao, S. Swaroop Vedula, Carol E. Reiley, Narges Ahmidi, Balakrishnan Varadarajan, Henry C. Lin, Lingling Tao, Luca Zappella, Benjamn Bejar, David D. Yuh, Chi Chiung Grace Chen, Rene Vidal, Sanjeev Khudanpur, and Gregory D. Hager. Language of surgery: A surgical gesture dataset for human motion modeling. *Modeling and Monitoring of Computer Assisted Interventions (M2CAI) 2014*, 2014.

[14] John S Garofolo, Lori F Lamel, William M Fisher, Jonathon G Fiscus, and David S Pallett. DARPA TIMIT acoustic-phonetic continuous speech corpus CD-ROM. NIST speech disc 1-1.1. *NASA STI/Recon technical report*, 1993.

[15] Felix A Gers, Jürgen Schmidhuber, and Fred Cummins. Learning to forget: Continual prediction with LSTM. *Neural computation*, 12(10):2451–2471, 2000.

[16] Alex Graves, Greg Wayne, and Ivo Danihelka. Neural turing machines. *arXiv preprint arXiv:1410.5401*, 2014.

[17] K. Greff, R. K. Srivastava, J. Koutník, B. R. Steunebrink, and J. Schmidhuber. LSTM: A search space odyssey. *IEEE Transactions on Neural Networks and Learning Systems*, 2016.

[18] Andrew K Halberstadt. *Heterogeneous acoustic measurements and multiple classifiers for speech recognition*. PhD thesis, Massachusetts Institute of Technology, 1998.
[19] Mikael Henaff, Arthur Szlam, and Yann LeCun. Orthogonal RNNs and long-memory tasks. *International Conference on Machine Learning (ICML)*, 2016.

[20] Sepp Hochreiter. Untersuchungen zu dynamischen neuronalen netzen. *Diploma, Technische Universität München*, page 91, 1991.

[21] Sepp Hochreiter and Jürgen Schmidhuber. Long short-term memory. *Neural computation*, 9(8):1735–1780, 1997.

[22] Jan Koutnik, Klaus Greff, Faustino Gomez, and Juergen Schmidhuber. A clockwork RNN. *International Conference on Machine Learning (ICML)*, pages 1863–1871, 2014.

[23] David Krueger, Tegan Maharaj, János Kramár, Mohammad Pezeshki, Nicolas Ballas, Nan Rosemary Ke, Anirudh Goyal, Hugo Larochelle, Aaron Courville, et al. Zoneout: Regularizing rns by randomly preserving hidden activations. *arXiv preprint arXiv:1606.01305*, 2016.

[24] Quoc V Le, Navdeep Jaitly, and Geoffrey E Hinton. A simple way to initialize recurrent networks of rectified linear units. *arXiv preprint arXiv:1504.00941*, 2015.

[25] Colin Lea, René Vidal, and Gregory D. Hager. Learning convolutional action primitives for fine-grained action recognition. *2016 IEEE International Conference on Robotics and Automation (ICRA)*, 2016.

[26] Yann LeCun, Léon Bottou, Yoshua Bengio, and Patrick Haffner. Gradient-based learning applied to document recognition. *Proceedings of the IEEE*, 86(11):2278–2324, 1998.

[27] K-F Lee and H-W Hon. Speaker-independent phone recognition using hidden Markov models. *IEEE Transactions on Acoustics, Speech, and Signal Processing*, 37(11):1641–1648, 1989.

[28] Tsungnan Lin, Bill G Horne, Peter Tino, and C Lee Giles. Learning long-term dependencies in NARX recurrent neural networks. *IEEE Transactions on Neural Networks*, 7(6):1329–1338, 1996.

[29] James Martens and Ilya Sutskever. Learning recurrent neural networks with hessian-free optimization. In *International Conference on Machine Learning (ICML)*, 2011.

[30] Yajie Miao, Mohammad Gowayyed, and Florian Metze. EESEN: End-to-end speech recognition using deep RNN models and WFST-based decoding. *Automatic Speech Recognition and Understanding (ASRU)*, pages 167–174, 2015.

[31] Aaron Van den Oord, Nal Kalchbrenner, and Koray Kavukcuoglu. Pixel recurrent neural networks. *International Conference on Machine Learning (ICML)*, 2016.

[32] Razvan Pascanu, Tomas Mikolov, and Yoshua Bengio. On the difficulty of training recurrent neural networks. *International Conference on Machine Learning (ICML)*, 28:1310–1318, 2013.

[33] Tony A. Plate. Holographic recurrent networks. *Advances in neural information processing systems (NIPS)*, 1993.

[34] David E Rumelhart, Geoffrey E Hinton, and Ronald J Williams. Learning representations by back-propagating errors. *Nature*, 323(6088):533–538, 1986.

[35] Sainbayar Sukhbaatar, Jason Weston, Rob Fergus, et al. End-to-end memory networks. *Advances in neural information processing systems (NIPS)*, 2015.

[36] Paul J Werbos. Generalization of backpropagation with application to a recurrent gas market model. *Neural networks*, 1(4):339–356, 1988.

[37] Paul J Werbos. Maximizing long-term gas industry profits in two minutes in lotus using neural network methods. *IEEE Transactions on Systems, Man, and Cybernetics*, 19(2):315–333, 1989.

[38] Paul J Werbos. Backpropagation through time: what it does and how to do it. *Proceedings of the IEEE*, 78(10):1550–1560, 1990.

[39] Jason Weston, Sumit Chopra, and Antoine Bordes. Memory networks. *International Conference on Learning Representations (ICLR)*, 2015.

[40] Ronald J Williams and David Zipser. A learning algorithm for continually running fully recurrent neural networks. *Neural computation*, 1(2):270–280, 1989.

[41] Yonghui Wu, Mike Schuster, Zhifeng Chen, Quoc V Le, Mohammad Norouzi, Wolfgang Macherey, Maxim Krikun, Yuan Cao, Qin Gao, Klaus Macherey, et al. Google’s neural machine translation system: Bridging the gap between human and machine translation. *arXiv preprint arXiv:1609.08144*, 2016.
1 Simpler Derivation for Simple RNNs

This Section is intended as an aid to Section 4.3.1 in the main paper. For simple RNNs, by examining Equation 2, we can immediately see that all partials \( \frac{\partial h_t'}{\partial h_t} \) are 0 except for the one satisfying \( t' = t - \tau + 1 \). This yields

\[
\frac{\partial^+ h_t}{\partial h_{t-\tau}} = \frac{\partial^+ h_t}{\partial h_{t-\tau+1}} \frac{\partial h_{t-\tau+1}}{\partial h_{t-\tau}} (1)
\]

Now, by applying Equation 12 again to \( \frac{\partial^+ h_t}{\partial h_{t-\tau+1}} \) and then to \( \frac{\partial^+ h_t}{\partial h_{t-\tau+2}} \), and so on, we trace out a path from \( t - \tau \) to \( t \), as shown in Figure 1, finally resulting the single term

\[
\frac{\partial h_t}{\partial h_{t-1}} \ldots \frac{\partial h_{t-\tau+2}}{\partial h_{t-\tau+1}} \frac{\partial h_{t-\tau+1}}{\partial h_{t-\tau}} (2)
\]

This term is associated with the only path from \( t - \tau \) to \( t \), with one factor per edge.

2 Surgical Activity Recognition: Experimental Details

We use the same experimental setup as [1], which currently holds state-of-the-art performance on these tasks. For kinematic inputs we use positions, velocities, and gripper angles for both hands. We also use their leave-one-user-out test setup, with 8 users in the case of JIGSAWS and 15 users in the case of MISTIC-SL. Finally we use the same hyperparameters: 1 hidden layer of 1024 units; dropout as defined in [7] with \( p = 0.5 \); 80 epochs of training with a learning rate of 1.0 for the first 40 epochs and having the learning rate every 5 epochs for the rest of training. As mentioned in the main paper, the primary difference is that we replaced their LSTM layer with our simple RNN, LSTM, or MIST RNN layer. Training is carried out by minimizing cross-entropy loss.

3 Experimental Setup (General)

Everything in this section holds for all experiments except surgical activity recognition, as in that case we mimicked [1] as closely as possible, as described above.

For MIST RNNs, we use delays 1, 2, 4, \ldots, 128. All weight matrices are initialized using a normal distribution with a mean of 0 and a standard deviation of \( 1/\sqrt{n_h} \), where \( n_h \) is the number of hidden units. All initial hidden states (for \( t < 1 \)) are initialized to 0. For optimization, gradients are computed using full backpropagation through time, and we use stochastic gradient descent with a momentum of 0.9, with gradient clipping as described by [6] at 1, and with a minibatch size of 100. Biases are generally initialized to 0, but we follow best practice for LSTM by initializing the forget-gate bias to 1 [2, 5]. To ensure fair comparisons, we avoid manual learning-rate tuning in its entirety. Instead, we run 50 trials for each experimental configuration. In each trial, the learning rate is drawn uniformly at random in log space between \( 10^{-4} \) and \( 10^1 \), and initial weight matrices are also redrawn at random.
We report results over the top 10% of trials according to validation-set error. (An alternative option is to report results over all trials. However, because the majority of trials yields bad performance for all methods, this simply blurs comparisons. See for example Figure 3 of [3], which compares these two options.)

4 Phoneme Recognition: Experimental Details

We follow [3] and extract 12 mel frequency cepstral coefficients plus energy every 10ms using 25ms Hamming windows and a pre-emphasis coefficient of 0.97. However we do not use derivatives, resulting in 13 inputs per frame. Each input sequence is individually shifted and scaled to have mean 0 and variance 1 over each dimension. We form our splits according to [4], resulting in 3696 sequences for training, 400 sequences for validation, and 192 sequences for testing. Training is carried out by minimizing cross-entropy loss. Means and standard deviations are computed using the top 5 randomized trials out of 50 (ranked according to performance on the validation set).

5 Copy Problem: Experimental Details

In our experiments, the \( L \) relevant symbols are drawn at random (with replacement) from the set \( \{0, 1, \ldots, 9\} \); \( D \) is always a multiple of 10; and \( L \) is chosen to be \( D/10 \). This way the simplest baseline of always predicting the blank symbol yields a constant error rate for all experiments. No input preprocessing of any kind is performed.

In each case, we generate 100,000 examples for training and 1,000 examples for validation. Training is carried out by minimizing cross-entropy loss.

References

[1] Robert DiPietro, Colin Lea, Anand Malpani, Narges Ahmidi, S Swaroop Vedula, Gyusung I Lee, Mija R Lee, and Gregory D Hager. Recognizing surgical activities with recurrent neural networks. International Conference on Medical Image Computing and Computer-Assisted Intervention, pages 551–558, 2016.

[2] Felix A Gers, Jürgen Schmidhuber, and Fred Cummins. Learning to forget: Continual prediction with LSTM. Neural computation, 12(10):2451–2471, 2000.

[3] K. Greff, R. K. Srivastava, J. Koutník, B. R. Steunebrink, and J. Schmidhuber. LSTM: A search space odyssey. IEEE Transactions on Neural Networks and Learning Systems, 2016.

[4] Andrew K Halberstadt. Heterogeneous acoustic measurements and multiple classifiers for speech recognition. PhD thesis, Massachusetts Institute of Technology, 1998.

[5] Rafal Jozefowicz, Wojciech Zaremba, and Ilya Sutskever. An empirical exploration of recurrent network architectures. International Conference on Machine Learning (ICML), 2015.

[6] Razvan Pascanu, Tomas Mikolov, and Yoshua Bengio. On the difficulty of training recurrent neural networks. International Conference on Machine Learning (ICML), 28:1310–1318, 2013.

[7] Wojciech Zaremba, Ilya Sutskever, and Oriol Vinyals. Recurrent neural network regularization. arXiv preprint arXiv:1409.2329, 2014.