Dynamical Isometry and a Mean Field Theory of LSTMs and GRUs

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Abstract

Training recurrent neural networks (RNNs) on long sequence tasks is plagued with difficulties arising from the exponential explosion or vanishing of signals as they propagate forward or backward through the network. Many techniques have been proposed to ameliorate these issues, including various algorithmic and architectural modifications. Two of the most successful RNN architectures, the LSTM and the GRU, do exhibit modest improvements over vanilla RNN cells, but they still suffer from instabilities when trained on very long sequences. In this work, we develop a mean field theory of signal propagation in LSTMs and GRUs that enables us to calculate the time scales for signal propagation as well as the spectral properties of the state-to-state Jacobians. By optimizing these quantities in terms of the initialization hyperparameters, we derive a novel initialization scheme that eliminates or reduces training instabilities. We demonstrate the efficacy of our initialization scheme on multiple sequence tasks, on which it enables successful training while a standard initialization either fails completely or is orders of magnitude slower. We also observe a beneficial effect on generalization performance using this new initialization.

1. Introduction

A common paradigm for research and development in deep learning involves the introduction of novel network architectures followed by experimental validation on a selection of tasks. While this methodology has undoubtedly generated significant advances in the field, it is hampered by the fact that the full capabilities of a candidate model may be obscured by difficulties in the training procedure. It is often possible to overcome such difficulties by carefully selecting the optimizer, batch size, learning rate schedule, initialization scheme, or other hyperparameters. However, the standard strategies for searching for good values of these hyperparameters are not guaranteed to succeed, especially if the trainable configurations are constrained to a low-dimensional subspace of hyperparameter space, which can render random search, grid search, and even Bayesian hyperparameter selection methods unsuccessful.

In this work, we argue that, for long sequence tasks, the trainable configurations of initialization hyperparameters for LSTMs and GRUs lie in just such a subspace, which we characterize theoretically. In particular, we identify precise conditions on the hyperparameters governing the initial weight and bias distributions that are necessary to ensure trainability. These conditions derive from the observation that in order for a network to be trainable, (a) signals from the relevant parts of the input sequence must be able to propagate all the way to the loss function and (b) the gradients must be stable (i.e. they must not explode or vanish exponentially).

As shown in Figure 1, training of recurrent networks with standard initialization on certain tasks begins to fail as the sequence length increases and signal propagation be-
comes harder to achieve. However, as we shall show, a suitably-chosen initialization scheme can dramatically improve trainability on such tasks.

We study the effect of the initialization hyperparameters on signal propagation for a very broad class of recurrent architectures, which includes as special cases many state-of-the-art RNN cells, including the GRU (Cho et al., 2014), the LSTM (Hochreiter & Schmidhuber, 1997), and the peephole LSTM (Gers et al., 2002). The analysis is based on the mean field theory of signal propagation developed in a line of prior work (Schoenholz et al., 2016; Xiao et al., 2018; Chen et al., 2018; Yang et al., 2019), as well as the concept of dynamical isometry (Saxe et al., 2013; Pennington et al., 2017; 2018) that is necessary for stable gradient backpropagation and which was shown to be crucial for training simpler RNN architectures (Chen et al., 2018). We perform a number of experiments to corroborate the results of the calculations and use them to motivate initialization schemes that outperform standard initialization approaches on a number of long sequence tasks.

2. Background and Related Work

2.1. Mean field analysis of neural networks

Signal propagation at initialization can be controlled by varying the hyperparameters of fully-connected (Schoenholz et al., 2016; Yang & Schoenholz, 2017) and convolutional (Xiao et al., 2018) feed-forward networks, as well as for simple gated recurrent architectures (Chen et al., 2018). In all these cases, such control was used to obtain initialization schemes that outperformed standard initializations on benchmark tasks. In the feed-forward case, this enabled the training of very deep architectures without the use of batch normalization or skip connections.

By forward signal propagation, we specifically refer to the persistence of correlations between the hidden states of networks with different inputs as a function of time (or depth in the feed-forward case), as will be made precise in Section 4.2. Backward signal propagation depends not only on the norm of the gradient, but also on its stability, which is governed by the state-to-state Jacobian matrix, as discussed in (Bengio et al., 1994). In our context, the goal of the backward analysis is to enhance the conditioning of the Jacobian by controlling the first two moments of its squared singular values. Forward signal propagation and the spectral properties of the Jacobian at initialization can be studied using mean field theory and random matrix theory (Poole et al., 2016; Schoenholz et al., 2016; Yang & Schoenholz, 2017; 2018; Xiao et al., 2018; Pennington et al., 2017; 2018; Chen et al., 2018; Yang et al., 2019). More generally, mean field analysis is also emerging as a promising tool for studying the dynamics of learning in neural networks and even obtaining generalization bounds in some settings (Mei et al., 2018).

While extending an analysis at initialization to a trained network might appear hopeless due to the complexity of the training process, intriguingly, it was recently shown that in the infinite width, continuous time limit neural networks exhibit certain invariances during training (Jacot et al., 2018), further motivating the study of networks at initialization. In fact, the general strategy of proving the existence of some property beneficial for training at initialization and controlling it during the training process is the core idea behind a number of recent global convergence results for over-parametrized networks (Du et al., 2018; Allen-Zhu et al., 2018), some of which (Allen-Zhu et al., 2018) also rely explicitly on control of forward and backward signal propagation (albeit not defined in the exact sense as in this work).

As neural network training is a nonconvex problem, using a modified initialization scheme could lead to convergence to different points in parameter space in a way that adversely affects the generalization error. We provide some empirical evidence that this does not occur, and in fact, the use of initialization schemes satisfying these conditions has a beneficial effect on the generalization error.

2.2. The exploding/vanishing gradient problem and signal propagation in recurrent networks

The exploding/vanishing gradient problem is a well-known phenomenon that hampers training on long time sequence tasks (Bengio et al., 1994; Pascanu et al., 2013). Apart from the gating mechanism, there have been numerous proposals to alleviate the vanishing gradient problem by constraining the weight matrices to be exactly or approximately orthogonal (Pascanu et al., 2013; Wisdom et al., 2016; Vorontsov et al., 2017; Jose et al., 2017), or more recently by modifying some terms in the gradient (Arpit et al., 2018), while exploding gradients can be handled by clipping (Pascanu et al., 2013). Another recently proposed approach to ensuring signal propagation in long sequence tasks introduces auxiliary loss functions (Trinh et al., 2018). This modification of the loss can be seen as a form of regularization. Chang et al. (2019) study the connections between recurrent networks and certain ordinary differential equations and propose the AntisymmetricRNN that can capture long term dependencies in the inputs. While many of these approaches have been quite successful, they typically require modifying the training algorithm, the loss function, or the architecture, and as such exist as complementary methods to the one we investigate here. We postpone the investigation of a combination of techniques to future work.
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| Vanilla RNN | Minimal RNN (Chen et al., 2018) | GRU (Cho et al., 2014) | peephole LSTM (Gers et al., 2002) | LSTM (Hochreiter & Schmidhuber, 1997) |
|-------------|---------------------------------|------------------------|----------------------------------|--------------------------------------|
| $s_t$       | $h_t'$                           | $h_t'$                 | $c_t'$                           | $h_t'$                               |
| $K$         | $\{f\}$                         | $\{f, r\}$            | $\{i, f, r, o\}$                 | $\{i, f, r, o\}$                     |
| $p$         | $s_t'$                           | $s_t'$                 | $\sigma(u_o) \circ \tanh(s_t')$ | $s_t'$                               |
| $g_k$       | .                               | .                      | .                                | .                                    |
| $f$         | $\sigma(u_f') \circ s_t'^{-1}$  | $\sigma(u_f') \circ s_t'^{-1}$ | $\sigma(u_f') \circ s_t'^{-1}$  | $\sigma(u_f') \circ \tanh(c_t')$    |

Table 1. A number of recurrent architectures written in the form 1. The LSTM cell state is unordered in order to emphasize that it can be written as a function of variables that are Gaussian at the large $N$ limit.

3. Notation

We denote matrices by bold upper case Latin characters and vectors by bold lower case Latin characters. $\mathcal{D} \mu$ denotes a standard Gaussian measure. The normalized trace of a random $N \times N$ matrix $A$, $\frac{1}{N} \mathcal{E}_{\mathcal{D}(A)},$ is denoted by $\tau(A)$. $\circ$ is the Hadamard product, $\sigma(\cdot)$ is a sigmoid function and both $\sigma(\cdot), \tanh(\cdot)$ act element-wise. We denote by $D_{\alpha}$ a diagonal matrix with $\alpha$ on the diagonal.

4. Mean field analysis of signal propagation and dynamical isometry

4.1. Model description and important assumptions

We present a general setup in this section and subsequently specialize to the case of the GRU, LSTM and peephole LSTM. This section follows closely the development in (Chen et al., 2018). We denote the state of a recurrent network at time $t$ by $s_t \in \mathbb{R}^N$ with $s_0 \sim \mathcal{D}_0$, and a sequence of inputs to the network $\{z^1, ..., z^T\}, \ z^t \in \mathbb{R}^N$. We also define sets of subscripts $K$ and pre-activations $u_k^t \in \mathbb{R}^N, k \in K$ defined by

$$u_k^t = W_k s_t^{t-1} + U_k z^t + b_k$$  \hspace{1cm} (1a)

where $W_k, U_k \in \mathbb{R}^{N \times N}, b_k \in \mathbb{R}^N$. We define additional variables given by

$$u_{k_2}^t = W_{k_2} D_{g_k(u_k)} s_t^{t-1} + U_{k_2} z^t + b_{k_2}$$ \hspace{1cm} (1b)

where $g_k : \mathbb{R}^N \rightarrow \mathbb{R}^N$ is an element-wise function and $u_k^t$ is defined as in eqn. (1a) \hspace{1cm} 2. In cases where there is no need to distinguish between variables of the form 1a and 1b we will refer to both as $u_k^t$. The state evolution of the network is given by

$$s^t = f(s^{t-1}, \{u_k^t\}, ..., \{u_k^t\}, x^t)$$ \hspace{1cm} (1c)

where $f$ is an element-wise, affine function of $s^{t-1}$. The output of the network at every time is given by $p(s^t, \{u_k^t\})$. These dynamics describe all the architectures studied in this paper, as well as many others, as detailed in Table 1. In the case of the peephole LSTM and GRU, eqn. (1c) will be greatly simplified.

In order to understand the properties of a neural network at initialization, we take the weights of the network to be random variables. Specifically, we assume $W_{k,ij} \sim \mathcal{N}(0, \sigma_k^2/\sqrt{N}), U_{k,ij} \sim \mathcal{N}(0, \nu^2_k/\sqrt{N}), b_{k,i} \sim \mathcal{N}(\mu_k, \rho_k^2)$ i.i.d. and denote $\Theta = \bigcup_k \{\sigma_k^2, \nu_k^2, \rho_k^2, \mu_k\}$. As in (Chen et al., 2018), we make the unified weights assumption $W_{k,ls} \sim \mathcal{N}(0, \sigma^2_k/N)$. Tied weights would increase the autocorrelation of states across time, but this might be dominated by the increase due to the correlations between input tokens when the latter is strong. Indeed, we provide empirical evidence that calculations performed under this assumption still have considerable predictive power in cases where it is violated.

4.2. Forward signal propagation

We now consider two sequences of normalized inputs $\{z^t_k\}, \{z^t_k\}$ with zero mean and covariance $R = \begin{pmatrix} 1 & \Sigma \end{pmatrix}$ fed into two copies of a network with identical weights, and resulting in sequences of states $\{s^t_k\}, \{s^t_k\}$. We are interested in the moments and correlations

$$\mu^t_s \equiv \mathbb{E}[s^t_{ia}]$$  \hspace{1cm} (2a)

$$Q^t_s \equiv Q^t_{s,aa} = \mathbb{E}[s^t_{i'a}s^t_{ia}]$$  \hspace{1cm} (2b)

$$\Sigma^2_{s}C_s^2 + (\mu^t_s)^2 = \mathbb{E}[s^t_{i'a}s^t_{ib}]$$  \hspace{1cm} (2c)

where we define $\Sigma^2_{s} = Q^t_s - (\mu^t_s)^2$ (and $\Sigma^2_{s}$ analogously).

At the large $N$ limit we can invoke a CLT to find

$$\begin{pmatrix} u^t_{k,ia} \\ u^t_{k,ib} \end{pmatrix} \sim \mathcal{N} \begin{pmatrix} \mu^t_k \\ \Sigma^2_{s}C_s^2 \begin{pmatrix} 1 \\ C_s^2 \end{pmatrix} \begin{pmatrix} 1 \\ C_s^2 \end{pmatrix} \end{pmatrix}$$ \hspace{1cm} (3)
where the second moment $Q_k^t$ is given by

$$Q_k^t = E[u_k^{t,1} u_k^{t,2}] = \sigma^2_k E[s_{i_a^{t,1}} s_{i_a^{t,2}}] + \nu_k^2 E[z_{i_a^{t,1}} z_{i_a^{t,2}}] + \rho_k^2 + \mu_k^2$$

$$\equiv \sigma^2_k Q_s^t + \nu_k^2 R + \rho_k^2 + \mu_k^2$$

(4a)

and the correlations $C_k^t$ by $C_k^t = \mu_k^2 = E[u_k^{t,1} u_k^{t,2}]$ and hence

$$C_k^t = \frac{\sigma^2_k (\Sigma^2_k C_s^t + \mu_k^2) + \nu_k^2 R \Sigma z_s + \rho_k^2}{Q_k^t - \mu_k^2}. \quad (4b)$$

(4c)

The variables $u_{k2i}^{t,1}$, $u_{k2i}^{t,2}$ given by 1b are also asymptotically Gaussian, with their covariance detailed in Appendix A for brevity of exposition. We conclude that

$$\left( \begin{array}{c} u_{k2i}^{t,1} \\ u_{k2i}^{t,2} \end{array} \right) \sim \mathcal{N} \left( \begin{array}{c} \mu_k \\ \Sigma_{k2} \end{array} \left( \begin{array}{cc} C_s^t & 1 \\ 1 & C_s^t \end{array} \right) \right)$$

and $u_{k2i}^{t,1}$, $u_{k2i}^{t,2}$ are distributed analogously with respect to $Q_{k2}, C_{k2}, \mu_{k2}$. We will subsequently drop the vector subscript $i$ since all elements are identically distributed and $f$, $g$, etc. act element-wise, and the input sequence index in expressions that involve only one sequence.

For any $l \leq t$, the $u_k^t$ are independent of $s^l$ at the large $N$ limit. Combining this with the fact that their distribution is determined completely by $\mu_s^{t-1}, Q_s^{t-1}, C_s^{t-1}$ and that $f$ is affine, one can rewrite eqn. (2) using eqn. (1) as the following deterministic dynamical system

$$(\mu_s^t, Q_s^t, C_s^t) = \mathcal{M}(\mu_s^{t-1}, Q_s^{t-1}, C_s^{t-1}, ..., \mu_s^{t}, Q_s^t, C_s^t)$$

(6)

where the dependence on $\Theta$ and the data distribution has been suppressed. In the peephole LSTM and GRU, the form will be greatly simplified to $\mathcal{M}(\mu_s^{t-1}, Q_s^{t-1}, C_s^{t-1})$.

In Appendix C we compare the predicted dynamics defined by eqn. (6) to simulations, showing good agreement.

One can now study the fixed points of eqn. (6) and the rate of convergence to these fixed points by linearizing around them. The fixed points are pathological, in the sense that any information that distinguishes two input sequences is lost upon convergence. Therefore, delaying the convergence to the fixed point should allow for signals to propagate across longer time horizons. Quantitatively, the rate of convergence to the fixed point gives an effective time scale for forward signal propagation in the network.

While the dynamical system is multidimensional and analysis of convergence rates should be performed by linearizing the full system and studying the smallest eigenvalue of the resulting matrix, in practice as in (Chen et al., 2018) this eigenvalue appears to always corresponds to the $C_s^t$ direction $\dagger$. Hence, if we assume convergence of $Q_s^t, \mu_s^t$ we need only linearize

$$C_s^t = \mathcal{M}(\mu_s^t, Q_s^t, C_s^{t-1})$$

(7)

where $\mathcal{M}_C$ also depends on expectations of functions of $\{u_k^t\}, ... \{u_k^{t-2}\}$ that do not depend on $C_s^{t-1}$. While this dependence is in principle on an infinite number of Gaussian variables as the dynamics approach the fixed point, $\mathcal{M}_C$ can still be reasonably approximated in the case of the LSTM as detailed in Section 4.5, while there is no such dependence for the peephole LSTM and GRU (See Table 1).

We study the dynamics approaching the fixed point by setting $C_s^t = C_s^* + \epsilon^t$ and writing

$$C_s^* + \epsilon^{t+1} = \mathcal{M}(\mu_s^t, Q_s^t, C_s^*) + \frac{\partial \mathcal{M}}{\partial C_s} \frac{d C_s}{d \epsilon} |_{C_s=C_s^*} \epsilon^t + O((\epsilon^t)^2)$$

and since $\mathcal{M}(\mu_s^t, Q_s^t, C_s^*) = C_s^*$,

$$\frac{\epsilon^{t+1}}{\epsilon^t} = \left[ \frac{\frac{\partial \mathcal{M}}{\partial C_s} \frac{d C_s}{d \epsilon}}{\frac{\partial \mathcal{M}}{\partial C_s} \frac{d C_s}{d \epsilon}} + \sum_k \frac{\partial \mathcal{M}}{\partial u_k} \frac{d u_k}{d \epsilon} \right]_{C_s=C_s^*} + O(1)$$

$$\equiv \chi C_s^*$$

(8)

We show that in the case of the peephole LSTM this map is convex in Appendix B. This can be shown for the GRU by a similar argument. It follows directly that it has a single stable fixed point in these cases.

The time scale of convergence to the fixed point is given by

$$\xi C_s^* = -\frac{1}{\log \chi C_s^*},$$

(9)

which diverges as $\chi C_s^*$ approaches 1 from below. Due to the detrimental effect of convergence to the fixed point described above, it stands to reason that a choice of $\Theta$ such that $\chi C_s^* = 1 - \delta$ for some small $\delta > 0$ would enable signals to propagate from the initial inputs to the final hidden state when training on long sequences.

### 4.3. Backwards signal propagation - the state-to-state Jacobian

We now turn to controlling the gradients of the network. A useful object to consider in this case is the asymptotic state-to-state transition Jacobian

$$J = \lim_{t \to \infty} \frac{\partial s^{t+1}}{\partial s^t}.$$

This matrix and powers of it will appear in the gradients of the output with respect to the weights as the dynamics...
approach the fixed point \((\text{specifically}, the\ \text{gradient of a network trained on a sequence of length } T \text{ will depend on a matrix polynomial of order } T \text{ in } J)\), hence we desire to control the squared singular value distribution of this matrix. The moments of the squared singular value distribution are given by the normalized traces

\[ m_{J JJ^T}, n = \tau((JJ^T)^n). \]

Since \(U_t, t' < t\) is independent of \(s^t, i\), if we index by \(k, k'\) the variables defined by eqn. (1a) and (1b) respectively we obtain

\[
J = \frac{\partial f}{\partial s_k} + \sum_{k'} \frac{\partial f}{\partial u_{k'}} W_k \left( D_g_{k'}(u_{k'}) + W_{k'} D_g_{k'}(u_{k'}) D_{s_k} \right).
\]

(10)

Under the untied assumption \(W_k, W_{k'}\) are independent of \(s^t, u^t\) at the large \(N\) limit, and are also independent of each other and their elements have mean zero. Using this and the fact that \(f\) acts element-wise, we have

\[ \tau(JJ^T) = \mathbb{E} \sum_{k \in K \cup \{0\}} a_k \] (11)

where

\[
a_k = \begin{cases} 
D_k^2 & k = 0 \\
\sigma_k^2 D_k^2 & \text{if } \mathbf{u}_k \text{ is given by (1a)} \\
\sigma_k^2 D_k^2 \left( \frac{g_k^2(u_k^t)}{\sigma_k^2} + \frac{g_k^2(u_k^t)}{\sigma_k^2} \right) & \text{if } \mathbf{u}_k \text{ is given by (1b)}
\end{cases}
\]

(12)

and \(D_0 = \frac{\partial f}{\partial s_k}, D_k = \frac{\partial f}{\partial u_{k'}}\). The values of \(D_0, D_k\) for the architectures considered in the paper are detailed in Appendix A. Forward and backward signal propagation are in fact intimately related, as the following lemma shows:

**Lemma 1.** For a recurrent neural networks defined by (1), the mean squared singular value of the state-to-state Jacobian defined in (11) and \(\chi C\), that determines the time scale of forward signal propagation (given by (8)) are related by

\[ m_{J JJ^T}, 1 = \chi C = 1, \Sigma_z = 1 \] (13)

**Proof.** See Appendix B. \(\Box\)

Controlling the first moment of \(J J^T\) is not sufficient to ensure that the gradients do not explode or vanish, since the variance of the singular values may still be large. This variance is a function of the first two moments and is given by

\[ \sigma_{JJ^T} = m_{J JJ^T}, 2 - m_{J JJ^T}, 1. \]

The second moment \(m_{J JJ^T}, 2\) can be calculated from (10), and is given by

\[ m_{J JJ^T}, 2 = \mathbb{E} \sum_{k,l \in K \cup \{0\}} 2a_k a_l - a_k^2 \] (14)

where the \(a_k\) are defined in (12). One could compute higher moments as well either explicitly or using tools from non-Hermitian random matrix theory.

### 4.4. Dynamical Isometry

The objective of the analysis is to ensure, at least approximately, that the following equations are satisfied simultaneously

\[ \chi C = 1 \] (15a)

\[ m_{J JJ^T}, 1 = 1 \] (15b)

\[ \sigma_{JJ^T} = 0. \] (15c)

We refer to these as dynamical isometry conditions. We demand that these equations are only satisfied approximately since for a given architecture, there may not be a value of \(\Theta\) that satisfies all the conditions. Additionally, even if such a value exists, the optimal value of \(\chi C\) for a given task may not be 1. There is some empirical evidence that if the characteristic time scale defined by \(\chi C\) is much larger than that required for a certain task, performance is degraded. In feed-forward networks as well, there is evidence that the optimal performance is achieved when the dynamical isometry conditions are only approximately satisfied (Pennington et al., 2017). Accounting for this observation is an open problem at present.

Convexity of the map (7) in the case of the peephole LSTM and GRU implies that for \(\Sigma = 1\), conditions (15a) and (15b) can only be satisfied simultaneously if \(C = 1\) (since (15b) implies \(dC/dC = 1\)).

For all the architectures considered in this paper, we find that \(D_0 = \sigma(u_k^t)\) while \(D_k\) are finite as \(\forall k : \sigma_k^2 \to 0\). Combining this with (11), (13), (14), we find that if \(\Sigma_z = 1\) the dynamical isometry conditions are satisfied if \(a_0 = 1, a_k \neq 0 = 0\), which can be achieved by setting \(\forall k : \sigma_k^2 = 0\) and taking \(\mu_f \to \infty\). This motivates the general form of the initializations used in Section 5.2

In the case of the peephole LSTM, since the \(\{u_k^t\}\) depend on the second moments of \(c_{t-1}\) and \(f\) is an affine function of \(c_{t-1}\), one can write a closed form expression for the dynamical system (6) in terms of first and second moments. In the standard LSTM however, the relevant state \(h^t\) depends on the cell state, which has non-trivial dynamics. The cell state differs substantially from other random variables that appear in this analysis since it cannot be expressed as a function of a finite number of variables that are Gaussian at the large \(N\) and \(t\) limit (see Table 1). Since

\[\text{In the case of the LSTM, we also want to prevent the output gate from taking very small values, as explained in Appendix A.2.}\]
that the density and even the likelihood have no closed
form from the stationary cell state distribution, despite the fact
In practice, one can overcome this difficulty by sampling
turn determines the distributions of $Y,Z$.

|Algorithm 1 LSTM hidden state moment fixed point iteration using cell state sampling |
|---|
|**FixedPointIteration**($\mu^{t-1}_s, Q^{t-1}_s, \Theta, n_s, n_{iters}$): |
| $Q^{t-1}_k \leftarrow \text{CalculateQK}(Q^{t-1}_k, \Theta)$ \{Using 4\} |
| Initialize $c \in \mathbb{R}^n$ |
| for $i \leftarrow 1$ to $n_{iters}$ do |
| $u_i, u_f, u_r \leftarrow \text{SampleUS}(Q^{t-1}_k, \Theta)$ \{Using 3\} |
| $c \leftarrow \text{UpdateC}(c, u_i, u_f, u_r)$ \{Using 16\} |
| end for |
| $(\mu^t_s, Q^t_s) \leftarrow \text{CalculateM}(\mu^{t-1}_s, Q^{t-1}_s, \Theta, c)$ \{Using 6\} |
| Return $(\mu^t_s, Q^t_s)$ |

at this limit the $u^t_i$ are independent, by examining the cell state update equation

$$c^t = \sigma(u^t_f) \circ c^{t-1} + \sigma(u^t_i) \circ \tanh(u^t_r)$$ \(16\)

we find that the asymptotic cell state distribution is that of a perpetuity, which is a random variable $X$ that obeys $X_d \sim XY + Z$ where $Y, Z$ are random variables and $d$ denotes equality in distribution. The stationary distributions of a perpetuity, if it exists, is known to exhibit heavy tails (Goldie, 1991). Aside from the tails, the bulk of the distribution can take a variety of different forms and can be highly multimodal, depending on the choice of $\Theta$ which in turn determines the distributions of $Y, Z$.

In practice, one can overcome this difficulty by sampling from the stationary cell state distribution, despite the fact that the density and even the likelihood have no closed form. For a given value of $Q_k$, the variables $u_k^t$ appearing in (16) can be sampled since their distribution is given by (5) at the large $N$ limit. The update equation (16) can then be iterated and the resulting samples approximate well the stationary cell state distribution for a range of different choices of $\Theta$, which result in a variety of stationary distribution profiles (see Appendix C3). The fixed points of (6) can then be calculated numerically as in the deterministic cases, yet care must be taken since the sampling introduces stochasticity into the process. An example of the fixed point iteration equation (6a) implemented using sampling is presented in Algorithm 1. The correlations between the hidden states can be calculated in a similar fashion. In practice, once the number of samples $n_s$ and sampling iterations $n_{iters}$ is of order 100 reasonably accurate values for the moment evolution and the convergence rates to the fixed point are obtained (see for instance the right panel of Figure 2). The computational cost of the sampling is linear in both $n_s, n_{iters}$ (as opposed to say simulating a neural network directly in which case the cost is quadratic in $n_s$).

5. Experiments

5.1. Corroboration of calculations

5.1.1. PADDED MNIST CLASSIFICATION

The calculations presented above predict a characteristic time scale $\xi$ (defined in (9)) for forward signal propagation in a recurrent network. It follows that on a task where success depends on propagation of information from the first time step to the final $T$-th time step, the network will not be trainable for $T \gg \xi$. In order to test this prediction, we consider a classification task where the inputs are sequences consisting of a single MNIST digit followed by $T - 1$ steps of i.i.d Gaussian noise and the targets are the digit labels. By scanning across certain directions in hyperparameter space, the predicted value of $\xi$ changes. We plot training accuracy of a network trained with untied weights after 1000 iterations for the GRU and 2000 for the LSTM, as a function of $T$ and the hyperparameter values, and overlay this with multiples of $\xi$. As seen in Figure 2, we observe
5.1.2. Squared Jacobian Spectrum Histograms

To verify the results of the calculation of the moments of the squared singular value distribution of the state-to-state Jacobian presented in Section 4.3 we run an untied peephole LSTM for 100 iterations with i.i.d. Gaussian inputs. We then compute the state-to-state Jacobian and calculate its spectrum. This can be used to compare the first two moments of the spectrum to the result of the calculation, as well as to observe the difference between a standard initialization and one close to satisfying the dynamical isometry conditions. The results are shown in Figure 3. The validity of this experiment rests on making an ergodicity assumption, since the calculated spectral properties require taking averages over realizations of random matrices, while in the experiment we instead calculate the moments by averaging over the eigenvalues of a single realization. The good agreement between the prediction and the empirical average suggests that the assumption is valid.

5.2. Long sequence tasks

One of the significant results of the calculation is that the results motivate critical initializations that dramatically improve the performance of recurrent networks on standard long sequence benchmarks, despite the fact that the calculation is performed using the untied assumption, at the large $N$ limit, and makes some rather unrealistic assumptions about the data distribution. The details of the initializations used are presented in Appendix C.

5.2.1. Unrolled MNIST and CIFAR-10

We unroll an MNIST digit into a sequence of length 786 and train a critically initialized peephole LSTM with 600 hidden units. We also train a critically initialized LSTM with hard sigmoid nonlinearities on unrolled CIFAR-10 images feeding in 3 pixels at every time step, resulting in sequences of length 1024. We also apply standard data augmentation for this task. We present accuracy on the test set in Table 2. Interestingly, in the case of CIFAR-10 the best performance is achieved by an initialization with a forward propagation time scale $\xi$ that is much smaller than the sequence length, suggesting that information sufficient for successful classification may be obtained from a subset of the sequence.

|                | MNIST | CIFAR-10 |
|----------------|-------|----------|
| standard LSTM  | 98.6  | 58.8     |
| h-detach LSTM  | 98.8  | -        |
| critical LSTM  | 98.9  | 61.8     |

Table 2. Test accuracy on unrolled MNIST and CIFAR-10.

5.2.2. Repeated Pixel MNIST and Multiple Digit MNIST

In order to generate longer sequence tasks, we modify the unrolled MNIST task by repeating every pixel a certain number of times and set the input dimension to 7. To create a more challenging task, we also combine this pixel repetition with concatenation of multiple MNIST digits (either 0 or 1), and label such sequences by a product of the original labels. In this case, we set the input dimension to 112 and repeat each pixel 10 times. We train a peephole LSTM with both a critical initialization and a standard initialization on both of these tasks using SGD with momentum. In this former task, the dimension of the label space is constant (and not exponential in the number of digits like in the latter). In both tasks, we observe three distinct phases. If the sequence length is relatively short the critical and standard initialization perform equivalently. As the sequence length is increased, training with a critical initialization is faster by orders of magnitude compared to the standard initialization. As the sequence length is increased further, training with a standard initialization fails, while training with a critical initialization still succeeds. The results are shown in Figure 4.

6. Discussion

In this work, we calculate time scales of signal propagation and moments of the state-to-state Jacobian at initialization for a number of important recurrent architectures. The cal-

\[^5\text{reproduced from (Arpit et al., 2018)}\]

\[^6\text{reproduced from (Trinh et al., 2018)}\]
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Figure 4. Training accuracy for unrolled, concatenated MNIST digits (top) and unrolled MNIST digits with replicated pixels (bottom) for different sequence lengths. Left: For shorter sequences the standard and critical initialization perform equivalently. Middle: As the sequence length is increased, training with a critical initialization is faster by orders of magnitude. Right: For very long sequence lengths, training with a standard initialization fails completely.

Another compelling issue is the persistence of the dynamical isometry conditions during training and their effect on the solution, for both feed-forward and recurrent architectures. Intriguingly, it has been recently shown that in the case of certain infinitely-wide MLPs, objects that are closely related to the correlations and moments of the Jacobian studied in this work are constant during training with full-batch gradient descent in the continuous time limit, and as a result the dynamics of learning take a simple form (Jacot et al., 2018). Understanding the finite width and learning rate corrections to such calculations could help extend the analysis of signal propagation at initialization to trained networks. This has the potential to improve the understanding of neural network training dynamics, convergence and ultimately perhaps generalization as well.

References

Allen-Zhu, Z., Li, Y., and Song, Z. A convergence theory for deep learning via over-parameterization. arXiv preprint arXiv:1811.03962, 2018.

Arpit, D., Kanuparthi, B., Kerg, G., Ke, N. R., Mitliagkas, I., and Bengio, Y. h-detach: Modifying the lstm gradient towards better optimization. arXiv preprint arXiv:1810.03023, 2018.

Bengio, Y., Simard, P., and Frasconi, P. Learning long-term
dependencies with gradient descent is difficult. *IEEE transactions on neural networks*, 5(2):157–166, 1994.

Chang, B., Chen, M., Haber, E., and Chi, E. H. AntisymmetricRNN: A dynamical system view on recurrent neural networks. In *International Conference on Learning Representations*, 2019. URL https://openreview.net/forum?id=ryxe0oCgFX.

Chen, M., Pennington, J., and Schoenholz, S. S. Dynamical isometry and a mean field theory of rnns: Gating enables signal propagation in recurrent neural networks. *arXiv preprint arXiv:1806.05394*, 2018.

Cho, K., van Merrienboer, B., Gulcehre, C., Bahdanau, D., Bougares, F., Schwenk, H., and Bengio, Y. Learning phrase representations using rnn encoder–decoder for statistical machine translation. In *Proceedings of the 2014 Conference on Empirical Methods in Natural Language Processing (EMNLP)*, pp. 1724–1734, 2014.

Du, S. S., Zhai, X., Poczos, B., and Singh, A. Gradient descent provably optimizes over-parameterized neural networks. *arXiv preprint arXiv:1810.02054*, 2018.

Gers, F. A., Schraudolph, N. N., and Schmidhuber, J. Learning precise timing with lstm recurrent networks. *Journal of machine learning research*, 3(Aug):115–143, 2002.

Glorot, X. and Bengio, Y. Understanding the difficulty of training deep feedforward neural networks. In *Proceedings of the thirteenth international conference on artificial intelligence and statistics*, pp. 249–256, 2010.

Goldie, C. M. Implicit renewal theory and tails of solutions of random equations. *The Annals of Applied Probability*, pp. 126–166, 1991.

Hochreiter, S. and Schmidhuber, J. Long short-term memory. *Neural computation*, 9(8):1735–1780, 1997.

Jacot, A., Gabriel, F., and Hongler, C. Neural tangent kernel: Convergence and generalization in neural networks. *arXiv preprint arXiv:1806.07572*, 2018.

Jose, C., Cissé, M., and Fleuret, F. Kronecker recurrent units. *arXiv preprint arXiv:1705.10142*, 2017.

Mei, S., Montanari, A., and Nguyen, P.-M. A mean field view of the landscape of two-layers neural networks. *arXiv preprint arXiv:1804.06561*, 2018.

Pascual, R., Mikolov, T., and Bengio, Y. On the difficulty of training recurrent neural networks. In *International Conference on Machine Learning*, pp. 1310–1318, 2013.

Pennington, J., Schoenholz, S., and Ganguli, S. Resurrecting the sigmoid in deep learning through dynamical isometry: theory and practice. In *Advances in neural information processing systems*, pp. 4785–4795, 2017.

Pennington, J., Schoenholz, S. S., and Ganguli, S. The emergence of spectral universality in deep networks. *arXiv preprint arXiv:1802.09979*, 2018.

Poole, B., Lahiri, S., Raghu, M., Sohl-Dickstein, J., and Ganguli, S. Exponential expressivity in deep neural networks through transient chaos. In *Advances in neural information processing systems*, pp. 3360–3368, 2016.

Saxe, A. M., McClelland, J. L., and Ganguli, S. Exact solutions to the nonlinear dynamics of learning in deep linear neural networks. *arXiv preprint arXiv:1312.6120*, 2013.

Schoenholz, S. S., Gilmer, J., Ganguli, S., and Sohl-Dickstein, J. Deep information propagation. *arXiv preprint arXiv:1611.01232*, 2016.

Trinh, T. H., Dai, A. M., Luong, T., and Le, Q. V. Learning longer-term dependencies in rnns with auxiliary losses. *arXiv preprint arXiv:1803.00144*, 2018.

Vorontsov, E., Trabelsi, C., Kadoury, S., and Pal, C. On orthogonality and learning recurrent networks with long term dependencies. In *International Conference on Machine Learning*, pp. 3570–3578, 2017.

Wisdom, S., Powers, T., Hershey, J., Le Roux, J., and Atlas, L. Full-capacity unitary recurrent neural networks. In *Advances in Neural Information Processing Systems*, pp. 4880–4888, 2016.

Xiao, L., Bahri, Y., Sohl-Dickstein, J., Schoenholz, S. S., and Pennington, J. Dynamical isometry and a mean field theory of cnns: How to train 10,000-layer vanilla convolutional neural networks. *arXiv preprint arXiv:1806.05393*, 2018.

Yang, G. and Schoenholz, S. Mean field residual networks: On the edge of chaos. In *Advances in neural information processing systems*, pp. 7103–7114, 2017.

Yang, G. and Schoenholz, S. S. Deep Mean Field Theory: Layerwise Variance and Width Variation as Methods to Control Gradient Explosion. *ICLR Workshop*, February 2018. URL https://openreview.net/forum?id=rJGY8Gbr-.00000.

Yang, G., Pennington, J., Rao, V., Sohl-Dickstein, J., and Schoenholz, S. S. A Mean Field Theory of Batch Normalization. In *International Conference on Learning Representations*, 2019. URL https://openreview.net/forum?id=SyMDXnCcF7.
Appendices

A. Details of Results

A.1. Covariances of \( u_{k_2} \)

The variables \( u_{k_2} \) are asymptotically Gaussian at the \( N \to \infty \), with

\[
Q_{k_2} = \sigma_{k_2}^2 \int g_k(u_a) D_k Q_s + \nu_{k_2}^2 R + \rho_{k_2}^2 + \mu_{k_2} \tag{17a}
\]

\[
C_{k_2}^t = \left( \frac{\sigma_{k_2}^2 \int g_k(u_a) g_k(u_a) D_k (\Sigma_s^2 C_s^t + \mu_s^2)}{Q_{k_2} - \mu_{k_2}^2} \right) \tag{17b}
\]

where \( D_k \) is a Gaussian measure on \((u_a, u_b)\) corresponding to the distribution in eqn. (3).

A.2. Dynamical isometry conditions for selected architectures

We specify the form of \( \chi_{C_s, \Sigma} \) and \( a \) for the architectures considered in this paper:

A.2.1. GRU

\[
\chi_{C_s, \Sigma} = \mathbb{E} \left[ \sigma(u_{fa}) \sigma(u_{fb}) + \sigma_f^2 \left( \tanh(u_{ra}) \tanh(u_{rb}) \right) \sigma'(u_{fa}) \sigma'(u_{fb}) \right. \\
+ \sigma_{r_2}^2 (1 - \sigma(u_{fa}))(1 - \sigma(u_{fb})) \tanh'(u_{ra}) \tanh'(u_{rb}) \left( \sigma(u_{ra}^*) \sigma(u_{rb}^*) \right) \\
\left. + \sigma_{r_1}^2 h_a^* h_b^* \sigma'(u_{ra})^* \sigma'(u_{rb})^* \right]
\]

\[
a = \begin{pmatrix}
\sigma^2(u_f^*) \\
\sigma_f^2 (\tanh^2(u_{r_2}^*) + Q_h^*) \sigma^2(u_f^*) \\
\sigma_{r_1}^2 \sigma_{r_2}^2 h_a^* h_b^* (1 - \sigma(u_f^*))^2 \tanh'^2(u_{r_2}^*) \sigma'^2(u_{r_1}^*) \\
\sigma_{r_2}^2 (1 - \sigma(u_f^*))^2 \tanh'^2(u_{r_2}^*) \sigma'^2(u_{r_1}^*)
\end{pmatrix}
\]

A.2.2. PEephole LSTM

\[
\chi_{C_s, \Sigma} = \mathbb{E} \left[ \sigma(u_{fa}) \sigma(u_{fb}) + \sigma_{f_1}^2 \sigma'(u_{fa}) \sigma'(u_{fb}) \tanh(u_{ra}) \tanh(u_{rb}) \right. \\
\left. + \sigma_{f_2}^2 C_a^* C_b^* \sigma'(u_{fa})^* \sigma'(u_{fb})^* + \sigma_{r}^2 \sigma(u_{ra}) \sigma(u_{rb}) \tanh'(u_{ra}) \tanh'(u_{rb}) \right]
\]

\[
a = \begin{pmatrix}
\sigma^2(u_f^*) \\
\sigma_{f_1}^2 \sigma'^2(u_f^*) \tanh^2(u_f^*) \\
\sigma_{f_2}^2 \sigma'^2(u_f^*) \\
\sigma_{r}^2 \sigma'^2(u_f^*) \tanh^2(u_f^*)
\end{pmatrix}
\]

A.2.3. LSTM

\[
\chi_{C_s, \Sigma} = \mathbb{E} \left[ \sigma(u_{fa}) \sigma(u_{fb}) + \sigma_{o_1}^2 \sigma'(u_{oa}) \sigma'(u_{ob}) \tanh(c_{a}^*) \tanh(c_{b}^*) \right. \\
\left. + \sigma(u_{oa}) \sigma(u_{ob}) \tanh'(c_{a}^*) \tanh'(c_{b}^*) \right]
\]

\[
a = \begin{pmatrix}
\sigma^2(u_f^*) \\
\sigma_{o_1}^2 \sigma'(u_{oa}) \sigma'(u_{ob}) \tanh'(c_{oa}^*) \tanh'(c_{oa}^*) \\
\sigma_{o_2}^2 C_a^* C_b^* \sigma'(u_{fa}) \sigma'(u_{fb})^* \\
\sigma_{r}^2 \sigma(u_{ra}) \sigma(u_{rb}) \tanh'(u_{ra}) \tanh'(u_{rb}) \right)
\]

\]

\[
+ \sigma_{o_2}^2 \sigma'(u_{oa}) \sigma'(u_{oa}) \tanh(u_{ra}) \tanh(u_{rb}) \\
+ \sigma_{o_1}^2 \sigma(u_{oa}) \sigma(u_{ob}) \tanh'(u_{ra}) \tanh'(u_{rb})
\end{pmatrix}
\]
When evaluating 8 in this case, we write the cell state as $c' = \tanh^{-1} \left( \frac{s^t}{\sigma(\sigma')^2} \right)$, and assume $\frac{\sigma(\sigma')}{\sigma(\sigma')^2} \approx 1$ for large $t$. The stability of the first equation and the accuracy of the second approximation are improved if $o'$ is not concentrated around 0.

B. Auxiliary Lemmas and Proofs

**Proof of Lemma 1.** Despite the fact that each $u_{ka}$ as defined in 1 depends in principle upon the entire state vector $s_a$, at the large $N$ limit due to the isotropy of the input distribution we find that these random variables are i.i.d. and independent of the state. Combining this with the fact that $f$ is an element-wise function, it suffices to analyse a single entry of $s^t = f(s^{t-1}, \{u^*_k\}, \ldots, \{u^*_k\})$, which at the large $t$ limit gives

$$
\mathcal{M}_C(\mu^*_s, Q^*_s, C_s) = \frac{\mathbb{E} [f(s_a, U^*_a) f(s_b, U^*_b)] - (\mu^*_s)^2}{Q^*_s - (\mu^*_s)^2}
$$

where $U^*_a = \{u^*_{ka} | k \in K, u^*_ka \sim \mathcal{N}(\mu_k, Q^*_k - \mu_k^2)\}$ and $U^*_b$ is defined similarly (i.e. we assume the first two moments have converged but the correlations between the sequences have not, and in cases where $f$ depends on a sequence of $\{u^*_k\}, \ldots, \{u^*_k\}$ we assume the constituent variables have all converged in this way). We represent $u^*_{ka}, u^*_{kb}$ via a Cholesky decomposition as

$$
u^*_{ka} = \Sigma_k z_{ka} + \mu_k^* \tag{18a}$$
$$u^*_{kb} = \Sigma_k \left( C_k^* z_{ka} + \sqrt{1 - (C_k^*)^2 z_{kb}} \right) + \mu_k^* \tag{18b}$$

where $z_{ka}, z_{kb} \sim \mathcal{N}(0, 1)$ i.i.d. We thus have $\frac{\partial u^*_{kb}}{\partial C_k} = \sqrt{Q_k^* - (\mu_k^*)^2} \left( z_{ka} - \frac{C_k}{\sqrt{1 - (C_k^*)^2}} z_{kb} \right)$. Combining this with the fact that $\int Dz g(z) z = \int Dz g'(z)$ for any $g(z)$, integration by parts gives for any $g_1, g_2$

$$
\frac{\partial}{\partial C_k} \int Dz_k Dz_k g_1(u^*_{ka}) g_2(u^*_{kb})
= \int Dz_k Dz_k g_1(u^*_{ka}) \left( \frac{\partial g_2(u^*_{kb})}{\partial u^*_{kb}} \right) \frac{\partial u^*_{kb}}{\partial C_k}
= \Sigma_k^2 \int Dz_k Dz_k \frac{\partial g_1(u^*_{ka})}{\partial u^*_{ka}} \frac{\partial g_2(u^*_{kb})}{\partial u^*_{kb}} \tag{19}
$$

Denoting $\Sigma_k^2 = Q_k^* - (\mu_k^*)^2$ and defining $\Sigma_k, \Sigma_{k_2}$ similarly, we have

$$
\frac{dC_{ka}}{dC_s} = \frac{\Sigma_{ka}^2}{\Sigma_k^2} \tag{20}
$$
Proof of Lemma 2.

For any odd function \(g(x)\), \(\begin{pmatrix} x \\ y \end{pmatrix} \sim \mathcal{N} \left( \begin{pmatrix} \mu \\ 1 \end{pmatrix}, \Sigma \begin{pmatrix} C & 1 \\ 1 & 1 \end{pmatrix} \right)\), \(0 \leq C \leq 1\) we have \(\mathbb{E}g(x)g(y) \geq 0\).

**Proof of Lemma 2.** For \(C = 1\) the proof is trivial. We now assume \(0 \leq C < 1\). We split up \(\mathbb{R}^2\) into four orthants and consider a point \((a, b)\) with \(a, b \geq 0\). We have \(g(a)g(b) = g(-a)g(-b) = -g(a)g(-b) = -g(-a)g(b) \geq 0\). We will show that \(p(a, b) + p(-a, -b) > p(a, -b) + p(-a, b)\) where \(p\) is the probability density function of \((x, y)\) and hence the points where the integrand is positive will contribute more to the integral than the ones where it is negative. Plugging these points into \(p(x, y)\) gives

\[
\frac{p(a, b) + p(-a, -b)}{p(a, -b) + p(-a, b)} = \frac{e^{-\alpha(a+\mu)^2 - 2C(a+\mu)(b+\mu) + (b+\mu)^2}}{e^{-\alpha(a+\mu)^2 - 2C(b+\mu)(a+\mu) + (b+\mu)^2}} + e^{-\alpha(a+\mu)^2 + 2C(b+\mu)(a+\mu) + (b+\mu)^2}
\]

where \(\alpha\) is some positive constant that depends on the determinant of the covariance (since \(C < 1\) the matrix is invertible and the determinant is positive).
where the last inequality holds for $0 \leq C < 1$. It follows that the positive contribution to the integral is larger than the negative one, and repeating this argument for every $(a, b)$ in the positive orthant gives the desired claim (if $a = 0$ or $b = 0$ the four points in the analysis are not distinct but the inequality still holds and the integrand vanishes in any case).

**Lemma 3.** The map $6$ is convex in the case of the peephole LSTM.

**Proof of Lemma 3.** We have

$$
\mathcal{M}(C_t^t) = \int f_t^t f_t^t ( (Q_c^t - (\mu_c^t)^2) C_c^t + \mu_c^t) + \int i_t^t i_t^t r_t^t r_t^t + 2 \int f_t^t \int r_t^t \mu_c^t - \mu_c^t
$$

From the definition of $u_{kb}^t$ and $C_k^t$ we have

$$
\frac{\partial u_{kb}^t}{\partial C_k^t} = \sqrt{Q_k^t - (\mu_k^t)^2} \left( z_{ka} - \frac{C_k^t}{\sqrt{1 - C_k^t}} z_{kb} \right)
$$

and using $\int D x g(x) x = \int D x g'(x)$ we then obtain for any $g(x)$

$$
\frac{\partial}{\partial C_k^t} \int \mathcal{D} z_{ka} \mathcal{D} z_{kb} g(u_{ka}^t) g(u_{kb}^t) = \int \mathcal{D} z_{ka} \mathcal{D} z_{kb} g(u_{ka}^t) g'(u_{kb}^t) \frac{\partial u_{kb}^t}{\partial C_k^t} = \sigma_k^2 (Q_c^t - \mu_c^t)
$$

(21)

$$(Q_c^t - \mu_c^t) \frac{\partial^2 \mathcal{M}(C_c)}{\partial C_c^2} = \frac{\partial^2}{\partial C_c^2} \left[ \int f_a f_b ((Q_c^t - (\mu_c^t)^2) C_c + \mu_c^t) + \int i_a i_b \int r_a r_b \right]
$$

$$
= \frac{\partial^2}{\partial C_c^2} \int f_a f_b ((Q_c^t - (\mu_c^t)^2) C_c + \mu_c^t) + 2 \frac{\partial}{\partial C_c} \int f_a f_b (Q_c^t - (\mu_c^t)^2)
$$

$$
+ \frac{\partial^2}{\partial C_c^2} \int r_a r_b + \frac{\partial}{\partial C_c} \frac{\partial}{\partial C_c} \int r_a r_b + \frac{\partial^2}{\partial C_c^2} \int r_a r_b
$$

From 21 and non-negativity of some of the integrands

$$
\geq \frac{\partial^2}{\partial C_c^2} \int f_a f_b ((Q_c^t - (\mu_c^t)^2) C_c + \mu_c^t) + \frac{\partial^2}{\partial C_c^2} \int r_a r_b + \int i_a i_b \frac{\partial^2}{\partial C_c^2} \int r_a r_b
$$

From Lemma 2 we have $\int r_a r_b \geq 0$ and $\frac{\partial^2}{\partial C_c^2} \int g_a g_b = \alpha \int g_a g_b \geq 0$ for $g = f, i, r$. We thus have

$$
\frac{\partial^2 \mathcal{M}(C_c)}{\partial C_c^2} \geq 0
$$
for $0 \leq C_c \leq 1$.

Convexity of this map has a number of consequences. One immediate one is that the map has at most one stable fixed point.

C. Additional Experiments and Details of Experiments

C.1. Dynamical system

We simulate the dynamics of 14b for a GRU using inputs with $\Sigma_z^t = 0$ for $t < 10$ and $\Sigma_z^t = 1$ for $t \geq 10$. The results show good agreement in the untied case between the calculation at the large $N$ limit and the simulation, as shown in Figure 5.

![Figure 5. Top: Dynamics of the correlation 6b for the GRU with 3 different values of $\mu_f$ as a function of time. The dashed line is the prediction from the mean field calculation, while the red curves are from a simulation of the network with i.i.d. Gaussian inputs. Left: Network with untied weights. Right: Network with tied weights. Bottom: The predicted fixed point of 6b as a function of different $\mu_f$. Left: Network with untied weights. Right: Network with tied weights.](image)

C.2. Heatmaps

In Figure 6 we present results of training on the same task shown in Figure 2 with tied weights, showing the deviations resulting from the violation of the untied weights assumption.

C.3. Sampling the LSTM cell state distribution

As described in Section 4.5, calculating the signal propagation time scale and the moments of the state-to-state Jacobian for the LSTM requires integrating with respect to the stationary cell state distribution. The method for doing this is described in Algorithm 1. As is shown in Figure 7, this distribution can take different forms based on the choice of initialization hyperparameters $\Theta$, but in all cases we have studied the proposed algorithm appears to provide a reasonable approximation to this distribution efficiently. The simulations are obtained by feeding a network of width $N = 200$ with i.i.d. Gaussian
Figure 6. Training accuracy on the padded MNIST classification task described in 5.1.1 at different sequence lengths $T$ and hyperparameter values $\Theta$ for networks with tied weights. The green curves are multiples of the forward propagation time scale $\xi$ calculated under the untied assumption. We generally observe improved performance when the predicted value of $\xi$ is high, yet the behavior of the network with tied weights is not part of the scope of the current analysis and deviations from the prediction are indeed observed.

Figure 7. Sampling from the LSTM cell state distribution using Algorithm 1, showing good agreement with the cell state distribution obtained by simulating a network with untied weights. The two panels correspond to two different choices of $\Theta$ inputs.

C.4. Critical initializations

Peephole LSTM:

$$\mu_i, \mu_r, \mu_o, \rho_i^2, \rho_f^2, \rho_r^2, \nu_i^2, \nu_f^2, \nu_o^2 = 0$$

$$\mu_f = 5$$

$$\sigma_i^2, \sigma_f^2, \sigma_r^2, \sigma_o^2 = 10^{-5}$$

LSTM (Unrolled CIFAR-10 task):

$$\mu_i, \mu_r, \mu_o, \rho_i^2, \rho_f^2, \rho_r^2, \nu_i^2, \nu_f^2, \nu_o^2 = 0$$

$$\nu_i^2, \nu_r^2, \sigma_o^2, \mu_f = 1$$

$$\sigma_i^2, \sigma_f^2, \sigma_r^2 = 10^{-5}$$

C.5. Standard initialization

LSTM and peephole LSTM:

Kernel matrices (corresponding to the choice of $\nu_k^2$): Glorot uniform initialization (Glorot & Bengio, 2010)
Recurrent matrices (corresponding to the choice of $\sigma^2_k$): Orthogonal initialization (i.i.d. Gaussian initialization with variance $1/N$ also used giving analogous performance)

$$\mu_i, \mu_r, \mu_o, \rho_i^2, \rho_f^2, \rho_r^2, \rho_o^2 = 0$$

$$\mu_f = 1$$

C.5.1. Long sequence tasks

Learning rate scan: 8 equally spaced points between $10^{-2}$ and $10^{-5}$. 