Exact information propagation through fully-connected feed forward neural networks

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Abstract

Neural network ensembles at initialisation give rise to the trainability and training speed of neural networks and thus support parameter choices at initialisation. These insights rely so far on mean field approximations that assume infinite layer width and study average squared signals. Thus, information about the full output distribution gets lost. Therefore, we derive the output distribution exactly (without mean field assumptions), for fully-connected networks with Gaussian weights and biases. The layer-wise transition of the signal distribution is guided by a linear integral operator, whose kernel has a closed form solution in case of rectified linear units for nonlinear activations. This enables us to analyze some of its spectral properties, for instance, the shape of the stationary distribution for different parameter choices and the dynamics of signal propagation.

1 Introduction

Deciding about the architecture before training neural networks is a big challenge. For fully-connected (Poole et al., 2016; Raghu et al., 2016; Schoenholz et al., 2017) and residual networks (Yang and Schoenholz, 2017), it has been shown that ensembles of random initialised networks are indicative of the trainability of an architecture. Specifically, the training success relates to the quality of mean field average information propagation. This insight has been used to determine two parameters: the variance of the bias and weight distribution at initialisation. They are chosen at the edge of chaos to guaranty enough expressivity of the networks and, at the same time, to avoid gradient explosion or vanishing. This way, the average eigenvalue of the signal input-output Jacobian in mean field neural networks is steered towards 1. Furthermore, a high concentration of the full spectral density of the Jacobian close to 1 seems to support higher training speeds (Pennington et al., 2017a,b). This property is referred to as dynamic isometry.

Despite their successful application in practice, rectified linear units (ReLUs) do not posses this property in conjunction with Gaussian weight initialisation (Pennington et al., 2017a). Yet, the results so far rely on mean field approximations that assume layers of infinite widths and draw conclusions about average squared signals at criticality. Thus, distribution information gets lost that could contain further hints about good initialisations. For instance, it might be indicative also of the variance of accuracies achieved after training. In addition, ReLUs achieve high expressivity already at small depths. Thus, good trainability might be reached (also for non-critical parameters) before the output signal distribution converges to a stationary distribution. Furthermore, the criterion to obtain the critical values for the variances seems less important for small depths, since the increase or decrease of signal norms stays within limited boundaries.

To extend the analysis of signal propagation properties of fully-connected network ensembles at initialisation with Gaussian weights and biases, we therefore derive exact equations for the output
signal distribution (which does not require mean field approximations). For general nonlinear activations, we find a linear transition operator that advances the signal distribution layer-wise. In case of ReLUs, we give an explicit formula for the corresponding integral kernel, which allows us to analyse some of its spectral properties and derive the shape of the stationary distribution. Interestingly, this distribution depends on the number of neurons in a layer. We show, how we can choose the shape of the stationary output signal distribution by the choice of weight variance. This enables us to also explore alternative parameters that lead to stationary distributions that are independent of the layer width. We compare the trainability of the corresponding network ensembles in experiments on MNIST.

2 Background and notation

We study fully-connected deep neural networks consisting of $L$ layers in addition to an input layer ($l = 0$). Each layer $l = 0, \ldots, L$ has $N_l$ neurons that are associated with components of a signal vector $\mathbf{x}^{(l)}$ and are connected with all neurons of the previous layer. These connections govern the signal propagation through the network, which is as usual defined by the following equations:

$$\mathbf{x}^{(l)} = \phi \left( \mathbf{h}^{(l)} \right), \quad \mathbf{h}^{(l)} = \mathbf{W}^{(l)} \mathbf{x}^{(l-1)} + \mathbf{b}^{(l)}$$

$$x_i^{(l)} = \phi \left( h_i^{(l)} \right), \quad h_i^{(l)} = \sum_{j=1}^{N_{l-1}} w_{ij}^{(l)} x_j^{(l-1)} + b_i^{(l)} \quad \text{for} \ l = 1, \ldots, L$$

where $\mathbf{h}^{(l)}$ is a pre-activation at layer $l$, $\mathbf{W}^{(l)}$ is a weight matrix, $\mathbf{b}^{(l)}$ is a bias vector, and $\phi$ is a nonlinear activation function. If not indicated otherwise, 1-dimensional functions are applied to vectors componentwise. To ease notation, we follow the convention to suppress the superscript $(l)$ and write, for instance, $x_i$ instead of $x_i^{(l)}$, $x_i$ instead of $x_i^{(l-1)}$, and $x_i$ instead of $x_i^{(l+1)}$, when the layer reference is clear from the context.

The challenge for practitioners is to decide a priori about the network architecture, i.e. the activation functions, the depth $L$ and the layer widths $N_l$. Then, also the parameters, i.e. the weights and biases, have to be initialized before training. A standard approach is to draw them independently at random from Gaussian distributions with zero mean. We assume that the weights in the same layer follow a distribution with the same standard deviation $\sigma_w^{(l)}$ and the biases with $\sigma_b^{(l)}$ (but usually drop the index $l$). Thus, we have initially: $w_{ij}^{(l)} \sim \mathcal{N} \left( 0, \sigma_w^{2} \right)$, $b_i^{(l)} \sim \mathcal{N} \left( 0, \sigma_b^{2} \right)$. This creates an ensemble of possible initial network configurations, where each configuration maps inputs $\mathbf{x}^{(0)}$ to outputs $\mathbf{x}^{(L)}$. This ensemble also includes the resulting network after training. Ideally, the initialized network is close to this target with high probability and can be reached fast in a small number of training steps.

The idea is to relate the architecture and parameter choice to properties of the initial network ensemble, for instance, how well it propagates signal (which is usually data independent). In practice, its trainability also depends on the task and data at hand, the training method, etc. and more configurations might lead to good or better results. Ensuring a priori good signal propagation properties of network ensembles can still provide orientation in parameter search and give insights into the general properties of deep neural networks. Several approaches in this spirit (Poole et al. 2016; Raghu et al. 2016; Schoenholz et al. 2017) have demonstrated a strong correspondence between training success and quality of mean field average information propagation. Correlations between signals corresponding to different initial inputs should not be perfectly preserved to ensure expressive power of a network ensemble. But they should also not be so chaotic that correlated signals become independent during propagation through layers. This is realized by a choice of parameters at the edge of chaos, where the average cosine difference between two signals corresponding to different inputs converges to a stable fixed point $1$. The convergence is even exponentially fast in depth. These dynamics are also linked to backpropagation so that gradients neither explode nor vanish with the right choice of parameters (Poole et al. 2016). According to this analysis, ReLUs in conjunction with zero mean Gaussian weights and biases have only one pair of critical parameters: $\sigma_b = 0$ and $\sigma_w = \sqrt{2/N_l}$. Those avoid exploding signal lengths (Glorot and Bengio 2010).

But they do not lead to dynamic isometry (Pennington et al. 2017a), i.e. the average spectrum of the input-output Jacobian is not concentrated around $1$ for higher depths and infinite width. Yet they lead
to network ensembles of high expressivity, as squared input signals converge exponentially fast to a fixed point so that only small depths are necessary. For such small depths, networks might still be well trainable for parameters different from the critical ones, as gradients and signal norms can be allowed to increase or decrease slightly for a small number of layers.

Our goal is to derive tools for analysis that relax the mean field assumptions and allow, in particular, for a more refined analysis of ReLUs. Specifically, we study which signal distribution properties provide a good environment for training success. For this purpose, we derive the layer-wise linear signal propagation operator. The final linear operator that maps an input distribution to the output distribution can be interpreted as Jacobian of the dynamics. We conjecture that its spectral properties could be even more indicative of trainability than the average spectrum of the input-output signal Jacobian as studied with the help of random matrix theory [Pennington et al., 2017a,b].

3 Theoretical results

In the remainder of this work, we focus on the analysis of fully-connected neural network ensembles with zero mean Gaussian weights. We thus make the following assumption.

Assumptions 1. An ensemble \( \{G\}_{D,N_l,\sigma,\sigma_w} \) of fully-connected feed forward neural networks consists of networks with depths \( L \), layer widths \( N_l \), \( l = 0, \ldots , L \), independently normally distributed weights and biases with \( w_{ij}^{(l)} \sim N(0, \sigma^2_w), b_i^{(l)} \sim N(0, \sigma^2_b) \), and non-decreasing activation function \( \phi : \mathbb{R} \rightarrow \mathbb{R} \).

Our main goal is to determine the output distribution of signals that propagate through such a neural network ensemble. In the following, we collect our insights in theorems. Their proofs can be found in the supplementary material.

3.1 Signal propagation for single inputs

In a mean field approach, the average squared signal norm would be propagated from layer to layer in a network of infinite width. Interestingly, the squared signal is exactly the variable that determines the distribution of an output signal component. To see this, let’s assume that the output signal \( x \) of the previous layer is given. Each pre-activation component \( h_i \) of the current layer is then normally distributed as \( h_i = \sum_{j=1}^{N_l} w_{ij} z_j + b_i \sim N\left(0, \sum_j \sigma^2_w \sigma^2_j + \sigma^2_b\right) \), since the weights and bias are independently normally distributed with zero mean. The non-linear transformation \( x_i = \phi(h_i) \) is then distributed as \( x_i \sim \Phi\left(\frac{\phi^{-1}(1)}{\sigma_i}\right) \), where \( \phi^{-1} \) denotes the generalized inverse of \( \phi \). \( \Phi \) is the cumulative distribution function (cdf) of the Standard normal, and \( \sigma^2 = \sigma^2_w |x|^2 + \sigma^2_b \). Thus, we only need to know the distribution of \( |x|^2 \) as input to compute the distribution of \( x_i \). The signal propagation is thus reduced to a 1-dimensional problem.

Theorem 1. Additionally to Assumption 1, we assume that the probability density \( p_0(z) \) of the squared input \( |x(0)|^2 = \sum_{i=1}^{N_0} x_i(0)^2 \) is known. Then, the distribution \( p_l(z) \) of the squared signal vector \( |x(l)|^2 \) depends only on the distribution of the previous layer as transformation by a linear operator \( T_l : L^1(\mathbb{R}_+) \rightarrow L^1(\mathbb{R}_+) \) so that \( p_l = T_l(p_{l-1}) \). \( T \) is defined as

\[
T_l(p)[z] = \int_0^\infty k_l(y, z)p(y) \, dy,
\]

where \( k_l(y, z) \) is the distribution of the squared signal \( z \) at layer \( l \) given the squared signal at the previous layer \( y \) so that \( k_l(y, z) = p_{\ast\ast}(h_y, z) \), where \( \ast \ast \) stands for convolution and \( p_{\phi(h_y)}(z) \) denotes the distribution of the transformed pre-activation \( h_y \), which is normally distributed as \( h_y \sim N\left(0, \sigma^2_w y^2 + \sigma^2_b\right) \). This distribution serves to compute the cumulative distribution function (cdf) of each signal component \( x_i \) as

\[
F_{x(i)}(x) = \int_0^\infty dz \, p_{l-1}(z)\Phi\left(\frac{\phi^{-1}(x)}{\sqrt{\sigma^2_w z + \sigma^2_b}}\right),
\]

(2)
Consequently, the expectation of the final squared signal norm depends on the initial input as:

$$F_{x_1^{(l)}, \ldots, x_{N_l}^{(l)}}(x) = \int_0^\infty dz \ p_{l-1}(z) \prod_{i=1}^{N_l} \Phi \left( \frac{x_i}{\sigma_z} \right),$$

(3)

where we use the abbreviation $\sigma_z = \sqrt{\sigma_w^2 \sigma_y^2 + \sigma_b^2}$.

First, we note the radial symmetry of the output distribution. It only depends on the squared norm of the input. For images, this would correspond to the pixel density. Further properties of the data cannot inform initialisation schemes that are solely based on the output distribution above.

Otherwise, the linear operators $T_i$ govern this distribution. Since $p_{\mathbf{x}(L)} = \prod_{l=1}^{L} T_l p_{\mathbf{x}(0)}$, the operator $\prod_{l=1}^{L} T_l$ can also be interpreted as the Jacobian corresponding to the function that maps the input distribution to the output distribution. Its spectral properties might be even more indicative of training speeds than the average spectrum of the input output signal Jacobian that is analyzed by random matrix theory approaches [Pennington et al., 2017a,b]. Note that the operators $T_i$ are identical for identical widths $N_l = N$. For any nonlinear activation function, $T_i$ can be approximated numerically on an equidistant grid. The convolution in the kernel definition can be computed efficiently with the help of Fast Fourier Transformations and the eigenvalues of the matrix approximating $T_i$ give rise to the dynamics of signal propagation. Specifically for rectified linear units (ReLUs), we can even derive a closed form solution for the integral kernel $k_i(y, z)$ of $T_i$ and derive some of its spectral properties. This allows us to reason about the shape of the stationary distribution of $T_i$, i.e. the limit output distribution for networks with increasing depth.

### 3.1.1 Rectified Linear Units (ReLUs)

For rectified linear units (ReLUs), i.e. $\phi(x) = \max(x, 0)$, Theorem 1 can be further advanced.

**Theorem 2.** For rectified linear units, the linear operator $T$ in Theorem 1 is defined by

$$k_i(y, z) = 0.5 N_l \left( \delta_0(z) + \sum_{k=1}^{N_l} \frac{N_l}{k} p_{x_k^2} \left( \frac{z - y}{\sigma_y^2} \right) \right)$$

(4)

with $\sigma_y = \sqrt{\sigma_w^2 y + \sigma_b^2}$. For $\sigma_b = 0$, the functions $f_m(y) = y^m \mathbf{1}_{[0, \infty)}(y)$ are eigenfunctions of $T_i$ for any $m \in \mathbb{R}$ (even though they are not elements of $L^1(\mathbb{R}^+)$ and thus not normalizable as probability measures) with corresponding eigenvalue $\lambda_{l,m} \in \mathbb{R}$:

$$T_i f_m = \lambda_{l,m} f_m \quad \text{with} \quad \lambda_{l,m} = 0.5 N_l^{m-1} \sum_{k=1}^{N_l} \left( \frac{N_l}{k} \right) \frac{\Gamma(k/2 - m - 1)}{\Gamma(k/2)}$$

(5)

For $\sigma_b \neq 0$, we found numerical cases in which no stationary distribution exists. According to mean field analysis, we would enter the chaotic regime. Yet, also the eigenfunctions for $\sigma_b = 0$ are not normalizable on $\mathbb{R}^+$. For $m < -1$, the antiderivative diverges in zero. Yet, when we discretize $T$ in numerical experiments, they can be normalized and the real eigenvectors representing probability distributions attain shapes $x^m$. Interestingly, with the choice of $\sigma^{(l)}_w$, we define the exponent $m$ of the eigenfunction corresponding to eigenvalue 1 and thus the shape of the output distribution that we expect after propagation through deep networks. Before we analyse the spectrum closer for different choices of $\sigma^{(l)}_w$, we first determine interesting choices based on average properties of the output signal distribution.

**Theorem 3.** For rectified linear units, the expectation value of the squared signal conditional on the squared signal of the previous layer is given by:

$$\mathbb{E} \left( |x^{(l)}|^2 | x^{(l-1)} = y \right) = (\sigma_w^2 y + \sigma_b^2) \frac{N_l}{2}.$$  

(6)

Consequently, the expectation of the final squared signal norm depends on the initial input as:

$$\mathbb{E} \left( |x^{(L)}|^2 | x^{(0)} = y \right) = |x^{(0)}|^2 \prod_{l=1}^{L} \frac{N_l \sigma_w^2}{2} + \sigma_b^2 \frac{N_l}{2} + \sum_{l=1}^{L} \sigma_b^2 \frac{N_l}{2} \prod_{n=l+1}^{L} \frac{N_n \sigma_w^2}{2}$$  

(7)
The expectation value and variance of a single signal component conditional on the squared signal norm of the previous layer are given by:

\[
E(x_i | |x|^2 = y) = \frac{1}{\sqrt{2\pi}} \sqrt{\sigma_w^2 + \sigma_b^2},
\]

\[
\text{Var}(x_i | |x|^2 = y) = \frac{\pi - 1}{2\pi} (\sigma_w^2 + \sigma_b^2).
\]

The last layer depends on the input as:

\[
E(x_i^{(L)} | x^{(0)}) \leq \frac{1}{\sqrt{2\pi}} \left[ |x^{(0)}|^2 \Pi_{l=1}^{L-1} \frac{N_l \sigma_{w,l}^2}{2} \sigma_{w,L}^2 \right. \\
\left. + \sigma_{w,L}^2 \left( \sigma_{w,L-1}^2 \frac{N_{L-1}}{2} + \sum_{i=1}^{L-1} \sigma_{b,l}^2 \frac{N_i \sigma_{w,l}}{2} \right) \right]^{1/2},
\]

\[
\text{Var}(x_i^{(L)} | x^{(0)}) = |x^{(0)}|^2 \frac{\pi - 1}{2\pi} \sigma_{w,L}^2 \Pi_{l=1}^{L-1} N_l \sigma_{w,l}^2 \\
\left. + \frac{\pi - 1}{2\pi} \left( \sigma_{w,L}^2 \left( \sigma_{w,L-1}^2 \frac{N_{L-1}}{2} + \sum_{i=1}^{L-1} \sigma_{b,l}^2 \frac{N_i \sigma_{w,l}}{2} \right) \right) \right]^{1/2}.
\]

A straightforward way to preserve the average squared signal or the squared output signal norm distribution, would be \( \sigma_b^{(l)} = 0 \) and \( \sigma_w^{(l)} = \sqrt{2/N_l} \). These are the known critical values provided by mean field analysis. While they preserve signal variance in forward propagation, they also avoid gradient explosion in back-propagation. An example is provided by Figure 1 for 9 layers each consisting of \( N_l = 200 \) neurons whose weight parameters have critical standard deviation. The variance is indeed preserved, while the average decreases for increasing depths. Yet, also different parameter choices could preserve the variance and might even preserve the average.

For instance, any arbitrary choice of the variances in the first layers can be compensated by the variance of the last layer. Furthermore, for networks of limited depths, we might not need to enforce strict average preservation. As long as the range of the output distribution stays within reasonable limits, training should not be hampered by exploding gradients. Alternatively, also the variance of the input distribution could be preserved instead of the average squared signal. Then, the choice of \( \sigma_b > 0 \) would become data dependent and not support a stationary signal distribution.

At which depth \( l \) a stationary distribution \( x^m \) is reached by layer-wise signal propagation so that \( T^l x^m \approx x^m \) is determined by the spectrum of \( T \). Figure 2 visualizes the general shape of the spectrum. For \( m = -1 \), the corresponding eigenvalue is independent of \( \sigma_w \) and given by \( \lambda = 1 - 0.5^N \). Thus, it approaches \( \lambda = 1 \) for an increasing number of neurons in a layer. Yet, there always exists another exponent \( m_{\text{crit}} \), for which \( \lambda = 1 \) holds exactly. This exponent depends on \( N_l \) and \( \sigma_w \) however. \( m_{\text{crit}} \) decreases with increasing \( N \) or decreasing \( \sigma_w \). For \( m_{\text{crit}} < m < -1 \), the corresponding eigenvalues are smaller than 1. For \( m < m_{\text{crit}} \), the eigenvalues increase rapidly so that \( x^m \) is not attractive for \( m < m_{\text{crit}} \).

These insights become especially relevant when layers of different widths are considered, for instance in case of autoencoders. Then signal operators have different stationary distributions at criticality.

Figure 1: Squared signal norm distribution at different depths for \( N_l = 200 \) and variance preserving \( \sigma_w = 0.1 \), \( \sigma_b = 0 \) for ReLUs. The initial distribution \( (L = 0) \) is defined by the MNIST dataset.
\( \sigma_w^{(l)} = \sqrt{2/N_l} \). The product of their eigenvalues needs to be 1 to determine the exponent \( m_{\text{crit}} \) corresponding to the stationary distribution. Neither of the two factors has to be critical to achieve this result.

Interestingly, the critical point is defined by \( m_{\text{crit}} \) for finite networks. Specifically, for the variance preserving values \( \sigma_b^{(l)} = 0 \) and \( \sigma_w = \sqrt{2/N_l} \), numerical experiments reveal a relation \( m_{\text{crit}} \approx -3.2559793 - 1.6207083 N_l \). Thus, for increasing \( N_l \), the eigenfunction approaches a \( \delta_0 \)-distribution. Thus, in the mean field limit \( N_l \to \infty \), the dynamic properties of \( T \) change and \( m = -1 \) corresponds to eigenvalue 1 independent of the considered \( \sigma_w \). Numerically, there is an earlier (finite \( N_l \)) transition towards this point when \( m_{\text{crit}} \) is small enough.

Numerically, this is basically realized for \( N_l = 200 \) already. We conjecture that a small \( m_{\text{crit}} \) is good for trainability, since it reduces the range of eigenvalues \( \lambda > 1 \), which can lead to instabilities and exploding signals. Thus, decreasing \( \sigma_w \) slightly could be advantageous. The spectrum consisting of many quite small eigenvalues points to a quite fast convergence of the output signal to a stationary distribution, since broader tails of the distribution are quickly damped and probability mass close to zero increases. The depths at which the neural networks can be trained might be quite limited in consequence.

To test our hypotheses, we consider next small experiments on MNIST.

### 4 Experiments: Classification on MNIST

We analyze the classification performance of different network architectures and parameter configurations in conjunction with ReLUs on MNIST (Lecun et al., 1998). Our goal is to gain insights whether further parameter configurations than the critical one \( \sigma_w = \sqrt{2/N} \) and \( \sigma_b = 0 \) can achieve similarly good results. In particular, we are interested in small perturbations of \( \sigma_w \) to understand whether some shifts in the stationary distribution or spectral properties can still support the trainability of fully connected networks at different width. Furthermore, we answer the question whether it is sufficient to guaranty overall stable output signal variance and expectation of squared signal norm by Equation \[7\]

### 4.1 Equal number of neurons

#### 4.1.1 At criticality: The influence of width and depths

First, we consider ReLUs and fully connected feed forward networks of different depth consisting of \( L \) hidden layers with the same number of neurons \( N_l = N \) and an additional classification layer (with sigmoids). Here, we focus on the minimization of the \( L^2 \)-error by Stochastic Gradient Descent (SGD), where the gradient backpropagation has similar properties as signal forward propagation. Other training algorithms might lead to different results and are also worth further exploration.

Figure 3a shows the classification test accuracy at mean field criticality (\( \sigma_w = \sqrt{2/N} \), \( \sigma_b = 0 \)) for different widths and depths. The width does not have a big influence on the trainability (at criticality), as the eigenvalues are almost identical in the studied range. Yet, only small depths lead to high accuracy. The performance decreases relatively fast starting from depths \( L = 3 \) or \( L = 4 \). While networks of larger width seem to perform slightly better for small depths, they seem to do worse than narrower ones for larger depths. Larger width implies slightly smaller eigenvalues for \( m < -2 \) and bigger ones for \( -2 < m < -1 \). The eigenvalues \( -2 < m < -1 \) are especially relevant for convergence to a stationary distribution. When they are bigger (for bigger \( N \)), convergence to \( x^{-m} \) for increasing depth \( L \) is slower for increasing width. The true stationary distribution at \( x^{m_{\text{crit}}} \) is more attractive.
\( \sigma_w = \sqrt{2/N} \).

(a) \( N = 200 \).

Figure 3: Classification test accuracy on MNIST for different widths \( N \), depths \( L \), and \( \sigma_b = 0 \).

(a) At criticality. (b) The critical \( \sigma_w = 0.1 \) (green triangles) is compared with small positive (blue squares) and negative (red circles) distortions.

4.1.2 Perturbations of criticality

Interestingly, decreasing \( \sigma_w \) has a different effect than increasing \( N \). All eigenvalues are decreased, also the ones corresponding to exponents \(-2 < m < -1\). We conjecture that this is the reason why a small decrease of the critical \( \sigma_w \) improves the trainability of networks for higher depths as shown in Figure 3b.

4.2 Two hidden layers

We furthermore test the influence of different widths, i.e. a network consisting of two hidden layers. In the first example, the layer closer to the input has \( N_1 = 100 \) neurons, the other one \( N_2 = 200 \). In the second example, those are swapped, i.e. \( N_1 = 200, N_2 = 100 \). The variance of the output signal at initialisation would therefore be preserved for \( \sigma_{b,1} = \sigma_{b,2} = 0 \) and \( \sigma_{w,1} = \sqrt{2/N_1}, \sigma_{w,2} = \sqrt{2/N_2} \).

Next, we study the influence of small perturbations of the weight standard deviations.

4.2.1 Perturbations at criticality

We perturb \( \sigma_{w,2} \) away from the mean field critical choice and adjust \( \sigma_{w,1} \) to still preserve the output variance by Equation 7, i.e. \( \sigma_{w,1} = 2/\left(\sigma_{w,2}\sqrt{N_1N_2}\right) \). The results are reported in Figure 4. First, we observe that also other choices then the mean field critical parameters lead to good trainability. While the differences are small, there seems to be a tendency that joint increases in \( \sigma_{w,2} \) and decreases \( \sigma_{w,1} \) improve the classification performance regardless of which of the two layers has a higher number of
neurons. Notably, $N_1 > N_2$ leads to consistently higher accuracies. We cannot explain this just by the spectral properties of $T_1 T_2$ or $T_2 T_1$, since both have the same eigenvalues and eigenfunctions. Yet, the operators themselves are not identical. A characterization of their full spectrum might provide valuable insights into the trainability of autoencoder and other architectures with different number of neurons per layer in the future.

Next, we also analyze perturbations that do not preserve the output signal variance. Figure 5 shows the results for our first example. Again, the differences are small, but indicate that performance can be improved by distortions that do not preserve the variance. In general, decreases of $\sigma_w,1$ seem to be beneficial. Yet, reductions of both do not lead to the best results, as we could have hypothesized based on our perturbations of fully connected layers with the same number of neurons. Best results are achieved by a critical choice $\sigma_w,2$ or even an increase that is slightly higher than a value that preserves the output signal variance at initialization.

5 Discussion

We have introduced a framework for the analysis of deep fully-connected feed forward neural networks at initialisation with zero mean normally distributed weights and biases. It is exact, does not rely on mean field approximations, provides distribution information of output and joint output signals, and applies to networks with arbitrary layer widths. With its help, we have analyzed rectified linear units (ReLUs) as activation functions in more depths.

We could derive a closed form solution for the layer-wise linear transition operator that advances squared signal norm distributions from layer to layer. Its spectral properties give rise towards the question which initialisation parameters lead to network configurations that usually lead to good training accuracies. While mean field analysis provides a single set of critical parameters for good training results, we have extended the number of possible good parameter choices and tested their performance and small perturbations in experiments on MNIST. They confirm our expectations that parameter choices that limit the number of large eigenvalues perform better.

In future, we would be interested in understanding what kind of spectral properties support faster training and how this influences the joint distribution of signals corresponding to different inputs. It is straightforward to extend our results to include Drop-Out dynamics as well. Yet, backpropagation dynamics will most likely not be covered exactly because of high dependencies between network weights. Still, the link is worth exploring and we hope to inspire further explorations of activation functions and the spectral properties of the linear signal transition operator they induce.

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