FREE PROBABILITY, NEWTON LILYPADS AND JACOBIANS OF NEURAL NETWORKS

REDA CHHAIBI, TARIQ DAOUDA, AND EZÉCHIEL KAHN

Abstract. Gradient descent during the learning process of a neural network can be subject to many instabilities. The spectral density of the Jacobian is a key component for analyzing robustness. Following the works of Pennington et al., such Jacobians are modeled using free multiplicative convolutions from Free Probability Theory. We present a reliable and very fast method for computing the associated spectral densities. This method has a controlled and proven convergence.

Our technique is based on an adaptative Newton-Raphson scheme, by finding and chaining basins of attraction: the Newton algorithm finds contiguous lilypad-like basins and steps from one to the next, heading towards the objective.

We demonstrate the applicability of our method by using it to assess how the learning process is affected by network depth, layer widths and initialization choices: empirically, final test losses are very correlated to our Free Probability metrics.

Contents

1. Introduction 2
1.1. Contributions 4
1.2. Structure of the paper 5
2. Free Probability 5
  2.1. Definitions and notations 5
  2.2. Product of rectangular free matrices 7
3. Theoretical resolution of the model 7
  3.1. The model 7
  3.2. Master equation 8
4. Numerical resolution 9
  4.1. On the classical Newton-Raphson scheme 10
  4.2. Kantorovich criterion 10
  4.3. Doubling strategies and chaining 11
5. Benchmarks and experiments 12
6. Conclusion 14
7. Acknowledgements 14

Appendix A. Supplementary material 15
  A.1. Table 15
  A.2. Proofs 16
    A.2.1. Proof of Theorem 2.3 16
    A.2.2. Proof of Theorem 3.1 17
  A.3. Moments of J 18
  A.4. Details on the experiment and Github repository 20

Date: November 2, 2021.

2010 Mathematics Subject Classification. Primary 60F99; Secondary 60G60, 81P15.

Key words and phrases. Machine learning, Robustness and design of neural networks, Free probability.
1. Introduction

Consider a feed-forward network of depth $L \in \mathbb{N}$, with $L$ full-connected layers. For each depth $\ell \in \{1, 2, \ldots, L\}$, the layer has activation vector $x_\ell \in \mathbb{R}^{N_\ell}$, where $N_\ell$ is the current width. The vector $x_0 \in \mathbb{R}^{N_0}$ takes in the neural network’s input, while $x_L \in \mathbb{R}^{N_L}$ gives the output. The vector of widths is written:

$$N := (N_0, N_1, \ldots, N_L),$$

and will appear in superscript to indicate the dependence in any of the $N_\ell$’s. The following recurrence relation holds between layers:

$$x_\ell = \phi_\ell \left( W_\ell^{(N)} x_{\ell-1} + b_\ell^{(N)} \right),$$

where $\phi_\ell$ is a choice of non-linearity applied entry-wise, $W_\ell^{(N)} \in M_{N_\ell,N_{\ell-1}}(\mathbb{R})$ is a weight matrix and $b_\ell^{(N)} \in \mathbb{R}^{N_\ell}$ is the vector of biases. We write $h_\ell := W_\ell^{(N)} x_{\ell-1} + b_\ell^{(N)}$ for the pre-activations.

The Jacobian computed during back-propagation can be written explicitly by using the chain rule. Indeed, we have:

$$J^{(N)} := \frac{\partial x_L}{\partial x_0} = \frac{\partial x_L}{\partial x_L-1} \frac{\partial x_1}{\partial x_0} = D_L^{(N)} W_L^{(N)} D_{L-1}^{(N)} W_{L-1}^{(N)} \cdots D_1^{(N)} W_1^{(N)} ,$$

where $D_\ell$’s are the diagonal matrices given by

$$(D_\ell^{(N)})_{i,i} = \phi_\ell'([h_\ell]_i).$$

Technically, a step of gradient descent updates weights and biases following

$$\left( W_\ell^{(N)}, b_\ell^{(N)} \right) \leftarrow \left( W_\ell^{(N)}, b_\ell^{(N)} \right) - \alpha \frac{\partial \mathcal{L}}{\partial (W_\ell^{(N)}, b_\ell^{(N)})} ,$$

for each $\ell = 1, \ldots, L$. Here $\alpha > 0$ is the learning rate and $\mathcal{L}$ is the loss on a minibatch. If the minibatch has size $B \in \mathbb{N}$, and corresponds a small sample $((X_i, Y_i) ; i = 1, \ldots, B)$ of the dataset, we have:

$$\mathcal{L} = \frac{1}{B} \sum_{i=1}^{B} d(x_L(X_i), Y_i) .$$

Here $d$ is a real-valued distance or similarity function, the $X_i$’s are the input vectors while the $Y_i$’s are the output vectors (e.g. labels in the case of classifier, $Y_i \approx X_i$ in the case of an autoencoder etc...).

The chain rule dictates:

$$\frac{\partial \mathcal{L}}{\partial (W_\ell^{(N)}, b_\ell^{(N)})}$$
\[
\frac{\partial L}{\partial x_L} = \frac{\partial L}{\partial x_L} \frac{\partial x_{L-1}}{\partial x_L} \cdots \frac{\partial x_{\ell+1}}{\partial x_L} \frac{\partial x_\ell}{\partial W^{(N)}_\ell, b^{(N)}_\ell}.
\]

where

\[
\frac{\partial L}{\partial x_L} = \frac{1}{B} \sum_{i=1}^{B} \partial_i d(x_L(X_i), Y_i) \in M_{1,N_L}(\mathbb{R}),
\]

\[
J^{(N)}_\ell = D^{(N)}_L W^{(N)}_L \cdots D^{(N)}_{\ell+1} W^{(N)}_{\ell+1} D^{(N)}_\ell \in M_{N_{\ell}, N_{\ell}}(\mathbb{R}).
\]

Therefore, for the sake of simplicity, we shall focus on the Jacobian \(J^{(N)}\) given in Eq. (1.1) since it has exactly the same form as the \(J^{(N)}_\ell\) given in Eq. (1.6). The issue is that a large product of (even larger) matrices can easily become unstable:

- If many singular values are \(\ll 1\), we have gradient vanishing.
- If many singular values are \(\gg 1\), we have gradient explosion.

**Intuition.** This instability is easily understood thanks to the naive analogy with the one-dimensional case. Indeed, the geometric progression \(q^n\) with \(n \to \infty\) is the archetype of a long product and it converges extremely fast, to either 0 if \(|q| < 0\) or to \(\infty\) if \(|q| > 1\).

A less naive intuition consists in observing that mini-batch sampling in Eq. (1.5) is very noisy. Without further information on the dataset and sampling procedure, it is fair to assume that \(\frac{\partial C}{\partial x_L}\) has a Gaussian behavior with covariance proportional to \(I_{N_L}\). Therefore, each gradient step \(\alpha \frac{\partial C}{\partial (W^{(N)}_\ell, b^{(N)}_\ell)}\) in Eq. (1.3) is approximately a Gaussian vector with covariance proportional to:

\[
\alpha^2 \left( \frac{\partial h_\ell}{\partial (W^{(N)}_\ell, b^{(N)}_\ell)} \right)^T J^{(N)}_\ell \left( J^{(N)}_\ell \right)^T \frac{\partial h_\ell}{\partial (W^{(N)}_\ell, b^{(N)}_\ell)}.
\]

Simplifying further, we see the importance of the spectrum of \((J^{(N)}_\ell)^T J^{(N)}_\ell\) for stability. Basically, eigenvectors of \((J^{(N)}_\ell)^T J^{(N)}_\ell\) are the directions along which the one-dimensional intuition applies.

This intuition is confirmed in the conclusion of [BSF94], using the language of hyperbolic attractors i.e. the presence of eigenvalues larger and smaller than one.

**Randomness.** Starting from the pioneering works of Glorot and Bengio [GB10] on random initializations, it was suggested that the spectral properties of \(J^{(N)}\) are an excellent indicator for stability and learning performance. In particular, an appropriate random initialization was suggested and since implemented in all modern ML frameworks [PGC+17, AAB+15].

Here are classical choices of random initializations. The biases \(b^{(N)}_\ell\) are taken as random vectors which entries are centered i.i.d. Gaussian random variables with standard deviation \(\sigma_b\). For the weights, we will consider the following matrix ensembles: the \([W^{(N)}_\ell]_{i,j}\) are drawn from i.i.d. centered random variables with variance \(\sigma_w^2 / N_\ell\) and finite fourth moment as in [PS20].

**Modeling spectrum thanks to Free Probability Theory.** Now, following the works of Pennington et al. [PSG18], the tools of Free Probability Theory (FPT) can
be used to quantitatively analyze the singular values of $J^{(N)}$ in the large width limit. The large width limit is particularly attractive when studying large deep networks, especially because free probability appears at relatively small sizes because of strong concentration properties [LLC+18].

For the purposes of this paragraph, we restrict ourselves to square matrices and assume $N_{\ell} = N$ for all $\ell = 1, \ldots, L$. In fact, FPT is concerned with the behavior of spectral measures as $N \to \infty$. For any diagonalizable $A_N \in M_N(\mathbb{R})$, the associated spectral measure on the real line is:

$$\mu_{A^{(N)}}(dx) := \frac{1}{N} \sum_{i=1}^{N} \delta_{a_i^{(N)}}(dx)$$

with the $a_i^{(N)}$’s being the eigenvalues of $A_N$. For ease of notation, the spectrum of (squared) singular values is written $\nu_{A^{(N)}} := \mu_{A^{(N)}}(A^{(N)})$. A fundamental assumption for invoking tools from Free Probability Theory, is the assumption of asymptotic freeness. Without defining the notion, which can be found in [MS17], let us describe the important computation it allows, discovered in the seminal work of Voiculescu [Voi87]. Given two sequences of square matrices $A^{(N)}$, $B^{(N)}$ in $M_N(\mathbb{R})$, with converging spectral measures:

$$\lim_{N \to \infty} \nu_{A^{(N)}} = \nu_A, \quad \lim_{N \to \infty} \nu_{B^{(N)}} = \nu_B,$$

we have that, under the assumption of asymptotic freeness:

$$\lim_{N \to \infty} \nu_{A^{(N)}B^{(N)}} = \nu_A \boxtimes \nu_B,$$

where $\boxtimes$ is a deterministic operation between measures called multiplicative free convolution. The $\boxtimes$ will be detailed in Section 2. The letter $A$ (as well as $B$) does not correspond to a limiting matrix but to an abstract operator, with associated spectral measure $\mu_A$ and measure of squared singular values $\nu_A$. For such limiting operators, we drop the superscript $(N)$.

Under suitable assumptions which are motivated and detailed later following the works of [PSG18, HN19, Pas20, PS20, CH21], for all $\ell = 1, \ldots, L$, the measures $\nu_{W_{\ell}^{(N)}}$ and $\nu_{D_{\ell}^{(N)}}$ will respectively converge to $\nu_{W_{\ell}}$ and $\nu_{D_{\ell}}$. Again the $W_{\ell}$’s and $D_{\ell}$’s are abstract operators which only make sense in the infinite width regime. In the limit, asymptotic freeness will also hold. Therefore, we will see that the measure of interest is:

$$\lim_{N \to \infty} \nu_{J^{(N)}} = \nu_J := \nu_{D_L} \boxtimes \nu_{W_L} \boxtimes \cdots \boxtimes \nu_{D_1} \boxtimes \nu_{W_1}. \quad (1.7)$$

The goal of this paper is to give a very fast and stable computation of this measure, in the more general setup of rectangular matrices. This allows for a number of insights on the stability of back-propagation and paves the road towards more automatic tuning of neural networks.

1.1. Contributions. More precisely, we aim at streamlining the approach of Pennington et al. by providing the tools for a systematic use of FPT. The contributions of this paper can be categorized as:

- Theoretical: At this level, the contribution is incremental. In Pennington et al., a constant width is assumed. We generalize the model to allow for a width profile, which reflects how neural networks are designed in practice. This requires us to develop a rectangular multiplicative free convolution.
We also do not assume that the non-linearity $\phi_\ell$ is the same throughout the neural network.

- Numerical: This is our main contribution. We propose and implement an efficient computational scheme for computing spectral densities. The method relies on adaptative inversions of $S$-transforms using the Newton-Raphson algorithm. If the Newton-Raphson scheme is only local, we achieve a global resolution by chaining basins of attractions, thanks to doubling strategies.

Interestingly, even in the FPT community, inverting $S$-transforms has been considered impossible to realize in practice [BGD08]. This misconception led to the use combinatorial methods that use moments, or fixed-point algorithms via the subordination method [ATV+20, MNN+20, Tar20]. In the ML community, Pennington et al. pioneered the application of FPT to the theoretical foundations of Machine Learning. Naturally, numerical performance was not the focus and a generic root finding procedure was proposed [PSG18, Algorithm 1].

In contrast our algorithm has guaranteed convergence and high performance, which allows for a large body of experiments. A complete implementation is provided in a Github repository:

https://github.com/redachhaibi/FreeNN

- Empirical: We ask whether the design of feed-forward neural networks can quantitatively benefit from the insights of FPT. To that endeavor, we analyze the correlation between the loss of of several randomly generated architectures and the quantiles of $\nu_J$, after a fixed number of epochs.

Remarkably, we find that the ultimate loss is very negatively correlated to the higher quantiles. This suggests that spread-out spectral distributions $\nu_J$ are more desirable, provided of course we avoid the explosive regime.

1.2. Structure of the paper. We start in Section 2 by stating facts from Free Probability Theory. Most of it is available in the literature, except the definition of the product of rectangular free matrices. There, we establish in the rectangular setting an analogue of Eq. (1.7) in Theorem 2.3. Although it is probably known to specialists, the specifics were never made explicit.

In Section 3, we explain in detail the FPT model for random neural networks. Then thanks to the results of [Pas20, PS20] and our rectangular setting, we show that the spectral measure of the Jacobian $J^{(N)}$ converges to $\nu_J$ and we encode the limit in explicit generating series in Theorem 3.1. This gives how $\nu_J$ can theoretically be recovered.

Section 4 presents the numerical resolution which inverts the generating series. There, we start by a quick primer on the classical Newton-Raphson scheme, give Kantorovich’s criterion for detecting (local) basins of attraction and then give our algorithm. By chaining different basins of attractions, we obtain a global resolution method.

Finally Section 5 benchmarks the numerical method and presents the experiment using feed-neural networks.

2. Free Probability

2.1. Definitions and notations. Free Probability Theory provides a framework to analyze eigenvalues and singular values of large random matrices. We now introduce various complex-analytic generating series which encode the measures and the basic operations on them. First, the Cauchy-Stieltjes transform of $\mu$, a probability measure
on $\mathbb{R}_+$ is:

$$G_\mu : \mathbb{C}_+ \to \mathbb{C}_-, \quad z \mapsto \int_{\mathbb{R}_+} \frac{\mu(dv)}{z-v},$$

where

$$\mathbb{C}_\pm := \{ z \in \mathbb{C} \mid \pm \Im z > 0 \}.$$  

The transform $G_\mu$ encodes the measure $\mu$ and reciprocally, the measure can be recovered thanks to:

**Lemma 2.1** (Cauchy-Stieltjes inversion formula – Theorem 6 in [MS17]). We have the weak convergence of probability measures:

$$\lim_{y \to 0} -\frac{1}{\pi} \Im G_\mu(x + iy)dx = \mu(dx).$$

The moment generating function is

$$M_\mu(z) = zG_\mu(z) - 1 = \sum_{k=1}^{+\infty} \frac{m_k(\mu)}{z^k}, \quad (2.1)$$

where for all $k \in \mathbb{N}$, $m_k(\mu) := \int_{\mathbb{R}} x^k \mu(dx)$ is the $k$-th moment of $\mu$. For $\mu \neq \delta_0$, $M_\mu$ is invertible in the neighborhood of $\infty$ and the inverse is denoted by $M_\mu^{(-1)}$. The S-transform of $\mu$ is defined as

$$S_\mu(m) = \frac{1 + m}{mM_\mu^{(-1)}(m)},$$

and is analytic in a neighborhood of $m = 0$. Furthermore, the variable $z$ will always denote an element of $\mathbb{C}_+$, while the variables $g$ and $m$ will denote elements in the image of $G_\mu$ and $M_\mu$.

For a diagonalizable matrix $A^{(N)} \in M_N(\mathbb{R})$, we write $S_{A^{(N)}} := S_{\mu_{A^{(N)}}}$, $G_{A^{(N)}} := G_{\mu_{A^{(N)}}}$, $M_{A^{(N)}} := M_{\mu_{A^{(N)}}}$.

A landmark result in the field introduces free multiplicative convolution in a natural way, and shows that this operation is linearized by the S-transform:

**Theorem 2.2** (Voiculescu, [Voi87]). Consider two sequences of positive matrices, each element in $M_N(\mathbb{R})$

$$(A^{(N)} ; N \geq 1), \quad (B^{(N)} ; N \geq 1),$$

such that:

$$\lim_{N \to \infty} \mu_{A^{(N)}} = \mu_A, \quad \lim_{N \to \infty} \mu_{B^{(N)}} = \mu_B.$$

Under the assumption of asymptotic freeness for $A^{(N)}$ and $B^{(N)}$, there exists a deterministic probability measure $\mu_A \boxtimes \mu_B$ such that:

$$\lim_{N \to \infty} \mu_{A^{(N)}B^{(N)}} = \mu_A \boxtimes \mu_B.$$

The operation $\boxtimes$ is the multiplicative free convolution. Moreover

$$S_{AB}(m) = S_A(m)S_B(m), \quad (2.2)$$

This convergence akin to a law of large numbers is the key ingredient which allows to build the deterministic model for the back-propagation of gradients in Eq. (1.7).
2.2. Product of rectangular free matrices. As a generalization of Eq. (2.2) to rectangular matrices, we state:

**Theorem 2.3.** Let \((p_N)_{N \geq 1}, (q_N)_{N \geq 1}, (r_N)_{N \geq 1}\) be three sequences of integers satisfying
\[
p_N, q_N, r_N \xrightarrow{N \to \infty} \infty, \quad \frac{r_N}{q_N} \xrightarrow{N \to \infty} c > 0 .
\]
Consider for all \(N \geq 1\) let \(A^{(N)}, B^{(N)}\) be random matrices of respective sizes \(p_N \times q_N\) and \(q_N \times r_N\) such that the (squared) singular laws of \(A^{(N)}, B^{(N)}\) converge weakly. Assuming that \(B^{(N)} (B^{(N)})^T\) and \((A^{(N)})^T A^{(N)}\) are asymptotically free, we have that in the limit \(N \to \infty\):
\[
S_{(AB)^T AB}(m) = S_{A^T A}(cm) S_{B^T B}(m) .
\]

**Proof.** See the supplementary material, Subsection A.2.1 \(\Box\)

Implicitly this defines a rectangular multiplicative free convolution, which could be denoted \(\boxtimes_c\) in the spirit of the rectangular free additive convolution [BG09]. But, in the current setting, this is not a good idea. Indeed, if one defines \(\mu_1 \boxtimes_c \mu_2\) as the measure whose \(S\)-transform is \(S_{\mu_1}(c \cdot)S_{\mu_2}\), then a quick computation shows that \(\boxtimes_c\) is not associative i.e. for a triplet \((\mu_1, \mu_2, \mu_3)\) of probability measures and a pair \((c_1, c_2) \in \mathbb{R}_+^* \times \mathbb{R}_+^*\), we generically have:
\[
\mu_1 \boxtimes_{c_1} (\mu_2 \boxtimes_{c_2} \mu_3) \neq (\mu_1 \boxtimes_{c_1} \mu_2) \boxtimes_{c_2} \mu_3 .
\]
A better idea is to treat the dimension ratio \(c\) as part the data:

**Definition 2.4.** On the set of pairs \((\mu, c)\) such that \(\mu\) is a probability measure on \(\mathbb{R}_+\) and \(c \in \mathbb{R}_+^*\), define the operation \(\boxtimes\) as:
\[
(\mu_1, c_1) \boxtimes (\mu_2, c_2) := (\nu, c_1c_2) ,
\]
where \(\nu\) is the unique probability measure such that \(S_\nu = S_{\mu_1}(c_2 \cdot)S_{\mu_2}\). This extends the classical definition as the usual free convolution is recovered with:
\[
(\mu_1, 1) \boxtimes (\mu_2, 1) := (\mu_1 \boxtimes \mu_2, 1) .
\]

Such an operation is associative and will allow a neat formulation of the measure of interest in the upcoming Theorem 3.1, entirely analogous to Eq. (1.7).

3. Theoretical resolution of the model

Let us start by describing the model and the underlying assumptions.

3.1. The model. Width profile: Pennington et al. [PSG18] consider \(N_\ell = N\) for \(\ell = 1, 2, \ldots, N\). Here, we consider that the width of layers is not constant across layers, which is mostly the case in practice. Indeed, modern architectures typically have very sophisticated topologies with layers varying in widths.

Let us assume that we are in the infinite width regime in the sense that \(N_\ell \to \infty\), for all \(\ell = 0, 1, 2, \ldots, L\) and:
\[
\frac{N_{\ell-1}}{N_\ell} \xrightarrow{N \to \infty} \lambda_\ell \geq 0 ,
\]
and let us denote \(\Lambda_\ell := \lim_{N \to \infty} \frac{N_\ell}{N} = \prod_{k=1}^\ell \lambda_k\), with the convention \(\Lambda_0 = 1\).

**FPT limits:** Let \(\mathcal{N}\) be a standard Gaussian random variable on the real line \(\mathbb{R}\):
\[
\mathbb{P}(\mathcal{N} \in dx) = \frac{e^{-x^2/2}}{\sqrt{2\pi}} dx .
\]
Here $D^{(N)}_\ell$ is diagonal with entries $\phi'_\ell([h_\ell])$ (see Eq. (1.2)), and the pre-activations
\[ h_\ell = W^{(N)}_\ell x_{\ell-1} + b^{(N)}_\ell = W^{(N)}_\ell \phi_\ell(h_{\ell-1}) + b^{(N)}_\ell \]
clearly depend on the previous layers. Because of this lack of independence, the standard results of FPT cannot be applied directly i.e. asymptotic freeness does not obviously hold. This is an important subtlety that is addressed in the upcoming Theorem 3.1. Based on an information propagation argument, the papers [PLR+16, SGGSD16] argue that the entries of $h_\ell$ behave as the i.i.d. samples of a Gaussian distribution with zero mean and variance $q_\ell$. A basic law of large numbers applied to Eq. (1.2) gives a limit for the empirical measure:
\[ \mu_{D^{(N)}_\ell} = \lim_{N_\ell \to \infty} \mu_{D^{(N)}_\ell} = \phi'_\ell \left( \sqrt{q_\ell N} \right). \]

Also the recurrence for the variance is:
\[ q_\ell = f_\ell (q_{\ell-1}) = \sigma^2_{W_\ell} \mathbb{E} \left[ \phi_\ell \left( \sqrt{q_{\ell-1} N} \right)^2 \right] + \sigma^2_{b_\ell}, \]
with initial condition $q^1 = \frac{\sigma^2_{W_1}}{N_1} \sum_{i=1}^{N_1} (x_{i0})^2 + \sigma^2_{b_1}.$

Recently Pastur et al. completed this heuristic thanks to a swapping trick – see [Pas20, Lemma 3.3] and [PS20, Remark 3.4]. They proved that, regarding the asymptotical spectral properties of $J^{(N)}$, one can replace each $D^{(N)}_\ell$ by a diagonal matrix with independent Gaussian entries $\sqrt{q_\ell} N$ independent from the rest. In that setting, one can apply the results on products of asymptotically free matrices which were given in Section 2.

**Theorem 3.1.** In terms of the rectangular multiplicative free convolution, the measure of (squared) singular values of $J^{(N)}$ converges to
\[ \nu_J = (\nu_{D_L}, 1) \boxtimes (\nu_{W_L}, \lambda_L) \boxtimes \cdots \boxtimes (\nu_{D_1}, 1) \boxtimes (\nu_{W_1}, \lambda_1). \]

Moreover, the S-transform of $J^T J$ in the infinite width regime verifies
\[ S_{J^T J}(m) = \prod_{\ell=1}^{L} \left[ S_{D^{(N)}_\ell} (\Lambda_\ell m) S_{W^{(N)}_\ell} (\Lambda_{\ell-1} m) \right]. \]

In particular, under the assumption that the entries of $W_\ell$ are i.i.d. :
\[ S_{J^T J}(m) = \prod_{\ell=1}^{L} \left( S_{D^{(N)}_\ell} (\Lambda_\ell m) \frac{1}{\sigma^2_{W_\ell}} \frac{1}{1 + \Lambda_\ell m} \right), \]
\[ M_{J^T J}^{(-1)}(m) = \frac{m+1}{m} \prod_{\ell=1}^{L} \frac{\sigma^2_{W_\ell} (1 + \Lambda_\ell m)}{S_{D^{(N)}_\ell} (\Lambda_\ell m)}. \]

**Proof.** See the supplementary material, Subsection A.2.2. □

### 3.2. Master equation.
In the end, we only need to fix width ratios and non-linearities to form $M_{J^T J}^{(-1)}(m)$, and get the master equation which we solve numerically thanks to an adaptive Newton-Raphson scheme.

The non-linearities ReLu, Hard Tanh and Hard Sine yield explicit formulas, which can be found in Table A.1 of the supplementary material. If $W_\ell$ has i.i.d. entries, one
finds the explicit master equation:

\begin{equation}
M^{(-1)}_{J^T J}(m) = \frac{m + 1}{m} \prod_{\ell=1}^{L} \sigma^{2}_{\mathcal{W}_{\ell}} (c_{\ell} + \Lambda_{\ell} m) ,
\end{equation}

where \( c_{\ell} = \frac{1}{2} \) when \( \phi_{\ell} \) is ReLu, \( c_{\ell} = C_{\ell} = \mathbb{P} \left( 0 \leq \mathcal{N} \leq \frac{1}{\sqrt{q'}} \right) \) if \( \phi_{\ell} \) is Hard Tanh and \( c_{\ell} = 1 \) if \( \phi_{\ell} \) is Hard Sine.

4. Numerical resolution

Here we describe the numerical scheme aimed at computing the spectral density of \( J^T J \) in Eq. (1.1). We use the following steps to compute the spectral density at a fixed \( x \in \mathbb{R}_{+} \):

- Because of the Cauchy-Stieltjes inversion formula given in Lemma 2.1, pick a small \( y > 0 \) in order to compute:
  \[-\frac{1}{\pi} \Im G_{J^T J}(z = x + iy) .\]
  The smaller the better, and in practice our method works for up to \( y = 10^{-9} \). Figure 4.1 shows the same target distribution but convolved with various Cauchy distributions \( y \mathcal{C} \) where \( y \in \{1, 10^{-1}, 10^{-4}\} \). This corresponds to computing the density \( \frac{-1}{\pi} \Im G_{\mu}(\cdot + iy) \) for different \( y \)'s.
- Because of Eq. 2.1, we equivalently need to compute \( M_{J^T J}(z) \).
- \( M^{(-1)}_{J^T J}(m) \) is available thanks to the master equation in Theorem (3.1). Therefore, we need to invert \( m \mapsto M^{(-1)}_{J^T J}(m) \).

\begin{figure}
\centering
\includegraphics[width=\textwidth]{figure4.1.png}
\caption{Plot of the probability density \( \frac{-1}{\pi} \Im G_{\mu}(\cdot + iy) \) for \( y \in \{1, 10^{-1}, 10^{-4}\} \). Here \( \mu \) is the multiplicative free convolution of three Marchenko-Pastur distributions, with different parameters.}
\end{figure}
The last step is the crucial one, and has been deemed hopeless by many mathematicians working in Free Probability Theory. In the words of [BGD08, p.218], “the operations which are necessary in this method (the inversion of certain functions, the extension of certain analytic functions) are almost always impossible to realise practically.”

4.1. **On the classical Newton-Raphson scheme.** We first use the classical Newton-Raphson scheme to invert the equation \( z = f(m) \) where \( z \in \mathbb{C}_+ \) is fixed and \( f \) is rational. A neat trick which leverages the fact that \( f \) is rational and that \( z \in \mathbb{C}_+ \) is to define:

\[
\varphi_z(m) := \frac{P(m)}{Q(m)} - z .
\]  

As such, we have:

\[
z = f(m) = \frac{P(m)}{Q(m)} \iff \varphi_z(m) = 0 .
\]

There are several advantages of doing that:

- Inversion is recast into finding the zero of a polynomial function.
- Since we have \( \lim_{z \to \infty} M(z) = 0 \), if \( z \) is large in modulus, \( m = 0 \) is a natural starting point for the algorithm when \( z \) is large.

The pseudo-code for the algorithm is given in 4.1.

**Algorithm 4.1** Newton-Raphson scheme for a rational function \( f \)

- **Name:** \textsc{newton\_raphson}
- **Input:**
  - Numerical precision: \( \varepsilon > 0 \) (Default: \( 10^{-12} \)),
  - Image value: \( z \in \mathbb{C}_+ \),
  - Polynomials: \( P, Q \) such that \( f = \frac{P}{Q} \),
  - (Optional) Guess: \( m_0 \in \mathbb{C}, \) (Default: \( m_0 = 0 \)).
- **Code:**
  
  \[
m \leftarrow m_0
  \]
  
  \[
\text{while True do}
  \]
  
  \[
\text{value} \leftarrow \varphi_z(m) \quad \# \text{See Eq. (4.1)}
  \]
  
  \[
\text{if } |\text{value}| < \varepsilon \text{ then}
  \]
  
  \[
\text{return } m
  \]
  
  \[
\text{end if}
  \]
  
  \[
\text{grad} \leftarrow \varphi'_z(m)
  \]
  
  \[
m \leftarrow m - \text{value}/\text{grad}
  \]
  
  \[
\text{end while}
  \]

It is well-known that the Newton-Raphson scheme fails unless the initial guess \( m_0 \in \mathbb{C} \) belongs to a basin of attraction for the method. And, provided such a guarantee, the Newton-Raphson scheme is exceptionally fast with a quadratic convergence speed. Kantorovich’s seminal work in 1948 provides such a guarantee locally.

4.2. **Kantorovich criterion.** Here we give the optimal criterion from [GT74] adapted to this paper. Fix \( z \in \mathbb{C}_+ \) and recall that \( \varphi_z \) in Eq. (4.1) is the map whose zero we want to find.
Theorem 4.1 (Kantorovich’s criterion, [Kan48]). Consider a starting point \( m_0 \in \mathbb{C} \), and define:

\[
\delta := \frac{|\varphi_z(m_0)|}{|\varphi'_z(m_0)|}, \quad \kappa := \frac{1}{|\varphi'_z(m_0)|}.
\]

If the starting point satisfies \( h := \delta \kappa \lambda < \frac{1}{2} \), where

\[
\lambda := \sup_{|m - m_0| \leq t^*} |\varphi''_z(m)|, \quad t^* := \frac{2\delta}{1 + \sqrt{1 - h}} < 2\delta.
\]

Then, the Newton-Raphson scheme, starting from \( m_0 \) converges to \( m^* \) such that \( \varphi_z(m^*) = 0 \). Furthermore, the convergence at each step is at least quadratic.

Therefore, we assume that we have at our disposal a function \( (z, m) \mapsto \text{is\_in\_basin}(z, m) \) which indicates if the Kantorovich criterion is satisfied for \( \varphi_z \) at any \( m \in \mathbb{C} \). It is particularly easy to program with \( \varphi_z \) polynomial.

4.3. Doubling strategies and chaining. Now we have all the (local) ingredients in order to describe a global strategy which solves in \( m \in \mathbb{C} \) the equation:

\[
\varphi_z(m) = 0.
\]

First, one has to notice that this problem is part of a family parametrized by \( z \in \mathbb{C}_+ \). And the solution is \( m \approx 0 \) for \( z \) large. Therefore, one can find a proxy solution for \( z \in \mathbb{C}_+ \) high enough. This is done thanks to a doubling strategy until a basin of attraction is reached.

Second, if a proxy \( (z, m) \) is available, we can use the Newton-Raphson algorithm to find a solution \( (z + \Delta z, m + \Delta m) \) starting from \( m \). To do so, we need \( \Delta z \) small enough. This on the other hand is done by dichotomy.

Tying the pieces together allows to chain the different basins of attraction and leads to Algorithm 4.2. Notice that in the description of the algorithm, we chose to make implicit the dependence in the function \( f \), since it is only passed along as a parameter. Technically, \( f \) is a parameter for all three functions \textsc{newton\_raphson}, \textsc{is\_in\_basin}, \textsc{newton\_lilypads}.
Algorithm 4.2 Newton lilypads, chaining basins of attraction

Name: NEWTON_LILYPADS

Input:
Image value: \( z_{\text{objective}} \in \mathbb{C}_+ \)
(Optional) Proxy: \( (z_0, m_0) \in \mathbb{C}_+ \times \mathbb{C} \)

Output: \( M(z_{\text{objective}}) \)

Code:

# Find a proxy \((z_0, m_0 = 0)\) using a doubling strategy, if None given
if \((z_0, m_0)\) is None then
  \( m \leftarrow 0 \)
  \( z \leftarrow z_{\text{objective}} \)
  while not \text{IS_IN_BASIN}(z, m) \do
    \( z \leftarrow z + i \Re(z) = \Re(z) + i 2 \Im(z) \)  # Double imaginary part
  end while
  \( m \leftarrow \text{NEWTON_RAPHSON}(z, \text{Guess} = m) \)
else
  \((z, m) \leftarrow (z_0, m_0)\)
end if

# Starts heading towards \( z_{\text{objective}} \) using dichotomy
while \( |z_{\text{objective}} - z| > 0 \) do
  \( \Delta z \leftarrow z_{\text{objective}} - z \)
  while not \text{IS_IN_BASIN}(z + \Delta z, m) \do
    \( \Delta z \leftarrow 0.5 \ast \Delta z \)
  end while
  \( z \leftarrow z + \Delta z \)
  \( m \leftarrow \text{NEWTON_RAPHSON}(z, \text{Guess} = m) \)
end while
return \( m \)

5. BENCHMARKS AND EXPERIMENTS

| \( N \)    | 100  | 200  | 400  | 1000 |
|-----------|------|------|------|------|
| Time (ms) | 38.1 | 57.4 | 95.4 | 220.7 |

Table 5.1. Table of computational time, on a laptop with an Intel Core i7-9850H CPU, for computing \( N \) density points. Nearest points are used as proxy for the Newton-Raphson scheme.

**Computational speed and precision:** A table of the computational time required for computing \( N \) density points is given in Table 5.1. Notice that the recorded time scales sublinearly with the number of required points. This is easily understood by the fact that smaller \( N \) requires the computation of more basins of attraction per point.

Figure 5.1 compares the output of our method versus a Monte-Carlo sampling with matrices of size \( N = 3000 \). Not only Monte-Carlo is imprecise because of the noise, but its performance scales very poorly with \( N \) since one needs to diagonalize ever larger matrices. Of course, Monte-Carlo remains the easiest method to implement.

**Experiment:** To leverage the numerical scheme, we designed the following experiment. Consider a classical Multi-Layer Perceptron (MLP) with \( L = 4 \) layers,
Figure 5.1. Plot of density of singular values for the Jacobian matrix $J$. The network has constant width and ReLu non-linearities. Monte-Carlo sampling uses matrices of size $N_\ell = N = 3000$. Computation time is 22467.3 ms with the same laptop as the one used for Table 5.1.

feed-forward and fully-connected with ReLu non-linearities. The MLP’s architecture is determined by the vector $\lambda = (\lambda_0, \lambda_1, \ldots, \lambda_L)$. The initialization follows the Xavier normal initialization [GB10] as implemented in Pytorch [PGC+17]. The gains of this initialization are determined by the vector $\sigma = (\sigma_1, \sigma_2, \ldots, \sigma_L)$.

By randomly sampling the vector $\lambda$, we explore the space of possible architectures. In other to have balanced architectures, we chose independent $\lambda_i$’s with $E(\lambda_i) = 1$. Likewise, we also sample different possible gains. Hence we find ourselves with several MLPs architectures each with it’s unique initialization. The spectral distributions are computed thanks to our Algorithm 4.2. We further train multiple instances for each MLP, thus obtaining a large sample of learning curves. Finally we calculate the correlations between the cross-entropy loss on the test set and the 10th and 90th percentile of the spectral distribution $\nu_J$ after 50 epochs of training on the MNIST datasets.

Results for the experiment on 200 networks can be seen in Table 5.2 and show a strong negative correlation between the higher quantiles and the test loss at the end of training. This suggests that a spread-out spectral distributions $\nu_J$ has a beneficial effect on network convergence.

Table 5.3 shows a lesser yet existing correlation between the final test loss and the 10th percentile. Therefore, learning does benefit from less vanishing of the Jacobian, but the benefit is surprisingly not as important as the spreading of the spectral distribution. More details on the experiments are provided in supplementary materials.
Table 5.2. Table indicating the correlation between the loss after training and the 90% quantile of $\nu_J$. The $p$-value is for a hypothesis test whose null hypothesis is that quantile and loss are uncorrelated.

| Correlation factor | Spearman | Pearson |
|--------------------|----------|---------|
| Value              | -0.851   | -0.938  |
| $p$-value          | 3.6e-20  | 5.6e-32 |

Table 5.3. Table indicating the correlation between the loss after training and the 10% quantile of $\nu_J$.

| Correlation factor | Spearman | Pearson |
|--------------------|----------|---------|
| Value              | -0.576   | -0.562  |
| $p$-value          | 3.6e-20  | 5.6e-32 |

6. Conclusion

In this paper, we gave an efficient numerical method in FPT geared towards the application in machine learning. The computation method itself is fast and reliable, which can be used to automatically tune some design choices in neural networks such as the width profile, and initialization variances. Empirically, we demonstrate that the loss of a feed-forward neural networks after training is highly (negatively) correlated to higher quantiles of the theoretically computed spectral distribution.

Finally a challenging problem would be to accommodate for skip-connections:

$$x_\ell = \varphi\left(\sum_{i=1}^{K-1} W^{(N)}_{\ell,i} x_{\ell-1} + b^{(N)}_{\ell}\right),$$

where $K$ is the maximum lag and $W^{(N)}_{\ell,i} \in M_{N_{\ell},N_{\ell-1}}$ is a weight matrix. Here the chain rule used for back-propagation changes in a fundamental way. The Jacobian cannot be approximated by a simple product of free matrices: the same free variable will appear at multiple locations.

7. Acknowledgements

R.C. recognizes the support of French ANR STARS held by Guillaume Cébron.

The authors would like to thank Mireille Capitaine, Guillaume Cébron and Fabrice Gamboa for fruitful conversations.
APPENDIX A. SUPPLEMENTARY MATERIAL

| Linear | ReLu | Hard Tanh | Hard sine / Triangle |
|--------|------|-----------|----------------------|
| $\phi_\ell(h)$ | $h$  | $[h]_+$  | $[h+1]_+-[h-1]_+-1$ | $\frac{2}{\pi} \arcsin \circ \sin(\frac{x}{2}h)$ |
| $M_{D_\ell^2}(z)$ | $\frac{1}{z-1}$ | $\frac{1}{2}$ | $\frac{1}{2}$ | $\frac{1}{2}$ |
| $m_k(D_\ell^2)$ | $1$ | $\frac{1}{z-1}$ | $\frac{1}{z-1}$ | $\frac{1}{z-1}$ |
| $S_{D_\ell^2}(m)$ | $1$ | $\frac{1}{z-1}$ | $\frac{1}{z-1}$ | $\frac{1}{z-1}$ |
| $g_\ell(q)$ | $q$ | $\frac{q}{2}$ | $2qC_\ell - \sqrt{\frac{2q}{\pi}}e^{-\frac{1}{2q}}$ | $\frac{1}{3} + \frac{4}{\pi^2} \sum_{n \geq 1} \frac{(-1)^n}{n^2} e^{-\frac{n^2}{2}}$ |

Table A.1. Table of formulas for moment generating functions and $S$-transforms.

A.1. Table. Let us now collect the various required formulas, and specialize them to a selection of non-linearities: ReLu, Hard Tanh and Hard Sine. These non-linearities are very tractable hence the choice. As discussed in the introduction, the empirical distribution of $D_\ell^{(N)}$ converges to the law of $\phi'_\ell(\sqrt{qN})$. From this observation was deduced in [PSG18] the following formula:

$$M_{D_\ell^2}(z) = \sum_{k \geq 1} \frac{m_k(D_\ell^2)}{z^k} = E \left[ \frac{\phi'_\ell(\sqrt{qN})^2}{z - \phi'_\ell(\sqrt{qN})^2} \right],$$

(A.1)

$$S_{D_\ell^2}(m) = \frac{1 + m}{mM_{D_\ell^2}^{(1)}(m)},$$

(A.2)

In Table 1.1, the reader shall find the formulae of $M_{D_\ell^2}$, $S_{D_\ell^2}$ and the recurrence relation given by $f_\ell$ where

$$f_\ell(q^{-1}) = \sigma^2_W g_\ell(q^{-1}) + \sigma^2_b,$$

with $g_\ell(q) := E \left[ \phi_\ell(\sqrt{qN})^2 \right].$

and

$$C_\ell = P \left( 0 \leq N \leq \frac{1}{\sqrt{q^\ell}} \right).$$

Proof of formulas in Table A.1 ReLu and Hard Tanh have already been computed in [PSG18].

Hard Sine: This is the most tricky formula to establish. If $\phi(x) = \frac{2}{\pi} \arcsin \circ \sin(\frac{x}{2}x)$ and $\hat{f}(\xi) = \int dx f(x)e^{i\xi x}$ is the Fourier transform on $f$, then the application of the Plancherel formula yields:

$$E \left[ \phi(\sqrt{qN})^2 \right] = \int_{-\infty}^{\infty} dx e^{-\frac{x^2}{2\pi q}} \phi^2(x).$$
\[= \frac{1}{2\pi} \int_{-\infty}^{\infty} d\xi \, \hat{\phi}^2(\xi)e^{-q\xi^2}.\]

But in term of Fourier series:
\[
\phi^2(x) = \sum_{n \in \mathbb{Z}} \left( \hat{\phi}^2 \right)_n e^{i\pi nx}
\]
as \(\phi^2(x) = x^2\) on \([-1, 1]\) and extended in order to become 2-periodic. In terms of Schwartz distributions:
\[
\hat{\phi}^2(\xi) = \sum_{n \in \mathbb{Z}} \left( \hat{\phi}^2 \right)_n (x \mapsto e^{i\pi nx}) = \sum_{n \in \mathbb{Z}} \left( \hat{\phi}^2 \right)_n 2\pi \delta_{-n}(d\xi).
\]

Hence:
\[
\mathbb{E} \left[ \phi \left( \sqrt{q}N \right)^2 \right] = \sum_{n \in \mathbb{Z}} \left( \hat{\phi}^2 \right)_n e^{-q\frac{n^2}{2}}.
\]

We conclude by computing the Fourier coefficients of \(\phi^2\).
\[
\left( \hat{\phi}^2 \right)_0 = \frac{1}{2} \int_{-1}^{1} dx \, x^2 = \frac{1}{3}.
\]
\[
\left( \hat{\phi}^2 \right)_n = \frac{1}{2} \int_{-1}^{1} dx \, x^2 \, e^{-i\pi nx} = \int_{0}^{1} dx \, x^2 \, \cos(\pi nx) = \frac{2}{(\pi n)^2} \left[ x \cos(n\pi x) \right]_0^1 - \frac{2}{(\pi n)^2} \int_{0}^{1} dx \, \cos(\pi nx) = \frac{2}{(\pi n)^2} (-1)^n.
\]

In the end:
\[
\mathbb{E} \left[ \phi \left( \sqrt{q}N \right)^2 \right] = \frac{1}{3} + \frac{4}{\pi^2} \sum_{n \geq 1} \frac{(-1)^n}{n^2} e^{-q\frac{n^2}{2}}.
\]

A.2. Proofs.

A.2.1. Proof of Theorem 2.3. For \(k \in \mathbb{N}\), we have:
\[
Tr \left[ \left( (A^{(N)}B^{(N)})^T A^{(N)}B^{(N)} \right)^k \right] = Tr \left[ \left( (B^{(N)})^T (A^{(N)})^T AB \right)^k \right] = Tr \left[ \left( B^{(N)} (B^{(N)})^T (A^{(N)})^T A \right)^k \right].
\]
As \((A^{(N)}B^{(N)})^T A^{(N)}B^{(N)} \in M_{r_N}(\mathbb{C})\) and \(B^{(N)} (B^{(N)})^T (A^{(N)})^T A^{(N)} \in M_{q_N}(\mathbb{C})\), this shows that
\[
M_{A^{(N)}B^{(N)}}^{-1} \left( A^{(N)}B^{(N)} \right)^T \left( A^{(N)} \right) (z) = \frac{q_N}{r_N} M_{B^{(N)}(B^{(N)})^T A^{(N)}}^{-1} \left( B^{(N)} \right)^T \left( A^{(N)} \right) (z),
\]
and then
\[
M_{A^{(N)}B^{(N)}}^{-1} \left( A^{(N)}B^{(N)} \right)^T \left( A^{(N)} \right) \left( m \right) = M_{B^{(N)}(B^{(N)})^T A^{(N)}}^{-1} \left( B^{(N)} \right)^T \left( A^{(N)} \right) \left( \frac{r_N}{q_N} m \right).
\]
Consequently,

\[
S_{(A^{(N)})^TB^{(N)}}(m) = \frac{1 + m}{mM^{(-1)}_{(A^{(N)})^TB^{(N)}}(m)}
\]

\[
= \frac{1 + m}{mM^{(-1)}_{B^{(N)}}(m)} \times \frac{1 + \frac{r_N}{q_N}m}{1 + \frac{r_N}{q_N}m}
\]

(A.3)

As \((A^{(N)})^T A^{(N)}\) and \(B^{(N)}(N)^T\) are asymptotically free, taking the limit \(N \to +\infty\) and applying Voiculescu’s Theorem 2.2, we get

\[
S_{(AB)^*AB}(m) = \alpha \frac{1 + m}{1 + \alpha m} S_{BB^*} (\alpha m) S_{A^*A} (\alpha m).
\]

Moreover, the above equality is true replacing \(A\) with the identity \(I\). \(S_I(m) = 1\) yields:

\[
S_{B^*B}(m) = \alpha \frac{1 + m}{1 + \alpha m} S_{BB^*} (\alpha m) .
\]

Finally we have

\[
S_{(AB)^*AB}(m) = S_{A^*A} (\alpha m) S_{B^*B}(m) .
\]

This concludes the proof.

A.2.2. Proof of Theorem 3.1. We assume that \(W_l\) have i.i.d. entries. Thanks to a swapping trick justified in [PS20], we can assume that the matrices \(D_l\) have i.i.d. entries independent from the rest of the network, distributed as \(\phi’(\sqrt{qL})\). Notice that we can also replace the \(D_l\)’s by deterministic matrices that use the quantiles of the same distribution. This together with standard results from FPT such as [MS17] gives asymptotic freeness – see [BC17] for a more general result reflecting the current state of the art. Therefore, we can apply Theorem 2.3.

Starting from Eq. 1.1 in the main paper, we get in the infinite width regime and by induction:

\[
S_{(J^{(N)})^T J^{(N)}}(m) = S_{(D_{(N)}^{L(N)}W_{(N)}^{L(N)}D_{L-1}^{(N)}W_{L-1}^{(N)}\ldots D_1^{(N)}W_1^{(N)})^T D_{(N)}^{L(N)}W_{(N)}^{L(N)}D_{L-1}^{(N)}W_{L-1}^{(N)}\ldots D_1^{(N)}W_1^{(N)}(m)}
\]

\[
= S_{(D_{(N)}^{L(N)}W_{(N)}^{L(N)}D_{L-1}^{(N)}W_{L-1}^{(N)}\ldots D_2^{(N)}W_2^{(N)})^T D_{(N)}^{L(N)}W_{(N)}^{L(N)}D_{L-1}^{(N)}W_{L-1}^{(N)}\ldots D_2^{(N)}W_2^{(N)}D_1^{(N)}(\lambda_1m)}
\]

\[
\times S_{(W_1^{(N)})^T W_1^{(N)}(m)}
\]

\[
= S_{(D_{(N)}^{L(N)}W_{(N)}^{L(N)}D_{L-1}^{(N)}W_{L-1}^{(N)}\ldots D_2^{(N)}W_2^{(N)})^T D_{(N)}^{L(N)}W_{(N)}^{L(N)}D_{L-1}^{(N)}W_{L-1}^{(N)}\ldots D_2^{(N)}W_2^{(N)}(\lambda_1m)}
\]

\[
\times S_{(D_1^{(N)})^2(\lambda_1m)S_{(W_1^{(N)})^T W_1^{(N)}(m)}
\]

\[
\vdots
\]

\[
= \prod_{\ell=1}^L \left[ S_{(D_{(N)}^{\ell})^2} \left( \prod_{k=1}^{\ell} \lambda_k m \right) S_{(W_{(N)}^{\ell})^T W_{(N)}^{\ell}} \left( \prod_{k=1}^{\ell-1} \lambda_k m \right) \right]
\]

\[
= \prod_{\ell=1}^L \left[ S_{(D_{(N)}^{\ell})^2} (\Lambda m) S_{(W_{(N)}^{\ell})^T W_{(N)}^{\ell}} (\Lambda_{\ell-1}m) \right] ,
\]
with the convention \( \Lambda_0 = \prod_{k=1}^{0} \lambda_k = 1 \).

Under the assumption that the entries of \( W_\ell \) are i.i.d., the Marcenko-Pastur Theorem gives

\[
S_{(W^{(N)}_\ell)^T W^{(N)}_\ell}(m) = \frac{1}{\sigma^2_{W_\ell}} \frac{1}{1 + \lambda_m},
\]

which leads to

\[
S_{(J^{(N)})^T J^{(N)}}(m) = \prod_{\ell=1}^{L} \left( S_{(D^{(N)}_\ell)^2} (\Lambda_m) \frac{1}{\sigma^2_{W_\ell}} \frac{1}{1 + \lambda_m} \right).
\]

We thus have

\[
M_{(J^{(N)})^T J^{(N)}}^{(-1)}(m) = \frac{m + 1}{m \prod_{\ell=1}^{L} \left( S_{(D^{(N)}_\ell)^2} (\Lambda_m) \frac{1}{\sigma^2_{W_\ell}} \frac{1}{1 + \lambda_m} \right)}
\]

\[
= \frac{m + 1}{m \prod_{\ell=1}^{L} \sigma^2_{W_\ell} (1 + \lambda_m) \prod_{\ell=1}^{L} S_{(D^{(N)}_\ell)^2} (\Lambda_m)}
\]

\[
= \frac{(m + 1) \prod_{\ell=1}^{L} \sigma^2_{W_\ell} (1 + \lambda_m)}{m \prod_{\ell=1}^{L} S_{(D^{(N)}_\ell)^2} (\Lambda_m)}.
\]

A.3. Moments of \( J \). We can reach an early understanding of the behavior of \( J \)'s singular values by computing mean and variance. For ease of notation, we write:

\[ m_k^{(s)}(A) = m_k(A^T A) \]

for any operator \( A \), which admits a measure of singular values. We have under the assumptions that the entries of \( W_\ell \) are i.i.d.:

\[(A.4) \quad m_1^{(s)}(J) = \prod_{\ell=1}^{L} \left( m_1^{(s)}(D_\ell) m_1^{(s)}(W_\ell) \right) = \prod_{\ell=1}^{L} (c_\ell \sigma^2_{W_\ell}),
\]

\[(A.5) \quad m_2^{(s)}(J) - m_1^{(s)}(J)
\]

\[= m_1^{(s)}(J)^2 \left( \sum_{\ell=1}^{L} \Lambda_\ell \left( \frac{m_2^{(s)}(D_\ell) - m_1^{(s)}(D_\ell)^2}{m_1^{(s)}(D_\ell)^2} + \frac{m_2^{(s)}(W_\ell) - m_1^{(s)}(W_\ell)^2}{m_1^{(s)}(W_\ell)^2} \right) \right)
\]

\[= \left( \prod_{\ell=1}^{L} c_\ell \sigma^4_{W_\ell} \right) \left( \sum_{\ell=1}^{L} \Lambda_\ell \left( \frac{1}{c_\ell} + \lambda_\ell \right) \right).
\]

Under the assumption that \( W^T_\ell W_\ell = \sigma_{W_\ell} I_{N_{\ell-1}} \), we find the same \( m_1^{(s)}(J) \) and:

\[(A.6) \quad m_2^{(s)}(J) - (m_1^{(s)}(J))^2
\]

\[= \sum_{\ell=1}^{L} \left( \Lambda_\ell \left( \frac{m_2^{(s)}(D_\ell)}{m_1^{(s)}(D_\ell)^2} - 2 \right) \right) \prod_{\ell=1}^{L} (c_\ell \sigma^4_{W_\ell})
\]

\[= \sum_{\ell=1}^{L} \left( \Lambda_\ell \left( \frac{1}{c_\ell} - 2 \right) \right) \prod_{\ell=1}^{L} (c_\ell \sigma^4_{W_\ell}).
\]

These formulas need to be interpreted:
Variance grows with $L$, showing increased instability with depth.
Larger layers, relative to $N_0$, give larger $\Lambda_\ell$’s and thus the same effect.

**Proof: Computations of moments.** The following remark is useful in the computation of moments.

**Remark A.1** (Moments). At the neighborhood of $z \sim \infty$:

$$M_\mu(z) = \frac{m_1(\mu)}{z} + \frac{m_2(\mu)}{z^2} + \mathcal{O}(z^{-3})$$

By inversion, at the neighborhood of $m \sim 0$:

$$M_\mu^{(-1)}(m) = \frac{m_1(\mu)}{m} + \mathcal{O}(1)$$

$$M_\mu^{(-1)}(m) = \frac{m_1(\mu)}{m} + \frac{m_2(\mu)}{m_1(\mu)} + \mathcal{O}(m)$$

Hence:

$$S_\mu(m) = \frac{1 + m}{m_1(\mu) + m \frac{m_2(\mu)}{m_1(\mu)} + \mathcal{O}(m^2)}$$

$$= \frac{1}{m_1(\mu)} (1 + m) \left(1 - m \frac{m_2(\mu)}{m_1(\mu)^2} + \mathcal{O}(m^2)\right)$$

$$= \frac{1}{m_1(\mu)} + \frac{m}{m_1(\mu)} \left(1 - \frac{m_2(\mu)}{m_1(\mu)^2}\right) + \mathcal{O}(m^2)$$

Thanks to this, we can prove Eq. (A.4) and (A.5). By Remark A.1 and Theorem 3.1, we have as $m \rightarrow 0$:

$$S_{f_\ell J}(m) = \prod_{\ell=1}^L \left[ S_{D_\ell^2} (\Lambda m) S_{W_\ell} (\Lambda m) \right]$$

$$= \prod_{\ell=1}^L \left[ \left( \frac{1}{m_1(D_\ell)} + m \frac{\Lambda_\ell}{m_1(D_\ell)} \left(1 - \frac{m_2(D_\ell)}{m_1(D_\ell)^2}\right) + \mathcal{O}(m^2)\right) \right.\left. \left( \frac{1}{m_1(W_\ell)} + m \frac{\Lambda_\ell}{m_1(W_\ell)} \left(1 - \frac{m_2(W_\ell)}{m_1(W_\ell)^2}\right) + \mathcal{O}(m^2)\right) \right]$$

$$= \left[ \prod_{\ell=1}^L \frac{1}{m_1(D_\ell)m_1(W_\ell)} \right] \prod_{\ell=1}^L \left[ 1 + m \Lambda_\ell \left(2 - \frac{m_2(D_\ell)}{m_1(D_\ell)^2} - \frac{m_2(W_\ell)}{m_1(W_\ell)^2}\right) + \mathcal{O}(m^2) \right]$$

Identifying the first order term, one finds indeed Eq. (A.4). Continuing the previous computation:

$$S_{f_\ell J}(m) = \frac{1}{m_1(J)} + m \frac{1}{m_1(J)} \left( \sum_{\ell=1}^L \Lambda_\ell \left(2 - \frac{m_2(D_\ell)}{m_1(D_\ell)^2} - \frac{m_2(W_\ell)}{m_1(W_\ell)^2}\right) \right) + \mathcal{O}(m^2)$$

Applying Remark A.1 again for $S_{f_\ell J}$, we get:

$$\sum_{\ell=1}^L \Lambda_\ell \left(2 - \frac{m_2(D_\ell)}{m_1(D_\ell)^2} - \frac{m_2(W_\ell)}{m_1(W_\ell)^2}\right) = 1 - \frac{m_2(J)}{m_1(J)^2}$$

which is equivalent to Eq. (A.5).
We conclude by specializing to classical weight distributions. Under the assumption that the entries of $W_\ell$ are i.i.d. we have $m_1^{(s)}(W_\ell) = \sigma_{W_\ell}^2$ and $m_2^{(s)}(W_\ell) = \sigma_{W_\ell}^4(1 + \lambda_\ell)$ which gives
\[
m_2^{(s)}(J) = \left(1 - \sum_{\ell=1}^{L} \left( \Lambda_\ell \left(1 - \frac{m_2^{(s)}(D_\ell)}{m_1^{(s)}(D_\ell)^2} - \lambda_\ell \right) \right) \right) \prod_{\ell=1}^{L} \left( m_1^{(s)}(D_\ell)^2 \sigma_{W_\ell}^4 \right)
\]
\[
m_2^{(s)}(J) - (m_1^{(s)}(J))^2 = \sum_{\ell=1}^{L} \left( \Lambda_\ell \left( \frac{m_2^{(s)}(D_\ell)}{m_1^{(s)}(D_\ell)^2} + \lambda_\ell - 1 \right) \right) \prod_{\ell=1}^{L} \left( m_1^{(s)}(D_\ell)^2 \sigma_{W_\ell}^4 \right).
\]

\[\square\]

A.4. Details on the experiment and Github repository. Recall that we have provided an anonymized Github repository at the address: https://github.com/redachhaibi/FreeNN

A.4.1. Description of the experiment. Recall that we considered a classical Multi-Layer Perceptron (MLP) with $L = 4$ layers, feed-forward and fully-connected with ReLu non-linearities. The MLP’s architecture is determined by the vector $\lambda = (\lambda_0, \lambda_1, \ldots, \lambda_L)$. The initialization follows the Xavier normal initialization [GB10] as implemented in Pytorch [PGC+17]. The gains of this initialization are determined by the vector $\sigma = (\sigma_1, \sigma_2, \ldots, \sigma_L)$.

First, we sample random architectures. We chose
- the $\lambda_i$ to be i.i.d. and uniform on the segment $[0.25; 1.75]$. As such the mean is $\mathbb{E}\lambda_i = 1$ in order to obtain relatively balanced architectures.
- all the gains $\sigma_i^2$ are taken as a single standard exponential random variable.

Secondly, we compute the spectral distributions predicted by FPT for each random architecture.

Thirdly, we train about 200 instances of MLPs and record the learning curves.

In the end, by considering FPT quantiles and the final train loss for each MLP, we obtain data which amenable to a bivariate statistical analysis. The scatter plots in Figures A.1 and A.2 completes the correlation tables given in the main text.

![FPT quantile at 0.1 vs Loss](image)

**Figure A.1.** Scatter plot of 90th percentile and test loss.
A.4.2. Final remarks. Our sampling procedure does not consider large fluctuations in the $\lambda_i$’s and focuses on balanced architectures. Likewise, the gains at initialization do not deviate much from the classical [GB10]. It is important to recognize that without the insight of FPT, the scalings applied to such initializations are already normalized so that spectral measures do converge.

As such, we never encounter truly problematic gradient vanishing or gradient explosion, which completely sabotage the convergence of the neural network. Our refined FPT metrics are arguably "second order corrections". Nevertheless, it is surprising the 90th percentile in Fig. A.2 highly correlates to the final loss after training. The test loss can double for lower FPT quantiles. In the end, tuning FPT metrics does not amount to second order corrections at the level of the final loss.

References

[AAB+15] Martín Abadi, Ashish Agarwal, Paul Barham, Eugene Brevdo, Zhifeng Chen, Craig Citro, Greg S. Corrado, Andy Davis, Jeffrey Dean, Matthieu Devin, Sanjay Ghemawat, Ian Goodfellow, Andrew Harp, Geoffrey Irving, Michael Isard, Yangqing Jia, Rafal Jozefowicz, Lukasz Kaiser, Manjunath Kudlur, Josh Levenberg, Dan Mané, Rajat Monga, Sherry Moore, Derek Murray, Chris Olah, Mike Schuster, Jonathon Shlens, Benoit Steiner, Ilya Sutskever, Kunal Talwar, Paul Tucker, Vincent Vanhoucke, Vijay Vasudevan, Fernanda Viégas, Oriol Vinyals, Pete Warden, Martin Wattenberg, Martin Wicke, Yuan Yu, and Xiaoqiang Zheng, *TensorFlow: Large-scale machine learning on heterogeneous systems*, 2015, Software available from tensorflow.org.

[ATV+20] Octavio Arizmendi, Pierre Tarrago, Carlos Vargas, et al., *Subordination methods for free deconvolution*, Annales de l’Institut Henri Poincaré, Probabilités et Statistiques, vol. 56, Institut Henri Poincaré, 2020, pp. 2565–2594.

[BC17] Serban T Belinschi and Mireille Capitaine, *Spectral properties of polynomials in independent wigner and deterministic matrices*, Journal of Functional Analysis 273 (2017), no. 12, 3901–3963.

[BG09] Florent Benaych-Georges, *Rectangular random matrices, related convolution*, Probability Theory and Related Fields 144 (2009), no. 3-4, 471–515.

[BGD08] Florent Benaych-Georges and Mérouane Debbah, *Free deconvolution: from theory to practice*, Paradigms for Biologically-Inspired Autonomic Networks and Services (2008), 201–224.
[BSF94] Yoshua Bengio, Patrice Simard, and Paolo Frasconi, *Learning long-term dependencies with gradient descent is difficult*, IEEE transactions on neural networks 5 (1994), no. 2, 157–166.

[CH21] Benoît Collins and Tomohiro Hayase, *Asymptotic freeness of layerwise jacobians caused by invariance of multilayer perceptron: The haar orthogonal case*, arXiv preprint arXiv:2103.13466 (2021).

[GB10] Xavier Glorot and Yoshua Bengio, *Understanding the difficulty of training deep feedforward neural networks*, Proceedings of the thirteenth international conference on artificial intelligence and statistics, 2010, pp. 249–256.

[GT74] WB Gragg and RA Tapia, *Optimal error bounds for the newton–kantorovich theorem*, SIAM Journal on Numerical Analysis 11 (1974), no. 1, 10–13.

[HN19] Boris Hanin and Mihai Nica, *Products of many large random matrices and gradients in deep neural networks*, Communications in Mathematical Physics (2019), 1–36.

[Kan48] LV Kantorovich, *On newton’s method for functional equations*, Dokl. Akad. Nauk SSSR, vol. 59, 1948, pp. 1237–1240.

[LLC+18] Cosme Louart, Zhenyu Liao, Romain Couillet, et al., *A random matrix approach to neural networks*, The Annals of Applied Probability 28 (2018), no. 2, 1190–1248.

[MNN+20] Mylène Maïda, Tien Dat Nguyen, Thanh Mai Pham Ngoc, Vincent Rivoirard, and Viet Chi Tran, *Statistical deconvolution of the free fokker-planck equation at fixed time*, arXiv preprint arXiv:2006.11899 (2020).

[MS17] James A Mingo and Roland Speicher, *Free probability and random matrices*, vol. 35, Springer, 2017.

[MS20] Leonid Pastur, *On random matrices arising in deep neural networks. gaussian case*, arXiv preprint arXiv:2001.06188 (2020).

[PAS+17] Adam Paszke, Sam Gross, Soumith Chintala, Gregory Chanan, Edward Yang, Zachary DeVito, Zeming Lin, Alban Desmaison, Luca Antiga, and Adam Lerer, *Automatic differentiation in pytorch*.

[PLR+16] Ben Poole, Subhaneil Lahiri, Maithra Raghu, Jascha Sohl-Dickstein, and Surya Ganguli, *Exponential expressivity in deep neural networks through transient chaos*, arXiv preprint arXiv:1606.05340 (2016).

[PS20] L. Pastur and V. Slavin, *On random matrices arising in deep neural networks: General i.i.d. case*, 2020.

[PSG18] Jeffrey Pennington, Samuel Schoenholz, and Surya Ganguli, *The emergence of spectral universality in deep networks*, International Conference on Artificial Intelligence and Statistics, 2018, pp. 1924–1932.

[SGGSD16] Samuel S Schoenholz, Justin Gilmer, Surya Ganguli, and Jascha Sohl-Dickstein, *Deep information propagation*, arXiv preprint arXiv:1611.01232 (2016).

[Tar20] Pierre Tarrago, *Spectral deconvolution of unitarily invariant matrix models*, arXiv preprint arXiv:2006.09356 (2020).

[Voi87] Dan Voiculescu, *Multiplication of certain non-commuting random variables*, JSTOR, 1987, pp. 223–235.