Eigenvalue Distribution of Large Random Matrices Arising in Deep Neural Networks: Orthogonal Case

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Abstract

The paper deals with the distribution of singular values of the input-output Jacobian of deep untrained neural networks in the limit of their infinite width. The Jacobian is the product of random matrices where the independent rectangular weight matrices alternate with diagonal matrices whose entries depend on the corresponding column of the nearest neighbor weight matrix. The problem was considered in [26] for the Gaussian weights and biases and also for the weights that are Haar distributed orthogonal matrices and Gaussian biases. Basing on a free probability argument, it was claimed that in these cases the singular value distribution of the Jacobian in the limit of infinite width (matrix size) coincides with that of the analog of the Jacobian with special random but weight independent diagonal matrices, the case well known in random matrix theory. The claim was rigorously proved in [22] for a quite general class of weights and biases with i.i.d. (including Gaussian) entries by using a version of the techniques of random matrix theory. In this paper we use another version of the techniques to justify the claim for random Haar distributed weight matrices and Gaussian biases.

1 Introduction

Artificial neural networks is an emerging and quite efficient technique with a wide variety of applications, see, e.g. [1] [2] [3] [8] [10] [12] [30] [33]. One of the basic ingredients of the networks is the iterative scheme

$$x^l := \{x^l_{ji}\}_{j_i=1}^{n_i}, \quad x^l_{ji} = \varphi(y^l_{ji}), \quad y^l := W^l x^{l-1} + b^l, \quad l = 1, \ldots, L,$$  \hspace{1cm} (1.1)

where

$$x^0 := \{x^0_{j0}\}_{j_0=1}^{n_0} \in \mathbb{R}^{n_0}$$  \hspace{1cm} (1.2)

is the data input to the network,

$$x^L := \{x^L_{jL}\}_{j_L=1}^{n_L} \in \mathbb{R}^{n_L}$$  \hspace{1cm} (1.3)

is its output,

$$W^l := \{W^l_{ji,j_{i-1}}\}_{j_i,j_{i-1}=1}^{n_i,n_{i-1}}, \quad l = 1, \ldots, L$$  \hspace{1cm} (1.4)
are \( n_l \times n_{l-1} \) rectangular synaptic weight matrices,

\[ b^l := \{ b_{jl} \}_{j=1}^{n_l}, \quad l = 1, \ldots, L \]  

(1.5)

are \( n_l \)-component bias vectors of the \( l \)th layer, \( n_l \) is the width of the \( l \)th layer, \( \varphi : \mathbb{R} \to \mathbb{R} \) is the component-wise nonlinearity (activating function) and \( L \) is the depth of the network. If \( L > 1 \), then it is a deep neural network (DNN).

Another basic ingredient of the DNN is the training which modifies the parameters (weight matrices \( W^l \) and biases \( b^l \)) on every step of the iterative scheme in order to reduce the misfit between the output data and the prescribed data by using a certain optimization procedure (based often on a version of least square method). Being multiply repeated in the DNN, the procedure provides an output \( x^L \) (a recognized pattern, a translated text, etc.) but also certain final parameters \( W^L \) and \( b^L \), which could have a quite non-trivial structure, see e.g. \[12\].

It is important for this paper that the theory deals also with untrained and/or random parameters of the DNN architecture, see, e.g. \[5, 7, 11, 13, 26, 28, 31, 34, 37\] and references therein. It is assumed in these works that the weight matrices and the bias vectors are independent and identically distributed (i.i.d.) in \( l \).

An important characteristic of the DNN is the input-output Jacobian (see \[26\] and references therein)

\[ J^L_{n_l} := \left\{ \frac{\partial x^L_{j_l}}{\partial x^0_{j_0}} \right\}_{j_0, j_l=1}^{n_l} = \prod_{l=1}^{L} D^l_{n_l} W^l_{n_l}, \quad n_L = \{ n_l \}_{l=1}^{L}, \]  

(1.6)

the \( n_L \times n_0 \) random matrix, where

\[ D^l_{n_l} := \{ D^l_{j_l k_l} \}_{j_l, k_l=1}^{n_l} = \varphi' \left( \sum_{j_{l-1}=1}^{n_l} W_{j_l j_{l-1}}^{l-1} x_{j_{l-1}}^{l-1} + b^l_{j_l} \right), \quad l = 1, \ldots, L \]  

(1.7)

are diagonal random matrices and \( n_L := \{ n_l \}_{l=1}^{L} \).

Having in mind that the widths \( n_L := \{ n_l \} \) of layers are usually large, one looks for the characteristics of Jacobian that are well defined in this asymptotic regime. Since the spectral properties of the Jacobian are strongly correlated with the success of training, one of such characteristics is the distribution of the singular values of \( J^L_{n_l} \), i.e., the square roots of eigenvalues of the \( n_L \times n_L \) positive definite matrix

\[ M^L_{n_l} := J^L_{n_l} (J^L_{n_l})^T, \]  

(1.8)

for networks with random weights and biases and for large widths of layers, see \[11, 13, 25, 26, 28, 31, 34, 37\] for various motivations, settings and results. More precisely, one studies the asymptotic regime determined by the simultaneous limits

\[ \lim_{n_l \to \infty} \frac{n_{l-1}}{n_l} = c_l \in (0, \infty), \quad n_l \to \infty, \quad l = 1, \ldots, L. \]  

(1.9)

Note, however, that many principal results and difficulties in their proofs are practically the same for the case of distinct \( n_l \to \infty, \quad l = 1, \ldots, L \) in (1.9) and for that where

\[ n := n_l = \cdots = n_L. \]  

(1.10)

Thus, we confine ourselves to this case writing everywhere below \( n \) instead of \( n_L \).
Denote \( \{\lambda_l^i\}_{i=1}^n \) the eigenvalues of the random matrix (1.8) and introduce its *Normalized Counting Measure (NCM)*

\[
\nu_{M^L} := n^{-1} \sum_{t=1}^n \delta_{\lambda_t^L}.
\]  

(1.11)

We will deal with the limit

\[
\nu_{M^L} := \lim_{n \to \infty} \nu_{M_n^L}.
\]  

(1.12)

Note that since \( \nu_{M_n^L} \) is a random measure, the meaning of the limit has to be indicated.

The problem has been considered in [26] (see also [1, 9, 11, 21, 25, 34, 37]) for two cases:

(i) \( b_l^i, l = 1, 2, \ldots, L \) are \( n \)-component random vectors i.i.d. in \( l \) and having i.i.d. Gaussian components and \( W_l^i, l = 1, 2, \ldots, L \) are \( n \times n \) random matrices i.i.d. in \( l \) and having i.i.d. Gaussian entries (see [22] for more general i.i.d. components and entries);

(ii) \( b_l^i, l = 1, 2, \ldots, L \) are as in (i) and \( W_l^i = O_l^i n \), \( l = 1, 2, \ldots, L, \) \( (1.13) \)

where \( O_l^i n \in SO(n) \), \( l = 1, 2, \ldots, L \) are \( n \times n \) random orthogonal matrices independent in \( l \) and having the normalized to unity Haar measure on \( SO(n) \) as its probability measure.

This paper deals with the case (ii).

In [26] compact formulas for the limit of the expectation

\[
\nu_{M^L} := \lim_{n \to \infty} \nu_{M_n^L}, \quad \nu_{M_n^L} := E\{\nu_{M_n^L}\}
\]  

(1.14)

of the NCM (1.11) and its Stieltjes transform

\[
f_{M^L}(z) := \int_0^\infty \frac{\nu_{M^L}(d\lambda)}{\lambda - z}, \quad z \in \mathbb{C} \setminus \mathbb{R}^+.
\]  

(1.15)

were proposed for both cases (i) and (ii) above. The formula for \( \nu_{M^L} \) in the case (ii) is given in (2.15) below. To write the formula for \( f_{M^L} \) in the case (ii) it is convenient to introduce the moment generating function

\[
m_{M^L}(z) := \sum_{k=1}^{\infty} m_k z^k, \quad m_k := \int_0^\infty \lambda^k \nu_{M^L}(d\lambda),
\]  

(1.16)

of \( \nu_{M^L} \) related to \( f_{M^L} \) as

\[
m_{M^L}(z) = -1 - z^{-1} f_{M^L}(z^{-1}).
\]  

(1.17)

Let

\[
K_n^i := (D_n^i)^2 = \{(D_{ji}^i)^2\}_{j=1}^n \]  

(1.18)

be the square of the \( n_l \times n_l \) random diagonal matrix (1.7) and let \( m_{K_l^i} \) be the moment generating function of the \( n \to \infty \) limit \( \nu_{K_l^i} \) of the expectation \( \nu_{K_l^i} \) of the NCM \( \nu_{K_l^i} \) of \( K_n^i \) (see (2.16)). Then we have according to formulas (14) and (16) in [26] in the case where \( \nu_{K_l^i} \), hence, \( m_{K_l^i} \) do not depend on \( l \) (see Remark 2.2 (i))

\[
m_{M^L}(z) = m_{K_l^i}((z^{1/L}) \Psi_L(m_{M^L}(z))),
\]  

\[
\Psi_L(z) = ((1 + z)/z)^{1-1/L}.
\]  

(1.19)
In other words, $m_{ML}$, hence, $f_{ML}$ of (1.15) – (1.17), satisfy a certain functional equation, the standard situation in random matrix theory and its applications, see e.g. [6, 15, 19, 20, 23] and formulas (3.12) – (3.14) below. Note that our notation is different from that of [26]: our $f_{ML}(z)$ of (1.15) is $-G_X(z)$ of (7) in [26] and our $m_{ML}(z)$ of (1.16) is $M_X(1/z)$ of (9) in [26].

These and other related results are obtained in [26] by using the claimed in this work asymptotic freeness of the diagonal matrices $D^l_n$, $l = 1, \ldots, L$ of (1.7) and the matrices $O^l$, $l = 1, \ldots, L$ of (1.11) and (1.13) (see, e.g. [4, 16] for the definitions and properties of asymptotic freeness). This leads directly to (2.15) and (1.19) in view of the multiplicative property of the moment generating functions (1.16) and the so-called $S$-transforms of $\nu_{K^l}$ and of $\nu_{O^l(O^l)^T}$, the mean limiting NCM’s of $R^l_n$ and of $O^l_n(O^l_n)^T$, also see Remark 2.2 (i) and Corollary 3.4.

There is, however, a subtle point in the claim made in [26]. Indeed, to the best of our knowledge the asymptotic freeness has been established so far for the random Gaussian and orthogonal random matrices $W^l$ and deterministic (more generally, random but $W^l$-independent) diagonal matrices, see e.g. the recent book [16], Chapters 1 and 4. On the other hand, the diagonal matrices $D^l_n$ in (1.7) depend explicitly on $(W^l, b^l_n)$ of (1.4) – (1.5) and, implicitly, via $x^{-l}$, on the all "preceding" $(W^{l'}, b^l_n)$, $l' = l - 1, \ldots, 1$. Thus, the proof of validity of (2.15) and (1.19) requires an additional argument. It was given in [21] for the Gaussian weights and biases and in [22] for a wide class of weights and biases with i.i.d. but not necessarily Gaussian entries and components. In this paper we justify the results of [26] for the orthogonal weights of (1.13) and Gaussian biases with i.i.d. components (for more general biases see Remark 3.11 below).

It is also worth noting that we prove that formula (1.12) is valid not only in the mean (see (1.14) and [26]), but also with probability 1 (recall that the measures in the r.h.s. of (1.12) are random) and that the limiting measure $\nu_{ML}$ in the l.h.s. of (1.12) coincides with $\nu_{ML}$ of (1.14), i.e., $\nu_{ML}$ is non-random.

Our approach is an updated version of that developed in [23], Sections 8 – 10 for the spectral analysis of random matrices whose randomness is due the classical compact groups viewed as probability spaces with the normalized to unity Haar measure. This shows that the matrices (1.8) are in the scope of random matrix theory, especially that part of the theory which was created by Dyson in the 1960s. Note that the justification of results of [26] for matrices with Gaussian and more general i.i.d. weight entries and bias components, given in [21] [22], is based an appropriately updated version of the tools of random matrix theory presented in [23], Chapter 7, 18 and 19, although this version and that of this paper are borrowed from different parts of random matrix theory and have not too much in common.

An additional motivation of the paper is that according to [26], the tight concentration of the entire spectrum of singular values of the input-output Jacobian (1.6) around the point 1 of the spectral axis can considerably enhance the efficiency of the network in question, especially on the initial steps of iteration procedure (see also [9, 11, 34]), and that the orthogonal weights provide this property most simply.

The paper is organized as follows. In the next section we prove the validity of (1.12) with probability 1, formulas (2.15) for $\nu_{ML} = \nu_{ML}$ and (1.19) of [26]. The proof is based on a natural inductive procedure allowing for the passage from the $l$th to the $(l + 1)$th layer and it is fairly similar to that in [21] [22]. This is because the passage procedure is almost independent of the probability properties of the weight entries provided that a formula relating the limiting (in the layer width) Stieltjes transforms of the NCM’s of two subsequent layers is known. This formula and a number of auxiliary results are proved in Section 3.

Note that to make the paper self-consistent we present here certain facts and arguments that have been already given in [21] [22], thus the paper is in part a review of these works.
2 Main Result and its Proof.

As was already mentioned in Introduction, the goal of the paper is to justify the results of [26] for the independent in $l$ and the Haar distributed orthogonal weights $O^l$'s and the independent in $l$ biases $b^l$'s with independent Gaussian components (see Remark 3.11 for more general biases).

More precisely, we consider the case of (1.2) – (1.5) where:

(i) all $b^l_n$ and $W^l_n$, $l = 1, \ldots, L$ in (2.1) – (2.2) are of the same size $n$ and $n \times n$ respectively, i.e., (1.10) holds true;

(ii) the bias vectors $b^l_n = \{b^l_{ji}\}_{ji=1}^n$, $l = 1, 2, \ldots, L$ are random i.i.d. in $l$ and for every $l$ their components are i.i.d Gaussian random variables with

$$E_b\{b^l_{ji}\} = 0, \quad E_b\{(b^l_{ji})^2\} = \sigma_b^2 > 0,$$

where $E_b\{\ldots\}$ denotes the expectation in the probability space of $b^l$;

(iii) the weight matrices $W^l_n$, $l = 1, 2, \ldots, L$ are also i.i.d in $l$ and for every $l$

$$W^l_n = O^l_n = \{O^l_{ji\bar{i}-1}\}_{ji\bar{i}=1}^n,$$

where $O^l_n$ is the random matrix with values in the group $SO(n)$ of orthogonal and unimodular ($\det O^l_n = 1$) matrices. The group plays the role of the probability space and the normalized to unity Haar measure on the group plays the role of the probability measure. In particular, we have

$$E_{O^l}\{O^l_{ji\bar{i}-1}\} = 0, \quad E_{O^l}\{O^l_{ji_1\bar{i}_1-1}O^l_{ji_2\bar{i}_2-1}\} = n^{-1}\delta_{ji_1\bar{i}_2}\delta_{ji_2\bar{i}_1} - \delta_{ji_1\bar{i}_2} - \delta_{ji_2\bar{i}_1},$$

where $E_{O^l}\{\ldots\}$ denotes the expectation with respect to the normalized to unity Haar measure on $SO(n)$.

For every $l$ we view $b^l_n$ as the first $n$ components of the semi-infinite random vector

$$\{b^l_{ji}\}_{ji=1}^\infty$$

whose independent Gaussian components satisfy (2.1) and we denote $\Omega_{b^l}$ the infinite-dimensional (product) probability space for (2.4).

Next, it follows from Proposition 3.5 (iii) that there exists an analogous infinite-dimensional space for the sequence

$$\{O^l_n\}_{n=1}^\infty.$$

We denote this space by $\Omega_{O^l}$ and by $E_{O^l}\{\ldots\}$ the expectation in this space.

As a result of the above construction of the infinite-dimensional probability spaces for weights and biases of the $l$th layer they are now defined for all $n = 1, 2, \ldots$ on the same infinite-dimensional product probability space

$$\Omega^l = \Omega_{b^l} \times \Omega_{O^l}.$$

Let also

$$\Omega_L = \Omega^L \times \Omega^{L-1} \times \cdots \times \Omega^1$$

be the infinite-dimensional probability space on which the recurrence (1.1) is defined for a given depth $L$. This will allow us to formulate various results on the large size asymptotic behavior of the eigenvalue distribution of matrices (1.8) as those valid with probability 1 in $\Omega_L$. We will denote $E\{\ldots\}$ the expectation in $\Omega_L$. 

5
In fact, it was argued in [26] for the Gaussian and the orthogonal weights (and proved in [21, 22] for the weights with the Gaussian and the i.i.d. entries) that the resulting eigenvalue distribution of random matrices (1.8) coincides with that of matrices of the same form where, however, the analogs of diagonal matrices (1.7) are random but independent of $W^l$. In this paper we prove an analogous result for orthogonal weights. Thus, we formulate first the corresponding results of random matrix theory which are largely known (see, e.g. [23], Section 10.4, [35], [24] and references therein)

Consider for every positive integer $n$: (i) the $n \times n$ random Haar distributed over the group matrices $O_n \in O(n)$ (see (2.2) – (2.3)) and defined for all $n$ of the same probability space $\Omega_O$ (see (2.5)); (ii) the $n \times n$ positive definite matrices $K_n$ and $R_n$ (that may also be random but independent of $O_n$ and defined on the same probability space $\Omega_{KR}$ for all $n$ (cf. (2.5))) and such that their Normalized Counting Measures $\nu_{K_n}$ and $\nu_{R_n}$ (see (1.11)) converge weakly (with probability 1 if random) as $n \to \infty$.

\begin{align*}
\nu_{K_n} \to \nu_K, \quad \nu_{R_n} \to \nu_R, \quad n \to \infty. 
\end{align*}

(2.8)

Set

\begin{align*}
M_n = K_n^{1/2} O_n R_n O_n^T K_n^{1/2}.
\end{align*}

(2.9)

According to random matrix theory (see, e.g. [23], Section 10.4, [24, 35] and Lemma 3.8 below), in this case and under certain conditions on $K_n$ and $R_n$ the Normalized Counting Measure $\nu_{M_n}$ of $M_n$ converges weakly with probability 1 (on $\Omega_O \times \Omega_{KR}$) as $n \to \infty$ to a non-random measure $\nu_M$ which is uniquely determined by the limiting measures $\nu_K$ and $\nu_R$ of (2.8) via a certain analytical procedure (see, e.g. formulas (1.15) and (3.12) – (3.14) below).

We can write down symbolically this fact as

\begin{align*}
\nu_M = \nu_K \boxtimes \nu_R
\end{align*}

(2.10)

to stress that the procedure defines a binary operation in the set of non-negative measures of total mass 1 and of support belonging to the positive semi-axis (see more in Corollary 3.4). The operation was studied in detail in free probability, [16], having the above random matrices as a basic analytic model, and is known there as the free multiplicative convolution.

It follows from [26] that the limiting Normalized Counting Measure (1.12) of random matrices (1.8), where the role of $K_n$ plays the matrix (1.13) that depends on matrices $O^l$’s of (2.2), can be found as the "product" with respect the operation (2.10) of $L$ measures $\nu_{K_l}$, $l = 1, \ldots, L$ which are the limiting Normalized Counting Measures of random matrices of (1.18) - (1.7) given in (2.16) - (2.17). This claim can be reformulated as follows. Write (1.8) with $W^l = O_n^l$, $l = 1, \ldots, L$ in (1.6) - (1.7) as

\begin{align*}
M_n^l = D_n^l O_n^l M_n^{l-1}(O_n^l)^T D_n^l
\end{align*}

(2.11)

and observe that $M_n^{l-1}$ is random but independent of $O_n^l$, hence can play the role of $R_n$ in (2.9). Thus, to be able to write (2.10), we have to assume that $D_n^l$ of (1.7) can be replaced by

\begin{align*}
D_n^l = \{D_n^l\delta_{jk}\}_{j,k=1}^n, \quad D_n^l = \varphi'\left((O_n^l x^{l-1})_j + b_n^l\right), \quad l = 1, \ldots, L,
\end{align*}

(2.12)

where $O_n^l$, $l = 1, \ldots, L$ are Haar distributed orthogonal matrices that are independent of $O_n^l$, $l = 1, \ldots, L$.

The goal of the paper is to justify this replacement in the limit $n \to \infty$ for the widths of layers.
Theorem 2.1 Let $M_n^L$ be the random matrix (1.8) defined by (1.1) – (1.7) and (1.10), where the weights $\{O_i^l\}_{l=1}^\infty$ are i.i.d. in $l$ and are $n \times n$ Haar distributed orthogonal matrices for every $n$ (see (2.2) – (2.3) and (2.4)), the biases $\{b_i^l\}_{l=1}^\infty$ are i.i.d. in $l$ and are $n$-component vectors with independent Gaussian components (see (2.1) and (2.4)) for every $n$ and the input vector $x_0^0$ (1.3) (deterministic or random) is such that there exists a finite limit

$$q^0 := \lim_{n \to \infty} q_n^0 > 0, \quad q_n^0 = n^{-1} \sum_{j=0}^n (x_j^0)^2 + \sigma_b^2.$$

(2.13)

Assume also that the $n$-independent nonlinearity $\varphi$ in (1.1) has a piece-wise differential derivative $\varphi'$ which is not zero identically and

$$\sup_{t \in \mathbb{R}} |\varphi(t)| = \Phi_0 < \infty, \quad \sup_{t \in \mathbb{R}} |\varphi'(t)| = \Phi_1 < \infty.$$  

(2.14)

Then the Normalized Counting Measure (NCM) $\nu_{M_n^L}$ of $M_n^L$ (see (1.11)) converges weakly with probability 1 in the probability space $\Omega_L$ of (2.7) to the non-random measure

$$\nu_{M_n^L} = \nu_{KL} \otimes \cdots \otimes \nu_{K1} \otimes \delta_1,$$

(2.15)

where the operation "$\otimes$" is the free multiplicative convolution, given in (2.10) (see also [4, 16] and Corollary 3.4 below), $\delta_1$ is the unit measure concentrated at 1 and

$$\nu_{K}((\Delta)) = \mathbb{P}\{((\varphi'(q_n-1)^{1/2}q)^2) \in \Delta\}, \quad \Delta \in \mathbb{R}, \quad l = 1, \ldots, L,$$

(2.16)

with the standard Gaussian random variable $\gamma$ and $q_l$ determined by the recurrence

$$q_l = (2\pi)^{-1/2} \int_{-\infty}^{\infty} \varphi^2(\gamma \sqrt{q_{l-1}}) e^{-\frac{\gamma^2}{2}} d\gamma, \quad l \geq 1,$$

(2.17)

where $q^0$ is given by (2.13).

Remark 2.2 (i) If

$$q_{L-1} = \cdots = q_0,$$

(2.18)

then $\nu_K := \nu_{ Kl}, \quad l = 1, \ldots, L$ and (2.15) becomes

$$\nu_{M_n^L} = \nu_K \otimes \cdots \otimes \nu_K \otimes \delta_1.$$  

(2.19)

An important case of (2.18) is where $q^0 = q^*$ and $q^*$ is a fixed point of (2.17), see [13, 28, 31] for a detailed analysis of (2.17) and its role in the deep neural networks setting.

(ii) If the input vectors (1.2) are random, then it is necessary to assume that they are defined on the same probability space $\Omega_{x^0}$ for all $n$ and that (2.13) is valid with probability 1 in $\Omega_{x^0}$, i.e., there exists

$$\Omega_{x^0} \subset \Omega_{x^0}, \quad \mathbb{P}\{\Omega_{x^0}\} = 1$$

(2.20)

where (2.13) holds. It follows then from the Fubini theorem that in this case the set $\Omega_L \subset \Omega_{x^0}, \quad \mathbb{P}\{\Omega_L\} = 1$ where Theorem 2.1 holds has to be replaced by the set $\Omega_{Lx^0} \subset \Omega_L \times \Omega_{x^0}, \quad \mathbb{P}\{\Omega_{Lx^0}\} = 1$. An example of this situation is where $\{x_j^0\}_{j=1}^n$ are the first $n$ components of an ergodic sequence (e.g. a sequence of i.i.d. random variables) with finite fourth moment. Here $q^0$ in (2.13) exists with probability 1 on the corresponding $\Omega_{x^0}$ and even is non-random just by ergodic theorem (the strong Law of Large Numbers in the case of i.i.d. sequence) and the theorem is valid with probability 1 in $\Omega_L \times \Omega_{x^0}$.
We present now the proof of Theorem 2.1.

**Proof.** We prove the theorem by induction in $L$. We have from (1.1) – (1.8) and (1.10) with $L = 1$ the following $n \times n$ random matrix

$$M^1_n = J^1_n J^1_n = D^1_n O^1_n O^1_n D^1_n = (D^1_n)^2 := K^1_n. \quad (2.21)$$

The matrix is a particular case with $R_n = 1_n$ of matrix (3.1) treated in Theorem 3.1 below. Since the NCM of $1_n$ is the Dirac measure $\delta_1$, conditions (3.2) – (3.3) of the theorem are evident. Condition (3.9) is just (2.13). It follows then from Corollary 3.4 that the assertion of our theorem, i.e., formula (2.15) with $q^0$ of (2.13), is valid for $L = 1$.

Consider now the case $L = 2$ of (1.1) – (1.8) and (1.10):

$$M^2_n = D^2_n O^2_n M^1_n (O^2_n)^T D^2_n, \quad (2.22)$$

Observe that the matrix is a particular case of matrix (3.1) of Theorem 3.1 with $M^1_n$ of (2.21) as $R_n, O^2_n$ as $O_n, D^2_n$ as $D_n$, $\{x_{j_1}\}_{j_1=1}^n$ as $\{x_{\alpha n}\}_{\alpha=1}^n$, $\Omega_1 = \Omega^1$ of (2.7) as $\Omega_{Rx}$ and $\Omega^2$ of (2.7) as $\Omega_{Ob}$, i.e., the case of the random but $\{O^2_n, b^2_n\}$ - independent $R_n$ and $\{x_{\alpha n}\}_{\alpha=1}^n$ in (3.1) as described in Remark 3.2 (i). Let us check that conditions (3.2) – (3.3) and (3.9) of Theorem 3.1 are satisfied for $M^2_n$ of (2.22) with probability 1 in the probability space $\Omega_1 = \Omega^1$ generated by $\{O^1_n, b^1_n\}$ for all $n$ and independent of the space $\Omega^2$ generated by $\{O^2_n, b^2_n\}$ for all $n$ (see (2.7)).

We will use the bounds:

$$||D^1_n|| \leq \Phi_1, \quad (2.23)$$

following from (1.7) and (2.14) and valid everywhere in $\Omega_1$ of (2.7) and

$$| \text{Tr} AB | \leq ||A|| \text{Tr} B, \quad (2.24)$$

valid for any matrix $A$ and a positive definite matrix $B$. According to the bounds, we have everywhere in $\Omega_1$:

$$n^{-1} \text{Tr} (M^1_n)^2 = n^{-1} \text{Tr} (K^1_n)^2 \leq \Phi_1^4. \quad (2.25)$$

We conclude that $M^1_n$, that plays here the role of $R_n$ of Theorem 3.1 and Remark 3.2 (i) according to (2.22), satisfies condition (3.2) with $r_2 = \Phi_1^4$ and with probability 1 in our case, i.e., on a certain $\Omega_{12} \subset \Omega_1$, $P(\Omega_{12}) = 1$.

Next, it follows from the above proof of the theorem for $L = 1$, i.e., in fact, from Theorem 3.1 that there exists $\Omega_{12} \subset \Omega_1$, $P(\Omega_{12}) = 1$ on which the NCM $\nu_{\Omega_{12}}$ converges weakly to a non-random limit $\nu_{\Omega_1}$, hence condition (3.3) is also satisfied with probability 1, i.e., on $\Omega_{12}$.

At last, according to Lemma 3.10 with $l = 1$ and (2.13), there exists $\Omega_{13} \subset \Omega_1$, $P(\Omega_{13}) = 1$ on which there exists

$$\lim_{n \to \infty} n^{-1} \sum_{j_1=1}^n (x_{j_1}^1)^2 + \sigma_b^2 = q^1 > \sigma_b^2,$$

and according to (1.1) and (2.14) we have uniformly in $n$: $|x_{j_1}^1| \leq \Phi_0$, $j_1 = 1, \ldots, n$, i.e., condition (3.9) is also satisfied.

Hence, we can apply Theorem 3.1 and Corollary 3.4 on the subspace

$$\overline{\Omega}_1 = \Omega_{11} \cap \Omega_{12} \cap \Omega_{13} \subset \Omega_1, \quad P(\overline{\Omega}_1) = 1$$

where all the conditions of the theorem are valid, i.e., $\overline{\Omega}_1$ plays the role of $\Omega_{Rx}$ of Remark 3.2 (i). The theorem implies that for every $\omega_1 \in \overline{\Omega}_1$ there exists subspace $\overline{\Omega}^2(\omega_1)$ of the space $\Omega^2$ generated
by \( \{O_n^2, b_n^2\} \) for all \( n \) and such that \( P(\Omega^2(\omega_1)) = 1 \) and formulas (2.15) - (2.17) are valid for \( L = 2 \). Then the Fubini theorem implies that the same is true on a certain \( \Omega_2 \subset \Omega_2, \ P(\Omega_2) = 1 \) where \( \Omega_2 \) is defined by (2.7) with \( L = 2 \).

This proves the theorem for \( L = 2 \). The proof for \( L = 3, 4, \ldots \) is analogous, since in general \( M_n^L \) and \( M_n^{L-1} \) are related by (2.11), hence \( M_n^{L-1} \) plays the role of \( R_n \) of Theorem 3.1. In particular, we have from (2.23) - (2.24) with \( L = 2 \)

\[
n^{-1} \text{Tr}(M^L)^2 \leq \Phi_1^4 n^{-1} \text{Tr}(M^{L-1})^2 \leq \Phi_1^{4L}, \quad L \geq 1.
\]

If \( x_0 \) is random, then it is necessary to add the argument given in Remark 2.2 (ii).

It follows then form Theorem 3.1 and Corollary 3.4 that the binary operation relating the limiting measures \( \nu_{M^L}, \nu_{K^L} \) and \( \nu_{M^{L-1}} \), hence, implying (2.15), is indeed the free multiplicative convolution given in (2.9) - (2.10).

The derivation of the functional equation (1.19) is given in [26].

Note that the above part of this section is rather close to that of Section 2 of [22] and is given here to make the paper more self-consistent.

An important property of the network Jacobian (1.6) is the tight concentration of its singular value spectrum, i.e., the spectrum of (1.8), around the point 1 of the spectral axis. This property of DNN is known as the dynamical isometry and implies that the corresponding Jacobian is well-conditioned, see [9, 11, 26, 34] and references therein. It is indicated in these works that the networks with the Gaussian weights \( W \)'s do not possess this property while the networks with orthogonal weights and certain non-linearities can achieve the dynamical symmetry as the depth \( L \) increases.

\[3\] Auxiliary Results.

Theorem 2.1 of previous section is proved by induction in the depth \( L \) of the network, see formulas (2.22) and (2.11). To pass from the depth \( (L - 1) \) to that \( L \) we need a formula relating the limiting NCM \( \nu_{M^L} \) of the matrix \( M_n^L \) and that \( \nu_{M^{L-1}} \) of \( M_n^{L-1} \) in the infinite width limit \( n \to \infty \). The corresponding result, Theorem 3.1, which could be of independent interest, as well as certain auxiliary results are proved in this section. In particular, functional equations relating the Stieltjes transforms of \( \nu_{M^L} \) and \( \nu_{M^{L-1}} \) in the limit \( n \to \infty \) are obtained (see (3.12) - (3.14)).

**Theorem 3.1** Consider for every positive integer \( n \) the \( n \times n \) random matrix

\[
M_n = D_n O_n R_n O_n^T D_n,
\]

where:

(a) \( R_n \) is a positive definite \( n \times n \) matrix such that

\[
\sup_n n^{-1} \text{Tr} R_n^2 = r_2 < \infty
\]

and

\[
\lim_{n \to \infty} \nu_{R_n} = \nu_R, \quad \nu_R(\mathbb{R}_+) = 1,
\]

where \( \nu_{R_n} \) is the Normalized Counting Measure of \( R_n \), \( \nu_R \) is a non-negative measure not concentrated at zero and \( \lim_{n \to \infty} \) denotes the weak convergence of probability measures;
On is the $n \times n$ orthogonal Haar distributed random matrix (see (2.2)), $b_n$ is the $n$-component random vector

$$b_n = \{b_j\}_{j=1}^n, \ E\{b_j\} = 0, \ E\{b_j^2\} = \sigma_b^2$$

(3.4)

with independent Gaussian components (see (2.1)) and for all $n$ the matrices $O_n$ and the vectors $b_n$ are viewed as defined on the same probability space

$$\Omega_{Ob} = \Omega_O \times \Omega_b,$$

(3.5)

where $\Omega_O$ and $\Omega_b$ are generated by (2.3) and (2.4);

(c) $D_n$ is the diagonal random matrix

$$D_n = \{\delta_{jk}D_{jn}\}_{j,k=1}^n, \ D_{jn} = \psi\left((O_nN)_{jn} + b_j\right),$$

(3.6)

where $\psi : \mathbb{R} \to \mathbb{R}$ is a piecewise continuous function that is not identically zero and such that

$$\sup_{x \in \mathbb{R}} |\psi(x)| = \Psi < \infty,$$

(3.7)

and the collection

$$x_n = \{x_{n\alpha}\}_{\alpha=1}^n \in \mathbb{R}_n$$

(3.8)

admits the limit

$$q = \lim_{n \to \infty} q_n > \sigma_b^2 > 0, \ q_n = n^{-1} \sum_{\alpha=1}^n (x_{n\alpha})^2 + \sigma_b^2.$$

(3.9)

Denote (cf. (1.18))

$$K_n = D_n^2.$$

(3.10)

Then the Normalized Counting Measure (NCM) $\nu_{M_n}$ of $M_n$ converges weakly with probability 1 in $\Omega_{Ob}$ of (3.5) to a non-random measure $\nu_M$, such that $\nu_M(\mathbb{R}) = 1$ and its Stieltjes transform

$$f_M(z) = \int_0^\infty \frac{\nu_M(d\lambda)}{\lambda - z}, \ z \in \mathbb{C} \setminus \mathbb{R}_+$$

(3.11)

can be obtained from a unique solution $(f_M, h_K, h_R)$ of the system of functional equations

$$(1 + zf_M(z))f_M(z) - h_K(z)h_R(z) = 0,$$

(3.12)

$$f_R(zf_M(z)/h_K(z)) = h_K(z),$$

(3.13)

$$f_K(zf_M(z)/h_R(z)) = h_R(z),$$

(3.14)

where $f_R$ and $f_K$ are the Stieltjes transforms of $\nu_R$ and $\nu_K$, $\nu_R$ is defined in (3.3) and

$$\nu_K(\Delta) = P\{(\psi(q^{1/2}\gamma + b_1))^2 \in \Delta\}, \ \Delta \in \mathbb{R},$$

(3.15)

with $q$ is given by (3.2), $\gamma$ is the standard Gaussian random variable. The system (3.12) – (3.14) is uniquely solvable in the class of triple $(f_M, h_K, h_R)$ of functions analytic outside the closed positive semi-axis, continuous and positive on the negative semi-axis and such that

$$\Re f(z) \Re z > 0, \ \Re z \neq 0; \ \sup_{\xi \geq 1} \xi f(-\xi) \in (0, \infty), \ f = f_M, h_K, h_R.$$  

(3.16)
Remark 3.2 To apply Theorem 3.1 to the proof of Theorem 2.1 we need a version of the former in which its "parameters", i.e., $R_n$ in \((3.1) - (3.3)\), (possibly) $\{x_{\alpha n}\}_{\alpha=1}^n$ in \((3.6)\) and $q$ in \((3.9)\) are random, defined for all $n$ on the same probability space $\Omega_{Rx}$, independent of $\Omega_{Ob}$ of \((3.4)\) and satisfying conditions \((3.2) - (3.3)\) and \((3.9)\) with probability 1 in $\Omega_{Rx}$, i.e., on a certain subspace (cf. \((2.20)\))

$$\Omega_{Rx} \subset \Omega_{Rx}, \quad P(\Omega_{Rx}) = 1.$$ \tag{3.17}

In this case Theorem 3.1 is valid with probability 1 in $\Omega_{Ob} \times \Omega_{Rx}$. The corresponding argument is standard in random matrix theory, see, e.g. of \([23]\)), Section 2.3 and Remark 2.2 (ii). The obtained limiting NCM $\nu_M$ is random in general due to the (possible) randomness of $\nu_R$ and $q$ in \((3.3)\) and \((3.9)\) which are defined on the probability space $\Omega_{Rx}$ (but do not depend on $\omega \in \Omega_{Ob}$). Note, however, that in the case of Theorem 2.1 the analogs of $\nu_R$ and $q$ are not random, thus the limiting measure $\nu_{M^n}$ is non-random as well.

Proof. Write \((3.1)\) as

$$M(O_n) := M(O_n, D_n(O_n x_n + b_n), R_n)$$ \tag{3.18}

and replace $O_n$ by $O_n O_n(x)$, where

$$O_n(x_n x_n = ||x_n|| e_n, \quad x_n = ||x_n|| O_n^T(x_n) e_n, \quad ||x_n||^2 = \sum_{\alpha=1}^n (x_{\alpha n})^2,$$ \tag{3.19}

with $e_n$ being the $n$th (last) vector of the canonical basis of $\mathbb{R}^n$.

Because of the orthogonal invariance of the Haar measure on $SO(n)$ the probability laws of $M_n(O_n)$ and $M_n(O_n O_n(x_n))$ coincide for any $x_n \in \mathbb{R}^n$. Thus, these matrices are statistically equivalent, i.e., all their statistical characteristics (various moments, the convergence with probability 1, etc.) are the same for any $x_n$. We will write this fact as

$$M_n(O_n) \equiv M_n^{(1)} := M_n(O_n O_n(x_n)).$$ \tag{3.20}

In particular, this is the case for the NCM’s and of $M_n(O_n)$ and $M_n^{(1)}$

$$\nu_{M_n(O)} \equiv \nu_{M_n^{(1)}},$$ \tag{3.21}

hence, it suffices to prove the convergence of $\nu_{M_n^{(1)}}$ with probability 1.

We have then from \((3.1)\) and \((3.20)\):

$$M_n^{(1)} = M_n(O_n, D_n(||x_n|| O_n e_n + b_n), R_n^{O_n(x_n)}),$$

$$R_n^{O_n(x_n)} = O_n(x) R_n O_n^T(x).$$ \tag{3.22}

We use now Proposition 3.5 (i) – (ii) to present $O_n$ as the product $V_n O_n$ \((3.33)\) of two independent orthogonal matrices $O_n$ and $V_n$ allowing us to write \((3.22)\) as

$$M_n^{(1)} = V_n M_n^{(2)} V_n^T,$$

$$M_n^{(2)} = M_n(O_n, D_n(||x_n|| V_n e_n + b_n), R_n^{O_n(x_n)}),$$

$$D_n^{V_n} = V_n^T D_n(||x_n|| V_n e_n + b_n) V_n.$$ \tag{3.23}

Since $M_n^{(1)}$ and $M_n^{(2)}$ are orthogonally equivalent, their spectra, hence, their NCM’s, coincide:

$$\nu_{M_n^{(1)}} = \nu_{M_n^{(2)}},$$ \tag{3.24}
Next, it follows from Lemma \[3.7\] that
\[\nu_{M_n^{(2)}} = \nu_{M_n^{(3)}} + O(1/n), \quad n \to \infty,\]  
(3.25)
where
\[M_n^{(3)} = [D_n^{V_n}([|x_n||V_n e_n + b_n|])O_{n-1}^1[R_n^{O_n(x)}]O_{n-1}^T[D_n^{V_n}([|x||V_n e_n + b_n|])].\]  
(3.26)
and for any \(n \times n\) matrix \(A\) we denote \([A]\) its \((n-1) \times (n-1)\) upper left block. Hence, \(M_{n-1}^{(3)}\) is a \((n-1) \times (n-1)\) matrix.

Combining (3.21) – (3.25), we obtain
\[\nu_{M_n^{(1)}} = \nu_{M_n^{(3)}} + O(1/n), \quad n \to \infty.\]

It is important that \(V_n\) and \(O_{n-1} = [O_n]\) are independent (see (3.33) – (3.37)) and that \(V_n\) is present only in \(D_n^{V_n}\) of (3.23).

We conclude that the initial problem to find the probability 1 the \(n \to \infty\) limit \(\nu_M\) of the NCM \(\nu_{M_n}\) of the matrix (3.1) reduces to the traditional problem of random matrix theory (see e.g. \[23\], Section 10, \[24, 35\] and Lemma \[3.8\] below) to find the \(n \to \infty\) limit of the NCM of a particular case \(M_{n}^{(3)}\) of (2.9) where the role of \(K_n = D_n^2\) and \(R_n\) play \([R_{n+1}]\) and \([D_{n+1}]\) respectively with \((n+1) \times (n+1)\) matrices
\[D_{n+1} = D_{n+1}^{V_{n+1}}([|x||V_{n+1} e_{n+1} + b_{n+1}|], \quad R_{n+1} = R_{n+1}^{O_{n+1}(x)},\]  
(3.27)
see (3.22) and (3.23).

It follows from (3.27), Lemma \[3.6\] (3.22) and the orthogonal invariance of the NCM of any real symmetric matrix that
\[\nu_{[R_{n+1}]} = \nu_{R_{n+1}} + O(1/n) = \nu_{R_{n+1}} + O(1/n).\]

Thus, we obtain the convergence of \(\nu_{[R_{n+1}]}\) with probability 1 of \(\nu_{[R_{n+1}]}\) to \(\nu_R\) given by (3.3).

Likewise, the NCM of \([D_{n+1}]\) equals the NCM of \(D_{n+1}\) in (3.27) up to \(O(1/n)\) and the NCM of \(D_{n+1}\) equals the NCM of \(D_{n+1}([|x||V_{n+1} e_{n+1} + b_{n+1}|]),\) because \(D_{n+1}\) is orthogonal equivalent to \(D_{n+1}([|x||V_{n+1} e_{n+1} + b_{n+1}|])\) (see (3.27) and (3.23)). The validity of condition (2.8) for \(\nu_{D_{n+1}}\) and the explicit form of the limiting measure follow from Lemma \[3.10\] .

As for condition (3.65), it is valid because of (3.2) for \(\nu_{[R_{n+1}]}\) and because of (3.15) and (3.7) for \(\nu_{[D_{n+1}]}\).

**Remark 3.3** As is noted at the beginning of Section 2, despite the fact that the matrices \(D^l\) of (1.7), hence \(K^l\) of (1.8), are random and depend on \(O^l\) of (2.2), the limiting eigenvalue distribution of \(M^L_n\) of (1.8) corresponds to the case where the analogs \(D_n\) of \(D^l_n\) of (1.7) are random but independent of \(O^l\) as in (2.9), see (2.16) and (3.15). The emergence of this remarkable property of \(M^L_n\) is well seen in the above proof.

Theorem \[3.1\] yields an analytic form of the binary operation (2.10) of the free multiplicative convolution via equations (3.12) – (3.14). It is convenient to write the equations in a compact form analogous to that of free probability theory \[4, 16\]. This, in particular, makes explicit the symmetry and the transitivity of the operation.
Corollary 3.4 Let $\nu_A$, $A = K, R, M$ be the probability measures (non-negative measures of the total mass 1) entering (3.12) – (3.14) and $m_A$, $A = K, R, M$ be their moment generating functions (see (1.16) – (1.17)). Then:

(i) the functional inverses $z_A$, $A = K, R, M$ of $m_A$, $A = K, R, M$ are related as follows

$$z_M(m) = z_K(m)z_R(m)(1 + m)m^{-1};$$

(3.28)

(ii) if $S_A(m) = z_A(m)(m + 1)/m$, $A = K, R, M$, (3.29)

is the $S$-transform of $\nu_A$, then

$$S_M(m) = S_K(m)S_R(m)$$

(3.30)

i.e., according to the terminology of free probability theory, $\nu_M$ is the free multiplicative convolution of $\nu_K$ and $\nu_R$ (see (2.10)).

Proof. Recall that given a non-negative measure $\nu$, $\nu(R) = 1$, its Stieltjes transform $f_\nu$ (see (1.15) and its moment generating function $m_\nu$ (see (1.16) are related as (cf. 1.17))

$$zf_\nu(z) = -(m_\nu(z^{-1}) + 1).$$

(3.31)

Note that the moment generating function is well defined by this formula even if $\nu$ has no finite moment of sufficiently high order. Besides, the formula shows that the functional inverse $z_\nu$ of $m_\nu$ is well defined in a neighborhood of the origin of the $m$-plane where $|\Im m| \geq \varepsilon|\Re m|$ for some $\varepsilon > 0$, because it follows from (1.15) that

$$f_\nu = z^{-1}(1 + o(d^{-1})), \quad f'_\nu = z^{-2}(1 + o(d^{-1})), \quad d = \text{dist}(z, R_+) \to \infty.$$ 

(3.32)

Let us prove (3.28). By using (3.31) for $\nu = \nu_A$, $A = M, R$ to pass from $f = f_A$, $A = M, R$ to $m = m_A$, $A = M, R$ in (3.13), we obtain

$$m_M(z^{-1}) = m_R(h_K(z)/(m_M(z^{-1}) + 1)).$$

An analogous argument for $A = M, K$, applied to (3.14), yields

$$m_M(z^{-1}) = m_K(h_R(z)/(m_M(z^{-1}) + 1)).$$

Changing in the both relations $z \to z^{-1}$ and applying to the first one the functional inverse $z_R$ of $m_R$ and to the second one the functional inverse $z_K$ of $m_K$, we get

$$(1 + m)z_R(m) = h_K(z_M^{-1}(m)), \quad (1 + m)z_K(m) = h_R(z_M^{-1}(m)),$$

hence,

$$(1 + m)^2z_K(m)z_R(m) = h_K(z_M^{-1}(m))h_R(z_M^{-1}(m)).$$

Now we use again (3.31) to write equation (3.12) as

$$z_M(m)m(m + 1) = h_K(z_M^{-1}(m))h_R(z_M^{-1}(m)).$$

Combining the last two relations, we obtain (3.28).

To obtain (3.30) we combine (3.29) and (3.28). ■

We will now give the list of results on orthogonal matrices, linear algebra and random matrix theory that are used in the proof of the theorem.

First is a collection of facts on the group $SO(n)$. 

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Proposition 3.5  Given a positive integer \( n \) consider the group \( SO(n) \) of \( n \times n \) orthogonal matrices with determinant 1. The following facts on \( SO(n) \) are valid.

(i) Viewing \( O_n \in SO(n) \) as the orthogonal transformation of \( \mathbb{R}^n \) with an orthogonal basis \( \{ e_j \}_{j=1}^n \) and denoting \( g_k(\theta) \) the rotation by the angle \( \theta \) in the \( (e_{k+1}, e_k) \) plane from \( e_{k+1} \) to \( e_k \) and

\[
g^{(k)} = g_1(\theta^k_1) \cdots g_1(\theta^k_j), \quad \theta^k_j \in [0, 2\pi), \quad \theta^k_j \in [0, \pi), \quad j \neq 1,
\]

we have

\[
O_n = V_n O_n, \quad (3.33)
\]

where

\[
V_n = g^{(n-1)} = V_n(\Theta_1), \quad O_n = g^{(n-2)} \cdots g^{(1)} = O_n(\Theta_2), \quad (3.34)
\]

i.e., \( V_n \) and \( O_n \) depend only on

\[
\Theta^{(1)}_n = \{ \theta^{(n-1)}_j \}_{j=1}^{n-1}, \quad \Theta^{(2)}_n = \{ \theta^{(k)}_j \}_{j,k=1}^{n-1} \quad (3.35)
\]

respectively, i.e., on the independent parametrization of the unit sphere \( S^{n-1} \) and of that of the group \( SO(n-1) \), and \( O_n \) is the block-diagonal matrix whose \( (n-1) \times (n-1) \) upper left block is a \( SO(n-1) \) matrix and lower right \( 1 \times 1 \) block is 1:

\[
O_n = O_{n-1} \oplus 1_1 = \begin{pmatrix} O_{n-1} & 0 \\ 0 & 1 \end{pmatrix}; \quad (3.36)
\]

(ii) If \( dO_n \) is the normalized Haar measure of \( SO(n) \), then

\[
dO_n = dV_n dO_{n-1}, \quad (3.37)
\]

where \( dV_n \) is the normalized measure on the manifold determined by \( \Theta_1 \), in fact the "uniform" probability distribution of the vector

\[
\xi_n = O_n e_n \quad (3.38)
\]

over \( S^{n-1} \) and \( dO_{n-1} \) is a probability measure on \( SO(n-1) \), in fact its normalized Haar measure of \( SO(n-1) \);

(iii) Let \( \Phi : SO(n) \to M_n(\mathbb{C}) \) be a map admitting a \( C^1 \) continuation into an open neighborhood of \( SO(n) \) in the whole algebra \( M_n(\mathbb{R}) \) of \( n \times n \) matrices and \( E_n \{ \ldots \} \) denotes the integration (expectation) with respect to the normalized to unity Haar measure on \( SO(n) \). Then we have

\[
E_n \{ \Phi'(O_n) \cdot A_n O_n \} = 0, \quad E_n \{ \Phi'(O_n) \cdot O_n A_n \} = 0, \quad \forall A_n \in A_n, \quad (3.39)
\]

where \( A_n \) is the space of \( n \times n \) real antisymmetric matrices and \( \Phi' \) is viewed as a linear map from \( M_n(\mathbb{R}) \) to \( M_n(\mathbb{C}) \), or, in the coordinate form

\[
\sum_{l=1}^n E_n \{ \Phi'_{ij}(O_n)(O_n)_{lk} - \Phi'_{lk}(O_n)(O_n)_{ij} \} = 0, \quad j, k = 1, \ldots, n, \quad (3.40)
\]

where

\[
\Phi'_{jk}(U) = \Phi'(U) \cdot \mathcal{E}^{(jk)} = \lim_{\varepsilon \to \infty} (\Phi(U + \varepsilon \mathcal{E}^{(jk)})) - \Phi(U) \varepsilon^{-1}, \quad \mathcal{E}^{(jk)} = \left\{ \mathcal{E}_{ab}^{(jk)} \right\}_{a,b=1}^{n}, \quad \mathcal{E}_{ab}^{(jk)} = \delta_{ab} \delta_{lk} \in M_n(\mathbb{R}), \quad (3.41)
\]

\[
\sum_{l=1}^n E_n \{ \Phi'_{ij}(O_n)(O_n)_{lk} - \Phi'_{lk}(O_n)(O_n)_{ij} \} = 0, \quad j, k = 1, \ldots, n
\]

where

\[
\Phi'_{jk}(U) = \Phi'(U) \cdot \mathcal{E}^{(jk)} = \lim_{\varepsilon \to \infty} (\Phi(U + \varepsilon \mathcal{E}^{(jk)})) - \Phi(U) \varepsilon^{-1}, \quad \mathcal{E}^{(jk)} = \left\{ \mathcal{E}_{ab}^{(jk)} \right\}_{a,b=1}^{n}, \quad \mathcal{E}_{ab}^{(jk)} = \delta_{ab} \delta_{lk} \in M_n(\mathbb{R}), \quad (3.41)
\]
i.e., \( \{E^{(jk)}\}_{j,k=1}^n \) is a basis in \( \mathcal{M}_n(\mathbb{R}) \):

(iv) We have in the above notation for a map \( \varphi : SO(n) \to \mathbb{C} \) and a sufficiently large \( n \)

\[
\text{Var}_n \{ \varphi \} := E_n \{ |\varphi|^2 \} - |E_n \{ \varphi \}|^2 
\leq \frac{C}{n} E_n \left\{ \sum_{1 \leq j < k \leq n} |\varphi'_{jk}|^2 \right\},
\]

(3.42)

where \( C \) is an absolute constant and

\[
\varphi'_j(O_n) = \varphi'(O_n) \cdot A^{(jk)} = \lim_{\varepsilon \to \infty} (\varphi(O_n(1_n + \varepsilon A^{(jk)})) - \varphi(O_n))\varepsilon^{-1},
\]

\[
A^{(jk)} = \{A_{ab}^{(jk)}\}_{a,b=1}^n, \quad A_{ab}^{(jk)} = \delta_{aj} \delta_{bk} - \delta_{ak} \delta_{bj},
\]

(3.43)

i.e., \( \{A^{(jk)}\}_{0 \leq j < k \leq n} \) is the basis of \( A_n \):

(v) There exists an infinite-dimensional probability space \( \Omega_O \) on which all \( O_n, n \geq 1 \), are simultaneously defined.

Items (i) and (ii) of proposition are structure properties of \( SO(n) \), see [36], Section IX.1 and [17], Chapters 2 and 5. Item (iii) follows from the invariance of the Haar measure of \( SO(n) \) with respect to the left \( O \to e^{\varepsilon A}O \) and the right \( O \to Oe^{\varepsilon A} \) shifts with \( \varepsilon \to 0 \), see [23], Section 8.1. Item (iv) is a version of the Poincaré inequality for \( SO(n) \), see [23], Section 8.1 and item (v) is again a structure property of \( SO(n) \), see [18], Section 2.10 and [23], Section 8.1.

**Lemma 3.6** Let \( T_n \) be an \( n \times n \) matrix and \( [T_n] \) be its upper left block, i.e., if \( P_n \) is the orthogonal projection on the last basis vector \( e_n \) of \( \mathbb{C}^n \) and \( Q_n \) is the complementary orthogonal projection, so that

\[
Q_n + P_n = 1_n,
\]

we can write

\[
[T_n] = [T_{Q_n}], \quad T_{Q_n} := Q_n T_n Q_n = \begin{pmatrix} [T_n] & 0 \\ 0 & 0 \end{pmatrix}.
\]

(3.44)

(3.45)

We have:

(i) if \( A_n \) is an \( n \times n \) hermitian matrix, then

\[
A_n = A_{Q_n} + R_3, \quad \text{rank } R_3 \leq 3;
\]

(3.46)

(ii) if \( A_n \) and \( B_n \) are \( n \times n \) hermitian matrices, \( X_n \) is an \( n \times n \) block-diagonal matrix

\[
X_n = \begin{pmatrix} [X_n] & 0 \\ 0 & 1 \end{pmatrix} = X_{Q_n} + P_n, \quad X_{Q_n} = Q_n X_n Q_n
\]

and

\[
C_n = A_n X_n^* B_n X_n A_n,
\]

(3.47)

(3.48)

then

\[
C_n = C_{Q_n} + R_6,
\]

(3.49)

where

\[
C_{Q_n} = \begin{pmatrix} [C_{Q_n}] & 0 \\ 0 & 0 \end{pmatrix}, \quad [C_{Q_n}] = [A_n][X_n^*][B_n][X_n][A_n]
\]

and

\[
\text{rank } R_6 \leq 6.
\]

(3.50)

(3.51)
Proof. (i) We will omit the subindex $n$ in the cases where it does not lead to confusion. We have from (3.44) and (3.45)

$$A = A_Q + QAP + PAQ + PAP.$$  (3.52)

Given $x, y \in \mathbb{C}^n$, define the rank-one matrix

$$L_{xy}u := (u, x)y, \forall u \in \mathbb{C}^n.$$  (3.53)

We obtain

$$QAP = L_{e_n, QAe_n}, PAQ = L_{Ae_n, e_n}, PAP = (Ae_n, e_n)L_{e_n, e_n} = (Ae_n, e_n)P,$$

implying that $A - A_Q$ is of rank 3 at most. This and the min-max principle of linear algebra yields (3.46).

(ii) Applying (3.46) to $C$ of (3.48), we get

$$C = C_Q + R_3, \text{ rank } R_3 \leq 3.$$  (3.54)

Next, we have from (3.44), (3.47), (3.48) and (3.50)

$$C_Q = C_Q + T_1 + T_2 + T_3,$$  (3.55)

where,

$$C_Q = A_QX^*_Q B_Q X_Q A_Q$$  (3.56)

and, in view of (3.53),

$$T_1 := A_QX^*_QBPAQ = L_{QAe_n, QAe_n},$$
$$T_2 := QAPBX_QA = L_{QAe_n, QAe_n},$$
$$T_3 := QAPBPAQ = (B_{e_n}, e_n)L_{QAe_n, QAe_n}.$$  (3.57)

All the factors on the right of (3.56) are of the form $T_Q$ in (3.45), $T = A, B, X$, hence the l.h.s. $C_Q$ is also of this form with $[C_Q]$ given by the r.h.s. of (3.50). In addition, since each $T_a, a = 1, 2, 3$ in (3.57) is of rank 1, we have that rank($T_1 + T_2 + T_3$) $\leq 3$. This, the min-max principle, (3.54) and (3.55) imply (3.51). 

Lemma 3.7 Let $M_n$ be defined in (3.7) – (3.9) and let

$$M_{n-1} = [S_n]O_{n-1}^T[K_n]O_{n-1}[S_n]$$  (3.58)

be $(n-1) \times (n-1)$ matrix, where $[S_n]$ is the $(n-1) \times (n-1)$ upper left block of $S_n$, $O_{n-1}$ is the Haar distributed $SO(n-1)$ matrix, $[K_n]$ is the $(n-1) \times (n-1)$ upper left block of $K_n$ := $(D_n^T)^2 = V_n^T K_n V_n$, where $V_n$ is given (3.33) – (3.35) and $K_n$ is given by (3.6). Denote $\nu_{M_n}$ and $\nu_{M_{n-1}}$ the NCM of $M_n$ and $M_{n-1}$. Then

$$\nu_{M_n}(\Delta) - \nu_{M_{n-1}}(\Delta) = O(1/n), n \rightarrow \infty.$$  (3.59)
Lemma 3.8

Let orthogonal matrix given by (3.34), (3.35) and (3.36). Denoting now \( \nu \), Normalized Counting Measures combining (3.62) and (3.64), we get

\[ K \text{ and } \]

Next, according to the same lemma, we have for the \( \nu_{M_n} \) and \( \nu_{(M_n)Q} \), then it follows from (3.61) and the min-max principle of linear algebra that

\[ \nu_{M_n} - \nu_{(M_n)Q} = O(1/n), \ n \to \infty. \]  

Next, according to the same lemma, we have for the \( (n-1) \times (n-1) \) upper left block \( [(M_n)_Q] \) of \( (M_n)_Q \)

\[ [(M_n)_Q] = [S_n]O_n^T[K_n^{V_n}]O_nS_n. \]  

Thus, if \( \nu_{M_n} \) and \( \nu_{(M_n)Q} \) are the NCM of \( M_n \) and \( (M_n)_Q \), then it follows from (3.62) and the min-max principle of linear algebra that

\[ \nu_{M_n} - \nu_{(M_n)Q} = O(1/n), \ n \to \infty. \]  

Next, according to the same lemma, we have for the \( (n-1) \times (n-1) \) upper left block \( [(M_n)_Q] \) of \( (M_n)_Q \)

\[ [(M_n)_Q] = [S_n]O_n^T[K_n^{V_n}]O_nS_n. \]  

Thus, if \( \nu_{M_n} \) and \( \nu_{(M_n)Q} \) are the NCM of \( M_n \) and \( (M_n)_Q \), then it follows from (3.62) and the min-max principle of linear algebra that

\[ \nu_{(M_n)_Q} - \nu_{(M_n)Q} = O(1/n), \ n \to \infty. \]  

Combining (3.62) and (3.64), we get

\[ |\nu_{M_n}(\Delta) - \nu_{(M_n)_Q}| = O(1/n), \ n \to \infty. \]  

Denoting now \( [(M_n)_Q] := M_{n-1} \) and using (3.63), we obtain (3.58). \( \blacksquare \)

The next lemma gives an explicit analytic form of the operation (2.10).

Lemma 3.8 Let \( M_n \) be the \( n \times n \) random matrix (2.9) where \( O_n \) is Haar distributed over \( SO(n) \) and \( K_n \) and \( R_n \) are \( n \times n \) positive definite random matrices independent of \( O_n \) and such that their Normalized Counting Measures \( \nu_{K_n} \) and \( \nu_{R_n} \) converge weakly with probability 1 as \( n \to \infty \) to the non-random limits \( \nu_K \) and \( \nu_R \) of (2.3) with \( \nu_K(\mathbb{R}+) = \nu_R(\mathbb{R}+) = 1 \) and

\[ \sup_n \int_0^\infty \lambda^2 \nu_{A_n}(d\lambda) < \infty, \ A = K, R. \]  

Then the Normalized Counting Measure \( \nu_{M_n} \) of \( M_n \) converges weakly with probability 1 as \( n \to \infty \) to a non-random limit \( \nu_M \) and its Stieltjes transform (see (3.11)) is a unique solution of (3.12) – (3.14) satisfying (3.16).

The lemma is known in fact, see [16] Section 4.3, [23], Section 10.4 and [35] for unitary matrices. A streamlined proof applicable to both unitary and orthogonal matrices is given in [24].

The next two lemmas deal with asymptotic properties of the activation vectors \( x^l \) in the \( l \)th layer, see (3.11). It is an extended version (treating the convergence with probability 1) of assertions proved in [13], [28], [31] for expectations.

The first lemma is a version of the Law of Large Numbers for random vectors that are uniformly distributed over \( S^{n-1} \).
Lemma 3.9 Let $\chi : \mathbb{R} \to \mathbb{R}$ be piece-wise continuous and

$$\sup_{x \in \mathbb{R}} |\chi(x)| = \hat{\chi} < \infty,$$

(3.66)

$\xi_n = \{\xi_{jn}\}_{j=1}^n \in \mathbb{S}^{n-1}$ be the random vector uniformly distributed over the sphere $\mathbb{S}^{n-1}$, $b = \{b_j\}_{j=1}^\infty$ (cf. (2.4)) be a collection of i.i.d. Gaussian random variables of zero mean and variance $\sigma_b^2$ and $\{a_n\}_{n=1}^\infty$ be a real valued sequence such that

$$\lim_{n \to \infty} a_n = a.$$

(3.67)

Denoting $\Omega_b$ the probability space generated by $b$ and writing $\xi_n = O_n e_n$, we can say that $b$ and $\{\xi_n\}_{n=1}^\infty$ are defined on the same probability space $\Omega_b = \Omega_O \times \Omega_b$ (cf. (2.4) – (2.5)). Set

$$\chi_n = \frac{1}{n} \sum_{j=1}^n \chi \left( n^{1/2} a_n \xi_{jn} + b_j \right).$$

(3.68)

and view it as a random variable in $\Omega_{Ob}$. Then we have with probability 1 in $\Omega_{Ob}$

$$\chi = \lim_{n \to \infty} \chi_n = \int_{-\infty}^{\infty} \chi (a \gamma + b) \frac{e^{-\gamma^2/2 - b^2/2\sigma_b^2}}{2\pi\sigma_b} d\gamma db.$$

(3.69)

Proof. Denote $E_{Ob}\{\ldots\}$ the expectation in $\Omega_{Ob}$ and $E_b\{\ldots\}$ and $E_O\{\ldots\}$ the expectation in $\Omega_b$ and $\Omega_O$ respectively, so that $E_{Ob} = E_O E_b$. Write

$$\chi_n = T_{1n} + T_{2n},$$

(3.70)

where

$$T_{1n} = \chi_n - E_b\{\chi_n\} = \frac{1}{n} \sum_{j=1}^n \chi \left( n^{1/2} a_n \xi_{jn} + b_j \right) - \frac{1}{n} \sum_{j=1}^n E_b\{\chi \left( n^{1/2} a_n \xi_{jn} + b_j \right)\}$$

(3.71)

and

$$T_{2n} = E_b\{\chi_n\} = \frac{1}{n} \sum_{j=1}^n E_b\{\chi \left( n^{1/2} a_n \xi_{jn} + b_j \right)\}.\quad (3.72)$$

For any fixed $\{\xi_{jn}\}_{j=1}^n \in \mathbb{S}^{n-1}$ the r.h.s. of (3.71) is the arithmetic mean of the bounded (see (3.66)) i.i.d. random variables of zero mean in $\Omega_b$. It follows then from a standard calculation and (3.66) that

$$E_b\{|T_{1n}|^4\} \leq 3\hat{\chi}^4/n^2.$$

Since the r.h.s. of this bound is independent of $\{\xi_{jn}\}_{j=1}^n \in \mathbb{S}^{n-1}$, we obtain

$$E_{Ob}\{|T_{1n}|^4\} \leq 3\hat{\chi}^4/n^2.$$

This and the Borel-Cantelli lemma imply that the limit

$$\lim_{n \to \infty} T_{1n} = 0.$$

(3.73)

holds with probability 1 in $E_{Ob}$.
Let us prove now that the almost sure limit of $T_{2n}$ of (3.72) equals the r.h.s. of (3.69). To this end we first rewrite $T_{2n}$ as

$$T_{2n} = \frac{1}{n} \sum_{j=1}^{n} \chi \left( n^{1/2} a \xi_{jn} \right) + T_{3n}$$

(3.74)

where

$$\chi(x) = E_b \{ \chi(x + b) \} = \int_{-\infty}^{\infty} \chi(x + b) \frac{e^{-b^2/\sigma_b^2}}{\sqrt{2\pi\sigma_b^2}} \, db$$

(3.75)

and

$$T_{3n} = \frac{1}{n} \sum_{j=1}^{n} \left( \chi \left( n^{1/2} a n \xi_{jn} \right) - \chi \left( n^{1/2} a \xi_{jn} \right) \right).$$

(3.76)

It follows from (3.66) and (3.75) that

$$\sup_{x \in \mathbb{R}} |\chi'(x)| := \chi_1 < \infty, \chi_1 = (2/\pi\sigma_b^2)^{1/2} \hat{\chi}_0,$$

(3.77)

hence, we have for $\{\xi_{jn}\}_{j=1}^{n} \in \mathbb{S}^{n-1}$ by Schwarz inequality

$$|T_{3n}| \leq \chi_1 n^{1/2}|a_n - a| \frac{1}{n} \sum_{j=1}^{n} |\xi_{jn}|$$

$$\leq \chi_1 n^{1/2}|a_n - a| \left( \frac{1}{n} \sum_{j=1}^{n} |\xi_{jn}|^2 \right)^{1/2} = \chi_1 |a_n - a|.$$  

(3.78)

Next, it follows from a direct calculation that if $\{\gamma_j\}_{j=1}^{n}$ is the collection of independent standard Gaussian random variables and

$$\Gamma_n^2 = \sum_{j=1}^{n} \gamma_j^2,$$

(3.79)

then

$$\xi_{jn} = \gamma_j / \Gamma_n, \; j = 1, \ldots n$$

(3.80)

(we thank A. Sodin for the indication on this nice fact).

Thus, we can write in view of (3.67), (3.74), (3.78) and (3.80)

$$T_{2n} = n^{-1} \sum_{j=1}^{n} \chi \left( a n^{1/2} \gamma_j / \Gamma_n \right) + o(1)$$

$$= n^{-1} \sum_{j=1}^{n} \chi (a \gamma_j) + T_{4n} + o(1), \; n \to \infty$$

(3.81)

where

$$T_{4n} = n^{-1} \sum_{j=1}^{n} \left( \chi \left( a n^{1/2} \gamma_j / \Gamma_n \right) - \chi (a \gamma_j) \right).$$

Repeating the argument leading to (3.78), we obtain

$$|T_{4n}| \leq \chi_1 a |n^{1/2} / \Gamma_n - 1| n^{-1} \sum_{j=1}^{n} |\gamma_j|$$

$$\leq \chi_1 |1 - \Gamma_n / n^{1/2}|$$
According to the strong Law of Large Numbers and (3.79), we have with probability 1
\[
\lim_{n \to \infty} \frac{\Gamma_n}{n^{1/2}} = \lim_{n \to \infty} \left( n^{-1} \sum_{j=1}^{n} |\gamma_j|^2 \right)^{1/2} = \left( \mathbb{E}\{\gamma_1^2\} \right)^{1/2} = 1,
\]
(3.82)
hence
\[
\lim_{n \to \infty} T_{4n} = 0
\]
with probability 1.

We are left with the proof that the first term of (3.81) tends to the r.h.s. of (3.69) with probability 1 as \(n \to \infty\). This follows immediately from the strong Law of Large Numbers since \(\{\gamma_j\}_{j=1}^{\infty}\) are the independent standard Gaussian random variables. 

We will use the lemma to prove formulas (2.16) and (2.17).

**Lemma 3.10** Let \(y^l = \{y^l_j\}_{j=1}^{n},\ l = 1, \ldots, L\) be post-affine random vectors defined in (1.1) – (1.3) with \(x^0\) satisfying (2.13), \(\chi : \mathbb{R} \to \mathbb{R}\) be a bounded piece-wise continuous function and \(\Omega_L\) be defined in (2.7). Set
\[
\chi_n^l = n^{-1} \sum_{j=1}^{n} \chi(y^l_j), \ l = 1, \ldots, L.
\]
(3.83)
Then there exists \(\Omega_l \subset \Omega_L, \ P(\Omega_l) = 1\) such that for every \(\omega_l \in \Omega_l, \ i.e.,\) with probability 1 in \(\Omega_L\), the limits
\[
\chi^l := \lim_{n \to \infty} \chi_n^l, \ l = 1, \ldots, L
\]
exist, are not random and equal
\[
\chi^l = \int_{-\infty}^{\infty} \chi((q^l)^{1/2} \gamma + b) \frac{e^{-\gamma^2/2-b^2/2\sigma_b^2}}{2\pi\sigma_b} d\gamma db, \ l = 1, \ldots, L,
\]
(3.84)
valid on \(\Omega_l\) with \(q^l\) defined recursively as
\[
q^l = \int_{-\infty}^{\infty} \varphi^2((q^{l-1})^{1/2} \gamma + b) \frac{e^{-\gamma^2/2-b^2/2\sigma_b^2}}{2\pi\sigma_b} + \sigma_b^2, \ l = 1, \ldots, L
\]
(3.85)
with \(q^0\) given in (2.13).

In particular, we have from the above with \(\chi = \psi\) the validity with probability 1 formula (2.16) (hence, (3.15)) for the weak limit \(\nu_{K^1_n}\) of the Normalized Counting Measure \(\nu_{K^1_n}\) of diagonal random matrix \(K^1_n\) of (1.18).

**Proof.** Consider the case where \(l = 1\) in (3.83):
\[
\chi_n^1 = \frac{1}{n} \sum_{j=1}^{n} \chi((O^1 x^0)_{j_1} + b_{j_1}^1).
\]
(3.87)
Since probability distribution of \(O^1\), i.e., the normalized to unity Haar measure on \(SO(n)\), is orthogonal invariant, we can replace \(O^1\) in (3.87) by \(O^1 O^0\) such that \(O^0 x^0 = e_n\) (cf. (3.19)). Hence, the random variable, obtained by using this replacement in (3.87), is stochastically equivalent to
that of (3.87), i.e., its probability distribution coincides with that of (3.87). We denote this random variable again \( \chi_n^1 \) and write

\[
\chi_n^1 = \frac{1}{n} \sum_{j=1}^{n} \chi(||x_j^0|| \xi_{nj} + b_{j1}),
\]

(3.88)

where \( \{\xi_{jn}\}_{j=1}^{n} = \xi_n \) is the unit vector uniformly distributed over the unit sphere \( S^{n-1} \). It follows then from the condition of the lemma that the random variable (3.88) satisfies the condition of Lemma 3.9 (condition (3.67) of the lemma is guaranteed by (2.13)). We conclude that (3.84) – (3.85) hold for \( l = 1 \).

Remark 3.11 Lemma 3.9 remains valid for any i.i.d. \( \{b_j\}_{j=1}^{\infty} \) such that the derivative \( p' \) of the density \( p \) of their common probability law \( P \) belongs to \( L^1(\mathbb{R}) \). Indeed, it is easy to see that in this case we have instead of (3.69)

\[
\sup_{x \in \mathbb{R}} |\nabla (x)| = \chi_1 < \infty, \quad \chi_1 = \hat{\chi}_0 ||p'||_{L^1(\mathbb{R})}
\]

and instead of (3.69)

\[
\chi := \lim_{n \to \infty} \chi_n = \int_{-\infty}^{\infty} \chi(a \gamma + b) \frac{e^{-\gamma^2/2-\beta^2/2\sigma_b^2}}{\sqrt{2\pi}} d\gamma P(db),
\]

where \( P \) is the common probability law of \( \{b_j\}_{j=1}^{\infty} \).

This leads to more general version of (3.85)

\[
\chi^l = \int_{-\infty}^{\infty} \chi(\gamma \sqrt{q_{l-1}^2 - \sigma_b^2} + b) \frac{e^{-\gamma^2/2}}{\sqrt{2\pi}} P(db), \quad l = 1, 2, \ldots,
\]
hence, of (3.86)
\[
q^l = \int_{-\infty}^{\infty} \varphi^2(\gamma \sqrt{q^l - 1 - \sigma^2_b + b}) \frac{e^{-\gamma^2/2}}{(2\pi)^{1/2}} P(db) + \sigma^2_b, \quad l = 2, 3, \ldots
\]
and of (2.16)
\[
\nu_K(\Delta) = P\{(\varphi'(q^l - 1 - \sigma^2_b)\gamma + b)\gamma \in \Delta\}, \quad \Delta \in \mathbb{R}, \quad l = 1, \ldots, L.
\]
with \(q^0\) is given by (2.13).

To have the validity of the lemma for general i.i.d. \(\{b_j\}_{j=1}^{\infty}\) of zero mean and variance \(\sigma^2_b\) we have to assume, for instance, that \(\chi\) has a bounded derivative.

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