THEORETICAL UNDERSTANDING OF BATCH-NORMALIZATION: A MARKOV CHAIN PERSPECTIVE

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Abstract. Batch-normalization (BN) is a key component to effectively train deep neural networks. Empirical evidence has shown that without BN, the training process is prone to unstabilities. This is however not well understood from a theoretical point of view. Leveraging tools from Markov chain theory, we show that BN has a direct effect on the rank of the pre-activation matrices of a neural network. Specifically, while deep networks without BN exhibit rank collapse and poor training performance, networks equipped with BN have a higher rank. In an extensive set of experiments on standard neural network architectures and datasets, we show that the latter quantity is a good predictor for the optimization speed of training.

1. Introduction

Depth is known to play an important role in the expressive power of a neural network [Tel16]. Yet, increased depth typically leads to a drastic slow down of learning with gradient based methods, which is commonly attributed to unstable gradient norms in deep networks [Hoc98]. One key component that has enabled to train neural networks regardless of their depth is batch normalization (BN) [IS15]. While the empirical success of this architectural change is uncontested, the underlying mechanism of BN as well as its interplay with stochastic gradient descent is still poorly understood from a theoretical point of view.

Ever since, an emerging line of research has contributed to a better understanding of the inner working of batch-normalization e.g. [BGSW18, KDL+18, JGH19, ALL18] but the community has not yet reached a general consensus on what exactly renders BN so effective when training deep nets with gradient based algorithms.

We address this question using tools from Markov chain theory. Since our aim is to study the behavior of BN in a broad perspective, we study a standard non-convolutional architecture. Taking inspiration from recent results from the mean-field theory literature [YPR+19], we also consider the use of residual connections that have shown to be effective for optimizing neural networks [HZRS16].

We therefore consider a standard $L$-layer multi-layer perceptron (MLP) equipped with residual connections. Given an input matrix $X \in \mathbb{R}^{d \times N}$ containing $N$ samples of dimensionality $d$, we denote the pre-activation matrices of all layers by $\{\hat{H}_\ell \in \mathbb{R}^{d_\ell \times N}\}_{\ell=1}^L$. They follow the recurrence

$$\hat{H}_{\ell+1} = \hat{H}_\ell + \gamma W_\ell F(\hat{H}_\ell),$$

where $\hat{H}_0 = X$, $W_\ell \in \mathbb{R}^{d_\ell \times d_{\ell-1}}$ is the weight matrix for layer $\ell$, and $F$ is an activation function which is applied element-wise to its input. For the sake of simplicity, we assume that every layer has the same number of hidden units, that is $d_1 = \cdots = d_L = d$. The parameter $\gamma \in \mathbb{R}^+$ regulates the strength of the non-residual term of each layer.
1.1. **Batch normalization.** Let \( \mathbf{1}_k \) be the \( k \)-dimensional all one vector. Given parameter vectors \( \alpha \in \mathbb{R}^d \) and \( \beta \in \mathbb{R}^d \), the batch normalization mapping, denoted by \( \text{BN}_{\alpha, \beta} : \mathbb{R}^{d \times N} \rightarrow \mathbb{R}^{d \times N} \), is defined as [IST15]:

\[
\text{BN}_{\alpha, \beta}(H) = \beta \circ \left( \text{diag}(M(H)) \right)^{-1/2} G(H) + \alpha \mathbf{1}_N^\top,
\]

where \( \circ \) is a row-wise product and the functions \( G \) and \( M \) are defined as:

\[
G(H) := H \left( I_N - \frac{1}{N} \mathbf{1}_N \mathbf{1}_N^\top \right)
\]

\[
M(H) := \frac{1}{N} HH^\top.
\]

Furthermore, the operator \( \text{diag} : \mathbb{R}^{d \times d} \rightarrow \mathbb{R}^{d \times d} \) sets all off-diagonal elements of a given matrix to 0.

Notably, the parameters \( \alpha \) and \( \beta \) are trainable, therefore allowing \( \text{BN} \) to simulate an affine operator.

The pre-activation matrices of a network equipped with \( \text{BN} \) layers evolve as

\[ H_{\ell+1} = \text{BN}_{\alpha_{\ell}, \beta_{\ell}}(H_{\ell} + \gamma W_{\ell} F(H_{\ell})). \]

1.2. **Advantages of normalized pre-activations.** In this work we address the fundamental question of how apparent differences between the above defined batch-normalized pre-activation matrices \( H_{\ell} \) and those of a vanilla network \( \hat{H}_{\ell} \) lead to totally different optimization behaviour in deep neural networks.

One obvious difference is that the rows of the matrices \( \{H_{\ell}\} \) are zero-mean and unit-variance across all layers, which does not hold for the matrices \( \{\hat{H}_{\ell}\} \). Yet, [STIM18] show in a comprehensive empirical investigation that this property cannot explain the superior optimization behaviour of batch normalized networks.

Building on an empirical observation from [BGSW18], who show that \( \text{BN} \) prevents deep nets from always predicting one single class after random initialization, we here highlight another key difference between the two networks that is particularly intriguing: For a vanilla network, the rank of the pre-activation matrices (i.e., \( \hat{H}_{\ell} \)) quickly becomes equal to one as the depth increases\(^1\). However, \( \text{BN} \) stabilizes the rank of the pre-activation matrices \( \{H_{\ell}\} \) for any depth (see Figure 1). In summary, we make two key contributions:

(i) We theoretically prove that \( \text{BN} \) indeed avoids rank collapse for any depth under standard initialization and in the case of both linear- and non-linear networks.

(ii) We empirically show that the rank is indeed a relevant quantity for gradient based learning across many real world datasets and network architectures.

1.3. **Theoretical results (i).** For vanilla linear networks, existing results from the literature on products of random matrices [Bou12] can directly be leveraged to show that the rank of \( \hat{H}_{\ell} \) tends to 1 for \( \ell \rightarrow \infty \) (see detailed statement in Lemma 4). However, these results do not apply to neural networks equipped with the non-linear \( \text{BN} \) operator. Leveraging tools from Markov chain theory, our main result proves that the rank of \( H_{\ell} \) scales with the network width as \( \Omega(\sqrt{d}) \).

We further extend this result to non-linear neural networks. In particular, we establish the lower-bound rank(\( H_{\ell} \)) \( \geq 2 \) for all odd activation functions \( F \) (such as hyperbolic tangent).

1.4. **Empirical results (ii).** We conduct a comprehensive set of experiments which show that the rank of the pre-activation matrices is indeed a crucial quantity for training deep networks after random initialization. More specifically, we show that both the rank and the final training accuracy quickly diminish in depth unless batch-normalization layers are incorporated into the architecture of both simple feed-forward and convolutional neural networks. To take this reasoning beyond mere correlations, we actively intervene with the rank of networks before training and

\[^1\]In the limit, this effect appears regardless of the presence of residual connections.
Figure 1. Rank comparison in forward pass: The vertical axis shows logarithm of the rank of batch-normalized (ln(rank$_{\tau}$($H_\ell$)), blue lines) and vanilla networks (ln(rank$_{\tau}$($\tilde{H}_\ell$)), orange lines) of width 32 (d) and increasing depth ($\ell$) for two values of $\gamma$. For numerical approximation of the rank, we normalize each matrix and zero-out singular values with absolute values less than 10$^{-9}$. We draw weights $\{W_\ell\}_{\ell=1}^L$ i.i.d. from a symmetric uniform distribution with variance one ($U[-\sqrt{3}, \sqrt{3}]$) and input a full rank matrix with Gaussian data.

Table 1. Summary of theoretical and experimental rank analysis for deep neural networks. Notably, rank$_{\tau}$, which is defined in Eq. (4), is a soft notion of rank which is robust for numerical experiments.

|                  | linear | tanh |
|------------------|--------|------|
| no BN            | Theory | rank$_{\tau}$($H_{\infty}$) = 1 (Lem. 4) |
|                  | Experiments | rank$_{\tau}$($H_{\ell}\geq k$) = 1 |
| BN               | Theory | rank$_{\tau}$($H_\ell$) $\geq \Omega(\sqrt{d})$ (Thm. 3) |
|                  | Experiments | rank$_{\tau}$($H_\ell$) $\geq \Omega(\sqrt{d})$ |

show that (a) one can break the training stability of BN by initializing in a way that reduces its rank preserving properties, and (b) a rank-increasing pre-training procedure for deep vanilla neural networks significantly accelerates learning even in deep networks. In a final experiment, we give some intuition by connecting the rank of a network to its information propagation properties.

2. Preliminaries

2.1. Rank lower bound. For each pre-activation $H \in \mathbb{R}^{d \times N}$, we define its matrix of second moments as $M(H) = \frac{1}{N}HH^\top$. Given the above map, we define the ratio function $r(H) : \mathbb{R}^{d \times N} \to \mathbb{R}$ as

$$r(H) = \text{Tr}(M(H))^2/\|M(H)\|_F^2,$$

which lower bounds the rank of $H$ as stated in the next lemma.

Lemma 1. For every matrix $H$, $\text{rank}(H) \geq r(H)$.

2.2. Soft rank. The computation of the rank typically suffers from numerical issues as singular values can be small but not exactly equal to zero. To circumvent this issue, we introduce a soft notion of the rank denoted by rank$_{\tau}(H)$. Let $\sigma_1, \ldots, \sigma_d$ be the singular values of $H$. Given $\tau \in \mathbb{R}^+$,
rank$_r(H)$ is defined as

$$
\text{rank}_r(H) = \sum_{i=1}^{d} 1(\sigma_i^2/N \geq \tau),
$$

which is the number of singular values whose absolute values are greater than $\sqrt{N/\tau}$. It is clear that rank$_r(H)$ is less than rank$(H)$ for all $H$ matrices.

2.3. **Underlying spaces.** Throughout this paper, we assume that $N$ is finite. Let $H$ be the space of all $d \times N$ matrices whose rows have equal norm $\sqrt{N}$. This space includes the set of pre-activation matrices of a neural network equipped with BN. $H$ is endowed with the Frobenius norm $\| \cdot \|_F$. Notably, $H$ is a compact space. One interesting property of $H \in H$ is that $r(H)$ provides a lower-bound on rank$_r(H)$. The next lemma establishes this bound.

**Lemma 2.** For all $H \in H$, rank$_r(H) \geq (1 - \tau)^2 r(H)$ holds for $\tau \in [0, 1]$.

We use notation $\mathcal{P}(H)$ for the space of all probability measures defined over $H$.

2.4. **Initialization.** This paper studies neural networks with standard randomly initialized weights $\{W_t\}$, whose elements are i.i.d. samples from a symmetric, zero-mean distribution such as in e.g. [GB10, HZRS15]. Let $\mu$ denote the probability law of $W_t$.

**Definition 1** (Distribution of weights). Let $W \in \mathbb{R}^{d \times d}$ be a random matrix. $W$ is drawn from distribution $\mu$ (i.e. $W \sim \mu$), if all elements of $W$ are drawn independently from the zero-mean and unit-variance distribution uniform$[\sqrt{3}, \sqrt{3}]$.

2.5. **Chain of pre-activation matrices.** We define the operator $\text{FBN}_\gamma : \mathbb{R}^{d \times N} \times \mathbb{R}^{d \times d} \to H$ as

$$
\text{FBN}_\gamma(H,W) = (\text{diag}(M(H_\gamma(W))))^{-1/2} H_\gamma(W),
$$

where $M : \mathbb{R}^{d \times N} \to \mathbb{R}^{d \times d}$ is defined in Eq. (2) and

$$
H_\gamma(W) = H + \gamma WF(H).
$$

The operator $\text{FBN}_\gamma$ applies the operator $\text{BN}_{0,1_d}$ to $H_\gamma(W)$. That is, we consider $\alpha$ and $\beta$ as fixed. Furthermore, we omit the mean-deduction (i.e., multiplication by $1_N 1_N^T$ in Eq. (1)) for simplicity. As shown in the appendix, this modification does not impair the performance of BN. Given $\text{FBN}_\gamma$, we define a Markov chain of pre-activation matrices.

**Definition 2.** The Markov chain of the pre-activation matrices of a neural network equipped with BN, denoted by $\{H^{(\gamma)}_\ell\}_{\ell \geq 1}, X, \mu$, is a chain that obeys $H^{(\gamma)}_{\ell+1} = \text{FBN}_\gamma(H^{(\gamma)}_\ell, W_\ell)$ and $H^{(\gamma)}_1 = \text{FBN}_\gamma(X, W_1)$ where $\{W_\ell\}_{\ell \geq 0}$ are drawn i.i.d. from $\mu$.

The invariant distribution associated with the chain is defined below.

**Definition 3.** $\nu_\gamma \in \mathcal{P}(H)$ is an invariant distribution associated with chain $\{H^{(\gamma)}_\ell\}_{\ell \geq 1}, X, \mu$, if

$$
\int g(H) d\nu_\gamma(H) = \int g(\text{FBN}_\gamma(H,W)) d\nu_\gamma(H) d\mu(W)
$$

holds for all bounded Borel functions $g$.

The invariant distribution $\nu_\gamma$ determines the limit of the average of $g(H^{(\gamma)}_\ell)$ for bounded Borel functions $g : H \to \mathbb{R}$. Under fairly weak assumptions, the chain of pre-activation matrices $\{H^{(\gamma)}_\ell\}, X, \mu$ obeys Birkhoffs Ergodicity [DMPS18]. Namely,

$$
\lim_{L \to \infty} \frac{1}{L} \sum_{\ell=1}^{L} g(H^{(\gamma)}_\ell) = \int g(H) d\nu_\gamma(H),
$$

holds almost surely.
3. Linear neural networks

We first focus on linear neural networks for which we have $F(H) = H$.

3.1. Main result. The next theorem presents our main result on the rank of the pre-activation matrices $\{H_\ell^{(\gamma)}\}_{\ell=1}^L$ (for a linear neural network equipped with BN).

**Theorem 3.** Suppose that $F(H) = H$, $\text{rank}(X) = d$, and $\gamma$ is sufficiently small (independent of $\ell$). Furthermore, assume the Markov chain $\{(H_\ell^{(\gamma)})_{\ell \geq 1}, X, \mu\}$ admits a unique invariant distribution. Then the following limit exists and

$$\lim_{L \to \infty} \frac{1}{L} \sum_{\ell=1}^L \text{rank}_\tau(H_\ell^{(\gamma)}) \geq \lim_{L \to \infty} \frac{(1 - \tau)^2}{L} \sum_{\ell=1}^L r(H_\ell^{(\gamma)}) \geq (1 - \tau)^2 \Omega(\sqrt{d})$$

holds almost surely for all $\tau \in [0, 1]$, under an additional technical assumption detailed in the Appendix.

Please see the Appendix for a detailed proof.

3.2. Implication on singular values. By setting for example $\tau = \frac{1}{2}$, the result of Theorem 3 states that the average number of singular values with absolute value greater than $\sqrt{N/2}$ is at least $\sqrt{d}/24$, regardless of the depth of the network. Thus, BN preserves at least a certain amount of variation in the data as the input is propagated forwards. For a comparison, replacing $\text{diag}(M)^{-1/2}$ by the full inverse $(M)^{-1/2}$ in Eq. (5) effectively constitutes a whitening of all pre-activation matrices, such that all $\{H_\ell^{(\gamma)}\}_{\ell=1}^L$ would be full rank ($d$). Yet, the whitening operation is (i) in itself not computationally feasible and (ii) back-propagating through the whitening operator is even more expensive. As such, BN can be seen as a computationally cheap approximation of whitening, which does not yield pre-activation matrices with full rank but still provides a relatively high rank scaling as $\Omega(\sqrt{d})$.

3.3. Experimental validations. We validate the result of Theorem 3 for $d = N$ and $\tau = 0.5$ in Fig. 2. The curves for different values of $\gamma$ clearly validate the $\Omega(\sqrt{d})$ dependency for $\lim_{L \to \infty} \frac{1}{L} \sum_{\ell=1}^L \text{rank}_\tau(H_\ell^{(\gamma)})/L$ predicted in the theorem. Although the established guarantee requires the step size to be small, the results of Figure 2 indicates that the established lower bound holds for a wider range of $\gamma$, including the case where no residual connections are used at all ($\gamma = \infty$).

Interestingly, this result also holds when the input matrix is close to being rank deficient in the sense that its rows are almost linearly dependent, i.e. each pairwise cosine similarity is almost one. In this case, we find that batch normalization is able to amplify small variations in the data. As can be seen in Figure 3, the pairwise eigengap between the first few eigenvalues decreases with the network depth. Note that, as suggested by our theory as well as the result of Figure 1 & 2, this network is still rank deficient since $\lambda_{\text{min}} \approx 0$ and hence such effects are not captured by the condition number. In that sense, a rank analysis is one step further towards an analysis of the entire eigenspectrum of the network. In the Appendix, we will provide further details on this observation and justify it through our Markov-chains-based analysis.

3.4. Necessary assumptions. The result of Theorem 3 relies on three key assumptions: (i) the input $X$ needs to be full rank, (ii) the markov chain must admit a unique invariant distribution and (iii) the weight matrices have to be drawn from a zero-mean distribution $\mu$. We believe that these assumptions are not only sufficient but also necessary to have a high rank. For example, consider the chain starting from a rank one matrix. In this case, the rank of all $\{H_\ell^{(\gamma)}\}_{\ell}$ is one as the rank cannot
Figure 2. Result of Theorem 3 for different values of $\gamma$, where $\gamma = \infty$ stands for networks without skip connections. Each point represents the average rank $1/2$ over depth ($L=10^6$) of networks of width $d \in \{8, 16, ..., 256\}$ as on the x-axis. Shaded areas are standard deviation.

Figure 3. Top 10 eigenvalues of $M_\ell = M(H_i^{(\gamma)})$ for increasing values of $\ell$. As can be seen, BN quickly amplifies smaller variations in the data while reducing the largest one. Possibly increase through the recurrence $F_{B_n \gamma}$. Furthermore, one can check that the chain starting from a rank one input admits many distinct stationary distributions (see the Appendix for details). Therefore, starting from a relatively high rank input is necessary for the desired lower-bound on the rank. Finally, we will show experimentally (Section 5.2) that the zero-mean property of the initialization law $\mu$ is not only essential for the theoretical result of Theorem 3 but also crucial for the performance of SGD on neural networks equipped with BN.
3.5. **Comparison with vanilla networks.** Now, we compare the predicted rank of $H_{\ell}$ with the rank of $\tilde{H}_\ell$ for the following linear network:

$$
\tilde{H}_\ell^{(\gamma)} = (I + \gamma W_\ell)H_{\ell-1}^{(\gamma)} = \left( \prod_{k=1}^{\ell} (I + \gamma W_k) \right) X.
$$

Since the norm of $\tilde{H}_\ell^{(\gamma)}$ is not necessarily bounded, we normalize it as $\tilde{H}_\ell^{(\gamma)} = \tilde{B}_\ell X / \|\tilde{B}_\ell\|$. Assuming that $\|X\|$ is bounded, $\|\tilde{H}_\ell^{(\gamma)}\|$ is bounded too. The next lemma characterizes the limit behaviour of $\{\tilde{H}_\ell^{(\gamma)}\}$.

**Lemma 4.** Suppose that the input $X$ is bounded and $\gamma \in (0, 1)$. Then, there exists a monotonically increasing sequence of integers denoted by $\ell_1 < \ell_2, \ldots < \ell_L$ such that $\{\tilde{H}_k^{(\gamma)}\}$ converges to a rank one matrix.

According to the empirical observations in Figure 1, the above result holds for the usual sequence of indices $\{\ell_k = k\}$, which indicates that $\{\tilde{H}_k^{(\gamma)}\}$ converges to a rank one matrix. This is a striking contrast to the the result of Theorem 3 established for a BN network.

The spectral distribution of products of random matrices with i.i.d. standard Gaussian elements has been studied extensively [BGSW18, LWZ+16, For13]. One can show that the gap between the top singular value and the second largest singular value increases with the number of products (i.e., $\ell$) in an exponential rate [For13, LWZ+16]. Hence, the normalized product of matrix converges to a rank one matrix. Lemma 4 extends this result to products of random matrices with a residual branch that is obtained by adding identity matrix to random matrices. Indeed, residual skip connections cannot avoid rank collapse for very deep neural networks, unless one is willing to incorporate a depth dependent down-scaling of the parametric branch as for example $\gamma = O(\frac{1}{d})$ [AZLS18]. BN layers, however, provably avoids rank collapse even for infinitely deep neural networks and without requiring the networks to become in some way closer and closer to identity (Theorem 3).

### 4. Non-linear Neural Networks

#### 4.1. Main results.** In this section, we consider batch normalized networks with odd activation functions $(-F(x) = F(-x))$. The next Theorem proves that the rank does not collapse, it is $\text{rank}(H_{\ell}^{(\gamma)}) \geq 2$.

**Theorem 5.** Suppose that $F$ is an odd and bounded function, namely $|F(x)| \leq B|x|$ for all $x \in \mathbb{R}$ and $B \geq 0$. If the Markov chain of pre-activation matrices $\{(H_\ell)_{\ell \geq 1}, X, \mu\}$ admits a unique invariant distribution, then

$$
\text{rank}(H_{\ell}^{(\gamma)}) \geq 2 \quad (7)
$$

holds almost surely for all integers $\ell$ and $\gamma \leq 1/(8Bd)$.

Compared to Theorem 3, the lower-bound of Theorem 5 is rather weaker since it is established in terms of the rank (instead of $\text{rank}_*\gamma$) and it does not scale with $d$. Yet, the established result relies on fairly weak assumptions on the activation function.

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$^2$The growth-rate of $i$-th singular value is determined by $i$-th Lyapunov exponent of product of random matrices. We refer readers to [For13] for more details on Lyapunov exponents.
4.2. **Experimental validations.** One can readily check that tangent hyperbolic function, which is a commonly used activation function, satisfies the assumptions of the last Theorem. Indeed, Fig. 4 confirms that the rank does not collapse to one for tanh networks equipped with BN. Interestingly, we again observe that the rank scales favourably with the network with (d) and the result holds for a much wider range of $\gamma$ than that predicted by the theory.

![Figure 4](image-url)

**Figure 4.** Experimental validation for $F = \tanh$. Horizontal axis is the logarithm of the number of hidden layers, i.e. $\log_2(L)$. We plot $\log_2\left(\frac{1}{T} \sum_{t=1}^{L} r(H_t^{(\gamma)})\right)$. The results suggest that the statement of Theorem 5 is valid but can be improved to match the $O(\sqrt{d})$ result for linear nets.

4.3. **Proof of Theorem 5.** The proof of Theorem 5 is simple and provides insights about the proof of Theorem 3. Recall that the weights $\{W_\ell\}$ are drawn from the distribution $\mu$, hence they obey an important property: element-wise symmetricity, i.e. $[W_\ell]_{ij}$ is distributed as $-[W_\ell]_{ij}$. Such an initialization enforces an interesting structural property for the invariant distribution $\nu_\gamma$, which we detail in the following.

4.4. **Symmetricity.** The symmetricity of the law of $\mu$ imposes a symmetric structure on the unique invariant distribution $\nu_\gamma$.

**Lemma 6.** Suppose that the chain $\{\{H_t\}_{t=1}^{\infty}, X, \mu\}$ (Def. 2) admits a unique invariant distribution $\nu_\gamma$ and $H$ is drawn from $\nu_\gamma$. If $F$ is an odd function, then the law of $H_i$: equates the law of $-H_i$: where $H_i$: denotes the $i$th row of matrix $H$.

The proof of the last lemma is provided in the Appendix. An important consequence of the symmetricity is that

$$\mathbb{E}_{H \sim \nu_\gamma} [[M(H)]_{ij}] = -\mathbb{E}_{H \sim \nu_\gamma} [[M(H)]_{ij}] = 0 \quad (8)$$

holds for all $i \neq j$. The above property enforces that $[M(H)]_{ij}^2$ is small and hence $\|M(H)\|_F^2$ is small as well. As rank$(M)$ is proportional to $1/\|M(H)\|_F^2$ (compare Eq. (3)), the rank stays large. The rest of the proof is based on this intuition.
4.5. **Ergodicity.** Given the uniqueness of the invariant distribution, we can invoke Birkhoff’s Ergodic Theorem for Markov Chains (Theorem 5.2.1 and 5.2.6 [DMPS18]) that yields

\[
\lim_{L \to \infty} \frac{1}{L} \sum_{\ell=1}^{L} [M(H_{\ell}^{(\gamma)})]_{ij} = \mathbb{E}_{H \sim \nu_{\gamma}} ([M(H)]_{ij}).
\]

This allows us to conclude the proof by a simple contradiction. Assume that \(\text{rank}(H_{k}^{(\gamma)})\) is indeed one. Then, as established in the following Lemma, in the limit all entries of \(M(H_{\ell}^{(\gamma)})\) are constant and either \(-1\) or \(1\).

**Lemma 7.** Suppose the assumptions of Lemma 5 hold. If \(\text{rank}(H_{k}^{(\gamma)}) = 1\) for an integer \(k\), then

\[
\lim_{L \to \infty} \frac{1}{L} \sum_{\ell=1}^{L} [M(H_{\ell}^{(\gamma)})]_{ij} \in \{1, -1\}
\]

holds.

The intuition for this lemma is simple: Suppose that \(\text{rank}(H) = 1\), then established rank bound from Lemma 4 gives that \(\|M_{\ell}\|_{F} = d^{2}\). Yet, the fact that BN yields matrices \(M_{\ell}\) where all diagonal elements are one and all off-diagonals are smaller than 1 in absolute value suggests that then \([M(H_{\ell})]_{ij} \in \{+1, -1\}\) for all \(i, j\) must hold. Finally, for sufficiently small \(\gamma\) one can easily prove that the sign of \([M(H_{\ell})]_{ij}\) and \([M(H_{\ell+1})]_{ij}\) are the same (Please find a detailed proof in the Appendix).

As a result, leveraging the ergodicity established in (66), we get that then

\[
\mathbb{E}_{H \sim \nu_{\gamma}} ([M(H)]_{ij}) \in \{+1, -1\}
\]

must also hold. However, this contradicts the consequence of the symmetricity (Eq. (8)) which states that for any \(j \neq i\) we have \(\mathbb{E}_{H \sim \nu_{\gamma}} ([M(H)]_{ij}) = -\mathbb{E}_{H \sim \nu_{\gamma}} ([M(H)]_{ij}) = 0\). Thus, the rank one assumption cannot hold, which proves the assertion.

5. **Importance of the rank for optimization**

5.1. **Correlating rank and training accuracy.** Our theoretical considerations as well as the simulations conducted in Figure 4 suggest that batch normalized networks keep a high rank while vanilla MLPs suffer from quickly occurring rank deficiency as the networks grow deeper. In order to put these results into perspective on real data, we train batch-normalized and vanilla MLPs of growing depth on the Fashion-MNIST dataset for 15'000 iterations with a batch-size 32 and grid-searched learning rate. Indeed, as can be seen in Figure 5 the vanilla networks are essentially unable to learn as soon as the number of layers is above 10. Batch-normalized networks, however, preserve a high rank across all network sizes and their training accuracy drops only very mildly as the networks reach depth 32.

5.2. **Beyond correlation: rank and optimization stability.** While Figures 2 & 5 clearly confirm our theoretical finding that batch-norm indeed yields a higher rank, it is still unclear whether the improved training ability of deep batch-normalized networks is really due to the improved rank or whether the previous results depict a mere correlation.

To settle this matter we conduct two further experiments, in which we show that: (i) The rank preserving property of batch normalization can be broken by initializing networks asymmetrically, leads to a deterioration of learning\(^3\) (ii) One can pre-train a randomly initialized vanilla MLP in such a way that the pre-activation matrix of the last layer become high rank, which allows previously un-trainable deep networks to learn.

\(^3\)Note that a symmetric initialization around zero is also important for our theoretical result (Lemma 6).
Figure 5. **Effect of depth on learning**: Fashion-MNIST on MLPs of depth 1-32, where each hidden layer has 128 units with ReLU activations in all networks. Average and 95% confidence interval of 5 independent runs.

Figure 6. **Pretraining**: Fashion-MNIST on MLPs of depth 32 and width 128. Blue line is a ReLU network with standard initialization. Other solid lines are pre-trained layer-wise with 25 (orange) and 75 (green) iterations to improve rank. Dashed lines are batchnorm networks with standard and asymmetric initialization. Average and 95% confidence interval of 5 independent runs.

For the results depicted in Figure 6 we train various MLPs of depth 32 on Fashion-MNIST. While the vanilla network is unable to learn after standard random initialization, we pre-train each layer of two further networks with a small number of stochastic gradient ascent steps (25 and
75) on the rank lower bound $r(M)$ in Eq. (3). Interestingly, this allows even deep MLPs to train without batchnorm. Furthermore, we train two MLPs with batchnorm but change the initialization for the second net from the standard PyTorch way $W_{l,i,j} \sim U\left(-\frac{1}{\sqrt{d_l}}, +\frac{1}{\sqrt{d_l}}\right)$ \cite{PGM19,GB10} to $W_{l,i,j} \sim U(0, +\frac{2}{\sqrt{d_l}})$, where $d_l$ is the layer size.

As can be seen to the right, this small change reduces the rank preserving quality of BN significantly, which is reflected in much slower learning behaviour. For all networks, we want to emphasize the clear trend that networks with higher rank perform much faster optimization, especially in the earlier epochs. Interestingly, as depicted in Figure 7, the above introduced asymmetric initialization does not only break batchnorm in the case of simple MLPs but even sophisticated modern day architectures such as VGG and ResNet networks are unable to fit the CIFAR-10 dataset after changing the initialization in this way.

5.3. Why the rank matters for gradient based learning. Finally, we provide a possible intuitive explanation of why rank one activations prevent randomly initialized networks from learning. Particularly, we argue that these networks essentially map all inputs to a very small
subspace such that most (if not all) such that the final classification layer can no longer disentangle the hidden representations. As a result, the gradients of that layer also align, yielding a learning signal that becomes independent of the input.

To be more precise, consider training on a dataset \(\{x_i, y_i\}_{i=1}^n\), where \(x_i \in \mathbb{R}^{d_{in}}\) and \(y_i \in \mathbb{R}^{d_{out}}\). Each column \(\hat{H}_{L,i}(W)\) of the pre-activations of the last hidden layer \(\hat{H}_L(W)\) (of any given network) is the latent representation of datapoint \(i\), which is fed into a final classification layer parametrized by \(W_L \in \mathbb{R}^{d_{out} \times d_h}\). We optimize \(\mathcal{L}(W)\), where \(W\) is a tensor containing all weights \(W_1, \ldots, W_L\):

\[
\min_W \mathcal{L}(W) = \sum_{i=1}^n \ell(y_i, W_L F(H_{L,i}(W))),
\]

where \(\ell: \mathbb{R}^{d_{out}} \to \mathbb{R}^+\) is a differentiable loss function. Now, if the pre-activation matrix becomes rank one (as predicted for vanilla MLPs by Lemma 4 and Fig. 1), one can readily check that the stochastic gradients of any neuron \(k\) in the last linear layer, i.e., \(\nabla_{W_{L,[k,\cdot]}} \mathcal{L}_i(W) = (\nabla \ell_i)_k F(H_{L,i})\), align for both linear and ReLU networks.

**Proposition 8.** Consider a network with rank one pre-activation in the last layer \(\hat{H}_L(W)\), then for any two datapoints \(i, j\) we have \(F(\hat{H}_{L,i}) = \alpha_{i,j} F(\hat{H}_{L,j})\), \(\alpha_{i,j} \in \mathbb{R}\) for both \(F(\hat{H}) = \hat{H}\) and \(F(H) = \max(\hat{H}, 0)\). Consequently,

\[
\nabla_{W_{L,[k,\cdot]}} \mathcal{L}_i(W) = \alpha_{i,j} (\nabla \ell_i)_k (\nabla \ell_j)_k \nabla_{W_{L,[k,\cdot]}} \mathcal{L}_j(W)
\]

hold \(\forall i, j\). That is, all stochastic gradients of neuron \(k\) in the final classification layer align along one single direction in \(\mathbb{R}^d\).

We call this effect **directional gradient vanishing**. To validate this claim, we again train CIFAR-10 on the VGG19 network from Figure 7 (top).

![VGG19: Training Accuracy](image1)

**Figure 8.** Directional gradient vanishing CIFAR-10 on a VGG19 network with BN, SGD, SGD with 100x learning rate and SGD on random data. Average and 95% confidence interval of 5 independent runs.

\(^4\)A single line in \(\mathbb{R}^d\) in the extreme case of rank one mappings
As expected, the network shows perfectly aligned gradients without BN (right hand side of Fig. 8), which renders it un-trainable. In a next step, we replace the input by images generated randomly from a uniform distribution between 0 and 255 and find that SGD takes almost the exact same path on this data (compare log accuracy on the left hand side). Thus, our results suggest that the commonly accepted vanishing gradient norm hypothesis is not descriptive enough since SGD does not take small steps into the right- but into a random direction after initialization in deep neural networks. As a result, even a 100x increase in the learning rate does not allow the network to train. We consider our observation as a potential starting point for novel theoretical analysis focusing on understanding the propagation of information through neural networks, whose importance has also been highlighted by [BGSW18].

6. DISCUSSIONS AND RELATED WORKS

Recently, different hypotheses for the effectiveness of batch normalization have emerged in the literature: decoupling optimization of direction and length of the parameters [KDL+18], auto-tuning of the learning rate for stochastic gradient descent [ALLIS], widening the learning rate range [BGSW18], alleviating sharpness of the Fisher information matrix [KAA19] and smoothing the optimization landscape [STIM18]. Yet, most of these justifications are still being debated within the community. For example, [STIM18] argue that under certain assumptions batch normalization simplifies optimization by smoothing the loss landscape but their analysis is on a per-layer basis and treats only the largest eigenvalue. Furthermore, recent empirical studies attribute the exact opposite effect to BN, e.g. on a ResNet20 [YGKM19].

Mostly related to our work is a side contribution made in [BGSW18] which empirically shows that vanilla networks tend to always predict one and the same class for any inputs after random initialization. Furthermore, they show that BN prevents this issue, thereby yielding gradients that are not dominated by a single output neuron. This reasoning is very much in line with our observations in Section 5 but a theoretical investigation of this effect was not undertaken in [BGSW18].

In this work we conduct a sound theoretical analysis of the effects of batch normalization on neural networks after random initialization. Towards this end we leverage strong mathematical tools from Markov chain - and Ergodic theory, as was done e.g. by [DDB17] for the convergence analysis of constant step size SGD. Both our theoretical analysis and the empirical findings in Section 5 underpin that preventing rank collapse of pre-activation matrices is (i) a key property of BN and (ii) of crucial importance for training deep networks with gradient based methods.

The latter observation is reflected in our experiments which show that on can accelerate optimization of deep vanilla neural networks by increasing the rank through a pre-training step. This result is particularly interesting for future research as it suggests a computationally viable alternative to BN in settings where batch normalization layers are commonly not applicable as for example during test time, for high resolution image tasks (where memory is a bottleneck) or when training recurrent- or generative neural networks. Furthermore, analyzing numerous recent alternative normalization techniques [BKH16, SK16, UVL16] and initialization schemes [SMG13, ACGH18, ZDM19] in terms of their rank preservation properties constitutes an interesting direction of future research.

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7. Appendix

7.1. Preliminaries. Let \( H \sim \nu \) denote random matrix \( H \in \mathcal{H} \) is drawn from distribution \( \nu \). Then, the expectation of a function \( g : \mathcal{H} \to \mathbb{R} \) with respect to \( \nu \) is denoted as

\[
\mathbb{E}_{H \sim \nu} [g(H)] = \int g(H) \nu(dH).
\]

(14)

If two random matrix \( A \) and \( B \) have the same probability law, we use the notation \( A \overset{d}{=} B \). Let \( \|M\|_F^2 \) denote the Frobenius norm of an arbitrary matrix \( M \).

Recall that \( \mathcal{H} \) denotes the space of \( d \times N \) matrices whose rows have equal norm \( \sqrt{N} \). The matrix \( M(H) = HH^\top / N \) obey the following interesting properties for all \( H \in \mathcal{H} \): (i) its diagonal elements are one (ii) the absolute value of its off-diagonal elements is less than one. Property (i) imposes trace (hence sum of eigenvalues) of \( M(H) \) to be \( d \). We will repeatedly use these properties in our analysis. Notably, this notation has been used in the definition of the invariance distribution in Def. \( 3 \).

We assume that weight matrices \( \{W_\ell\}_\ell^L \) are drawn i.i.d. from distribution \( \mu \) defined below.

7.2. Lower bounds on (soft) rank. Recall that we introduced the ratio \( r(H) = \text{Tr}(M(H))^2 / \|M(H)\|_F^2 \) in Eq. (3) that bounds rank\((H)\) (stated in Lemma 1) and soft rank \( \text{rank}_\tau(H) \) (stated in Lemma 2). This section establishes these lower bounds.

Proof of Lemma 1. Let \( M := M(H) = HH^\top / N \). Since the eigenvalues of \( H \) are obtained by a constant scaling factor of squared singular values of \( H \), these two matrices have the same rank. We now establish a lower bound on rank\((M)\). Let \( \lambda \in \mathbb{R}^d \) contains eigenvalues of matrix \( M \) hence \( \|\lambda\|_1 = \text{Tr}(M) \) and \( \|\lambda\|_2^2 = \|M\|_F^2 \). Given \( \lambda \), we define the vector \( w \in \mathbb{R}^d \) as

\[
w_i = \begin{cases} 
1/\|\lambda\|_0 & : \lambda_i \neq 0 \\
0 & : \lambda_i = 0
\end{cases}
\]

(15)

The rest of the proof is based on a straightforward application of Cauchy-Schwartz

\[
|\langle \lambda, w \rangle| \leq \|\lambda\|_2 \|w\|_2
\]

(16)

\[
\implies \|\lambda\|_1 / \|\lambda\|_0 \leq \|\lambda\|_2 / \|\lambda\|_0^{1/2}
\]

(17)

\[
\implies \|\lambda\|_1 / \|\lambda\|_2 \leq \|\lambda\|_0^{1/2}
\]

(18)

Replacing \( \|\lambda\|_2 = \|M\|_F \) and \( \|\lambda\|_1 = \text{Tr}(M) \) into the above equation concludes the result. Note that the above proof technique has been used in the planted sparse vector problem \cite{BS16}.

\( \square \)

Proof of Lemma 2. The proof is similar to the proof of Lemma 1. Let \( \lambda \in \mathbb{R}_+^d \) be a vector containing the eigenvalues of the matrix \( M(H) = HH^\top / N \). Let \( \sigma \in \mathbb{R}_+^d \) contain singular values of \( H \). Then, one can readily check that \( \sigma_i^2 / N = \lambda_i \). Furthermore, \( \|\lambda\|_1 = d \) holds since \( H \in \mathcal{H} \). By definition, we have

\[
\text{rank}_\tau(H) = h_\tau(\lambda) := \sum_{i=1}^d 1(\sigma_i^2 / N \geq \tau) = \sum_{i=1}^d 1(\lambda_i \geq \tau).
\]

(19)

We define a vector \( w \in \mathbb{R}^d \) with entries

\[
w_i = \begin{cases} 
1/h_\tau(\lambda) & : \lambda_i \geq \tau \\
0 & : \text{otherwise}
\end{cases}
\]

(20)
Then, we use Cauchy-Schwartz to get
\begin{equation}
|\langle \lambda, w \rangle| \leq \|\lambda\|_2 \|w\|_2.
\end{equation}
It is easy to check that \( \|w\|_2 = h_r(\lambda)^{-1/2} \) holds. Furthermore,
\begin{equation}
h_r(\lambda)|\langle w, \lambda \rangle| = \sum_{|\lambda_i| \geq \tau} |\lambda_i|
\end{equation}
\begin{equation}
\geq \|\lambda\|_1 - d\tau
\end{equation}
\begin{equation}
\geq (1 - \tau)\|\lambda\|_1 \quad \|\lambda\|_1 = d
\end{equation}
Replacing this into the bound of Eq. (21) yields
\begin{equation}
\text{rank}_r(H) = h_r(\lambda) \geq (1 - \tau)^2\|\lambda\|_1^2/\|\lambda\|_2^2 = (1 - \tau)^2r(H)
\end{equation}
\[\Box\]

7.3. Analysis for Vanilla Linear Networks. In this section, we prove Lemma 4 that states the rank vanishing problem for vanilla linear networks. Since the proof relies on existing results on products of random matrices (PRM) [Bou12], we first shortly review these results. Let \( T \) be the set of \( d \times d \) matrices. Then, we review two notions for \( T \): contractiveness and strong irreducibility.

**Definition 4** (Contracting set [Bou12]). \( T \) is contracting if there exists a sequence \( \{M_n \in T, n \geq 0\} \) such that \( M_n/\|M_n\| \) converges to a rank one matrix.

**Definition 5** (Invariant union of proper subspaces [Bou12]). Consider a family of finite proper linear subspace \( V_1, \ldots, V_k \subset \mathbb{R}^d \). The union of these subspaces is invariant with respect to \( T \), if \( MV \in V_1 \) or \( V_2 \) or \( \ldots \) or \( V_k \) holds for \( \forall v \in V_1 \) or \( V_2 \) or \( \ldots \) or \( V_k \) and \( \forall M \in T \).

**Example 9.** Consider the following sets
\[
T = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad V_1 = \text{span}(\begin{pmatrix} 0 \\ 1 \end{pmatrix}), \quad V_2 = \text{span}(\begin{pmatrix} 1 \\ 0 \end{pmatrix})
\]
then, union of \( V_1 \) and \( V_2 \) is invariant with respect to \( T \) because \( \alpha T v_1 \in V_2 \) and \( \alpha T v_2 \in V_1 \) hold for \( \alpha \neq 0 \).

**Definition 6** (Strongly irreducible set [Bou12]). The set \( T \) is strongly irreducible if there does not exist a finite family of proper linear subspaces of \( \mathbb{R}^d \) such that their union is invariant with respect to \( T \).

For example, the set \( T \) defined in Example 9 is not strongly irreducible.

**Lemma 10** (Thm 3.1 of [Bou12]). Let \( W_1, W_2, \ldots \) be random \( d \times d \) matrices drawn independently from a distribution \( \mu \). Let \( B_n = \prod_{k=1}^n W_k \). If the support of \( \mu \) is strongly irreducible and contracting, then any limit point of \( \{B_n/\|B_n\|\}_{n=1}^\infty \) is a rank one matrix almost surely.

This result allows us to prove Lemma 4.

**Proof of Lemma 4**. Recall the structure of the random weight matrices as \( \hat{W}_k = I + \gamma W_k \) where the coordinates \( \hat{W}_k \) are i.i.d. from uniform\([−\sqrt{3}, \sqrt{3}]\) (i.e. with variance 1). Let \( m \) be a random integer that obeys the law \( p(m = k) = 2^{-k} \). Given the random variable \( m \), we define the random matrix \( Y = \prod_{k=1}^m \hat{W}_k \) and use the notation \( \mu' \) for its law. Let \( \{Y_i = \prod_{j=1}^{m_i} \hat{W}_{k_i} \}_{i=1}^k \) be drawn i.i.d. from \( \mu' \). Then, \( C_k := Y_k \ldots Y_2 Y_1 \) is distributed as \( B_{\ell_k} := \hat{W}_{\ell_k} \ldots \hat{W}_2 \hat{W}_1 \) for \( \ell_k = \sum_{i=1}^k m_i \). We prove that every limit point of \( \{C_k/\|C_k\|\} \) converges to a rank one matrix, which equates the convergence
of limit points of \( \{ B_{t_k}/\|B_{t_k}\| \} \) to a rank one matrix. To this end, we prove that the support of \( \mu' \) denoted by \( T_{\mu'} \) is contractive and strongly contractive. Then, Lemma 10 implies that the limit points of \( \{ C_k/\|C_k\| \} \) are rank one.

**Contracting.** Let \( e_1 \in \mathbb{R}^d \) be the first standard basis vector. Since \( A_n := (I + \gamma e_1 e_1^\top)^n \in T_{\mu'} \) and its limit point \( \{ A_n/\|A_n\| \} \) converges to a rank one matrix, \( T_{\mu'} \) is contractive.

**Strong irreducibility.** Consider an arbitrary family of linear proper subspaces of \( \mathbb{R}^d \) as \( \{ V_1, \ldots, V_q \} \). Let \( \nu \) be an arbitrary unit norm vector which belongs to one of the subspaces \( \{ V_i \}_{i=1}^q \). Given \( \nu \), we define an indexed family of matrices \( \{ M_\alpha \in T_{\mu'} | \alpha \in \mathbb{R}^d, |\alpha_i| \leq 1 \} \) such that

\[
M_\alpha = I + \frac{\gamma}{d} \sum_{i=1}^d \alpha_i e_i \nu^\top \in T_{\mu'},
\]

where \( e_i \) is the i-th standard basis \( ^5 \). Then, we get

\[
M_\alpha \nu = \nu + \frac{\gamma}{d} \sum_{i=1}^d \alpha_i e_i
\]

Therefore, \( \{ M_\alpha \nu | |\alpha_i| \leq 1 \} \) is not contained in any union of finite proper \((m < k)\)-dimensional linear subspace of \( \mathbb{R}^d \), hence \( T_{\mu'} \) is strongly irreducible.

7.4. **Initialization consequences.** Recall that weight matrices are assumed to be random with law \( \mu \). More precisely, we assume that the elements of the weight matrices \( \{ W_\ell \}_\ell \) are drawn i.i.d. from the zero-mean and unit-variance distribution uniform\([-\sqrt{3}, \sqrt{3}]\). This distribution obeys two important properties: (i) elements of matrices are drawn i.i.d and (ii) distribution of each element is symmetric, namely \( W_{ij} \) is distributed as \( -W_{ij} \). Here, we prove that these two properties impose an interesting structure on the invariant distribution of the chain \( \{ \{ H_\ell \}, X, \mu \} \) defined in Def. 2.

**Invariance and i.i.d. initialization.** Leveraging the i.i.d. assumption on the elements of the weight matrices \( \{ W_\ell \} \), the next lemma proves that this property imposes a structural permutation invariance on the law of the unique invariant distribution \( \nu_\gamma \) associated with the chain \( \{ \{ H_\ell^{(\gamma)} \}, X, \mu \} \).

**Lemma 11.** Suppose that the chain \( \{ \{ H_\ell \}_{\ell=1}^\infty, X, \mu \} \) (Def. 3) admits a unique invariant distribution \( \nu_\gamma \) (Def. 3). If \( H \) is drawn from \( \nu_\gamma \), the law of \( H \) and \( \Pi H \) are the same for any permutation matrix \( \Pi \in \mathbb{R}^{d \times d} \).

In other words, \( \nu_\gamma \) inherits the permutation invariance of the weights, which is due to the i.i.d. sampling of the weight elements. Notably, the above result holds for any choice of activation \( F \) used in the chain recurrence in Eq. [5].

**Proof of lemma 7.** Given two random matrices \( A \) and \( B \), \( A \overset{d}{=} B \) indicates that the random matrices \( A \) and \( B \) have the same probability law. The proof is a direct consequence of the independence of the elements of \( W_\ell \) that implies \( \Pi^\top W \Pi \overset{d}{=} W \) holds for a random matrix \( W \) with i.i.d elements. Let \( H \) is drawn from unique invariant distribution \( \nu_\gamma \), then

\[
H \overset{d}{=} H_+ \overset{d}{=} \left( \mathrm{diag}(H_{1/2} H_{1/2}^\top/N) \right)^{-1/2} H_{1/2}, \quad H_{1/2} := H + \gamma \Pi^\top W F(H)
\]

By multiplying both sides with \( \Pi \), we get

\[
\Pi H \overset{d}{=} \Pi \left( \mathrm{diag} \left( H_{1/2} H_{1/2}^\top/N \right) \right)^{-1/2} \Pi^\top \hat{H}_{1/2}, \quad \hat{H}_{1/2} := \Pi H + \gamma W F(\Pi H)
\]

Notably, the absolute value of each element of \( \frac{1}{d} \sum_{i=1}^d \alpha_i e_i v^\top \) is less than 1, hence this matrix belongs to the support of \( \mu \).
where we used the fact that $\Pi F(H) = F(\Pi H)$ since $F$ is applied to the matrix $H$ element-wise. Since $\Pi^\top \Pi = \Pi \Pi^\top = I$ holds, we get

\begin{align}
(30) \quad \text{diag} \left( H_{1/2}^\top H_{1/2}^\top \right) &= \text{diag} \left( \left( H + \gamma \Pi^\top W \Pi F(H) \right) \left( H + \gamma \Pi^\top W \Pi F(H) \right)^\top \right) \\
&= \text{diag} \left( \left( \Pi^\top \Pi H + \gamma \Pi^\top W \Pi F(H) \right) \left( \Pi^\top \Pi H + \gamma \Pi^\top W \Pi F(H) \right)^\top \right) \\
(31) \quad &= \text{diag} \left( \Pi^\top \tilde{H}_{1/2}^\top \tilde{H}_{1/2}^\top \Pi \right) \\
&= \Pi^\top \text{diag} \left( \tilde{H}_{1/2}^\top \tilde{H}_{1/2}^\top \right) \Pi \\
(32) \quad &= \Pi^\top \Pi \Pi^\top \\
&= \Pi \Pi^\top \Pi \\
(33) \quad &= \Pi \Pi^\top \\
&= \Pi \\
\end{align}

Replacing this into Eq. (29) yields

\begin{align}
(34) \quad \Pi H &= \Pi^\top \left( \Pi \Pi^\top \text{diag} \left( \tilde{H}_{1/2}^\top \tilde{H}_{1/2}^\top / N \right) \Pi \right)^{-1/2} \Pi^\top \tilde{H}_{1/2} \\
(35) \quad &= \Pi \Pi^\top \left( \text{diag} \left( \tilde{H}_{1/2}^\top \tilde{H}_{1/2}^\top / N \right) \right)^{-1/2} \Pi \Pi^\top \tilde{H}_{1/2} \\
(36) \quad &= \left( \text{diag} \left( \tilde{H}_{1/2}^\top \tilde{H}_{1/2}^\top / N \right) \right)^{-1/2} \tilde{H}_{1/2}
\end{align}

where we exploit the orthogonality of the permutation matrix in the second line. Hence, the law of $\Pi H$ is invariant. Since the invariant distribution is assumed to be unique, $\Pi H \overset{d}{=} H$ holds \hfill \Box

**Symmetry analysis.** Here, we provide the proof of Lemma 6 that relates the symmetry of $\mu$ to a symmetric structure for the invariant distribution $\nu_\gamma$. This proof also relies on the uniqueness of the invariant distribution.

**Proof of Lemma 6** The proof is similar to the proof of lemma 11. Let $S$ be a sign filling matrix: it is diagonal and its diagonal elements are in $\{+1, -1\}$. Then $SW \overset{d}{=} W$ holds for a random matrix $W$ whose distribution is coordinate-wise i.i.d. and symmetric. Let $H$ be drawn from the invariant distribution of the chain denoted by $\nu_\gamma$; Leveraging the invariance property, we get

\begin{align}
H \overset{d}{=} & \left( \text{diag} \left( H_{1/2}^\top H_{1/2}^\top / N \right) \right)^{-1/2} H_{1/2}, \quad H_{1/2} := H + \gamma S WS F(H) \\
\end{align}

By multiplying both sides with $S$, we get

\begin{align}
SH \overset{d}{=} & \left( \text{diag} \left( H_{1/2}^\top H_{1/2}^\top / N \right) \right)^{-1/2} \tilde{H}_{1/2}, \quad \tilde{H}_{1/2} := SH + \gamma WF(SH)
\end{align}

Note that we use the fact that diagonal matrices commute in the above derivation. Since $F$ is assumed to be odd, $SF(H) = F(SH)$ holds. Furthermore, $S^2 = I$ holds. Considering these facts, we get

\begin{align}
(37) \quad \text{diag} \left( H_{1/2}^\top H_{1/2}^\top \right) &= \text{diag} \left( \left( H + \gamma S WS F(H) \right) \left( H + \gamma S WS F(H) \right)^\top \right) \\
(38) \quad &= \text{diag} \left( \left( SH + \gamma WS F(H) \right) \left( SH + \gamma WS F(H) \right)^\top \right)
\end{align}
Recall the established lower bound on the rank \( \tau(H) \) holds hence \( \tau(H) \) holds for all \( H \in \mathcal{H} \). Therefore, \( \|M(H)\|_F^2 \) directly influences \( \tau(H) \) (and also \( \tau(H) \)) according to Lemmas 1 and 2. Here, we characterize the change in \( \|M(H)\|_F^2 \) after applying the FBN, \( \gamma \) to \( H \). Assuming that \( F \) is linear, the preactivation matrices obey the following recurrence
\[
H_+ = (\text{diag}(M(H_+(W))))^{-1/2} H_+(W), \quad H_+(W) = (I + \gamma W) H.
\]
Let \( M = M(H) \) and \( M_+ = M(H_+) \). The next lemma estimates the expectation (taken over the randomness of \( W \)) of the difference between the Frobenius norms of \( M_+ \) and \( M \).

**Lemma 12.** If \( W \sim \mu \) (defined in Def. [7]), then
\[
(\mathbb{E}_W\|M_+\|_F^2 - \|M\|_F^2) / (\gamma^2) = 2d^2 - 2\|M\|_F^2 - 8\text{Tr}(M^2) + 8\text{Tr}(\text{diag}(M^2)^2) + O(\gamma)
\]
holds.

The proof of the above lemma is based on a straightforward Taylor expansion of the BN non-linear operator. We postpone the detailed proof to the end of this section. The above equation seems complicated at the first glance, yet it provides some interesting insights.

**Interlude: intuition behind Lemma 12** In order to gain more understanding of the implications of the result derived in Lemma 12, we make the simplifying assumption that all the rows of matrix \( M \) have the same norm. We emphasize that this assumption is purely for intuition purposes and is not necessary for the proof of our main theorem. Under such an assumption, the next proposition shows that the change in the Frobenius norm directly relates to the spectral properties of matrix \( M \).

**Proposition 13.** Suppose that all the rows of matrix \( M \) have the same norm. Let \( \lambda \in \mathbb{R}^d \) contains eigenvalues of matrix \( M \). Then,
\[
\text{Tr}(M^3) = \|\lambda\|_3^3, \quad \text{Tr}(\text{diag}(M^2))^2 = \|\lambda\|^4 / d, \quad \|M\|_F^2 = \|\lambda\|_2^2
\]
holds hence
\[
\delta_F(M) = \delta_F(\lambda) := 2d^2 - 2\|\lambda\|^2_2 - 8\|\lambda\|_3^3 + 8\|\lambda\|^4_4 / d.
\]
We postpone the proof to the end of this section. The main difference between Lemma 12 and the last proposition is that the result of the last proposition is based on spectral properties of \( M \).

Based on the above proposition, we can explain the reasoning behind an interesting empirical observation we report in Figure 3. This figure plots the eigenvalues of the matrix \( M(H_\ell) \) starting from a matrix \( M(H_0) \) whose leading eigenvalue is large and all other eigenvalues are very small. We
observe that some small eigenvalues of \(M(H^{(3)})_\gamma\) grows with \(\ell\), while the leading eigenvector decreases. In the next example, we show that the result of the last proposition predicts this observation.

**Example 14.** Suppose that \(M\) is a matrix whose rows have the same norm. Let \(\lambda_1 \geq \lambda_2, \ldots, \lambda_d\) be the eigenvalues associated with the matrix \(M\) such that \(\lambda_2 = \lambda_{d-1} = \gamma^2\) and \(\lambda_1 = d - \gamma^2(d-1)\). In this setting, Prop. 13 implies that \(E\|M_+\|_F^2 < \|M\|_F^2 - \gamma^4d^2\) for a sufficiently small \(\gamma\). This change has two consequences in expectation: (i.) the leading eigenvalue of \(M_+\) is \(O(-\gamma^4d)\) smaller than the leading eigenvalue of \(M\), and (ii.) some small eigenvalues of \(M_+\) are greater than those of \(M\) (see Fig. 3).

We provide a more detailed justification for the above statement at the end of this section. This example illustrates that the change in Frobenius norm (characterized in Lemma 12) can predict the change in the eigenvalues of \(M(H^{(3)})_\gamma\) (singular values of \(H^{(3)}\)) and hence the desired rank. Inspired by this, we base the proof of Theorem 3 on leveraging the invariance property of the unique invariant distribution with respect to Frobenius norm — i.e. setting \(g(H) = \|M(H)\|_F^2\) in Def. 3.

**An observation: regularity of the invariant distribution** We now return to the result derived in Lemma 12 that characterizes the change in Frobenius norm of \(M(H)\) after applying \(FBN_\gamma\) (in Eq. (5)) to \(H\). We show how such a result can be used to leverage the invariance property with respect to the Frobenius norm. First, we observe that the term \(\text{Tr}(M(H)^3)\) in the expansion can be shown to dominate the term \(\text{Tr}((\text{diag}(M(H)^2))^2)\) in expectation. The next definition states this dominance formally.

**Definition 7.** (Regularity constant \(\alpha\)) Let \(\nu\) be a distribution over \(H \in \mathcal{H}\). Then regularity constant associated with \(\nu\) is defined as the following ratio:

\[
\alpha = \mathbb{E}_{H \sim \nu} \left[ \text{Tr}(\text{diag}(M(H)^2)^2) \right] / \left( \mathbb{E}_{H \sim \nu} \left[ \text{Tr}(M(H)^3) \right] \right).
\]

The next lemma states that the regularity constant \(\alpha\) associated with the invariant distribution \(\nu_\gamma\) is always less than one. Our analysis will in fact directly rely on \(\alpha < 1\).

**Lemma 15.** Suppose that the chain of pre-activation matrices \(\{\{H^{(3)}\}_\gamma, X, \mu\}\) (in Def. 2) admits the unique invariant distribution \(\nu_\gamma\) (in Def. 3). Then, the regularity constant of \(\nu_\gamma\) (in Def. 7) is less than one.

**Proof.** We use a proof by contradiction where we suppose that the regularity constant of distribution \(\nu_\gamma\) is greater than one, then we prove that it can not be invariant with respect to Frobenius norm.

If the regularity constant \(\alpha\) is greater than one, then

\[
\mathbb{E}_{H \sim \nu_\gamma} \left[ -\text{Tr}(M(H)^3) + \text{Tr}((\text{diag}(M(H)^2))^2) \right] \geq 0
\]

holds. According to Theorem 3, the rank of \(M(H)\) is at least 2. Since the sum of the eigenvalues is constant \(d\), the leading eigenvalue is less than \(d\). This leads to

\[
\|M(H)\|_F^2 = \sum_i \lambda_i^2 \leq \max_i \lambda_i \left( \sum_j \lambda_j \right) \leq d \max \lambda_i < d^2.
\]

Plugging the above inequality together with inequality 52 into the established bound in Lemma 12 yields

\[
\mathbb{E}_{W,H \sim \nu_\gamma} \left[ \|M(H^+)\|_F^2 - \|M(H)\|_F^2 \right] > 0
\]

for a sufficiently small \(\gamma\). Therefore, \(\nu_\gamma\) does not obey the invariance property for \(g(H) = \|M(H)\|_F^2\) in Def. 3. \(\square\)
We can experimentally estimate the regularity constant $\alpha$ using the Ergodicity of the chain. Assuming that the chain is Ergodic\footnote{The uniqueness of the invariant distribution implies Ergodicity (see Theorem 5.2.1 and 5.2.6 \cite{DMPS18}).},

\begin{equation}
\lim_{L \to \infty} \frac{1}{L} \sum_{\ell=1}^{L} g(H_{\ell}^{(\gamma)}) = \mathbb{E}_{H \sim \nu_{\gamma}} [g(H)]
\end{equation}

holds almost surely for every Borel bounded function $g : \mathcal{H} \to \mathbb{R}$. By setting $g_1(H) = \text{Tr}(M(H)^3)$ and $g_2(H) = \text{Tr} (\text{diag}(M(H)^2)^2)$, we can estimate $\mathbb{E}_{H \sim \nu_{\gamma}} [g_i(H)]$ for $i = 1$, and 2. Given these estimates, $\alpha$ can be estimated. Our experiments in Fig. 9 show that the regularity constant of invariant distribution $\nu_{\gamma}$ is less than 0.9 for $d > 10$.

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{fig9.png}
\caption{Regularity constant of the invariant distribution. The vertical axis is the estimated regularity constant $\alpha$ and the horizontal axis is $d$. We use $L = 10^5$ (in Eq. (54)).}
\end{figure}

**Interlude: intuition behind the regularity** We highlight the regularity constant does not necessarily relates to the desired rank property in Theorem 3. This is illustrated in the next example that shows how the regularity constant relates to the spectral properties of $M(H)$.

**Example 16.** Suppose that the support of distribution $\nu$ contains only matrices $H \in \mathcal{H}$ for which all rows of $M(H)$ have the same norm. If the regularity constant of $\nu$ is greater than or equal to one, then all non-zero eigenvalues of matrix $M(H)$ are equal.

A detailed justification of the above statement is presented at the end of this section. This example shows that the regularity constant does not necessarily relate to the rank of $H$, but instead it is determined by how much non-zero eigenvalues are close to each other. We believe that a sufficient variation in non-zero eigenvalues of $M(H)$ imposes the regularity of the law of $H$ with a constant less than one (i.e. $\alpha < 1$ in Def. 7). The next example demonstrates this.

**Example 17.** Suppose the support of distribution $\nu$ contains matrices $H \in \mathcal{H}$ for which all rows of $M(H)$ have the same norm. Let $\lambda \in \mathbb{R}^d$ contains sorted eigenvalues of $M(H)$. If $\lambda_1 = \Theta(d^3)$ and $\lambda_i = o(d^3)$ for $i > 1$ and $\beta < 1$\footnote{According to definition, $\lim_{d \to \infty} o(d^3)/\Theta(d^3) = 0$}, then the regularity constant $\alpha$ associated with $\nu$ is less than 0.9 for a sufficiently large $d$.

We later provide further details about this example.

**Invariance consequence** The next lemma establishes a key result on the invariant distribution $\nu_{\gamma}$.
Lemma 18. Suppose that the chain \( \{\{H^{(\gamma)}\}, X, \mu\} \) (see Def. [2]) admits the unique invariant distribution \( \nu_\gamma \) (see Def. [3]). If the regularity constant associated with \( \nu_\gamma \) is \( \alpha < 1 \) (defined in Def. [7]), then

\[
\mathbb{E}_{H \sim \nu_\gamma} \left[ \| M(H) \|_F^2 \right] \leq d^{3/2}/\sqrt{1-\alpha}
\]

holds.

Proof. Leveraging invariance property in Def. [3]

\[
\mathbb{E}_{W,H \sim \nu_\gamma} \left[ \| M(H) \|_F^2 - \| M(H) \|_F^2 \right] = 0
\]

holds where the expectation is taken with respect to the randomness of \( W \) and \( \nu_\gamma \). Invoking the result of Lemma [12] we get

\[
\mathbb{E}_{H \sim \nu_\gamma} \left[ 2d^2 - 2\| M(H) \|_F^2 - 8\text{Tr}(M(H)^3) + 8\text{Tr}(\text{diag}(M(H)^2)) \right] + O(\gamma) = 0
\]

Having a regularity constant less than one for \( \nu_\gamma \) implies

\[
0 \leq 2d^2 - \mathbb{E}_{H \sim \nu_\gamma} \left[ 2\| M(H) \|_F^2 - 8(1-\alpha)\text{Tr}(M(H)^3) \right]
\]

holds for sufficiently small \( \gamma \). Let \( \lambda \in \mathbb{R}^d \) be a random vector containing the eigenvalues of the random matrix \( M(H) \)\(^9\). The eigenvalues of \( M^3 \) are \( \lambda^3 \), hence the invariance result can be written alternatively as

\[
0 \leq 2d^2 - \mathbb{E} \left[ 2\| \lambda \|_3^2 - 8(1-\alpha)\| \lambda \|_3 \right].
\]

The above equation leads to the following interesting spectral property:

\[
\mathbb{E}\| \lambda \|_3^2 \leq d^2/(1-\alpha).
\]

A straightforward application of Cauchy-schwarz yields:

\[
\| \lambda \|_2^2 = \sum_i \lambda_i^2 = \sum_i \lambda_i^{3/2} \lambda_i^{3/2} \leq \sqrt{\sum_i \lambda_i} \sqrt{\sum_j \lambda_j} \leq \sqrt{d\| \lambda \|_3^2}
\]

Given (i) the above bound, (ii) an application of Jensen’s inequality, (iii) and the result of Eq. (60), we conclude with the desired result:

\[
\mathbb{E}_{H \sim \nu_\gamma} \left[ M(H) = \mathbb{E} \left[ \| \lambda \|_2^2 \right] \right] \leq \mathbb{E} \sqrt{d\| \lambda \|_3^2} \leq \mathbb{E} \sqrt{d\| \lambda \|_3^2} \leq d^{3/2}/\sqrt{1-\alpha}
\]

\[\square\]

Notably, the invariant distribution is observed to have a regularity constant less than 0.9 (in Fig. [9]) for sufficiently large \( d \). This implies that an upper-bound \( O(d^{3/2}) \) is achievable on the Frobenius norm. Leveraging Ergodicity (with respect to Frobenius norm in Eq. (54)), we experimentally validate the result of the last lemma in Fig. [10].

**Proof of the Main Theorem** Here, we give a formal statement of the main Theorem that contains all required additional details (which we omitted for simplicity in the original statement).

**Theorem 19 (Formal statement of Theorem [3]).** Suppose that \( F(H) = H \), \( \text{rank}(X) = d \), and \( \gamma \) is sufficiently small. Furthermore, assume that the Markov chain \( \{\{H^{(\gamma)}\}_{\ell \geq 1}, X, \mu\} \) admits a unique invariant distribution. Then, the regularity constant \( \alpha > 0 \) associated with \( \nu_\gamma \) (see Def. [7]) is less than one and the following limits exist such that

\[
\lim_{L \to \infty} \frac{1}{L} \sum_{\ell=1}^L \text{rank}_\gamma (H^{(\gamma)}_\ell) \geq \lim_{L \to \infty} \frac{1-\tau^2}{L} \sum_{\ell=1}^L \tau(H^{(\gamma)}_\ell) \geq (1-\tau)^2(1-\alpha)^{1/2}\sqrt{d}
\]

\[\text{This result is obtained by setting } g(H) = \| M(H) \|_F^2 \text{ in Def. [3]}\]

\[\text{Note that } H \in \mathcal{H} \text{ is a random matrix whose law is } \nu_\gamma, \text{ hence } \lambda \in \mathbb{R}^d \text{ is also a random vector.}\]
holds almost surely for all $\tau \in [0, 1]$. Assuming that the regularity constant $\alpha$ does not increase with respect to $d$, the above lower-bound is proportional to $(1 - \alpha)^{1/2}\sqrt{d} = \Omega(\sqrt{d})$.

Remarkably, we experimentally observed (in Fig. 9) that the regularity constant $\alpha$ is decreasing with respect to $d$. Examples 16 and 17 provide insights about the regularity constant. We believe that it is possible to prove that constant $\alpha$ is non-increasing with respect to $d$, hence lower-bound $\Omega(\sqrt{d})$ is achievable on the rank.

Proof of Theorem 3. Lemma 15 proves that the regularity constant $\alpha$ is less than one for the unique invariant distribution. Suppose that $H \in \mathcal{H}$ is a random matrix whose law is the one of the unique invariant distribution of the chain. For $H \in \mathcal{H}$, we get $\text{Tr}(M(H)) = d$. A straightforward application of Jensen’s inequality yields the following lower bound on the expectation of $r(H)$ (i.e. the lower bound on the rank):

$$E[r(H)] = E\left[\frac{\text{Tr}(M(H))^2}{\|M(H)\|^2_F}\right] = E\left[\frac{d^2}{\|M(H)\|^2_F}\right] \geq \frac{d^2}{E[\|M(H)\|^2_F]}$$

where the expectation is taken over the randomness of $H$ (i.e. the invariant distribution). Invoking the result of Lemma 18, we get an upper-bound on the expectation of the Frobenius norm – in the right-side of the above equation. Therefore,

$$E[r(H)] \geq \sqrt{(1 - \alpha)d}$$

holds. The uniqueness of the invariant distribution allows us to invoke Birkhoffs Ergodic Theorem for Markov Chains (Theorem 5.2.1 and 5.2.6 [DMPS18]) to get

$$\lim_{L \to \infty} \frac{1}{L} \sum_{\ell=1}^{L} r(H_\ell^{(\gamma)}) = E[r(H)] \geq \sqrt{(1 - \alpha)d}.$$  

The established lower bound on $\text{rank}_r(H_\ell^{(\gamma)})$ – in terms of $r(H_\ell^{(\gamma)})$ – in Lemma 2 concludes

$$\lim_{L \to \infty} \frac{1}{L} \sum_{\ell=1}^{L} \text{rank}_r(H_\ell^{(\gamma)}) \geq \lim_{L \to \infty} \frac{(1 - \tau)^2}{L} \sum_{\ell=1}^{L} r(H_\ell^{(\gamma)}) \geq (1 - \tau)^2 \sqrt{(1 - \alpha)d}.$$  

\[\boxed{\text{This is the technical assumption required for Theorem 3}}\]
Postponed proofs.

**Proof of Lemma 12** The proof is based on a Taylor expansion of the Bn non-linear recurrence function. Let’s review Bn recurrence:

\[ H_+ = (\text{diag}(M(H_{\gamma})))^{-1/2} H_{\gamma}, \quad H_{\gamma} = (I + \gamma W)H \]

Consider the covariance matrices \( M = M(H) \) and \( M_+ = M(H_+) \) which obey

\[ M_{\gamma} := M(H_{\gamma}) = M + \Delta M, \quad \Delta M := \gamma WM + \gamma M W^T + \gamma^2 WMW^T \]

For the sake of simplicity, we use the compact notation \( g := g_{ij} \) for \( i \neq j \). We further introduce the set of indices \( S = \{ii, ij, jj\} \). A taylor expansion of \( g \) at \( M \) yields

\[ \mathbb{E}_W [g(M_{\gamma})] = g(M) + \sum_{pq \in S} \left( \frac{\partial g(M)}{\partial M_{pq}} \right) \mathbb{E}_W [\Delta M_{pq}] + \frac{1}{2} \sum_{pq, km \in S} \left( \frac{\partial^2 g(M)}{\partial M_{pq} \partial M_{km}} \right) \mathbb{E}_W [\Delta M_{pq} \Delta M_{km}] + O(\gamma^3). \]

Note that the choice of element-wise distribution uniform\([-\sqrt{3}, \sqrt{3}]\) allows us to deterministically bound the Taylor remainder term by \( O(\gamma^3) \). Now, we compute derivatives and expectations appeared in the above expansion individually. Let us start with the term \( T_1 \). The first-order partial derivative term in \( T_1 \) is computed bellow.

\[ \frac{\partial g(M)}{\partial M_{pq}} = \begin{cases} -M_{ij}^2/(M_{ii} M_{jj}) & \text{if } pq = \{ii, jj\} \\ 2M_{ij}/(M_{ii} M_{jj}) & \text{if } pq = \{ij\} \end{cases} \]

The expectation term in \( T_1 \) is

\[ \mathbb{E}_W [\Delta M_{pq}] = \begin{cases} 0 & \text{if } pq = \{ij\} \\ \gamma^2 \sum_{k=1}^d M_{kk} = \gamma^2 d & \text{if } pq = \{ii, jj\} \end{cases} \]

Given the above formula, we reach the following compact expression for \( T_1 \):

\[ T_1 = -2\gamma^2 dg(M). \]

The compute \( T_2 \) we need to compute second-order partial derivatives of \( g \) and also estimate the following expectation:

\[ \mathbb{E}_W [\Delta M_{pq} \Delta M_{km}] = \gamma^2 \left( \mathbb{E}_W \left[\left[WM + M W^T\right]_{pq} \left[WM + M W^T\right]_{km}\right]\right) + O(\gamma^3). \]

We now compute \( K_{pq, km} \) in the above formula

\[ K_{\alpha, \beta} = \begin{cases} \sum_{k} M_{kj}^2 + \sum_{n} M_{kn}^2 & \alpha = \{ij\}, \beta = \{ij\} \\ 2 \sum_{k} M_{kj} M_{ki} & \alpha = \{ij\}, \beta = \{ii\} \\ 4 \sum_{k} M_{ki}^2 & \alpha = \{ii\}, \beta = \{ii\} \\ 0 & \alpha = \{ii\}, \beta = \{jj\} \end{cases} \]
The second-order partial derivatives of \( g \) read as

\[
\frac{\partial^2 g(M)}{\partial M_\alpha \partial M_\beta} = \begin{cases} 
  2 & \alpha = \{ij\}, \beta = \{ij\} \\
  -2M_{ij} & \alpha = \{ij\}, \beta = \{ii\} \\
  +2M_{ij}^2 & \alpha = \{ii\}, \beta = \{ii\} \\
  M_{ij}^2 & \alpha = \{jj\}, \beta = \{ii\} 
\end{cases}
\]

(77)

Now, we replace the computed partial derivatives and the expectations into \( T_2 \):

\[
T_2 = \sum_k M_{kj}^2 + \sum_n M_{in}^2 - 8 \sum_k M_{kj}M_{ij}M_{ki} + 4 \sum_k M_{ij}^2 M_{ki}^2 + 4 \sum_k M_{ij}^2 M_{kj}^2
\]

(78)

Plugging terms \( T_1 \) and \( T_2 \) into the Taylor expansion yields

\[
\mathbb{E}_W [g_{ij}(M_+) - g_{ij}(M)] / (\gamma^2) = \sum_k M_{kj}^2 + \sum_n M_{in}^2 - 8 \sum_k M_{kj}M_{ij}M_{ki} + 4 \sum_k M_{ij}^2 M_{ki}^2 + 4 \sum_k M_{ij}^2 M_{kj}^2 + O(\gamma)
\]

(79)

Summing over \( i \neq j \) concludes the proof (note that the diagonal elements are one for the both of matrices \( M \) and \( M_+ \)). \( \square \)

**Proof of Proposition 13.** Consider the spectral decomposition of matrix \( M \) as \( M = U \text{diag}(\lambda) U^T \), then \( M^k = U \text{diag}(\lambda^k) U^T \). Since \( \text{Tr}(M^k) \) is equal to the sum of the eigenvalues of \( M^k \), we get

\[
\text{Tr}(M^k) = \sum_{i=1}^d \lambda_i^k = \|\lambda\|_k^k
\]

(80)

for \( k = 2 \) and \( k = 3 \). The sum of the squared norm of rows of \( M \) is equal to the Frobenius norm of \( M \). Assuming that the rows have equal norm, we get

\[
\sum_{k=1}^d M_{ik}^2 = \sum_{i=1}^d \sum_{k=1}^d M_{ik}^2 / d = \|M\|_F^2 / d = \|\lambda\|_2^2 / d.
\]

(81)

Therefore,

\[
\text{Tr}(\text{diag}(M^2))^2 = \sum_{i=1}^d \left( \sum_{k=1}^d M_{ik}^2 \right)^2 = \|\lambda\|_2^4 / d
\]

(82)

holds.

\( \square \)

**Details of Example 14.** Under the assumptions stated in Example 14, we get

\[
\|\lambda\|_2^2 \approx d^2 - 2\gamma^2 d, \quad \|\lambda\|_3^2 \approx d^3 - 3\gamma^2 d^2, \quad \|\lambda\|_4^2 \approx d^4 - 4\gamma^2 d^3
\]

(83)

where the approximations are obtained by a first-order Taylor approximation of the norms at \( \lambda' = (d, 0, \ldots, 0) \), and all small terms \( o(\gamma^2) \) are omitted. Using the result of Proposition 13, we get

\[
\mathbb{E} [\|M_+\|_F^2] - \mathbb{E} [\|M\|_F^2] \approx \gamma^2 \delta_F(\lambda) \approx O(-\gamma^4 d^2)
\]

(84)

Let \( \lambda_+ \) be the eigenvalues of matrix \( M_+ \), then

\[
\sum_{i=1}^d \mathbb{E}[\lambda_+^2] - \lambda_i^2 = O(-\gamma^4 d^2) \implies \max_i \mathbb{E}[\lambda_+^2] - \lambda_i^2 \leq O(-\gamma^4 d^2) + \sum_{i=2}^d \lambda_i^2 \leq O(-\gamma^4 d^2) + \gamma^4 d = O(-\gamma^4 d^2)
\]

(85)
Let \( j = \arg \max_i \mathbb{E} \left[ |\lambda_i|^2 \right] \). A straight-forward application of Jensen’s inequality yields

\[
(86) \quad \mathbb{E} \left[ |\lambda_j|^2 \right] \leq \sqrt{\mathbb{E} \left[ |\lambda_j|^2 \right]} \leq \lambda_1 - O(\gamma^4 d)
\]

Hence the leading eigenvalue of \( M_+ \) is smaller than the one of \( M \). Since the sum of eigenvalues \( \lambda_+ \) and \( \lambda \) are equal, some of the eigenvalues \( \lambda_+ \) are greater than those of \( \lambda \) (in expectation) to compensate \( \mathbb{E}[\lambda_+] < \lambda_1 \). \( \square \)

**Details of Example 16.** Invoking Prop. 13 we get

\[
(87) \quad \mathbb{E} \left[ \text{Tr}(M (H)^3) \right] = ||\lambda||^3, \quad \mathbb{E} \left[ \text{diag}(M (H)^2)^2 \right] = ||\lambda||^2 / d
\]

where \( \lambda \in \mathbb{R}^d \) contains eigenvalues of \( M(H) \). Since \( H \in \mathcal{H} \), \( ||\lambda||_1 = d \). If the regularity constant is greater than or equal to one, then

\[
(88) \quad ||\lambda||^3 \leq ||\lambda||^2 / d = ||\lambda||^2 / ||\lambda||_1.
\]

A straightforward application of Cauchy-Schwartz yields:

\[
(89) \quad ||\lambda||^2_2 = \sum_{i=1}^{d} \sum_{j=1}^{d} \lambda_i^2 \lambda_j^2 = \sum_{i=1}^{d} \sum_{j=1}^{d} (\lambda_i \lambda_j)^{1/2} (\lambda_i \lambda_j)^{3/2} \leq \sqrt{\left( \sum_{i,j} \lambda_i \lambda_j \right) \left( \sum_{i,j} \lambda_i^3 \lambda_j^3 \right)} = ||\lambda||_1 ||\lambda||^3_3
\]

The above result together with inequality 88 obtains

\[
(90) \quad ||\lambda||^3_3 = ||\lambda||^2_2 / d = ||\lambda||^2_2 / ||\lambda||_1.
\]

The above equality is met only when all non-zero eigenvalues are equal. \( \square \)

**Details of Example 17.** Since \( \lambda_1 = \Theta(d^3) \) and \( \lambda_{i>1} = o(d^3) \), we get

\[
(91) \quad ||\lambda||^3_3 = \Theta(d^3), \quad ||\lambda||^2_2 = \Theta(d^{2\beta}).
\]

Thus, Prop. 13 yields

\[
(92) \quad \mathbb{E} \left[ \text{Tr}(M^3) \right] = \Theta(d^{3\beta}), \quad \mathbb{E} \left[ \text{Tr}(\text{diag}(M^2)^2) \right] = ||\lambda||^2_2 / d = \Theta(d^{4\beta-1})
\]

Therefore,

\[
(93) \quad \alpha = \lim_{d \to \infty} \frac{\mathbb{E} \left[ \text{Tr}(\text{diag}(M^2)^2) \right]}{\mathbb{E} \left[ \text{Tr}(M^3) \right]} = O(d^{\beta-1}) = 0
\]

Thus, \( \alpha \) is less than 0.9 for sufficiently large \( d \). \( \square \)

7.6. **Analysis for Non-linear Networks.** This section focuses on completing the proof of Theorem 5 for non-linear BN networks which shows that the rank of pre-activation matrix is greater than 2.

**Notations.** Recall map \( \text{FBN}_\gamma \) introduced in Eq. (5):

\[
\text{FBN}_\gamma(H, W) = (\text{diag} \left( M(H_\gamma(W)) \right))^{-1/2} \ H_\gamma(W), \quad H_\gamma(W) = H + \gamma WF(H)
\]

Now, we formulate the change in the covariance matrix \( M(H) \) after applying \( \text{FBN} \). We first define the following matrix

\[
(94) \quad M_+(H, W) := M(H_\gamma(W)) = M(H) + \Delta M(H, W, \gamma)
\]

where

\[
(95) \quad \Delta M(H, W, \gamma) := \gamma W K(H) + \gamma K(H)^TW^T + \gamma^2 WP(H)W^T, \quad P(H) = F(H)F(H)^T / N
\]
and $K(H) = HF(H)/N$ as $P(H) = F(H)F(H)^\top/N$. Given the above notation, one can compute $M(F_{BN,\gamma}(H,W))$:

\begin{equation}
(M(F_{BN,\gamma}(H,W)))_{ij} = [(\text{diag}(M_+(H,W)))^{-1/2}M_+(H,W)(\text{diag}(M_+(H,W)))^{-1/2}]_{ij}
\end{equation}

\begin{equation}
\frac{M_+(H,W)_{ij}}{\sqrt{M_+(H,W)_{ii}}M_+(H,W)_{jj}}
\end{equation}

The next lemma establishes an upper-bound on the absolute value of the elements of $\Delta M(H,W,\gamma)$.

**Lemma 20.** Suppose the random matrix $W \in \mathbb{R}^{d \times d}$ is drawn from $\mu$ and $|F(x)| \leq B|x|$ for $x \in \mathbb{R}$, then

\begin{equation}
|\Delta M(H,W,\gamma)|_{ij} \leq 2\sqrt{3d}B\gamma + 3d^2B^2\gamma^2.
\end{equation}

**Proof.**

According to the definition in Eq. 95 and by the triangle inequality we have

\begin{equation}
|\Delta M(H,W,\gamma)|_{ij} \leq \gamma|WK(H)|_{ij} + \gamma|\Delta H|_{ij} + \gamma^2|WP(H)W^\top|_{ij}.
\end{equation}

Furthermore, since $W$ is drawn from $\nu$, we know that $|W|_{ij} \leq \sqrt{3}$ holds. Therefore,

\begin{equation}
|WK(H)|_{ij} \leq 3d\max_{pq} |K(H)_{pq}|
\end{equation}

\begin{equation}
|WP(H)W^\top|_{ij} \leq 3d^2\max_{pq} |P(H)_{pq}|
\end{equation}

Then we bound $|P(H)_{ij}|$ and $|K(H)_{ij}|$ for $H \in \mathcal{H}$ using Cauchy Schwarz inequality as well as the fact that each row $H$ is of length $\sqrt{N}$:

\begin{equation}
|P(H)_{ij}| = |\langle F(H)_{ik}, F(H)_{kj} \rangle/N \leq \|F(H)_{ik}\|_2\|F(H)_{kj}\|_2/N \leq B\|H_{ik}\|_2\|H_{kj}\|_2/N \leq B^2.
\end{equation}

\begin{equation}
|K(H)_{ij}| = |\langle F(H)_{ik}, H_{kj} \rangle/N \leq \|F(H)_{ik}\|_2\|H_{kj}\|_2/N \leq B\|H_{ik}\|_2\|H_{kj}\|_2/N \leq B.
\end{equation}

Combining Eq. 100 & 101 proves the assertion. \hfill \Box

**Postponed proofs for Theorem 5.** Here we present a more detailed version of Lemma 7 that is used in the proof of Thm. 5.

**Lemma 21 (Restated Lemma 7).** Suppose the assumptions of Lemma 5 hold. If $\text{rank}(H_k^{(\gamma)}) = 1$ for an integer $k$, then $M(H_k^{(\gamma)}) = M(H_k^{(\gamma)})$ holds for all $\ell > k$. Furthermore, all elements of all matrices $\{M(H_{\ell}^{(\gamma)})\}_{\ell \geq k}$ have absolute value one, hence

\begin{equation}
\lim_{L \to \infty} \frac{1}{L} \sum_{\ell=1}^{L} |M(H_{\ell}^{(\gamma)})|_{ij} \in \{1, -1\}
\end{equation}

holds.

**Proof of Lemma 7.** Suppose that $\text{rank}(H_k) = 1$, then $\text{rank}(H_{\ell}) = 1$ for all $\ell \geq k$ as the sequence $\{\text{rank}(H_{\ell})\}$ is non-increasing.\footnote{Recall FBN, (in Eq. 5) is obtained by matrix multiplications, hence it does not increase the rank.} Invoking the established rank bound from Lemma 1, we get

\begin{equation}
\text{rank}(H_{\ell}) = \frac{\text{Tr}(M(H_{\ell}))^2}{\|M(H_{\ell})\|_F^2} \leq \text{rank}(H_{\ell}) = 1.
\end{equation}

Since $H_{\ell} \in \mathcal{H}$, the matrix $M(H_{\ell}) = H_{\ell}H_{\ell}^\top/N$ exhibits particular properties: (i.) its diagonal elements are one and (ii.) the absolute value of any off-diagonal element is not greater than 1. Property (i.) directly yields $\text{Tr}(M(H_{\ell})) = d$. Replacing this into the above equation gives that $\|M(H_{\ell})\|_F^2 \geq d^2$ must hold for the rank of $H_{\ell}$ to be one. Yet, recalling property (ii.), this can only be the case if $M(H_{\ell})|_{ij} \in \{+1, -1\}$ for all $i, j$. 
We now prove that the sign of \([M(H_\ell)]_{ij}\) and \([M(H_{\ell+1})]_{ij}\) are the same for \([M(H_\ell)]_{ij} \in \{+1, -1\}\). Given \(H_{\ell+1} = F_{BN_\gamma}(H_\ell, W)\), the sign of \([M(H_{\ell+1})]_{ij}\) equates that of \([M_+(H_\ell, W)]_{ij}\) (recall Eq. (96)). According to the definition,

\[
[M_+(H_\ell, W)]_{ij} = [M(H_\ell)]_{ij} + [\Delta M(H_\ell, W)]_{ij}
\]

holds, where \(|[\Delta M(H_\ell, W)]_{ij}|\) is bounded by the result of Lemma 20. For \(\gamma \leq 1/(8Bd)\), this bound yields \(|[\Delta M(H, W)]_{ij}| \leq \frac{1}{2}\). Therefore, the sign of \([M_+(H_\ell, W)]_{ij}\) is equal to the one of \([M(H_\ell)]_{ij}\). Since furthermore \([M_+(H_\ell, W)]_{ij} \in \{1, -1\}\) holds, we conclude that all elements of \(M_\ell\) remain constant for all \(\ell \geq k\), which yields the limit stated in Eq. 102.

\[\square\]

7.7. Notes on assumptions and settings. Uniqueness of the invariant distribution. Our analysis relies on the uniqueness of the invariant distribution and also starting the chain from an input matrix \(X\) whose rank is \(d\). Consider starting the chain from a rank one matrix; then, Lemma 21 proves that matrix \(M(H_\ell^{(\gamma)})\) is a constant rank one covariance matrix with \(\pm 1\) elements. In this case, the invariant distribution is not unique and depends on the starting rank one matrix \(X\). Therefore, our established lower bounds in Theorems 3 and 5 do not hold.

Mean deduction for \(B_n\). As mentioned in Section 2, we omit the mean deduction in \(B_{n\alpha,\beta}\) (i.e. the multiplication by \(1_N 1_N^\top\) in Eq. (1)) for the sake of simplicity. Fig. 11 shows that the mean-deduction does not change: (i) the performance of \(B_{n\beta}\) (ii) the established lower-bound on the rank of pre-activation matrices (i.e. quantity \(r(H)\) in Eq. 3). Hence, we believe that the results of Theorems 3 and 5 extend to \(B_n\) equipped with the mean deduction.

\[13\] This is also observed by [SK16].