Entropy Maximization with Depth: A Variational Principle for Random Neural Networks

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Abstract

To understand the essential role of depth in neural networks, we investigate a variational principle for depth: Does increasing depth perform an implicit optimization for the representations in neural networks? We prove that random neural networks equipped with batch normalization maximize the differential entropy of representations with depth up to constant factors, assuming that the representations are contractive. Thus, representations inherently obey the principle of maximum entropy at initialization, in the absence of information about the learning task. Our variational formulation for neural representations characterizes the interplay between representation entropy and architectural components, including depth, width, and non-linear activations, thereby potentially inspiring the design of neural architectures.

1 Introduction

Depth is an essential component of neural networks. Increasing depth boosts the performance of deep neural networks in such a way that they have become the baseline algorithms in various domains, including image classification [16], reinforcement learning [17], and protein structure prediction [22]. The excellent performance of deep neural networks has even inspired going beyond finitely deep neural networks [6]. The benefits of depth are not limited to fully optimized networks. Indeed, even with a majority of random parameters, neural networks with batch normalization can achieve surprisingly good performance as their depth grows [14]. These observations called for studying the role of depth in random neural networks.

Random neural networks have been extensively studied in the literature [9, 33, 2, 28, 8, 7]. However, this literature does not reveal the power of depth since it relies on laboratory neural networks: [8, 7] use linear activations, [9, 33, 2] use networks with infinite width, and [28] does not consider batch normalization. We investigate the role of depth for standard modern random neural networks with batch normalization, finite width, and non-linear activations.

Hidden representations across layers form a stochastic process. We research a variational principle for this process that formulates the role of depth. [21] establishes such a formulation for Ito processes, including Langevin dynamics. We prove that random networks also admit a variational
formulation: The entropy of hidden representations increases with depth. Thus, increasing depth implicitly implements the standard principle of maximum entropy.

The proposed variational formulation bridges an explanatory gap between statistical mechanics and deep neural networks. The fundamental postulate of statistical mechanics asserts that an isolated system in equilibrium has maximum entropy and is used to derive standard Boltzman’s distribution [15]. [19] draws a correspondence between information entropy and thermodynamics, arguing that the maximum entropy principle provides a natural prior for statistical mechanics. We show that deep neural networks also obey this principle. The following Theorem states our main contribution.

Theorem 1 (Informal). In a multi-layer perceptron with ReLU or odd activations equipped with batch normalization, and random Gaussian weight matrices, if the chain of hidden representations is $\alpha$-contractive ($\alpha < 1$, Assumption 7), (normalized) differential entropies of hidden representations obeys

$$\text{Entropy}_{\text{depth}} \geq \text{Entropy}_{\text{max}} - \log(1/\lambda) - O\left(\alpha^{\text{depth}} + \frac{\text{batch-size}^3 \log(\text{width})}{\lambda^2 (1 - \alpha) \text{width}}\right)^{\frac{1}{2}},$$

where $\lambda \in (0, 1]$ determines the gap with $\text{Entropy}_{\text{max}}$, defined in Definition 4, as the maximum entropy subject to the batch size and network width.

Theorem 1 enables us to adjust the entropy level with the design of the network architecture. The established lower bound for entropy decreases with a polynomial rate with width and an exponential rate with depth, up to a constant gap with the information-theoretic limit. With odd activations, for which $\lambda = 1$, networks can achieve the maximum entropy as they grow in depth and width. However, ReLU activations reduce entropy by $\lambda = \frac{1}{2}$, corresponding to zeroing-out negative representations. Note that the batch-size in batch normalization is distinct from the size of the dataset, and is typically smaller than the width. We will demonstrate that the standard Doeblin’s condition [30] from Markov chain theory ensures the required contraction in the above Theorem.

The established variational principle is imposed by batch normalization. [18] proposes batch normalization to keep the variance and mean of representations constant across layers, which significantly enhances training. Despite its conceptual simplicity, the inner workings of batch normalization have remained largely unresolved [25, 24, 8, 7]. [8] conjectures that batch normalization
avoids the rank collapse of hidden representation with depth that significantly influences training performance. We prove this conjecture as an application of our results.

The established entropy analysis relies on a novel Gaussian approximation for the distribution of hidden representations. Under the settings of Theorem 1, we prove that in deep random neural networks endowed with batch normalization, the output distribution is within \( O(\alpha \text{depth} + \frac{\text{batch-size}}{\text{width}^2}) \) total variation distance to a Gaussian distribution. Furthermore, for a broad class of activations, notably tanh, and ReLU, the Gaussian approximation is almost isotropic. To the best of our knowledge, this is the first non-asymptotic Gaussian approximation for standard deep neural networks with non-linear activations and a finite width. The existing literature relies on either linear activations [8] or the asymptotic regime of infinite width [9]. [27] pioneered studies of neural networks in the regime of infinite width. These studies establish the elegant link between parametric learning with neural networks and non-parametric learning with Gaussian processes. The proposed Gaussian approximate is a step towards extending this link to standard networks with a finite width.

2 Contraction of representations

2.1 Notations

We use \( f(x) \lesssim g(x) \) and equivalently \( f(x) = O(g(x)) \), to imply existence of constants \( c,C \) such that for all \( x \geq c \), \( f(x) \leq Cg(x) \). We use capital letters to denote matrices. For an \( n \times m \) matrix \( M \), we use \( \|M\| \) to denote its spectral norm, i.e., \( \|M\| := \max_{\|v\|_2 \leq 1} \|Mv\|_2 \). \( \|M\|_F \) denotes the Frobenius norm \( \|M\|_F = (\sum_{i,j} m_{ij}^2)^{1/2} \), and \( \text{tr}(M) \) to denotes its trace \( \sum_{i=1}^n M_{ii} \) if it is \( n \times n \). Also, we use the compact notation \( 1_{n \times n} \) for the \( n \times n \) all-ones matrix.

Throughout the manuscript, we use bold-face fonts to denote random variables. If \( x \) and \( y \) follow probability measures \( x \sim \mu_1, y \sim \mu_2 \) over a measurable space \( S \), the total variation distance is defined as

\[
d_{tv}(\mu, q) := \inf_{\gamma} \int \chi(x \neq y) \gamma(dx, dy), \quad \text{such that} \quad \int_S \gamma(\cdot, dy) = \mu_1, \int_S \gamma(dx, \cdot) = \mu_2.
\]

With a slight abuse of notation, \( d_{tv}(x, y) = d_{tv}(x, q) = d_{tv}(\mu, y) = d_{tv}(\mu, q) \). The differential entropy of a random variable \( X \) over the space \( X \) and with probability density function \( f_X \), is denoted by \( \mathcal{H}(X) \) or \( \mathcal{H}(f_X) \), and defined as

\[
\mathcal{H}(f_X) = \mathcal{H}(X) := \mathbb{E}[-\log(f_X(X))] = -\int_X f_X(x) \log f_X(x) dx.
\]

Naturally, the entropy of random vectors increases with its dimension. To achieve a dimension-free entropy, we introduce normalized entropy.

**Definition 1** (Normalized entropy). *For a random vector \( x \) with dimension overall \( D \), define the normalized entropy as \( \overline{\mathcal{H}}(x) := \frac{1}{D} \mathcal{H}(x) \).*

In the case of random matrix \( H \in \mathbb{R}^{d \times n} \), its normalized entropy is \( \overline{\mathcal{H}}(H) = \frac{1}{dn} \mathcal{H}(H) \).

2.2 Fixed point Theorem

Consider a non-empty complete metric space \( \Omega \) endowed with a metric \( d \), and a given map \( T : \Omega \to \Omega \). Brouwer’s fixed point theorem establishes the existence of fixed point \( X_* \) that obeys \( T(X_*) = X_* \).
Theorem 2 (Brouwer’s fixed point theorem [5]). For $T : S \rightarrow S$ where $S$ is a convex compact set, there exists a fixed point $X_\ast \in S$ such that $T(X_\ast) = X_\ast$.

Banach fixed point Theorem establishes the convergence of $X_{k+1} = T(X_k)$ to its fixed point for a contractive $T$. The map $T$ is $\alpha$-contracting if $d(T(X), T(Y)) \leq \alpha d(X,Y)$ holds for all $X,Y \in \Omega$ and $\alpha \in (0,1)$. Banach fixed point Theorem establishes $X_k \rightarrow X_\ast$ as $k \rightarrow \infty$.

Theorem 3 (Banach fixed point theorem [3]). If $T$ is $\alpha$-contracting, then there exists a unique $X_\ast \in \Omega$ such that $T(X_\ast) = X_\ast$. Furthermore, $d(X_k, X_\ast) = O(\alpha^k d(X_0, X_\ast))$.

2.3 Hidden layer representations form a Markov chain

Let $H_0 \in \mathbb{R}^{d \times n}$ denote the input matrix that consists of $n$ samples in $\mathbb{R}^d$. $H_\ell \in \mathbb{R}^{d \times n}$ denotes the hidden representation of these samples at layer $\ell$ of a network with a constant width $d$ across the layer with normalization denoted by $N$. These representations form a time homogeneous Markov chain as

$$H_{\ell+1} := W_\ell A_\ell, \quad A_{\ell+1} := \frac{1}{\sqrt{d}} F \circ N(H_\ell),$$

(representation chain)

where $F$ is the activation that acts element-wise, and $W_\ell \in \mathbb{R}^{d \times d}$ are random weight matrices with i.i.d. Gaussian elements. Our analysis covers not only the batch normalization used for theoretical analyses [7, 8] denoted by $N_1$, but also the standard batch normalization used in practice [18] denoted by $N_2$:

- $N_1$: Normalization. $N_1'$ projects $\mathbb{R}^n$ onto the $n$-sphere with radius $\sqrt{n}$: $N_1(v) := \frac{v}{\|v\|/\sqrt{n}}$, and also admits matrix-inputs: $[N_1(A)]_i = N_1(A_i)$.

- $N_2$: Normalizing with mean reduction. $N_2'$ centers before normalization $N_2(v) := N_1(v - \frac{1}{n} \sum_i v_i)$, and similarly acts row-wise on matrices $[N_2(A)]_i = N_2(A_i)$.

We will characterize the distribution of random matrices $H_1, \ldots, H_\ell$ for various $F$, and $N$. In particular, we will demonstrate applications of our theoretical analysis for ReLU$(x) = \max(0, x)$, and also the family of odd activations denoted by $F_{\text{odd}}$.

Definition 2. Define the following function classes

- Sub-linear $F_{\text{sub-lin}} := \{F : |F(x)| \leq |x|\}$.

- Odd $F_{\text{odd}} := \{F : F(-x) = F(x)\}$.

Observe that the hyperbolic tangent used in practice, and linear activations for theoretical studies [8, 7] belong to $F_{\text{odd}}$.

2.4 Contraction of hidden representations with depth

Let $\{\mu_\ell\}_{\ell \in \mathbb{N}}$ denote the distribution of the chain of hidden representations $\{H_\ell\}_{\ell \in \mathbb{N}}$. Since the chain is homogeneous in $\ell$, $\{\mu_\ell\}_{\ell}$ obeys a linear iteration as

$$\mu_{\ell+1} = \int k(\cdot, y) \mu_\ell(y) (dy),$$

(distributional iteration)
where $k$ is the Markov kernel associated with the chain of hidden representations. Recall the Markov kernel is an extension of transition probability to Markov chains with infinite state spaces [13]. Our analysis relies on the contraction of $\mu_\ell$ in total variation stated in the following assumption.

**Assumption 1 (Contraction).** The **distributional iteration** is $\alpha$-contracting in total variation.

A sufficient condition for the contraction is Doeblin’s condition [11]. Doeblin’s condition, which is also called minorisation condition [30], ensures the chain explore the entire state space [13]: There exist a measure $\nu$ and a constant $\alpha \in (0, 1)$ such that

$$k(B, y) \geq (1 - \alpha)\nu(B),$$

for all Borel set $B$ and $y$. Doeblin’s condition has been extensively studied in Markov chain theory [30, 31, 26, 29, 20, 12]. For example, Gibbs sampler and state-space models [13], hierarchical Poisson modes [31], and other Markov chain Monte Carlo [20] are known to obey Doeblin’s condition — hence they are contractive. For contractive distributional iteration, Banach fixed-point Theorem ensures the convergence of distributions to a unique stationary distribution denoted by $\pi$. In upcoming sections, we characterize this stationary distribution.

### 3 Variational formulation

#### 3.1 Stationary moments

To characterize the distribution of hidden representations, we leverage the stationary moments of hidden representation.

**Definition 3 (β-Stationary).** Given a random vector $w \sim N(0, C_*)$, the matrix $C_* \in \mathbb{R}^{n \times n}$ is β-stationary, if it obeys

$$\mathbb{E} \left[ \phi(w)\phi(w)^\top \right] = C_*, \quad \text{tr}(C_*) = \beta n.$$  

(stationary condition)

Observe that $C_* = 0$ is the 0-stationary for any function that $F(0) = 0$. The Proposition 4 and Proposition 5 demonstrate existence of non-trivial, i.e. $\beta > 0$-stationary moments, for networks with odd and ReLU activations respectively. The high level idea is to define $C_*$ with constant diagonal and off-diagonal elements, show that $C_*' := \mathbb{E}\phi(w)\phi(w)^\top$ has constant diagonal and off-diagonals, and leverage Brouwer’s fixed point theorem to show a stationary $C_*$ (find the detailed proof in the appendix).

**Proposition 4 (Odd activations).** Suppose $F \in \mathcal{F}_{odd} \cap \mathcal{F}_{sub-lin}$. For a network with $\phi := F \circ N_1$, there exists $\beta_F := \Omega(\inf_{x \geq 1} F^2(x))$ such that $\beta_F I_n$ is $\beta_F$-stationary.

Leveraging Brouwer’s fixed-point theorem, the following Proposition characterizes stationary moments of networks with ReLU activation.

**Proposition 5 (ReLU activations).** For $\phi := \text{ReLU} \circ N_2$, there exists $0 \leq \rho \leq \frac{1}{2}$, such that

$$\frac{1}{2}((1 - \rho)I_n + \rho 1_{n \times n})$$

is $(\frac{1}{2})$-stationary.
3.2 Differential entropy maximization

We formulate the maximum achievable entropy for hidden representations as a variational problem.

Definition 4. The maximum entropy $H_{\text{max}}$ is the maximum differential entropy amongst all probability measures $\mu$ over $d \times n$ matrices, with bounded trace:

$$H_{\text{max}} := \max_{\mu} \left\{ H(\mu) : \int_{\mathbb{R}^{d \times n}} \text{tr}(A^T A) \mu(dA) \leq n \right\},$$

and we define ${\overline{H}}_{\text{max}}$ as the normalized maximum entropy (with dimension) ${\overline{H}}_{\text{max}} := \frac{1}{nd} H_{\text{max}}$.

The above variational problem admits a closed-form solution presented in the following lemma.

Lemma 6. $H_{\text{max}} = \frac{n d}{2} (1 + \ln(2\pi))$ and ${\overline{H}}_{\text{max}} = \frac{1}{2} (1 + \ln(2\pi))$.

3.3 Entropy maximization with depth

Using the stationary moments, we analyze the entropy of representations in random networks. The following theorem proves the entropy increases with depth. The proof of this Theorem is postponed to Section 6.

Theorem 7 (Restated Theorem 1). Suppose the chain of hidden representations obeys Assumption 1, the activation is sub-linear $F \in F_{\text{sub-lin}}$, and $C_*$ is $\beta$-stationary; then,

$$\overline{H}(H_{\ell+1}/\beta) \geq \overline{H}_{\text{max}} - \log(1/\lambda_1) - O \left( \frac{\alpha^{\ell} + \frac{n^3 \log(d)}{\lambda_1^2(1-\alpha)d}}{\frac{1}{2}} \right),$$

where $\lambda_1 := \lambda_1(C_*)$ denotes the smallest eigenvalue of $C_*$.

Note that dividing $H_{\ell+1}$ by $\beta = \frac{1}{n} \text{tr}(C_*)$ ensures that the trace constraint in Definition 4 is met.

The last theorem characterizes the entropy for a wide family of neural networks with non-linear activations. For example, incorporating Propositions 4, and 5 into the entropy lower bound yields:

• **Odd activations.** For $\phi = F \circ N_1$ for $F \in F_{\text{odd}}$ with $\beta_F$ introduced in Proposition 4,

$$\overline{H}(H_{\ell+1}^{(\text{odd})}/\beta_F) \geq \overline{H}_{\text{max}} - O \left( \frac{\alpha^{\ell} + \frac{n^3 \log(d)}{(1-\alpha)d}}{\frac{1}{2}} \right).$$

• **ReLU.** For $\phi = \text{ReLU} \circ N_2$,

$$\overline{H}(2H_{\ell+1}^{(\text{ReLU})}) \geq \overline{H}_{\text{max}} - \ln(2) - O \left( \frac{\alpha^{\ell} + \frac{n^3 \log(d)}{(1-\alpha)d}}{\frac{1}{2}} \right).$$

Therefore, the ReLU activation reduces the entropy bound by $\ln(2)$, as it zeroes out (almost half) of coordinates in random representations.

The last Theorem provides an information-theoretic view of the underlying mechanism of depth. By increasing entropy, deep neural networks compress irrelevant information in inputs. Let $I(x;y)$
denote the mutual information between random variables $x$ and $y$, which measures relevant information of $x$ about $y$. The last theorem implies $I(\text{input}, H_\ell/\beta)$ implicitly decreases with depth up to adjustable constants:

$$(nd)^{-1}I(H_\ell/\beta; \text{input}) = \overline{H}(H_\ell/\beta) - \overline{H}(H_\ell/\beta|\text{input})$$

$$= \overline{H}(H_\ell/\beta) \mp \overline{H}_{\max} - \overline{H}(H_\ell/\beta|\text{input})$$

$$\leq 2 \times (\text{bound in Theorem 7}).$$

According to the information bottleneck principle, pruning irrelevant information is essential for learning \cite{34}. The information bottleneck principle formulates the learning objective as generating representations $H$ that minimizes

$$I(\text{input}; H) - \gamma I(H; \text{labels}).$$

Pruning irrelevant information decreases the first term. While minimizing the second term implies capturing relevant information about labels. We can omit the second term at initialization since the network is agnostic to labels. In that regard, deep networks with increasing entropy obey the information bottleneck principle.

4 Normalization with depth

The entropy characterization relied on the Gaussian approximation of hidden representations established in the following theorem (see Section 6 for the proof).

**Theorem 8.** Suppose the chain of hidden representations obeys Assumption 7 $F \in \mathcal{F}_{sub-lin}$, and $C_*$ is $\beta$-stationary; then,

$$d_{TV}(H_\ell, G) \lesssim \alpha^\ell + \frac{n^3 \log d}{(1-\alpha)d} \|C_*^{-1}\|^2,$$

(normal approximation)

holds for $G \in \mathbb{R}^{d \times n}$ whose rows are i.i.d. $\mathcal{N}(0, C_*)$.

Thus, the distribution of hidden representations contracts to a Gaussian distribution within an $\epsilon$ total variation distance, where $\epsilon$ vanishes as $d \to \infty$ and $\ell \to \infty$. Mean-field studies of neural networks in \cite{9} also confirm the Gaussian outputs for $d \to \infty$. However, there are rare Gaussian approximations for standard neural networks with finite width and batch normalization. To the best of our knowledge, \cite{7} proposes the only non-asymptotic result established for neural networks with linear activations. Gaussian contraction in the last theorem holds for a wide family of activations. Leveraging the established characterizations for stationary moments by Propositions 4 and 5 we demonstrate the generality of Gaussian approximation for ReLU and odd activations:

**Odd activations.** Let $\phi = F \circ N_1$ for $F \in \mathcal{F}_{\text{odd}} \cap \mathcal{F}_{\text{sub-lin}}$, $d_{TV}(H_\ell, G) \lesssim \alpha^\ell + \frac{n^3 \log d}{d \beta^2(1-\alpha)}$.

**ReLU.** For $\phi = \text{ReLU} \circ N_2$, $d_{TV}(H_\ell, G) \lesssim \alpha^\ell + \frac{8n^3 \log d}{d(1-\alpha)}$.

The result for odd activations recovers the Gaussian approximation bound for linear activation established by \cite{7} (with a worse dependency on $n$).

Remarkably, Gaussian distributions admit the maximum entropy principle under mild conditions. Leveraging this property, we established the entropy bound in Theorem 7 (see Section 6 for the proof).
5 Batch normalization avoids the rank collapse issue

Batch normalization interacts with learning neural networks in various ways: influencing input-output Jacobians [4], adjusting the learning-rate [1, 4], influencing the gradient explosion [37], changing the landscape properties of the training loss [32, 23], and avoiding the rank collapse of hidden representations [8, 7]. We demonstrate how to prove these observations with our analysis, thereby shedding light on batch normalization’s inner workings. In particular, we show the application of our results in the rank analysis. Without batch normalization, the rank of hidden representations collapses to one with depth, in that training significantly slows [8]. In stark contrast, we prove batch normalization avoids the rank collapse issue [8].

Lemma 9 (Concentration with total variation). \( A^\top_\ell A_\ell - C_* \) is concentrated around the \( \beta \)-stationary \( C_* \):

\[
P \left( \| A^\top_\ell A_\ell - C_* \| \geq t \right) \leq \frac{d_{tv}(W_\ell A_\ell, G)}{\|C_*^{-1}\|^2 t^2},
\]

for a random matrix \( G \in \mathbb{R}^{d \times n} \) with i.i.d. rows sampled from \( \mathcal{N}(0, C_*) \).

The proof of the last lemma is postponed to the Appendix. The existing theoretical analysis for the rank collapse is limited to networks with linear activations [8]. Combining Theorem 8, stationary moments for ReLU and odd activations, and the last lemma, concludes that hidden representations remain full-rank with high probability. For \( \phi = F \circ N_1 \) with \( F \in \mathcal{F}_{\text{odd}} \), the minimum eigenvalue of \( A^\top_\ell A_\ell \) is \( \Omega(\beta_F) \) with high probability for \( d = \Omega(n^{3/2}(\min\{\beta_F, 1\})^{-4}) \) and \( \ell = \Omega((nd)^{-1} \min\{\beta_F, 1\}^{-1}) \). For \( \phi = \text{ReLU} \circ N_2 \), the minimum eigenvalue of \( A^\top_\ell A_\ell \) is greater than a constant with high probability as long as \( d = \Omega(n^{3/2}) \) and \( \ell = \Omega((nd)^{-1}) \).

6 Proofs

6.1 Proof of Theorem 8 (normalization)

The main idea behind the proof is based on proposing a distribution with remains approximately invariant after passing through the first layer of the networks. Such an invariance enables us to approximate the invariant distribution of representations. The next lemma represents the almost invariant distribution.

Lemma 10 (An almost invariant distribution). Let \( W \in \mathbb{R}^{d \times d} \) be random matrices whose elements are i.i.d. Gaussian. Suppose that \( G \in \mathbb{R}^{d \times n} \) is a Gaussian matrix whose rows are i.i.d. \( \mathcal{N}(0, C_*) \) for a \( \beta \)-stationary \( C_* \), and \( F \in \mathcal{F}_{\text{sub-lin}} \); then,

\[
d_{tv} \left( \frac{1}{\sqrt{d}} W \phi(G), G \right) \leq \frac{13n^3 \ln(d)}{d} \|C_*^{-1}\|^2.
\]

This lemma states that \( G \) stays in its local neighborhood after passing through a single layer of the random network. Let \( \pi \) denote the unique invariant distribution for the chain of hidden representations \( \{H_\ell\}_\ell \). The result of the last lemma yields

\[
d_{tv}(G, \pi) \leq d_{tv} \left( G, \frac{1}{\sqrt{d}} W \phi(G) \right) + d_{tv} \left( \frac{1}{\sqrt{d}} W \phi(G), \pi \right)
\]
\[
\leq \epsilon + d_{tv} \left( \frac{1}{\sqrt{d}} W \phi(G), \pi \right),
\]
where $\epsilon := \frac{13n^3 \ln(d)}{d} \|C^{-1}\|^2$. Leveraging the contractive property in Assumption 1, we get
\[
d_{tv}\left(\frac{1}{\sqrt{d}} W \phi(G), \pi\right) = d_{tv}\left(\frac{1}{\sqrt{d}} W \phi(G), \int k(., y)d\pi(y)\right) \leq \alpha d_{tv}(G, \pi),
\]
where we used Assumption 1 for the last inequality. Combining the last two inequalities, we get $d_{tv}(G, \pi) \leq \frac{\epsilon}{(1-\alpha)^2}$. Therefore, the almost invariant distribution approximates $\pi$. Invoking Banach fixed point Theorem completes the proof:
\[
d_{tv}(H_{t+1}, G) \leq d_{tv}(H_{t+1}, \pi) + d_{tv}(G, \pi) = O\left(\alpha^t + \frac{\epsilon}{(1-\alpha)}\right).
\]

6.2 Proof of Lemma 10
Define $A := \frac{1}{\sqrt{d}} \phi(G)$, $C := A^\top A$, and let $g_i$ and $w_i$ for $i = 1, \ldots, d$ denote rows of $G$ and $W$ respectively. The proof is based on a coupling between $G$ and $WA$, conditioned on $A$. Define product measure $\gamma_A = \gamma_A^\otimes n$, where $\gamma_A$ is the optimal coupling between $g_1 \sim \mathcal{N}(0, C_*)$ and $Aw_1 \sim \mathcal{N}(0, A^\top A)$. Note that Theorem 4.1 by [36] ensures the existence of the optimal coupling $\gamma_A$. According to definition, this coupling gives an upper-bound on total variation as
\[
d_{tv}(WA, G) \leq \int \mathbb{1}(WA \neq GA_*) \gamma_A^\otimes n(dG, dW)\mathbb{P}(dA),
\]
where $\mathbb{1}$ denotes indicator, and $\mathbb{P}$ denotes the probability density for random matrix $A$. We introduce the event $S_t = \{A \in \mathbb{R}^{d \times n} : \|A^\top A - C_*\| \leq t\}$. Using $S_t$ and its complement $S_t^c$, we get
\[
d_{tv}(WA, G) \leq \int_{A \in S_t} \mathbb{1}(WA \neq G) \gamma_A^\otimes n(dW, dG)\mathbb{P}(dA) + \int_{A \notin S_t} \mathbb{1}(WA \neq G) \gamma_A^\otimes n(dW, dG)\mathbb{P}(dA)
\]
\[
\leq n \int_{A \in S_t} \mathbb{1}(g_1 \neq Aw_1) \gamma_A(dw_1, dg_1)\mathbb{P}(dA) + \mathbb{P}(S_t^c)
\]
\[
= n \sup_{A \in S_t} d_{tv}(g_1, Aw_1) + \mathbb{P}(S_t^c).
\]
We can bound the first term by invoking Theorem 1.1 by [10] as $d_{tv}(Aw_1, g_1) \leq \frac{3n^2}{2} \|C_*^{-1}\|^2t^2$. The second term $\mathbb{P}(S_t^c)$ is a tail-probability as $\mathbb{P}(\|A^\top A - C_*\| \geq t)$, we can bound this term via matrix Bernstein inequality (see Appendix A for a detailed derivation):
\[
\mathbb{P}(S_t^c) = \mathbb{P}(\|A^\top A - C_*\| \geq t) \leq (2n) \exp\left(\frac{-dt^2}{4n(1 + t/3)}\right).
\]
Replacing bounds with $t = \sqrt{\frac{8n \ln(d)}{d}}$ into the total variation bound concludes the proof.

6.3 Proof of Theorem 7
The main idea is: Controlling $\mathcal{H}(WA) - \mathcal{H}(G)$ by the concentration of $C_\ell := A^\top A$. Recall $G \in \mathbb{R}^{d \times n}$ with rows $g_1, \ldots, g_d \sim i.i.d. \mathcal{N}(0, C_*)$, and $W := W_\ell \in \mathbb{R}^{d \times d}$ with i.i.d. Gaussian elements.
Let $\mathbb{P}$ denote density of $A_\ell$. Observe that $H_{\ell+1}$ is equal in distribution to $WA_\ell$. By independence of rows of $W$ and $G$ we get

$$\Delta \mathcal{H} := \mathcal{H}(G) - \mathcal{H}(W A_\ell | A_\ell)$$

$$= \mathcal{H}(G) - \int_{R^{d\times n}} \mathbb{P}(dA) \mathcal{H}(WA)$$

$$= d \int_{R^{d\times n}} \mathbb{P}(dA) \log \det \left( C^{-1}_* (A^\top A) \right)$$

$$\triangleright \text{rows of } W, G \text{ are iid}$$

$$\leq d \int_{R^{d\times n}} \mathbb{P}(dA) \log \det \left( C^{-1}_* (A^\top A - I) \right)$$

$$\triangleright \log \det(\Sigma) \leq \text{tr}(\Sigma - I)$$

$$\leq nd \|C^{-1}_*\| \int_{R^{d\times n}} \mathbb{P}(dA) \| A^\top A - C_* \|$$

$$\triangleright \text{tr} (\Sigma \Sigma') \leq n \|\Sigma\| \|\Sigma'\|$$

$$\leq nd \|C^{-1}_*\| \int_{t \geq 0} dt \mathbb{P} \left( \| A^\top A - C_* \| \geq t \right)$$

$$\triangleright S_t := \{ A \in \mathbb{R}^{d \times n} : \| A^\top A - C_* \| \leq t \}.$$ 

For some $t_0 \geq 0$, we can divide the integration and invoke Lemma 9 to bound the second term:

$$\Delta \mathcal{H} \leq nd \|C^{-1}_*\| \left( \int_{t=0}^{t_0} dt \mathbb{P} (S^c_t) + \int_{t \geq t_0} dt \mathbb{P} (S^c_t) \right)$$

$$\lesssim nd \|C^{-1}_*\| \left( t_0 + \int_{t \geq t_0} \|C^{-1}_*\|^{-2} t^{-2} d_{tv}(H_{\ell+1}, G) \right) dt.$$

By integration with respect to $t$ and setting $t_0 := \|C^{-1}_*\|^{-1} d_{tv}(H_{\ell+1}, G)^{\frac{1}{2}}$, we can invoke Theorem 8 to get

$$\Delta \mathcal{H} \lesssim nd \left( \alpha^\ell + \|C^{-1}_*\|/2 n^3 \log (d)/(1 - \alpha)d \right)^{\frac{1}{2}}.$$

Since the mutual information is non-negative, we get

$$\mathcal{H}(WA_\ell) = \mathcal{H}(W A_\ell | A_\ell) + \mathcal{I}(W A_\ell, A_\ell).$$

Recall that $\mathcal{H}(G) = \frac{nd}{2} (1 + \log(2\pi) + \frac{1}{d} \log \det(C_*))$. Since $\frac{1}{n} \log \det(C_*) \geq -\log \|C^{-1}_*\|$, we have

$$\mathcal{H}(H_{\ell+1}) \gtrsim \frac{nd}{2} (1 + \log(2\pi) + \log \|C^{-1}_*\|) - nd\mathcal{O} \left( \alpha^\ell + \|C^{-1}_*\|^2 n^3 \log (d)/(1 - \alpha)d \right)^{\frac{1}{2}}.$$ 

Dividing $H_{\ell+1}$ by $nd$ and scaling by $\beta = \frac{1}{n} \text{tr}(C_*)$, and using $\lambda_1 := \lambda_1(C_*)$ to denote smallest eigenvalue, we have

$$\bar{\mathcal{H}}(H_{\ell+1}/\beta) \gtrsim \bar{\mathcal{H}}_{\max} + \log(1/\lambda_1) - \mathcal{O} \left( \alpha^\ell + \frac{n^3 \log (d)}{\lambda_1^2 (1 - \alpha)d} \right)^{\frac{1}{2}}.$$ 

10
7 Discussion

We have established a variational formulation for the role of depth in random neural networks with batch normalization: The entropy of hidden representations increases with depth up to constants. Is this entropy increase achieved by a gradient flow in the space of probability measures? This question is inspired by the variational formulation for Ito processes established by [21]. According to this formulation, the distribution of Ito processes, which obey Fokker–Planck equation, can be viewed as a gradient flow minimizing a free energy functional.

The established entropy bound in Theorem [1] proves the entropy increase up to constants that are adjustable with architectural components, including width, depth, and activation function. However, our analysis does not cover convolutional and pooling layers. Convolutional layers may impose a particular inductive bias on the distribution of hidden representation, thereby influencing the learning performance. Hence, extending the variational formulation to networks with convolutional layers is essential.

Our analysis relies on the contraction of hidden representations in total variation stated in Assumption [1]. As discussed in Section [2], the standard Doeblin’s condition is sufficient for the contraction [21]. We conjecture that it is possible to prove Doeblin’s condition for the chain of hidden representations: Gaussian weights and full-rank inputs allow the exploration required in Doeblin’s condition, thereby ensuring the contraction of the distribution of the hidden representation.

We connect our analysis to the rank of hidden representations linked to the learning performance [8]. However, this link is not proven. It is interesting to theoretically investigate the role of the entropy or the rank of hidden representations in optimization. We conjecture that the entropy of hidden representation imposes a particular structure on the gradient of training loss. Studying this structure should shed light on the learning mechanism for neural networks.

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Appendix

Numerical illustration. Figure 1 illustrates the entropy increase with depth. We generate the chain of hidden representations in representation chain with \( W_\ell = (1-\gamma)I_d + \gamma G_\ell \), where \( G_\ell \in \mathbb{R}^{d \times d} \) is a random matrix with i.i.d. Gaussian random coordinates with \( \gamma = 0.01 \) modulating the residual connections. For this simulation, we use \( n = 3, d = 1000, F = \tanh \). Each point in the plot is one of the rows of matrix \( A_\ell \) for \( \ell \in \{1, 20, 100\} \). The simulation starts with input matrix \( H_0 \in \mathbb{R}^{d \times n} \) with a low entropy level, to allow us to observe the entropy increase with depth.

Maximum Entropy. Recall the definition of maximum entropy:

Definition 5 (Restated Definition 4). The maximum entropy \( H_{\text{max}} \) is the maximum differential entropy amongst all probability measures \( \mu \) over \( d \times n \) matrices, with bounded trace:

\[
H_{\text{max}} := \max_{\mu} \left\{ H(\mu) : \int_{\mathbb{R}^{d \times n}} \text{tr}(A^\top A)\mu(dA) \leq n \right\},
\]

and we define \( \overline{H}_{\text{max}} \) as the normalized maximum entropy (with dimension) \( \overline{H}_{\text{max}} := \frac{1}{nd}H_{\text{max}} \).

We will prove the Lemma 6 restated below which establishes the closed form solution of the above variational problem.

Lemma 11 (restated Lemma 6). \( H_{\text{max}} = \frac{nd}{2}(1 + \ln(2\pi)) \) and \( \overline{H}_{\text{max}} = \frac{1}{2}(1 + \ln(2\pi)) \).

Proof. First we prove the bound for \( d = 1 \), and then extend it to \( d > 1 \). Let \( x \in \mathbb{R}^n \) be a random vector with density \( q \). Define \( C := \mathbb{E}_q x^\top x \), which satisfies \( \text{tr}(C) \leq \beta n \). Let \( p := \mathcal{N}(0, C) \).

Special case \( d = 1 \). Observe that the only variable-dependent term in expansion of \( p(x) \) is the quadratic component \( \log p(x) = \text{const} + x^\top C^{-1}x \). The constant terms not affected by the distribution, while quadratic terms in \( x^\top C^{-1}x \) are equal in expectation due to identity \( \mathbb{E}_p x^\top C^{-1}x = \mathbb{E}_q x^\top C^{-1}x \). Therefore, \( \mathbb{E}_p \log p(x) = \mathbb{E}_q \log p(x) \). We get

\[
0 \leq D_{\text{KL}}(p \parallel q) = \int_x p(x) \log \frac{p(x)}{q(x)} dx \leq \int_x q(x) \log(q(x))dx - \int_x q(x) \log(p(x))dx = -\mathcal{H}(q) + \mathcal{H}(p) \Rightarrow \mathcal{H}(q) \leq \mathcal{H}(p) = \frac{n}{2}(1 + \ln(2\pi)) + \frac{1}{2} \log \det(C).
\]

Since \( \sum_{i=1}^n \lambda_i(C) = \text{tr}(C) \leq n\beta \), \( \log \det(C) \) is maximized when all eigenvalues are equal to \( \beta \), resulting in

\[
\mathcal{H}(p) \leq \mathcal{H}(q) = \frac{n}{2}(1 + \ln(2\pi) + \log \beta).
\]
General case $d \geq 1$. $\text{tr}(\mathbb{E}X^\top X) \leq n$: for an arbitrary measure $p$ over $d \times n$ matrices, put $C := \mathbb{E}_p X^\top X$. For rows $i \in \{1, \ldots, d\}$ of $X$, let $C_i := \mathbb{E}_p X_i^\top X_i$ denote the associated covariance. Observe that $\text{tr}(C) = \sum_{i=1}^d \text{tr}(C_i)$. From the case $d = 1$, we can bound the entropy of rows $X_i$ by setting $\beta_i := \text{tr}(C_i)$, which obeys $\sum_{i=1}^d \beta_i \leq n$. The entropy of matrix $H(X)$ is bounded by the sum of entropy of its rows $\sum_{i=1}^d H(X_i)$. Invoking $d = 1$ case, this is bounded by $\sum_{i=1}^d \log(\beta_i)$, which maximizes when the $\beta_i$s are all equal to 1:

$$H(p) \leq \sum_{i=1}^d \frac{n}{2} (1 + \ln(2\pi) + \log \beta_i) \leq \frac{nd}{2} (1 + \ln(2\pi)). \quad (8)$$

Stationary moments. Recall our analysis relies on stationary moments.

**Definition 6** ($\beta$-Stationary). Given a random vector $w \sim \mathcal{N}(0, C_*)$, the matrix $C_* \in \mathbb{R}^{n \times n}$ is $\beta$-stationary, if it obeys

$$\mathbb{E}\left[\phi(w)\phi(w)^\top\right] = C_*, \quad \text{tr}(C_*) = \beta n. \quad \text{(stationary condition)}$$

**Proposition 12** (Restated Proposition 4). Suppose $F \in \mathcal{F}_{\text{odd}} \cap \mathcal{F}_{\text{sub-lin}}$. For a network with $\phi := F \circ N_1$, there exists $\beta_F := \Omega(\inf_{x \geq 1} F^2(x))$ such that $\beta_F I_n$ is $\beta_F$-stationary.

**Proof.** Define

$$\beta_F := \mathbb{E}\left[F^2\left(\frac{w_1}{\sqrt{n} \sum_{j=1}^n w_j^2}\right)\right], \quad w_i \overset{\text{i.i.d.}}{\sim} \mathcal{N}(0, 1). \quad (9)$$

We will prove that $C = \beta_F I_n$ is $\beta_F$-stationary.

Define $X := F(N_1(W))$ where rows of random matrix $W \in \mathbb{R}^{d \times n}$ are i.i.d. from $\mathcal{N}(0, I_n)$. Let $C' = \mathbb{E}X^\top X$. Since the law of $W$ is symmetric with respect to sign and $F \in \mathcal{F}_{\text{odd}}$, the off-diagonal elements of $C'$ are zero $C_{ij} = 0, \forall i \neq j$. Since the law of $X$ is invariant with respect to permutations of rows all the diagonal elements are equal with $\beta_F := C_{11} = \mathbb{E}||X_1||_2^2$. Finally, note that due to scale-invariance of $N_1$, $\mathbb{E}X^\top X = C'$ holds for $X = \phi(W(\beta I_n))$. Therefore, $C = \beta I_n$ satisfies the invariant stationary condition.
To finalize the proof, we need to a lower bound on $\beta_F$. We have

$$\beta_F = \mathbb{E} F^2 \left( \frac{w_1}{\sqrt{\frac{1}{n} \sum_{i=1}^{n} w_i^2}} \right) \geq \inf_{x \geq 1} F^2(x) \mathbb{P} \left( \frac{w_1}{\sqrt{\frac{1}{n} \sum_{i=1}^{n} w_i^2}} \geq 1 \right) \geq \inf_{x \geq 1} F^2(x) \lim_{n \to \infty} \mathbb{P}(z_{n-1} \leq 1) = \frac{3}{10} \inf_{x \geq 1} F^2(x),$$

where $z_{n-1} := \frac{1}{n-1} \sum_{i=2}^{n} w_i^2$.

In equation (14) observe that $z_{n-1}$ follows F-distribution with parameters $(n-1, 1)$, and the density of F-distribution increases with $n$ on interval $[1, \infty)$. This allows us to take the limit $n \to \infty$. In the limit, the density of $\frac{1}{n-1} \sum_{i=2}^{n} z_i$ becomes the Dirac measure $\delta(1)$. Finally, in equation (16) we use the cumulative distribution function of a standard normal $\mathbb{P}(I_1 \leq c) = \frac{1}{2}(1 + \text{erf}(c/\sqrt{2}))$ to lower bound the probability $\mathbb{P}(w_1 \geq 1) = (1 - \text{erf}(1/\sqrt{2})) \geq \frac{3}{10}$. □

**Proposition 13 (Restated Proposition 5).** For $\phi := \text{ReLU} \circ N_2$, there exists $0 \leq \rho \leq \frac{1}{2}$, such that $\frac{1}{2} ((1-\rho)I_n + \rho 1_{n \times n})$ is $(\frac{1}{4})$-stationary.

**Proof.** The proof is based on the application of the Brouwer fixed point theorem. Define $C(\rho) := \frac{1}{2} ((1-\rho)I_n + \rho 1_{n \times n})$. Observe that $C_i(\rho) = \frac{1}{2}$ for diagonal $i \in \{1, \ldots, n\}$, and $C_{ij}(\rho) = \rho$ for off-diagonal elements. We prove that there exists a $\rho \in [0, \frac{1}{4}]$ such that $C(\rho)$ satisfies the stationary condition.

Let $w \sim \mathcal{N}(0, C(\rho))$. Define $\bar{w} := \frac{1}{n} \sum_{i=1}^{n} w_i$, $\tilde{w} := (w_i - \bar{w})_{i \leq n}$. Put $x := N_2(\bar{w})$. Observe that $x = \sqrt{n} \tilde{w} / \|\tilde{w}\|$. We refer to the following definitions:

- **Diagonals.** The definition of $N_2$ directly implies

  $$\|x\|^2 = \frac{1}{n} \sum_{i=1}^{n} \tilde{w}_i^2 = n \implies \mathbb{E} \sum_{i=1}^{n} x_i^2 = \sum_{i=1}^{n} \mathbb{E} x_i^2 = n. \quad (17)$$

  Note that we use the fact that $x_1, \ldots, x_n$ are identically distributed, hence $\mathbb{E} x_i^2 = \mathbb{E} x_1^2$ holds. Since the laws of $w_i$ and $x_i$ are symmetric with respect to sign-flip, we get $\mathbb{E} F(x_i)^2 = \mathbb{E} x_1^2 \mathbb{P}(x_i \geq 0) = \frac{1}{2}$.

- **Off-diagonals.** According to definitions, we have

  $$\sum_{i,j \leq n, i \neq j} x_i x_j = \frac{1}{n} \sum_{i,j \leq n, i \neq j} \tilde{w}_i \tilde{w}_j = \frac{(\sum_{i=1}^{n} \tilde{w}_i)^2 - \sum_{i=1}^{n} \tilde{w}_i^2}{\frac{1}{n} \sum_{k=1}^{n} \tilde{w}_k^2} = -n. \quad (18)$$
Note that we exploit \( \sum_i \bar{w}_i = 0 \) (see the definition). Since \( E x_i x_j = E x_1 x_2, E x_i x_j = -\frac{1}{n-1} \), yields
\[
-\frac{1}{n-1} = E[|x_i x_j| |x_i x_j > 0]P(x_i x_j > 0) - E[|x_i x_j| |x_i x_j < 0]P(x_i x_j < 0). \tag{19}
\]

By Cauchy Swartz inequality we have \( E[|x_i x_j|] \leq \sqrt{E x_i^2 E x_j^2} = 1 \), which yields
\[
E[|x_i x_j| |x_i x_j > 0]P(x_i x_j > 0) + E[|x_i x_j| |x_i x_j < 0]P(x_i x_j < 0) \leq 1
\]
\[
\implies \quad E[|x_i x_j| |x_i x_j > 0]P(x_i x_j > 0) \leq \frac{1}{2}
\tag{20}
\]
\[
\implies \quad EF(x_i)F(x_j) = \frac{1}{2}E[|x_i x_j| |x_i x_j > 0]P(x_i x_j > 0) \leq \frac{1}{4}. \tag{21}
\]

In the last step, we use the fact that the joint distribution \((x_i, x_j)\) is equal to the joint distribution \((-x_i, -x_j)\).

Define \( g(\rho) := EF(x_i)F(x_j) \) where \( x_i, x_j \) depend on \( \rho \) according to definition. The above derivation implies that \( g \) maps the compact convex set \( \rho \in [0, \frac{1}{4}] \) to itself \( g(\rho) \in [0, \frac{1}{4}] \). Invoking Brouwer fixed point theorem, we get \( g(\rho) = \rho \) for at least one \( \rho \in [0, \frac{1}{4}] \). Since \( E[|F(x_i)F(x_j)|] \) are equal for all \( j \neq k \), we conclude that \( E[C(\rho)] = C(\rho) \).

\[\square\]

### A Concentration analysis

Now, we provide more details for the proof of Lemma \[10\]. Recall that we leverage a particular matrix concentration in the proof sketch. We provide more details on this concentration. Let define \( x_i := \phi(g_i) \) for \( i \in \{1, \ldots, d\} \). Since \( x_i \) are identically distributed, and \( C_* \) obeys stationary condition we have
\[
Ex_i^\top x_i = Ex_i \sim N(0, I_n) \phi(A_* g_i) \phi(A_* g_1)^\top = C_*, i \in \{1, \ldots, d\}. \tag{23}
\]

This implies that \( C \) is the sample average with expectation \( C_* \). The matrix Bernstein inequality \[35\] states that if sample covariances are uniformly \( L \)-bounded deviation from their mean, and \( v(C_*) \) denotes the matrix variance
\[
\|x_i^\top x_i - C_*\| \leq L, \quad v(C_*) = \|E(x^\top x - C_*)^\top (x^\top x - C_*)\|, \tag{24}
\]
then we have
\[
\mathbb{P}(\|C_* - C\| \geq t) \leq (2n) \exp \left( \frac{-dt^2/2}{v(C_*) + Lt/3} \right). \tag{25}
\]

In order to invoke the matrix Bernstein inequality, we need to bound spectral norms \( \|x_i x_i^\top\| \). Recall \( \phi := F \circ N \), where \( N \) projects into the unit ball with radius \( \sqrt{n} \), and by assumption \( |F(a)| \leq |a| \) for all values. Therefore, the \( \ell^2 \) norm of sample vectors will be bounded \( \|x_i\|_2^2 = \|\phi(A_* g_i)\|_2^2 \leq n \),
implying that $\|x_i x_i^\top\| \leq n$ for all $i$. We are now equipped to quantify $v(C_\star)$, $L$, $\|C_\star\|$, in the matrix Bernstein inequality as follows

\begin{align*}
\|C_\star\| &= \|Ex_1 x_1^\top\| \leq \E \|x_1^\top x_1\| \leq n \\
\forall i \leq d : \|x_i^\top x_i - C_\star\| &\leq \|x_i\|_2^2 + \|C_\star\| \leq 2n =: L.
\end{align*}

With $v(C_\star) = 2n$ and $L = 2n$, we get

\begin{equation}
\P(\|C_\star - C\| \geq t) \leq (2n) \exp \left( \frac{-dt^2}{4n(1 + t/3)} \right).
\end{equation}

\begin{align*}
d_{tv}(WA, G) &\leq \frac{3n^2}{2} \|C_\star^{-1}\|^2 t^2 + (2n) \exp \left( \frac{-dt^2}{4n(1 + t/3)} \right) .
\end{align*}

Because this bound is true for for any $t$, we can set $t := \sqrt{\frac{8n \ln(d)}{d}}$ to get

\begin{align*}
d_{tv}(WA, G) &\leq \frac{12n^3 \ln(d)}{d} \|C_\star^{-1}\|^2 + (2n) \exp \left( \frac{-4 \ln(d)}{8n(1 + \sqrt{2 \ln(d)}/d)} \right) \\
&\leq \frac{12n^3 \ln(d)}{d} \|C_\star^{-1}\|^2 + (2n) \exp(- \ln(d)) \\
&= \frac{12n^3 \ln(d)}{d} \|C_\star^{-1}\|^2 + \frac{2n}{d} \\
&\leq \frac{13n^3 \ln(d)}{d} \|C_\star^{-1}\|^2.
\end{align*}

**B Proof of Lemma 9**

**Lemma 14 (Restated Lemma 9).** $A_\ell^\top A_\ell$ is concentrated around the $\beta$-stationary $C_\star$:

\begin{equation}
\P(\|A_\ell^\top A_\ell - C_\star\| \geq t) \leq \frac{d_{tv}(W_\ell A_\ell, G)}{\|C_\star^{-1}\|^2 t^2},
\end{equation}

for a random matrix $G \in \R^{d \times n}$ with i.i.d. rows $N(0, C_\star)$.

**Proof.** Define $S_\ell$ as set of matrices $A$ that $A^\top A$ is closer than $t$ from $C_\star$, and let $S_\ell^c$ denote its complement:

\begin{equation}
S_\ell := \{ A \in \R^{d \times n} : \|A^\top A - C_\star\| \leq t \}, \quad t \geq 0.
\end{equation}
Let \( \gamma_A \) denote the optimal coupling for \( W_A \) and \( G \). Using this coupling, we get

\[
d_{tv}(W_A, G) = \int 1(WA \neq G) \gamma_A(dW, dG) \mathbb{P}(dA) \tag{37}
\]

\[
\geq \int_{A \in S_t} 1(WA \neq G) \gamma_A(dW, dG) \mathbb{P}(dA) \tag{38}
\]

\[
\geq \mathbb{P}(S^c_t) \inf_{A \notin S_t} \int 1(WA \neq G) \gamma_A(dW, dG) \tag{39}
\]

\[
= \mathbb{P}(S^c_t) \inf_{A \notin S_t} d_{tv}(W_A, G) \tag{40}
\]

\[
\geq \mathbb{P}(S^c_t) \inf_{A \notin S_t} \|C^{-1} \mathbb{F} A - I\|^2_F \tag{41}
\]

\[
= \mathbb{P}(S^c_t) \inf_{A \notin S_t} \|C^{-1} \mathbb{F} A - C_*\|^2_F \tag{42}
\]

\[
\geq \mathbb{P}(S^c_t) \|C_*^{-1}\|^2_F \inf_{A \notin S_t} \|A^T A - C_*\|^2 \tag{43}
\]

\[
= \mathbb{P}(S^c_t) \|C_*^{-1}\|^2 \tag{44}
\]

where use Theorem 1.1 by [10] to get a lower-bound on the total variation in Eq. 41