WHY ARE DEEP NETS REVERSIBLE: A SIMPLE THEORY, WITH IMPLICATIONS FOR TRAINING

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ABSTRACT

Generative models for deep learning are promising both to improve understanding of the model, and yield training methods requiring fewer labeled samples.

Recent works use generative model approaches to produce the deep net’s input given the value of a hidden layer several levels above. However, there is no accompanying “proof of correctness” for the generative model, showing that the feedforward deep net is the correct inference method for recovering the hidden layer given the input. Furthermore, these models are complicated.

The current paper takes a more theoretical tack. It presents a very simple generative model for RELU deep nets, with the following characteristics: (i) The generative model is just the reverse of the feedforward net: if the forward transformation at a layer is $A$ then the reverse transformation is $A^T$. (This can be seen as an explanation of the old weight tying idea for denoising autoencoders.) (ii) Its correctness can be proven under a clean theoretical assumption: the edge weights in real-life deep nets behave like random numbers. Under this assumption —which is experimentally tested on real-life nets like AlexNet— it is formally proved that feed forward net is a correct inference method for recovering the hidden layer.

The generative model suggests a simple modification for training: use the generative model to produce synthetic data with labels and include it in the training set. Experiments are shown to support this theory of random-like deep nets; and that it helps the training.

1 INTRODUCTION

Discriminative/generative pairs of models for classification tasks are an old theme in machine learning (Ng and Jordan, 2001). Generative model analogs for deep learning may not only cast new light on the discriminative backpropagation algorithm, but also allow learning with fewer labeled samples. A seeming obstacle in this quest is that deep nets are successful in a variety of domains, and it is unlikely that problem inputs in these domains share common families of generative models.

Some generic (i.e., not tied to specific domain) approaches to defining such models include Restricted Boltzmann Machines (Freund and Haussler, 1994; Hinton and Salakhutdinov, 2006) and Denoising Autoencoders (Bengio et al., 2006; Vincent et al., 2008). Surprisingly, these suggest that deep nets are reversible: the generative model is a essentially the feedforward net run in reverse. Further refinements include Stacked Denoising Autoencoders (Vincent et al., 2010), Generalized Denoising Auto-Encoders (Bengio et al., 2013b) and Deep Generative Stochastic Networks (Bengio et al., 2013a).

In case of image recognition it is possible to work harder —using a custom deep net to invert the feedforward net—and reproduce the input very well from the values of hidden layers much higher up, and in fact to generate images very different from any that were used to train the net (e.g., (Mahendran and Vedaldi, 2015)).
To explain the contribution of this paper and contrast with past work, we need to formally define the problem. Let \( x \) denote the data/input to the deep net and \( z \) denote the hidden representation (or the output labels). The generative model has to satisfy the following: **Property (a)**: Specify a joint distribution of \( x, z \), or at least \( p(x|z) \). **Property (b)**: A proof that the deep net itself is a method of computing the (most likely) \( z \) given \( x \). As explained in Section 1.1, past work usually fails to satisfy one of (a) and (b).

The current paper introduces a simple mathematical explanation for why such a model should exist for deep nets with fully connected layers. We propose the random-like nets hypothesis, which says that real-life deep nets—even those obtained from standard supervised learning—are “random-like,” meaning their edge weights behave like random numbers. Notice, this is distinct from saying that the edge weights actually are randomly generated or uncorrelated. Instead we mean that the weighted graph has bulk properties similar to those of random weighted graphs. To give an example, matrices in a host of settings are known to display properties—specifically, eigenvalue distribution—similar to matrices with Gaussian entries; this so-called Universality phenomenon is a matrix analog of the Law of Large Numbers. The random-like properties of deep nets needed in this paper (see proof of Theorem 2.3) involve a generalized eigenvalue-like property.

If a deep net is random-like, we can show mathematically (Section 3) that it has an associated simple generative model \( p(x|z) \) (Property (a)) that we call the shadow distribution, and for which Property (b) also automatically holds in an approximate sense. (Our proof currently works for up to 3 layers, though experiments show Property (b) holds for even more layers.) Our generative model makes essential use of dropout noise and RELUs and can be seen as providing (yet another) theoretical explanation for the efficacy of these two in modern deep nets.

Note that Properties (a) and (b) hold even for random (and hence untrained/useless) deep nets. Empirically, supervised training seems to improve the shadow distribution, and at the end the synthetic images are somewhat reasonable, albeit cruder compared to say (Mahendran and Vedaldi, 2015).

The knowledge that the deep net being sought is random-like can be used to improve training. Namely, take a labeled data point \( x \), and use the current feedforward net to compute its label \( z \). Now use the shadow distribution \( p(x|z) \) to compute a synthetic data point \( \tilde{x} \), label it with \( z \), and add it to the training set for the next iteration. We call this the SHADOW method. Experiments reported later show that adding this to training yields measurable improvements over backpropagation + dropout for training fully connected layers. Furthermore, throughout training, the prediction error on synthetic data closely tracks that on the real data, as predicted by the theory.

### 1.1 Related Work and Notation

Deep Boltzmann Machine (Hinton et al., 2006) is an attempt to define a generative model in the above sense, and is related to the older notion of autoencoder. For a single layer, it posits a joint distribution of the observed layer \( x \) and the hidden layer \( h \) of the form \( \exp(-h^T A x) \). This makes it reversible, in the sense that conditional distributions \( x | h \) and \( h | x \) are both easy to sample from, using essentially the same distributional form and with shared parameters. Thus a single layer net indeed satisfies properties (a) and (b). To get a multilayer net, the DBN stacks such units. But as pointed out in (Bengio, 2009), this does not yield a generative model per se since one cannot ensure that the marginal distributions of two adjacent layers match. If one changes the generative model to match up the conditional probabilities, then one loses reversibility. Thus the model violates one of (a) or (b). We know of no prior solution to this issue.

In (Lee et al., 2009b) the RBM notion is extended to convolutional RBMs. In (Nair and Hinton, 2010), the theory of RBMs is extended to allow rectifier linear units, but this involves approximating RELU’s with multiple binary units, which seems inefficient. (Our generative model below will sidestep this inefficient conversion to binary and work directly with RELUs in forward and backward direction.) Recently, a sequence of papers define hierarchichal probabilistic models (Ranganath et al., 2015; Kingma et al., 2014; Patel et al., 2015) that are plausibly reminiscent of standard deep nets. Such models can be used to model very lifelike distributions on documents or images, and thus some of them plausibly satisfy Property (a). But they are not accompanied by any proof that the feedforward deep net solves the inference problem of recovering the top layer \( z \), and thus don’t satisfy (b).
The paper of ([Arora et al., 2014]) defines a consistent generative model satisfying (a) and (b) under some restrictive conditions: the neural net edge weights are random numbers, and the connections satisfy some conditions on degrees, sparsity of each layer etc. However, the restrictive conditions limit its applicability to real-life nets. The current paper doesn’t impose such restrictive conditions.

Finally, several works have tried to show that the deep nets can be inverted, such that the observable layer can be recovered from its representation at some very high hidden layer of the net ([Lee et al., 2009a]). The recovery problem is solved in the recent paper ([Mahendran and Vedaldi, 2015]) also using a deep net. While very interesting, this does not define a generative model (i.e., doesn’t satisfy Property (a)). Adversarial nets ([Goodfellow et al., 2014]) can be used to define very good generative models for natural images, but don’t attempt to satisfy Property (b). (The discriminative net there doesn’t do the inference but just attempts to distinguish between real data and generated one.)

**Notation:** We use $\| \cdot \|$ to denote the Euclidean norm of a vector and spectral norm of a matrix. Also, $\| x \|_\infty$ denotes infinity (max) norm of a vector $x$, and $| x |_0$ denotes the number of non-zeros. The set of integers $\{ 1, \ldots, p \}$ is denoted by $[ p ]$. Our calculations use asymptotic notation $O(\cdot)$, which assumes that parameters such as the size of network, the total number of nodes (denoted by $N$), the sparsity parameters (e.g $k_j$’s introduced later) are all sufficiently large. (But $O(\cdot)$ notation will not hide any impractically large constants.) Throughout, the “with high probability event $E$ happens” means the failure probability is upperbounded by $N^{-c}$ for constant $c$, as $N$ tends to infinity. Finally, $\tilde{O}(\cdot)$ notation hides terms that depend on $\log N$.

### 2 Single Layer Generative Model

For simplicity let’s start with a single layer neural net $h = r(W^T x + b)$, where $r$ is the rectifier linear function, $x \in \mathbb{R}^n, h \in \mathbb{R}^m$. When $h$ has fewer nonzero coordinates than $x$, this has to be a many-to one function, and prior work on generative models has tried to define a probabilistic inverse of this function. Sometimes —e.g., in context of denoising autoencoders— such inverses are called reconstruction if one thinks of all inverses as being similar. Here we abandon the idea of reconstruction and focus on defining many inverses $\tilde{x}$ of $h$. We define a shadow distribution $P_{W,\rho}$ for $x|h$, such that a random sample $\tilde{x}$ from this distribution satisfies Property (b), i.e., $r(W^T \tilde{x} + b) \approx h$ where $\approx$ denotes approximate equality of vectors.

To understand the considerations in defining such an inverse, one must keep in mind that the ultimate goal is to extend the notion to multi-level nets. Thus a generated “inverse” $\tilde{x}$ has to look like the output of a 1-level net in the layer below. As mentioned, this is where previous attempts such as DBN or denoising autoencoders run into theoretical difficulties.

From now on we use $x$ to denote both the random variable and a specific sample from the distribution defined by the random variable. Given $h$, sampling $x$ from the distribution $P_{W,\rho}$ consists of first computing $r(\alpha W h)$ for a scalar $\alpha$ and then randomly zeroing-out each coordinate with probability $1 - \rho$. (We refer to this noise model as “dropout noise.”) Here $\rho$ can be reduced to make $x$ as sparse as needed; typically $\rho$ will be small. More formally, we have (with $\odot$ denoting entry-wise product of two vectors):

$$x = r(\alpha W h) \odot n_{\text{drop}},$$  

where $\alpha = 2/(\rho n)$ is a scaling factor, and $n_{\text{drop}} \in \{ 0, 1 \}^n$ is a binary random vector with following probability distribution where ($| n_{\text{drop}} |_0$ denotes the number of non-zeros of $n_{\text{drop}}$).

$$\Pr[|n_{\text{drop}}|_0 = \rho | n_{\text{drop}} |_0].$$  

Model [1] defines the conditional probability $\Pr[x|h]$ (Property (a)). The next informal claim (made precise in Section 2.2) shows that Property (b) also holds, provided the net (i.e., W) is random-like, and $h$ is sparse and nonnegative (for precise statement see Theorem 2.3).

**Theorem 2.1** (Informal version of Theorem 2.3). If entries of $W$ are drawn from i.i.d Gaussian prior, then for $x$ that is generated from model [1], there is a threshold $\theta \in \mathbb{R}$ such that $r(W^T x + \theta 1) \approx h$, where $1$ is the all-$1$’s vector.
Section\textsuperscript{2} shows that this 1-layer generative model composes layer-wise while preserving Property (b). The main reason this works is that the above theorem makes minimal distributional assumptions about $h$. (In contrast with RBMs where $h$ has a complicated distribution that is difficult to match to the next layer.)

### 2.1 Why random-like nets hypothesis helps theory

Continuing informally, we explain why the random-like nets hypothesis ensures that the shadow distribution satisfies Property (b). It’s helpful to first consider the linear (and deterministic) generative model sometimes used in autoencoders, $\hat{x} = Wh$ — also a subcase of \textsuperscript{1} where $\rho = 1$ and the rectifier linear $r(\cdot)$ is removed.

Suppose the entries of $W$ are chosen from a distribution with mean 0 and variance 1 and are independent of $h$. We now show $h = W^T \hat{x}$ is close to $h$ itself up to a proper scaling\textsuperscript{1}.

A simple way to show this would be to write $\hat{h} = W^T Wh$, and then use the fact that for random Gaussian matrix $W$, the covariance $W^T W$ is approximately the identity matrix. However, to get better insight we work out the calculation more laboriously so as to later allow an intuitive extension to the nonlinear case. Specifically, rewrite a single coordinate $h_i$ as a linear combination of $\hat{x}_j$’s:

$$
\hat{h}_i = \sum_{j=1}^{n} W_{ji} \hat{x}_j.
$$

By the definition of $\hat{x}_j$, each term on the RHS of (3) is equal to

$$
W_{ji} \hat{x}_j = W_{ji} \sum_{\ell=1}^{m} W_{j\ell} h_{\ell} = W_{ji}^2 h_i + W_{ji} \sum_{\ell \neq j} W_{j\ell} h_{\ell}.
$$

We split the sum this way to highlight that the first subgroup of terms reinforce each other since $\mu_j = W_{ji}^2 h_i$ is always nonnegative. Thus $\sum_j \mu_j$ accumulates into a large multiple of $h_i$ and becomes the main “signal” on the the RHS of (3). On the other hand, the noise term $\eta_j$, though it would typically dominate $\mu_j$ in (4) in magnitude, has mean zero. Moreover, $\eta_j$ and $\eta_t$ for different $j, t$ should be rather independent since they depend on different set of $W_{ij}$’s (though they both depend on $h$). When we sum equation (4) over $j$, the term $\sum_j \eta_j$ attenuates due to such cancellation.

$$
\hat{h}_i = \sum_{j=1}^{n} \mu_j + \sum_{j=1}^{n} \eta_j \approx n h_i + R
$$

where we used that $\sum_j W_{ji}^2 \approx n$, and $R = \sum_j \eta_j$. Since $R$ is a sum of random-ish numbers, due to the averaging effect, it scales as $\sqrt{mn}$. For large $n$ (that is $\gg m$), the signal dominates the noise and we obtain $\hat{h}_i \approx n h_i$. This argument can be made rigorous to give the proposition below, whose proof appears in Section\textsuperscript{A}.

**Proposition 2.2** (Linear generative model). Suppose entries $W$ are i.i.d Gaussian. Let $n > m$, and $h \in \{0,1\}^m$, and $\hat{x}$ is generated from the deterministic linear model $x = Wh$, then with high probability, the recovered hidden variable $\hat{h} = W^T \hat{x}$ satisfies that $\|\hat{h} - h\|_\infty \leq O\left(\sqrt{m/n}\right)$.

The biggest problem with this simple linear generative model is that signal dominates noise in (5) only when $n \gg m$. That is, the feed-forward direction must always reduce dimensionality by a large factor, say 10. This is unrealistic, and fixed in the nonlinear model, with RELU gates playing an important “denoising” role.\textsuperscript{1} Since RELU function $r$ satisfies for any nonnegative $\alpha$, $r(\alpha x) = \alpha r(x)$, readers should from now on basically ignore the positive constant scaling, without loss of generality.
2.2 Formal proof of Single-layer Reversibility

Now we give a formal version of Theorem 2.1. We begin by introducing a succinct notation for model (1), which will be helpful for later sections as well. Let \( t = \rho n \) be the expected number of non-zeros in the vector \( \eta_{\text{drop}} \), and let \( s_t(\cdot) \) be the random function that drops coordinates with probability \( 1 - \rho \), that is, \( s_t(z) = z \odot \eta_{\text{drop}} \). Then we rewrite model (1) as

\[
x = s_t(r(\alpha Wh))
\]

We make no assumptions on how large \( m \) and \( n \) are except to require that \( k < t \). Since \( t \) is the (expected) number of non-zeros in vector \( x \), it is roughly — up to logarithmic factor — the amount of “information” in \( x \). Therefore the assumption that \( k < t \) is in accord with the usual “bottleneck” intuition, which says that the representation at higher levels has fewer bits of information.

The random-like net hypothesis here means that the entries of \( W \) independently satisfy \( W_{ij} \sim \mathcal{N}(0, 1) \).

\[
W_{ij} \sim \mathcal{N}(0, 1)
\]

(7)

Also we assume the hidden variable \( h \) comes from any distribution \( D_h \), that is supported on nonnegative \( k \)-sparse vectors for some \( k \), where none of the nonzero coordinates are very dominant. (Allowing a few large coordinates wouldn’t kill the theory but the notation and math gets hairier.) Technically, when \( h \sim D_h \),

\[
h \in \mathbb{R}^n_{\geq 0}, \quad |h|_0 \leq k \text{ and } |h|_\infty \leq \beta \cdot \|h\| \quad \text{almost surely}
\]

(8)

where \( \beta = O(\sqrt{\log k}/k) \). The last assumption essentially says that all the coordinates of \( h \) shouldn’t be too much larger than the average (which is \( 1/\sqrt{k} \cdot \|h\| \)). As mentioned earlier the weak assumption on \( D_h \) is the key to layerwise composability.

**Theorem 2.3** (Reversibility). Suppose \( t = \rho n \) and \( k \) satisfy that \( k < t < k^2 \). For \((1 - n^{-5})\) measure of \( W \)'s, there exists offset vector \( b \), such that the following holds: when \( h \sim D_h \) and \( \Pr[x|h] \) is specified by model (1), then with high probability over the choice of \((h, x)\),

\[
\|r(W^T x + b) - h\|^2 \leq \tilde{O}(k/t) \cdot \|h\|^2.
\]

(9)

The next theorem says that the generative model predicts that the trained net should be stable to dropout.

**Theorem 2.4** (Dropout Robustness). Under the condition of Theorem 2.3, suppose we further drop 1/2 fraction of values of \( x \) randomly and obtain \( x_{\text{drop}} \), then there exists some offset vector \( b' \), such that with high probability over the randomness of \((h, x_{\text{drop}})\), we have

\[
\|r(2W^T x_{\text{drop}} + b') - h\|^2 \leq \tilde{O}(k/t) \cdot \|h\|^2.
\]

(10)

To parse the theorems, we note that the error is on the order of the sparsity ratio \( k/t \) (up to logarithmic factors), which is necessary since information theoretically the generative direction must increase the amount of information so that good inference is possible. In other words, our theorem shows that under our generative model, feedforward calculation (with or without dropout) can estimate the hidden variable up to a small error when \( k \ll t \). Note that this is different from usual notions in generative models such as MAP or MLE inference. We get direct guarantees on the estimation error which neither MAP or MLE can guarantee.\(^2\)

Furthermore, in Theorem 2.4 we need to choose a scaling of factor 2 to compensate the fact that half of the signal \( x \) was dropped. Moreover, we remark that an interesting feature of our theorems is that we show an almost uniform offset vector \( b \) (that is, \( b \) has almost the same entries across coordinate) is enough. This matches the observation that in the trained Alex net (Krizhevsky et al. 2012), for most of the layers the offset vectors are almost uniform\(^3\). In our experiments (Section 4), we also found restricting the bias terms in RELU gates to all be some constant makes almost no change to the performance.

\(^2\)Under the situation where MLE (or MAP) is close to the true \( h \), our neural-net inference algorithm is also guaranteed to be close to both MLE (or MAP) and the true \( h \).

\(^3\)Concretely, for the simple network we trained using implementation of [Jia et al. 2014], for 5 out of 7 hidden layers, the offset vector is almost uniform with mean to standard deviation ratio larger than 5. For layer 1, the ratio is about 1.5 and for layer 3 the offset vector is almost 0.
We devote the rest of the sections to sketching a proof of Theorems 2.3 and 2.4. The main intermediate step of the proof is the following lemma, which will be proved at the end of the section:

**Lemma 2.5.** Under the same setting as Theorem 2.3, with high probability over the choice of \( h \) and \( x \), we have that for \( \delta = O(1/\sqrt{\tau}) \),

\[
\|W^T x - h\|_\infty \leq \delta \|h\|.
\]

Observe that since \( h \) is \( k \)-sparse, the average absolute value of the non-zero coordinates of \( h \) is \( \tau = \|h\|/\sqrt{k} \). Therefore the entry-wise error \( \delta \|h\| \) on RHS of (11) satisfies \( \delta \|h\| = \epsilon \tau \) with \( \epsilon = O(\sqrt{k/\tau}) \). This means that \( W^T h \) (the hidden state before offset and RELU) estimates the non-zeros of \( h \) with entry-wise relative error \( \epsilon \) (in average), though the relative errors on the zero entries of \( h \) are huge. Therefore, even though we get a good estimate of \( h \) in \( \ell_\infty \) norm, the \( \ell_2 \) norm of the difference \( W^T x - h \) could be as large as \( \epsilon \tau \sqrt{n} = \tilde{O}(\sqrt{m/\tau} \|h\|) \) which could be larger than \( \|h\| \).

It turns out that the offset vector \( b \) and RELU have the denoising effects that reduce errors on the non-support of \( h \) down to 0 and therefore drive the \( \ell_2 \) error down significantly. The following proof of Theorem 2.3 (using Lemma 2.5) formalizes this intuition.

**Proof of Theorem 2.3.** Let \( \hat{h} = W^T x \). By Lemma 2.5, we have that \( |\hat{h}_i - h_i| \leq \delta \|h\| \) for any \( i \). Let \( b = -\delta \|h\| \). For any \( i \) with \( h_i = 0 \), \( \hat{h}_i + b \leq h_i + \delta \|h\| + b \leq 0 \), and therefore \( r(\hat{h}_i + b) = 0 = h_i \). On the other hand, for any \( i \) with \( h_i \neq 0 \), we have \( |\hat{h}_i + b - h_i| \leq |b| + |\hat{h}_i - h_i| \leq 2\delta \|h\| \). It follows that \( |r(\hat{h}_i + b) - r(h_i)| \leq 2\delta \|h\| \). Since \( h_i \) is nonnegative, we have that \( |r(\hat{h}_i + b) - h_i| \leq 2\delta \|h\| \). Therefore the \( \ell_2 \) distance between \( r(W^T x + b) = r(\hat{h} + b) \) and \( h \) can be bounded by \( \|r(\hat{h} + b) - h\|^2 = \sum_{i:h_i \neq 0} |r(\hat{h}_i + b) - h_i|^2 \leq 4k\delta^2 \|h\|^2 \). Plugging in \( \delta = O(1/\sqrt{\tau}) \) we obtain the desired result.

Theorem 2.4 is a direct consequence of Theorem 2.3, essentially due to the dropout nature of our generative model (we sample in the generative model which connects to dropout naturally). See Section A for its proof. We conclude with a proof sketch of Lemma 2.5. The complete proof can be found in Section A.

**Proof Sketch of Lemma 2.5.** Here due to page limit, we give a high-level proof sketch that demonstrates the key intuition behind the proof, by skipping most of the tedious parts. See section A for full details.

By a standard Markov argument, we claim that it suffices to show that w.h.p over the choice of \((W, h, x)\) the network is reversible, that is, \( \Pr_{x, h, W} \) [equation 9] holds \( \geq 1 - n^{10} \). Towards establishing this, we note that equation 9 holds for any positive scaling of \( h, x \) simultaneously, since RELU has the property that \( r(\beta z) = \beta \cdot r(z) \) for any \( \beta \geq 0 \) and any \( z \in \mathbb{R} \). Therefore WLOG we can choose a proper scaling of \( h \) that is convenient to us. We assume \( \|h\|^2 = k \). By assumption 8, we have that \( \|h\|_\infty \leq O(\sqrt{\log K}) \).

Define \( \hat{h} = \alpha W^T x \). Similarly to (3), we fix \( i \) and expand the expression for \( \hat{h}_i \) by definition,

\[
\hat{h}_i = \alpha \sum_{j=1} W_{ji} x_j
\]

Suppose \( n_{\text{drop}} \) has support \( T \). Then we can write \( W_{ji} x_j \) as

\[
W_{ji} x_j = W_{ji} r\left( \sum_{\ell=1}^m W_{ji} h_\ell \right) \cdot n_{\text{drop}, j} = W_{ji} r(W_{ji} h_i + \eta_j) \cdot 1_{j \in T},
\]

where \( \eta_j = \sum_{\ell \neq j} W_{ji} h_\ell \). Though \( r(\cdot) \) is nonlinear, it is piece-wise linear and more importantly still Lipschitz. Therefore intuitively, RHS of (13) can be “linearized” by approximating \( r(W_{ji} h_i + \eta_j) \) by \( 1_{\eta_j > 0} \cdot (W_{ji} h_i + r(\eta_j)) \). Note that this approximation is not accurate only when \( |\eta_j| \leq |W_{ji} h_i| \), which happens with relatively small probability, since \( \eta_j \) typically dominates \( W_{ji} h_i \) in magnitude.

Then \( W_{ji} x_j \) can be written approximately as \( 1_{\eta_j > 0} \cdot (W_{ji}^2 h_i + W_{ji} r(\eta_j)) \), where the first term corresponds to the bias and the second one corresponds to the noise (variance), similarly to the argument in the linear generative model case in Section 2.1.
Figure 1: Generative-discriminative pair: a) defines the conditional distribution \( \Pr[x|h^{(\ell)}] \); b) defines the feed-forward function \( \hat{h}^{(\ell)} = \text{NN}(x) \).

Using the intuition above, one can formally prove (as in the full proof in Section A) that \( \mathbb{E}[W_{ij} x_j] = \frac{1}{2}h_i \pm O(1/k^{3/2}) \) and \( \text{Var}[W_{ij} x_j] = O(\sqrt{k}/t) \). By a concentration inequality\(^4\) for the sum \( \tilde{h}_i = \alpha \sum_{j=1}^n W_{ij} x_j \), one can show that with high probability \( (1 - n^{-10}) \) we have \( |\tilde{h}_i - h_i| \leq O(\sqrt{k}/t) \). Taking union bound over all \( i \in [n] \), we obtain that with high probability, \( \|\tilde{h} - h\|_\infty \leq O(\sqrt{k}/t) \). Recall that \( \|h\|_\infty \) was assumed to be equal to \( k \) (WLOG). Hence we obtain that \( \|\tilde{h} - h\|_\infty \leq O(\sqrt{1/t} \|h\|_\infty) \) as desired.

3 FULL MULTILAYER MODEL

We describe the multilayer generative model for the shadow distribution associated with an \( \ell \)-layer deep net with RELUs. The feed-forward net is shown in Figure 3 (b). The \( j \)-th layer has \( n_j \) nodes, while the observable layer has \( n_0 \) nodes. The corresponding generative model is in Figure 3 (a). The number of variables at each layer, and the edge weights match exactly in the two models, but the generative model runs from top to down.

The generative model uses the hidden variables at layer \( j \) to produce the hidden variables at \( j - 1 \) using exactly the single-layer generative analog of the corresponding layer of the deep net. It starts with a value \( h^{(\ell)} \) of the top layer, which is generative from some arbitrary distribution \( D_{\ell} \) over the set of \( k_\ell \)-sparse vectors in \( \mathbb{R}^{n_\ell} \) (e.g., uniform \( k_\ell \) subset as support, followed by Gaussian distribution on the support). Then using weight matrix \( W_{\ell-1} \), it generates the hidden variable \( h^{(\ell-1)} \) below using the same stochastic process as described for one layer in Section 2. Namely, apply a random sampling function \( s_{k_{\ell-1}}(\cdot) \) (or equivalently add dropout noise with \( \rho = 1 - k_{\ell-1}/n^{\ell-1} \)) on the vector \( \rho (\alpha_{\ell-1} W_{\ell-1} h^{(\ell)}) \), where \( k_{\ell-1} \) is the target sparsity of \( h^{(\ell-1)} \), and \( \alpha_{\ell-1} = 2/k_{\ell-1} \) is a scaling constant. Repeating the same stochastic process (with weight \( W_j \), random sampling function \( s_{k_j}(\cdot) \)), we generate \( x \) at the bottom layer. In formula, we have

\[
x = s_{k_0}(\rho (\alpha_0 W_0 s_{k_0}(\rho (\alpha_1 W_1 \cdots))))
\]

We can prove Property (b) (that the feedforward net inverts the generative model) formally for 2 layers by adapting the proof for a single layer. The proof for 3 layers works under more restricted conditions. For more layers the correctness seems intuitive too but a formal proof seems to require proving concentration inequalities for a fairly complicated and non-linear function. We have verified empirically that Property (b) holds for up to 6 layers.

\(^4\)Note that to apply concentration inequality, independence between random variables is needed. Therefore technically, we need to condition on \( h \) and \( T \) before applying concentration inequality, as is done in the full proof of this lemma in Section A.
We assume the random-like matrices $W_j$’s to have standard gaussian prior as in (7), that is,
\[
W_j \text{ has i.i.d entries from } \mathcal{N}(0, 1)
\]  
(15)
We also assume that the distribution $D_\ell$ produces $k_\ell$-sparse vectors with not too large entries almost surely as in (8), that is, $h^{(1)}_i, h^{(1)}_f \in \mathbb{R}_{\geq 0}^{n_\ell}$, $|h^{(1)}_i|_0 \leq k_\ell$ and $|h^{(1)}_f|_\infty \leq O \left( \sqrt{\log N/(k_\ell)} \right)$ a.s. (Note that $N \triangleq \sum_{j} n_j$ is the total number of nodes in the architecture.)

Under this mathematical setup, we prove the following reversibility and dropout robustness results, which are the 2-layers analog of Theorem 2.3 and Theorem 2.4.

**Theorem 3.1 (2-Layer Reversibility and Dropout Robustness).** For $\ell = 2$, and $k_2 < k_1 < k_0 < k_2$, for 0.9 measure of the weights $(W_0, W_1)$, the following holds: There exists constant offset vector $b_0, b_1$ such that when $h^{(2)} \sim D_2$ and $\Pr[x \mid h^{(2)}]$ is specified as model (14), then network has reversibility and dropout robustness in the sense that the feedforward calculation (defined in Figure 3b) gives $\tilde{h}^{(2)}$ satisfying
\[
\forall i \in [n_2], \quad \mathbb{E} \left[ |h^{(2)}_i - \tilde{h}^{(2)}_i|^2 \right] \leq \epsilon r^2
\]  
(16)
where $\tau = \frac{1}{k_2} \sum_i h_i^{(2)}$ is the average of the non-zero entries of $h^{(2)}$ and $\epsilon = \tilde{O}(k_2/k_1)$. Moreover, the network also enjoys dropout robustness as in Theorem 2.4.

To parse the theorem, we note that when $k_2 \ll k_1$ and $k_1 \ll k_0$, in expectation, the entry-wise difference between $h^{(2)}$ and $\tilde{h}^{(2)}$ is dominated by the average single strength of $h^{(2)}$.

However, we note that we prove weaker results than in Theorem 2.3 – though the magnitudes of the error in both Theorems are on the order of the ratio of the sparsities between two layers, here only the expectation of the error is bounded, while Theorem 2.3 is a high probability result. In general we believe high probability bounds hold for any constant layers networks, but seemingly proving that requires advanced tools for understanding concentration properties of a complex non-linear function. Just to get a sense of the difficulties of results like Theorem 3.1, one can observe that to obtain $\tilde{h}^{(2)}$ from $h^{(2)}$ the network needs to be run twice in both directions with RELU and sampling. This makes the dependency of $\tilde{h}^{(2)}$ on $h^{(2)}$ and $W_2$ and $W_1$ fairly complicated and non-linear.

Finally, we extend Theorem 3.1 to three layers with stronger assumptions on the sparsity of the top layer – We assume additionally that $\sqrt{k_3} k_2^2 < k_0$, which says that the top two layer is significantly sparser than the bottom layer $k_0$. We note that this assumption is still reasonable since in most of practical situations the top layer consists of the labels and therefore is indeed much sparser. Weakening the assumption and getting high probability bounds are left to future study.

**Theorem 3.2 (3-layers Reversibility and Dropout Robustness, informally stated).** For $\ell = 3$, when $k_3 < k_2 < k_1 < k_0 < k_2$ and $\sqrt{k_3} k_2^2 < k_0$, the 3-layer generative model has the same type of reversibility and dropout robustness properties as in Theorem 3.1.

4 Experiments

We present experimental results that support our theory.

**Verification of the random-like nets hypothesis.** Testing the fully connected layers in a few trained networks showed that the edge weights are indeed random-like. For instance Figure 3 in the appendix shows the statistics for the the second fully connected layer in AlexNet (after 60 thousand training iterations). Edge weights fit a Gaussian distribution, and bias in the RELU gates are essentially constant (in accord with Theorem 2.3) and the distribution of the singular values of the weight matrix is close to the quartercircular law of random Gaussian matrices.

**Generative model.** We trained a 3-layer fully connected net on CIFAR-10 dataset as described below. Given an image and a neural net our shadow distribution can be used to generate an image. Figure 2 shows the generated image using the initial (random) deep net, and from the trained net after 100,000 iterations.
Improved training using synthetic data. Our suggestion is to use the shadow distribution to produce synthetic images together with labels and add them to the training set (named SHADOW). Figure 2 clarifies that the generated images are some kind of noisy version of the original. Thus the method is reminiscent of dropout, except the “noise” is applied to the original image rather than at each layer of the net. We trained feedforward networks with two hidden layers, each containing 5000 hidden units, using the standard datasets MNIST (handwritten digits) (LeCun et al., 1998), and CIFAR-10 and CIFAR-100 (32x32 natural images) (Krizhevsky and Hinton, 2009). A similar testbed was recently used in (Neyshabur et al., 2015), who were also testing their proposed algorithm for fully connected deep nets. During each iteration, for each real image one synthetic image is generated from the highest hidden layer using the shadow distribution. The loss on the synthetic images is weighted by a regularization parameter. (This parameter and the learning rate were chosen by cross validation; see the appendix for details.) All networks were trained both with and without dropout. When training with dropout, the dropout ratio is 0.5.

Figure 3 shows the test errors of networks trained by backpropagation alone, by backpropagation and dropout, and by our SHADOW regularization combined with backpropagation and dropout. Error drops much faster with our training, and a small but persistent advantage is retained even at the end. In the appendix, we also show that SHADOW outperforms backpropagation alone, and the error on the synthetic data tracks that on the real data, as predicted by the theory.

5 CONCLUSIONS

We have highlighted an interesting empirical finding, that the weights of neural nets obtained by standard supervised training behave similarly to random numbers. We have given a mathematical proof that such mathematical properties can lead to a very simple explanation for why neural nets have an associated generative model, and furthermore one that is essentially the reversal of the forward computation with the same edge weights. (This associated model can also be seen as some theoretical explanation of the empirical success of older ideas in deep nets such as weight tying and dropout.)

The model leads to a natural new modification for training of neural nets with fully-connected layers: in addition to dropout, train also on synthetic data generated from the model. This is shown to give some improvement over plain dropout. Extension of these ideas for convolutional layers is left for future work.

Theoretically explaining why deep nets satisfy the random-like nets hypothesis is left for future work. Possibly it follows from some elementary information bottleneck consideration ((Tishby and Zaslavsky, 2015)).
Another problem for future work is to design provably correct algorithms for deep learning assuming the input is generated exactly according to our generative model. This could be a first step to deriving provable guarantees on backpropagation.

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APPENDIX

A COMPLETE PROOFS FOR ONE-LAYER REVERSIBILITY

Proof of Lemma 2.5. We claim that it suffices to show that w.h.p\(^7\) over the choice of \((W, h, x)\) the network is reversible (that is, \([9]\) holds),

\[
\Pr_{x, h, W} \{\text{equation } [9] \text{ holds} \} \geq 1 - n^{10}.
\]

Indeed, suppose \([17]\) is true, then using a standard Markov argument, we obtain

\[
\Pr_{W} \left[ \Pr_{x, h} \{\text{equation } [9] \text{ holds } | W \} > 1 - n^{-5} \right] \geq 1 - n^5,
\]

as desired.

Now we establish \([17]\). Note that equation \([9]\) (and consequently statement \([17]\)) holds for any positive scaling of \(h, x\) simultaneously, since RELU has the property that \(r(\beta z) = \beta \cdot r(z)\) for any \(\beta \geq 0\) and any \(z \in \mathbb{R}\). Therefore WLOG we can choose a proper scaling of \(h\) that is convenient to us. We assume \(|h|^2 = k\).

By assumption \([8]\), we have that \(|h|_{\infty} \leq O(\sqrt{\log k})\).

Define \(\hat{h} = \alpha W^T x\). Similarly to \([13]\), we fix \(i\) and expand the expression for \(\hat{h}_i\) by definition and obtain \(\hat{h}_i = \alpha \sum_{j=1}^n W_{ji} x_j\). Suppose \(n_{\text{drop}}\) has support \(T\). Then we can write \(x_j\) as

\[
x_j = r(\sum_{\ell=1}^m W_{j\ell} h_\ell) \cdot n_{\text{drop}, j} = r(W_{ji} h_i + \eta_j) \cdot 1_{j \in T},
\]

where \(\eta_j \triangleq \sum_{\ell \neq j} W_{ji} h_\ell\). Though \(r(\cdot)\) is nonlinear, it is piece-wise linear and more importantly still Lipschitz. Therefore intuitively, RHS of \([13]\) can be “linearized” by approximating \(r(W_{ji} h_i + \eta_j)\) by \(1_{\eta_j > 0} \cdot (W_{ji} h_i + r(\eta_j))\). Note that this approximation is not accurate only when \(|\eta_j| \leq |W_{ji} h_i|\), which happens with relatively small probability, since \(\eta_j\) typically dominates \(W_{ji} h_i\) in magnitude.

Using the intuition above, we can formally calculate the expectation of \(W_{ji} x_j\) via a slightly tighter and more sophisticated argument: Conditioned on \(h\), we have \(W_{ji} \sim \mathcal{N}(0, 1)\) and \(\eta_j = \sum_{\ell \neq j} W_{ji} h_\ell \sim \mathcal{N}(0, \sigma^2)\) with \(\sigma^2 = |h|^2 - h_j^2 = k - h_j^2 \geq \Omega(k)\). Therefore we have \(\log \sigma = \frac{1}{2} \log(\Omega(k)) \geq h_j\) and then by Lemma \([5, 1]\) (\(W_{ji}\) here corresponds to \(w\) in Lemma \([1\text{]}\) \(\eta_j\) to \(\xi\) and \(h_j\) to \(h\)), we have \(\mathbb{E}[W_{ji} x_j | h] = \mathbb{E}[W_{ji} r(W_{ji} h_j + \eta_j) | h] = \frac{1}{2} h_i \pm O(1/k^{3/2})\).

It follows that

\[
\mathbb{E}[\hat{h}_i | h] = \sum_{j \in T} \mathbb{E}[W_{ji} r(W_{ji} h_j + \eta_j) | h] = \frac{\alpha |T|}{2} h_i \pm O(\alpha t/k^{3/2})
\]

Taking expectation over the choice of \(T\) we obtain that

\[
\mathbb{E}[\hat{h}_i | h] = \frac{\alpha t}{2} h_i \pm O(\alpha n/k^{3/2}) = h_i \pm O(1/(k^{3/2}))
\]

(Recall that \(t = \rho n\) and \(\alpha = 2/(\rho m)\). Similarly, the variance of \(\hat{h}_i | h\) can be bounded by \(\text{Var}[\hat{h}_i | h] = O(k/t)\) (see Claim \(A.2\)). Therefore we expect that \(\hat{h}_i\) concentrate around its mean with fluctuation \(\pm O(\sqrt{k}/t)\). Indeed, by by concentration inequality, we can prove (see Lemma \(A.1\) in Section \(A\) that actually \(\hat{h}_i | h\) is sub-Gaussian, and therefore conditioned on \(h\), with high probability \((1 - n^{-10})\) we have \(|\hat{h}_i - h_i| \leq \)

5We use w.h.p as a shorthand for “with high probability” in the rest of the paper.
\(\tilde{O}(\sqrt{k/t} + 1/k^{3/2})\), where the first term account for the variance and the second is due to the bias (difference between \(\mathbb{E}[\hat{h}_i]\) and \(h_i\)).

Noting that \(k < t < k^2\) and therefore \(1/k^{3/2}\) is dominated by \(\sqrt{k/t}\), take expectation over \(h\), we obtain that \(\Pr[|\hat{h}_i - h_i| \geq \tilde{O}(\sqrt{k/t})] \leq n^{-10}\). Taking union bound over all \(i \in [n]\), we obtain that with high probability, \(\|\hat{h}_i - h_i\|_{\infty} \leq \tilde{O}(\sqrt{k/t})\). Recall that \(\|h\|\) was assumed to be equal \(k\) without loss of generality. Hence we obtain that \(\|\hat{h}_i - h_i\|_{\infty} \leq \tilde{O}(\sqrt{1/t})\|h\|\) as desired.

**Proof of Theorem 2.4** Recall that in the generative model already many bits are dropped, and nevertheless the feedforward direction maps it back to \(h\). Thus dropping some more bits in \(x\) doesn’t make much difference. Concretely, we note that \(x^{\text{drop}}\) has the same distribution as \(s_{t/2}(r(\alpha Wh))\). Therefore invoking Theorem 2.3 with \(t\) being replaced by \(t/2\), we obtain that there exists \(b'\) such that \(\|r(2W^Tx^{\text{drop}} + b') - h\|^2 \leq \tilde{O}(k/t) \cdot \|h\|\).

**Lemma A.1.** Under the same setting as Theorem 2.3 let \(\hat{h} = \alpha W^T h\). Then we have
\[
\Pr[|\hat{h}_i - h_i| \geq \tilde{O}((\sqrt{k/t} + 1/k^{3/2}) | h)] \leq n^{-10}
\]

**Proof of Lemma A.1** Recall that \(\hat{h}_i = \sum_{j \in T} \alpha W_{ji} r(W_{ji} h_j + \eta_j)\). For convenience of notation, we condition on the randomness \(h\) and \(T\) and only consider the randomness of \(W\) implicitly and omit the conditioning notation. Let \(Z_j\) be the random variable \(\alpha W_{ji} x_j = \alpha W_{ji} r(W_{ji} h_j + \eta_j)\). Therefore \(Z_j\) are independent random variables (conditioned on \(h\) and \(T\)). Our plan is to show that \(Z_j\) has bounded Orlicz norm and therefore \(\hat{h}_i = \sum_j Z_j\) concentrates around its mean.

Since \(W_{ji}\) and \(x_j\) are Gaussian random variables with variance 1 and \(\|h\| = \sqrt{\kappa}\), we have that \(\|W_{ji}\|_{\psi_2} = 1\) and \(\|x_j\|_{\psi_2} \leq \sqrt{\kappa}\). This implies that \(W_{ji}x_j\) is sub-exponential random variables, that is, \(\|W_{ji}x_j\|_{\psi_1} \leq O(\sqrt{\kappa})\). That is, \(Z_j\) has \(\psi_1\) orlicz norm at most \(O(\alpha \sqrt{\kappa})\). Moreover by Lemma D.2 we have that \(\|Z_j - \mathbb{E}[Z_j]\|_{\psi_1} \leq O(\alpha \sqrt{\kappa})\). Then we are ready to apply bernstein inequalities for sub-exponential random variables (Theorem D.1) and obtain that for some universal constant \(c\),
\[
\Pr\left[\left|\sum_{j \in T} Z_j - \mathbb{E}\left[\sum_{j \in T} Z_j\right]\right| > c\sqrt{|T|\alpha \sqrt{k} \log n}\right] \leq n^{-10}.
\]

Equivalently, we obtain that
\[
\Pr\left[|\hat{h}_i - \mathbb{E}[\hat{h}_i]| > c\sqrt{|T|k/t^2 \log n} | h, T\right] \leq n^{-10}.
\]

Note that with high probability, \(|T| = (1 \pm o(1))t\). Therefore taking expectation over \(T\) and taking union bound over \(i \in [n]\) we obtain that for some absolute constant \(c\),
\[
\Pr\left[\forall i \in [n], |\hat{h}_i - \mathbb{E}[\hat{h}_i]| > c\sqrt{k/t \log n} | h\right] \leq n^{-8}.
\]

Finally note that as shown in the proof of Theorem 2.3 we have \(\mathbb{E}[\hat{h}_i | h] = h_i \pm 1/k^{3/2}\). Combining with the equation above we get the desired result.
Claim A.2. Under the same setting as in the proof of Theorem 2.3. The variance of \( \hat{h}_i \) can be bounded by

\[
\text{Var}[\hat{h}_i | h] \leq O(k/t)
\]

Proof. Using Cauchy-Schwartz inequality we obtain

\[
\text{Var}[W_{ji} x_j | h] \leq \mathbb{E}[W_{ji}^2 x_j^2 | h] \\
\leq \mathbb{E}[W_{ji}^4 | h]^{1/2} \mathbb{E}[x_j^4 | h]^{1/2} \leq O(k)
\]

It follows that

\[
\text{Var}[\hat{h}_i | h] = \mathbb{E} \left[ \sum_{j \in T} \alpha^2 \text{Var}[W_{ji} x_j | h] \right] \leq \alpha^2 t \cdot O(k) = O(k/t),
\]

We note that a tighter calculation of the variance can be obtained using Lemma B.1. ☐

B Auxiliary Lemmas for One Layer Model

We need a series of lemmas for the one layer model, which will be further used in the proof of two layers and three layers result.

As argued earlier, the particular scaling of the distribution of \( h \) is not important, and we can assume WLOG that \( \|h\|^2 = k \). Throughout this section, we assume that for \( h \sim D_h \), \( h \in \mathbb{R}^n_+, \|h\| \leq k \), \( \|h\| = k \), and \( |h|_\infty \leq O(\sqrt{\log N}) \) almost surely (20)

Lemma B.1. Suppose \( w \in \mathcal{N}(0, 1) \) and \( \xi \sim \mathcal{N}(0, \sigma^2) \) are two independent variables. For \( \sigma = \Omega(1) \) and \( 0 \leq h \leq \log(\sigma) \), we have that \( \mathbb{E}[w \cdot r(wh + \xi)] = \frac{h}{2} \pm \tilde{O}(1/\sigma^3) \) and \( \mathbb{E}[w^2 \cdot r(wh + \xi)^2] \leq 3h^2 + \sigma^2 \).

Proof. Let \( \phi(x) = \frac{1}{\sigma \sqrt{2\pi}} \exp(-\frac{x^2}{2\sigma^2}) \) be the density function for random variable \( \xi \). Let \( C_1 = \mathbb{E}[|\xi|/\sigma] = \frac{\sigma}{2} \int_0^\infty \phi(x) x dx \). We start by calculating \( \mathbb{E}[r(wh + \xi) | w] \) as follows:

\[
\mathbb{E}[w \cdot r(wh + \xi) | w] = w \int_{-\infty}^\infty \phi(x)(wh + x) dx \\
= w \int_0^\infty \phi(x)(wh + x) dx + w \int_{-\infty}^0 \phi(x)(wh + x) dx \\
= \frac{C_1}{2} + \frac{w^2 h}{2} + w \int_{-\infty}^0 \phi(y)(wh - y) dy \\
\]

Therefore we have that

\[
\mathbb{E}[\mathbb{E}[w \cdot r(wh + \xi) | w]] = \frac{h}{2} + \mathbb{E}[G(w)]
\]

Thus it remains to understand \( G(w) \) and bound its expectation. We calculate the derivative of \( G(w) \): We have that \( G(w) \) can be written as
\[ G(w) = w^2 h \int_0^w \phi(y) dy - w \int_0^w \phi(y) y dy \]

and its derivative is
\[ G(w)' = 2wh \int_0^w \phi(y) dy + w^2 h^2 \phi(wh) - \int_0^w \phi(y) y dy - w^2 h^2 \phi(wh) \]
\[ = 2wh \int_0^w \phi(y) dy - \int_0^w \phi(y) y dy \]

The it follows that
\[ G(w)'' = 2h \int_0^w \phi(y) dy + 2wh^2 \phi(wh) - w^2 \phi(wh) \]
\[ = 2h \int_0^w \phi(y) dy + wh^2 \phi(wh) \]

Moreover, we can get the third derivative and forth one
\[ G(w)''' = 3h^2 \phi(wh) + wh^3 \phi'(wh) \]

and
\[ G(w)^{(4)} = 4h^3 \phi'(wh) + wh^4 \phi''(wh) \]

Therefore for \( h \leq 10 \log(\sigma) \) and \( w \) with \( |w| \leq 10 \log(\sigma) \), using the fact that \( \phi'(wh) = \frac{1}{\sqrt{2\pi} wh} \exp(-\frac{w^2 h^2}{2wh}) \frac{wh}{\sigma^2} \) and similarly, \( \phi''(wh) \leq \frac{1}{\sigma^4} \). It follows that \( G(w)^{(4)} \leq O(\frac{w^4}{\sigma^4}) \) for any \( w \leq 10 \log(\sigma) \).

Now we are ready to bound \( \mathbb{E}[G(w)] \): By Taylor expansion at point 0, we have that
\[ G(w) = \frac{h^2 \phi(0)}{2} w^3 + \frac{G(\zeta)^{(4)}}{24} w^4 \]
for some \( \zeta \) between 0 and \( w \). It follows that for \( |w| \leq 10 \log(\sigma) \),
\[ |G(w) - \frac{h^2 \phi(0)}{2} w^3| \leq O(1/\sigma^3), \]
and therefore we obtain that
\[ \mathbb{E}[G(w) \mid |w| \leq 10 \log(\sigma)] - \mathbb{E}\left[ \frac{h^2 \phi(0)}{2} w^3 \mid |w| \leq 10 \log(\sigma) \right] \leq \mathbb{E}\left[ G(w) - \frac{h^2 \phi(0)}{2} w^3 \mid |w| \leq 10 \log(\sigma) \right] \leq O(1/\sigma^3) \]

Since \( w |w| \leq 10 \log(\sigma) \) is symmetric, we have \( \mathbb{E}\left[ \frac{h^2 \phi(0)}{2} w^3 \mid |w| \leq 10 \log(\sigma) \right] = 0 \), and it follows that
\[ \mathbb{E}[G(w) \mid |w| \leq 10 \log(\sigma)] \leq O(1/\sigma^3). \]
Moreover, note that \( |G(w)| \leq O(w^3 h^2) \leq O(\log^2(\sigma) w^3) \), then we have that
\[ \mathbb{E}[G(w) \mid |w| \geq 10 \log(\sigma)] \Pr[|w| \geq 10 \log(\sigma)] \leq \sigma^{-4} \int_{|w| \geq 10 \log(\sigma)} O(\log^2(\sigma) w^3) \exp(-w^2/2) dw \leq O(1/\sigma^3) \]

Therefore altogether we obtain
\[ \mathbb{E}[G(w)] = \mathbb{E}[G(w) \mid |w| \geq 10 \log(\sigma)] \Pr[|w| \geq 10 \log(\sigma)] + \mathbb{E}[G(w) \mid |w| \leq 10 \log(\sigma)] \Pr[|w| \leq 10 \log(\sigma)] = \widetilde{O}(1/\sigma^3) + O(1/\sigma^3) = \widetilde{O}(1/\sigma^3). \]

Finally we bound the variance of \( w \cdot r(wh + \xi) \). We have that
\[ \mathbb{E}[w^2 \cdot r(wh + \xi)] \leq \mathbb{E}[w^2 \cdot (wh + \xi)^2] = h^2 \mathbb{E}[w^4] + \mathbb{E}[w^2] \mathbb{E}[\xi^2] = 3h^2 + \sigma^2. \]

as desired.
Lemma B.2. For any \( a, b \geq 0 \) with \( a, b \leq 5 \log \sigma \) and random variable \( u, v \sim \mathcal{N}(0, 1) \) and \( \xi \in \mathcal{N}(0, \sigma^2) \), we have that
\[
\left| \mathbb{E}[uv \cdot r(au + bv + \xi)^2] - \mathbb{E}[ur(au + bv + \xi)] \mathbb{E}[vr(au + bv + \xi)] \right| = O(1).
\]

Proof. Let \( t = \sqrt{a^2 + b^2} \) in this proof. We first represent \( u = \frac{1}{t}(ax + by) \) and \( v = \frac{1}{t}(bx - ay) \), where \( x = \frac{1}{t}(au + bv) \) and \( y = \frac{1}{t}(bu - av) \) are two independent Gaussian random variables drawn from \( \mathcal{N}(0, 1) \). We replace \( u, v \) by the new parameterization,
\[
\mathbb{E}[uv \cdot r(au + bv + \xi)^2] = \mathbb{E}\left[ \frac{1}{t^2} (ax + by)(bx - ay)r(tx + \xi)^2 \right]
\]
\[
= \mathbb{E}\left[ \frac{1}{t^2} abx^2r(tx + \xi)^2 \right] - \mathbb{E}\left[ \frac{1}{t^2} abr(tx + \xi)^2 \right]
\]
\[
= \mathbb{E}\left[ \frac{1}{t^2} ab(x^2 - 1)r(tx + \xi)^2 \right]
\]
where we used the fact that \( \mathbb{E}[y] = 0 \) and \( y \) is independent with \( x \) and \( \xi \).

Then we expand the expectation by conditioning on \( x \) and taking expectation over \( \xi \):
\[
(x^2 - 1) \mathbb{E}[r(tx + \xi)^2 | x] = (x^2 - 1) \int_{tx}^{\infty} (tx + y)^2 \phi(y) dy
\]
\[
= (x^2 - 1) \left( \int_{0}^{tx} (tx + y)^2 \phi(y) dy + (x^2 - 1) \int_{0}^{\infty} (tx + y)^2 \phi(y) dy \right)
\]
\[
= (x^2 - 1) \int_{0}^{tx} (tx + y)^2 \phi(y) dy + (x^2 - 1)(C_0 t^2 x^2 + 2C_1 tx + C_2)
\]
\[
\triangleq H(x) + (x^2 - 1)(C_0 t^2 x^2 + 2C_1 tx + C_2)
\]
where \( C_0 = \int_{0}^{\infty} \phi(y) dy = \frac{1}{2} \), and \( C_1, C_2 \) are two other constants (the values of which we don’t care) that don’t depend on \( x \). Therefore by Lemma B.3 we obtain that \( |\mathbb{E}[H(x)]| \leq \tilde{O}(1/\sigma) \) and therefore taking expectation of the equation above we obtain that
\[
\mathbb{E}[(x^2 - 1) \mathbb{E}[r(tx + \xi)^2 | x]] = \mathbb{E}[H(x)] + \mathbb{E}[(x^2 - 1)(C_0 t^2 x^2 + 2C_1 tx + C_0)]
\]
\[
= 2C_2 t^2 \pm \tilde{O}(1/\sigma) = t^2 \pm \tilde{O}(1/\sigma)
\]
Therefore we have that \( \mathbb{E}[uv \cdot r(au + bv + \xi)^2] = \mathbb{E}\left[ \frac{1}{t^2} ab(x^2 - 1)r(tx + \xi)^2 \right] = \tilde{O}(1) \). Using the fact that \( \mathbb{E}[ur(au + bv + \xi)] \leq \tilde{O}(1) \) and \( \mathbb{E}[vr(au + bv + \xi)] \leq \tilde{O}(1) \), we obtain that
\[
|\mathbb{E}[uv \cdot r(au + bv + \xi)^2] - \mathbb{E}[ur(au + bv + \xi)] \mathbb{E}[vr(au + bv + \xi)]| = \tilde{O}(1).
\]

Lemma B.3. Suppose \( z \sim \mathcal{N}(0, 1) \), and let \( \phi(x) = \frac{1}{2\sqrt{2\pi}} \exp\left(-\frac{x^2}{2\sigma^2}\right) \) be the density function of \( \mathcal{N}(0, \sigma^2) \) where \( \sigma = \Omega(1) \). For \( r \leq 10 \log \sigma \), define \( G(z) = \int_{0}^{r} (rz - y)^2 \phi(y) dy \), and \( H(z) = (z^2 - 1)G(z) \). Then we have that \( \mathbb{E}|H(z)| \leq \tilde{O}(1/\sigma) \)

Proof. Our technique is to approximate \( H(z) \) using taylor expansion at point close to 0, and then argue that since \( z \) is very unlikely to be very large, so the contribution of large \( z \) is negligible. We calculate the derivate
of $H$ at point $z$ as follows:

$$H(z)' = 2zG(z) + (z^2 - 1)G'(z)$$
$$H(z)'' = 2G(z) + 4zG'(z) + (z^2 - 1)G''(z)$$
$$H(z)''' = 6G'(z) + 6zG''(z) + (z^2 - 1)G'''(z)$$

Moreover, we have that the derivatives of $G$

$$G'(z) = \int_0^r 2r(z - y)\phi(y)dy$$
$$G''(z) = \int_0^r 2r^2\phi(y)dy$$
$$G'''(z) = 2r^3\phi(rz)$$

Therefore we have that $G'(0) = G''(0) = 0$ and $H'(0) = H''(0) = 0$. Moreover, when $r \leq 10\log \sigma$ and $z \leq 10\log \sigma$ and we have that bound that $|H''(z)| \leq \tilde{O}(1/\sigma)$. Therefore, we have that for $z \leq 10\log \sigma, |H(z)| \leq \tilde{O}(1/\sigma)$, and therefore we obtain that $\mathbb{E}[H(z) | |z| \leq 10\log \sigma] \text{Pr}[|z| \leq 10\log \sigma] \leq \tilde{O}(1/\sigma)$. Since $|H(z)| \leq \tilde{O}(1) \cdot z^4$ for any $z$, we obtain that for $z \geq 10\log \sigma$, the contribution is negligible: $\mathbb{E}[H(z) | |z| > 10\log \sigma] \text{Pr}[|z| > 10\log \sigma] \leq \tilde{O}(1/\sigma^2)$. Therefore altogether we obtain that $|\mathbb{E}[H(z)]| \leq \tilde{O}(1/\sigma)$.

The following two lemmas are not used for the proof of single layer net, though they will be useful for proving the result for 2-layer net. The following lemma bound the correlation between $\hat{h}_i$ and $\hat{h}_j$.

**Lemma B.4.** Let $\hat{h} = W^T_x$, and $D_h$ satisfies (20), then for any $i, j$, we have that $|E[\hat{h}_i \hat{h}_j] - E[\hat{h}_i] E[\hat{h}_j]| \leq \tilde{O}(1/t)$.

**Proof.** We expand the definition of $\hat{h}_i$ and $\hat{h}_j$ directly.

$$\mathbb{E}[\hat{h}_i \hat{h}_j] = \alpha^2 \mathbb{E} \left[ \left( \sum_{u \in S} W_{ui}x_u \right) \left( \sum_{v \in S} W_{vj}x_v \right) \right]$$
$$= \alpha^2 \sum_{u \in S} \mathbb{E} [W_{ui}W_{vi}x_u^2] + \alpha^2 \sum_{u \neq v} \mathbb{E} [W_{ui}W_{vj}x_u x_v]$$
$$= \alpha^2 \sum_{u \in S} \mathbb{E} [W_{ui}W_{vi}x_u^2] + \alpha^2 \sum_{u \neq v} \mathbb{E} [W_{ui}x_u] \mathbb{E} [W_{vj}x_v]$$
$$= \alpha^2 \sum_{u \in S} (\mathbb{E} [W_{ui}W_{vi}x_u^2] - \mathbb{E}[W_{ui}x_u] \mathbb{E}[W_{vj}x_v]) + \alpha^2 \sum_{u \neq v} \mathbb{E} [W_{ui}x_u] \mathbb{E} [W_{vj}x_v]$$
$$= \alpha^2 \sum_{u \in S} (\mathbb{E} [W_{ui}W_{vi}x_u^2] - \mathbb{E}[W_{ui}x_u] \mathbb{E}[W_{vj}x_v]) + \mathbb{E}[\hat{h}_i] \mathbb{E}[\hat{h}_j]$$

where in the third line we use the fact that $W_{ui}x_u$ is independent with $W_{vj}x_v$, and others are basic algebra manipulation. Using Lemma B.4 we have that

$$|\mathbb{E} [W_{ui}W_{vi}x_u^2] - \mathbb{E}[W_{ui}x_u] \mathbb{E}[W_{vj}x_v]| \leq \tilde{O}(1)$$

Therefore we obtain that

$$|\mathbb{E}[\hat{h}_i \hat{h}_j] - \mathbb{E}[\hat{h}_i] \mathbb{E}[\hat{h}_j]| = \alpha^2 \tilde{O}(t) = \tilde{O}(1/t)$$
The following lemmas shows that the

**Lemma B.5.** Under the single-layer setting of Lemma B.4, let \( K \) be the support of \( h \). Then for any \( k \)-dimensional vector \( u_K \) such that \( |u_K|_\infty \leq \tilde{O}(1) \), we have that

\[
\mathbb{E}[|u_K^T(h_K - \mathbb{E}h_K)|^2] \leq \tilde{O}(k^2/t)
\]

**Proof.** We expand our target and obtain,

\[
\mathbb{E}[|u_K^T(h_K - \mathbb{E}h_K)|^2] = \mathbb{E}[\sum_{i \in K} u_i(h_i - \mathbb{E}h_i)^2]
\]

\[
= \sum_{i \in K} \mathbb{E}[u_i^2(h_i - \mathbb{E}h_i)^2] + \mathbb{E}\left[\sum_{i \neq j} u_iu_j(h_i - \mathbb{E}h_i)(h_j - \mathbb{E}h_j)\right]
\]

\[
= \sum_{i \in K} \mathbb{E}[(h_i - \mathbb{E}h_i)^2] \cdot \tilde{O}(1) + \max_{i \neq j} \{\mathbb{E}|h_i| \mathbb{E}|h_j|\} \cdot \tilde{O}(1) \cdot k^2
\]

By Lemma A.2, we have that \( \mathbb{E}[(h_i - \mathbb{E}h_i)^2] \leq \tilde{O}(|h|^2/t) \). By Lemma B.4, therefore we obtain that \( \max_{i \neq j} \{\mathbb{E}|h_i| \mathbb{E}|h_j|\} \leq \tilde{O}(1/t) \). Using the fact that \( |h|^2 \leq \tilde{O}(k) \),

\[
\mathbb{E}[|u_K^T(h_K - \mathbb{E}h_K)|^2] \leq \tilde{O}(k^2/t)
\]

\[\square\]

C  **MULTILAYER REVERSIBILITY AND DROPOUT ROBUSTNESS**

We state the formal version of Theorem 3.1 here. Recall that we assume the distribution of \( h^{(\ell)} \) satisfies that

\[
h^{(\ell)} \in \mathbb{R}_{\geq 0}^n, |h^{(\ell)}|_0 \leq k_\ell \text{ and } |h^{(\ell)}|_\infty \leq O\left(\sqrt{\log N/(k_\ell)}\right) \text{ a.s.} \tag{21}
\]

**Theorem C.1 (2-Layer Reversibility and Dropout Robustness).** For \( \ell = 2 \), and \( k_2 < k_1 < k_0 < k_2^2 \), there exists constant offset vector \( b_0, b_1 \) such that with probability \( .9 \) over the randomness of the weights \( (W_0, W_1) \) from prior (15), and \( h^{(2)} \sim D_2 \) that satisfies (21), and observable \( x \) generated from the 2-layer generative model (14), the hidden representations obtained from running the network feedforwardly

\[
\tilde{h}^{(1)} = r(W_0^T x + b_1), \text{ and } \tilde{h}^{(2)} = r(W_1^T h^{(1)} + b_2)
\]

are entry-wise close to the original hidden variables

\[
\forall i \in [n_2], \quad \mathbb{E}\left[|\tilde{h}^{(2)}_i - h^{(2)}_i|^2\right] \leq \tilde{O}(k_2/k_1) \cdot \tilde{h}^{(2)}
\tag{22}
\]

\[
\forall i \in [n_1], \quad \mathbb{E}\left[|\tilde{h}^{(1)}_i - h^{(1)}_i|^2\right] \leq \tilde{O}(k_1/k_0) \cdot \tilde{h}^{(1)}
\tag{23}
\]

where \( \tilde{h}^{(2)} = \frac{1}{k_2} \sum_i h^{(2)}_i \) and \( \tilde{h}^{(1)} = \frac{1}{k_1} \sum_i h^{(1)}_i \) are the average of the non-zero entries of \( h^{(2)} \) and \( h^{(1)} \).

Moreover, there exists offset vector \( b'^1 \) and \( b'^2 \), such that when hidden representation is calculated feedforwardly with dropping out a random subset \( \mathcal{G}_0 \) of size \( n_0/2 \) in the observable layer and \( \mathcal{G}_2 \) of size \( n_1/2 \) in the first hidden layer:

\[
\tilde{h}^{(1)}\text{drop} = r(2W_0^T(x \odot n^0_{\text{drop}}) + b'^1), \text{ and } \tilde{h}^{(2)} = r(2W_1^T(h^{(1)} \odot n^1_{\text{drop}}) + b'^2)
\]

are entry-wise close to the original hidden variables in the same form as equation (22) and (23). (Here \( n^0_{\text{drop}} \) and \( n^1_{\text{drop}} \) are uniform random binary vector of size \( n_0 \) and \( n_1 \), which governs which coordinates to be dropped).
For the ease of math, we use a cleaner notation and setup as in Section 3. Suppose there are two hidden layers $g \in \mathbb{R}^p$ and $h \in \mathbb{R}^m$ and one observable layer $x$. We assume the sparsity of top layer is $q$, and we assume in our generative model that $h = s_k(r(\beta U g))$ and $x = s_t(r(\alpha W h))$ where $U$ and $W$ are two random matrices with standard normal entries.

Let $\tilde{h} = r(W^T x + b)$ and $\tilde{g} = r(U^T h + c)$, where $b$ and $c$ two offset vectors. Our result in the last section show that $\tilde{h} \approx h$, and in the section we are going to show $\tilde{g} \approx g$. The main difficulty here is that the value of $h$ and $\tilde{h}$ depends on the randomness of $U$ and therefore the additional dependency and correlation introduced makes us hard to write $\tilde{g}$ as a linear combination of independent variables. Here we aim for a weaker result and basically prove that $\mathbb{E}[|g_r - \tilde{g}_r|^2]$ is small for any index $r \in [p]$.

**Theorem C.2.** When $q < k < t < q^2$, and any fixed $g \in \mathbb{R}^p$ with $|g|_0 \leq q$ and $\|g\|_2 = \Theta(\sqrt{q})$ and $|g|_\infty \leq \tilde{O}(1)$, for $\alpha = \frac{q}{2}$, $\beta = 2/k$ and some $b$, and $c$, with high probability over the randomness of $W$, $\tilde{g}$ satisfies that for any $r \in [p]$,

$$\mathbb{E}[|g_r - \tilde{g}_r|^2] \leq \tilde{O}(q/k)$$

**Proof.** We fix an index $r \in [p]$, and consider $g_r$ and $\tilde{g}_r$. Moreover, we fix the choice of random sampling function $s_k(\cdot)$ to the function $s_k(x) = [x_K, 0]$ where $K$ and $T$ be subsets of $[m]$ and $[n]$, with size $k$ and $t$, respectively. Let $\tilde{g}_r = U_r^T \tilde{h}$ where $U_r$ is the $r$-th column of $U$, that is, $\tilde{g}_r$ is the version before shift and rectifier linear. Further more, let’s assume $U_r^T h = u^T = [u_1, \ldots, u_m]$ and $u_K$ is the its restriction to subset $K$. Therefore, $\tilde{g}_r$ can be written as

$$\tilde{g}_r = u^T \tilde{h} = u^T h + u^T (h - \tilde{h})$$

(24)

By Lemma 2.5 (applying to the layer between $g$ and $h$), we know that with high probability over the randomness of $U$, $|u^T h - g_r| \leq \tilde{O} \left( \sqrt{q/k} \right)$. We conditioned on the event $E$ that $|u^T h - g_r| \leq \tilde{O} \left( \sqrt{q/k} \right)$, and that $\|u\|_\infty \leq \tilde{O}(1)$ in the rest of the proof (note that event $E$ happens with high probability).

Now it suffices to prove that $u^T (h - \tilde{h})$ is small. First of all, we note that with high probability over the randomness of $W$, $\tilde{h}$ matches $h$ on the support, therefore we can write $u^T (h - \tilde{h}) = u^T K (h_K - h_K')$, which turns out to be essential for bounding the error. We further decompose it into

$$u^T K (h_K - h_K') = u^T K (h_K - \mathbb{E}[h_K]) + u^T K (\mathbb{E}[h_K] - h_K') + u^T K (h_K - \mathbb{E}[h_K]),$$

(25)

and bound them individually.

First of all, we note that $h_i$ is typically of magnitude $\beta \sqrt{q}$ where $q$ is the sparsity of $g$, and $\|h\| = \tilde{O} \left( \sqrt{q} \right)$. We first scale down $h$ by $\beta \sqrt{q}$ and then $h/(\beta \sqrt{q})$ meets the scaling of equation (20). We are going to apply Lemmas in Section B with $h/(\beta \sqrt{q})$.

by equation 19, we have that $|\mathbb{E}[h_i]/(\beta \sqrt{q}) - h_i/(\beta \sqrt{q})| \leq \tilde{O}(1/(q^{3/2}))$, and therefore $|\mathbb{E}[h_K] - h_K|_1 \leq \tilde{O}((\beta \sqrt{q})^{-1}/(q^{3/2}k) \cdot k) = \tilde{O}(1/q)$.

Therefore $u^T K (h_K - \mathbb{E}[h_K]) \leq |u|_\infty |\mathbb{E}[h_K] - h_K|_1 \leq \tilde{O}(1/q)$. Moreover, we note that $h_K - \mathbb{E}[h_K] = b 1_K$ is a constant vector and therefore $u^T (h_K - h_K') = b'$ for a constant $b$ (which depends on $r$ and $u$ implicitly).

Finally we bound the term $u^T K (h_K - \mathbb{E}[h_K])$. We invoke Lemma B.5 (with $h/(\beta \sqrt{q})$) and obtain that

$$\mathbb{E}[||u^T K (h_K - \mathbb{E}[h_K])||^2 | h, E] \leq \tilde{O}(k^2/t)$$

It follows that

$$\mathbb{E}[||u^T K (h_K - \mathbb{E}[h_K])||^2 | h, E] \leq \tilde{O}(q/t)$$

Note that the small probability event has only negligible contribution to the the expectation, therefore bounding the difference and marginalize over $h$, we obtain that $\mathbb{E}[||u^T K (h_K - \mathbb{E}[h_K])||^2] \leq \tilde{O}(q/t)$. Therefore we
have bounded the three terms in RHS of (25). \( E[\hat{y}_r - u^T \hat{h}]^{2} \leq \tilde{O}(1/q + q/k) = \tilde{O}(q/k) \). Note that 

\( g = r(\hat{g} + b) \), therefore for any \( b = \epsilon 1 \) with \( \epsilon \leq \tilde{O}(q/k) \), we obtain that \( E[\|\hat{y} - g\|_\infty^2] \leq \tilde{O}(q/k) \).

\[ \square \]

C.1 Proof Sketch of Theorem 3.2

As argued in Section 3, the drawback of not getting high probability bound in the 2-layer Theorems is that we lose the denoising property of rectifier linear. Note that since \( |g_r - g_r| \) is only small in expectation, passing through the rectifier linear we obtain \( r(\hat{g} + c) \), and we can’t argue that \( r(\hat{g} + c) \) matches the support \( g \) theoretically. (Though experimentally and intuitively, we believe that choosing \( c \) to be proportional to the noise would remove the noise on all the non-support of \( g \).)

However, bounding the error in a weaker way we could obtain Theorem 3.2. The key idea is that the in a three layer network described as in Section 3, the inference error of \( h^{(3)} \) come from three sources: the error caused by incorrectly recover \( h^{(1)} \), \( h^{(2)} \) and the error of reversing the third layer \( W_2 \). The later two sources error reduces to two and one layer situation and therefore we can bound them. For the first source of error, we note that by Theorem 3.2 the

D Toolbox

**Definition 1** (Orlicz norm \( \| \cdot \|_{\psi_\alpha} \)). For \( 1 \leq \alpha < \infty \), let \( \psi_\alpha(x) = \exp(x^\alpha) - 1 \). For \( 0 < \alpha < 1 \), let \( \psi_\alpha(x) = x^\alpha - 1 \) for large enough \( x \geq x_\alpha \), and \( \psi_\alpha \) is linear in \([0, x_\alpha]\). Therefore \( \psi_\alpha \) is convex. The Orlicz norm \( \psi_\alpha \) or a random variable \( X \) is defined as

\[
\|X\|_{\psi_\alpha} \triangleq \inf\{c \in (0, \infty) \mid E[|X|/c] \leq 1\} \tag{26}
\]

**Theorem D.1** (Bernstein’ inequality for subexponential random variables (Lecue, 2009). There exists an absolute constant \( c > 0 \) for which the following holds: Let \( X_1, \ldots, X_n \) be \( n \) independent mena zero \( \psi_1 \) random variables. Then for every \( t > 0 \),

\[
Pr\left[\sum_{i=1}^{n} X_i > t\right] \leq 2 \exp\left(-c \min\left(\frac{t^2}{n\bar{v}}, \frac{t}{M}\right)\right)
\]

where \( M = \max_i \|X_i\|_{\psi_\alpha} \) and \( \bar{v} = n^{-1} \sum_i \|X_i\|_{\psi_\alpha}^{-1} \).

**Lemma D.2.** Suppose random variable \( X \) has \( \psi_\alpha \) orlicz norm \( a \), then \( X - E[X] \) has \( \psi_\alpha \) orlicz norm at most \( 2a \).

**Proof.** First of all, since \( \psi_\alpha \) is convex and increasing on \([0, \infty)\), we have that \( E[\psi_\alpha(|X|/a)] \geq \psi_\alpha(E[|X|]/a) \). Then we have that

\[
E\left[\psi_\alpha\left(\frac{|X - E[X]|}{2a}\right)\right] \leq E[\psi_\alpha\left(\frac{|X|}{2a}\right) + E|X|/a)] \leq E\left[\frac{1}{2}\psi_\alpha(|X|/a) + \frac{1}{2}\psi_\alpha(|E[X]|/a)\right] \leq E[\psi_\alpha(|X|/a)] \leq 1
\]

where we used the convexity of \( \psi_\alpha \) and the fact that \( E[\psi_\alpha(|X|/a)] \geq \psi_\alpha(|E[X]|/a) \). \( \square \)

E Experimental Details and Additional Results

**Verification of the random-like nets hypothesis.** Figure 4 plots some statistics for the the second fully connected layer in AlexNet (after 60 thousand training iterations). Figure 4(a) shows the histogram of the edge weights, which is close to that of a Gaussian distribution. Figure 4(b) shows the bias in the RELU gates. The bias entries are essentially constant (in accord with Theorem 2.3) mostly within the interval
Figure 4: Some statistics of the parameters in the second fully connected layer of AlexNet.

Figure 4(c) shows that the distribution of the singular values of the weight matrix is close to the quartercircular law of random Gaussian matrices.

**Improved training using synthetic data.** The network we trained takes images $x$ as input and computes three layers $h_1, h_2,$ and $h_3$ by

$$h_1 = r(W_1^T x + b_1), \quad h_2 = r(W_2^T h_1 + b_2), \quad h_3 = W_3^T h_2 + b_3,$$

where $h_1$ and $h_2$ have 5000 nodes, and $h_3$ have 10 for CIFAR-10 and MNIST or 100 nodes for CIFAR-100 (corresponding to the number of classes in the dataset). We generated synthetic data $\tilde{x}$ from $h_2$ by

$$h_1 = r(W_2^T \tilde{h}_2), \quad x' = r(W_1^T h_1).$$

Then $x'$ was used for training along with $x$.

For training the networks, we used mini-batches of size 100 and the learning rate of $4^{\alpha} \times 0.001$, where $\alpha$ is an integer between $-2$ and $2$. When training with our regularization, we used a regularization weight $2^\beta$, where $\beta$ is an integer between $-3$ and $3$. To choose $\alpha$ and $\beta$, 10000 randomly chosen points that are kept out during the initial training as the validation set, and we picked the ones that reach the minimum validation error at the end. The network was then trained over the entire training set. All the networks were trained both with and without dropout. When training with dropout, the dropout ratio is 0.5.

Figure 3 in the main text shows the test errors with SHADOW combined with backpropagation and dropout. Here we additionally show the performance with SHADOW combined with backpropagation alone, and also show the test error on the synthetic data generated from the test set. The error drops much faster with SHADOW, and a significant advantage is retained even at the end. The test error on the synthetic data tracks that on the real data, which aligns with the theory.

**Variants of the SHADOW regularization** Instead of using $\tilde{h}_2$ to generate the synthetic data, one can also use other layers. Figure 6 compares the results when using $h_3$ and $\tilde{h}_2$. The error when using $h_3$ is similar or better than that using $\tilde{h}_2$. This indicates that the images generated from $h_3$ can play a similar role as those generated from $\tilde{h}_2$.

One can also use sampling when generating synthetic images from the hidden layers. More precisely, one can use

$$h_1 = r(W_2^T \tilde{h}_2) \odot n_{\text{drop}}, \quad x' = r(W_1^T h_1) \odot n_{\text{drop}}$$

where the sampling ratio is 0.5. This adds more noise to the synthetic data and can also act as a regularization, since the true distribution should be robust to such noise, as suggested by the success of dropout regularization. Other prior knowledge about the true distribution can also be incorporated, such as smoothness of the images:

$$h_1 = r(W_2^T \tilde{h}_2), \quad x' = r(W_1^T h_1), \quad x'' = \text{Smooth}(x')$$

(28)
Figure 5: Testing error of networks trained with and without our regularization for three datasets. Dropout was not used. “error on synthetic” is the testing error on the synthetic data generated from the test set.

Figure 6: Testing error of networks trained with our regularization on CIFAR-10 using the hidden layer $\tilde{h}_2$ or $\tilde{h}_3$ to generate synthetic data.

where Smooth operator sets each pixel of $x''$ to be the average of the pixels in its $3 \times 3$ neighborhood. The performances of these variants are shown in Figure 7. With sampling, there is larger variance but the error is similar to that without sampling, in accord with our theory. With smoothing, the error has larger variance at the beginning but the final error is lower than that without smoothing.
Figure 7: Testing error of networks trained with variants of our regularization on CIFAR-10. SHADOW: uses the hidden layer $h_2$ to generate synthetic data for training. SHADOW+sampling: also uses $\tilde{h}_2$ but randomly sets half of the entries to zeros when generating synthetic data. SHADOW+smoothing: also uses $\tilde{h}_2$ but smooths the synthetic data before using them for training.