On the Regularization Properties of Structured Dropout

Ambar Pal
Connor Lane
René Vidal
Benjamin D. Haeffele
Mathematical Institute for Data Science, Johns Hopkins University, Baltimore, MD USA
{ambar, clane, rvidal, bhaeffele}@jhu.edu

Abstract

Dropout and its extensions (e.g. DropBlock and DropConnect) are popular heuristics for training neural networks, which have been shown to improve generalization performance in practice. However, a theoretical understanding of their optimization and regularization properties remains elusive. Recent work shows that in the case of single hidden-layer linear networks, Dropout is a stochastic gradient descent method for minimizing a regularized loss, and that the regularizer induces solutions that are low-rank and balanced. In this work we show that for single hidden-layer linear networks, DropBlock induces spectral $k$-support norm regularization, and promotes solutions that are low-rank and have factors with equal norm. We also show that the global minimizer for DropBlock can be computed in closed form, and that DropConnect is equivalent to Dropout. We then show that some of these results can be extended to a general class of Dropout-strategies, and, with some assumptions, to deep non-linear networks when Dropout is applied to the last layer. We verify our theoretical claims and assumptions experimentally with commonly used network architectures.

1 Introduction

Dropout is a widely-used heuristic for training deep neural networks (NN), which involves setting to zero the output of a random subset of hidden neurons at each training iteration. The improved generalization performance of Dropout in practice has led to many variants of dropout \cite{DBLP:journals/corr/abs-1802-05301,DBLP:journals/corr/abs-1710-03980,DBLP:journals/corr/abs-1805-08344,sparselayer,contextualdrop,mutualdropout}. However, despite the popularity and improved empirical performance of Dropout-style techniques, several theoretical questions remain regarding their optimization and regularization properties, e.g.: What objective function is minimized by general Dropout-style techniques? Do these techniques converge to a global minimum? Does Dropout-style regularization induce an explicit regularizer? What is the inductive bias of Dropout-style regularization?

Related Work. Recent work has considered some of these questions in the case of single-layer linear neural networks trained with the squared loss. For example, \cite{DBLP:journals/corr/abs-1710-03980} show that Dropout is a stochastic gradient descent (SGD) method for minimizing the following objective:

$$\min_{U,V} \mathbb{E}_z \|Y - \frac{1}{\theta} U \text{diag}(z) V^T X\|_F^2. \quad (1)$$

Here $X \in \mathbb{R}^{b \times N}$ and $Y \in \mathbb{R}^{a \times N}$ denote the training set, $U \in \mathbb{R}^{a \times d}$ and $V \in \mathbb{R}^{b \times d}$ are the weight matrices, $N$ is the dataset size, $d$ is number of hidden neurons, and $z$ is a vector of Dropout variables whose $i$th entry $z_i \sim \text{Ber}(\theta)$ is i.i.d. Bernoulli with parameter $\theta$. Moreover, \cite{DBLP:journals/corr/abs-1710-03980} shows that Dropout induces explicit regularization in the form of a squared nuclear norm, which is known to induce low-rank solutions. Specifically, \cite{DBLP:journals/corr/abs-1710-03980} shows that the optimization problem \cite{DBLP:journals/corr/abs-1710-03980} reduces to

$$\min_{U,V} \|Y - UV^T X\|_F^2 + \frac{1 - \theta}{\theta} \sum_{i=1}^d \|u_i\|_2^2 \|X^T v_i\|_2^2, \quad (2)$$

which in turn is related to $\min_{Z} \|Y - Z\|_F^2 + \lambda \|Z\|_*$, where $Z = UV^T X$ and $\|Z\|_*$ is the nuclear norm. In addition, \cite{DBLP:journals/corr/abs-1710-03980} shows that the optimal weights $(U, V)$ can be found in polynomial time and are balanced, i.e., the product of the norms of incoming and outgoing weights, $\|u_i\|_2 \|v_i\|_2$, is the same for all neurons.

Paper Contributions. In this paper, we significantly generalize these results to more general Dropout schemes and more general neural network architectures. We will first study DropBlock, an alternative to Dropout for convolutional networks which was recently proposed in \cite{DBLP:journals/corr/abs-1710-03980} and displays improved performance compared to Dropout in practice. Instead of zeroing the output of each neuron independently, DropBlock introduces a structural dropping pattern by zeroing a block of neurons within a local neighborhood together.
to reflect the strong correlations in responses for neighboring pixels in a CNN. Specifically, for a block-size \( r \), we will look at the following optimization problem:

\[
\min_{U,V} \left\| Y - \frac{1}{\theta} U (\text{diag}(w) \otimes I_d) V^\top X \right\|^2_F, \tag{3}
\]

where \( \otimes \) denotes the Kronecker product and \( w \) are the stochastic Bernoulli variables with one entry \( w_i \sim \text{Ber}(\theta) \) getting applied simultaneously to a block of columns in \((U, V)\) of size \( r \). We will study the DropBlock optimization problem \( \text{(3)} \) in detail, understanding the explicit regularizer induced by DropBlock and the properties of the optimal solutions. Specifically, we will show that DropBlock induces low-rank regularization in the form of a \( k \)-support norm on the singular values of the solution, which is known to have some favorable properties compared to the \( \ell_1 \)-norm \( \| \cdot \|_1 \). This provides a step towards explaining the superior performance of DropBlock in practice, as compared to Dropout, which induces an \( \ell_2 \)-norm on the singular values. We will then prove that the solutions to \( \text{(3)} \) are such that the norms of the factors are balanced, i.e., products of corresponding blocks of \( r \) columns of \( U \) and \( V \) have equal Frobenius norms. Combining these results will allow us to get a closed form solution to \( \text{(3)} \).

We will then extend our analysis to more general dropping strategies where we will allow arbitrary sampling distributions for the Dropout variables, and obtain the explicit regularizer for this general case. We will also extend our analysis to Dropout applied to the last layer of a deep neural network, and show that this as well as many existing results in the literature can be readily extended to this scenario. We will end with a short result on an equivalence between Dropout and DropConnect, which is a different way of performing Dropout. Extensive experiments will be used to validate the theoretical results and assumptions whenever necessary.

## 2 DropBlock Analysis

In this section, we study the optimization and regularization properties of DropBlock, a variant of Dropout where blocks of neurons are dropped together. In this setting, we let \( d \) be the final hidden layer dimension and let \( r \) be the size of the block that is dropped. We make the simplifying assumption that the blocks form a partition of the neurons in the final hidden layer, which requires the hidden dimension \( d \) to be a multiple of \( r \). This is typically a minor assumption when \( d \gg r \). Then at each iteration, we sample a binary vector of \( k = d/r \) i.i.d. \( \text{Ber}(\theta) \) random variables \( w \in \{0,1\}^k \) and set the corresponding block of variables in \( z \in \{0,1\}^d \) to the value of \( w_i \), i.e., \( z_i = w_i \) for \((i-1)r < j \leq ir\). This sampling scheme, which we refer to as \( \text{DropBlockSample}(\theta, r) \), captures the key principle behind DropBlock by dropping a block of neighboring neurons at a time and is a very close approximation of DropBlock (which does not assume the blocks need to be non-overlapping) when \( d \gg r \). The resulting DropBlock algorithm that we will study is specified in Algorithm \( \text{[I]} \). Note that the Dropout Algorithm can be obtained as a particular case of the DropBlock Algorithm \( \text{[I]} \) with the block size set to \( r = 1 \).

### 2.1 Regularizer Induced by DropBlock

We first show that the DropBlock Algorithm \( \text{[I]} \) can be interpreted as applying SGD to the objective in \( \text{(3)} \). To that end, recall that the gradient of the expected value is equal to the expected value of the gradient. Thus, the gradient of \( \left\| Y - \frac{1}{\theta} U (\text{diag}(w) \otimes I_d) V^\top X \right\|^2_F \) with respect to \( U \) and \( V \) for a random sample of \( w \) provides a stochastic gradient for the objective in \( \text{(3)} \). Steps 7 and 8 of Algorithm \( \text{[I]} \) compute such gradients.

Having shown that DropBlock is an SGD method for minimizing \( \text{(3)} \), the next step is to understand the regularization properties of DropBlock. The following Lemma \( \text{[II]} \) shows that the Dropblock optimization problem is equivalent to a deterministic formulation with a regularization term, which we denote by \( \Omega_{\text{DropBlock}} \). That is, DropBlock induces explicit regularization.

**Lemma 2.1.** The stochastic DropBlock objective \( \text{(3)} \) is equivalent to a regularized deterministic objective:

\[
\mathbb{E}_w \left\| Y - \frac{1}{\theta} U (\text{diag}(w) \otimes I_d) V^\top X \right\|^2_F = \left\| Y - UV^\top X \right\|^2_F + \Omega_{\text{DropBlock}}(U, X^\top V), \tag{4}
\]

\( \text{[II]} \)

The complete proofs of all our results are given in the Supplementary Material.
where $\Omega_{\text{DropBlock}}$ is given by

$$
\Omega_{\text{DropBlock}}(U, X^\top V) = \frac{1 - \theta}{\theta} \sum_{i=1}^{k} \|U_i V_i^\top X\|_F^2
$$

(5)

with $U_i \in \mathbb{R}^{n \times d}$ and $V_i \in \mathbb{R}^{b \times r}$ denoting the $i$th blocks of $r$ consecutive columns in $U$ and $V$ respectively and $k = \frac{d}{r}$ denoting the number of blocks.

As expected, when we set $r = 1$, i.e. when we drop blocks of 1 neuron independently, $\Omega_{\text{DropBlock}}$ reduces to Dropout regularization in (2). Therefore, DropBlock regularization generalizes Dropout regularization in (2) by taking the sum over the squared Frobenius norms of rank-$r$ submatrices. But what is the effect of this modification? Specifically, can we characterize the regularization properties of $\Omega_{\text{DropBlock}}$, and how it controls the capacity of the network?

### 2.2 Capacity Control Property of DropBlock

In this subsection we first study whether DropBlock is capable of constraining the capacity of the network alone. That is, if the network were allowed to be made arbitrarily large, would DropBlock regularization be sufficient to constrain the capacity of the network?

It is clear from the definition of $\Omega_{\text{DropBlock}}$ that for any non-zero $(U, V)$ the function will be strictly positive. However, it is not clear if the function increases with $d$. Lemma 2.2 shows that when the Dropout probability, $1 - \theta$, is constant with respect to $d$, $\Omega_{\text{DropBlock}}$ can be made arbitrarily small (approaching 0 in the limit) by making the width $d$ of the final layer arbitrarily large.

**Lemma 2.2.** Given any matrix $A$, if the number of columns, $d$, in $(U, V)$ is allowed to vary, with $\theta$ held constant, then

$$
\inf_{d} \inf_{U \in \mathbb{R}^{n \times d}, V \in \mathbb{R}^{b \times d}} \Omega_{\text{DropBlock}}(U, X^\top V) = 0.
$$

(6)

The above Lemma implies that DropBlock alone cannot constrain the capacity of the network with a fixed Dropout probability, $1 - \theta$, since for any output of the network, $A$, one can find a factorization into $UV^\top X$ with an arbitrarily small value of the regularization function provided $d$ can be large. We note that this result is also true for regular Dropout (which is a special case of DropBlock) with a fixed Dropout probability.

In what follows, we show that if the Dropout probability, $1 - \theta$, increases as the number of columns, $d$, in $(U, V)$ increases, then DropBlock is capable of constraining network capacity. Specifically, let us denote the retain probability for dimension $d$ as:

$$
\bar{\theta}(d) = \frac{\tilde{\theta}(r)}{\tilde{\theta}(r) + (1 - \tilde{\theta})d}.
$$

(7)

where $\bar{\theta}(r)$ denotes the value of the DropBlock parameter when there is only one block, and $d = r$. With $\theta = \bar{\theta}(d)$, Lemma 2.2 gives us the following deterministic equivalent of the DropBlock objective:

$$
f(U, V, d) = \|Y - UV^\top X\|_F^2 + \frac{d}{r} \frac{1 - \tilde{\theta}}{\tilde{\theta}} \sum_{i=1}^{k} \|U_i V_i^\top X\|_F^2
$$

(8)

In order to understand the effect of $d$ on the regularizer, given a matrix $A$, we wish to find a factorization $A = UV^\top X$ of size $d$ such that $(U, X^\top V)$ minimizes the value of the regularizer. Formally, we accomplish this by defining a function $\Lambda(A)$ as follows,

$$
\Lambda(A) = \frac{1 - \bar{\theta}}{\bar{\theta}} \inf_{d \in \mathbb{R}^{n \times d}, V \in \mathbb{R}^{b \times d}} \inf_{A = UV^\top X} \frac{d}{r} \sum_{i=1}^{k} \|U_i V_i^\top X\|_F^2.
$$

(9)

Note that due to the definition of $\Lambda(A)$ in (9), one can define a function $\tilde{F}(A)$ as

$$
\tilde{F}(A) = \|Y - A\|_F^2 + \Lambda(A)
$$

(10)

and by construction $\tilde{F}(A)$ will have the property that it globally lower bounds $f(U, V, d)$ — i.e., $\tilde{F}(A) \leq f(U, V, d)$ for all $(U, V, A)$ such that $UV^\top X = A$, with equality for $(U, V, A)$ that achieve the infimum in (9). As a result, $\tilde{F}(A)$ provides a useful analysis tool to study the properties of solutions to the problem of interest $f(U, V, d)$ as it provides a lower bound to our problem of interest in the output space (i.e., $UV^\top X$).

While it is simple to see that $\tilde{F}(A)$ is a lower bound of our problem of interest, it is not clear whether $\tilde{F}(A)$ is a useful lower bound or whether the minimizers to $\tilde{F}$ can characterize minimizers of $f$. In the following analysis, we will prove that the answer to both questions is positive, that $\tilde{F}(A)$ is a tight lower bound of $f$, generalizing existing results in the literature [2, 7], and show that solutions to $\tilde{F}(A)$ can be computed in closed form.

### 2.3 DropBlock Induces k-support Norm Regularization

Based on the above discussion, we now analyze characteristics of the global minimizers of $\tilde{F}(A)$. Unfortunately, $\Lambda(A)$ is not necessarily convex w.r.t. $A$, which complicates the analysis of the global minimizers of $\tilde{F}(A)$, so instead we consider the convex envelope of $\Lambda(A)$. We will show later that this is not a restriction, and the lower convex envelope will be a tight bound to our problem of interest (6). Recall that the lower convex envelope [10] of a function $h(x)$ is the largest convex function $g(x)$ such that $\forall x, g(x) \leq h(x)$, and is given by the Fenchel double dual (i.e., the Fenchel
dual of the Fenchel dual). For $\Lambda(A)$, the following result provides the lower convex envelope. Note that in this sub-section, we will assume that $X$ has full column rank. This is typically a minor assumption since if $X$ is not full rank adding a very small amount of noise will make $X$ full rank.

Theorem 2.3. When $X$ has full column rank in (9), the lower convex envelope of the DropBlock regularizer $\Lambda(A)$ in (9), is given by

$$\Lambda^{\ast\ast}(A) = \frac{1 - \tilde{\theta}}{\theta} \left( \sum_{i=1}^{\rho^* - 1} a_i^2 + \frac{(\sum_{i=\rho^*}^{d} a_i)^2}{r - \rho^* + 1} \right),$$

where $\rho^*$ is the integer in $\{1, 2, \ldots, r\}$ that maximizes (11), and $a_1 \geq a_2 \geq \ldots \geq a_d$ are the singular values of $A$.

Note that the quantity $\rho^*$ mentioned in (11) is purely a property of the matrix $A$, the hidden dimension $d$ and the block size $r$, and is determined completely in time $d \log d$, given a SVD of $A$.

We now note some connections to recent literature. The form of the solution (11) is particularly interesting because it is a matrix norm that has recently been discovered in the sparse prediction literature by (1), where it is called the $k$-Support Norm and provides the tightest convex relaxation of sparsity combined with an $\ell_2$ penalty. When applied to the singular values of a matrix (as is the case here), it is called the Spectral $k$-Support Norm, as studied recently in (6).

Why is the $k$-Support norm good? We are often interested in obtaining sparse or low-rank solutions to problems, as they have been shown to generalize well and are useful in discarding irrelevant features. Specifically, if we are learning a vector $w$, we can get sparse solutions by constraining the $\ell_0$ norm of $w$, that is the number of non-zero entries in $w$. However, $\| \cdot \|_0$ is not a convex function (and hence not a norm), and it is hard to project onto the set $S_0 = \{ w : \|w\|_0 \leq k \}$. Hence, typically we relax the regularizer to be the $\ell_1$ norm, which has nice properties. However, constraining the $\ell_1$ norm does not yield a convex relaxation of $S_0$, in the sense that $\|w\|_0$ might be small while $\|w\|_1$ is large. However, additionally constraining the $\ell_2$ norm fixes this problem, as the convex hull of the set $S_{0,2} = \{ w : \|w\|_0 \leq k, \|w\|_2 \leq 1 \}$ is a subset of $S_{1,2} = \{ w : \|w\|_1 \leq \sqrt{k}, \|w\|_2 \leq 1 \}$, i.e. $\text{conv}(S_{0,2}) \subseteq S_{1,2}$. This motivates the use of the elastic-net regularizer in literature. Recently, researchers have looked at whether $S_{1,2}$ is the tightest convex relaxation of $S_{0,1}$, and found that it is not. Specifically, (1) show that this tightest convex envelope can be obtained in closed form as a norm, which they call the $k$-Support norm of $w$.

The $k$-Support Norm is essentially a trade-off between an $\ell_2$ penalty on the largest components, and an $\ell_1$ penalty on the remaining smaller components. In our case, we can look at (11) to see that when $\rho^* = 1$, $\Lambda^{\ast\ast}(A)$ reduces to $\frac{2}{r} (\sum_{i=1}^{d} a_i^2) = \frac{2}{r} \|A\|_F^2$, which is (a scaling of) the nuclear norm (squared) of $A$. On the other hand, when the block size $r$ is larger, $\rho^*$ will take higher values, implying the regularizer $\Lambda^{\ast\ast}(A)$ will move closer to $c_0 \sum_{i=1}^{d} a_i^2 = c_0 \|A\|_F^2$, which is (a scaling of) the squared Frobenius norm of $A$. From this discussion, the DropBlock regularizer can thus be seen to be acting as an interpolation between (squared) nuclear norm regularization when the block size is small to (squared) Frobenius norm regularization when the block size becomes very large. Further, (1, 6) observe that regularization using the $k$-Support norm achieves better performance than other forms of regularization on some real-world datasets and this might be a step towards theoretically explaining the superior performance of DropBlock compared to Dropout, as was observed experimentally in (5).

Continuing our analysis, with the convex envelope of $\Lambda(A)$, we can construct a convex lower bound of the DropBlock objective $f(U, V, d)$, as follows:

$$F(A) = \|Y - A\|_F^2 + \Lambda^{\ast\ast}(A)$$

with the relationship $F(A) \leq \tilde{F}(A) \leq f(U, V)$ for all $(U, V, A)$ such that $UV^\top = A$. However, it is currently unclear whether $F$ is a useful lower bound for $f$. We will now show that the function $F(\cdot)$ is a tight lower bound for the non-convex function $f(\cdot, \cdot, \cdot)$.

2.4 DropBlock Induces Balanced Weights

In order to characterize the minimizers of $f(U, V, d)$, we first need to define the notion of balanced factors:

Definition 2.4. The matrix pair $(U, V)$ is balanced if the norms of the products of the corresponding blocks of $U$ and $V$ are equal. In other words, $\|U_iV_i^\top X\|_F = \|U_2V_2^\top X\|_F = \ldots = \|U_rV_r^\top X\|_F$, where $U_i$ and $V_i$ denote the $i$th blocks of $r$ consecutive columns in $U$ and $V$ respectively.

The following result shows that all minimizers of $f(U, V, d)$ are balanced. The intuition behind the proof is that whenever $(U, V)$ are not balanced, we can add additional blocks of neurons in a particular way that makes the block-product-norms $\|U_iV_i^\top X\|_F$ more balanced and reduces the objective.

Theorem 2.5. If $(U^*, V^*, d^*)$ is a minimizer of (8), then $(U^*, V^*)$ is balanced.

Theorem 2.5 provides a characterisation of the minimizers of the DropBlock objective (8), saying that all
the summands in the regulariser are equal at optimality. With this result, we will be able to link the minimizers of $f$ and $F$, and hence find the regularization induced by DropBlock.

**Theorem 2.6.** If $(U^*, V^*, d^*)$ is a global minimizer of the factorized problem $f$, then $A^* = U^*V^*\top X$ is a global minimizer of the lower bound $F$. Furthermore, the lower bound is tight, i.e. we have $f(U^*, V^*, d^*) = F(A^*)$.

Theorem 2.6 provides a link between the hard non-convex problem of interest, $f$, and the convex lower bound, $F$, and gives us a guarantee that we can verify solutions to $f$ by showing they are solutions to $F$. Hence, we now focus our attention on characterizing solutions of $F(A)$.

We now complete the analysis by deriving a closed form solution for the global minimum of $F(A)$.

**Theorem 2.7.** When $X$ has full column rank in (9), the global minimizer of $F(A)$ is given by $A_{p,\lambda} = U_Y \text{diag}(a_{p,\lambda}) V_Y\top$, where $Y = U_Y \text{diag}(m)V_Y\top$ is an SVD of $Y$, and $a_{p,\lambda}$ is given by

$$a_{p,\lambda} = \begin{cases} \left(\frac{m_1}{\beta + 1}, \frac{m_1}{\beta + 1}, \ldots, \frac{m_1}{\beta + 1}, 0, \ldots, 0\right) & \text{if } \lambda \leq \rho - 1 \\ \frac{m_1}{\beta + 1}, \frac{m_2}{\beta + 1}, \ldots, \frac{m_\rho - 1}{\beta + 1}, m_{\rho} - \frac{\beta}{\epsilon} S, m_{\rho+1} - \frac{\beta}{\epsilon} S, \ldots, \frac{m_{\rho + 1}}{\beta + 1}, & \text{if } \lambda \geq \rho. \end{cases}$$

The constants are $\beta = 1 - \frac{\rho - 1}{\rho}$, $S = \sum_{i=1}^{\rho} m_i$, $c = r + \beta \lambda + (\beta + 1)(1 - \rho)$, $\rho \in \{1, 2, \ldots, r - 1\}$ and $\lambda \in \{1, 2, \ldots, d\}$ are chosen such that they minimize $F(A_{p,\lambda})$.

Note that the constants mentioned in Theorem 2.7 depend purely on the matrix $Y$, and can be computed in time $O(d^2)$ given the singular values $m_i$. Finally, the following Corollary completes the picture by showing that the solution computed in Theorem 2.7 recovers the value of the global minimizer of the Dropout objective $f(\cdot, \cdot, \cdot)$:

**Corollary 2.8.** If $A^*$ is a global minimizer of the lower convex envelope $F$, and $(U^*, V^*, d^*)$ is a global minimizer of the non-convex objective $f$, then we have $F(A^*) = \hat{F}(A^*) = f(U^*, V^*, d^*)$ with $A^* = U(V^*)\top X$.

Having understood the properties of one particular generalization of dropout for a single hidden-layer linear network, we will now show how our methods can be generalised to other Dropout variants applied to the last layer of an overparameterized neural network.

**Lemma 3.1.** The Generalized Dropout objective (13) is approximated by a single stochastic sample of the Dropout variables, $z$, in this setting, we can obtain the deterministic form of (13), which is a generalisation of Lemma 2.7.

**Figure 1:** Top: Stochastic DropBlock training with SGD is equivalent to the deterministic Objective [3]. Bottom: DropBlock converges to the global minimum computed in Theorem 2.7.

### 3 Generalized Dropout Framework

In general, Dropout-style algorithms applied to the last layer of a Deep Neural Network proceed in a stochastic manner, where at each iteration of training one randomly selects a subset of neurons to set to zero, then performs one iteration of (stochastic) gradient descent with the outputs of the selected neurons held at zero. This leads us to consider a NN training problem with a squared-loss of the form

$$\min_{U, F} \|Y - U\text{diag}(\mu)^{-1}\text{diag}(z)g(U)(X)\|_F^2$$

(13)

where we follow the notation in the introduction, along with $g_U$ denotes the output of the second to last layer of a NN with weight parameters $\Gamma$ (i.e., the $j^{th}$ column of $g_\Gamma$ is the output of second to last layer of the network given input $x_j$), $U \in \mathbb{R}^{d \times d}$, with $d$ being the size of the output of the second to last layer, is the weight matrix for the final linear layer, and $\mu \in \mathbb{R}^d$ is a vector of the means of the Dropout variables, $\mu_i = \mathbb{E}[z_i]$ (note that in expectation, the output of the $i^{th}$ hidden unit of $g_U$ is scaled by $\mathbb{E}[z_i]$), so to counter this effect, we rescale the output by $\mathbb{E}[z_i]^{-1}$.

We will assume that the Dropout variables $z$ are stochastically sampled at each iteration of the algorithm from an arbitrary probability distribution $S$, with covariance matrix $\text{Cov}(z, z)$ noted as $C$ and non-zero mean $\mu$, so one iteration of a typical Dropout algorithm can be interpreted as performing one iteration of stochastic gradient descent on (13), where the gradient of (13) is approximated by a single stochastic sample of the Dropout variables, $z$. In this setting, we can obtain the deterministic form of (13), which is a generalisation of Lemma 2.7.
is equivalent to a regularized deterministic objective:

\[ \mathbb{E}_x \| \mathbf{y} - \mathbf{u} \text{diag}(\mu)^{-1} \text{diag}(\mathbf{z}) g_\Gamma(\mathbf{x}) \|_F^2 = \| \mathbf{y} - \mathbf{u} g_\Gamma(\mathbf{x}) \|_F^2 + \Omega_{\mathbf{C}, \mu}(\mathbf{u}, g_\Gamma(\mathbf{x})^\top) \]  

(14)

The generalized Dropout regularizer, \( \Omega_{\mathbf{C}, \mu}(\mathbf{u}, \mathbf{v}) \), is found to be as follows:

\[ \Omega_{\mathbf{C}, \mu}(\mathbf{u}, \mathbf{v}) = \sum_{i,j=1}^d c_{i,j} \frac{(\mathbf{u}_i^\top \mathbf{u}_j)(\mathbf{v}_i^\top \mathbf{v}_j)}{\mu_i \mu_j} = (\mathbf{C}, \mathbf{u}^\top \mathbf{u} \odot \mathbf{v}^\top \mathbf{v}) \]

(15)

where \((\mathbf{u}_i, \mathbf{v}_i)\) denotes the \(i\)th columns of matrices \(\mathbf{U}\) and \(\mathbf{V}\) (here we have defined \(\Omega_{\mathbf{C}, \mu}\) for general matrices \((\mathbf{U}, \mathbf{V})\), but typically we will have \(\mathbf{V} = g_\Gamma(\mathbf{x})^\top\)), \(c_{i,j}\) denotes the entry of \(\mathbf{C}\) in row \(i\), column \(j\), and \(d\) is the dimension of the final hidden layer (i.e., the number of rows of \(g_\Gamma\)). Additionally, in [15], for notational simplicity, we define the Characteristic Matrix \(\mathbf{C}\) from entries of the mean and covariance of \(\mathbf{z}\) as

\[ \mathbf{c}_{i,j} = \frac{c_{i,j}}{\mu_i \mu_j} \]

(16)

Notice that \(\mathbf{C}\) completely determines the regularization properties of any Dropout scheme. For example, in classical Dropout, the entries of \(\mathbf{z}\) are i.i.d. Bernoulli variables with mean \(\theta\), which gives that \(\mathbf{C}\) is diagonal with diagonal entries \(c_{i,i} = \theta(1 - \theta)\) and \(\mu_i = \theta\), hence \(\mathbf{C}\) is diagonal with diagonal entries \(\mathbf{c}_{i,i} = \frac{\mathbf{1}_r^\top}{\theta}\). For DropBlock with block-size \(r\), we have \(\mathbf{C} = \frac{1 - \theta}{\theta} \text{BklDiag}(\mathbf{1}, \mathbf{1}^\top, \ldots, \mathbf{1}, \mathbf{1}^\top)\), where \(\text{BklDiag}(\cdot)\) denotes forming a block diagonal matrix with the function arguments along the diagonal and \(\mathbf{1}_r\) denotes an \(r\)-dimensional vector of all ones. In the case of Dropout, we recover an immediate simple corollary for the regularization induced by Dropout in the final layer of non-linear networks:

**Corollary 3.2.** For regular Dropout applied to objective [13] the following equivalence holds:

\[ \mathbb{E}_x \| \mathbf{y} - \mathbf{u} \text{diag}(\mu)^{-1} \text{diag}(\mathbf{z}) g_\Gamma(\mathbf{x}) \|_F^2 = \| \mathbf{y} - \mathbf{u} g_\Gamma(\mathbf{x}) \|_F^2 + \sum_{i=1}^d \| \mathbf{u}_i \|_2^2 g_\Gamma(\mathbf{x})^2 \]

(17)

where \(g_\Gamma(\mathbf{x}) \in \mathbb{R}^N\) denotes the output of the \(i\)th neuron of \(g_\Gamma\) (i.e., the \(i\)th row of \(g_\Gamma(\mathbf{x})\)).

Given this result, a simple interpretation of Dropout in the final layer of the network is that it adds a form of weight-decay both to the weight parameters in the final layer, \(\mathbf{U}\), and the output of \(g_\Gamma\). Additionally, from this result it is relatively simple to show the following characterization on the regularization that is induced by Dropout applied to the final layer of a network. Note that the following result (Lemma 3.3) can be shown using similar arguments to those used in previous work [2] along with a sufficient capacity assumption.

**Proposition 3.3.** If the network architecture, \(g_\Gamma\), has sufficient capacity to span \(\mathbb{R}^{d \times N}\) (i.e., given any matrix \(\mathbf{Q} \in \mathbb{R}^{d \times N}\), \(\exists \mathbf{F}\) such that \(g_\Gamma(\mathbf{x}) = \mathbf{Q}\)) and \(d \geq \min\{a, N\}\), then the global optimum of [13] with
with parameter $\theta$ drawn independently from the Bernoulli distribution. 

$Z$ samples a random matrix of the connection weights to zero independently with elements.

Dropout, but instead of setting the outputs of hidden

4 DropConnect Analysis

DropConnect, proposed in [11], is very similar to Dropout, but instead of setting the outputs of hidden neurons to zero, DropConnect instead sets elements of the connection weights to zero independently with probability $1 - \theta$. Hence, the DropConnect algorithm samples a random matrix $Z \in \mathbb{R}^{B \times d}$, with each $z_{i,j}$ drawn independently from the Bernoulli distribution with parameter $\theta$. For Dropconnect applied to the second-last layer weights $V$ of a deep network parameterized as $UV^T g_\theta(X)$, the optimization problem then becomes the following:

$$\min_{U, V, \theta} \mathbb{E}_Z \left\| Y - \frac{1}{\theta} U(Z \odot V)^T g_\theta(X) \right\|_F^2 \quad (19)$$

We show that DropConnect induces the same regularization as Dropout. Specifically, the regulariser induced in (19) is same as vanilla Dropout on the last layer [45].

**Theorem 4.1.** For Dropconnect applied to the second-last layer weights $V$ of a deep network parameterized as $UV^T g_\theta(X)$, the following equivalence holds:

$$\mathbb{E}_Z \left\| Y - \frac{1}{\theta} U(Z \odot V)^T g_\theta(X) \right\|_F^2 = \left\| Y - UV^T g_\theta(X) \right\|_F^2 + \frac{1 - \theta}{\theta} \sum_{i=1}^d \|u_i\|_2^2 \|g_\theta(X)^Tv_i\|_2^2$$

where $g_\theta(X) \in \mathbb{R}^N$ denotes the output of the $i^{th}$ neuron of $g_\theta$ (i.e., the $i^{th}$ row of $g_\theta(X)$).

Taking $g_\theta(X) = X$ in Theorem 4.1 then gives us the following result for a single layer linear network. **Corollary 4.2.** For single layer linear networks, the stochastic DropConnect objective [19] is equivalent to the vanilla Dropout deterministic objective:

$$\mathbb{E}_Z \left\| Y - \frac{1}{\theta} U(Z \odot V)^T X \right\|_2^2 = \left\| Y - UV^T X \right\|_2^2 + \frac{1 - \theta}{\theta} \sum_{i=1}^d \|u_i\|_2^2 \|X^Tv_i\|_2^2 \quad (20)$$

Note that by an identical line of arguments as made in [2, 7] the above result also implies that DropConnect induces low-rank solutions in linear networks.

5 Experiments

In this section, we conduct experiments in training single hidden layer linear networks as well as multilayer nonlinear networks to validate the theory developed so far.

5.1 Shallow Network Experiments

We first create a simple synthetic dataset $D_{syn}$ by taking 1000 i.i.d samples of $x$ from a 100-dimensional standard normal distribution. Then, $y \in \mathbb{R}^{80}$ is generated as $y = Mx$, where $M = U_{true} V_{true}^T$. To ensure a reliable comparison, all the experiments start with the same choice of $U_0 = U_{init} \in \mathbb{R}^{80 \times 50}$ and $V_0 = V_{init} \in \mathbb{R}^{100 \times 50}$. The entries of all the matrices $U_{true}, V_{true}, U_{init}, V_{init}$ are sampled elementwise from $\mathcal{N}(0, 1)$. 
Verifying Deterministic Formulations  We first verify the correctness of the deterministic formulations for various dropout schemes analyzed in this paper, i.e., (5) and (20), in the top panels of Figure 1 and Figure 3. In Figure 1, the curve labelled \( \text{DropBlock Stochastic} \) is the training objective plot, i.e., it plots the value of the DropBlock stochastic objective (3) as the training progresses via Algorithm 1. For generating the curve labelled \( \text{DropBlock Deterministic} \), we take the current iterate, i.e., \( U_i, V_i \), and plot the Deterministic DropBlock objective obtained in Lemma 2.1 at every iteration. The deterministic equivalent of the DropConnect objective is similarly verified in Figure 3. Both the figures show plots for \( \theta = 0.5 \), and the plots for more values of \( \theta \) are deferred to the Appendix. It can be seen that the expected value of DropConnect and DropBlock over iterations matches the values derived in our results. Additionally, the bottom panel of Figure 3 shows that Dropout and DropConnect have the same expected value of the objective at each iteration.

Verifying Convergence to the Global Minimum  

We next verify convergence of DropBlock to the theoretical global minimum computed in Theorem 2.7. The bottom panel of Figure 1 plots the deterministic DropBlock objective as the training progresses, showing convergence to the computed theoretical global minimum. It can be seen that the training converges to the DropBlock Global minimum computed in Theorem 2.7, as proven.

5.2 Deep Network Experiments

In order to test our predictions on common network architectures, we modify the standard ResNet-50 architecture by removing the last layer and inserting a fully-connected (FC) layer to reduce the hidden layer dimensionality to 80 (to make the experiments consistent with the Synthetic Experiments). Hence, the network architecture now is, \( x \rightarrow \text{Resnet-50 Layers} \rightarrow \text{FC} \rightarrow \text{Dropout} \rightarrow \text{FC} \rightarrow y \). We then train the entire network on small datasets \( D_{\text{MNIST}}, D_{\text{CIFAR10}} \) with DropBlock applied to the last layer with a block size of 5. Figure 2 shows that the solution found by gradient descent is very close to the lower bound predicted by Theorem 2.7. The objective value is plotted on the left, and the singular values of the final predictions matrix \( U_{GR}(X) \) are plotted on the right in decreasing order. Note that qualitatively the singular values of the final predictions matrix closely match the theoretical prediction, with the exception of the least significant singular value, which we attribute to the highly non-convex network training problem not converging completely to the true global minimum.

5.3 Effect of DropBlock approximation

The original DropBlock method [5] allows dropping blocks at arbitrary locations, in this paper we made an approximation by constraining the block locations to a grid, as explained in the introduction. This approximation is a minor constraint, and the block retaining probability \( \theta \) can be scaled appropriately to recover the original behavior. DropBlockOriginal with the same \( \theta \) as DropBlock would lead to a higher effective dropping rate. This can be corrected by solving for \( \theta'_{\text{DropBlock}} \) such that the probability of dropping any neuron in DropBlock with retain probability \( \theta'_{\text{DropBlock}} \) is same as the probability of dropping a neuron in DropBlockOriginal with retain probability \( \theta_{\text{DropBlockOriginal}} \). Specifically, referring to notation in Section 2 under the Original DropBlock scheme, the probability of \( z_i = 0 \) is same as the probability of (none of the \( w_j = 1 \)) over all \( j \) where \( |i - j| \leq k \). This probability is \( (1 - \theta_{\text{DropBlockOriginal}})^{2k-1} \). Under our approximation, the probability of \( z_i = 0 \) is \( 1 - \theta_{\text{DropBlock}} \). Equating these quantities, we can solve for \( \theta'_{\text{DropBlockOriginal}} \) as \( \theta'_{\text{DropBlockOriginal}} = 1 - (1 - \theta_{\text{DropBlock}})^{2k-1} \). As can be seen in Fig 4, DropBlockOriginal with the appropriate correction is approximately the same as DropBlock, as the green, blue, orange curves are very close in log-scale at iteration \( 10^5 \).

6 Conclusion

In this work, we have analysed the regularization properties of structured Dropout training of neural networks, and characterized the global optimum obtained for some classes of networks and structured Dropout strategies. We showed that DropBlock induces spectral \( k \)-Support norm regularization on the weight matrices, providing a potential way of theoretically explaining the empirically observed superior performance of DropBlock as compared to Dropout. We also proved that Dropout training is equivalent to DropConnect training for some network classes. Finally, we showed that our techniques can be extended
to other generic Dropout strategies, and to Deep Networks with Dropout-style regularization applied to the last layer of the network, significantly generalizing prior results.

7 Acknowledgments

This work was supported by NSF 1618485 and IARPA DIVA D17PC00345

References

[1] A. Argyriou, R. Foygel, and N. Srebro. Sparse prediction with the $k$-support norm. In Advances in Neural Information Processing Systems, pages 1457–1465, 2012.

[2] J. Cavazza, B. Haeffele, C. Lane, P. Morerio, V. Murino, and R. Vidal. Dropout as a low-rank regularizer for matrix factorization. In International Conference on Artificial Intelligence and Statistics, volume 84, pages 435–444, 2018.

[3] Y. Gal, J. Hron, and A. Kendall. Concrete dropout. In Advances in Neural Information Processing Systems, 2017.

[4] X. Gastaldi. Shake-shake regularization. In arXiv preprint arXiv:1705.07485, 2017.

[5] G. Ghiasi, T.-Y. Lin, and Q. V. Le. Dropblock: A regularization method for convolutional networks. In Advances in Neural Information Processing Systems, pages 10750–10760, 2018.

[6] A. M. McDonald, M. Pontil, and D. Stamos. Spectral k-support norm regularization. In Advances in Neural Information Processing Systems, pages 3644–3652, 2014.

[7] P. Mianjy, R. Arora, and R. Vidal. On the implicit bias of dropout. In International Conference on Machine Learning, 2018.

[8] P. Morerio, J. Cavazza, R. Volpi, R. Vidal, and V. Murino. Curriculum dropout. In IEEE International Conference on Computer Vision, Oct 2017.

[9] S. J. Rennie, V. Goel, and S. Thomas. Annealed dropout training of deep networks. In 2014 IEEE Spoken Language Technology Workshop (SLT), 2014.

[10] R. T. Rockafellar. Convex analysis. Princeton university press, 2015.

[11] L. Wan, M. Zeiler, S. Zhang, Y. Le Cun, and R. Fergus. Regularization of neural networks using dropconnect. In International Conference on Machine Learning, pages 1058–1066, 2013.

[12] Y. Yamada, M. Iwamura, T. Akiba, and K. Kise. Shakedrop regularization for deep residual learning. In arXiv preprint arXiv:1802.02375, 2018.

[13] K. Zolna, D. Arpit, D. Suhubdy, and Y. Bengio. Fraternal dropout. In arXiv preprint arXiv:1711.00066, 2017.
A Notation and Assumptions

Matrices are denoted by boldface uppercase letters $Z$, vectors by boldface lowercase letters $z$ and scalars by lowercase letters $z$. Unless otherwise stated, scalars and their corresponding matrices and vectors are represented by the same character. For example, scalars $z_{i,j}$ make up the vector $z_j$ and the vectors $z_i$ make up the columns of the matrix $Z$. $I_d$ represents the identity matrix having dimensions $d \times d$. The subscript form $z_k$ on a matrix $Z$ denotes the $k^{th}$ column of $Z$. Given a matrix $Z$, $Z_i$ will denote the $i^{th}$ submatrix of $Z$ formed by sampling a set of columns from $Z$, where the sampling will be clear from context. A colon in the subscript, $z_{i:j}$ denotes a vector formed by the elements $z_i, z_{i+1}, \ldots, z_{j-1}, z_j$. For NNs, we weight matrices are noted with $U, V$, with the output of the neural network being an input $x$ being $U V^T x$, and $Y$ will denote the target outputs $Y$ of the network given training data, $X$, as the input. $d$ will be the number of units in the hidden layer hidden layer, $b$ will denote the input-data dimension, and $a$ will be the dimension of the output. Hence, $U \in \mathbb{R}^{a \times d}$, $V \in \mathbb{R}^{b \times d}$. The Hadamard product and the Kronecker product are denoted by $\odot$ and $\otimes$, respectively. Given a matrix $M$, the Frobenius norm of $M$ is denoted by $\|M\|_F$, and the inner product between two matrices $M, N$ is denoted by $(M, N)$ and defined as $Tr(MN^T)$. Given a function $f : \mathbb{R} \to \mathbb{R}$ defined on scalars, $f(Q)$ will denote applying the function entry-wise to each entry of the matrix $Q$.

B Proofs for Section 2

Lemma 2.1 Restated) The stochastic DropBlock objective (3) is equivalent to a regularized deterministic objective:

$$
\mathbb{E}_w \left\| Y - \frac{1}{\theta} U (\text{diag}(w) \odot I_d^Z) V^T X \right\|^2_F = \| Y - U V^T X \|^2_F + \Omega_{\text{DropBlock}}(U, X^T V)
$$

where $\Omega_{\text{DropBlock}}$ is given by

$$
\Omega_{\text{DropBlock}}(U, V) = \frac{1 - \theta}{\theta} \sum_{i=1}^k \| U_i V_i^T X \|^2_F
$$

with $U_i \in \mathbb{R}^{a \times r}$ and $V_i \in \mathbb{R}^{b \times r}$ denoting the $i^{th}$ blocks of $r$ consecutive columns in $U$ and $V$ respectively and $k = \frac{dr}{d}$ denoting the number of blocks.

Proof. This result is an instance of the more general result in Theorem 3.1 and hence we will just specify the Covariance matrix $C$, mean vector $\mu$, and mapping $g_r(X)$ to be used in order to apply Theorem 3.1

Recall from the main text that the entries of $w$ are sampled i.i.d. from $\text{Ber}(\theta)$. Now, the mean $\mu$ is given by $\mathbb{E}_w [\text{diag}(w) \odot I_d^Z] = \theta I_r \odot I_d^Z = \theta I_d$. To compute the covariance matrix, observe that the random variables $z_i, z_j$ are uncorrelated when $i, j$ lie in different blocks. Hence, for such pairs, $c_{ij} = 0$. Now, when $i, j$ are within the same block ($i$ might equal $j$), either both are dropped with probability $1 - \theta$, or none of them is. Hence, $\text{Cov}(z_i, z_j) = \mathbb{E}[z_i z_j] - \mathbb{E}[z_i] \mathbb{E}[z_j] = \theta - \theta^2 = \theta(1 - \theta)$. Note that this implies that $C$ is block diagonal with blocks $\frac{1 - \theta}{\theta} I_1, I_1^T$. Finally, we take $g_r(X) = V^T X$. Applying Theorem 3.1 now, we get the required result.

Lemma 2.2 Restated) Given any matrix $A$, if the number of columns, $d$, in $(U, V)$ is allowed to vary, with $\theta$ held constant, then

$$
\inf_{d} \inf_{U \in \mathbb{R}^{m \times d}, V \in \mathbb{R}^{n \times d}} \Omega_{\text{DropBlock}}(U, X^T V) = 0
$$

Proof. Let $A = U V^T X$ be a factorization of $A$ into $d$ sized factors $U \in \mathbb{R}^{a \times d}, V \in \mathbb{R}^{b \times d}$. Construct $\hat{U} \in \mathbb{R}^{a \times 2d}, \hat{V} \in \mathbb{R}^{b \times 2d}$ by concatenating $U$ and $V$ along the $2^{nd}$ axis, as $U = \frac{1}{\sqrt{2}} [U \ U]$ and $V = \frac{1}{\sqrt{2}} [V \ V]$. Observe that $\hat{U} \hat{V}^T X = A$, but

$$
\Omega_{\text{DropBlock}}(U, X^T V) = \sum_{i=1}^d \| U_i V_i^T X \|^2_F = 2 \sum_{i=1}^d \left\| \frac{U_i}{\sqrt{2}} \frac{V_i}{\sqrt{2}} X \right\|^2_F = \frac{1}{2} \Omega_{\text{DropBlock}}(U, X^T V)
$$
Hence, by increasing the size of the factorization, we have been able to reduce the regularizer value by half, while maintaining the value of the product. This process can be continued indefinitely to make the value of $\Omega_{\text{DropBlock}}$ go arbitrarily close to zero.

**Theorem 2.5 (Restated)** With $f$ defined as $[8]:$

$$f(U, V, d) = \|Y - UV^T X\|_F^2 + \frac{d}{r} \Omega_{\text{DropBlock}}(U, X^TV)$$

If $(U^*, V^*, d^*)$ is a minimizer of $f$, then $(U^*, V^*)$ is balanced.

**Proof.** Fix a factorization $(U, V, d)$ and suppose $(U, V)$ is not balanced. We will then construct a new factorization $(\bar{U}, \bar{V}, d + d)$ such that $\bar{U}\bar{V}^TX = UV^TX$, while $(d + d)\Omega_{\text{DropBlock}}(\bar{U}, X^T\bar{V}) < d\Omega_{\text{DropBlock}}(U, X^TV)$, showing that $(U, V, d)$ is not a global minimizer.

First, define a vector $\alpha \in \mathbb{R}^d$ containing the scale of each factor, $\alpha_i = \|U_iV_i^TX\|_F$. Secondly, let $(\bar{U}_i, \bar{V}_i)$ denote the $i$th normalised factor, $\bar{U}_i = (\frac{1}{\alpha_i})^{\frac{1}{2}}U_i$, $\bar{V}_i = (\frac{1}{\alpha_i})^{\frac{1}{2}}V_i$.

Note that since $(U, V)$ is not balanced, we know that $d\Omega_{\text{DropBlock}}(U, X^TV) = d\|\alpha\|_2^2 > \|\alpha\|_1^2$. The last inequality holds because for any $C > 0$, $\frac{C}{2}1$ is the unique minimum $\ell_2$-norm element over the scaled standard simplex $C\Delta^d$, with $\|\frac{C}{2}1\|_2^2 = C^2$, and we know $\alpha \in \|\alpha\|_1 \Delta^d$.

Now, for a fixed $\hat{d} > 0$, we construct $(\hat{U}, \hat{V})$ of size at most $\hat{d} + d$ by replicating each $(\bar{U}_i, \bar{V}_i)$ in proportion to $\alpha_i$. Specifically, let $r_i = \lfloor \frac{\alpha_i}{\|\alpha\|_1}\hat{d} \rfloor$ and $\gamma_i = \frac{\alpha_i}{\|\alpha\|_1}\hat{d} - r_i < 1$. Then for each $i = 1, \ldots, d$, $\hat{U}$ contains $r_i$ copies of $(\frac{\|\alpha\|_1}{\hat{d}})^{\frac{1}{2}}\bar{U}_i$ followed by one “remainder” factor $(\frac{\gamma_i\|\alpha\|_1}{\hat{d}})^{\frac{1}{2}}\bar{U}_i$. Similarly for $\hat{V}$.

More explicitly,

$$\hat{U} = \left[ (\frac{\|\alpha\|_1}{\hat{d}})^{\frac{1}{2}} \left( \begin{array}{c} 1 \end{array} \right) \right] \left( \begin{array}{c} 1 \end{array} \right) \bar{U}_1 \cdots \left( \begin{array}{c} 1 \end{array} \right) \left( \begin{array}{c} 1 \end{array} \right) \bar{U}_d$$

$$\hat{V} = \left[ (\frac{\|\alpha\|_1}{\hat{d}})^{\frac{1}{2}} \left( \begin{array}{c} 1 \end{array} \right) \left( \begin{array}{c} 1 \end{array} \right) \bar{V}_1 \cdots \left( \begin{array}{c} 1 \end{array} \right) \left( \begin{array}{c} 1 \end{array} \right) \bar{V}_d \right].$$

Then observe that $(\hat{U}, \hat{V})$ are of size $\sum_i r_i + d \leq \hat{d} + d$. And we have by construction

$$\hat{U}\hat{V}^TX = \sum_{i=1}^d \frac{\|\alpha\|_1(r_i + \gamma_i)}{\hat{d}} (\bar{U}_i\bar{V}_i^TX) = \sum_{i=1}^d \alpha_i(\bar{U}_i\bar{V}_i^TX) = UV^TX$$

$$(\hat{d} + d)\Omega_{\text{DropBlock}}(\hat{U}, X^T\hat{V}) = (\hat{d} + d) \left( \frac{\|\alpha\|_1}{\hat{d}} \right)^2 \sum_{i=1}^d r_i + (\hat{d} + d) \sum_{i=1}^d \left( \frac{\gamma_i\|\alpha\|_1}{\hat{d}} \right)^2 < \left( \frac{\hat{d} + d}{\hat{d}} \right)^2 \|\alpha\|_1^2.$$

Taking $\hat{d}$ sufficiently large so that $\|\alpha\|_1^2 \left( \frac{\hat{d} + d}{\hat{d}} \right)^2 \leq d\|\alpha\|_2^2 = d\Omega_{\text{DropBlock}}(U, X^TV)$, we see that

$$(\hat{d} + d)\Omega_{\text{DropBlock}}(\hat{U}, X^T\hat{V}) < d\Omega_{\text{DropBlock}}(U, X^TV)$$

and this completes the proof.

**Theorem 2.6 (Restated)** If $(U^*, V^*, d^*)$ is a global minimizer of the factorized problem $f$, then $A^* = U^*V^T$ $X$ is a global minimizer of the following convex lower bound $F$.

$$F(A) = \|Y - A\|_F^2 + \Theta(A) \quad \text{where} \quad \Theta(A) \triangleq \inf_{d, U \in \mathbb{R}^{m \times d}, V \in \mathbb{R}^{n \times d}} \left( \sum_{i=1}^d \|U_iV_i^TX\|_F \right)^2$$

Furthermore, the lower bound is tight, i.e. we have $f(U^*, V^*, d^*) = F(A^*)$. Moreover, the same statements also hold for the lower convex envelope $F$. 
Proof. Fix \((U, V, d)\) and let \(A = UV^T\). Suppose \(A\) does not minimize the lower bound \(\bar{F}\). Then, there exists \(A'\) and \(\epsilon > 0\) such that \(F(A') \leq \bar{F}(A) - \epsilon\). Now, choose \(U', V', d'\) such that \(A' = U'V'^T\) and \((\sum_i \|U'_i V'^T_i X_i\|_F^2)^2 \leq \Theta(A') + \epsilon/3\). Apply Theorem 2.3 to approximately balance and obtain \((\tilde{U}, \tilde{V}, \tilde{d}, \tilde{d}')\) such that \((\tilde{d} + \tilde{d}')\Omega_{\text{DropBlock}}(\tilde{U}, X^T \tilde{V}) < (\sum_i \|U'_i V'^T_i X_i\|_F^2)^2 + \epsilon/3\). It follows that:

\[
f(\tilde{U}, \tilde{V}, \tilde{d} + \tilde{d}') < F(A') + 2\epsilon/3 \leq F(A) - \epsilon/3 \leq f(U, V, d) - \epsilon/3,
\]

showing that \((U, V, d)\) is not a global minimizer of \(f\).

So, we have shown that for any global minimizer \((U^*, V^*, d^*)\) of the factorized objective \(f\), \(A^* = U^*V^*^T\) must also be a global minimizer of \(\bar{F}\). Since by Theorem 2.5 \((U^*, V^*, d^*)\) must be balanced, we know the objectives must also be equal, \(\bar{F}(A^*) = f(U^*, V^*, d^*)\).

Finally, because \(F\) is the lower convex envelope of \(\bar{F}\), and \(\bar{F}\) lower bounds \(f\), we must have \(\bar{F}(A) \leq F(A) \leq \bar{F}(A) \leq f(U, V, d)\) for all \(A\) and \((U, V, d)\) such that \(A = UV^T\). Then what we have shown for \(\bar{F}\) must also hold for \(F\).

**Theorem 2.3** (Restated) The lower convex envelope of the DropBlock regularizer \(\Lambda(A)\) in \(\mathcal{F}\), is given by

\[
\Lambda^{**}(A) = \frac{1 - \bar{\theta}}{\theta} \left( \sum_{i=1}^{a^*_1 - 1} a_i^2 + \frac{\left(\sum_{i=r^*}^d a_i\right)^2}{r - r^* + 1} \right),
\]

where \(r^*\) is the integer in \(\{1, 2, \ldots, r\}\) that maximizes \(\frac{2}{\theta} \Lambda(A)\), and \(a_1 \geq a_2 \geq \ldots \geq a_d\) are the singular values of \(A\).

**Proof.** We begin by noting that if the lower convex envelope of a function \(f(x)\) is given by \(g(x)\), then the lower convex envelope of \(\alpha f(x)\) is given by \(\alpha g(x)\) for a constant \(\alpha \geq 0\). We will use this fact to simplify the presentation of the following proof, by finding the lower convex envelope of \(\bar{\Lambda}(A)\) such that \(\Lambda(A) = \frac{2}{\hat{\theta}} \bar{\Lambda}(A)\), since \(\bar{\theta}\) is a constant. Hence, \(\bar{\Lambda}(A)\) is defined as,

\[
\bar{\Lambda}(A) = \inf_{\substack{U \in \mathbb{R}^{m \times d}, V \in \mathbb{R}^{n \times d}, \quad \frac{d}{r} \sum_{i=1}^{k} \|U_i V_i^T X_i\|_F^2, \quad A = UV^T X}}
\]

Computing the Fenchel-Conjugate of \(\bar{\Lambda}(A)\),

\[
\bar{\Lambda}^*(Q) = \sup_{A} \left( Q, A - \inf_{\substack{U \in \mathbb{R}^{m \times d}, V \in \mathbb{R}^{n \times d}, \quad \frac{d}{r} \sum_{i=1}^{k} \|U_i V_i^T X_i\|_F^2, \quad A = UV^T X}} \right)
\]

Then,

\[
\bar{\Lambda}^*(Q) = \sup_{U, V, d} \left( Q, UV^T X - \frac{d}{r} \sum_{i=1}^{k} \|U_i V_i^T X_i\|_F^2 \right)
\]

\[
= \sup_{U, V, d} \left( Q, \sum_{i=1}^{k} U_i V_i^T X_i - \frac{d}{r} \sum_{i=1}^{k} \|U_i V_i^T X_i\|_F^2 \right)
\]

\[
= \sum_{i=1}^{k} \sup_{U_i, V_i, d} \left( Q, U_i V_i^T X_i - \frac{d}{r} \|U_i V_i^T X_i\|_F^2 \right)
\]

\[
= \sum_{i=1}^{k} \left( Q, U_i V_i^T X_i - \frac{d}{r} \|U_i V_i^T X_i\|_F^2 \right)
\]

In the above, \((27)\) follows because we can separate the maximization over the pairs \((U_i, V_i)\). The value of all these maximization problems are the same. Let \(U_i V_i^T X = \Sigma N_i^T\) be a singular value decomposition of the product \(U_i V_i^T X\), with \(\Sigma = \text{diag}(\sigma)\). Since \(U_i, V_i\) each have \(r\) columns, we know that the number of non-zero
entries in $\sigma$ is atmost $r$, i.e. $\|\sigma\|_0 \leq r$, hence the problem (27) now reduces to:

$$
\tilde{\Lambda}^*(Q) = k \cdot \sup_{\|\sigma\|_0 \leq r, d, M, N} \left( \langle Q, M\text{diag}(\sigma)N^\top \rangle - \frac{d}{r} \|M\text{diag}(\sigma)N^\top\|_F^2 \right)
$$

$$
= k \cdot \sup_{\|\sigma\|_0 \leq r, d, M, N} \left( \langle \text{diag}(\sigma_Q), \text{diag}(\sigma) \rangle - \frac{d}{r} \|\sigma\|_2^2 \right)
$$

$$
= k \cdot \sup_{\|\sigma\|_0 \leq r, d} \sigma_Q^\top \sigma - \frac{d}{r} \|\sigma\|_2^2
$$

$$
= \frac{1}{4} \sum_{i=1}^r \sigma_i^2(Q)
$$

(29)

In the above, (28) follows from the Von-Neumann trace inequality, when $Q = M_Q\text{diag}(\sigma_Q)N_Q^\top$, and $\sigma$ has the same ordering as $\sigma_Q$ and $M^\top M_Q = N_Q^\top N = I_d$. To obtain (29), we use $d = k \cdot r$. Note that there is an implicit sufficient rank assumption for obtaining (29), i.e. there should be a choice of $U_iV_i$ such that the top $r$ singular values of $U_iV_i^\top X$ are the same as $\sigma_Q$. We compute the double dual now.

The basic geometric idea behind the computation of the double dual is to understand the shape of the constraint set, and the level sets of the objective function (29). The constraint set $x_1 \geq x_2 \geq \ldots \geq x_d$ is a cone in $d$ dimensions.

$$
\tilde{\Lambda}^{**}(A) = \sup_X \left( \langle A, X \rangle - \frac{1}{4} \sum_{i=1}^r \sigma_i^2(X) \right)
$$

(30)

$$
= \sup_X \left( \sum_{i=1}^d a_i x_i - \frac{1}{4} \sum_{i=1}^r x_i^2 \right) \text{ s.t. } x_1 \geq x_2 \geq \ldots \geq x_d \geq 0
$$

(31)

To simplify notation, in (31), we denote the singular values of $A$ by $a_i$ and the singular values of $X$ by $x_i$, with $a_1 \geq a_2 \geq \ldots \geq a_d$. Note that we have used the Von-Neumann inequality to obtain (31) from (30), and hence, the SVD of $X$ is given by $U_A\text{diag}(x_{sol})V_A^\top$ where $A = U_A\text{diag}(a) V_A^\top$ is the SVD of $A$.

To study (31), we first note that the variables $x_{r+1}, \ldots, x_d$ are bounded only by the order constraints and non-negativity constraints on $x_1$. Since all the $a_i \geq 0$, the objective (31) is linear and monotonically increasing in any of the variables $x_{r+1}, \ldots, x_d$. Hence, in any optimal solution to (31), each of $x_{r+1}$ takes the maximum value possible within constraints, and we have $x_r = x_{r+1} = \ldots = x_d$ at optimality. We have the following simplified problem now:

$$
\sup_X \left( \sum_{i=1}^{r-1} a_i x_i + x_r \sum_{i=r}^d a_i - \frac{1}{4} \sum_{i=1}^r x_i^2 \right) \text{ s.t. } x_1 \geq x_2 \geq \ldots \geq x_r \geq 0
$$

(32)

Notice that the solution to the optimization problem (32) does not change if we drop the constraints among the first $r-1$ variables. Hence, (32) is same as:

$$
\sup_X \left( \sum_{i=1}^{r-1} a_i x_i + x_r \sum_{i=r}^d a_i - \frac{1}{4} \sum_{i=1}^r x_i^2 \right) \text{ s.t. } \min(x_1, x_2, \ldots, x_r) = x_r \geq 0
$$

(34)

Now, assume that the minimum among $x_i$ is $x_r$. We consider two cases, $\rho = 1$, and $\rho > 1$. For the case when $\rho = 1$, or when all of the $x_i$ are equal, we see that the optimization problem is:

$$
\sup_{x_1} \left( x_1 \sum_{i=1}^d a_i - \frac{r}{4} x_1^2 \right) \text{ s.t. } x_1 \geq 0
$$

(35)

This has the solution $x_1 = \frac{3}{r} \sum_{i=1}^d a_i$.
Now, consider the case when \( \rho > 1 \). Recall that \( \rho \leq r \). WLOG, let the solution vector \( x \) have the form 
\( (x_1, x_2, x_3, \ldots, x_\rho, x_\rho, \ldots, x_\rho) \), with \( x_{\rho-1} > x_\rho \).

**Claim 1:** We claim that \( x_i = 2a_i \) for \( i = 1, 2, \ldots, \rho - 1 \). Since there is no upper constraint on \( x_1 \), and \( x_1 \) contributes the factor \( a_1 x_1 - \frac{1}{4} x_1^2 \), we see that \( x_1 = 2a_1 \) at optimality. Now, assume inductively that the claim is true for \( x_1, \ldots, x_i \). Consider \( x_{i+1} \). Since \( x_i \geq x_{i+1} \) and \( x_i = 2a_i \), we know that the constraint on \( x_{i+1} \) is \( 0 \leq x_{i+1} \leq 2a_i \).

Observe that \( x_{i+1} \) contributes the factor \( a_{i+1} x_{i+1} - \frac{1}{4} x_{i+1}^2 \) to the sum, which has the maximum at \( x_{i+1} = 2a_{i+1} \). As \( 0 \leq 2a_{i+1} \leq 2a_i \), this lies in the permissible range for \( x_{i+1} \), and we see that \( x_{i+1} = 2a_{i+1} \). This proves the claim via induction.

**Claim 2:** We claim that \( x_\rho = 2 \sum_{i=\rho}^d a_i \). Observe that \( x_\rho \) contributes the factor \( x_\rho \sum_{i=\rho}^d a_i - \frac{1}{4}(r-\rho+1) x_\rho^2 \) to the sum, which has the maximum at \( \alpha = \frac{2}{r-\rho+1} \sum_{i=\rho}^d a_i \). Along with the permissible range \( 0 \leq x_\rho \leq 2a_{\rho-1} \), we see that if \( \alpha > 2a_{\rho-1} \), then the maximum occurs at \( x_\rho = 2a_{\rho-1} = x_{\rho-1} \), which violates the assumption \( x_{\rho-1} > x_\rho \). Hence, \( \alpha \leq 2a_{\rho-1} \), and \( x_\rho = \alpha \).

To summarise, given \( \rho \), the solution \( x \) has the following closed form:

\[
\begin{pmatrix}
2a_1, 2a_2, \ldots, 2a_{\rho-1}, \frac{2}{r-\rho+1} \sum_{i=\rho}^d a_i, \ldots, \frac{2}{r-\rho+1} \sum_{i=\rho}^d a_i
\end{pmatrix}
\]  
(36)

The objective value at the solution [36] is:

\[
\sum_{i=1}^{\rho-1} a_i x_i + x_r \sum_{i=\rho}^d a_i - \frac{1}{4} \sum_{i=1}^{r} x_i^2
\]

\[
= \sum_{i=1}^{\rho-1} (a_i x_i - \frac{1}{4} x_i^2) + x_\rho \sum_{i=\rho}^d a_i - \frac{r - \rho + 1}{4} a_\rho^2
\]

\[
= \sum_{i=1}^{\rho-1} a_i^2 + \frac{2}{r-\rho+1} \sum_{i=\rho}^d a_i - (r - \rho + 1) \left( \sum_{i=\rho}^d a_i \right)^2
\]

\[
= \sum_{i=1}^{\rho-1} a_i^2 + \frac{\left( \sum_{i=\rho}^d a_i \right)^2}{r-\rho+1}
\]  
(37)

To find the value of \( \rho \), it suffices to evaluate \( \rho = \{1, 2, \ldots, d\} \) to get the value \( \rho^* \) that maximizes (37). Finally, bringing the multiplier back, we have the following expression for \( \Lambda^{**}(A) \):

\[
\Lambda^{**}(A) = \frac{1-\theta}{\theta} \Lambda^{**}(A)
\]

\[
= \frac{1-\theta}{\theta} \left( \sum_{i=1}^{\rho^*-1} a_i^2 + \frac{\left( \sum_{i=\rho}^d a_i \right)^2}{r-\rho^*+1} \right)
\]

**Theorem 2.7 (Restated)** The global minimizer of \( F(A) \) is given by \( A_{\rho,\lambda} = U \text{diag}(a_{\rho,\lambda}) V_Y^T \), where \( Y = U \text{diag}(m) V_Y \) is an SVD of \( Y \), and \( a_{\rho,\lambda} \) is given by

\[
a_{\rho,\lambda} = \begin{cases}
(m_1, m_2, \ldots, m_\lambda, 0, \ldots, 0) & \text{if } \lambda \leq \rho - 1 \\
(m_1, m_2, \ldots, m_\lambda, m_{\rho+1}, m_{\rho+1}, \ldots, m_{\lambda}) & \text{if } \lambda \geq \rho \text{ and } \rho \in \{1, 2, \ldots, r-1\}
\end{cases}
\]

The constants are \( \beta = \frac{1-\theta}{\theta} \), \( S = \sum_{i=\rho}^d m_i, \) \( c = r + \beta \lambda + (\beta + 1)(1 - \rho) \), \( \rho \in \{1, 2, \ldots, r-1\} \) and \( \lambda \in \{1, 2, \ldots, d\} \) are chosen such that they minimize \( F(A_{\rho,\lambda}) \).
Proof. We now use the solution for $\Lambda^\ast$ computed above to find the global minimizer of the convex lower bound defined in (12) as $F(A) = \|M - A\|^2_F + \Lambda^\ast(A) = \|M - A\|^2_F + \beta\Lambda^\ast(A)$, with $\beta = \frac{1 - \theta}{\sigma}$. 

\[
\min_X \|A - X\|^2_F + \beta\Lambda^\ast(X) 
= \min_X \|\sigma_A - \sigma_X\|^2_F + \beta\sum_{i=1}^d x_i^2 + \beta\left(\frac{\sum_{i=\rho}^d x_i^2}{r - \rho + 1}\right) 
= \min_X \sum_{i=1}^\lambda (a_i - x_i)^2 + \sum_{i=\lambda+1}^d a_i^2 + \beta\sum_{i=1}^\lambda x_i^2 + \frac{\sum_{i=\rho}^d x_i^2}{r - \rho + 1} 
\tag{38}
\]

Note that in moving from (38) to (39), we used the Von-Neumann inequality, and took $X = U_A \text{diag}(x)V_A^\top$ where $A = U_A \text{diag}(a)V_A^\top$ is an SVD of $A$. Assume there are $\lambda$ non-zero elements in the solution of (39). The objective now becomes:

\[
\min_X \sum_{i=1}^\lambda (a_i - x_i)^2 + \sum_{i=\lambda+1}^d a_i^2 + \beta\sum_{i=1}^\lambda x_i^2 + \sum_{i=\rho}^d x_i^2 + \frac{\sum_{i=\rho}^d x_i^2}{r - \rho + 1} 
\tag{40}
\]

From the KKT conditions for (40), we have $x_1, x_2, \ldots, x_\lambda > 0$ and $x_\lambda = x_{\lambda+1} = \ldots = x_d = 0$. We consider two cases, $\lambda \leq \rho$ and $\lambda > \rho$. Firstly, consider the case when $\lambda \leq \rho - 1$. From the KKT conditions we have the following solution for this case:

\[
2(x_i - a_i) + 2\beta x_i = 0 \implies x_{1:\lambda} = \frac{1}{\beta + 1} a_{1:\lambda} 
\tag{41}
\]

For $\lambda > \rho$, the objective becomes

\[
\min_X \sum_{i=1}^\lambda (a_i - x_i)^2 + \sum_{i=\lambda+1}^d a_i^2 + \beta\sum_{i=1}^\lambda x_i^2 + \frac{\sum_{i=\rho}^d x_i^2}{r - \rho + 1} 
\tag{42}
\]

For the first $\rho - 1$ variables, $x_{1:\rho-1}$, the KKT conditions give the same solution as in (41), i.e. $x_{1:\rho-1} = \frac{1}{\beta + 1} a_{1:\rho-1}$. For $x_i$ with $\rho \leq i \leq \lambda$, we need to solve a system of linear equations, as follows:

\[
2(x_i - a_i) + 2\beta\sum_{i=\rho}^d x_i = 0 
\implies \left( I_{\lambda-\rho+1} - \frac{\beta}{r - \rho + 1} 11^\top \right) x_{\rho:\lambda} = a_{\rho:\lambda} 
\implies x_{\rho:\lambda} = \left( I_{\lambda-\rho+1} - \frac{\beta}{r - \rho + 1} 11^\top \right) a_{\rho:\lambda} 
\implies x_{\rho:\lambda} = \left( a_{\rho:\lambda} - \frac{\beta \sum_{i=\rho}^\lambda a_i}{r + \beta \lambda - (\beta + 1)\rho + (\beta + 1)} \right) 
\tag{43}
\]

For (43), we use the Sherman-Morrison Matrix Identity i.e. $(I_d + \alpha 11^\top)^{-1} = I_d - \frac{\alpha}{1 + \alpha} 11^\top$. The $+$ subscript on (44) denotes applying the thresholding operation $x_i = \text{Max}(x_i, 0)$ to all entries of the vector.

Note that we do not know $\lambda$ or $\rho$ at this point. However, from the solution (43) (44), we know that the optimal pair $(\lambda^\ast, \rho^\ast)$ achieves the minimum value of $F(X)$, given the solution $X = U_A \text{diag}(x)V_A^\top$. Hence, to compute this optimal pair, we can evaluate all $O(d^2)$ possibilities for $(\lambda, \rho)$ given $A$.

\[
\textbf{Corollary 2.8 (Restated)} \text{ If } A^\ast \text{ is a global minimizer of the lower convex envelope } F, \text{ and } (U^\ast, V^\ast, d^\ast) \text{ is a global minimizer of the non-convex objective } f, \text{ then we have } F(A^\ast) = \hat{F}(A^\ast) = f(U^\ast, V^\ast, d^\ast) \text{ with } A^\ast = U(V^\ast)^\top X. 
\]
For regular Dropout, we have

\[ P \text{.} \]

**Proof.** By Theorem 2.5 we know that if \((U^*, V^*, d^*)\) is a global minimizer of \(f\), then with \(A^* = U(V^*)^\top X\), we have \(\bar{F}(A^*) = f(U^*, V^*, d^*)\). Additionally, we know that \(A^*\) is a global minimizer of \(\bar{F}\). Now, by construction, we know that \(F\) is the lower convex envelope of \(\bar{F}\). Also, \(\bar{F}\) is a non-negative function defined over the space of real matrices. Hence, by the properties of the lower convex envelope \([10]\), we know that \(F\) and \(\bar{F}\) have the same value at \(A^*\).

\[ \square \]

C  Proofs for Section 3

**Theorem 3.1 (Restated)** The Generalized Dropout objective \([13]\) is equivalent to a regularized deterministic objective:

\[
\mathbb{E}_z \| Y - U \text{diag}(\mu)^{-1} \text{diag}(z) g_r(X) \|_F^2 = \| Y - U g_r(X) \|_F^2 + \Omega_{C, \mu}(U, g_r(X)^\top) \]

where the generalized Dropout regularizer, \(\Omega_{C, \mu}(U, V)\) is:

\[
\Omega_{C, \mu}(U, V) = \sum_{i,j=1}^d c_{i,j} \frac{(u_i^\top u_j)(v_i^\top v_j)}{\mu_i \mu_j} = \langle C, U^\top U \odot V^\top V \rangle,
\]

**Proof.** We generalize the Dropout analysis to get a deterministic equivalent for the objective when \(z\) is drawn from an arbitrary distribution \(S\).

\[
\mathbb{E}_z \| Y - U \text{diag}(\mu)^{-1} \text{diag}(z) g_0(X) \|_F^2 \\
= \| Y - U \text{diag}(\mu)^{-1} \text{diag}(z) V^\top \|_F^2 \\
= \mathbb{E}_z \| Y - U \text{diag}(\mu)^{-1} \text{diag}(z) V^\top \|_F^2 + 1^\top \text{Var} [ Y - U \text{diag}(\mu)^{-1} \text{diag}(z) V^\top ] 1 \\
= \| Y - U \text{diag}(\mu)^{-1} \text{diag}(\mu) V^\top \|_F^2 + 1^\top \text{Var} [ U \text{diag}(\mu)^{-1} \text{diag}(z) V^\top ] 1 \\
= \| Y - U V^\top \|_F^2 + 1^\top \text{Var} \left[ \sum_{i=1}^d \frac{z_i}{\mu_i} u_i v_i^\top \right] 1 \\
= \| Y - U V^\top \|_F^2 + \sum_{i,j=1}^d 1^\top \text{Covar} \left( \frac{z_i}{\mu_i} u_i v_i^\top, \frac{z_j}{\mu_j} u_j v_j^\top \right) 1 \\
= \| Y - U V^\top \|_F^2 + \sum_{i,j=1}^d \frac{\langle u_i v_i^\top, u_j v_j^\top \rangle}{\mu_i \mu_j} \text{Covar}(z_i z_j) \\
= \| Y - U V^\top \|_F^2 + \sum_{i,j=1}^d c_{i,j} \frac{\langle u_i v_i^\top, u_j v_j^\top \rangle}{\mu_i \mu_j}
\]

In [45], we have substituted \(g_0(X) = V^\top\) for ease of presentation. Then, in [46], we have used the identity \(\mathbb{E}[a^2] = \mathbb{E}[a]^2 + \text{Var}[a]\) applied to each element of the matrix \(A\), which gives that \(\mathbb{E}[\|A\|_F^2] = \|\mathbb{E}[A]\|_F^2 + 1^\top \text{Var}[A] 1\). We have used the matrix equivalent of the identity \(\text{Var}(a_1 + a_2 + \ldots + a_d) = \sum_{i,j} \text{Covar}(a_i, a_j)\) in [47].

**Corollary 3.2 (Restated)** For regular Dropout applied to objective \([13]\) the following equivalence holds:

\[
\mathbb{E}_z \| Y - U \text{diag}(\mu)^{-1} \text{diag}(z) g_r(X) \|_F^2 = \| Y - U g_r(X) \|_F^2 + \sum_{i=1}^d \| u_i \|_2^2 \| g_r(X) \|_2^2
\]

where \(g_r(X) \in \mathbb{R}^N\) denotes the output of the \(i^{th}\) neuron of \(g_r\) (i.e., the \(i^{th}\) row of \(g_r(X)\)).

**Proof.** For regular Dropout, we have \(z \sim_i \text{i.i.d.} \text{Bernoulli}(\theta)\). Hence, the covariance matrix is given by \(c_{i,i} = \theta(1 - \theta)\) and \(c_{i,j} = 0\) when \(i \neq j\). Further, \(\mu_i = \theta\) for all \(i\). Using Theorem 3.1 with this choice of \(\mu, C\) we get the result.
Lemma 3.3 (Restated) If the network architecture, \( g \), has sufficient capacity to span \( \mathbb{R}^{d \times N} \) (i.e., given any matrix \( Q \in \mathbb{R}^{d \times N} \), \( \exists \bar{\Gamma} \) such that \( g_{\bar{\Gamma}}(X) = Q \)) and \( d \geq \min\{a, N\} \), then the global optimum of (13) with \( z \sim \text{Bernoulli}(\theta) \) is given by:

\[
\min_{U, \Gamma} \mathbb{E}_{z} \left\| Y - U \text{diag}(\mu)^{-1} \text{diag}(z) g_{\Gamma}(X) \right\|_F^2 = \min_{A} \left\| Y - A \right\|_F^2 + \frac{1 - \theta}{\theta} \| A \|_*^2
\]

where \( \| A \|_* \) denotes the nuclear norm of \( A \).

Proof. From Corollary 3.2, we have for Dropout,

\[
\mathbb{E}_{z} \left\| Y - U \text{diag}(\mu)^{-1} \text{diag}(z) g_{\Gamma}(X) \right\|_F^2 = \left\| Y - U g_{\Gamma}(X) \right\|_F^2 + \sum_{i=1}^{d} \| u_i \|_2^2 \| v_i \|_2^2
\]

Since the network is sufficiently overparameterized such that for any \( V \in \mathbb{R}^{N \times d} \) there exists \( \bar{\Gamma} \) such that \( g_{\bar{\Gamma}}(X) = V^T \), we can replace \( g_{\Gamma}(X) \) by \( V \) and optimize over \( V \). Now, we can use arguments similar to [7] to obtain the result:

\[
\min_{U, V} \left\| Y - UV^T \right\|_F^2 + \sum_{i=1}^{d} \| u_i \|_2^2 \| v_i \|_2^2 = \min_{A} \left\| Y - A \right\|_F^2 + \| A \|_*^2
\]

D Proofs for Section 4

Theorem 4.1 (Restated) For Dropconnect applied to the second-last layer weights \( V \) of a deep network parameterized as \( UV^T g_{\Gamma}(X) \), the following equivalence holds:

\[
\mathbb{E}_{Z} \left\| Y - \frac{1}{\theta} U (Z \odot V)^T g_{\Gamma}(X) \right\|_F^2 = \left\| Y - UV^T g_{\Gamma}(X) \right\|_F^2 + \frac{1 - \theta}{\theta} \sum_{i=1}^{d} \| u_i \|_2^2 \| g_{\Gamma}(X)^T v_i \|_2^2
\]

where \( g_{\Gamma}(X) \in \mathbb{R}^N \) denotes the output of the \( i \)-th neuron of \( g_{\Gamma} \) (i.e., the \( i \)-th row of \( g_{\Gamma}(X) \)).

Proof. We show that DropConnect induces a deterministic objective. The proof performs algebraic manipulations to evaluate the expectation of the objective over \( Z \) first and then \( x \). For ease of presentation, we substitute...
\(M = g_\Gamma(X)\), and hence evaluate \(E_Z \|Y - \frac{1}{\theta}U(Z \odot V)^\top M\|^2_F\).

\[
E_Z \left\| Y - \frac{1}{\theta}U(Z \odot V)^\top M \right\|^2_F = \left\| E_Z \left[ Y - \frac{1}{\theta}U(Z \odot V)^\top M \right] \right\|^2_F + 1^\top \text{Var}_Z \left[ Y - \frac{1}{\theta}U(Z \odot V)^\top M \right] = \left\| Y - \frac{1}{\theta}U(E_Z(Z \odot V)^\top M) \right\|^2_F + \frac{1}{\theta^2} 1^\top \text{Var}_Z [U(Z \odot V)^\top M] \tag{52}
\]

\[
E_Z \left\| Y - \frac{1}{\theta}U(\theta V)^\top M \right\|^2_F + \frac{1}{\theta^2} 1^\top \text{Var}_Z \left[ \sum_{k=1}^d u_k (M^\top(Z \odot V))_k \right] = \left\| Y - \frac{1}{\theta}U(\theta V)^\top M \right\|^2_F + \frac{1}{\theta^2} 1^\top \text{Var}_Z \left[ \sum_{k=1}^d u_k M^\top(Z \odot V)_k \right] \tag{53}
\]

\[
E_Z \left\| Y - UV^\top M \right\|^2_F + \frac{1}{\theta^2} \sum_{k=1}^d 1^\top \text{Var}_{z_k} [u_k M^\top(z_k \odot v_k)] = \left\| Y - UV^\top M \right\|^2_F + \frac{1}{\theta^2} \sum_{k=1}^d (\theta)(1 - \theta)\|u_k\|^2\|M^\top v_k\|^2_F \tag{54}
\]

\[
E_Z \left\| Y - UV^\top M \right\|^2_F + \frac{1 - \theta}{\theta} \sum_{k=1}^d \|u_k\|^2\|M^\top v_k\|^2_F = \left\| Y - UV^\top M \right\|^2_F + \frac{1 - \theta}{\theta} \sum_{k=1}^d \|u_k\|^2\|M^\top v_k\|^2_F \tag{56}
\]

In (52), we have used the identity \(E[a^2] = E[a]^2 + \text{Var}[a]\) applied to each element of the matrix \(A = Y - \frac{1}{\theta}U(Z \odot V)^\top M\), which gives that \(E[\|A\|^2_F] = \|E[A]\|^2_F + 1^\top \text{Var}[A]\). Each of the columns of \(Z\) are independent, which implies each of the summands in (53) are independent. Hence, the variance and the summation can be interchanged, and (54) follows. Further, since each element of a column of \(Z\) is independent, (55) follows.

\section*{E Extended Experiments}

\textbf{Verifying Deterministic Formulations} We verify the correctness of the deterministic formulations for various dropout schemes analyzed in this paper, i.e. (5) and (20), in the top panels of Figure 5 and Figure 6. In Figure 5, the curve labelled \textit{DropBlock Stochastic} is the training objective plot, i.e. it plots the value of the DropBlock stochastic objective (3) as the training progresses via Algorithm 1. For generating the curve labeled \textit{DropBlock Deterministic}, we take the current iterate, i.e. \(U_i, V_i\), and plot the Deterministic DropBlock objective obtained in Lemma 2.1 at every iteration. The deterministic equivalent of the DropConnect objective is similarly verified in Figure 6. It can be seen that the expected value of DropConnect and DropBlock over iterations matches the values derived in our results. Additionally, the bottom panel of Figure 6 shows that Dropout and DropConnect have the same expected value of the objective at each iteration.
Figure 5: Top: Stochastic DropBlockGrid training with SGD is equivalent to the deterministic Objective [5]. Bottom: DropBlockGrid converges to the global minimum computed in Theorem 2.7.

Figure 6: Comparing DropConnect to DropOut. Top: Stochastic DropConnect training with SGD is equivalent to the deterministic Objective [20]. Bottom: DropConnect training is equivalent to Dropout training for the squared loss.