Explicit regularization and implicit bias in deep network classifiers trained with the square loss

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Abstract

Deep ReLU networks trained with the square loss have been observed to perform well in classification tasks. We provide here a theoretical justification based on analysis of the associated gradient flow. We show that convergence to a solution with the absolute minimum norm is expected when normalization techniques such as Batch Normalization (BN) or Weight Normalization (WN) are used together with Weight Decay (WD). The main property of the minimizers that bounds their expected error is the norm: we prove that among all the close-to-interpolating solutions, the ones associated with smaller Frobenius norms of the unnormalized weight matrices have better margin and better bounds on the expected classification error. With BN but in the absence of WD, the dynamical system is singular. Implicit dynamical regularization – that is zero-initial conditions biasing the dynamics towards high margin solutions – is also possible in the no-BN and no-WD case. The theory yields several predictions, including the role of BN and weight decay, aspects of Papyan, Han and Donoho’s Neural Collapse and the constraints induced by BN on the network weights.

1 Introduction

In the case of exponential-type loss functions a mechanism of complexity control underlying generalization was identified in the asymptotic margin maximization effect of minimizing exponential-type loss functions [1, 2, 3]. However, this mechanism

- cannot explain the good empirical results that have been recently demonstrated using the square loss [4];
- cannot explain the empirical evidence that convergence for cross-entropy loss minimization depends on initialization.

This puzzle motivates our focus in this paper on the square loss. More details and sketches of the proofs can be found in [5].

Here we assume commonly used GD-based normalization algorithms such as BN [6] (or WN [7]) together with weight decay (WD), since they appear to be essential for reliably training
deep networks (and were used by [4]. We also consider, however, the case in which neither BN nor WD are used showing that a dynamic “implicit regularization” effect for classification is still possible with convergence strongly depending on initial conditions.

1.1 Notation
We define a deep network with $L$ layers with the usual coordinate-wise scalar activation functions $\sigma(z) : \mathbb{R} \rightarrow \mathbb{R}$ as the set of functions $g(W; x) = (W_L \sigma(W_{L-1} \cdots \sigma(W_1 x)))$, where the input is $x \in \mathbb{R}^d$, the weights are given by the matrices $W_k$, one per layer, with matching dimensions. We sometime use the symbol $W$ as a shorthand for the set of $W_k$ matrices $k = 1, \cdots, L$. There are no bias terms: the bias is instantiated in the input layer by one of the input dimensions being a constant. The activation nonlinearity is a ReLU, given by $\sigma(x) = x_+ = \max(0, x)$. Furthermore,

- we define $g(x) = \rho f(x)$ with $\rho$ defined as the product of the Frobenius norms of the weight matrices of the $L$ layers of the network and $f$ as the corresponding network with normalized weight matrices $V_k$ (because the ReLU is homogeneous [3]);

- in the following we use the notation $f_n$ meaning $f(x_n)$, that is the output of the normalized network for the input $x_n$;

- we assume $||x|| = 1$;

- separability is defined as correct classification for all training data, that is $y_n f_n > 0$, $\forall n$. We call average separability when $\sum y_n f_n > 0$.

1.2 Regression and classification
In our analysis of the square loss, we need to explain when and why regression works well for classification, since the training minimizes square loss but we are interested in good performance in classification (for simplicity we consider here binary classification). Unlike the case of linear networks we expect several global zero square loss minima corresponding to interpolating solutions (in general degenerate, see [9] and reference therein). Although all interpolating solutions are optimal solutions of the regression problem, they will in general have different margins and thus different expected classification performance. In other words, zero square loss does not imply by itself neither large margin nor good expected classification. Notice that if $g$ is a zero loss solution of the regression problem, then $g(x_n) = y_n$, $\forall n$. This is equivalent to $\rho f_n = y_n$ where $f_n$ is the margin for $x_n$. Thus the norm $\rho$ of a minimizer is inversely related to its average margin. In fact, for an exact zero loss solution of the regression problem, the margin is the same for all training data $x_n$ and it is equal to $\frac{1}{\rho_{eq}}$. Starting from small initialization, GD will explore critical points with $\rho$ growing from zero, as we will show. Thus interpolating solutions with small norm $\rho_{eq}$ (corresponding to the best margin) may be found before large $\rho_{eq}$ solutions which have worse margin. If the weight decay parameter is non-zero and large enough, there is independence

\footnote{This was the main concern of the first version of [5].}
from initial conditions. Otherwise, a near-zero initialization is required, as in the case of linear networks, though the reason is quite different and is due to an implicit bias in the dynamics of GD.

2 Dynamics and Generalization

Our key assumption is that the main property of batch normalization (BN) and weight normalization (WN) – the normalization of the weight matrices – can be captured by the gradient flow on a loss function modified by adding Lagrange multipliers.

Gradient descent on a modified square loss

\[
\mathcal{L} = \sum_n (\rho f_n - y_n)^2 + \nu \sum_k ||V_k||^2
\]

with \( ||V_k||^2 = 1 \) is in fact exactly equivalent to “Weight Normalization”, as proved in [3], for deep networks.

This dynamics can be written as \( \dot{\rho}_k = V_k^T \dot{W}_k \) and \( \dot{V}_k = \rho S \dot{W}_k \) with \( S = I - V_k V_k^T \). This shows that if \( W_k = \rho_k V_k \) then \( \dot{V}_k = \frac{1}{\rho_k} \dot{W}_k \) as mentioned in [3]. The condition \( ||V_k||^2 = 1 \) yields, as shown in [5], \( \nu = -\sum_n (\rho^2 f_n^2 - \rho y_n f_n) \). Here we assume that the BN module is used in all layers apart the last one, that is we assume \( \rho_k = 1 \), \( \forall k < L \) and \( \rho_L = \rho \) where \( L \) is the number of layers.

As we will show, the dynamical system associated with the gradient flow of the Lagrangian Equation 1 is “singular”, in the sense that normalization is not guaranteed at the critical points. Regularization is needed, and in fact it is common to use in gradient descent not only batch normalization but also weight decay. Weight decay consists of a regularization term \( \lambda ||W_k||^2 \) added to the Lagrangian yielding

\[
\mathcal{L} = \sum_n (\rho f_n - y_n)^2 + \nu \sum_k ||V_k||^2 + \lambda \rho^2.
\]

The associate gradient flow is then the following dynamical system

\[
\dot{\rho} = -2\sum_n \rho (f_n)^2 - \sum_n f_n y_n - 2\lambda \rho \tag{3}
\]

\[
\dot{V}_k = 2\rho \sum_n [(\rho f_n - y_n)(V_k f_n - \frac{\partial f_n}{\partial V_k})] \tag{4}
\]

\[\text{It is important to observe here that batch normalization – unlike Weight Normalization – leads not only to normalization of the weight matrices but also to normalization of each row of the weight matrices [3] because it normalizes separately the activity of each unit \( i \) and thus – indirectly – the \( W_{i,j} \) for each \( i \) separately. This implies that each row \( i \) in \( (V_k)_{i,j} \) is normalized independently and thus the whole matrix \( V_k \) is normalized (assuming the normalization of each row is the same 1 for all rows). The equations in the main text involving \( V_k \) can be read in this way, that is restricted to each row.}\]
where the critical points $\dot{\rho} = 0, \dot{V}_k = 0$ are singular for $\lambda = 0$ but are not singular for any arbitrarily small $\lambda > 0$. In particular, normalization is then effective at $\rho_{eq}$ unlike in the $\lambda = 0$ case. As a side remark, SGD, as opposed to gradient flow, may help (especially with label noise) to counter to some extent the singularity of the $\lambda = 0$ case, even without weight decay, because of the associated random fluctuations around the pathological critical point.

The equilibrium value at $\dot{\rho}_k = 0$ is

$$\rho_{eq} = \frac{\sum_n y_n f_n}{\lambda + \sum_n f_n^2}. \quad (5)$$

Observe that $\dot{\rho} > 0$ if $\rho$ is smaller than $\rho_{eq}$ and if average separability holds. Recall also that zero loss “global” minima (in fact arbitrarily close to zero for small but positive $\lambda$) are expected to exist and be degenerate [9].

If we assume that the loss (with the constraint $||V_k|| = 1$) is a continuous function of the $V_k$, then there will be at least one minimum of $\mathcal{L}$ at any fixed $\rho$, because the domain $V_k$ is compact. This means that for each $\rho$ there is at least a critical point of the gradient flow of $V_k$, implying that for each critical $\rho$ for which $\dot{\rho} = 0$, there is at least one critical point of the dynamical system in $\rho$ and $V_k$.

Around $\dot{V}_k = 0$ we have

$$\sum_n (\rho f_n - y_n) \frac{\partial f_n}{\partial V_k} = \sum_n (\rho f_n - y_n)(V_{eq}^k f_n), \quad (6)$$

where the terms $(\rho f_n - y_n)$ will be generically different from zero if $\lambda > 0$.

The conclusions of this analysis can be summarized in

**Observation 1** Assuming average separability, and gradient flow starting from small norm $\rho(0) = \epsilon > 0$, $\rho(t)$ grows monotonically until a minimum is reached at which $\rho_{eq} = \frac{\sum_n y_n f_n}{\lambda + \sum_n f_n^2}$. This dynamics is expected even in the limit of $\lambda = 0$, which corresponds to exact interpolation of all the training data at a singular critical point.

and

**Observation 2** Minimizers with small $\rho_{eq}$ correspond to large average margin $\sum y_n f_n$. In particular, suppose that the gradient flow converges to a $\rho_{eq}$ and $V_{eq}^k$ which correspond to zero square loss. Among all such minimizers the one with the smallest $\rho_{eq}$ (typically found first during the GD dynamics when $\rho$ increases from $\rho = 0$), corresponds to the (absolute) minimum norm – and maximum margin – solutions.

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3For $\lambda = 0$ the zero loss critical point is pathological, since $V_k = 0$ even when $(V_k f_n - \frac{\partial L}{\partial V_k})$ implying that an un-normalized interpolating solution satisfies the equilibrium equations. Numerical simulations show that even for linear degenerate networks convergence is independent of initial conditions only if $\lambda > 0$. 

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In general, there may be several critical points of the $V_k$ for the same $\rho_{eq}$ and they are typically degenerate (see references in [10]) with dimensionality $W - N$, where $W$ is the number of weights in the network may be degenerate. All of them will correspond to the same norm and all will have the same margin for all of the training points.

Since usually the maximum output of a multilayer network is $<< 1$, the first critical point for increasing $\rho$ will be when $\rho$ becomes large enough to allow the following equation to have solutions

$$\sum_n y_n f_n = \rho(\lambda + \sum_n f_n^2).$$

(7)

If gradient flow starts from very small $\rho$ and there is average separability, $\rho$ increases monotonically until such a minimum is found. If $\rho$ is large, then $\dot{\rho} < 0$ and $\rho$ will decrease until a minimum is found.

For large $\rho$ and very small $\lambda$, we expect many solutions under GD. The emerging picture is a landscape in which there are no zero-loss minima for $\rho < \rho_{min}$. With increasing $\rho$ from $\rho = 0$ there will be zero square-loss degenerate minima with the minimizer representing an almost interpolating solution (for $\lambda > 0$). We expect, however, that depending on the value of $\lambda$, there is a bias towards minimum $\rho_{eq}$ even for large $\rho$ initializations and certainly for small initializations.

All these observations are also supported by our numerical experiments. Figure 1, 2, 3, and 4 show the case of gradient descent with batch normalization and weight decay, which corresponds to a well-posed dynamical system for gradient flow; the other figures show the same networks and data with BN without WD and without both BN and WD. As predicted by the analysis, the case of BN+WD is the most well-behaved, whereas the others strongly depend on initial conditions.

To show that $\rho$ indeed controls the expected error we use classical bounds that lead to the following theorem

**Observation 3** With probability $1 - \delta$

$$L(f) \leq c_1 \rho R_N(\tilde{F}) + c_2 \epsilon(N, \delta)$$

(8)

where $c_1, c_2$ are constants that reflect the Lipschitz constant of the loss function (for the square loss this requires a bound on $f(x)$) and the architecture of the network. The Rademacher average $R_N(\tilde{F})$ depends on the normalized network architecture and $N$. Thus for the same network and the same data, the upper bound for the expected error of the minimizer is smaller for smaller $\rho$.

The theorem proves the conjecture in [11] that for deep networks, as for kernel machines, minimum norm interpolating solutions are the most stable.

\footnote{It is interesting to recall [9] that for SGD – unlike GD – the algorithm will stop only when $\ell_n = 0 \ \forall n$, which is the global minimum and corresponds to perfect interpolation. For the other critical points for which GD will stop, SGD will never stop but just fluctuate around the critical point.}
2.1 Predictions

- In a recent paper Papyan, Han and Donoho\cite{12} described four empirical properties of the terminal phase of training (TPT) deep networks, using the cross-entropy loss function. TPT begins at the epoch where training error first vanishes. During TPT, the training error stays effectively zero, while training loss is pushed toward zero. Direct empirical measurements expose an inductive bias they call neural collapse (NC), involving four interconnected phenomena. (NC1) Cross-example within-class variability of last-layer training activations collapses to zero, as the individual activations themselves collapse to their class means. (NC2) The class means collapse to the vertices of a simplex equiangular tight frame (ETF). (NC3) Up to rescaling, the last-layer classifiers collapse to the class means or in other words, to the simplex ETF (i.e., to a self-dual configuration). (NC4) For a given activation, the classifier’s decision collapses to simply choosing whichever class has the closest train class mean (i.e., the nearest class center \[NCC\] decision rule). We show in \cite{5} that these properties of the Neural Collapse\cite{12} seem to be predicted by the theory of this paper for the global (that is, close-to-zero square-loss) minima, irrespectively of the value of \[\rho_{eq}\]. We recall that the basic assumptions of the analysis are Batch Normalization and Weight Decay. Our predictions are for the square loss but we show that they should hold also in the case of crossentropy, explored in \cite{12}.

- At a close to zero loss critical point of the flow, \[\nabla_{V_k} f(x_j) = V_k f(x_j)\] with \[x_j\] in the training set, which are powerful constraints on the weight matrices to which training converges. A specific dependence of the matrix at each layer on matrices at the other layers is thus required. In particular, there are specific relations for each layer matrix \[V_k\] of the type,
Figure 2: ConvNet with Batch Normalization and Weight Decay Dynamics of $\rho$ from experiments in Figure 1. First row: small initialization (0.1). Second row: medium initialization (1). Third row: large initialization (5). A dashed rectangle denotes the previous subplot’s domain and range in the new subplot.
Figure 3: **ConvNet with Batch Normalization and Weight Decay** Dynamics of the average of $|f_n|$ from experiments in Figure 1. First row: small initialization (0.1). Second row: medium initialization (1). Third row: large initialization (5). A dashed rectangle denotes the previous subplot’s domain and range in the new subplot.
Figure 4: **ConvNet with Batch Normalization and Weight Decay** Margin of all training samples.

Figure 5: **ConvNet with Batch Normalization but no Weight Decay** Binary classification on two classes from CIFAR-10, trained with MSE loss. The model is a very simple network with 4 layers of convolutions. ReLU nonlinearity is used. Batch normalization is used without parameters (affine=False in PyTorch). The weight matrices of all layers are initialized with zero-mean normal distribution, scaled by a constant such that the Frobenius norm of each matrix is either 0.1 or 5. We run SGD with batch size 128, constant learning rate 0.01 and momentum 0.9 for 1000 epochs. No data augmentation. Every input to the network is scaled such that it has Frobenius norm 1. This is a single run but it is typical for the parameter values we used.
Figure 6: **ConvNet with Batch Normalization but no Weight Decay.** Dynamics of $\rho$ from experiments in Figure 5. Top row: small initialization (0.1). Bottom row: large initialization (5). The plot starts with $\rho(0) = 0$ despite an initialization of $\rho_k = 0$ because the the scaling factor of BN starts from 0. A dashed rectangle denotes the previous subplot’s domain and range in the new subplot.
explanation in the Appendix,

\[ V_{k,f} = [V_L D_{L-1}(x)V_{L-1} \cdots V_{k+1} D_k(x)]^T D_{k-1}(x)V_{k-1} D_{k-2}(x) \cdots D_1(x)V_1 x \quad (9) \]

where the \( D \) matrices are diagonal with components either 0 or 1, depending on whether the corresponding ReLU unit is on or off.

As described in [5] for linear networks, a class of possible solutions to these constraint equations are projection matrices; another one are orthogonal matrices and more generally orthogonal Stiefel matrices on the sphere. These are sufficient but not necessary conditions to satisfy the constraint equations. Interestingly, randomly initialized weight matrices (an extreme case of the NTK regime) are approximately orthogonal.

3 Explicit Regularization and Implicit Dynamic Bias

We have established here convergence of the gradient flow to a minimum norm solution for the square loss, when gradient descent is used with BN (or WN) and WD. This result assumes explicit regularization (WD) and is thus consistent with [13], where it is proved that implicit regularization with the square loss cannot be characterized by any explicit function of the model parameters. We also show, however, that in the absence of WD and BN good solutions for binary classification can be found because of the bias in the dynamics of GD toward small norm solution
Figure 8: **ConvNet with Batch Normalization but no Weight Decay**: Histogram of $|f_n|$ over time. Top figure: initial $\rho_k = 0.1$. Bottom figure: initial $\rho_k = 5$. 
introduced by near-zero initial conditions. Again, this is consistent with [13], because we identify an implicit bias in the dynamics which is relevant for classification.

For the exponential loss, BN is strictly not needed since minimization of the exponential loss maximizes the margin and minimizes the norm without BN, independently of initial conditions. Thus under the exponential loss, we expect a margin maximization bias for $t \to \infty$ as shown in [14], independently of initial conditions. The effect however can require very long times and unreasonably high precision to have significant effect in practice.

If there exist several almost-interpolating solutions with the same norm $\rho_{eq}$, they also have the same margin for each of the training data. Though they have the same norm and the same margin on each of the data point, they may in principle have different ranks of the weight matrices or of the rank of the local Jacobian $\partial f/\partial V_k$ (at the minimum $W^*$). Notice that in deep linear networks the GD dynamics biases the solution towards small rank solutions, since large eigenvalues converge much faster the small ones [15]. It is unclear whether the rank has a role in our analysis of generalization and we conjecture it does not.

Why does GD have difficulties in converging in the absence of BN+WD, especially for very deep networks? For square loss, the best answer is that good tuning of the learning rate is important and BN together with weight decay was shown to provide a remarkable autotuning [8]. A related answer is that regularization is needed to provide stability, including numerical stability.

4 Summary

The main results of the paper analysis can be summarized in the following

**Lemma 1** If the gradient flow with normalization and weight decay converges to an interpolating solution with near-zero square loss, the following properties hold:

1. The global minima in the square loss with the smallest $\rho$ are the global minimum norm solutions and have the best margin and the best bound on expected error;

2. Conditions that favour convergence to such minimum norm solutions are batch normalization with weight decay ($\lambda > 0$) and small initialization (small $\rho$);

3. initialization with small $\rho(0)$ can be sufficient to induce a bias in the dynamics of GD leading to large margin minimizers of the square loss;

4. The condition $\partial f(x_j)/\partial V_k = V_k f(x_j)$ which holds at the critical points of the SGD dynamics that are global minima, is key in predicting several properties of the Neural Collapse [12];

5. the same condition represents a powerful constraint on the set of weight matrices at convergence.
4.1 Discussion

The role of the Lagrange multiplier term $\nu \sum_k ||V_k||^2$ in Equation [1] is different from a standard regularization term because $\nu$, determined by the constraint $||V_k|| = 1$ can be positive or negative, depending on the sign of the error $\nu = -\sum_n (\rho^2 f_n^2 - \rho y_n f_n)$. Thus the $\nu$ term acts as a regularizer when the norm of $V_k$ is larger than 1 but has the opposite effect for $||V_k|| < 1$, thus constraining each $V_k$ to the unit sphere. For the exponential loss, the situation is different and $\nu$ in $\nu \sum_k ||V_k||^2$ acts as a positive regularization parameter, albeit a vanishing one (for $t \to \infty$).

Are there any implications of the theory sketched here for mechanisms of learning in cortex? Somewhat intriguingly, some form of normalization, often described as a balance of excitation and inhibition, has long been thought to be a key function of intracortical circuits in cortical areas [16]. One of the first deep models of visual cortex models, HMAX, explored the biological plausibility of specific normalization circuits with spiking and non-spiking neurons. It is also interesting to note that the Oja rule describing synaptic plasticity in terms of changes to the synaptic weight is the Hebb rule plus a normalization term that corresponds to a Lagrange multiplier.

The main problems left open by this paper are:

- The analysis is so far restricted to gradient flow. It should be extended to gradient descent along the lines of [8].
- It is remarkable that for the case of no BN and no WD, the dynamical system still yields good results, provided initialization is small. The case of BN+WD is the only one which seems rather independent of initial conditions in our experiments.
- In this context, an extension of the analysis to SGD may also be critical for providing a satisfactory analysis of convergence.

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Figure 9: ConvNet, no Batch Normalization, no Weight Decay. Binary classification on two classes from CIFAR-10, trained with MSE loss. The model is a very simple network with 4 layers of fully-connected Layers. The ReLU nonlinearity is used. The weight matrices of all layers are initialized with zero-mean normal distribution, scaled by a constant such that the Frobenius norm of each matrix is either 5, 15 or 30. We run SGD with batch size 128, constant learning rate 0.1 and momentum 0.9 for 1000 epochs. No data augmentation. Every input to the network is scaled such that it has Frobenius norm 1.
Figure 10: **ConvNet, no Batch Normalization, no Weight Decay.** Dynamics of $\rho$ from experiments in Figure 9. First row: small initialization (5). Second row: large initialization (15). Third row: extra large initialization (30). A dashed rectangle denotes the previous subplot’s domain and range in the new subplot. More details to be added.
Figure 11: **ConvNet, no Batch Normalization, no Weight Decay.** Margin of all training samples