Implicit dynamic regularization in deep networks

Tomaso Poggio, Qianli Liao

Abstract

Square loss has been observed to perform well in classification tasks, at least as well as cross-entropy for which an asymptotic analysis is available. However, a theoretical justification is lacking. Here we discuss several observations on the dynamics of gradient descent under the square loss in RELU networks. We show how convergence to a local minimum norm solution is expected when normalization techniques such as Batch Normalization (BN) or Weight Normalization (WN) are used, in a way which is similar to the behavior of linear degenerate networks under GD, though the reason why zero-initial conditions are need for good generalization is different.
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Abstract

Square loss has been observed to perform well in classification tasks, at least as well as cross-entropy [1] for which an asymptotic analysis is available (see [2] and references therein). However, a theoretical justification is lacking. Here we discuss several observations on the dynamics of gradient flow under the square loss in RELU networks. We show how convergence to a local minimum norm solution is expected when normalization techniques such as Batch Normalization (BN) or Weight Normalization (WN) are used, in a way which is similar to the behavior of linear degenerate networks under GD, though the reason for zero-initial conditions is different. The properties of the minimizer that bounds its expected error are its norm and the rank of the local Jacobian, because among all the interpolating solutions the ones associated with small Frobenius norms of the weight matrices have better margin and better bounds on the expected classification error.

1 Introduction: why square loss

We start from the assumption that an explanation of the ability of deep RELU networks to be predictive requires the identification of a hidden mechanism of complexity control at work during the training of deep networks[1].

In the case of exponential-type loss functions such a mechanism has been identified in the asymptotic margin maximization effect of minimizing exponential-type loss functions [4, 5, 6]. However, this mechanism

• cannot explain the good empirical results that can be obtained using the square loss [1][2]
• cannot explain non-asymptotic convergence for cross-entropy loss minimization and its dependence on initialization.

This is the motivation for focusing here on the square loss.

In the paper we assume commonly used GD-based optimization algorithms such such as BN or WN, since such mechanisms seem essential for reliably training deep networks[7].

1 Complexity control should ensure CV stability of the solution (good stability implies good test error[4]).
2 Assuming that specific forms of gradient descent used in such experiments – such as momentum or batch normalization – are not hiding complexity control effects.
Our explanation for an implicit regularization in overparametrized deep nonlinear networks is similar to why GD converges to a minimal norm solution in the case of overparametrized linear systems. Crucially, our explanation requires normalization techniques such as BN or WN. We know that for overparametrized linear systems GD converges to the minimum norm solution for zero initial conditions but also that in the presence of normalization of the weights – by BN or similar algorithms – the convergence is independent of initial conditions (see Appendix E.1). Thus it is natural to conjecture that this same mechanism ensures generalization in a nonlinear system which can be linearized around a (degenerate) minimum.

In addition, we need to explain why regression works well for classification. Why and under which conditions there is a bias for larger margin solutions? We will show that the bias for large margin interpolating solutions (that minimize the square loss) depends on small initialization. The observation is that the norm $\rho$ of a minimizer (product of the Frobenius norms of the weight matrices of the network layers) is inversely related to its average margin (for definition of margin see \[E.3\]). Furthermore, under the assumption of separability, if $\rho$ is small, it will grow monotonically until a minimum is reached. Starting from small initialization, GD will explore minima with $\rho$ growing from zero. Thus small $\rho$ interpolating solutions which have the best margin can be found before large $\rho$ interpolating solutions (associated with NTK) with worse margin. Thus for best classification a small initialization is required here, as in the linear case, though the reason is quite different.

This note is a preliminary communication with more details, proofs and experiments to follow in a future update. We first provide the equations describing the dynamics of GD. Then we will describe results and conjectures. Details and experiments are in the Appendix.

2 The dynamics of GD in $\rho$ and $V_k$

2.1 Gradient descent

The natural approach to training deep networks for binary classification using the square loss is to use stochastic gradient descent to find the weights $W_k$ that minimize $L = \frac{1}{N} \sum_n \ell_n^2 = \frac{1}{N} \sum_n (g(x_n) - y_n)^2$, with $y = \pm 1$. In this note, we consider the flow associated with gradient descent instead of stochastic gradient descent.

2.2 Notation

- 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 (because the RELU is homogeneous \[E.8\]);
- in the following we use the notation $f_n$ meaning $f(x_n)$, that is the normalized network;
- we assume $||x|| = 1$ implying $||f(x)|| \leq 1$ at convergence;

\[3\]Minimizing the norm minimizes stability
2.3 Dynamics under normalization

Gradient descent on $L = \mathcal{L} + \lambda \sum_k V_k^2 = \sum_n (\rho f_n - y_n)^2 + \lambda \sum_k ||V_k||^2$ with $||V_k||^2 = 1$ is completely equivalent to “Weight Normalization”, as shown in [6], for deep networks. This dynamics can also 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 [7].

We assume that the dynamics captures the key normalization property of batch normalization though not several of the details (see discussions in [6]). Thus we assume that for network trained with BN, following the spirit of the analysis of [7], $\rho_k = 1, \ \forall k < L$ and $\rho_L = \rho$ where $L$ is the number of layers, yielding

$$\dot{\rho} = -2[\sum_n \rho (f_n)^2 - \sum_n f_n y_n] = -2 \sum_n \ell_n f_n,$$

where $\ell_n = \rho f_n - y_n$ and

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

More details about the derivation of the Equations are in A (see also [6]).

**Equilibrium values**

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

$$\rho_{eq} = \frac{\sum_n y_n f_n}{\sum_n f_n^2}.$$  

Observe that $\dot{\rho}_k > 0$ as long as $\rho$ is smaller than its equilibrium value and separability holds (in fact it is enough that $\sum_n f_n y_n > 0$).

Notice that, in general, classification with maximum margin is not minimum norm interpolation of the labels (see Appendix B.1).

At equilibrium – that is when $V_k = 0$ – we have

$$\sum_n (\rho f_n - y_n) \frac{\partial f_n}{\partial V_k} = \sum_n (\rho f_n - y_n) (V_{eq} f_n).$$

Notice that $\dot{\rho} = 0$ implies $\sum \ell_n f_n = 0$. Then $\dot{V}_k = 0$ implies $\sum \ell_n \frac{\partial f_n}{\partial V_k} = 0$; this latter condition implies the first one (multiply both sides by $V_k^T$).

In the appendix C we describe the very interesting dynamics associated with the un-normalized case. If under BN, during GD, other layers in addition to the last have $\rho_k$ different from 1 (which happens in practice), the dynamics shows some of the interesting properties described in the appendix, which favor even more small initializations to reach solutions with larger margin. The dynamics of Equation 19 is that the smaller $\rho_{t=0}$ is, the longer it takes to $\rho$ to grow (this

\[4\] In the case of $V_k$ the learning rate is different for WN vs. no-WN but the equilibrium values are again the same.
phenomenon becomes stronger with a larger number of layers $L$). Thus $\rho$ is constrained by the nonlinear dynamics to be very small for a transient phase $T$ of GD iterations ($T$ is longer with more layers and longer with smaller initialization).

Appendix D describes a few additional properties of the dynamics of the normalized weights.

The conclusions of this analysis can be summarized in

**Observation 1** Assuming separability, and GD starting from $\rho$ close to $\rho = 0$, $\rho$ grows monotonically until a minimum is reached at which $\rho_{eq} = \frac{\sum y_n f_n}{\sum f_n^2}$.

and

**Observation 2** Minimizers with small $\rho_{eq}$ correspond to large average margin $\sum y_n f_n$.

These two observations on the dynamics of the normalized weights are supported by our numerical experiments (see Figures).

### 3 Additional properties of minima and margin

In order to see the full implications of the two observations above we need two additional results. Since the global minima to which GD converges are typically degenerate (see references in [8]) with dimensionality $W - N$, where $W$ is the number of weights in the network, we need to characterize the convergence of the minimizer. In addition, the relation between margin – defined in terms of $\rho$ – and expected error must be formalized.

The first question leads to the following conjecture:

**Observation 3** The conjecture is that for each global minimum of the square loss $W^*$, gradient descent with BN converges to a minimizer with weights $W(X)$ (where $X$ is the training set) which depends on the pseudoinverse of the Jacobian $\frac{\partial f}{\partial W}$ at $W^*$ that has minimum norm (locally).

The conjecture is supported by the Theorem and the other arguments in Appendix E. We do not have a full proof.

The second question can be answered by using classical bounds that lead (see Appendix F) to the following theorem

**Observation 4** With probability $1 - \delta$

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

(5)

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

4
4 SGD and Generalization in Deep Networks: a proposal

Consider a minimum of GD for which the square loss is zero and $\dot{V}_k = 0$. Clearly critical points of $\rho$ do not exist if $\rho$ is too small. Since usually the maximum output of a network depending on the number of layers is $<< 1$) the first critical point for increasing $\rho$ will be when $\rho$ is large enough to allow the following equation to have solutions

$$\sum_n y_n f_n = \rho \sum_n f_n^2.$$  

(6)

If gradient descent starts from very small $\rho$ and there is 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 $\rho$, we expect many solutions under GF. The existence of many solutions is related to arguments showing the existence of NTK-based solutions: intuitively the last layer is enough in an extreme case – given enough overparametrization in the previous layers – to provide solutions for any set of random weights in the previous layers (for large $\rho$ and small $f_i$). Furthermore the intermediate layer do not need to change much under GD in the iterations immediately after initialization. The emerging picture is a landscape in which there cannot be interpolating minima for $\rho < 1$ and in practice for rather significantly larger $\rho$ than 1. With increasing $\rho$ from $\rho = 0$ there will be a global degenerate (see [9] ) minimum with the minimizer representing an interpolating solution with relatively large $\rho$ may be seen as an implicit constraint corresponding to

$$\min_{W_k} L = \sum (\rho f(x_i) - y_i)^2 \quad \text{s.t.} \rho \leq C$$

(7)

which is Ivanov regularization, which is itself “equivalent” to Tikhonov regularization with appropriate $\lambda(\rho)$.

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5 $\rho \geq 1$ for a critical point to exist because the critical point with smallest $\rho$ is for $\rho = 1$, $f_n y_n = 1$.

6 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.

7 Part of this behavior can be explained by the logistic equation in which the coefficients change with time, with $y_n f_n$ decreasing slowly. As a consequence, the rate of increase of $\rho$ decreases, though the asymptotic value of $\rho = \frac{\sum y_n f_n}{\sum f_n^2}$ increases.
Our claim is that since $\rho$ always increases from zero, after separability is reached, up to an equilibrium value, small initialization allow the gradient flow to find minima with small $\rho$ (and large margin), whereas large initialization makes this much more difficult because of the many minima encountered for decreasing $\rho$ at large $\rho$. Once a small $\rho$ minimum is found, then the behavior with BN or WN is similar to iterative gradient descent in the case of linear networks (see for instance [10]) with convergence to the local minimum norm solution\(^8\).

The summary is as follows. Assume that we have separation and that $\rho$ is small. $\rho$ will eventually grow (and $f_n$ will become smaller), until $\sum \rho f_n^2 = \sum y_n f_n$. Consider instead the case of a large $\rho$ initialization: $\rho$ will decrease until $\sum \rho f_n^2 = \sum y_n f_n$. There are many $V_k$ such that $f_n$ satisfying the condition are now easy to find. Of course, though they are perfectly good minimizers of the square loss, they are not good for classification because their $f_n$ are smaller and so the margins $y_n f_n$.

5 Summary

- Convergence to a local minimum norm solution is expected when normalization techniques such as Batch Normalization (BN) or Weight Normalization (WN) are used, in a way which is similar to the behavior of linear degenerate networks under GD.

- The bias towards large margin interpolating solutions (of minimum norm) depends on zero-initial conditions. Thus zero initial conditions induce GD to explore first the small

\(^8\)In the nonlinear case, the same behavior could be expected once GD is close to a minimum because around a degenerate minimum (local or global), the loss should be locally equivalent to a Morse-Bott function (we are thinking about a positive definite Hessian in some directions and degenerate in the others).
Figure 2: Results with a convolution network and batch normalization: Dynamics of $\rho$ from experiments in Figure 1. 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.
Figure 3: Results with a convolution network and batch normalization: Margin of all training samples

norm, large margin solutions and only later the large norm, small margin ones. The expected error of the minimum norm solution is bounded by the rank of the local Jacobian $\frac{\partial f_n}{\partial V_k}$ (at the minimum $W^*$), associated with the pseudoinverse in the solution. More relevant is that the bounds of Theorem 4 relate small $\rho$ margins to better bounds on the expected error.

• Equation 3 is a critical point for the dynamics of $\rho$ under GD but NOT under SGD. In the case of SGD the asymptotic value of $\rho$ for fixed $\sum f_i y_i$ can be expected to fluctuate randomly around the $\frac{\sum y_n f_n}{\sum f_n^2}$. Similar comments also apply to the dynamics of $V_k$.

• If we assume that the loss $L = \frac{1}{N} (\sum_n \rho^2 f_n^2 - 2 \sum_n y_n \rho f_n + N)$ is a continuous function of the $V_k$, then it will have at least one minimum at any fixed $\rho$, because its domain $V_k$ is compact. This means that for each $\rho$ there is at least a critical point for $V_k$.

• For GD under the exponential loss, in addition to the same initial dynamic regularization, we expect a margin maximization effect at long times as shown in [2]. Thus deep nets under the square loss are more likely to overfit at long times than under exponential-type loss functions (unless momentum or regularization is used). As a consequence, early stopping is more likely to be effective for the square loss than for exponential-type loss functions.

• Suppose we control $\rho_k$ independently of $V_k$ and of equation 19 can we find $\rho(t)$ schedules leading to solutions with better generalization?
Figure 4: Results with a convolution network and batch normalization: Histogram of $|f_n|$ over time. Top figure: initial $\rho_k = 0.1$. Bottom figure: initial $\rho_k = 5$. 

9
Notice that in the case of BN \( \frac{\partial g_n(W)}{\partial W_k} = \rho \frac{\partial f_n(V)}{\partial V_k} \) for \( k \neq L \) and \( \frac{\partial g_n(W)}{\partial W_L} = \frac{\partial f_n(V)}{\partial V_L} \) otherwise. This suggests that for all layers apart the final one, the Jacobians are \( \frac{\partial f_n(V)}{\partial V_k} = \frac{1}{\rho} \frac{\partial g_n(W)}{\partial W_k} \).

It seems that square loss reaches solutions with good test error in multiclass CIFAR10 faster than cross-entropy. Continuing GD, however, yields overfitting for the square loss (and worse test error) but not for cross-entropy. This is interesting because it validates the asymptotic complexity control we described in [11]. This suggests that in the experiments of Belkin et al. early stopping may play a role to obtain results with the square loss case that are as good or better than cross-entropy.

There are open questions, one of which is as follows. Under the assumption of early separability during the first iterations of GD, small initialization ensures that \( \rho \) grows for small values thus exploring first large margin minima. Why does GD have difficulties in converging in the absence of BN, especially for very deep networks? At the moment, the best answers are that

- BN is needed to ensure convergence to the minimum local norm
- good tuning of the learning rate is important and BN ensures autotuning [7].

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References


Figure 5: 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. 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 Batch
normalization. No weight decay. No data augmentation. Every input to the network is scaled
such that it has Frobenius norm 1.

A Gradient flow for $\rho$ and $V_k$

Gradient descent on $L = \frac{1}{N}(\sum_n g_n^2 - 2 \sum_n y_n g_n + N)$ (using $g_n = g(x_n)$) gives

$$\dot{W}_k = -\frac{2}{N} \sum_n (g_n - y_n) \frac{\partial g_n}{\partial W_k}$$

that is

$$\dot{W}_k = -\frac{\partial L}{\partial W_k} = -\frac{2}{N} \sum_n g_n \frac{\partial g_n}{\partial W_k} + \frac{2}{N} \sum_n y_n \frac{\partial g_n}{\partial W_k}$$

(9)

We now derive the dynamics of the norm and of the normalized weights. We define $g(x) = \rho f(x)$. $\rho$ is the product of the Frobenius norms of the weight matrices of the L layers in the
network. $f$ is the corresponding network with normalized weight matrices (because the RELU
is homogeneous [6]. In the following we use the notation $f_n$ meaning $f(x_n)$. We also assume
$||x|| = 1$ implying $||f(x)|| \leq 1$ at convergence;

A.1 Dynamics under normalization

Gradient descent on $L = \mathcal{L} + \lambda \sum_k V_k^2 = \sum_n (\rho f_n - y_n)^2 + \lambda \sum_k ||V_k||^2$ with $||V_k||^2 = 1$ is completely

Gradient descent on $L$ wrt $\rho_k$ gives, assuming $\rho = \rho_k^L$

$$\dot{\rho}_k = -\frac{\partial L}{\partial \rho_k} = -2 \sum_n (\rho_k^L f_n - y_n) f_n \rho_k^{L-1} = -2 \rho_k^{L-1} \left[ \sum_n \rho_k^L (f_n)^2 - \sum_n f_n y_n \right]$$

(10)

while assuming that $\rho_k = 1$, $\forall k < L$ and $rho_L = \rho$ gives
Figure 6: Dynamics of $\rho$ from experiments in Figure 5. 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.
\[ \dot{\rho} = -2 \sum_n \ell_n f_n. \quad (11) \]

Gradient descent on \( L \) wrt \( V_k \) gives
\[ \dot{V}_k = -\frac{\partial L}{\partial V_k} = -2 \sum_n (\rho f_n - y_n) \rho \frac{\partial f_n}{\partial V_k} - 2\lambda V_k. \quad (12) \]

Because of the constraint imposed via Lagrange multipliers \( ||V_k||^2 = 1 \), \( V_k^T \dot{V}_k = 0 \), which gives
\[ \lambda = -\sum_n (\rho^2 f_n^2 - \rho y_n f_n). \]

In summary, gradient descent on \( L \) wrt \( \rho \) and \( V_k \) gives
\[ \dot{\rho} = -2 \left[ \sum_n \rho (f_n)^2 - \sum_n f_n y_n \right] = -2 \sum_n \ell_n f_n. \quad (13) \]
where \( \ell_n = \rho f_n - y_n \) and
\[ \dot{V}_k = 2 \sum_n [(\rho f_n - y_n) \rho (\frac{\partial f_n}{\partial V_k}) + 2V_k \rho f_n (\rho f_n - y_n)] = 2\rho \sum_n [(\rho f_n - y_n) (V_k f_n - \frac{\partial f_n}{\partial V_k})] \quad (14) \]

Without BN \( \frac{\partial g_n(W)}{\partial W_k} = \frac{\rho}{\rho_k} \frac{\partial f_n(V)}{\partial V_k} \); with BN this becomes \( \frac{\partial g_n(W)}{\partial W_k} = \rho \frac{\partial f_n(V)}{\partial V_k} \), \( \forall k < L \) and
\[ \frac{\partial g_n(W)}{\partial W_k} = \frac{\partial f_n(V)}{\partial V_k}. \]

This dynamics – where there is a “vanishing” Lagrange multiplier \( \lambda \) – can also be written as
\[ \dot{\rho}_k = V_k^T \dot{W}_k \text{ and } \dot{V}_k = \rho S \dot{W}_k \text{ with } S = I - V_k V_k^T. \] This shows that if \( W_k = \rho_k V_k \) then \( \dot{V}_k = \frac{1}{\rho_k} \dot{W}_k \) as mentioned in [7].

Notice that \( \dot{\rho} = 0 \) if \( y_n f_n = 1 \) and \( \rho_k = 1; \rho_{eq} \) in Equation 3 is a critical point for the dynamics of \( \rho \) under GD. In the case of SGD the asymptotic value of \( \rho \) for fixed \( \sum f_i y_i \) may fluctuate randomly around the \( \sum y_n f_n \). Furthermore, the lowest possible value of \( \rho_k \) at equilibrium (\( \dot{\rho}_k = 0 \)) is \( \rho_k = 1 \) which can be achieved if \( y_n f_n \) is either \( 1 \) or \( 0 \). Values \( y_n f_n = 1, \rho = 1 \) are stationary points of the dynamics of \( V_k \) given by \( \dot{V}_k = 0 \): they are minimizers with zero square loss.
B Maximum margin and minimum norm

Lemma 1 [6] The maximizer of the margin when $\|V_k\| = 1$ is the minimum norm solution when the margin is $\geq 1$.

B.1 In general classification with maximum margin is not minimum norm interpolation of the labels (Lorenzo)

Minimum norm regression of binary labels is

$$\min_{W_k} \frac{1}{2} \|W_k\|^2, \quad \forall k \text{ subj. to } y_i f(W_K, \ldots, W_1; x_i) = 1, \quad i = 1, \ldots, N.$$  \hfill (15)

Minimum norm binary classification is

$$\min_{W_k} \frac{1}{2} \|W_k\|^2, \quad \forall k \text{ subj. to } y_i f(W_K, \ldots, W_1; x_i) \geq 1, \quad i = 1, \ldots, N.$$  \hfill (16)

Clearly classification involves minimizing over a larger class of functions than regression. The result will be in general different.

Observation 5 Minimum norm binary classification under the square loss with margin 1 (implying $f_V(x_i) \geq 1 \forall i$) is not (in general) interpolation of all the data.

Notice that hard margin SVM is a case in point: the SVs interpolate their data point, but other non-support vectors have margin greater than one.

C Un-normalized GD

Here we assume (for simplicity of derivations) that at initialization all the layers have the same norm, that is $\rho_k$ is the same for all $k$ at initialization. Because of this assumption we can use the following

Lemma 2 $\frac{\partial \rho^2}{\partial t}$ is independent of $k$.

to claim that all $\rho_k$ are the same at all times. Thus $\rho = \rho_k^L$, where $L$ is the number of layers.

Proof Consider $\frac{\partial \|W_k\|^2}{\partial t}$. The calculation follows the case for the exponential loss:

$$\frac{\partial \|W_k\|^2}{\partial t} = 2W_k \frac{\partial W_k}{\partial t} = 4 \sum_n g_n^2 + 4 \sum_n g_n$$  \hfill (17)

because of the structural lemma. Thus the time evolution of $\rho^2 = \|W_K\|^2$ is independent of $k$.

Then we obtain the dynamical system

$$\dot{\rho}_k = -\frac{\partial L}{\partial \rho_k} = -2 \sum_n (\rho_k^L f_n - y_n) f_n \rho_k^{L-1} = -2 \rho_k^{L-1} \left[ \sum_n \rho_k^L (f_n)^2 - \sum_n f_n y_n \right]$$  \hfill (18)
which can be rewritten in terms of \( \rho = \rho_k^L \) using \( \dot{\rho} = \sum_k \frac{\partial \rho_k}{\partial \rho_k} \dot{\rho_k} \) as

\[
\dot{\rho} = 2L \rho^2 L_k \sum_n f_n y_n - \sum_n \rho(f_n)^2
\]

(19)

which is an equation of the type known as “differential logistic equation” used for instance to model sigmoidal population growth. It has an interesting dynamics as shown in the simulations in the appendix (look at \( \rho \) for small initialization during the first 50 or so iterations). This is less the case for the BN dynamics of Equation 1.

The dynamics of Equation 19 is that the smaller \( \rho_t = 0 \) is, the longer it takes to \( \rho \) to grow (this phenomenon increase with larger number of layers \( L \)). Thus \( \rho \) is constrained by the nonlinear dynamics to be very small for a transient phase \( T \) of GD iterations (as we mentioned, \( T \) is longer with more layers and longer with smaller initialization) and then to grow slowly while \( f_n \) grows towards 1 (implying that \( \sum f_n^2 \) approaches \( \sum y_n f_n \)). The first part was analyzed in [12] for a similar dynamics.

D Dynamics and equilibria for \( V_k \) and \( \rho \)

Equation 4 suggests the following form for \( V_k^{eq} \) close to the minimum (when \( V_k = 0 \))

\[
V_k^{eq} = \sum_n \lambda_n \frac{\partial f_n}{\partial V_k}
\]

(20)

Notice that in general not all of the \( N \) terms in Equation 20 are different from zero or independent of each other (an upper bound is set by the rank of Jacobian \( \frac{\partial f_n}{\partial V_k} \)). As an example consider the degenerate linear case when \( f \) is a linear function.

D.1 Weight decay

Adding a term \( \lambda |W_k|^2 \) to the Lagrangian corresponding to weight decay will change the dynamics of \( \rho \) but not the dynamics of \( V_k \). The Equation for \( \rho \) becomes

\[
\dot{\rho}_k = -2\rho_k^L - \sum_n f_n (f_n)^2 - \sum_n y_n f_n - 2\lambda \rho
\]

(21)

and

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

(22)

with an equilibrium given by

\[\text{Since assuming that } \sum \lambda_n \neq \text{zero we obtain } V_k^{eq} = \sum_n \frac{\partial f_n}{\partial \rho_k} \lambda_n \div \sum_n \lambda_n f_n \]

\[\text{Equation 20 has the same general form as provided by the Fritz-John lemma for the solution of a constrained optimization problem.}\]
\[ \rho_{eq} = \frac{\sum y_n f_n}{\lambda + \sum f_n^2}. \] (23)

Notice that label noise – suggested by [13] – may play a role somewhat similar to a regularization \( \lambda \) by making \( \sum y_n f_n \) smaller, thus also decreasing the equilibrium \( \rho \) and biasing the final solution to have larger margin.

E Degenerate minima, rank and minimum norm

Consider a K-layers network \( f(W; x_i) \) parametrized by its weights \( W \).

We first consider a simple setup with simplifying assumptions. We discuss later how to weaken the requirements.

Consider the zero-loss, interpolating equations

\[ F(X, Y, W) = 0 \] (24)

where \( Z = X, Y \) is the training set, \( W \) is the set of weights across layers and \( F(X, Y, W) \) is a set of \( N \) equations, one for each of the \( N \) data points (columns of \( X \) and \( Y \)), that is

\[ F_j(X, Y, W) = f(W; x_j) - y_j, \quad j = 1, \ldots, N. \]

We assume \( X \in \mathbb{R}^{N_x}, Y \in \mathbb{R}^{N_y} \) and \( W \in \mathbb{R}^D \). Under assumptions of differentiability of \( F \), Equation 24 defines a mapping \( W(X, Y) \) in the neighborhood of the solution \( X^*, Y^*, W^* \) such that \( F(X, Y, W(X, Y)) = 0 \) in that neighborhood.

We state here an implicit function theorem for selections (reformulated from [14]) that does not require the Jacobian to be invertible

**Theorem 3** Consider the function \( F : X \times W \to Y \), that is \( F : \mathbb{R}^{N_x} \times \mathbb{R}^D \to \mathbb{R}^{N_y} \) with \( N_x = N_y = N < D \) along with the associated solution mapping

\[ S : X \to W \in \mathbb{R}^D | F(W, Z) = 0. \] (25)

Let \( F(W, Z) = 0 \) so that \( W^* \in S(Z^*) \). Assume that \( F \) is strictly differentiable at \( (X^*, W^*) \) and suppose that the partial Jacobian \( \nabla W F(X^*, W^*) \) is of rank \( M \leq N \). Then the mapping \( S \) has a “local selection” \( s \) around \( X^* \) for \( W^* \) which is strictly differentiable with Jacobian

\[ \nabla s(X) = A^T (AA^T)^{-1} \nabla_X f, \]

where \( A = \nabla_W F(W^*, X^*) \).

Notice that Brower’s invariance of domain theorem says that the inverse \( A^{-1} \) since \( N_y < D \) fails to have a localization which is single-valued. However, though multivalued, \( A^{-1} \) may contain a function with the property of single-valued localization for the case \( N_y = D \). Such functions are called “selections” [14]. In our case, \( \nabla_X W \) depends on the pseudoinverse of \( \nabla_W f \). Notice that the rank of \( \frac{\partial f}{\partial W} \) may be much less than full rank \( N \)

\[ ^{11} \text{In the appendix on minimizing the norm we show that when we minimize the norm subject to margin constraints, } W \text{ depends only on a subset of } X, \text{ the so called support vectors that are on the margin.} \]

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The relevance of the theorem for this paper is the statement about the existence of a differentiable function $W(x_1, \ldots, x_n)$ around the minimum $W^*$ and about its rank $M$, which depends on the rank of the Jacobian $\frac{\partial f}{\partial W}$.

Without WN or BN, gradient descent may converge to the degenerate minimum $W^*$ but in general without converging to the minimum norm (pseudoinverse) solution because $W$ will contain non-zero components outside the range of $A^T$. They correspond to non-zero initial conditions for convergence determined by the Jacobian. However, normalization algorithms such as WN or BN ensure that GD will converge to the local, linear pseudoinverse (see Appendix). Notice that BN or WN are not required for this to happen in the classification case of exponential loss functions; however, their presence induces convergence to a minimum norm solution to happen faster than the asymptotic effect of the exponential loss.

Notice that the rank of the product of two matrices is the minimum of the two ranks: this helps interpreting the implications of the statement in the theorem that $\nabla s(X) = A^T(AA^T)^{-1} \nabla_X f$. Notice also that the rank of $\nabla s(X)$ is an upper bound on the $CV_{\text{loo}}$ stability of the network since it corresponds to the number of independent training data to which $W^*$ sensitive. Thus the larger is the number of $y_n f_n$ that are significantly larger than zero, the better is the stability. Finally notice that if GD converges then $V_k = \frac{\partial f}{\partial V_k} = \nabla_{V_k} f$ as shown in the next subsections. The arguments in the previous section suggest that convergence will be to the $\rho V_k$ of minimum norm.

### E.1 Convergence of Linear Networks with Normalization

Consider the separable case of a linear network ($f(x) = \rho v^T x$) the dynamics is with $\ell_n = e^{-\rho y_n v^T x_n}$ for the exponential loss and $\ell_n = (\rho v^T x_n - y_n)$ for the square loss

\[
\dot{\rho} = \frac{1}{\rho} \sum_{n=1}^{N} \ell_n y_n v^T x_n \tag{26}
\]

and

\[
\dot{v} \propto \sum_{n=1}^{N} \ell_n (x_n - vv^T x_n). \tag{27}
\]

Let us assume that $\sum_{n=1}^{N} \ell_n y_n \neq 0$. Thus

\[
\dot{v} \propto \sum_{j=1}^{N} \alpha_j (I - vv^T) x_j. \tag{28}
\]

If gradient descent converges to $\dot{v} = 0$, the solution $v$ must satisfy $vv^T x = x$, where $x = \sum_{j=1}^{N} \alpha_j x_j$. Assume $||x|| = 1$. Then $v = x$. Since the operator $T$ in $v(t+1) = Tv(t)$ associated with equation \[28\] is not expanding [15] (because $v$ has unit norm), there is a fixed point $v = x$ which is independent of initial conditions.

\[\text{12}\text{For hard margin linear support vector machines we conjecture?? that the minimal number of SVs must be smaller than the rank of the data matrix}\]
**E.2 Convergence of Networks with Normalization**

Consider

$$\dot{V}_k = \propto (I - V_k V_k^T) \sum_{n=1}^{N} (y_n - \rho f_n) \frac{\partial f_n}{\partial V_k}.$$  \hspace{1cm} (29)

Let us define $$\alpha_j = (y_n - \rho f_n)$$ and an “average” $$f = \sum_j \alpha_j f_j$$. Then $$(I - V_k V_k^T) \frac{\partial f}{\partial V_k} = \dot{V}_k$$. If there is convergence that is $$\dot{V}_k = 0$$ then $$V_k f = \frac{\partial f}{\partial V_k}$$.

**F Margins, \( \rho \) and expected error**

Assuming that small initialization provides a bias towards solution with “large” margin, the next step is to use simple bounds [15] to claim better expected error (and better stability) for those solutions.

A typical generalization bound that holds with probability at least \((1 - \delta)\), \(\forall f \in \mathbb{F}\) has the form [15]:

$$|L(f) - \hat{L}(f)| \leq c_1 \mathbb{R}_N(\mathbb{F}) + c_2 \sqrt{\frac{\ln(\frac{1}{\delta})}{2N}}$$  \hspace{1cm} (31)

where $$L(f) = \mathbb{E}[\ell_{\text{gamma}}(f(x), y)]$$ is the expected loss, is the empirical loss, $$\mathbb{R}_N(\mathbb{F})$$ is the empirical Rademacher average of the class of functions $$\mathbb{F}$$ measuring its complexity; $$c_1, c_2$$ are constants that reflect the Lipschitz constant of the loss function and the architecture of the network. The loss function here is the ramp loss $$\ell_{\text{gamma}}(f(x), y)$$ defined as

$$\ell_{\text{gamma}}(y, y') = \begin{cases} 1 & \text{if } yy' \leq 0, \\ 1 - \frac{yy'}{\gamma} & \text{if } 0 \leq yy' \leq \gamma, \\ 0 & \text{if } yy' \geq \gamma. \end{cases}$$

We define $$\ell_{\text{gamma}=0}(y, y')$$ as the standard 0–1 classification error and observe that $$\ell_{\text{gamma}=0}(y, y') < \ell_{\text{gamma}>0}(y, y')$$.

As in the linear case we now consider two solutions with zero empirical loss of the square loss regression problem obtained with the same RELU deep network and corresponding to two different minima with two different $$\rho$$s. Let us call them $$\rho_a f^a(x)$$ and $$\rho_b f^b(x)$$. Using the notation of this paper, the functions $$f_a$$ and $$f_b$$ correspond to networks both with normalized weight matrices at each layer.

Let us assume that $$\rho_a < \rho_b$$.

We now use the observation that, because of homogeneity of the networks, the empirical Rademacher complexity satisfies the property,

$$\mathbb{R}_N(\mathbb{F}) = \rho \mathbb{R}_N(\bar{\mathbb{F}}),$$  \hspace{1cm} (32)
where $F$ is the space of functions of our unnormalized networks and $\tilde{F}$ denotes the corresponding normalized networks. This observation allows us to use the bound Equation 31 and the fact that the empirical $\hat{L}_\gamma$ for both functions is zero (if $\gamma < \rho_a$) to write

$$L_0(f^a) = L_0(F^a) \leq c_1 \rho_a \mathbb{R}_N(\tilde{F}) + c_2 \sqrt{\frac{\ln(\frac{1}{\delta})}{2N}}$$

and

$$L_0(f^b) = L_0(F^b) \leq c_1 \rho_b \mathbb{R}_N(\tilde{F}) + c_2 \sqrt{\frac{\ln(\frac{1}{\delta})}{2N}}.$$

The bounds have the form

$$L_0(f^a) \leq A \rho_a + \epsilon \quad (33)$$

and

$$L_0(f^b) \leq A \rho_b + \epsilon \quad (34)$$

Thus the bound for the expected error $L_0(f^a)$ is better than the bound for $L_0(f^b)$.

### F.1 The Linear Case

Consider two different linear problem where the interpolating minimizers of the square loss are respectively $F^a(x) = \rho_a f^a(x) = \rho_a v^T a x$ and $F^b(x) = \rho_b f^b(x) = \rho_b v^T b x$ with $||v_a|| = ||v_b|| = 1$. Let us assume that $\rho_a < \rho_b$. We then know (from Lemma 15 in Akshay+Lorenzo+Poggio) that the upper bound on the $CV_{\text{loo}}$ stability for $f_b$ is $\rho_b$ and for $f_a$ is $\rho_a$. Thus the bound on stability and expected error of $f_a$ vs. $f_b$ is $\rho_a / \rho_b$ times smaller.

### F.2 Remarks

It would be interesting to avoid the use of the margin bounds and connect directly the lower margin (and large norm) solutions to lower stability. A possible way to proceed is to use the argument in section F.1 applying it to the Jacobian $\nabla s(X)$. Another approach would be to connect the regression setup of this paper with a constrained optimization in which results such as the Fritz John lemma could be applied.

Notice that stability (and expected error) is upper bounded by the rank of the Jacobian at $W^*$ which is at most $N$. Equation 20 shows that $V_k$ depends on the $\frac{\partial f}{\partial V_k}$ with $M$ non-zero coefficients, where $M$ is related to the rank of the Jacobian of $f(X; V)$ wrt $V_k$. In particular, if $M = N_y$ that is the number of data points, the $CV_{\text{loo}}$ stability of such a solution will be poor. On the other hand, if $M \ll N_y$, then we expect good stability and low expected error.

Notice also is that $\rho$ is by itself a measure of complexity of the hypothesis space; interestingly small $\rho$ roughly correlates with large “average” margin here that is with $\sum y_n f_n / \sum f_n^2$.

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13Furthermore, the Rademacher complexity of the space of functions associated with normalized networks of the same architecture is the same (see [17]).

14Every choice of a leave-one-out example will induce a change in $V_k$

15The former is the case of CiFAR with random labels; the latter is the case of CIFAR with natural labels.
G Networks with Normalization under Exponential Loss

Consider

\[ \dot{V}_k = \propto N \sum_{n=1}^{N} e^{-\rho y_n f_n} y_n \left( \frac{\partial f_n}{\partial V_k} - V_k V_k^T \frac{\partial f_n}{\partial V_k} \right) = (I - V_k V_k^T) \sum_{n=1}^{N} e^{-\rho y_n f_n} y_n \frac{\partial f_n}{\partial V_k}. \] (35)

Let us define \( \alpha_j = y_j e^{-\rho y_j f_j} \) and an “average” \( f = \sum_j \alpha_j f_j \). Then \( (I - V_k V_k^T) \frac{\partial f}{\partial V_k} = \dot{V}_k \). If there is convergence that is \( \dot{V}_k = 0 \) then

\[ V_k f = \frac{\partial f}{\partial V_k}. \] (36)

Notice that the solution is given in an implicit way assuming convergence since \( f \) depends on \( V_k \).