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Tomaso Poggio and Qianli Liao

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Generalization in deep network classifiers trained with the square loss

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Abstract

Square loss has been observed to perform well in classification tasks. However, a theoretical justification is lacking, unlike the cross-entropy [1] case for which an asymptotic analysis has been proposed (see [2] and [3] and references therein). Here we discuss several observations on the dynamics of gradient flow under the square loss in ReLU networks. We show that convergence to a solution with the absolute minimum norm is expected when normalization techniques such as Batch Normalization[4] (BN) or Weight Normalization[5] (WN) are used together with Weight Decay (WD). In the absence of BN+WD, good solutions for classification may still be achieved because of the implicit bias towards small norm solutions in the GD dynamics introduced by close-to-zero initial conditions. 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. 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

1.1 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 mechanism of complexity control at work during the training of deep networks.

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 [6, 2, 7]. However, this mechanism

- cannot explain the good empirical results that have been recently demostrated using the square loss[8];
- 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.

Here we *assume* commonly used GD-based normalization algorithms such such as BN (or WN) together with weight decay (WD), since such mechanisms seem essential for reliably training deep networks (and were used by [8])[9]. Crucially, our analysis depends on these assumptions[1].

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). A few preliminary remarks are helpful for understanding. Unlike the case of linear networks we expect several global zero square loss minima corresponding to interpolating solutions (in general degenerate, see [10] 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. Why and when we expect the solutions of the regression problem to have large margin? We will show that the bias for large margin interpolating solutions depends on weight decay and initialization of the weights close to zero. As we will define later more formally, the function corresponding to a deep network can be written as $g(x_n) = \rho f_n$ where $g(x_n)$ is the output of the network for the training example x_n, ρ is the product of the Frobenius norms of the weight matrices of the network and $f_n = f(x_n)$ is the output of the normalized network for the input x_n. Notice that if g is a zero loss solution of the regression problem, then $g(x_n) = y_n, \quad \forall n$. This is equivalent to $\rho f_n = y_n$ where f_n is the *margin* for x_n. Thus the norm ρ of a minimizer is inversely related to its average margin (see Appendix C). 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 $\frac{1}{\rho_{eq}}$. As we will see in the next section, under the assumption of separability (with BN and weight decay or without), if ρ is small at initialization, it will grow monotonically under GD until a critical point of the gradient flow dynamics is reached. In other words, starting from small initialization, GD will explore critical points with ρ growing from zero. Thus quasi-interpolating solutions with small ρ_{eq} (corresponding to the best margin) may be found before large ρ_{eq} quasi-interpolating solutions which have worse margin (and are likely to be associated with the NTK regime). If the weight decay parameter is large enough, there may be independence from initial conditions. Otherwise, a small initialization is required, as in the case of linear networks, though the reason is quite different.

[1] We know that for overparametrized linear systems GD converges to the minimum norm solution if the weights are initialized close to zero values.

2 The dynamics of GD in ρ and V_k

2.1 Notation

We define[2] a deep network with L layers with the usual coordinate-wise scalar activation functions $\sigma(z): \quad \mathbf{R} \to \mathbf{R}$ as the set of functions $g(W;x) = (W_L\sigma(W_{L-1}\cdots\sigma(W_1x)))$, where the input is $x \in \mathbf{R}^d$, 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 ρ 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 [7]);
- in the following we use the notation f_n meaning $f(x_n)$, that is the ouput of the normalized network for the input x_n;
- we assume $||x|| = 1$ implying[3] $|f(x)| \leq 1$ at convergence;
- the following structural property of the gradient of deep ReLU networks is useful (Lemma 2.1 of [11]):

$$\sum_{i,j} \frac{\partial g(W;x)}{\partial W_k^{i,j}} W_k^{i,j} = g(W;x); \tag{1}$$

  for $k = 1, \cdot, L$. Equation 1 can be rewritten as an inner product between W_k *as vectors*:

$$(W_k, \frac{\partial g(W;x)}{\partial W_k}) = g(W;x) \tag{2}$$

  where W_k is here the vectorized representation of the weight matrices W_k for each of the different layers. We use this vectorized notation in a few places, hoping it will not confuse the reader. Notice that Equation 1 must be used with care: the W_k matrix depends on x and on the network!

- we assume that $L \geq 2$. The main reason is to avoid the case of linear networks with a unique minimizer of the square loss;
- *separability* is defined as correct classification for all training data, that is $y_n f_n > 0, \quad \forall n$. We call *average separability* when $\sum y_n f_n > 0$.

[2] For more details about basic properties, see [7].

[3] Because $f(x)$ has the form of products of matrices of norm 1 (see Equation 50.

2.2 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 $\mathcal{L} = \frac{1}{N}\sum_n \ell_n^2 = \frac{1}{N}\sum_n^N (g(x_n) - y_n)^2$, with $y = \pm 1$. In this note, we consider the *gradient flow* associated with gradient descent.

2.3 Dynamics under normalization and weight decay

Gradient descent on a modified loss

$$\mathcal{L} = \sum_n (\rho f_n - y_n)^2 + \nu \sum_k ||V_k||^2 \tag{3}$$

with $||V_k||^2 = 1$ is equivalent to "Weight Normalization", as proved in [7], 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 [9].

The *key assumption* in this paper is that the dynamics above with Lagrange multipliers, captures the key normalization property of batch normalization, though not all of its details (see Appendix A and discussions in [7] and also [9]). Thus *we assume that for network trained with BN*, following the spirit of the analysis of [9], $\rho_k = 1, \quad \forall k < L$ and $\rho_L = \rho$ where L is the number of layers. 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 [7] 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. The normalization of each weight matrix yields, as shown in Appendix 2.3, $\nu = -\sum_n (\rho^2 f_n^2 - \rho y_n f_n)$.

As we will show, the dynamical system associated with the gradient flow of the Lagrangian of Equation 3 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 (see Appendix E.1) consists of a regularization term $\lambda ||W_k||^2$ added to the Lagrangian yielding

$$\mathcal{L} = \sum_n (\rho f_n - y_n)^2 + \nu \sum_k ||V_k||^2 + \lambda \rho^2. \tag{4}$$

The associate gradient flow is then the following well-defined dynamical system

$$\dot{\rho} = -2[\sum_n \rho (f_n)^2 - \sum_n f_n y_n] - 2\lambda\rho \tag{5}$$

$$\dot{V}_k = 2\rho \sum_n [(\rho f_n - y_n)(V_k f_n - \frac{\partial f_n}{\partial V_k})] \tag{6}$$

where the critical points $\dot{\rho} = 0, \quad \dot{V_k} = 0$ are not singular for any arbitrarily small $\lambda > 0$. For $\lambda = 0$ the zero loss critical point is pathological, since $\dot{V_k} = 0$ even when $(V_k f_n - \frac{\partial f_n}{\partial V_k}) \neq 0$ implying that a un-normalized interpolating solution can satisfy the equilibrium equations. Numerical simulations show that even for linear degenerate networks convergence is independent of initial conditions only if $\lambda > 0$. In particular, normalization is then effective at ρ_{eq}, unlike the $\lambda = 0$ case. As a side remark, SGD, as opposed to gradient flow, may help (especially with label noise) to counter the singularity of the $\lambda = 0$ case, even without weight decay, because of the associated random fluctuations around the pathological critical point.

2.3.1 Equilibrium values

The equilibrium value at $\dot{\rho_k} = 0$ is[4] (see Appendix E.1)

$$\rho_{eq} = \frac{\sum_n y_n f_n}{\lambda + \sum_n f_n^2}. \tag{7}$$

Observe that $\dot{\rho} > 0$ if ρ is smaller than ρ_{eq} and if average separability holds. Recall also that zero loss "global" minima (in fact arbitrarily close to zero for small but positive λ) are expected *to exist and be degenerate* [10].

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 ρ, because the domain V_k is compact.* This means that for each ρ there is at least a critical point[5] of the gradient flow of V_k, implying that for *each critical ρ for which $\dot{\rho} = 0$, there is at least one critical point of the dynamical system in ρ and V_k.*

Around $\dot{V_k} = 0$ we have

$$\sum_n (\rho f_n - y_n) \frac{\partial f_n}{\partial V_k} = \sum_n (\rho f_n - y_n)(V_k^{eq} f_n), \tag{8}$$

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

In appendix D we describe the interesting dynamics associated with the unnormalized case (when ρ_k are all the same $\forall k, \quad k = 1, \cdots, L$). If during GD (with BN), other layers, in addition to the last, have ρ_k different from 1 (which happens in practice), the dynamics will show some of the interesting properties described in appendix D, which favor small initializations to reach solutions with greater margin. The dynamics of Equation 28 is that the smaller $\rho_{t=0}$ is, the longer it takes to ρ to grow (this phenomenon becomes stronger with a larger number of layers L). Thus ρ 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 E describes a few additional properties of the dynamics of the normalized weights.

The conclusions of this analysis can be summarized in

[4] Notice that $\dot{\rho} = 0$ is equivalent to $\sum \ell_n f_n = 0$. Thus the two conditions together – $\dot{\rho} = 0$ and $\dot{V_k} = 0$ – imply $\sum \ell_n \frac{\partial f_n}{\partial V_k} = 0$.

[5] If $V_k f_n = \frac{\partial f_n}{\partial V_k}$ then $\dot{V_k} = 0$ but this is not a critical point for the system ρ, V_k unless $\dot{\rho} = 0$.

Observation 1 *Assuming average separability, and gradient flow starting from $\rho = \epsilon$ with small $\epsilon > 0$, ρ grows monotonically until a minimum is reached at which $\rho_{eq} = \frac{\sum_n y_n f_n}{\lambda + \sum_n f_n^2}$. In the limit $\lambda = 0$, the minimum of the square loss approaches zero, corresponding to exact interpolation of all the training data.*

and

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

In general, there may be several critical points of the V_k for the same ρ_{eq} and they are typically degenerate (see references in [12]) 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. The dynamic leading to ρ_{eq} and V_k^{eq} requires an analysis not just of gradient flow but of SGD and of the associated Fokker-Planck equation.

3 Dynamics

Consider a minimum of GD for which the square loss is close to zero and $\dot{V}_k = 0$. Clearly critical points of ρ cannot exist if ρ is too small[6]. Since usually the maximum output of a multilayer network is $<< 1$, the first critical point for increasing ρ will be when ρ becomes large enough to allow the following equation to have solutions

$$\sum_n y_n f_n = \rho(\lambda + \sum_n f_n^2). \tag{9}$$

If gradient flow starts from very small ρ and there is *average separability*, ρ increases monotonically until such a minimum is found[7]. If ρ is large, then $\dot{\rho} < 0$ and ρ will decrease until a minimum is found.

For large ρ and very small or zero λ, we expect several solutions under GD[8]. The existence of several solutions is related to arguments showing the existence of NTK-based solutions: intuitively the last layer is enough in an extreme case – if the last layer before the linear classifier is overparametrized wrt training data – to provide solutions for *any* set of random weights in the

[6] $\rho \geq 1$ for a critical point to exist because the critical point with smallest possible ρ is for $\rho = 1, f_n y_n = 1$.

[7] This analysis is for gradient flow. A satisfactory theory requires an analysis of gradient descent along the lines of [9]

[8] It is interesting to recall [10] that for SGD – unlike GD – the algorithm will stop only when $\ell_n = 0 \quad \forall n$, 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 may fluctuate around the critical point.

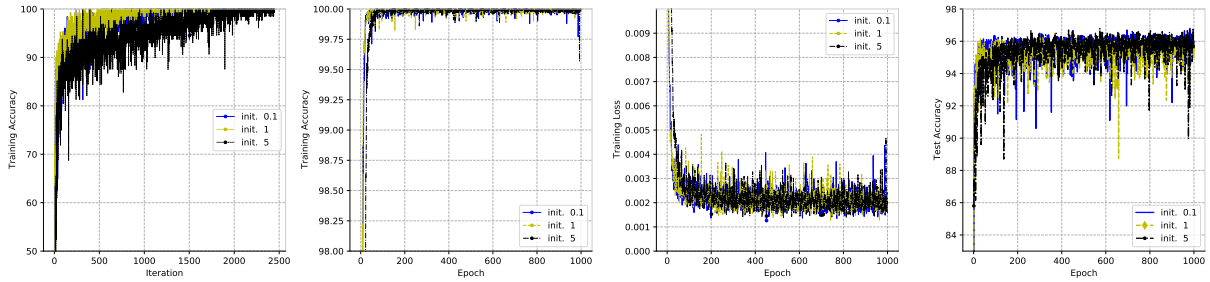


Figure 1: ***ConvNet with Batch Normalization and Weight Decay*** *Binary classification on two classes from CIFAR-10, trained with MSE loss. The model is a very simple network with 4 layers of fully-connected Layers. ReLU nonlinearity is used. Batch normalization is used. The weight matrices of all layers are initialized with zero-mean normal distribution, scaled by a constant such that the Frobenius norm of each matrix is 5. We use weight decay of 0.01. We run SGD with batch size 128, constant learning rate 0.1 and momentum 0.9 for 1000 epochs. No weight decay. No data augmentation. Every input to the network is scaled such that it has Frobenius norm 1.*

previous layers (for large ρ 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 are no zero-loss minima for $\rho < \rho_{min}$ (which, in practice, means $\rho_{min} >> 1$). With increasing ρ from $\rho = 0$ there will be zero square-loss degenerate (see [10]) minima with the minimizer representing an interpolating (for $\lambda = 0$) or almost interpolating solution (for $\lambda > 0$)[9]. We expect, however, that if λ is sufficiently large there will be a strong bias towards the minimum ρ_{eq}, even for large ρ initializations.

All these observations are also supported by our numerical experiments. Figure 1, 2, 3, 4 and 5 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.

4 Generalization in Deep Networks

In this section we prove formally that ρ, which is inversely related to the margin, as we discussed, indeed controls the expected error. We use classical bounds that lead (see Appendix F) to the following theorem

[9]Notice that the equilibrium value of ρ is a measure of "sparsity": small ρ corresponds to f_i being close to either 1 or zero (ρ is in the order of $\frac{1}{f_i}$).

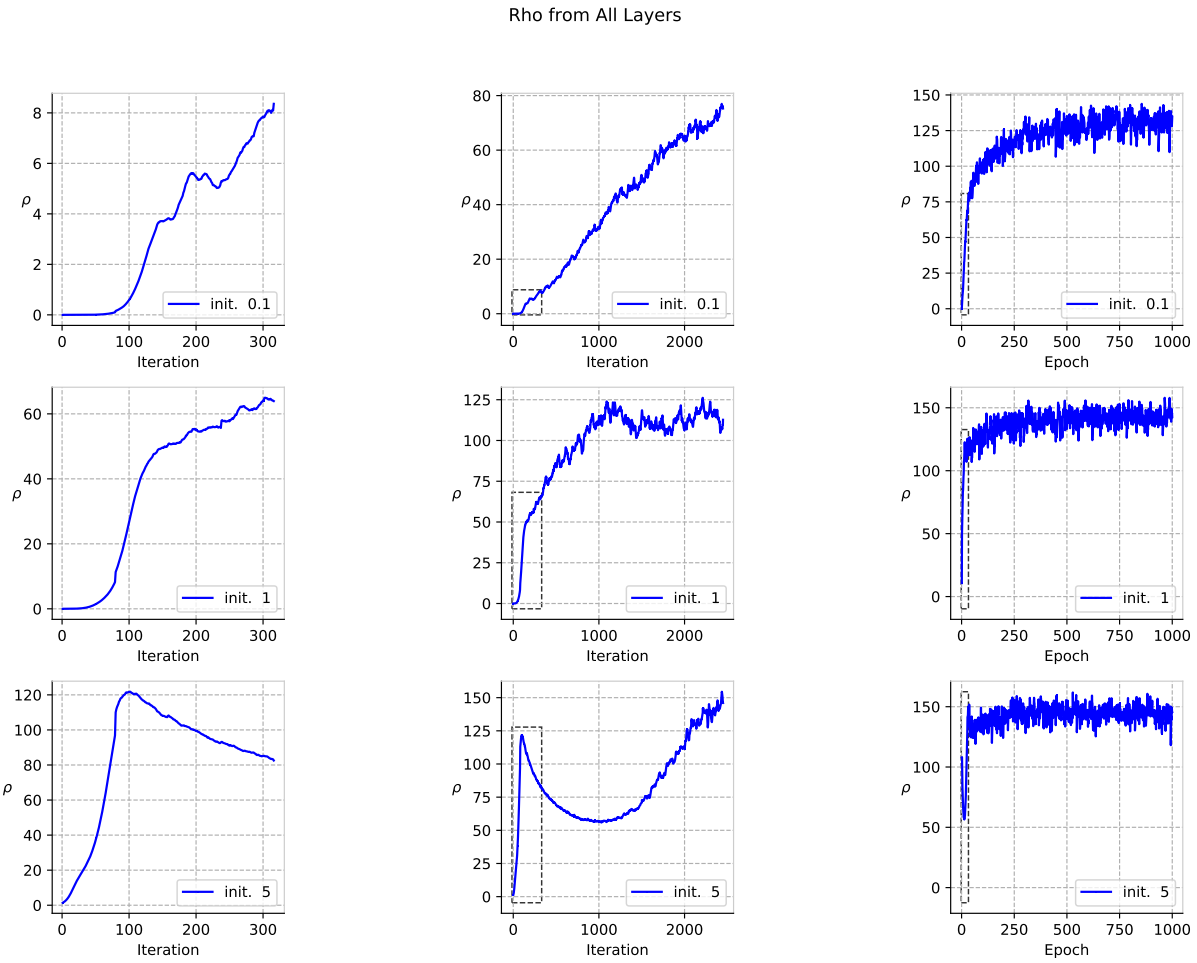


Figure 2: ***ConvNet with Batch Normalization and Weight Decay*** *Dynamics of ρ from experiments in Figure 1. First row: small initialization (0.1). Second row: medium initialization (1). Third row: large initialization (5). A dashed rectangle denotes the previous subplot's domain and range in the new subplot.*

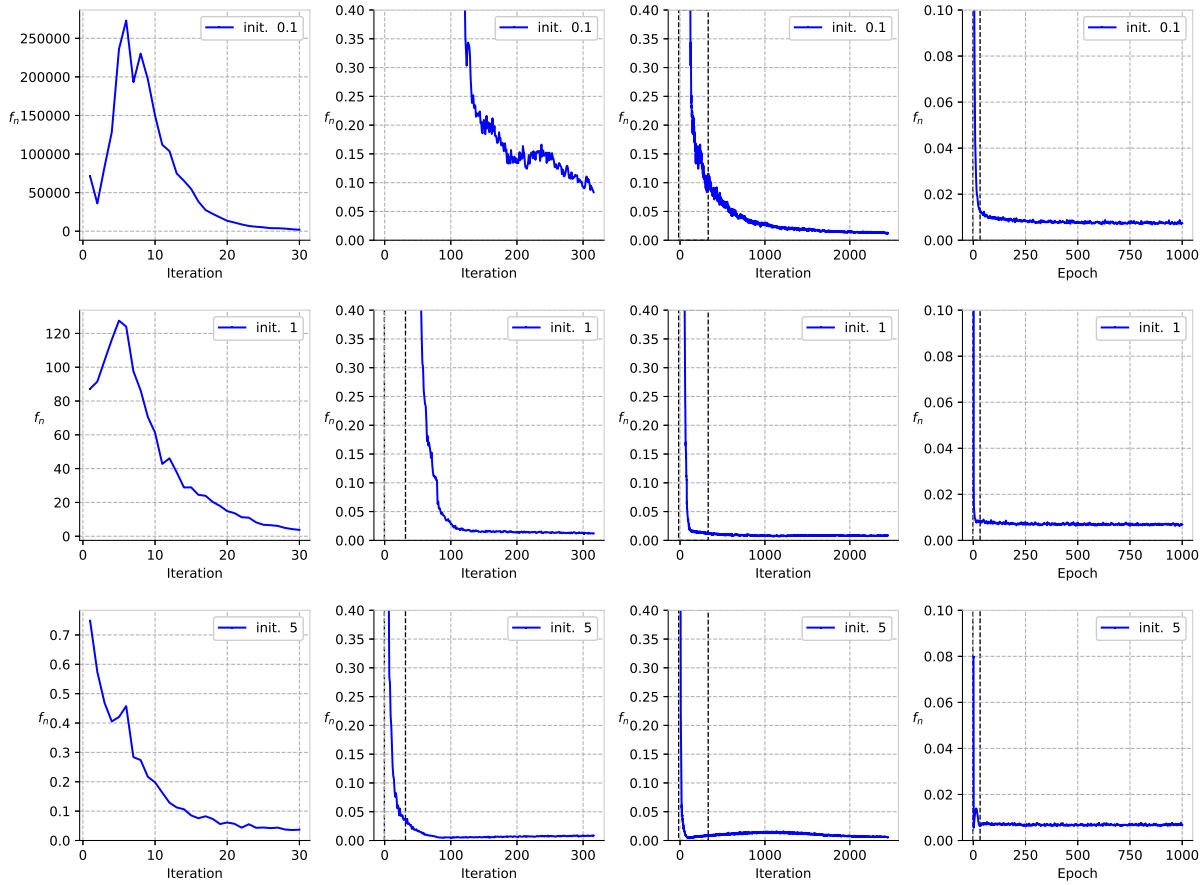


Figure 3: ***ConvNet with Batch Normalization and Weight Decay*** *Dynamics of the average of $|f_n|$ from experiments in Figure 1. First row: small initialization (0.1). Second row: medium initialization (1). Third row: large initialization (5). A dashed rectangle denotes the previous subplot's domain and range in the new subplot.*

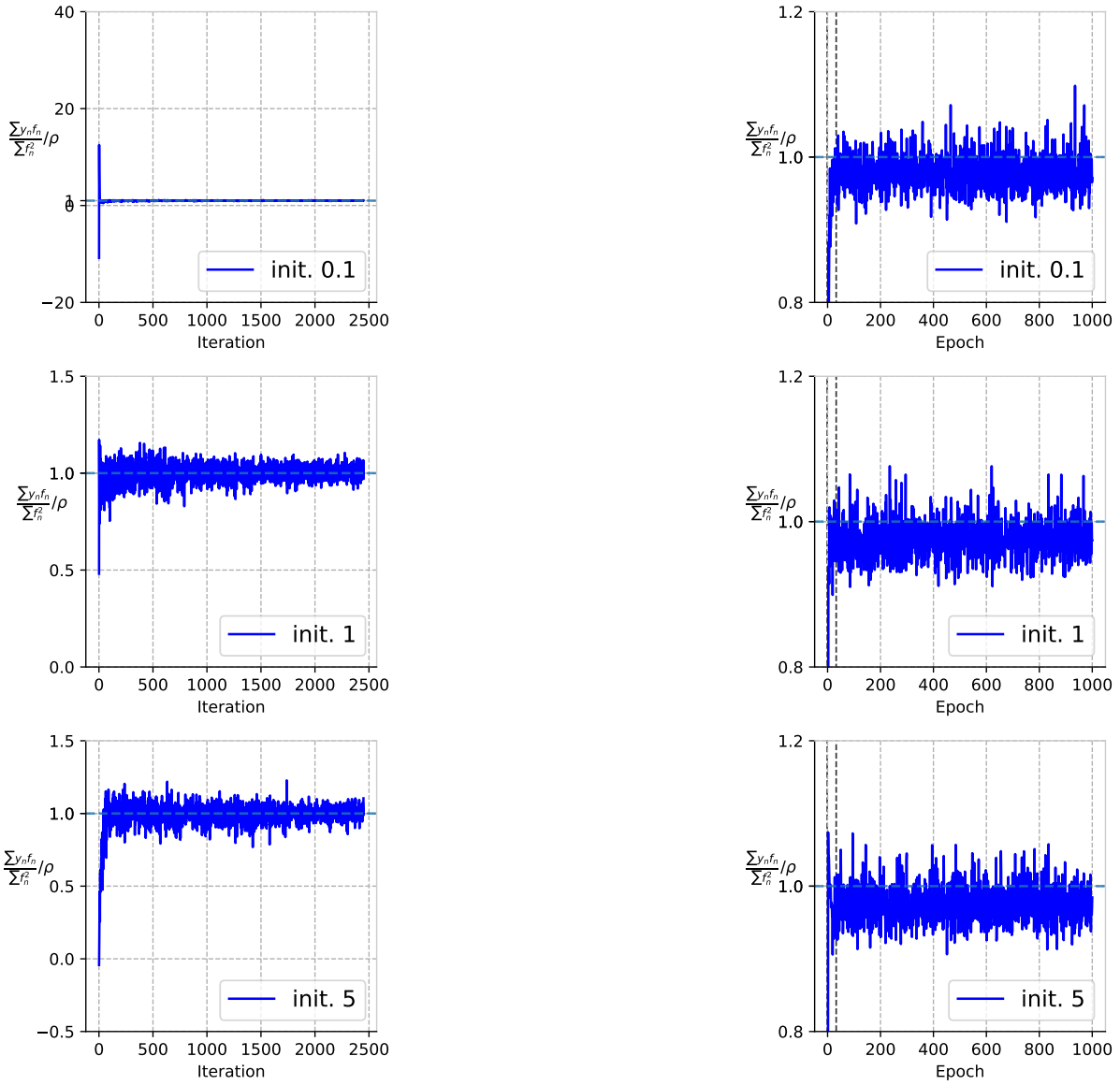


Figure 4: ***ConvNet with Batch Normalization and Weight Decay*** *Ratio of* $\frac{\sum y_n f_n}{\sum f_n^2}$ *and* ρ. *First row: small initialization (0.1). Second row: medium initialization (1). Third row: large initialization (5).*

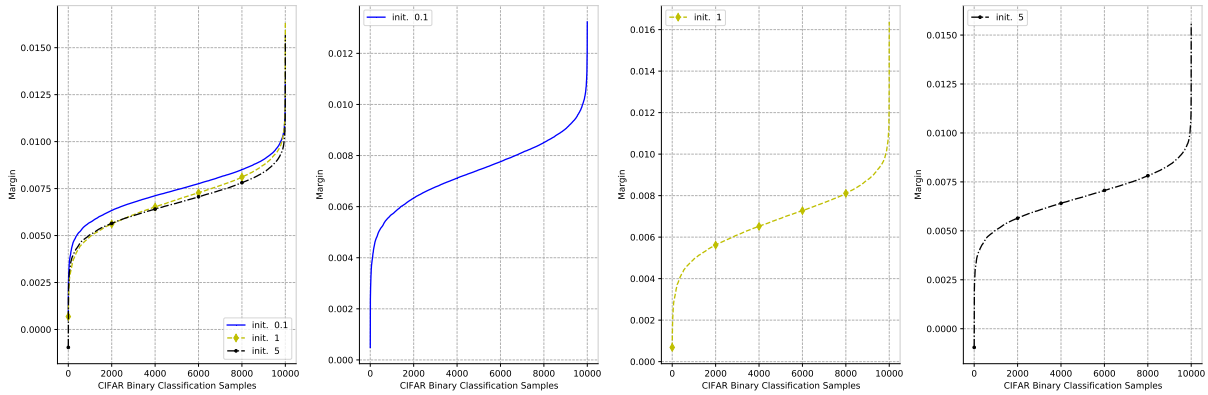


Figure 5: ***ConvNet with Batch Normalization and Weight Decay*** *Margin of all training samples.*

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

$$L(f) \leq c_1 \rho \mathbb{R}_N(\tilde{\mathbb{F}}) + c_2 \epsilon(N, \delta) \tag{10}$$

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* $\mathbb{R}_N(\tilde{\mathbb{F}})$ *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* ρ*.*

The theorem proves the conjecture in [13] that for deep networks, as for kernel machines, *minimum norm interpolating solutions are the most stable.*

5 Predictions

- In a recent paper Papyan, Han and Donoho[14] 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 Appendix G that

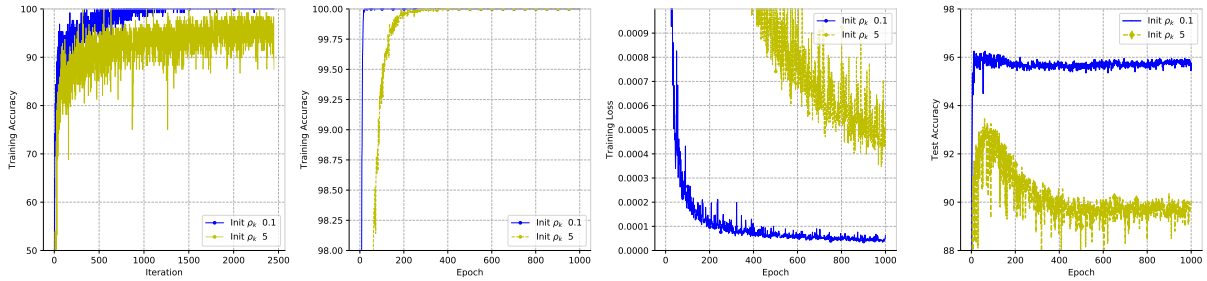


Figure 6: ***ConvNet with Batch Normalization but no Weight Decay*** *Binary classification on two classes from CIFAR-10, trained with MSE loss. The model is a very simple network with 4 layers of convolutions. ReLU nonlinearity is used. Batch normalization is used without parameters (affine=False in 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.*

these *properties of the Neural Collapse[14] 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 ρ_{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 (in the Appendix) that they should hold also in the case of crossnetropy, explored in [14].

- At a close to zero loss critical point of the flow, Equations 36 become (see Appendix E.3) $\nabla_{V_k} f(x_j) = V_k f(x_j)$ 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, explained in the Appendix,

$$V_k f = [V_L D_{L-1}(x) V_{L-1} \cdots V_{k+1} D_k(x)]^T D_{k-1}(x) V_{k-1} D_{k-2}(x) \cdots D_1(x) V_1 x, \qquad (11)$$

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 the Appendix *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. The current analysis (in Appendix H) of the constraint equation is quite limited since it holds only for deep linear networks: a full analysis is still missing. Interestingly, randomly initialized weight matrices (an extreme case of the NTK regime) are approximately orthogonal.

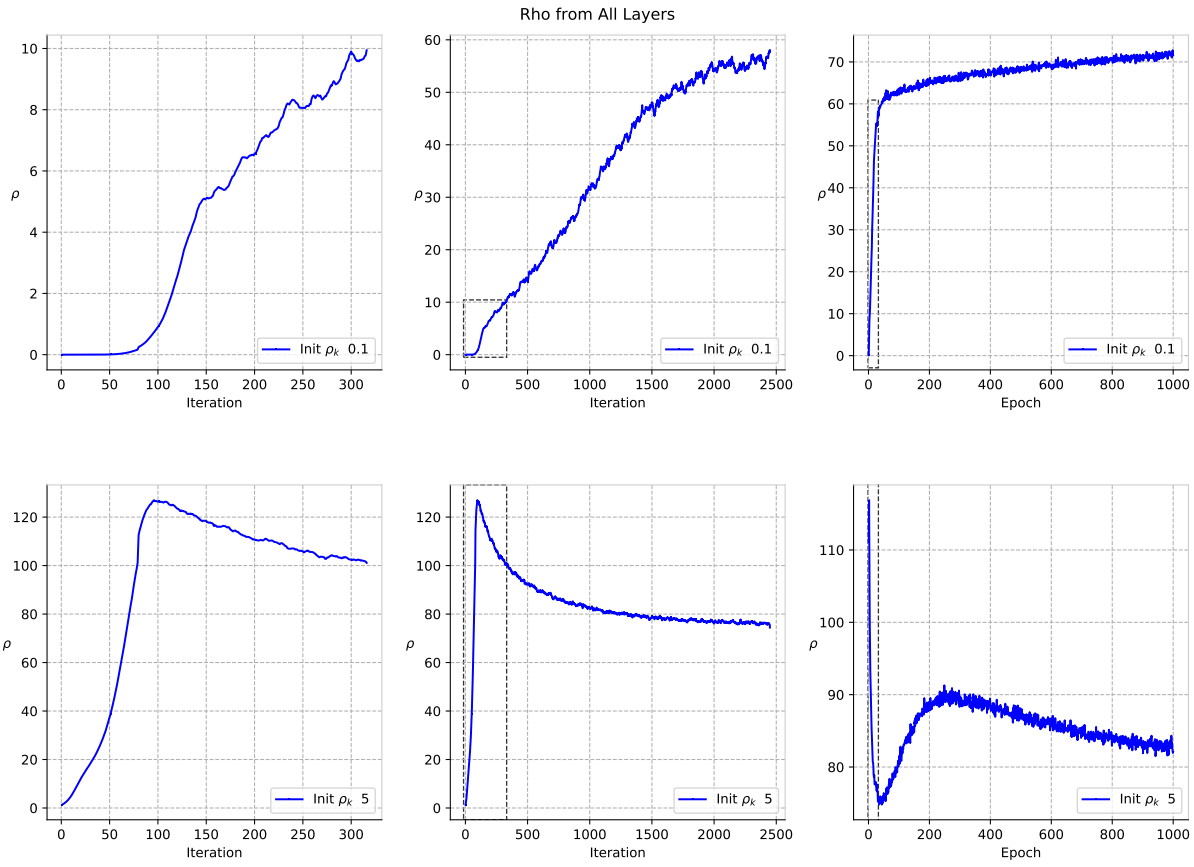


Figure 7: ***ConvNet with Batch Normalization but no Weight Decay***. *Dynamics of ρ from experiments in Figure 6. Top row: small initialization (0.1). Bottom row: large initialization (5). The plot starts with $\rho(0) = 0$ despite an initialization of $\rho_k = 0$ because the the scaling factor of BN starts from 0. A dashed rectangle denotes the previous subplot's domain and range in the new subplot.*

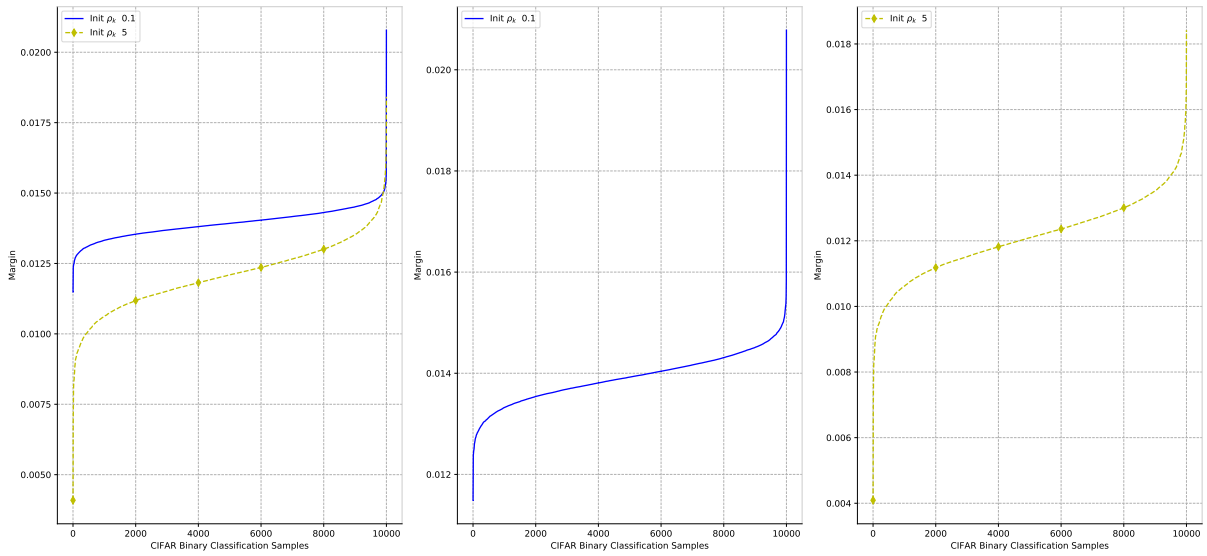


Figure 8: ***ConvNet with Batch Normalization but no Weight Decay***. *Margin of all training samples (see previous figures). If the solution were to correspond to exactly zero square loss, the margin distribution would be an horizontal line.*

6 Summary

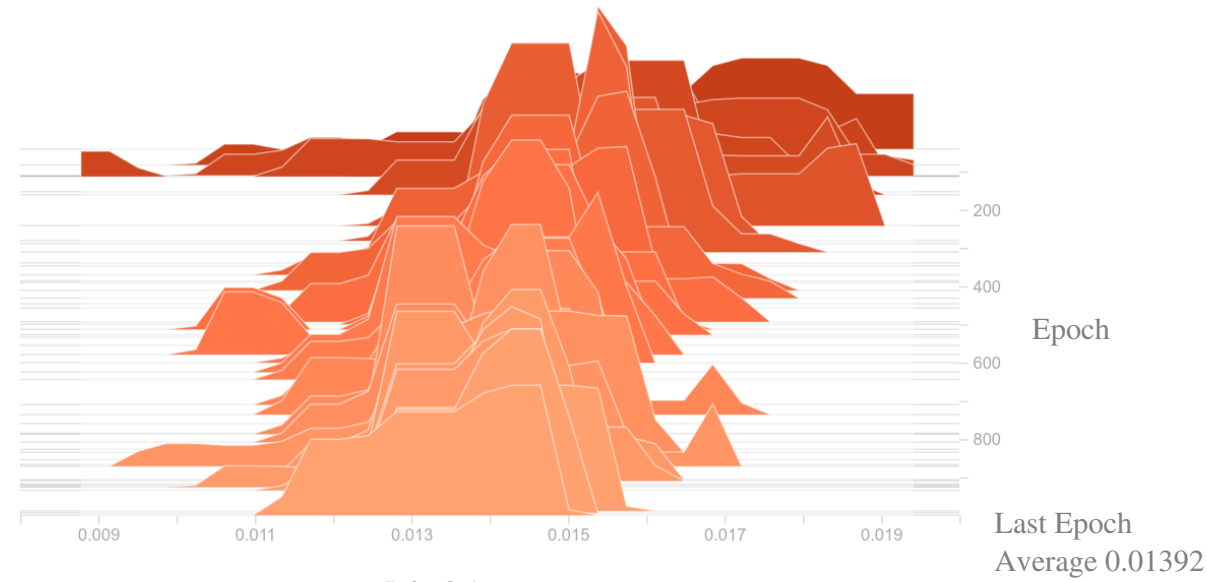
The main results of the paper analysis can be summarized in the following

Lemma 1 *If the gradient flow with normalization and weight decay converges to an interpolating solution with near-zero square loss (for $\lambda > 0$), the following properties hold:*

1. *The global minima in the square loss with the smallest ρ 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 weight decay λ (with BN) and small initialization (small ρ);*
3. *The condition $\frac{\partial f(x_j)}{\partial V_k} = V_k f(x_j)$ which holds at the critical points of the SGD dynamics that are global minima, is key in predicting several properties of the Neural Collapse[14];*
4. *the same condition represents a powerful constraint on the set of weight matrices at convergence.*

6.1 Remarks

- Suppose we control ρ_k independently of V_k and of equation 28: can we find $\rho(t)$ schedules leading more reliably to good solutions independently of initial conditions?



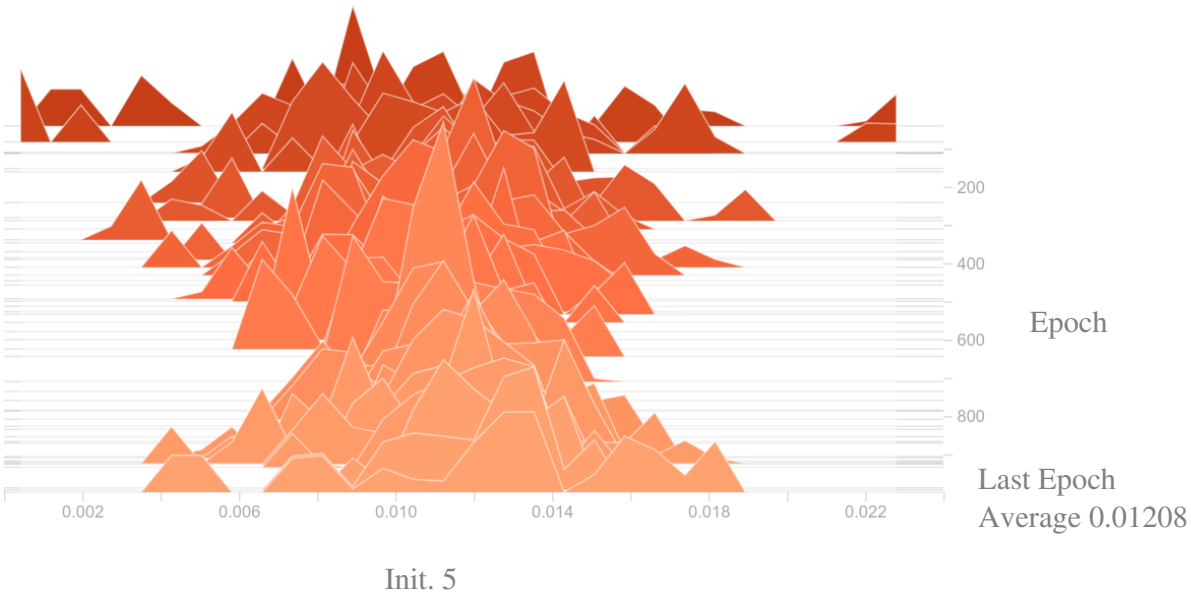


Figure 9: ***ConvNet with Batch Normalization but no Weight Decay****: Histogram of* $|f_n|$ *over time. Top figure: initial* $\rho_k = 0.1$*. Bottom figure: initial* $\rho_k = 5$*.*

- The role of the Lagrange multiplier term $\nu \sum_k ||V_k||^2$ in Equation 3 is different from a standard regularization term because ν, 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 ν 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 constraing each V_k to the unit sphere. For the exponential loss the situation is different and ν in $\nu \sum_k ||V_k||^2$ acts as a positive regularization parameter, albeit a vanishing one (for $t \to \infty$).

- For the square loss, convergence of the gradient flow to a minimum norm solution independently of initial conditions requires BN or WN and WD, unlike the case of linear networks. For the exponential loss, BN is strictly not needed since minimization of the exponential loss maximizes the margin and minimizes the norm without BN. Thus under the exponential loss, we expect a margin maximization effect for $t \to \infty$, as shown in [3], independently of intial conditions. Deep nets under the square loss are more likely to overfit at long times than under exponential-type loss functions (unless weight decay is used). As a consequence, early stopping is more likely to be effective for the square loss than for exponential-type loss functions. Empirically, it seems that square loss reaches solutions with good test error in multiclass CIFAR10 faster than cross-entropy. Continuing GD, however, sometime 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 [15]. It also suggests that in the experiments of [8], early stopping may play a role to obtain results with the square loss case that are as good or better than cross-entropy. We conjecture that the overfitting phenomenon is related to the singular nature of the global critical point when the weight decay λ is zero or too small (see Equations 5 and 6).

- If there exist several almost-interpolating solutions with the same norm ρ_{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 have different ranks of the weight matrices or of the rank of the local Jacobian $\frac{\partial f_n}{\partial V_k}$ (at the minimum W^*). Notice that in deep linear networks the GD dynamics seems to bias the solution towards small rank solutions, since large eigenvalues converge much faster the small ones [16]. It in unclear whether the rank has a role in our analysis of generalization.

- Small initialization ensures that ρ grows for small values thus exploring first large margin minima – assuming that average separability is reached early, during the first iterations of GD. Why does GD have difficulties in converging in the absence of BN, especially for very deep networks? At the moment, 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 [9].

- The normalization Equation 3 is a precise model of WN. Normalization of the weight matrices V_k is also an effect of BN. However, *BN is also normalizing each row of each* V_k

matrix, as we mentioned earlier[10].

- 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[17]. 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 exteded to *gradient descent* along the lines of [9].
  - The behavior of gradient descent around the global minima should be analyzed in the limit for $\lambda \to 0$. Equation 6 contains two terms, one reflecting the normalization and the other the regression error. Zero regression error implies that normalization fails at the critical point for $\lambda = 0$. It is remarkable that for $\lambda = 0$ or even more surprisingly 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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[10]The normalization may change during training between each training example because of the role of the D matrices, effectively switching on and off some weights in the network, depending on x_n and on whether BN is before or after the RELU nonlinearity (as pointed out by A. Banbuski).

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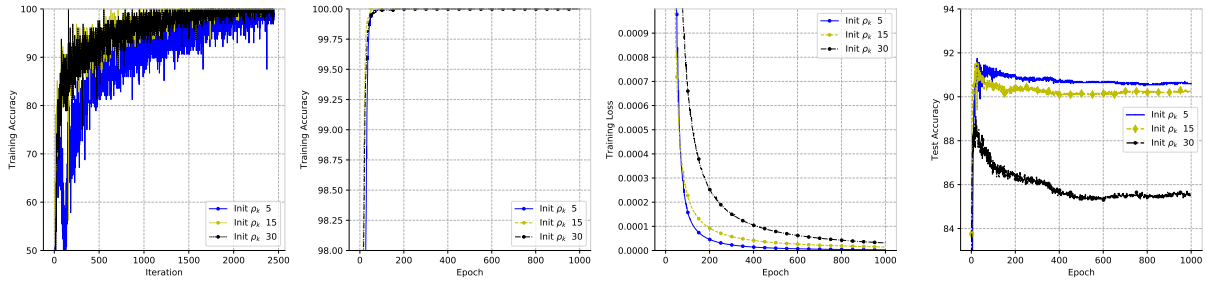

Figure 10: ***ConvNet, no Batch Normalization, no Weight Decay***. *Binary classification on two classes from CIFAR-10, trained with MSE loss. The model is a very simple network with 4 layers of fully-connected Layers. The ReLU nonlinearity is used. The weight matrices of all layers are initialized with 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.*

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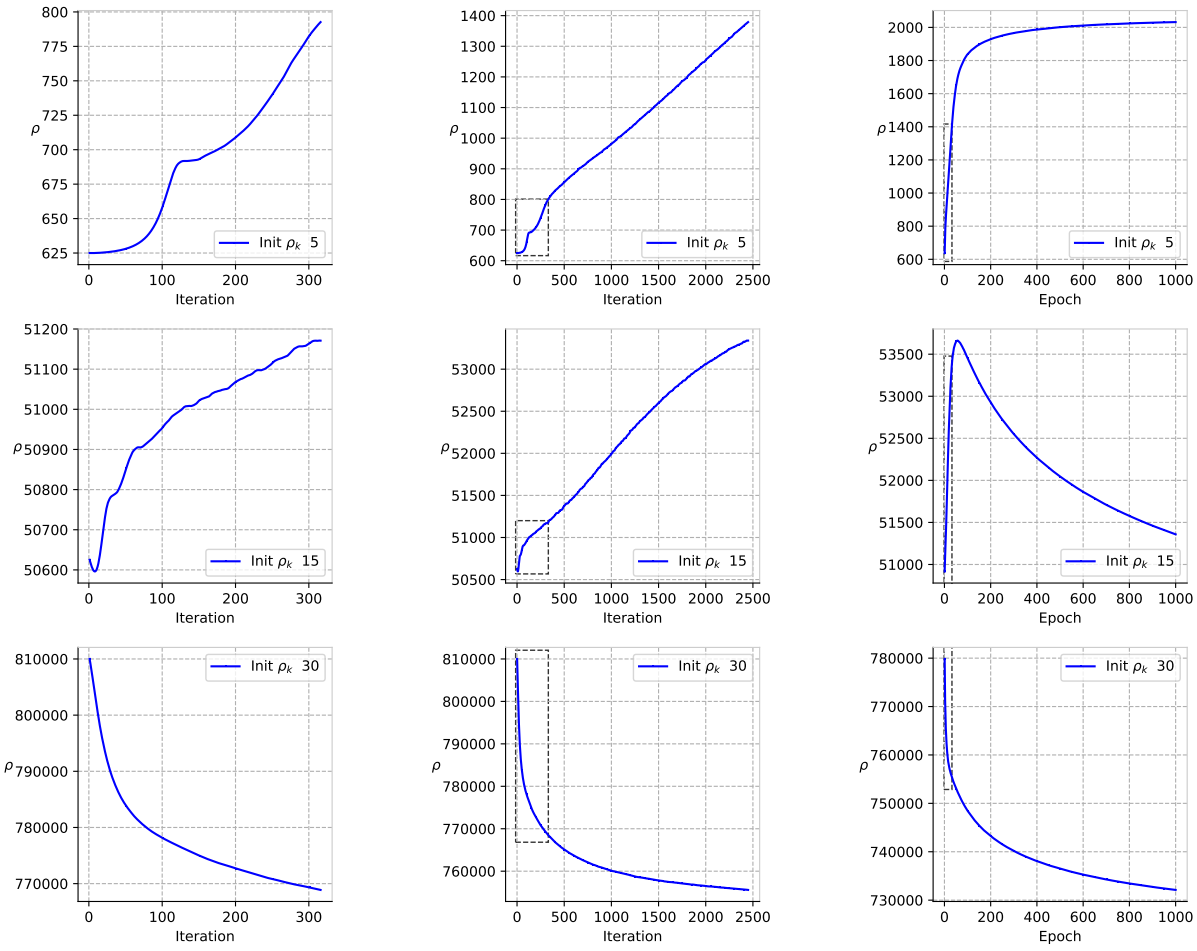

Figure 11: ***ConvNet, no Batch Normalization, no Weight Decay***. *Dynamics of ρ from experiments in Figure 10. First row: small initialization (5). Second row: large initialization (15). Third row: extra large initialization (30). A dashed rectangle denotes the previous subplot's domain and range in the new subplot. More details to be added.*

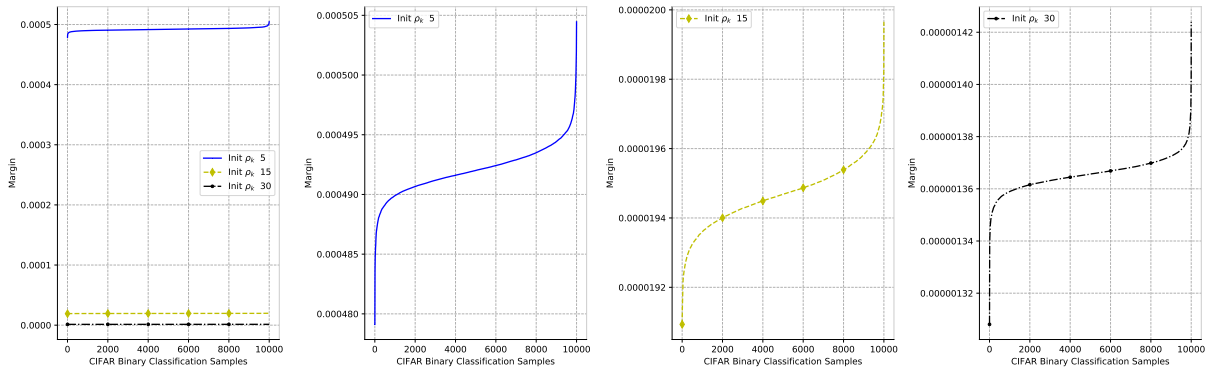

Figure 12: ***ConvNet, no Batch Normalization, no Weight Decay***. *Margin of all training samples*

A Normalization during Gradient Descent (from [7]

A.1 Weight Normalization

For each layer (for simplicity of notation and consistency with the original weight normalization paper), weight normalization [5] defines v and g in terms of $w = g\frac{v}{|v|}$. The dynamics on g and v is induced by the gradient dynamics of w as follows (assuming $\dot{w} = -\frac{\partial L}{\partial w}$

$$\dot{g} = \frac{v^T}{||v||}\dot{w} \tag{12}$$

and

$$\dot{v} = \frac{g}{||v||}S\dot{w} \tag{13}$$

with $S = I - \frac{vv^T}{||v||^2}$.

We claim that this is the same dynamics obtained from tangent gradient for $p = 2$. In fact, compute the flows in ρ, v from $w = \rho v$ as

$$\dot{\rho} = \frac{\partial w}{\partial \rho}\frac{\partial L}{\partial w} = v^T\dot{w} \tag{14}$$

and

$$\dot{v} = S\rho\dot{w} \tag{15}$$

Clearly the dynamics of this algorithm is the same as standard weight normalization if $||v||_2 = 1$, because then Equations 12 and 13 become identical to Equations 14 and 15 with g corresponding to ρ. We now observe, multiplying Equation 13 by v^T, that $v^T\dot{v} = 0$ because $v^TS = 0$, implying that $||v||^2$ is constant in time. Thus if $||v|| = 1$ at initialization, it will not

change (at least in the noiseless case). Thus *the dynamics of Equations 12 and 13 is the same dynamics as Equations 14 and 15*. It is also easy to see that the dynamics above is not equivalent to the standard dynamics on the w (see [7].

A.2 Batch Normalization

Batch normalization [4] for unit i in the network normalizes the input vector of activities to unit i – that is it normalizes $X^j = \sum_j W^{i,j} x_j$, where x_j are the activities of the previous layer. Then it sets the activity to be

$$Y^j = \gamma \cdot \hat{X}^j + \beta = \gamma \frac{X^j - \mu_B}{\sqrt{\sigma_B^2 + \epsilon}} + \beta,$$

where γ, β are learned subsequently in the optimization and

$$\mu_B = \frac{1}{N} \sum_{n=1}^{N} X_n \qquad \sigma_B^2 = \frac{1}{N} \sum_{n=1}^{N} (X_n - \mu_B)^2.$$

Note that both μ_B and σ_B^2 are vectors, so the division by $\sqrt{\sigma_B^2 + \epsilon}$ has to be understood as a point-wise Hadamard product $\odot(\sigma_B^2 + \epsilon)^{-1/2}$. The gradient is taken wrt the new activations defined by the transformation above.

Unlike Weight Normalization, the Batch Normalization equations do not include an explicit computation of the partial derivatives of L with respect to the new variables in terms of the standard gradient $\frac{\partial L}{\partial w}$. The reason is that Batch Normalization works on an augmented network: a BN module is added to the network and partial derivatives of L with respect to the new variables are directly computed on its output. Thus the BN algorithm uses only the derivative of L wrt the old variables as a function of the derivatives of L wrt new variables in order to update the parameters below the BN module by applying the chain rule. Thus we have to estimate what BN *implies* about the partial derivatives of L with the respect to the new variables as a function of the standard gradient $\frac{\partial L}{\partial w}$.

To see the nature of the dynamics implied by batch normalization we simplify the original Equations (in the Algorithm 1 box in [4]). Neglecting μ_B and β and γ, we consider the core transformation as $\hat{X} = \frac{X}{\sigma_B}$ which, assuming fixed inputs, becomes $\hat{X} = \frac{X}{|X|}$ which is mathematically identical with the transfomation considered in [7]. In a similar way the dynamics of $w = \frac{\partial L}{\partial w}$ induces the following dynamics on $\hat{X}$:

$$\dot{\hat{X}} = \frac{\partial \hat{X}}{\partial X} \dot{X} \tag{16}$$

where $\dot{x} = \nabla_x L$. We consider $X \in \mathbb{R}^{N \times D}$. In the $D = 1$ case, we get

$$\frac{\partial \hat{X}}{\partial X} = (\sigma_B^2 + \epsilon)^{-1/2} \left[-\frac{1}{N} \hat{X} \hat{X}^T + I \right].$$

In the general D-dimensional vector case, this generalizes to

$$\frac{\partial \hat{X}}{\partial X} = (\sigma_B^2 + \epsilon)^{-1/2} \left[-\frac{1}{N} \hat{X}^T \odot \hat{X} + I \right].$$

Notice that $I - \hat{X}\hat{X}^T = S$. Since $x = W x_{input}$ this shows that batch normalization is closely related to *gradient descent algorithms with unit L_2 norm constraint of the tangent gradient type*. Because of the simplifications we made, there are other differences between BN and weight normalization, some of which are described in the remarks below.

Remarks

1. Batch normalization, does not control directly the norms of $W_1, W_2, \cdots, W_K$ as WN does. Instead it controls the norms

$$||x||, ||\sigma(W_1 x)||, ||\sigma(W_2 \sigma(W_1 x))||, \cdots \tag{17}$$

2. In the multilayer case, BN controls separately the norms $||V_i||$ of the weights into unit i, instead of controlling the overall Frobenius norm of the matrix of weights as WN does. Of course control of the $||V_i||$ implies control of $||V||$ since $||V||^2 = \sum_i ||V_i||_i^2$.

B Gradient flow for ρ and V_k

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

$$\dot{W}_k = -\frac{2}{N} \sum_n (g_n - y_n) \frac{\partial g_n}{\partial W_k} \tag{18}$$

that is

$$\dot{W}_k = -\frac{\partial L}{\partial W_k} = -\frac{2}{N} \sum_n g_n \frac{\partial g_n}{\partial W_k} + \frac{2}{N} \sum_n y_n \frac{\partial g_n}{\partial W_k} \tag{19}$$

We now derive the dynamics of the norm and of the normalized weights. We define $g(x) = \rho f(x)$. ρ 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 [7]). 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;

B.1 Dynamics under normalization

Gradient flow on $\mathcal{L} = \sum_n (\rho f_n - y_n)^2 + \nu \sum_k ||V_k||^2 + \lambda \rho^2$ with $||V_k||^2 = 1$ is completely equivalent (for $\lambda = 0$) to "Weight Normalization"[7] for deep networks.

Assuming that $\rho_k = 1, \quad \forall k < L$ and $\rho_L = \rho$, gradient flow on L wrt ρ gives,

$$\dot{\rho} = -2\sum_n \ell_n f_n - 2\lambda\rho \tag{20}$$

Gradient flow on L wrt V_k gives

$$\dot{V_k} = -\frac{\partial L}{\partial V_k} = -2\sum_n (\rho f_n - y_n)\rho \frac{\partial f_n}{\partial V_k} - 2\lambda V_k. \tag{21}$$

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

In summary, gradient flow on L wrt ρ and V_k gives

$$\dot{\rho} = -2[\sum_n \rho (f_n)^2 - \sum_n f_n y_n] - 2\lambda\rho = -2\sum_n \ell_n f_n - 2\lambda\rho. \tag{22}$$

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

$$\dot{V_k} = 2\sum_n [(\rho f_n - y_n)\rho(-\frac{\partial f_n}{\partial V_k}) + 2V_k \rho f_n (\rho f_n - y_n)] = 2\rho \sum_n [(\rho f_n - y_n)(V_k f_n - \frac{\partial f_n}{\partial V_k})] \tag{23}$$

Without BN and without WD $\frac{\partial g_n(W)}{\partial W_k} = \frac{\rho}{\rho_k}\frac{\partial f_n(V)}{\partial V_k}$; with BN but without weight decay this becomes $\frac{\partial g_n(W)}{\partial W_k} = \rho \frac{\partial f_n(V)}{\partial V_k}$, $\quad \forall k < L$ and $\frac{\partial g_n(W)}{\partial W_L} = \frac{\partial f_n(V)}{\partial V_k}$.

This dynamics – where there is a "vanishing" Lagrange multiplier ν – 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 [9].

Notice that $\dot{\rho} = 0$ if $y_n f_n = 1$ and $\rho_k = 1$; ρ_{eq} is a critical point for the dynamics of ρ under GD. In the case of SGD the asymptotic value of ρ for fixed $\sum f_i y_i$ may fluctuate randomly around the $\frac{\sum_n y_n f_n}{\sum_n f_n^2}$. Furthermore, the lowest possible value of ρ_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.

C Maximum margin and minimum norm

Lemma 2 *[7] The maximizer of the margin under the constraint $||V_k|| = 1$ is the minimum norm solution under the constraint $y_n f_n \geq 1, \quad \forall n$.*

Minimum norm regression of binary labels is

$$\min_{W_k} \frac{1}{2}\|W_k\|^2, \qquad \forall k \quad \text{subj. to} \quad y_i f(W_K, \cdots, W_1; x_i) = 1, \qquad i = 1, \ldots, N. \tag{24}$$

Minimum norm binary classification is

$$\min_{W_k} \frac{1}{2}\|W_k\|^2, \qquad \forall k \quad \text{subj. to} \quad y_i f(W_K, \cdots, W_1; x_i) \geq 1, \qquad i = 1, \ldots, N. \tag{25}$$

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

Observation 4 *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. This indicates that there should be better algorithm to train deep networks for classification than regression.

D Unnormalized GD

Here we assume gradient flow without BN (and without weight decay), assuming, for simplicity, that at initialization all the layers have the same norm, that is ρ_k is the same for all k at initialization. Because of this assumption we can use the following

Lemma 3 $\frac{\partial \rho_k^2}{\partial t}$ *is independent of* k*.*

to claim that all ρ_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:

$$\frac{\partial ||W_k||^2}{\partial t} = 2W_k \frac{\partial W_k}{\partial t} = \frac{4}{N} \sum_n g_n^2 + \frac{4}{N} \sum_n g_n \tag{26}$$

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

$$\dot{\rho_k} = -\frac{\partial L}{\partial \rho_k} = -2L \sum_n (\rho_k^L f_n - y_n) f_n \rho_k^{L-1} = -2\rho_k^{L-1} [\sum_n \rho_k^L (f_n)^2 - \sum_n f_n y_n] \tag{27}$$

which can be rewritten in terms of $\rho = \rho_k^L$ using $\dot{\rho} = \sum_k \frac{\partial \rho}{\partial \rho_k} \dot{\rho_k}$ as

$$\dot{\rho} = 2L\rho^{\frac{2L-2}{L}} [\sum_n f_n y_n - \sum_n \rho (f_n)^2] \tag{28}$$

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 ρ for small initialization during the first 50 or so iterations).

The dynamics of Equation 28 is that the smaller $\rho_{t=0}$ is, the longer it takes to ρ to grow (this phenomenon increases with increasing number of layers L). Thus ρ 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 $\sum y_n f_n$). Part of this dynamics was analyzed by Shalev-Schwartz [16] in a different context.

If the initial conditions are $\rho_{t=0} \approx 0$, $\rho(t)$ will eventually grow (most of the time, when it does not go to zero), but slowly for a longish time. 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 ρ decreases, though the asymptotic value of $\rho = \frac{\sum y_n f_n}{\sum f_n^2}$ increases. until a critical point of the flow is reached

Compare this with the case in which ρ is large at initialization: then ρ may decrease until a critical point is reached. As we already noticed, there are plenty of critical points at large ρ (stationary points for ρ and V_k) because under appropriate overparametrization, almost every perturbations of the weights before the linear classifier at the top yields a different interpolating solution. Of course, in the presence of significant weight decay the gradient flow may escape these minima.

E Dynamics and equilibria for V_k and ρ

When $\lambda > 0$ the terms $\ell_n = (\rho f_n - y_n) \neq 0$ in Equation 8. It is then reasonable to assume that $\alpha_n > 0$ and that V^{eq} *at the minimum* can be written as

$$V_k^{eq} = \sum^N \alpha_n \frac{\partial f_n}{\partial V_k} \tag{29}$$

where $\alpha_n = \frac{\rho f_n - y_n}{\sum_n (\rho f_n - y_n) f_n}$[11].

E.1 Weight decay and label noise

Adding a term $\lambda ||W_k||^2$ to the Lagrangian corresponding to weight decay changes the dynamics of ρ but not the dynamics of V_k. The Equation for ρ becomes (with BN and WD) Equation 7, that is

$$\dot{\rho} = -2[\sum_n \rho (f_n)^2 - \sum_n f_n y_n] - 2\lambda\rho \tag{30}$$

which has an equilibrium given by

$$\rho_{eq} = \frac{\sum_n y_n f_n}{\lambda + \sum_n f_n^2}. \tag{31}$$

Notice that label noise (adding $\pm\delta$ – with δ a small random real number to the labels), as suggested by Jason Lee and coworkers[18], may play a role somewhat similar to a regularization

[11] Notice that in general not all of the N terms in Equation 29 are different from zero[12] 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.

λ by eliminating interpolation[13]. Both label noise and weight decay introduce a bias towards small ρ_{eq} minima – and thus better generalization – even for large initializations.

E.2 Convergence of Linear Networks with Normalization and Regularization

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–

$$\dot{\rho} = \frac{2}{\rho} \sum_{n=1}^{N} \ell_n y_n v^T x_n - 2\lambda\rho \tag{32}$$

and

$$\dot{v} \propto \sum_{n=1}^{N} \ell_n (x_n - v v^T x_n). \tag{33}$$

If $\lambda > 0$ it is reasonable to assume $\sum_{n=1}^{N} \ell_n y_n \neq 0$. Thus

$$\dot{v} \propto \sum_{j=1}^{N} \alpha_j (I - v v^T) x_j. \tag{34}$$

If gradient flow converges to $\dot{v} = 0$, the solution v must satisfy $v v^T x = x$, 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 34 is not expanding [19] (because v has unit norm), there is a fixed point $v = x$ which is *independent of initial conditions*. Numerical simulation show that this is not true for $\lambda = 0$.

E.3 Convergence of Networks with Normalization

Consider

$$\dot{V}_k =\propto (I - V_k V_k^T) \sum_{n=1}^{N} (y_n - \rho f_n) \frac{\partial f_n}{\partial V_k}. \tag{35}$$

Let us define $\alpha_n = (y_n - \rho f_n)$ and an "average" $\frac{\hat{\partial f}}{\partial V_k} = \sum_j \alpha_j \frac{\partial f_j}{\partial V_k}$. If $\lambda > 0$ then $\alpha_n \neq 0, \quad \forall n$. Then $(I - V_k V_k^T) \frac{\hat{\partial f}}{\partial V_k} = \dot{V}_k$. If there is convergence, that is $\dot{V}_k = 0$, then it makes sense to assume that in most cases

$$V_k \hat{f} = \frac{\partial \hat{f}}{\partial V_k} \tag{36}$$

with $\hat{f} = V^T \frac{\hat{\partial f}}{\partial V_k}$[14].

[13]Label noise also makes $\sum_n f_n y_n$ smaller, decreasing the equilibrium ρ and biasing the final solution to have larger margin

[14]If $V_k^T \frac{\partial f_n}{\partial V_k} = f_n$ with the same V_k for all n, *then* $\hat{f} = \sum_j \alpha_j f_j$. The equation provides constraints on the weights V_k and the other layer weights at convergence.

$$(\rho f_n - y_n)\frac{\partial f_n}{\partial V_k} = (\rho f_n - y_n)(V_k^{eq} f_n), \quad \forall n = 1, \cdots, N. \tag{37}$$

Thus, assuming $\lambda > 0$, in most cases at equilibrium the following holds

$$V_k^{eq} = \sum \alpha_n \frac{\partial f_n}{\partial V_k}, \tag{38}$$

with $\alpha_n = \frac{\rho f_n - y_n}{\sum (\rho f_n - y_n) f_n}$. SGD with minibatches of size 1 (the argument can be extended to other sizes $< N$) has stationary points given by [10]

$$0 = (I - V_k V_k^T)\ell(x_n)\frac{\partial f(x_n)}{\partial V_k}, \quad \forall n. \tag{39}$$

which implies (for $\lambda > 0$)

$$\frac{\partial f(x_n)}{\partial V_k} = V_k f(x_n), \quad \forall n. \tag{40}$$

F Margins, ρ and expected error

Assuming that weight decay, small initialization and $\lambda > 0$ provide a bias towards solution with "large" margin, the next step is to use simple bounds [20] to claim better expected error (and better stability) for those solutions.

A typical generalization bound that holds with probability at least $(1 - \delta)$, $\forall g \in \mathbb{G}$ has the form [20]:

$$|L(g) - \hat{L}(g)| \leq c_1 \mathbb{R}_N(\mathbb{G}) + c_2 \sqrt{\frac{\ln(\frac{1}{\delta})}{2N}} \tag{41}$$

where $L(g) = \mathbf{E}[\ell_{gamma}(g(x), y)]$ is the expected loss, $\hat{L}(g$ is the empirical loss, $\mathbb{R}_N(\mathbb{G})$ is the empirical Rademacher average of the class of functions $\mathbb{G}$ 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* $\ell_{gamma}(g(x), y)$ defined as

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

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

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 ρs. Let us call them $g^a(x) = \rho_a f^a(x)$ and $g^b(x) = \rho_b f^b(x)$. Using the notation of this

paper, the functions f_a and f_b correspond to networks 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,

$$\mathbb{R}_N(\mathbb{G}) = \rho \mathbb{R}_N(\mathbb{F}), \tag{42}$$

where $\mathbb{G}$ is the space of functions of our unnormalized networks and $\mathbb{F}$ denotes the corresponding normalized networks[15]. This observation allows us to use the bound Equation 41 and the fact that the empirical $\hat{L_\gamma}$ *for both functions is the same* to write $L_0(f^a) = L_0(F^a) \leq c_1 \rho_a \mathbb{R}_N(\tilde{\mathbb{F}}) + c_2 \sqrt{\frac{\ln(\frac{1}{\delta})}{2N}}$ and $L_0(f^b) = L_0(F^b) \leq c_1 \rho_b \mathbb{R}_N(\tilde{\mathbb{F}}) + c_2 \sqrt{\frac{\ln(\frac{1}{\delta})}{2N}}$. The bounds have the form

$$L_0(f^a) \leq A\rho_a + \epsilon \tag{43}$$

and

$$L_0(f^b) \leq A\rho_b + \epsilon \tag{44}$$

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

Similar results can be obtained taking into account different $\hat{L}(f)$ for the normalized f^a and f^b under different γ in Equation 41, that is

$$|L(f) - \hat{L}(f)| \leq c_1 \mathbb{R}_N(\tilde{\mathbb{F}}) + c_2 \sqrt{\frac{\ln(\frac{1}{\delta})}{2N}}. \tag{45}$$

It is unclear whether these bounds are meaningful in practice. It is likely there exist better ways to bound the expected error.

G Towards Predicting NC1 to NC4 (with A. Banburski)

We sketch here a proof of how our theoretical framework predicts the four properties NC1 to NC4 in the retricted case of *binary classification* under the square loss. In a network with L layers the last layer activations for an input $x_{i,c}$ where c is the class – here we consider just two classes $c = +1$ or $c = -1$ – are called $h_{i,c}$ by [14]. To conform to their notation we consider in this section a slightly different network from the one considered in the paper. Until now, we assumed that the network has one scalar output which is ideally ± 1. Here we consider instead a network with two outputs, one representing the positive class and the other the negative one both trained to take the value $+1$ for the respective class. Thus the last layer weights are $V_L^{c=+1} = -V_L^{c=-1}$. Convergence to a global minimum, that is $\dot{V_k} = 0$, $\dot{rho} = 0$, implies $f^c(x_{i,c}) = 1$ independently of i, because $\rho f_i = \frac{1}{\rho_{eq}}$. The key observation is that $h_{i,c}^T = \frac{\partial f(x_{i,c})}{\partial V_L^c}$.

[15] Furthermore, the Rademacher complexity of the space of functions associated with normalized networks of the same architecture is the same (see [21]).

Corollary 4 *Equations 5 and 6 imply NC1, NC2, NC3, NC4.*

Proof

- NC1: since $V_k f_c(x_i) = \frac{\partial f_c(x_i)}{\partial V_k}$ at convergence (see Equation 38) $h^T(x_{i,c}) = V_L^c f^c(x_i)$ at convergence. Since $f^c(x_i)$ does not depend on i at convergence, $V_L^c f^c(x_i)$ does not depend on i implying that the standard deviation of $h_{i,c}$ wrt i converges to zero when $\dot{V}_k$ and $\dot{\rho}$ converge to zero.
- NC2: in the binary case $h_{+1} \to V_L^T$ and $h_{-1} \to -V_L^T$ (see above). Thus $\mu_1 = V^T$ and $\mu_2 = -V^T$. This is the special binary case of NC2.
- NC3: since $h(x_{i,c}) = V_L^T f_c(x_i)$ and f_c does not depend on i, at convergence h is proportional to V_L^T.
- NC4: the result of [22], as shown by [14], implies together with NC1 and NC2, that NC3 and NC4 hold. Since our theory (in the previous sections), implies the result of [22], it also implies NC4.

We note that for the square loss these results apply to each global minimum, irrespectively of its ρ_{eq}. For the exponential loss a similar argument may be used. In particular, we assume that for a sufficiently large and fixed ρ, SGD reaches $\dot{V}_k = 0$ which implies $V_k f_n = \frac{\partial f}{\partial V_k}, \quad \forall n$. We assume that this is the absolute minimum of the exponential loss for that fixed ρ. Because of overparametrization, such global minima must be degenerate (see [10], that is such that the minimizing network f has the same maximum margin for all training data: $y_n f_n = y_1 f_1, \quad \forall n$ at the minimum. The same conclusion is reached using the following argument. Consider the gradient flow corresponding to GD under the exponential loss

$$\begin{aligned} \dot{\rho_k} &= \frac{\rho}{\rho_k} \sum_n e^{-\rho y_n f(V;x_n)} y_n f(V;x_n) \\ \dot{V_k} &= \rho \sum_n e^{-\rho y_n f(V;x_n)} y_n S_k \frac{\partial f(V;x_n)}{\partial V_k}. \end{aligned} \tag{46}$$

Without loss of generality let us assume that the training data f_n are ranked at $t = T_0$ according to increasing normalized margin, that is $f_1 \le f_2 \le \cdots \le f_N$. Let us define $B_n^k = B_k(V;x_n) = y_n(\frac{\partial f(V;x_n)}{\partial V_k} - V_k f(V;x_n))$. Then the equilibrium condition becomes for each weight matrix k

$$\sum_n^N e^{-\rho(t) y_n f_n} B_n^k = 0. \tag{47}$$

Equation 47 cannot be satisfied unless $f_1 = f_i, \quad \forall i$, since $\rho(t)$ is continuously increasing, implying that all the f_n must converge to the same asymptotic value. *Thus an asymptotic equilibrium for which $\dot{V}_k = 0$ implies that asymptotically $f_1 = f_i, \quad \forall i = 2, \cdots, N$: the margin becomes the same for all training data.*

H Remarks on Constraints on the Weight Matrices

The condition we have derived in the main theory

$$V_k f_n = \frac{\partial f_n}{\partial V_k}, \quad \forall k = 1, \cdots, L, \quad \forall n \tag{48}$$

imposes a strong set of constraints on the weights of the network, since $\frac{\partial f}{\partial V_k}$ depends on all weight matrices with the exception of V_k. Suppose

$$f(x) = (V_L \sigma(V_{L-1} \cdots \sigma(V_1 x))) \tag{49}$$

where $\sigma(x) = \sigma'(x)x$. The equation can be rewritten for each training example as

$$f(x_j) = V_L D_{L-1}(x_j) V_{L-1} \cdots\cdots V_{k+1} D_k(x_j) V_k \cdots D_1(x_j) V_1 x_j \tag{50}$$

where $D_k(x_j)$ is a diagonal matrix with 0 and 1 entries depending on whether the corresponding RELU is active or not for the specific input x_j, that is $D_{k-1}(x_j) = diag[\sigma'(N_k(x_j)]$ with $N_k(x_j)$ the input to layer k.

Call $V_L D_{L-1}(x) V_{L-1} \cdots V_{k+1} D_k(x) = a^T$ and $D_{k-1}(x) V_{k-1} D_{k-2}(x) \cdots D_1(x) V_1 x = b$. Then $f(x) = a^T V_k b$ and $\frac{\partial f}{\partial V_k} = ab^T$. As sanity checks, $f^T = b^T V_k^T a = f$; furthermore, the structural lemma Equation 1 gives

$$\sum_{i,j} \frac{\partial f(V;x)}{\partial V_k^{i,j}} V_k^{i,j} = \sum_{i,j} a^i b^j V_k^{i,j} = f(x). \tag{51}$$

Then Equation 48 becomes

$$V_k f = [V_L D_{L-1}(x) V_{L-1} \cdots V_{k+1} D_k(x)]^T D_{k-1}(x) V_{k-1} D_{k-2}(x) \cdots D_1(x) V_1 x \tag{52}$$

Let us now make some strong assumptions to get some intutition about the potential impact of the constraints on the weight matrices.

Assumptions

- Let us assume that all $V_k \quad \forall k = 1, \cdots (L-1) \in \mathbb{R}^{p,p}$ have the same dimensions, whereas $V_L \in \mathbb{R}^{1,p}$.
- We assume linear deep networks *at training time*, that is without RELUs. This is inspired by the observation that *if solutions V_k are found that satisfy Equation 52 then they will also satisfy the same Equations when the matrices D_k are replaced by I*, while the converse is not true.

  The intuition is that this big oversimplification may still be interesting, because the "training" equations above have to hold for all the x_n in the training set. This implies that the D matrices at each level are likely to eventually have 1 in each position of the diagonal across the whole of the training set. Of course, this will not hold completely and for all layers, especially if $p > N$ and especially for the layers at the top of the network, in which case the presence of the D_k makes the constraint Equation 48 effectively weaker.

Under these three assumptions, let us consider two natural types of solutions that are consistent with Equation 48.

H.1 V_k as projection matrices

A class of solution which is consistent with the constraints represented by Equation 48 is

$$V_1 = V_2 = \cdots = V_{L-1} \tag{53}$$

and

$$V_L = D_{L-1}(x)V_{L-1} \cdot \cdots \cdot V_{k+1}D_k(x)V_k \cdots D_1(x)V_1 x = \frac{\partial f}{\partial V_L} \tag{54}$$

In order for this to be true, the $V_k \quad k < L$ matrices can be projection matrices (P is a projection if $P^2 = P$; it is an orthogonal projection if $P = P^T$). Then, all the weight matrices are proportional to each other apart from the weight matrix of the last (L) layer which must be a vector proportional to the vector of activities of the units in layer $L - 1$.

If we assume that feedforward networks with T layers converge to this type of solution, the interesting *prediction is that recurrent networks (therefore with weight sharing across layers) under T iterations should be identical to forward networks with T layers (without weight sharing).*

H.2 V_k as orthogonal matrices

Another possible set of solutions consists of matrices V_k (assuming the weight matrices are all square matrices)each proportional to an orthogonal matrix. The constraint Equations 48 suggest the structure of a group since V_k is proportional to the product of similar matrices.

A key property of orthogonal matrices is that $V_k^T = V_k^{-1}$. Because of this property the constraint equations are always satisfied. For instance assume $f(x) = V_4V_3V_2V_1x$ with the matrices being orthogonal. Then it is easy to check that the constraint equations yield $V_3 \propto \frac{\partial f}{\partial V_3} = V_4^T(V_2V_1)^T$ and $V_2 \propto (V_4V_3)^T(V_1)^T$. Together they satisfy $V_3 = V_3$.

We observe that the underlying reason for restricting this class of solutions to the orthogonal group is BN or WN, since they are equivalent to constrained optimization with Lagrange multipliers. As observed in [23] regularization of each weight matrix of a linear network reduces the symmetry group of the loss function from $GL_p(\mathbb{R})$) to the orthogonal group $O_p(\mathbb{R})$. Furthemore, it is interesting to notice, as they do, that

- Orthogonal matrices are the determinant ± 1 matrices of minimal Frobenius norm (the squared determinant is the product of the squared singular values);
- Orthogonal matrices are the inverse matrices of minimum total squared Frobenius norm (sum of the squared singular values);
- A square matrix is orthogonal *iff* $A^{-1} = A^T$;
- Orthogonal matrices diagonalize any symmetric real-valued matrix $A = U\Lambda U^T$.

There is a large number of papers (for a random one see [24] and references therein) discussing the advantages of orhogonality for generalization in deep networks and probably as many papers proposing regularization-like algorithms in order to impose orthogonality in the weight matrices in a deep network. More generally, the discussion above should be extended from orthogonal matrices to non-square matrices in an orthogonal Stiefel manifold on the sphere. As far as we know, this appendix represents the first time that commonly used normalization algorithms, such as BN, are shown to bias weight matrices towards being orthogonal (or projection) vectors. It is natural to conjecture that additional properties of deep networks may be derived from the rich structure induced by this bias. On the other hand, we cannot expect weight matrices to be orthogonal in real networks because of the role of the RELUs, which is not taken into account in the simplified analysis above, and because BN in practice does not exactly normalizes the weight matrices[16].

H.3 Diagonal networks (with A. Banburski)

Diagonal networks have been recently analyzed in a number of theoretical papers (see [16] and references therein) and are particularly interesting here for two reasons which we show below: diagonal initializations are preserved by gradient descent and the D-matrices corresponding to the RELUs stages commute.

First, notice that gradient updates are given by

$$w_{t+1} - wt = -\eta \sum_n \ell(f(w; x_n), y_n)' \nabla_{w_t} f(w; x_n) \tag{55}$$

and so an update to any off-diagonal weight will be non-zero only if $\nabla_{w_t} f(w; x_n)$ for that weight is non-zero. We trivially find that

$$\frac{\partial f(x)}{\partial W_k^{ij}} = W_L D_{L-1}(x) W_{L-1} \cdots W_{k+1}^{i\cdot} D_k(x) D_{k-1}(x) W_{k-1}^{j\cdot} D_{k-2}(x) \cdots D_1(x) W_1 x. \tag{56}$$

This means that a off-diagonal layer-k entry (i, j) update depends on a term in f that has an i-th column in layer $k+1$ and j-th row in layer $k-1$. But if at time $t = 0$ the off-diagonal terms $i \neq j$ vanish, then the off-diagonal gradient update also vanishes for $t = 1$ and similarly for all subsequent times. Hence GD preserves diagonal initial conditions.

Assuming the same setting of square matrices as in the previous subsections, we can immediately see the usefulness of the diagonal assumption, from the simple fact that diagonal square matrices commute, so we can write

$$f = V_L \dots V_1 D_{L-1}(x) \dots D_1(x) x = V_L \dots V_1 \tilde{x} \qquad \text{with} \qquad \tilde{x} = D_{L-1}(x) \dots D_1(x) x,$$

i.e. we can push all the nonlinearities to the end and absorb them now into a single nonlinear transformation of the data x. This then allows us to deal with the sum over all training examples: by defining $\hat{x} = \sum_n \alpha_n \tilde{x}_n$ we have $\hat{f} = V_L \dots V_1 \hat{x}$.

[16] Normalization of each row exactly to norm 1 implies normalization of the matrix to M where M is the number of rows. However, normalization of each row to different constants does not lead to orthogonality.

We can now write the equation at the critical point here as

$$\frac{\partial \hat{f}}{\partial V_k^i} = V_L^i \cdots V_{k+1}^i V_{k-1}^i \cdots \hat{x^i}$$

and

$$V_k^i \hat{f} = V_k^i V_L \cdots V_{k+1} V_k V_{k-1} \cdots \hat{x}$$

where we now can label the diagonal layers with a single index i. Let us look at a specific example of a 4-layer network now, $\hat{f} = V_4 V_3 V_2 V_1 \hat{x}$. The equations are of the form

$$V_4^i \hat{f} = V_3^i V_2^i V_1^i \hat{x}^i$$

and similarly for other layers. Solving these, we get the very interesting constraints $\hat{f}^2 = (V_2^i V_1^i \hat{x}^i)^2 = (V_3^i V_1^i \hat{x}^i)^2 = \ldots$, or that some $V_k^i = 0$. This gives us that at the critical point, $V_k^i = \pm \frac{\hat{x}^i}{\hat{f}}$ or $V_k^i = 0$.

Putting back the definitions for the different expressions, we get that at the critical points, the normalized weights are given by

$$V_k^i = \pm \frac{\sum_n \alpha_n D_{L-1}(x_n^i) \ldots D_1(x_n^i) x_n^i}{\sum_n \alpha_n f(V; x_n)}, \tag{57}$$

with $i = 1, \ldots, p$ being one of the input channels (and the diagonal path trhough the network). Notice that the dependence on the layer k is only in the $\pm$ sign.