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# How Gradient Descent Separates Data with Neural Collapse: A Layer-Peeled Perspective

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## Abstract

1        In this paper, we study the inductive bias of the neural features and parameters  
2        from neural networks with cross-entropy loss. We study a surrogate model named  
3        unconstrained layer peeled model (ULPM), which helps us to illustrate that the  
4        features and classifiers in the last layer of the neural network will converge to  
5        a certain neural collapse structure [29], where the cross-example within-class  
6        variability of the last-layer features collapse to zero and the class-means converge  
7        to a Simplex Equiangular Tight Frame (ETF). We illustrate that the ULPM with  
8        cross-entropy loss enjoys a benign global landscape on this model where all the  
9        critical points are strict saddle points except the only global minimizers which  
10       exhibit neural collapse phenomenon. Empirically we show that our results also  
11       hold during the training of neural networks in real world tasks when explicit  
12       regularization or weight decay is not included.

## 13    1 Introduction

14    Deep learning has achieved state-of-the-art per-  
15    formances in various applications [21], from  
16    computer vision [17], to natural language  
17    processing[6] and even scientific discovery [24,  
18    42]. Despite the empirical successes achieved,  
19    how gradient descent or its variants leads deep  
20    neural networks to be biased towards solutions  
21    with good generalization performance on the  
22    test set is still a major open question. To de-  
23    velop a theoretical foundation for deep learn-  
24    ing, many works have studied the implicit  
25    bias of gradient descent in different settings  
26    [22, 1, 38, 34, 26, 3].

27    It is well-acknowledged that well-trained end-  
28    to-end deep architectures have the ability to ef-  
29    fectively extract features relevant to the given label. Although theoretical analysis of deep learning  
30    has several achievements in recent years [2, 13], most of the works that aim to analyze properties  
31    of the final output function fail to understand the feature learned. Recently in [29], authors observe  
32    that the within-class cross-sample features will collapse to the mean and the mean will converge  
33    to an Equiangular Tight Frame (ETF) during the terminal phase of training, *i.e.* after achieving  
34    zero training error and interpolating the in-sample training data. Such phenomenon, namely Neural  
35    Collapse (NC) [29], provides a clear view of how the last layer features in the neural network involve  
36    after interpolation and enables us to understand the benefit of training after achieving zero training  
37    error to achieve better properties in generalization and robustness. To theoretically analyze the neuron

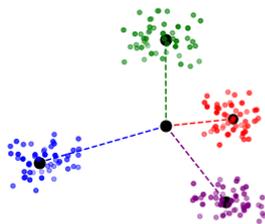


Figure 1: Illustration of Neural Collapse [29].

collapse phenomenon, [9, 25, 40] propose the Layer-Peeled Model (LPM) as a simplification for neural networks, where the last-layer features are modeled as free optimization variables. In particular, in a  $K$ -class classification problem using a neural network with  $d$  neurons in the last hidden layer, a corresponding class of LPMs can be defined through the form

$$\begin{aligned} \min_{\mathbf{W}, \mathbf{H}} \frac{1}{N} \sum_{i=1}^N \mathcal{L}(\mathbf{W}\mathbf{h}_i, \mathbf{y}_i) \\ \text{s.t. } \frac{1}{2} \|\mathbf{W}\|_F^2 \leq C_1, \frac{1}{2} \|\mathbf{H}\|_F^2 \leq C_2 \end{aligned} \quad (1)$$

for some positive constant  $C_1, C_2$ . Here  $\mathbf{W} = [\mathbf{w}_1, \mathbf{w}_2, \dots, \mathbf{w}_K]^\top \in \mathbb{R}^{K \times d}$  is the weight of the final linear classifier,  $\mathbf{H} = [\mathbf{h}_1, \mathbf{h}_2, \dots, \mathbf{h}_N] \in \mathbb{R}^{d \times N}$  is the feature of the last layer and  $\mathbf{y}_i$  is the corresponding label. The intuition behind LPM is that the modern deep networks are often highly over-parameterized, with the capacity to learn any representations of the input data. It has been shown that equiangular tight frame (ETF), *i.e.* feature with neural collapse, is the only global optimum of the LPM objective (1) [9, 25, 40]. However, even for this simplified model, the non-convexity nature of it makes the analysis highly non-trivial. In this paper we aim to understand *how gradient descent separates data with neural collapse*. To do this, we build a connection between the neural collapse with the recently proposed normalized margin [26, 39]. In [26], the authors shows that, using gradient descent, the direction of the weight converges to the direction that maximizes the  $\ell_2$ -margin of the data while the norm of the weight diverges to  $+\infty$  in homogeneous neural networks. Based on these results, we introduce neural collapse margin and use it provide a convergence result to the first order stationary point of the minimum-norm separation problem. Furthermore, we illustrate that the cross-entropy loss enjoys a benign global landscape where all the critical points are strict saddles in the tangent space except the only global minimizers which exhibit neural collapse phenomenon. The analysis provides insights on how gradient descent separates data during the training of neural networks with neural collapse and the benefit of training after interpolation on generalization and robustness. We verify our insights via empirical experiments.

| Reference    | Contribution                          | Feature Norm Constraint | Feature Norm Regularization | Loss Function      |
|--------------|---------------------------------------|-------------------------|-----------------------------|--------------------|
| [29]         | Empirical Results                     | ✗                       | ✗                           | Cross-Entropy Loss |
| [9]          | Global Optimum                        | ✓                       | ✗                           | Cross-Entropy Loss |
| [40]         | Global Optimum                        | ✓                       | ✗                           | Cross-Entropy Loss |
| [25]         | Global Optimum                        | ✓                       | ✗                           | Cross-Entropy Loss |
| [27, 30, 14] | Training Dynamics                     | ✗                       | ✗                           | $\ell_2$ Loss      |
| [44]         | Landscape Analysis                    | ✗                       | ✓                           | Cross-Entropy Loss |
| This paper   | Training Dynamics+ Landscape Analysis | ✗                       | ✗                           | Cross-Entropy Loss |

Table 1: Comparison of Recent Analysis for Neural Collapse. We provide strongest theoretical results with minimum modification on the training objective function.

Besides, [27] and a concurrent paper [44] also provide landscape and optimization analysis to study neural collapse phenomenon, we summarize the connection and difference with our paper in Table 1. Our result doesn't introduce any extra feature norm constraint or feature norm regularization, which are not commonly used in the realistic deep learning. We put the detailed discussion in Section 5.2.

## 1.1 Contribution

We summarize our contribution as follows.

- We build a relationship between the max-margin analysis [34, 28, 26] with the neural collapse and provide the inductive bias analysis to the feature rather than the output function.
- Previous works only prove that Gradient Descent on homogeneous neural networks will converge to the KKT point of the corresponding minimum-norm separation problem. However, the minimum-norm separation problem is still a highly non-convex problem. In this paper, we prove that the ULPM cases enjoys a benign landscape and characterize the neural collapse property of the global minimizer.

- We show that although the gradient descent on cross entropy loss will push the parameters to infinity, the landscape in the tangent space has no spurious minimum thus many optimization algorithms will converge only along the neural collapse directions .

## 1.2 Related Work

**Inductive Bias of Gradient Descent:** To understand how gradient or its variants descent helps deep learning to find solutions with good generalization performance on the test set. A recent line of research have studied the implicit bias of gradient descent in different settings. As example, gradient descent is biased towards model have smaller weight [22, 1, 38] and will converge to large margin solution [34, 28, 26, 7, 15] while using logistic loss. For linear networks, [3, 32, 12] have shown that gradient descent will find out a low rank approximation.

**Loss Landscape Analysis:** Although the practical optimization problems encountered in machine learning are often nonconvex, recent works have shown that critical points other than the good ones always lies in the balanced superpositions of symmetric copies of the ground truth according to the hidden symmetries in the objective function [35, 43] which leads to a benign global landscape. In particular, these landscapes do not exhibit spurious local minimizers or flat saddles and can be optimized easily via gradient based methods [10]. The examples including phase retrieval [37], low-rank matrix recovery [11, 10], dictionary learning [36, 31, 20], blind deconvolution [19].

## 2 Preliminaries and Problem Setup

### 2.1 Preliminaries

We consider a dataset with  $K$  classes:  $\bigcup_{k=1}^K \{\mathbf{x}_{k,i}\}_{i=1}^{n_k}$ . For simplicity, we assume the dataset is balanced, *i.e.*  $n_1 = \dots = n_K = n$ . A standard fully connected neural network can be represented as:

$$f(\mathbf{x}; \mathbf{W}_{full}) = \mathbf{b}_L + \mathbf{W}_L \sigma(\mathbf{b}_{L-1} + \mathbf{W}_{L-1} \sigma(\dots \sigma(\mathbf{b}_1 + \mathbf{W}_1 \mathbf{x}))). \quad (2)$$

Here  $\mathbf{W}_{full} = (\mathbf{W}_1, \mathbf{W}_2, \dots, \mathbf{W}_L)$  denote the weight matrices in each layer and  $(\mathbf{b}_1, \mathbf{b}_2, \dots, \mathbf{b}_L)$  are the bias terms,  $\sigma(\cdot)$  stands for the nonlinear activation function, for example, ReLU or sigmoid. Let  $\mathbf{h}_{k,i} = \sigma(\mathbf{b}_{L-1} + \mathbf{W}_{L-1} \sigma(\dots \sigma(\mathbf{b}_1 + \mathbf{W}_1 \mathbf{x}_{k,i}))) \in \mathbb{R}^d$  denote the last layer feature for data  $\mathbf{x}_{k,i}$  and  $\bar{\mathbf{h}}_k = \frac{1}{n} \sum_{i=1}^n \mathbf{h}_{k,i}$  the feature mean within in the  $k$ -th class. Without loss of generality, we can absorb the bias term into the weight matrix by adding a scalar into each feature vectors, so we will ignore the bias term in the following analysis. Let  $\mathbf{W} \in \mathbb{R}^{K \times d} = \mathbf{W}_L = [\mathbf{w}_1, \mathbf{w}_2, \dots, \mathbf{w}_K]^\top$  be the weight of the final linear classifier. Neural collapse is the phenomenon that the final layer feature will convergence to a simplex equiangular tight frame (ETF):

**Definition 2.1.** A symmetric matrix  $M \in \mathbb{R}^{K \times K}$  is said to be simplex equiangular tight frame (ETF) if

$$M = \sqrt{\frac{K}{K-1}} \mathbf{Q} (\mathbf{I}_K - \frac{1}{K} \mathbf{1}_K \mathbf{1}_K^\top). \quad (3)$$

Where  $\mathbf{Q} \in \mathbb{R}^{K \times K}$  is an orthogonal matrix.

The four criteria of neural collapse can be formulated precisely as

- **(NC1) Variability collapse:** As training progresses, the within-class variation of the activation becomes negligible as these activation collapse to their class-means  $\bar{\mathbf{h}}_k = \frac{1}{n} \sum_{i=1}^n \mathbf{h}_{k,i}$ .

$$\|\mathbf{h}_{k,i} - \bar{\mathbf{h}}_k\| = 0, \quad \forall 1 \leq k \leq K$$

- **(NC2) Convergence to Simplex ETF:** The vectors of the class-means (after centering by their global-mean converge to having equal length, forming equal-sized angles between any given pair, and being the maximally pairwise-distanced configuration constrained to the previous two properties.

$$\cos(\bar{\mathbf{h}}_k, \bar{\mathbf{h}}_j) = -\frac{1}{K-1}, \quad \|\bar{\mathbf{h}}_k\| = \|\bar{\mathbf{h}}_j\|, \quad \forall k \neq j$$

- **(NC3) Convergence to self-duality:** The linear classifiers and class-means will converge to each other, up to rescaling.

$$\exists C \text{ s.t. } \mathbf{w}_k = C \bar{\mathbf{h}}_k, \quad \forall 1 \leq k \leq K$$

- **(NC4) Simplification to Nearest Class-Center** For a given deepnet activation  $\mathbf{h} = \sigma(\mathbf{b}_{L-1} + \mathbf{W}_{L-1}\sigma(\dots\sigma(\mathbf{b}_1 + \mathbf{W}_1\mathbf{x}))) \in \mathbb{R}^d$ , the network classifier converges to choose whichever class has the nearest train class-mean

$$\arg \min_k \langle \mathbf{w}_k, \mathbf{h} \rangle \rightarrow \arg \min_k \|\mathbf{h} - \bar{\mathbf{h}}_k\|,$$

107 In this paper, we say a point  $\mathbf{W} \in \mathbb{R}^{K \times d}$ ,  $\mathbf{H} \in \mathbb{R}^{d \times nK}$  satisfies neural collapse conditions or is  
 108 neural collapse solution if these four criteria are all satisfied for  $(\mathbf{W}, \mathbf{H})$ .

## 109 2.2 Problem Setup

110 In this paper, we mainly focus on the neural collapse phenomenon, which is only related to the  
 111 classifiers and features in the last layer. Since general analysis on the highly non-smooth and non-  
 112 convex neural network is difficult, here we peel down the last layer of neural network and propose  
 113 the following **Unconstrained Layer-Peeled Model (ULPM)** as a simplification to capture the main  
 114 characteristic related to neural collapse during the training dynamics. Similar simplification is  
 115 common used in previous theoretical works [25, 9, 40, 44], but ours don't have any constraint or  
 116 regularization on features and stands closer to realistic neural network models. We need to mention  
 117 that although [27] also study the unconstrained model, their analysis is highly dependent on the  $\ell_2$   
 118 loss function which is rarely used in classification task while ours can address the most popular cross  
 119 entropy loss.

120 Let  $\mathbf{W} = [\mathbf{w}_1, \mathbf{w}_2, \dots, \mathbf{w}_K]^\top \in \mathbb{R}^{K \times d}$  and  $\mathbf{H} = [\mathbf{h}_{1,1}, \dots, \mathbf{h}_{1,N}, \mathbf{h}_{2,1}, \dots, \mathbf{h}_{K,N}] \in \mathbb{R}^{d \times KN}$   
 121 be the matrices of classifiers and features in the last layer, where  $K$  is the number of classes and  $N$   
 122 is the number of data points in each classes. The Unconstrained Layer-Peeled Model is defined as  
 123 following:

$$\min_{\mathbf{W}, \mathbf{H}} \mathcal{L}(\mathbf{W}, \mathbf{H}) = - \sum_{k=1}^K \sum_{i=1}^n \log \left( \frac{\exp(\mathbf{w}_k^\top \mathbf{h}_{k,i})}{\sum_{j=1}^K \exp(\mathbf{w}_j^\top \mathbf{h}_{k,i})} \right) \quad (4)$$

124 Here we do not have any constrain or regularization on features, which corresponds to the absence  
 125 of weight decay in deep learning training. The objective function (4) is generally non-convex on  
 126  $(\mathbf{W}, \mathbf{H})$  and we aim to study the landscape of the objective function (4). Furthermore, we consider  
 127 the gradient flow of the the objective function

$$\frac{d\mathbf{W}(t)}{dt} = \frac{\partial \mathcal{L}(\mathbf{W}(t), \mathbf{H}(t))}{\partial \mathbf{W}}, \quad \frac{d\mathbf{H}}{dt} = \frac{\partial \mathcal{L}(\mathbf{W}(t), \mathbf{H}(t))}{\partial \mathbf{H}}.$$

128 We also trace the the dynamic of the loss function  $\mathcal{L}(t) := \mathcal{L}(\mathbf{W}(t), \mathbf{H}(t))$  and study the convergence  
 129 of  $(\mathbf{W}(t), \mathbf{H}(t))$ .

130 **Notations.** We denote  $\|\cdot\|_F$  the Frobenius norm,  $\|\cdot\|_2$  the matrix spectral norm,  $\|\cdot\|_*$  the nuclear  
 131 norm,  $\|\cdot\|$  the vector  $l_2$  norm and  $tr(\cdot)$  the trace of matrices. We use  $[K] := \{1, 2, \dots, K\}$  to denote  
 132 the set of indices up to  $K$ .

## 133 3 Main Results

134 In this section, we present our main results about the training dynamics and landscape analysis about  
 135 (4). We organize the section as follows: First in Section 3.1.1, we show the relationship between  
 136 margin and neural collapse in our surrogate model. Inspired by this relationship, we propose a  
 137 minimum-norm separation problem (5) and show the connection between the convergence direction  
 138 of gradient flow and the KKT point of (5). In addition, we explicitly solve the global optimum of  
 139 (5) and show it must satisfy neural collapse conditions. However, due to the non-convexity, we find  
 140 an Example 3.1 in Section 3.2 which shows that there exist some bad KKT points such that simple  
 141 gradient flow will get stuck in them and not converge to neural collapse solution which is proved  
 142 to be optimal in Theorem 3.3. Then we present our second-order analysis result in Theorem 3.4 to  
 143 show that those bad points will exhibit decreasing directions in the tangent space thus if we add some  
 144 noise in the training algorithm (e.g. use stochastic gradient descent), our algorithm can escape from  
 145 those directions and can only converge to the neural collapse solutions.

### 146 3.1 Convergence To The First-Order Stationary Point

#### 147 3.1.1 Neural Collapse Margin

148 Before we state our convergence result, let's first discuss the relationship between margin and neural  
 149 collapse. By building the relationship between them we can have a better intuition about why gradient  
 150 flow can converge to neural collapse solution since the convergence to max-margin solutions has been  
 151 studied in many literature [22, 26, 1, 38]. Recall the margin of a single data point  $\mathbf{x}_{k,i}$  and associated  
 152 feature  $\mathbf{h}_{k,i}$  as  $q_{k,i}(\mathbf{W}, \mathbf{H}) := \mathbf{w}_k^\top \mathbf{h}_{k,i} - \max_{j \neq k} \mathbf{w}_j^\top \mathbf{h}_{k,i}$ . [5, 4]. To bridge the margin theory with  
 153 neural collapse phenomenon, we define the following neural collapse margin:

154 **Definition 3.1.** We define the the **Neural Collapse Margin** for the entire dataset as  $q_{\min}(\mathbf{W}, \mathbf{H}) =$   
 155  $\min_{k \in [1, K], i \in [1, n]} q_{k,i}(\mathbf{W}, \mathbf{H})$ .

156 The following lemma shows that the neural collapse margin is an indicator of the neural collapse  
 157 phenomenon in the sense that collapsed margin minimize the neural collapse margin. Thus we can  
 158 trace the neural collapse margin to study the convergence to the neural collapse solution.

**Lemma 3.1** (Neural Collapse Margin as an Indicator of Neural Collapse). *The neural collapse margin always smaller than*

$$q_{\min}(\mathbf{W}, \mathbf{H}) \leq \frac{\|\mathbf{W}\|_F^2 + \|\mathbf{H}\|_F^2}{2(K-1)\sqrt{n}}$$

159 and  $(\mathbf{W}, \mathbf{H})$  must satisfies the neural collapse conditions when the inequality above is reduced to an  
 160 equality.

#### 161 3.1.2 Convergence Results

162 Now we present our result about the convergence of gradient flow on the ULPM (4). Following [26],  
 163 we link gradient flow on cross-entropy loss with a minimum-norm separation problem.

164 **Theorem 3.1.** *For problem (4), let  $(\mathbf{W}(t), \mathbf{H}(t))$  be the path of gradient flow at time  $t$ , if there  
 165 exist a time  $t_0$  such that  $\mathcal{L}_{CE}(\mathbf{W}(t_0), \mathbf{H}(t_0)) < \log 2$ , then any limit point of  $\{(\hat{\mathbf{H}}(t), \hat{\mathbf{W}}(t)) :=$   
 166  $(\frac{\mathbf{H}(t)}{\sqrt{\|\mathbf{W}(t)\|_2^2 + \|\mathbf{H}(t)\|_2^2}}, \frac{\mathbf{W}(t)}{\sqrt{\|\mathbf{W}(t)\|_2^2 + \|\mathbf{H}(t)\|_2^2}})\}$  is along the direction of an Karush-Kuhn-Tucker (KKT)  
 167 point of the following minimum-norm separation problem:*

$$\begin{aligned} & \min_{\mathbf{W}, \mathbf{H}} \frac{1}{2} \|\mathbf{W}\|_F^2 + \frac{1}{2} \|\mathbf{H}\|_F^2 \\ & \text{s.t. } \forall k \neq j \in [K], i \in [n], \quad \mathbf{w}_k^\top \mathbf{h}_{k,i} - \mathbf{w}_j^\top \mathbf{h}_{k,i} \geq 1. \end{aligned} \quad (5)$$

168 *Remark 3.1.* Indeed, the problem (5) can be reorganized to maximize neural collapse margin such  
 169 that the norm is constrained to be lower than a certain value. The proof is as follows, for all feasible  
 170 solutions  $(\mathbf{W}, \mathbf{H})$ , we can find that  $\forall \alpha \geq q_{\min}(\mathbf{W}, \mathbf{H})^{-1/2}$ ,  $\alpha(\mathbf{W}, \mathbf{H})$  are still feasible thus the  
 171 minimum objective value is  $\frac{\frac{1}{2}\|\mathbf{W}\|_F^2 + \frac{1}{2}\|\mathbf{H}\|_F^2}{q_{\min}(\mathbf{W}, \mathbf{H})^{1/2}}$  along the direction of  $(\mathbf{W}, \mathbf{H})$ . Then take minimum  
 172 among all the directions we can find the minimum is attained if and only if  $(\mathbf{W}, \mathbf{H})$  attains the  
 173 maximum neural collapse margin on the sphere  $\{(\mathbf{W}, \mathbf{H}) : \|\mathbf{W}\|_F^2 + \|\mathbf{H}\|_F^2 \leq C\}$

174 The Theorem 3.1 indicates that the convergent direction of gradient flow is restricted to those  
 175 max-margin directions, which usually enjoy some good properties on robustness or generalization  
 176 performance. Generally speaking, the KKT conditions are not sufficient to obtain global optimality  
 177 since the minimum-norm separation problem (5) is non-convex. Moreover, in some certain occasions,  
 178 KKT conditions may be even not necessary for global optimum. However, we can have a precise  
 179 characterization about the optimum from another perspective, the following result shows that the  
 180 global optimum of this problem satisfies neural collapse conditions.

181 **Theorem 3.2.** *Every global optimum of the minimum-norm separation problem (5) is also a KKT  
 182 point and it satisfies the neural collapse conditions.*

183 To illustrate how does (5) related to (4) and gain insight about Theorem 3.1, we provided the following  
 184 lemmas to show that when  $t$  is sufficient large, the  $(\mathbf{W}(t), \mathbf{H}(t))$  is an  $(\epsilon, \delta)$  approximate KKT point  
 185 after appropriate scaling, where the  $(\epsilon, \delta)$  converges to zero when  $t \rightarrow \infty$ . Then as shown in [8] we  
 186 know that the limit of these  $(\epsilon, \delta)$  approximate KKT point is exact KKT point. Detailed definition of  
 187 KKT points and approximate KKT points can be found in appendix.

**Lemma 3.2.** *If there exist a time  $t_0$  such that  $\mathcal{L}(\mathbf{W}(t_0), \mathbf{H}(t_0)) < \log 2$ , then for any  $t > t_0$   $(\tilde{\mathbf{W}}(t), \tilde{\mathbf{H}}(t)) := (\mathbf{W}(t), \mathbf{H}(t))/q_{\min}(\mathbf{W}(t), \mathbf{H}(t))^{1/2}$  is a  $(\epsilon, \delta)$ -approximate KKT point of the following minimum-norm separation problem. More precisely, we have*

$$\epsilon = \sqrt{\frac{2(1-\beta(t))}{C}}, \delta = \frac{K}{2Cq_{\min}(t)}$$

where:

$$\beta = \frac{\text{tr}(\mathbf{W}^\top \nabla_{\mathbf{W}} \mathcal{L}(\mathbf{W}, \mathbf{H})) + \text{tr}(\mathbf{H}^\top \nabla_{\mathbf{H}} \mathcal{L}(\mathbf{W}, \mathbf{H}))}{\sqrt{\|\mathbf{W}\|_F^2} + \|\mathbf{H}\|_F^2} \sqrt{\|\nabla_{\mathbf{W}} \mathcal{L}(\mathbf{W}, \mathbf{H})\|_F^2} + \|\nabla_{\mathbf{H}} \mathcal{L}(\mathbf{W}, \mathbf{H})\|_F^2}$$

188 is the angle between  $(\mathbf{W}, \mathbf{H})$  and its corresponding gradient and  $C$  is a positive constant.

189 **Lemma 3.3.** *If there exist a time  $t_0$  such that  $\mathcal{L}_{CE}(\mathbf{W}(t_0), \mathbf{H}(t_0)) < \log 2$ , then we have:*

$$\beta(t) \rightarrow 1, \quad q_{\min}(t) \rightarrow \infty \text{ as } t \rightarrow \infty \quad (6)$$

190 which implies that  $\epsilon \rightarrow 0$  and  $\delta \rightarrow 0$  when time  $t$  goes to infinity.

### 191 3.2 Second-Order Landscape Analysis

192 Due to the non-convex nature of the objective (4), we can't achieve such global solution efficiently.  
193 The global optimality condition shown in Theorem 3.2 still can't guarantee convergence to neural  
194 collapse. In this section, we aim to show that this non-convex optimization problem is actually not  
195 scary.

196 Different from previous landscape analysis of non-convex problem, where people aim to show that  
197 the objective has a negative directional curvature around any stationary point [35, 43], once features  
198 can be perfectly separated, the ULPM objective (4) will always decrease along the direction of the  
199 current point and the optimum is attained only in infinity. Although growing along all of those  
200 perfectly separation directions can let the loss function decreasing to 0, the speed of decreasing are  
201 quite different and there exists an optimal direction with fastest decreasing speed. However, simple  
202 first-order analysis may fail to interpret how does gradient flow move among these directions and we  
203 need second-order analysis to help us fully characterize the realistic training dynamics. Here is an  
204 example illustrating our motivation.

205 **Example 3.1** (A Motivating Example). Consider the case when  $K = 4, n = 1$ , let  $(\mathbf{W}, \mathbf{H})$  be the  
206 following point:

$$\mathbf{W} = \mathbf{H} = C \begin{bmatrix} 1 & -1 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & 0 & 1 & -1 \\ 0 & 0 & -1 & 1 \end{bmatrix} \quad (7)$$

207 One can easily verify that this  $(\mathbf{W}, \mathbf{H})$  enables our model to classify all of the features perfectly.  
208 Further more, we can show it is along the direction of a KKT point of the minimum-norm separation  
209 problem (5) by construct the Lagrangian multiplier  $\Lambda = (\lambda_{ij})_{i,j=1}^K$  as following:

$$\Lambda = \begin{bmatrix} 0 & 0 & \frac{1}{2} & \frac{1}{2} \\ 0 & 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 \end{bmatrix} \quad (8)$$

210 And the gradient of  $(\mathbf{W}, \mathbf{H})$  is

$$\nabla_{\mathbf{W}} \mathcal{L}(\mathbf{W}, \mathbf{H}) = \nabla_{\mathbf{H}} \mathcal{L}(\mathbf{W}, \mathbf{H}) = -C \frac{2 + 2e^{-2C^2}}{2 + 2e^{-2C^2} + 2e^{2C^2}} \begin{bmatrix} 1 & -1 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & 0 & 1 & -1 \\ 0 & 0 & -1 & 1 \end{bmatrix} \quad (9)$$

211 We can find that the directions of gradient and the parameter align with each other (*i.e.*  
212  $\mathbf{W} // \nabla_{\mathbf{W}} \mathcal{L}(\mathbf{W}, \mathbf{H}), \mathbf{H} // \nabla_{\mathbf{H}} \mathcal{L}(\mathbf{W}, \mathbf{H})$ ), which implies simple gradient descent get stuck in this  
213 direction and only grow the parameter norm. However, if we construct:

$$\mathbf{W}' = \mathbf{H}' = C \begin{bmatrix} 1 & \alpha & \beta & \beta \\ \alpha & 1 & \beta & \beta \\ \beta & \beta & 1 & \alpha \\ \beta & \beta & \alpha & 1 \end{bmatrix}, \quad \alpha^2 + 2\beta^2 = 1, \alpha < 0, \beta < 0 \quad (10)$$

214 Then  $\forall \epsilon > 0$ , we can choose appropriate  $\alpha, \beta$  such that (see detailed computation in Appendix):

$$\begin{aligned} \|\mathbf{W}'\|_F^2 &= \|\mathbf{W}\|_F^2, \|\mathbf{H}'\|_F^2 = \|\mathbf{H}\|_F^2, \\ \|\mathbf{W}' - \mathbf{W}\|_F^2 + \|\mathbf{H}' - \mathbf{H}\|_F^2 &< \epsilon, \mathcal{L}(\mathbf{W}', \mathbf{H}') \leq \mathcal{L}(\mathbf{W}, \mathbf{H}) \end{aligned} \quad (11)$$

215 The results in (11) indicate that  $(\mathbf{W}', \mathbf{H}')$  is a saddle point on the sphere and there exists many better  
216 direction  $(\mathbf{W}', \mathbf{H}')$  staying very close to the original direction  $(\mathbf{W}, \mathbf{H})$ . Although simple gradient  
217 descent will always move along the original direction, once we add some noise in the training (e.g.  
218 stochastic gradient descent), the optimization algorithm can find this better direction and escape the  
219 original bad direction.

220 In Example 3.1, we show that there does exist some suboptimal KKT point of the minimum-norm  
221 separation problem (5), but there also exist some better points close to it thus stochastic gradient  
222 method can easily escape from them. In the following theorem, we will show that the best directions  
223 are neural collapse solutions in the sense that the loss function is lowest among all the growing  
224 directions.

225 **Theorem 3.3.** *The optimal value of loss function (4) on a sphere is attained (i.e.  $\mathcal{L}(\mathbf{W}, \mathbf{H}) \leq$   
226  $\mathcal{L}(\mathbf{W}', \mathbf{H}')$ ,  $\forall \|\mathbf{W}'\|_F^2 + \|\mathbf{H}'\|_F^2 = \|\mathbf{W}\|_F^2 + \|\mathbf{H}\|_F^2$ ) if only if the  $(\mathbf{W}, \mathbf{H})$  satisfies neural collapse  
227 conditions and  $\|\mathbf{W}\|_F = \|\mathbf{H}\|_F$ .*

228 *Remark 3.2.* Note that the second conditions is necessary since neural collapse conditions don't  
229 specify the norm ratio of  $\mathbf{W}$  and  $\mathbf{H}$ . That is, if  $(\mathbf{W}, \mathbf{H})$  satisfies neural collapse conditions,  
230  $(\alpha\mathbf{W}, \beta\mathbf{H})$ ,  $\forall \alpha, \beta \in \mathbb{R}$  will also satisfies them but only some certain  $\alpha, \beta$  are optimal.

231 Now we turns to those points that don't satisfy neural collapse conditions. To formalize our discussion  
232 in the motivating Example 3.1, we first introduce the tangent space:

233 **Definition 3.2** (tangent space). The tangent space of  $(\mathbf{W}, \mathbf{H})$  is defined to be a set of directions that  
234 are orthogonal to  $(\mathbf{W}, \mathbf{H})$  :

$$\mathcal{T}(\mathbf{W}, \mathbf{H}) = \{\Delta\mathbf{W} \in \mathbb{R}^{K \times d}, \Delta\mathbf{H} \in \mathbb{R}^{d \times nK} : \text{tr}(\mathbf{W}^\top \Delta\mathbf{W}) + \text{tr}(\mathbf{H}^\top \Delta\mathbf{H}) = 0\} \quad (12)$$

235 Our next result justify our observation in the Example 3.1 that for every suboptimal points, there exist  
236 a direction in the tangent space such that move along this direction will leads to a lower objective  
237 value.

238 **Theorem 3.4.** *If  $(\mathbf{W}, \mathbf{H})$  is not the optimal solutions in Theorem 3.3, then  $\exists(\Delta\mathbf{W}, \Delta\mathbf{H}) \in$   
239  $\mathcal{T}(\mathbf{W}, \mathbf{H})$ ,  $M > 0$  such that*

$$\forall 0 < \delta < M, \mathcal{L}(\mathbf{W} + \delta\Delta\mathbf{W}, \mathbf{H} + \delta\Delta\mathbf{H}) \leq \mathcal{L}(\mathbf{W}, \mathbf{H}) \quad (13)$$

240 . *Further more, it implies that  $\forall \epsilon > 0$ ,  $\exists(\mathbf{W}', \mathbf{H}')$  such that:*

$$\begin{aligned} \|\mathbf{W}'\|_F^2 + \|\mathbf{H}'\|_F^2 &= \|\mathbf{W}\|_F^2 + \|\mathbf{H}\|_F^2, \\ \|\mathbf{W}' - \mathbf{W}\|_F^2 + \|\mathbf{H}' - \mathbf{H}\|_F^2 &< \epsilon, \mathcal{L}(\mathbf{W}', \mathbf{H}') \leq \mathcal{L}(\mathbf{W}, \mathbf{H}) \end{aligned} \quad (14)$$

241 *Remark 3.3.* The result in (13) give us a decreasing direction orthogonal to the direction of  $(\mathbf{W}, \mathbf{H})$ ,  
242 as shown in Example 3.1, the gradient might be parallel to  $(\mathbf{W}, \mathbf{H})$ , the decreasing direction must be  
243 obtained by analyze the Hessian matrices and it further indicates that these points are exactly saddle  
244 points in the tangent space, a formal statement and definition can be found in appendix. For a large  
245 family of stochastic optimization algorithm , the projection of noise onto this decreasing direction  
246 is not zero with probability 1, so its those algorithms will escape the bad point and no longer move  
247 along this direction within a small number of iterations.

## 248 4 Empirical Results

249 **Gradient Descent on the ULPM Objective.** We first conduct experiments on the ULPM objective  
250 (4) to support the results of convergence towards Neural Collapse in our theories. We set  $N = 10$ ,  
251  $K = 5$ ,  $d = 20$  and use gradient descent with learning rate 5 to run  $10^5$  epochs. We characterize  
252 the dynamics of the training procedure in Figure 2, through four aspects: (1) variation of the  
253 centered class-mean features' norms (i.e.,  $\text{Std}(\|\mathbf{h}_k - \bar{\mathbf{h}}\|) / \text{Avg}(\|\mathbf{h}_k - \bar{\mathbf{h}}\|)$ ) and the variation of the  
254 classifier's norms (i.e.,  $\text{Std}(\|\bar{\mathbf{w}}_k\|) / \text{Avg}(\|\bar{\mathbf{w}}_k\|)$ ). (2) Within-class variation of last layer features  
255 (i.e.,  $\text{Avg}(\|\mathbf{h}_{k,i} - \mathbf{h}_k\|) / \text{Avg}(\|\mathbf{h}_{k,i} - \bar{\mathbf{h}}\|)$ ). (3) The cosines between pairs of last layer features (i.e.,

256  $\text{Avg}(|\cos(\bar{\mathbf{h}}_k, \bar{\mathbf{h}}_{k'}) + 1/(K-1)|)$ ) and that of the classifiers (*i.e.*,  $\text{Avg}(|\cos(\bar{\mathbf{w}}_k, \bar{\mathbf{w}}_{k'}) + 1/(K-1)|)$ ),  
 257 (4) The distance between normalized centered classifier and normalized last layer feature (*i.e.*,  
 258  $\text{Avg}(|(\bar{\mathbf{h}}_k - \bar{\mathbf{h}})/\|\bar{\mathbf{h}}_k - \bar{\mathbf{h}}\| - \bar{\mathbf{w}}_k/\|\bar{\mathbf{w}}_k\|)|)$ ). Empirically we observe that logarithm of the two  
 259 variations of norms (in the first aspect) decrease approximately at rate  $O(1/(\log(t)))$ , and the  
 260 remaining quantities decrease approximately at rate  $O(1/(\log(t)))$ .

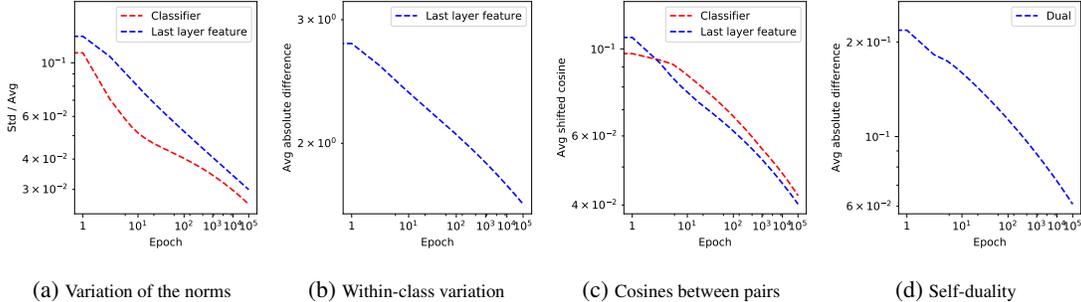


Figure 2: Training dynamics in ULPM. The  $x$ -axis in the figures are set to have  $\log(\log(t))$  scales and the  $y$ -axis in the figures are set to have  $\log$  scales. (a) The dynamics of the variation of the centered class-mean features’ norms (shown in blue) and the variation of the classifier’s norms (shown in red). We observe that the logarithm of both terms decrease at rate  $O(1/(\log(t)))$ . (b) The dynamics of the within-class variation of last layer features. Logarithm of the variation converge approximately at rate  $O(1/\log(t))$ . (c) The dynamics of the cosines between pairs of last layer features (shown in blue) and that of the classifiers (shown in red). Logarithm of both terms converge approximately at rate  $O(1/\log(t))$ . (d) The dynamics of the distance between normalized centered classifier and normalized last layer feature. Logarithm of the quantity converge approximately at rate  $O(1/\log(t))$  to the point of self-duality.

261 **Realistic Training.** We also extend our theory to realistic neural network training on benchmark  
 262 dataset. To evaluate our theory, we train the VGG-13 [33] on FashionMNIST [41] without weight  
 263 decay and track the convergence speed of the last layer feature to the neural collapse solution every few  
 264 epochs to see how it changes during the terminal phase training. Observe that all the aforementioned  
 265 quantities either decrease or stay in small values during the training process, providing implications  
 266 that neural collapse can occur with sufficient training epochs.

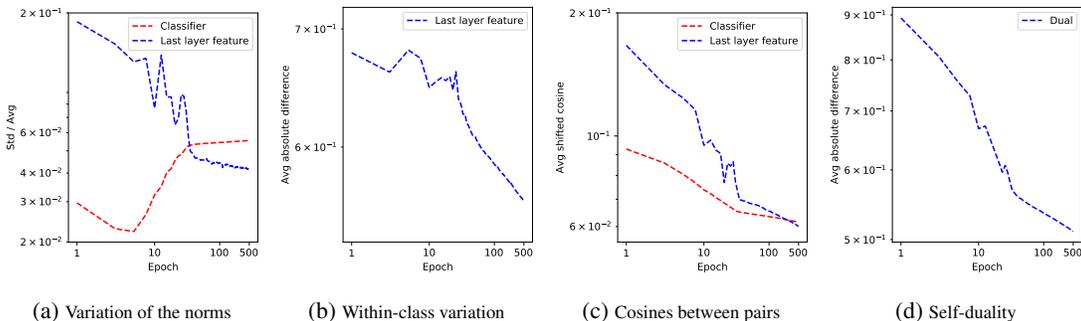


Figure 3: Training VGG-13 without weight decay on FashionMNIST. The  $x$ -axis in the figures are set to have  $\log(\log(t))$  scales and the  $y$ -axis in the figures are set to have  $\log$  scales. (a) Variation of the centered class-mean features’ norms and that of the classifier’s norms are below 0.1 after 500 epochs. (b) Logarithm of the within-class variation of last layer features decreases approximately linearly with respect to  $\log(\log(t))$  after 100 epochs. (c) The cosines between pairs of last layer features and that of the classifiers decrease and are below 0.1 after 500 epochs. (d) The distance between normalized centered classifier and normalized last layer feature decreases during training towards self-duality.

## 267 5 Conclusion and Discussion

### 269 5.1 Conclusion

270 To understand the inductive bias of neural feature from gradient descent training, we build a connection  
 271 between large margin inductive bias with neural collapse phenomenon and study a unconstrained

272 layer-peeled model in this paper. We proved that the gradient flow of the ULPM convergences  
273 to KKT point of a minimum-norm separation problem where the global optimum satisfies neural  
274 collapse conditions. Although the ULPM is nonconvex, we show that ULPM have a nice landscape  
275 where all the stationary point is a strict saddle point in the tangent space except the global neural  
276 collapse solution. Our study helps to demystify the neural collapse phenomenon, which shed light on  
277 the generalization and robustness properties during the terminal phase of training deep networks in  
278 classification problems.

## 279 5.2 Relationship with Other Results

280 Theoretical analysis of neural collapse are first provided by [25, 40, 9], they show that the neural  
281 collapse solution is the only global minimum of the simplified non-convex objective function. In  
282 particular, [40, 25] study a continuous integral form of the loss function and show that the feature  
283 learnt should be a uniform distribution on sphere. A more realistic discrete setting are studied in  
284 [9], where the constraint is on the whole feature matrix rather than individual features. All these  
285 results only relies on Jensen inequality on output logits thus can be generalized to other convex in  
286 logit losses. Our result utilize the implicit bias of the exponential like loss function to remove the  
287 feature norm constraint which is not practicable in real applications.

288 Though the global optimum shares good property [9], the ULPM objective is still highly non-convex.  
289 Regards optimization, [27, 30, 14] analyze the unconstrained feature model with  $\ell_2$  loss and establish  
290 convergence results to collapsed feature for gradient descent. However they fail to generalize on  
291 other more practical loss functions used in classification tasks. The analysis highly relies on the  $\ell_2$   
292 loss which turns the training dynamic to an ODE in eigenvalues.

293 The most relevant paper is a *concurrent* breakthrough work [44], which provide a landscape analysis  
294 about the regularized unconstrained feature model. [44] turns the feature norm constraint in [9] into  
295 feature norm regularization and still preserves the neural collapse global optimum. At the same  
296 time, [44] also show that the modified regularized objective shares a benign landscape, where all  
297 the critical points are strict saddles except the global one. Although our paper and [44] discover  
298 similar landscape results, we believe our characterization stays closer to the real algorithms used in  
299 the following two ways

- 300 • The same as [25, 40, 9], [44] only utilize the convexity in logits of the loss function. However,  
301 our analysis also explores the exponential-like property of the cross-entropy loss which will  
302 enlarge the norm of the feature. The large feature will provide better approximation to the  
303 true neural collapse problem of the normalized feature via approximating the max function  
304 via gradually scaled exponential function.
- 305 • We doesn't introduce any constraints or regularization on the feature norm, which is not  
306 applied in the realist training. Regularization on feature introduce in [44] is still different  
307 from the weight decay regularization [18]. However weight decay on homogeneous neural  
308 network is equivalent to gradient descent with scaling step size on unregularized objective  
309 [23, 42].

310 We summarize analysis of neural collapse in Table 1.

## 311 5.3 Limitation and Future Work

312 The convergence to neural collapse is super slow. [16] provide a loss dependent learning rate schedule  
313 and leads to  $O(1/t)$  convergence rate for linear regression. It's interesting to investigate can this  
314 methodology being generalized to our setting. On the other hand, although we have shown that the  
315 ULPM have a nice landscape, we still leave the global convergence of (stochastic) gradient descent  
316 as future work for we want to provide global convergence of gradient descent combined with a plug  
317 in feature extractor.

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425 **Checklist**

- 426 1. For all authors...
- 427 (a) Do the main claims made in the abstract and introduction accurately reflect the paper's  
428 contributions and scope? [Yes]
- 429 (b) Did you describe the limitations of your work? [Yes]
- 430 (c) Did you discuss any potential negative societal impacts of your work? [N/A]
- 431 (d) Have you read the ethics review guidelines and ensured that your paper conforms to  
432 them? [Yes]
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- 434 (a) Did you state the full set of assumptions of all theoretical results? [Yes]
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440 chosen)? [Yes]
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- 459 (c) Did you include the estimated hourly wage paid to participants and the total amount  
460 spent on participant compensation? [N/A]