

A PROOFS OF SECTION 3.1

A.1 PROOF OF THEOREM 2 AND CORRESPONDING RESULTS

Recall an ETF defined by

$$M = \sqrt{\frac{K}{K-1}} P \left(I_K - \frac{1}{K} \mathbf{1}_K \mathbf{1}_K^T \right) = \sqrt{\frac{K}{K-1}} \left(P - \frac{1}{K} \sum_{k=1}^K P_k \mathbf{1}_K^T \right),$$

where $P = [P_1, \dots, P_K] \in \mathbb{R}^{p \times K}$ is a partial orthogonal matrix with $P^T P = I_K$. Rewrite $M = [M_1, \dots, M_K]$. Let the label $y = (y_1, \dots, y_K)^T \in \{0, 1\}^K$ be represented by the one-hot encoding, that is, $y_k = 1$ and $y_j = 0$ for $j \neq k$ if y belongs to the k -th class.

Definition 6 (Classification problem under Neural Collapse). *Let there be K classes. The distribution $\mathbb{P}[x = M_k | y_k = 1] = 1$ for $k = 1, \dots, K$.*

Proof of Theorem 2 Let $W = [W_1, \dots, W_K]^T \in \mathbb{R}^{K \times p}$. Consider the output function $f_W(x) = Wx \in \mathbb{R}^K$. Suppose that $y_k = 1$. Then, the cross-entropy loss is defined by

$$\ell(f_W(x), y) = -\log \left(\frac{e^{W_k^T x}}{\sum_{k'=1}^K e^{W_{k'}^T x}} \right).$$

The corresponding empirical risk is

$$R_n(M, W) = \sum_{k=1}^K -n_k \log \left(\frac{e^{W_k^T M_k}}{\sum_{k'=1}^K e^{W_{k'}^T M_k}} \right).$$

Note that

$$\nabla_W \ell(f_W(x), y) = (\text{SoftMax}(f_W(x)) - y) x^T,$$

where $\text{SoftMax} : \mathbb{R}^K \rightarrow \mathbb{R}^K$ is the SoftMax function defined by

$$\text{SoftMax}(z)_i = \frac{e^{z_i}}{\sum_{j=1}^K e^{z_j}}, \quad \text{for all } z \in \mathbb{R}^K.$$

We obtain

$$\nabla_W R_n(M, W) = \sum_{k=1}^K n_k (\text{SoftMax}(f_W(M_k)) - y^k) M_k^T,$$

where y^k is the label of the k -th class. For zero initialization, we have

$$\text{SoftMax}(f_0(M_k)) = \frac{1}{K} \mathbf{1}_K$$

and

$$\nabla_W (R_n(M, W)) \Big|_{W=0} = \sum_{k=1}^K n_k \left(\frac{1}{K} \mathbf{1}_K - y^k \right) M_k^T. \quad (2)$$

Now we consider one step NoisyGD from 0 with learning rate $\eta = 1$:

$$\widehat{W} = - \sum_{k=1}^K n_k \left(\frac{1}{K} \mathbf{1}_K - y^k \right) M_k^T + \Xi,$$

where $\Xi \in \mathbb{R}^{K \times p}$ with Ξ_{ij} drawn independently from a normal distribution $\mathcal{N}(0, \sigma^2)$.

Consider $x = M_k$. It holds

$$f_{\widehat{W}}(x) = \widehat{W} M_k = - \sum_{k'=1}^K n_{k'} \left(\frac{1}{K} \mathbf{1}_K - y^{k'} \right) M_{k'}^T M_k + \Xi M_k.$$

Since

$$\Xi M_k \sim \mathcal{N}(0, \sigma^2 \|M_k\|_2^2 I_K) \quad \text{and} \quad \|M_k\|_2^2 = 1$$

we have

$$\widehat{W} M_k \sim \mathcal{N}(\boldsymbol{\mu}_{n,K}, \sigma^2 I_K),$$

where $\boldsymbol{\mu}_{n,K} = -\sum_{k'=1}^K n_{k'} \left(\frac{1}{K} \mathbf{1}_K - y^{k'}\right) M_{k'}^T M_k$. Note that

$$M_{k'}^T M_k = \frac{K}{K-1} \left(\delta_{k,k'} - \frac{1}{K}\right).$$

We obtain

$$(\boldsymbol{\mu}_{n,K})_j = \begin{cases} n/K, & j = k, \\ -\frac{n(K-2)}{K^2(K-1)}, & j \neq k, \end{cases}$$

for $n_{k'} = n/K$ (balanced data). By the union bound, the mis-classification error is

$$(K-1) \mathbb{P} \left[\mathcal{N}(n/K, \sigma^2) < \mathcal{N}\left(-\frac{n(K-2)}{K^2(K-1)}, \sigma^2\right) \right] = (K-1) \Phi \left(-\frac{n}{K\sigma} \left(1 + \frac{K-2}{K(K-1)}\right) \right)$$

□

Proof sketches of the insights. Note that in Equation equation 2 the gradient is a linear function of the feature map thanks to the zero-initialization while for least-squares loss, one can derive a similar gradient as Equation equation 2. Thus, the proof can be extended to the least squares loss directly. Moreover, by replacing n_k with $n_k \eta$ in equation 2 one can extend the results to any η .

A.2 PROOF OF THEOREM 3

Recall the re-parameterization for $K = 2$. Precisely, an equivalent neural collapse case gives $M = [-e_1, e_1]$ with $e_1 = [1, 0, \dots, 0]^T$. Furthermore, we consider the re-parameterization with $y \in \{-1, 1\}$, $\theta \in \mathbb{R}^p$ and the decision rule being $\hat{y} = \text{sign}(\theta^T x)$. Then, the logistic loss is $\log(1 + e^{-y \cdot \theta^T x})$.

Proof of Theorem 3 According to the re-parameterization, for the class imbalanced case, we have

$$\hat{\theta} = -\eta \left(\frac{n}{2} \cdot 0.5 \cdot \begin{pmatrix} -1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} + \frac{n}{2} \cdot 0.5 \cdot \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} + \mathcal{N}(0, \frac{G^2}{2\rho} I_p) \right) = -\eta \left(\begin{pmatrix} n/2 \\ 0 \\ \vdots \\ 0 \end{pmatrix} + \mathcal{N}(0, \frac{G^2}{2\rho} I_p) \right).$$

The rest of the proof is similar to that of Theorem 2

For the class-imbalanced case, assume that we have αn data points have with label +1 while the rest $(1 - \alpha)n$ points have label -1. Then, the gradient is

$$\hat{\theta} = -\eta \left(\frac{n\alpha}{2} \cdot \begin{pmatrix} -1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} + \frac{n(1-\alpha)}{2} \cdot \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} + \mathcal{N}(0, \frac{G^2}{2\rho} I_p) \right) = -\eta \left(\begin{pmatrix} n/2 \\ 0 \\ \vdots \\ 0 \end{pmatrix} + \mathcal{N}(0, \frac{G^2}{2\rho} I_p) \right).$$

Thus, the same conclusion holds.

□

A.3 PROOF OF THEOREM 4

In this section, we consider a broad pre-training on a gigantic dataset with K_0 classes. The downstream task is a K -class classification problem with $K \leq K_0$. Let $P = [P_1, \dots, P_{K_0}] \in \mathbb{R}^{p \times K_0}$ be a partial orthogonal matrix with $P^T P = I_{K_0}$. Let

$$M_0 = \sqrt{\frac{K_0}{K_0 - 1}} P \left(I_{K_0} - \frac{1}{K_0} \mathbf{1}_{K_0} \mathbf{1}_{K_0}^T \right) = \sqrt{\frac{K_0}{K_0 - 1}} \left(P - \frac{1}{K_0} \sum_{k=1}^{K_0} P_k \mathbf{1}_{K_0}^T \right).$$

Denote $M = [M_1, \dots, M_K]$ with each M_k being a column of M_0 . Note that

$$M_{k'}^T M_k = \frac{K_0}{K_0 - 1} \left(\delta_{k,k'} - \frac{1}{K_0} \right).$$

We have

$$\mu_{n,K} := - \sum_{k'=1}^K n_{k'} \left(\frac{1}{K} \mathbf{1}_K - y^{k'} \right) M_{k'}^T M_k.$$

For $j \neq k$, we have

$$(\mu_{n,K})_j = -\frac{n}{K} \left[\frac{1}{K} + \frac{K-1}{K(K_0-1)} - \frac{K-2}{K(K_0-1)} \right] = -\frac{n(K_0-2)}{K^2(K_0-1)}.$$

For $j = k$, it holds

$$(\mu_{n,K})_j = -\frac{n}{K} \left[\frac{1}{K} - 1 - \frac{K-1}{K(K_0-1)} \right] = \frac{n(K-1)K_0}{K^2(K_0-1)}.$$

By the union bound, the mis-classification error is

$$(K-1) \mathbb{P} \left[\mathcal{N}((\mu_{n,K})_k, \sigma^2) < \mathcal{N}((\mu_{n,K})_1, \sigma^2) \right] = (K-1) \Phi \left(\frac{n C_{K,K_0}}{\sigma} \right)$$

with $C_{K,K_0} = \frac{1}{K} \left[\frac{K \cdot K_0 - 2}{K^2(K_0 - 1)} \right]$.

B RESULTS FOR PERTURBING THE TESTING DATA

B.1 FIXED PERTURBATION

Recall that the output of DP-GD has the form $\hat{\theta} = \mathcal{N}(-\frac{m}{2}, \sigma^2)$. One has

$$\hat{\theta}^T(e+v) = \frac{n}{2} + \mathcal{N}\left(0, \frac{G^2(p\epsilon^2 + 1)}{2\rho}\right).$$

The sample complexity can be derived similarly as previous sections, which is dimension dependent.

B.2 RANDOM PERTURBATION

Let's say in prediction time, the input data point can be perturbed by a small value in ℓ_∞ . If we allow the perturbation to be adversarial chosen, then there exists v satisfying $\|v\|_\infty \leq \beta$ such that

$$\hat{\theta}^T(x+v) = \frac{n}{2} + \frac{G}{\sqrt{2\rho}} Z_1 - \sum_{i=1}^p |Z_i| \frac{G\beta}{\sqrt{2\rho}}$$

where $Z_1, \dots, Z_n \sim \mathcal{N}(0, 1)$ i.i.d. Note that the additional term scales as $O(p \frac{G\beta}{\sqrt{\rho}})$, which can alter the prediction if $p \asymp n$ even if ρ is a constant (weak privacy).

The number of data points needed to achieve $1 - \delta$ robust classification under neural collapse is $O\left(\frac{G \max\{p\epsilon, 1\} \sqrt{\log(1/\delta)}}{\sqrt{2\rho}}\right)$.

C RESULTS FOR PERTURBING THE TRAINING DATA

C.1 FIXED PERTURBATION

Without loss of generality, we assume $0 < \alpha < 1/2$. Consider the class imbalanced case with $n_{-1} = \alpha n$ and $n_{+1} = (1 - \alpha)n$. The gradient for $\theta_0 = 0$ is

$$\nabla \mathcal{L}(\theta_0) = \alpha n \cdot 0.5 \cdot -(-e_1 + v) + (1 - \alpha)n \cdot 0.5 \cdot (e_1 + v) = \frac{n}{2}e_1 + \frac{(1 - 2\alpha)n}{2}v.$$

Thus, the output is

$$\hat{\theta} = -\eta \left(\frac{n}{2}e_1 + \frac{(1 - 2\alpha)n}{2}v + \mathcal{N}(0, \sigma^2) \right)$$

The sensitivity is $G = \sqrt{1 + \|v\|_2}$ and σ^2 is taken to be $G^2/2\rho$ to achieve ρ -zCDP. Moreover, we have

$$\hat{\theta}^T e_1 = -\frac{n}{2} - \frac{(1 - 2\alpha)n}{2}v_1 + \mathcal{N}(0, \sigma^2).$$

Thus, the mis-classification error is

$$\mathbb{P}[\hat{\theta}^T e_1 > 0] = \Phi \left(\frac{n[1 - (1 - 2\alpha)v_1]}{2\sigma} \right) \leq e^{-\frac{n^2(1 - \beta + 2\alpha\beta)^2\rho}{4G^2}}.$$

As a result, the sample complexity to achieve $1 - \gamma$ accuracy is

$$n = O \left(\sqrt{\frac{4G^2 \log \frac{1}{\delta}}{(1 - \beta + 2\alpha\beta)^2 \cdot \rho}} \right)$$

The sensitivity $G = \sqrt{1 + \epsilon^2 p}$ here is dimension-dependent.

C.2 RANDOM PERTURBATION

Now we consider the random perturbation. Denote $\{v_i\}_{i=1}^n \subseteq \mathbb{R}^p$ a sequence of i.i.d. copies of a random vector v . Consider the binary classification problem with training set $\{(x_i, y_i)\}_{i=1}^n$. Here $x_i = e_1 + v_i$ if $y_i = 1$ and $x_i = -e_1 + v_i$ if $y_i = -1$. Then, the loss function is $\mathcal{L}(\theta) = \frac{1}{n} \sum_{i=1}^n \log \left(1 + e^{-y_i \theta^T x_i} \right)$. The one-step iterate of DP-GD from 0 outputs

$$\hat{\theta} = -\eta \sum_{i=1}^n (-y_i x_i) + \mathcal{N}(0, \sigma^2 I_p)$$

with $\sigma^2 = G^2/2\rho$ and $G = \sup_{v_i} \sqrt{1 + \|v_i\|_2}$. Assume that v_i is symmetric, that is $y_i v_i$ has the same distribution as $-y_i v_i$. Then, it holds

$$\sum_{i=1}^n y_i x_i = n e_1 + \sum_{i=1}^n v_i =: \mu_n.$$

The mis-classification error is now given by

$$\mathbb{P}[\hat{\theta}^T e_1 < 0] = \mathbb{P}[\mathcal{N}(\mu_n^T e_1, \sigma^2) < 0].$$

Assume that $\|v_i\|_\infty = \epsilon < 1$. Then, we have $\mu_n^T e_1 \geq n - \epsilon n$ and the sample complexity is $O \left(\sqrt{\frac{4G^2 \log(1/\delta)}{(1 - \epsilon)^2 \rho}} \right)$. with $G = \sqrt{1 + \epsilon^2 p}$.

D REMEDY TO NON-ROBUSTNESS

D.1 DETAILS OF THE NORMALIZATION

Consider the case where the feature is shifted by a constant offset v . The feature of the k -th class is

$$\tilde{x}_i = x_i - \frac{1}{n} \sum_{i=1}^n x_i = \tilde{M}_k = M_k + v$$

with M_k being the k -th column of the ETF M .

The offset v can be canceled out by considering the differences between the features. That is, we train with the feature $\tilde{M}_k - \frac{1}{K} \sum_{j=1}^K \tilde{M}_j$ for the k -th class. In fact, let P_k be the k -th column of P and we have

$$\begin{aligned} \tilde{M}_k - \frac{1}{K} \sum_{j=1}^K \tilde{M}_j &= M_k - \frac{1}{K} \sum_{j=1}^K M_j \\ &= \sqrt{\frac{K}{K-1}} \left[\left(P_k - \frac{1}{K} \sum_{i=1}^K P_i \right) - \frac{1}{K} \sum_{j=1}^K \left(P_j - \frac{1}{K} \sum_{i=1}^K P_i \right) \right] \\ &= \sqrt{\frac{K}{K-1}} \left(P_k - \frac{1}{K} \sum_{j=1}^K P_j \right) = M_k. \end{aligned}$$

D.2 PROOF OF THEOREM 5

Proof of Theorem 5 Consider the case with $K = 2$ and a projection vector $\hat{P} = (e_1 + \Delta)$ with some perturbation $\Delta = (\Delta_1, \dots, \Delta_p)$ such that $\|\Delta\|_\infty \leq \beta_0$ for some $0 < \beta_0 \ll p$. \hat{P} can be generated by the pre-training dataset or the testing dataset. Consider training with features $\tilde{x}_i = \hat{P}x_i$. Then, the sensitivity of the NoisyGD is $G = \sup_v |\hat{P}^T(e_1 + v)| = 1 + \beta + \beta|\Delta_1| + \beta(\sum_{j=1}^p |\Delta_j|) \leq 1 + \beta(1 + \beta_0 + p\beta_0)$. The output of Noisy-GD is then given by

$$\hat{\theta} = -\hat{P} \cdot \left(\sum_{i=1}^n y_i \tilde{x}_i \right) + \mathcal{N}(0, \sigma^2).$$

Moreover, for any testing data point $e_1 + v$, define

$$\hat{\mu}_n = - \left(\sum_{i=1}^n y_i \tilde{x}_i \right) \hat{P}^T (e_1 + v) = (e_1 + V)^T \hat{P} \hat{P}^T (e_1 + v)$$

with $V = \frac{1}{n} \sum_{i=1}^n v_i =: (V_1, \dots, V_p)$.

We now divide $\hat{\mu}_n$ into four terms and bound each term separately.

For the first term $e_1^T \hat{P} \hat{P}^T e_1$, it holds

$$e_1^T \hat{P} \hat{P}^T e_1 = (1 + e_1^T \Delta_1)^2 \leq (1 - \beta_0)^2.$$

For the second term $V^T \hat{P} \hat{P}^T e_1$, we have

$$V^T \hat{P} \hat{P}^T e_1 = V_1 + V^T \Delta$$

Note that V_1 is the average of n i.i.d. random variables bounded by β . By Hoeffding's inequality, we obtain

$$|V_1| \leq \frac{\beta \log \frac{2}{\gamma}}{\sqrt{n}}, \text{ with probability at least } 1 - \gamma.$$

Similarly, with confidence $1 - \gamma$, it holds

$$|V^T \Delta| \leq \frac{p\beta\beta_0 \log \frac{2}{\gamma}}{\sqrt{n}}.$$

The third term $e_1^T \widehat{P} \widehat{P}^T v$ can be bounded as

$$|e_1^T \widehat{P} \widehat{P}^T v| = (1 + \Delta_1) \left(\sum_{j=1}^p v_j (1 + \Delta_j) \right) \leq (1 + \beta_0) \left(\beta + \beta_0 \sqrt{p \log \frac{2}{\gamma}} \right),$$

where the last inequality is a result of the Hoeffding's inequality by assuming that each coordinate of v are independent of each others. Moreover, without further assumptions on the independence of each coordinate of v , we have

$$|e_1^T \widehat{P} \widehat{P}^T v| = (1 + \Delta_1) \left(\sum_{j=1}^p v_j (1 + \Delta_j) \right) \leq (1 + \beta_0) (\beta + \beta_0 p).$$

Using the Hoeffding's inequality again, for the last term $V^T \widehat{P} \widehat{P}^T (e_1 + v)$, it holds

$$|V^T \widehat{P} \widehat{P}^T (e_1 + v)| \leq \frac{(\beta + \beta_0 \sqrt{p})(1 + \beta + \beta_0 + \beta \beta_0 \sqrt{p}) \log \frac{4}{\gamma}}{\sqrt{n}}$$

with confidence $1 - \gamma$ if we assume that all coordinates of v are independent of each other. Without further assumptions on the independence of each coordinate of v , we have

$$|V^T \widehat{P} \widehat{P}^T (e_1 + v)| \leq \frac{(\beta + \beta_0 p)(1 + \beta + \beta_0 + \beta \beta_0 p) \log \frac{2}{\gamma}}{\sqrt{n}}.$$

□

E SOME CALCULATIONS ON RANDOM INITIALIZATION

E.1 GAUSSIAN INITIALIZATION WITHOUT OFFSET

For Gaussian initialization $\xi = (\xi_1, \dots, \xi_p) \sim \mathcal{N}(0, I_p)$, we have

$$\begin{aligned} \hat{\theta} &= \xi - \eta \left(\frac{n}{2} \cdot \frac{-e^{-\xi_1}}{1 + e^{-\xi_1}} \cdot \begin{bmatrix} -1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \right) + \frac{n}{2} \cdot \frac{-e^{-\xi_1}}{1 + e^{-\xi_1}} \cdot \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} + \mathcal{N}(0, \frac{G^2}{2\rho} I_p) \\ &= \xi + \eta \left(\frac{e^{-\xi_1}}{1 + e^{-\xi_1}} \cdot \begin{bmatrix} n \\ 0 \\ \vdots \\ 0 \end{bmatrix} + \mathcal{N}(0, \frac{G^2}{2\rho} I_p) \right) \end{aligned}$$

The sensitivity is $\frac{e^{-\xi_1}}{1 + e^{-\xi_1}} < 1$. Consider $x = (-1, 0, \dots, 0)^T$. We have

$$\widehat{\theta}^T x = -\xi_1 + \eta \left(-\frac{ne^{-\xi_1}}{1 + e^{-\xi_1}} \right) + \mathcal{N}(0, \frac{G^2}{2\rho}) =: \mu_{\xi_1, n} + \mathcal{N}(0, \frac{G^2}{2\rho}).$$

The mis-classification error is

$$\begin{aligned} \mathbb{P}[\widehat{\theta}^T x > 0] &= \mathbb{E}_{\xi_1 \sim \mathcal{N}(0,1)} \mathbb{P} \left[\mathcal{N} \left(\mu_{\xi_1, n}, \frac{G^2}{2\rho} \right) > 0 \mid \xi_1 \right] \\ &= \mathbb{E}_{\xi_1 \sim \mathcal{N}(0,1)} \left[\Phi \left(\frac{\sqrt{2\rho} \mu_{\xi_1, n}}{G} \right) \right] \end{aligned}$$

E.2 GAUSSIAN INITIALIZATION WITH OFF-SET

Denote $x_1 = -e_1 + v$ and $x_2 = e_1 + v$ with $\|v\|_\infty \leq \beta$. For the logistic loss $\ell(y, \theta^T x) = \log(1 + e^{-y\theta^T x})$, we have

$$g(\theta, y \cdot x) := \nabla_\theta \ell(y, \theta^T x) = \frac{e^{-y\theta^T x}}{1 + e^{-y\theta^T x}} (-yx).$$

Denote

$$g_1(\theta) = g(\theta, -1 \cdot x_1) = \frac{e^{\theta^T x_1}}{1 + e^{\theta^T x_1}} x_1$$

and

$$g_2(\theta) = g(\theta, 1 \cdot x_2) = \frac{e^{-\theta^T x_2}}{1 + e^{-\theta^T x_2}} (-x_2).$$

If we shift the feature by some vector v , then the loss function is

$$R_n = \frac{n}{2} \log(1 + e^{\theta^T x_1}) + \frac{n}{2} \log(1 + e^{-\theta^T x_2}).$$

And the gradient is

$$\nabla_\theta R_n(\theta) = \frac{n}{2} (g_1(\theta) + g_2(\theta)).$$

Thus, the output of one-step NoiseGD is given by

$$\hat{\theta} = \theta_0 - \frac{\eta n}{2} [g_1(\theta_0) + g_2(\theta_0) + \mathcal{N}(0, \sigma^2)].$$

Let $\mu_\xi = \xi - \frac{\eta n}{2} [g_1(\xi) + g_2(\xi)]$. Then, we have

$$\mu_\xi^T e_1 = \xi_1 - \frac{\eta n e^{\xi^T x_1}}{2 + 2e^{\xi^T x_1}} (-1 + v_1) + \frac{\eta n e^{\xi^T x_2}}{2 + 2e^{\xi^T x_2}} (1 + v_1).$$

And the mis-classification error is

$$\mathbb{E}_\xi \left(\Phi \left(-\frac{\sqrt{2\rho} \mu_\xi^T e_1}{G} \right) \right).$$