PREVENTING COLLAPSE IN CONTRASTIVE LEARNING WITH ORTHONORMAL PROTOTYPES (CLOP)

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ABSTRACT

Contrastive learning has emerged as a powerful method in deep learning, excelling at learning effective representations through contrasting samples from different distributions. However, dimensional collapse, where embeddings converge into a lower-dimensional space, poses a significant challenge, especially in semi-supervised and self-supervised setups. In this paper, we first theoretically analyze the effect of large learning rates on contrastive losses that solely rely on the cosine similarity metric, and derive a theoretical bound to mitigate this collapse. Building on these insights, we propose **CLOP**, a novel semi-supervised loss function designed to prevent dimensional collapse by promoting the formation of orthogonal linear subspaces among class embeddings. Unlike prior approaches that enforce a simplex ETF structure, CLOP focuses on subspace separation, leading to more distinguishable embeddings. Through extensive experiments on real and synthetic datasets, we demonstrate that CLOP enhances performance, providing greater stability across different learning rates and batch sizes.

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1 INTRODUCTION

028 Recent advancements in deep learning have positioned Contrastive Learning as a leading 029 paradigm, largely due to its effectiveness in learning representations by contrasting samples from different distributions while aligning those from the same distribution. Prominent models in 031 this domain include SimCLR Chen et al. (2020a), Contrastive Multiview Coding (CMC) Tian et al. (2020a), VICReg Bardes et al. (2021), BarLowTwins Zbontar et al. (2021), among oth-033 ers Wu et al. (2018); Henaff (2020); Li et al. (2020). These models share a common two-034 stage framework: representation learning and fine-tuning. In the first stage, representation learning is performed in a self-supervised manner, where the model is trained to map inputs to em-035 beddings using contrastive loss to separate samples from different labels. In the second stage, 036 fine-tuning occurs under a supervised setup, where labeled data is used to classify embeddings 037 correctly. For practical applicability, a small amount of labeled data is required in the finetuning stage to produce meaningful classifications, making the overall pipeline semi-supervised.

Empirical evidence demonstrates that these models, even with limited labeled data (as low as 10%), can achieve performance comparable to fully-supervised approaches on moderate to large datasets Jaiswal et al. (2020).

046 Despite the effectiveness of con-047 trastive learning on largely unlabeled 048 datasets, a common issue encoun-049 tered during the training process is 050 **Dimensional Collapse**. As pointed 051 out by Jing et al. (2021); Fu et al. (2022); Rusak et al. (2022); Xue et al. 052 (2023); Gill et al. (2024); Tao et al. (2024); Hassanpour et al. (2024), this

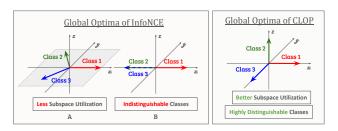


Figure 1: Illustration of global optima for InfoNCE and **CLOP** (this paper). For InfoNCE, global optima are reached when the model merges samples of the same class into a single embedding, whether the class arrangement is ETF (A) or co-linear (B). In contrast, the proposed CLOP introduces a novel regularizer that encourages embeddings to occupy a highly separable, full-rank space.

054 phenomenon describes the collapse of output embeddings from the neural network into a lower-055 dimensional space, reducing their spatial utility and leading to indistinguishable classes (see Fig-056 ure 1.B). There are two main approaches to resolve this issue: augmentation modification Jing et al. 057 (2021); Xue et al. (2023); Fu et al. (2022); Tao et al. (2024) and loss modification Fu et al. (2022); 058 Rusak et al. (2022); Hassanpour et al. (2024). In this paper, we propose an additional term in the loss function to address the issue of collapse. Our approach to deal with Dimensional collapse involves selecting prototypes similarly to Zhu et al. (2022); Gill et al. (2024). The key distinction lies in the 060 fact that, while their approach enforces the embeddings to conform to a simplex Equiangular Tight 061 Frame (ETF) hyperplane, our method aims to push the embeddings toward distinct orthogonal linear 062 subspaces, allowing them to occupy the full-rank space (see Figure 1 for intuition). This result in 063 more distinguishable subspace clusters, which can be more effectively learned by the downstream 064 classifier. 065

The main contributions of this paper can be summarized in three perspectives. First, we theoret-066 ically identify the impact of an overly large learning rate on contrastive learning loss that is based 067 solely on cosine similarity as the metric. We provide a theoretical bound for the learning rate to 068 avoid collapse for k classes under specified conditions. Furthermore, we simplify this bound to a 069 constant O(1). Second, we analyze the results under moderate learning rates and observe that the embeddings naturally lie on a hyperplane, which reduces spatial usage and makes it more difficult 071 for the downstream classifier to learn effectively. Finally, with these findings, we propose a novel 072 loss term, CLOP, which involves pulling a partial training dataset towards a few orthonormal pro-073 totypes. This loss is applicable in both semi-supervised and fully-supervised contrastive learning 074 settings, where a subset of labeled data is available for training. Through extensive experiments, we 075 demonstrate the performance superiority of CLOP. Specifically, we show that CLOP is significantly more stable across different learning rates and smaller batch sizes. 076

Paper Organization In Section 2, we begin by discussing the necessary background, including recent advancements in both self-supervised and supervised contrastive learning, as well as the analysis of the Dimensional collapse phenomenon in deep learning and contrastive learning, in particular. In Section 3, we present our theoretical analysis of Dimensional collapse. Next, in Section 4, we introduce our proposed model, CLOP. Lastly, we present the experimental results on CIFAR-100 and Tiny-ImageNet in Section 5.

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2 RELATED WORK

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Contrastive learning has gained prominence in deep learning for its ability to learn meaningful rep-089 resentations by pulling together similar (positive) pairs and pushing apart dissimilar (negative) pairs 090 in the embedding space. Positive pairs are generated through techniques like data augmentation, 091 while negative pairs come from unrelated samples, making contrastive learning particularly effec-092 tive in self-supervised tasks like image classification. Pioneering models such as SimCLR Chen 093 et al. (2020a), CMC Tian et al. (2020a), VICReg Bardes et al. (2021), and Barlow Twins Zbon-094 tar et al. (2021) share the objective of minimizing distances between augmented versions of the 095 same input (positive pairs) and maximizing distances between unrelated inputs (negative pairs). 096 SimCLR maximizes agreement between augmentations using contrastive loss, while CMC extends this to multi-view learning Chen et al. (2020a); Tian et al. (2020a). VICReg introduces variance-098 invariance-covariance regularization without relying on negative samples Bardes et al. (2021), and Barlow Twins reduce redundancy between different augmentations Zbontar et al. (2021). 099

100 Recent innovations have improved contrastive learning across various domains. For instance, meth-101 ods like structure-preserving quality enhancement in CBCT images Kang et al. (2023) and false 102 negative cancellation Huynh et al. (2022) have enhanced image quality and classification accuracy. 103 In video representation, cross-video cycle-consistency and inter-intra contrastive frameworks Wu & 104 Wang (2021); Tao et al. (2022) have shown significant gains. Additionally, contrastive learning has 105 advanced sentiment analysis Xu & Wang (2023), recommendation systems Yang et al. (2022), and molecular learning with faulty negative mitigation Wang et al. (2022b). Xiao et al. (2024) introduces 106 GraphACL, a novel framework for contrastive learning on graphs that captures both homophilic and 107 heterophilic structures without relying on augmentations.

108 2.1 CONTRASTIVE LOSS

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In unsupervised learning, Wu et al. (2018) introduced InfoNCE, a loss function defined as:

$$\mathcal{L}_{infoNCE} = -\sum_{i \in I} \log \frac{\exp(\mathbf{z}_i^\top \mathbf{z}_{j(i)}/\tau)}{\sum_{a \neq i} \exp(\mathbf{z}_i^\top \mathbf{z}_a/\tau)}$$
(1)

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where \mathbf{z}_i is the embedding of sample i, j(i) its positive pair, and τ controls the temperature.

116 Recent refinements focus on (1) component modifications, (2) similarity adjustments, and (3) novel approaches. Li et al. (2020) use EM with k-means to update centroids and reduce mutual information 117 loss, while Wang et al. (2022a) add L2 distance to InfoNCE, though both underperform state-of-the-118 art (SOTA) techniques. Xiao et al. (2020) reduce noise with augmentations, and Yeh et al. (2022) 119 improve gradient efficiency with Decoupled Contrastive Learning, though neither surpasses SOTA. 120 In similarity adjustments, Chuang et al. (2020) propose a debiased loss, and Ge et al. (2023) use 121 hyperbolic embeddings, but neither outperforms SOTA. Novel methods include min-max InfoNCE 122 Tian et al. (2020b), Euclidean-based losses Bardes et al. (2021), and dimension-wise cosine similar-123 ity Zbontar et al. (2021), achieving competitive performance without softmax-crossentropy. 124

125 2.2 SEMI-SUPERVISED AND SUPERVISED CONTRASTIVE LEARNING

127 Semi-supervised contrastive learning effectively leverages both labeled and unlabeled data to learn 128 meaningful representations. Zhang et al. (2022) introduced a framework with similarity cocalibration to mitigate noisy labels by adjusting the similarity between pairs. Inoue & Goto (2020) 129 proposed a Generalized Contrastive Loss (GCL), unifying supervised and unsupervised learning 130 for speaker recognition, while Kim et al. (2021) combined contrastive self-supervision with con-131 sistency regularization in SelfMatch. In domain adaptation, Singh (2021) utilized class-wise and 132 instance-level contrastive learning to minimize domain gaps, while Liu & Abdelzaher (2021) devel-133 oped a method for Human Activity Recognition (HAR) using semi-supervised contrastive learning 134 to achieve state-of-the-art performance. In medical image segmentation, Hua et al. (2022) intro-135 duced uncertainty-guided voxel-level contrastive learning, and Hu et al. (2021) combined global 136 self-supervised and local supervised contrast for improved label efficiency. For automatic speech 137 recognition (ASR), Xiao et al. (2021) reduced reliance on large labeled datasets while maintaining 138 high accuracy using semi-supervised contrastive learning. In 3D point cloud segmentation, Jiang 139 et al. (2021) presented a pseudo-label contrastive framework, while Shen et al. (2021) employed 140 contrastive learning for intent discovery in conversational datasets with minimal labeled data.

141 Supervised contrastive learning, initially proposed by Khosla et al. (2020), extends contrastive loss 142 to fully supervised settings, significantly improving task performance. Graf et al. (2021) further ex-143 plored its relationship with cross-entropy loss, highlighting its advantages in feature learning, while 144 Cui et al. (2021) introduced learnable class centers to balance class representations. Domain-specific 145 applications include recommendation systems, where supervised contrastive learning enhances item representations Yang et al. (2022), and product matching, where it improves matching accuracy 146 Peeters & Bizer (2022). It has also been extended to natural language processing as a fine-tuning 147 objective for pre-trained models Gunel et al. (2020). To address imbalanced datasets and noisy 148 labels, Targeted Supervised Contrastive Learning (TSC) focuses on under-represented classes in 149 long-tailed recognition Li et al. (2022b), while Selective-Supervised Contrastive Learning (Sel-CL) 150 selectively learns from clean data to improve performance under noisy supervision Li et al. (2022a). 151

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2.3 DIMENSIONAL COLLAPSE

154 Dimensional collapse is a notable phenomenon in deep learning, particularly during the terminal 155 phase of training. Several works have focused on establishing a theoretical foundation for under-156 standing dimensional collapse through geometric and optimization properties. Zhu et al. (2021) 157 provide a geometric framework that highlights the alignment of classifiers and features in neural 158 networks with a Simplex ETF structure. Similarly, Mixon et al. (2022) explore it from the perspec-159 tive of unconstrained features, showing that collapse naturally occurs without explicit regularization. Ji et al. (2021) extend this with an unconstrained layer-peeled model, linking collapse to optimiza-160 tion processes. Yaras et al. (2022) use Riemannian geometry to show that collapse solutions are 161 global minimizers. Extensions of dimensional collapse to more complex settings include Jiang et al.

(2023), who broaden its study to networks with a large number of classes. Rangamani et al. (2023) analyze intermediate phases of collapse, while Tirer et al. (2023) show that practical networks rarely achieve exact collapse, yet approximate collapse still occurs. Galanti et al. (2021) explore its role in transfer learning, demonstrating improvements in generalization. Zhong et al. (2023) apply dimensional collapse to imbalanced semantic segmentation, highlighting its impact on class separation and feature alignment.

168 For dimensional collapse in contrastive learning, Jing et al. (2021) examine dimensional collapse in 169 self-supervised learning. They attribute this to strong augmentations distorting features and implicit 170 regularization driving weights toward low-rank solutions. To address this, they propose DirectCLR, 171 which optimizes the representation space and outperforms SimCLR on ImageNet by better pre-172 venting collapse. Similarly, Xue et al. (2023) explore how simplicity bias leads to class collapse and feature suppression, with models favoring simpler patterns over complex ones. They suggest 173 increasing embedding dimensionality and designing augmentation techniques that preserve class-174 relevant features to counter this bias and promote diverse feature learning. Similarly, Fu et al. (2022) 175 emphasize the role of data augmentation and loss design in preventing class collapse, proposing a 176 class-conditional InfoNCE loss term that uniformly pulls apart individual points within the same 177 class to enhance class separation. In supervised contrastive learning, Gill et al. (2024) propose loss 178 function modifications to follow an ETF geometry by selecting prototypes that form this structure. 179 In graph contrastive learning, Tao et al. (2024) introduce a whitening transformation to decorrelate 180 feature dimensions, avoiding collapse and enhancing representation capacity. In medical image seg-181 mentation, Hassanpour et al. (2024) address dimensional collapse through feature normalization and 182 whitening approach to preserve feature diversity. Finally, Rusak et al. (2022) investigate the pref-183 erence of contrastive learning for content over style features, leading to collapse. They propose to leverage adaptive temperature factors in the loss function to improve feature representation quality. 184

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3 Theoretical Analysis

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The first part of this section delves into a theoretical examination of *complete collapse*, which refers 189 to the phenomenon where all embeddings converge to a single point in contrastive learning. Initially, 190 we show that complete collapse is a local minimum for the InfoNCE loss by showing that linear 191 embeddings result in a zero gradient (Lemma 1). This result is demonstrated using the InfoNCE loss, 192 but it can be applied to the majority of current loss functions that rely solely on cosine similarity 193 as a similarity metric. This holds across various settings, including unsupervised Henaff (2020); 194 Chen et al. (2020a); Cui et al. (2021); Xiao et al. (2020); Yeh et al. (2022); Wang et al. (2022a), 195 semi-supervised Hu et al. (2021); Shen et al. (2021), and supervised contrastive learning Khosla 196 et al. (2020); Cui et al. (2021); Peeters & Bizer (2022); Li et al. (2022b). Subsequently, we discuss 197 the effect of a large learning rate in producing complete collapse. We derive an upper-bound on the 198 learning rate to avoid collapse under mild assumptions (Theorem 1).

In the latter part of this section, we examine the phenomenon of *dimensional collapse*, where the embedding space of a model progressively shrinks to a lower-dimensional subspace (Lemma 2). We describe how cosine-similarity optimization drives this collapse without achieving the formation of a Simplex Equiangular Tight Frame (ETF). Specifically, we demonstrate that under gradient descent, which minimizes the total class cosine similarity loss \mathcal{L}_{class} , the embeddings — initially spanning the full space — contract into a lower-dimensional subspace where they are not equidistant (not ETF).

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3.1 LARGE LEARNING RATE CAUSES COMPLETE COLLAPSE

The concept of the InfoNCE loss, as defined in Eq. (1), aims to encourage the embeddings to form distinguishable clusters in high-dimensional space, thereby facilitating classification for downstream models. However, in Lemma 1, we demonstrate that the worst-case scenario — where all embeddings become identical or co-linear — also constitutes a local optimum for the InfoNCE loss. This includes non-unique global optima, which we will further explore in Section 3.2. This observation suggests that, from a theoretical perspective, InfoNCE exhibits instability, as both the best and worst solutions can lead to stationary points.

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Lemma 1. Let $\mathcal{F} : \mathbb{R}^m \to \mathbb{R}^{m'}$ be a family of Contrastive Learning structures, where m and m' denote the dimensions of the inputs and embeddings, respectively. If a function $f \in \mathcal{F}$ is trained using the InfoNCE loss, then there exist infinitely many local minima where all embeddings produced by f are all equal or <u>co-linear</u>.

The proof of Lemma 1 relies on the observation that the embeddings are only compared against each other. If all embeddings are either identical or co-linear, the gradient vanishes due to the lack of angular differences, as well as the normalization process. The full proof of Lemma 1 is presented in Appendix C.

The remainder of this section focuses on the causes of reaching local minima. In particular, we examine the role of a large learning rate in causing complete collapse. To understand the dynamics of contrastive learning, it is crucial to consider two forces acting on each embedding: the *gravitational force* within the same class and the *repulsive force* between different classes. Contrary to the common belief that the gravitational force is responsible for inducing collapse, we observe that the primary cause of complete collapse in contrastive learning is the overshooting of the repulsive force.

233 Figure 2 illustrates this phenomenon. For 234 simplicity of analysis, assume that the 235 model has successfully merged samples 236 from the same class into a single class em-237 bedding. Each light blue dot represents 238 one class embedding, while the dark blue 239 dot represents the mean of all class em-240 beddings. In practice, the mean is un-241 likely to be located at the center of the 242 space. The purpose of the repulsive force is to arrange the class embeddings more 243 uniformly across the space and center the 244 mean of the class embeddings, as shown in 245 Figure 2.B with a small learning rate. 246

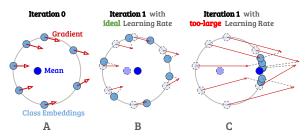


Figure 2: Illustration of the effect of repulsive force in contrastive learning. Light blue dots represent the individual class embedding, while the dark blue dot represents the mean of all class embeddings.

However, when the learning rate is too high, the repulsive force causes the class embeddings to
overshoot, as shown in Figure 2.C with a large learning rate. Due to the normalization operation
inherent in contrastive learning, the class embeddings tend to converge, which ultimately results
in the local minima characterized as complete collapse, as stated in Lemma 1. This overshooting
phenomenon necessitates the upper-bounding of the learning rate to better regulate the repulsive
force, ensuring optimal space utilization of class embeddings.

In Theorem 1, we establish an upper bound for the learning rate of the gradient descent step, where k represents the total number of class embeddings. This result is derived under the same assumption that embeddings of the same class are aggregated into a single class embedding by the upstream model. As shown in Figure 2, the shift in the class embedding mean is a critical phenomenon associated with complete collapse. Consequently, the upper bound is obtained by constraining the movement of the class embedding mean, ensuring that the mean in the next step remains strictly non-increasing.

Theorem 1. Consider k class embeddings uniformly distributed on the surface of an mdimensional unit ball, where $m \ge k > 2$. The upper bound on the learning rate μ for the gradient descent step, to minimize cosine similarity scores between class embeddings while preventing the class embedding mean from increasing by a ratio of $(1 + \varepsilon)$, is given by:

$$(1-\eta)^2 \le \left(1 + \frac{\eta}{k-1} - \frac{2\eta}{k} - 2\frac{\eta^2}{k(k-1)} + \frac{\eta^2 k}{(k-1)^2}\right)(1+\varepsilon)^2.$$
 (2)

Setting $\varepsilon = 0$ guarantees a non-increasing mean, and provides an O(1) upper bound for the learning rate.

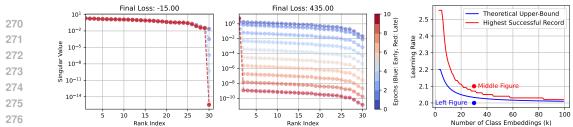


Figure 3: Numerical experiment conducted on tightness of Theorem 1. Left & Middle: Singular value spectra of X at different training epochs (color-coded from blue to red). The Left panel shows successful optimization with a learning rate of 2.0, while the Middle panel demonstrates optimization failure (complete collapse) at a learning rate of 2.1. Right: The maximum learning rates preventing collapse over 5 consecutive trials, for varying class embedding sizes, are plotted against the theoretical upper bound ($\varepsilon = 0$) from Theorem 1.

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The proof proceeds by establishing an upper bound on the norm of each class embedding, which is dependent on the step size after a gradient descent step. This enables us to derive an upper bound for the shifted mean. By comparing the upper bound of the shifted mean with the original mean, we guarantee that the mean remains non-increasing throughout the gradient descent process, thus preventing complete collapse. The detailed proof of Theorem 1 can be found in Appendix D.

To study the tightness of our bound, we perform numerical experiments to determine the highest learning rate possible without resulting in complete collapse. The results are presented in Figure 3, where we apply gradient descent to minimize the cosine similarity between each vector on a 100-dimensional unit ball. Specifically, let the class embedding matrix be denoted as $\mathbf{X} := [\mathbf{x}_1, \dots, \mathbf{x}_k] \in \mathbb{R}^{100 \times k}$. Assuming the model has successfully collapsed the samples from each class into a single class embedding, the InfoNCE loss (Eq. (1)) can be simplified to:

$$\mathcal{L}_{class}(\mathbf{X}) := -\sum_{i \neq j} [\mathbf{X}^{\top} \mathbf{X}]_{ij}.$$
(3)

297 The left and middle figures of Figure 3 show the singular value spectrum of the same 30 class 298 embeddings, with learning rates of 2.0 and 2.1, respectively. It is important to note that, according 299 to Theorem 1, the upper bound for non-increasing class embedding means is 2.03. The left figure 300 demonstrates successful learning with a low final loss, while the middle figure—where the learning 301 rate is just 0.1 higher—results in complete collapse, as the singular values are nearly zero for all 302 ranks except the first. Notably, collapse occurs early in training in the middle figure, aligning with the expectation from Figure 2, which suggests that overshooting may occur when the of Figure 3 303 are well-distributed across the space. Additionally, although the left figure successfully minimizes 304 the total cosine similarity, there are signs of dimensional collapse, as the singular value of the last 305 dimension gradually drops to zero. This indicates that adjusting the learning rate alone cannot 306 prevent dimensional collapse, a topic we will explore further in Section 3.2. 307

In the right figure of Figure 3, we plot the maximum learning rates that prevent collapse over 5 consecutive trials for varying number of class embeddings, comparing them to the theoretical upper bound from Theorem 1. The theoretical upper bound closely aligns with the highest successful learning rate recorded. The reason our bound is tighter than the highest recorded successful learning rate is that we guarantee the class embedding mean is non-increasing over gradient steps (i.e., $\varepsilon = 0$), providing the safest bound for the learning rate.

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315 3.2 COSINE-SIMILARITY CAUSES DIMENSIONAL COLLAPSE

316 There are three widely discussed methods for arranging k class embeddings in an m-dimensional 317 space, where m > k, to achieve optimal spatial utility. The first method is the Simplex Equiangular 318 Tight Frame (ETF), as introduced in Zhu et al. (2021); Graf et al. (2021). This approach arranges the 319 vectors on a hyperplane such that all vectors are equidistant from each other. ETF is frequently used 320 to explain the phenomenon of dimensional collapse observed in the final layer of a neural network. 321 The second method involves arranging k vectors to be mutually orthogonal. The third method divides the k vectors into equal-sized groups, where within each group, the vectors form pairs that 322 point in opposite directions. Additionally, the vectors from different groups are orthogonal to each 323 other.

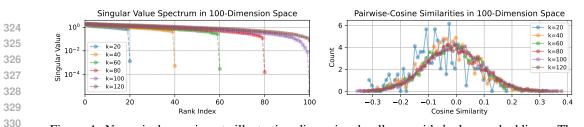


Figure 4: Numerical experiments illustrating dimensional collapse with k class embeddings. The results show that minimizing total cosine similarity via gradient descent leads to convergence within a subspace of rank k - 1 (left), while failing to preserve equal distances between the vectors (right).

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While the second "orthogonal" method yields the most distinguishable classes from a linear algebra standpoint, the first "simplex ETF" and third "inverted groups" methods achieve the optimal value of the InfoNCE-equivalent \mathcal{L}_{class} , given as -k. This result is obtained under the same conditions outlined in Section 3.1, where the model effectively consolidates samples from the same class into a unified class embedding. However, none of these configurations are commonly observed in contrastive learning via gradient descent. Instead, a more common outcome is that the initially full-rank embedding space gradually collapses into a lower-dimensional subspace, where the embeddings are no longer equidistant. In this section, we take a microscopic perspective to explore how individual embeddings adjust to minimize total cosine similarity.

This observation is validated by a simple numerical experiment, where we minimize the pairwise cosine similarity \mathcal{L}_{class} among all class embeddings using gradient descent. The class embeddings are randomly initialized from a Gaussian distribution and normalized to unit norm at each iteration. As shown in Figure 4, the results demonstrate that gradient descent consistently converges to a subspace of rank k - 1, where the pairwise similarities vary significantly.

Building on this observation, we present Lemma 2 to illustrate that, in the case of full rank, the optimal movement for each individual class embedding is to align itself within the subspace spanned by all other class embeddings. Consequently, the class embedding closest to the others is most likely to be pushed into this subspace, eventually reaching a local optimum by forming a zero-mean subspace of rank k - 1.

Lemma 2. Let $\mathbf{X} = {\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_{k-1}}$ be a set of k-1 linearly-independent unit-norm class embeddings in an m-dimensional space, where $m \ge k$. The optimal arrangement of the additional individual class embedding \mathbf{x}_k that minimize the total cosine similarity score \mathcal{L}_{class} (Eq. (3)) will result in \mathbf{x}_k being linearly dependent on the remaining class embeddings in \mathbf{X} .

Lemma 2 can be proven by constructing two matrices, **X** and **X'**, each consisting of k vectors. One matrix is full rank, while the other has rank k - 1. The only difference between **X** and **X'** is that the vector \mathbf{x}_k in **X** lies in a distinct dimension, whereas \mathbf{x}'_k in **X'** is the normalized projection of \mathbf{x}_k onto the subspace spanned by the remaining vectors in both **X** and **X'**. It can be shown that $\mathcal{L}_{class}(\mathbf{X}) > \mathcal{L}_{class}(\mathbf{X}')$. The complete proof is provided in Appendix E.

4 OUR MODEL: CONTRASTIVE LEARNING WITH ORTHONORMAL PROTOTYPES (CLOP)

To avoid the issue of complete collapse and dimensional collapse, we introduce a novel approach (CLOP) that promotes point isolation by adding an additional term to the loss function for contrastive learning. Specifically, we initialize a group of *orthonormal prototypes*, serving as the target for each class, following the same idea of class embeddings. The number of orthonormal prototypes matches the total number of classes in the dataset. We then maximize the similarity between the orthonormal prototypes and the labeled samples in the training set.

Formally, let S be the labeled training set containing pairs of embeddings and labels, denoted as $S = \{(\mathbf{z}_i, y_i) \mid i \in \{1, ..., |S|\}\}$. The set of prototypes, denoted as C, is defined as $C = \{\mathbf{c}_1, ..., \mathbf{c}_k\}$, where k represents the number of classes in the dataset. To generate the prototypes C, we randomly

sample k i.i.d. vectors from an m'-dimensional space, where $|\mathbf{z}_i| = m'$. Subsequently, we apply singular value decomposition (SVD) to obtain the orthonormal basis, denoted as C. This ensures that each prototype \mathbf{c}_i is initialized as a unit vector, orthogonal to all other prototypes, at the beginning of the training process. The CLOP loss is formulated as follows:

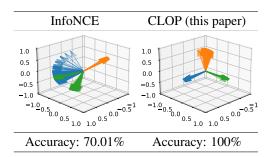
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where \mathcal{L}_{CL} represents the primary contrastive learning loss (e.g., InfoNCE, DCL, SupCon), and $s(\cdot, \cdot)$ denotes the similarity metric, typically chosen to be the same metric used in \mathcal{L}_{CL} .

 $\mathcal{L}_{\text{CLOP}} = \mathcal{L}_{CL} + \lambda \sum_{i=1}^{|\mathcal{S}|} (1 - s(\mathbf{z}_i, \mathbf{c}_{y_i})),$

390 The primary objective of the CLOP loss is to align all embeddings corresponding to the same class 391 towards a common target prototype, \mathbf{c}_{y_i} . Beyond the "gravitational force" and "repulsive force" 392 provided by the main contrastive loss, the CLOP loss introduces a supervised "pulling force" that 393 prevents collapse by isolating labeled embeddings into their own dimensions. It is important to note 394 that, without additional constraints, samples outside of set \mathcal{S} may still converge to other unspecified 395 embeddings, potentially collapsing into a rank-1 subspace. However, a fundamental assumption in contrastive learning is that augmented samples are treated as being drawn from the same distribution 396 as the original input data from the same class. Thus, the "gravitational force" between embeddings of 397 the same class should pull unsupervised embeddings toward the target *class embedding* prototypes. 398

399 To illustrate the effectiveness of CLOP in miti-400 gating embedding collapse, we conduct a straight-401 forward experiment using synthetically generated data. We begin by initializing 500 input samples 402 in a 3-dimensional space, categorized into three 403 distinct classes. Samples within each class are 404 initialized within the same linear subspace, with 405 random Gaussian noise (mean 0, variance 0.05) 406 added. A 3-layer Feedforward Neural Network 407 (FFN) is then trained following SimCLR frame-408 work. For the baseline methods (InfoNCE, DCL, 409 BarlowTwin, VICreg), the model is first trained 410 using a self-supervised approach, where data aug-411 mentation is performed by adding random Gaus-412 sian noise (mean 0, variance 0.05) and randomly inverting the sign of the samples with a probability 413 of 0.5. Following this training phase, the 10% la-414 beled samples are used to train a K-Nearest Neigh-415 bors (KNN) classifier (with k = 5), simulating the 416 fine-tuning phase, to predict the labels of the re-417 maining unlabeled samples. For methods employ-418 ing CLOP, the same 10% labeled samples are used 419 for the CLOP loss during the initial training phase. 420



(4)

Figure 5: Impact of avoiding dimensional collapse with CLOP (proposed method) on InfoNCE for contrastive learning. A 3-layer FFN is trained on synthetic data with 10% labeled samples, and the output embeddings are visualized in 3D. KNN classification accuracy (k = 5) is reported, where the model is trained on 10% labeled data and tested on the remaining unlabeled data.

The output embeddings and KNN accuracy are partially presented in Table 5 and fully detailed in Ta-421 ble 5 within Appendix B. The color of each point in the output embedding visualizations corresponds 422 to its ground truth label. As discussed in previous sections, methods utilizing sample-wise cosine 423 similarity (e.g., InfoNCE and DCL) are expected to push the embeddings into a lower-dimensional 424 subspace. This effect is clearly visible for InfoNCE in Table 5 and DCL in Table 5. Consistent 425 with CLOP's goal of addressing dimensional collapse, we observe that the embeddings trained with 426 CLOP show more distinct boundaries between classes, with each class being more orthogonal to the 427 others. The accuracy results further corroborate the improvement in embedding quality facilitated 428 by CLOP. Additionally, even for methods like VICReg and Barlow Twins (Table 5), which CLOP is 429 not specifically designed for, we observe better learning outcomes when CLOP is applied. While the accuracy improvement for VICReg is marginal, the embedding visualizations clearly demonstrate 430 that CLOP helps distribute the embeddings more evenly, potentially enhancing the model's ability 431 to generalize to future tasks.

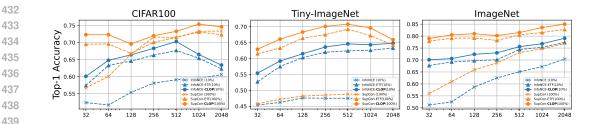


Figure 6: Top-1 classification accuracy across different batch sizes. The percentage of labels used for supervised training is indicated in the legend.

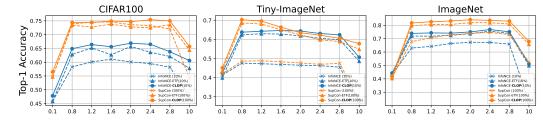


Figure 7: Top-1 classification accuracy across different different learning rates. The percentage of labels used for supervised training is indicated in the legend.

5 EXPERIMENT

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455 In this section, we present the experimental results for image classification, conducted with various 456 batch sizes and learning rates on the CIFAR-100 Krizhevsky et al. (2009), Tiny-ImageNet Le & 457 Yang (2015), and full ImageNet Deng et al. (2009) datasets. For baseline methods, we implement 458 the InfoNCE Wu et al. (2018) with a supervised linear classifier for semi-supervised learning and the SupCon Khosla et al. (2020) for fully-supervised learning. All experiments are performed us-459 ing the SimCLR Chen et al. (2020a) framework with ResNet-50 He et al. (2016). In addition to 460 these baselines, we introduce our novel loss function, CLOP, which incorporates a hand-tuned hy-461 perparameter, $\lambda = 1$, as defined in the formulation (see Eq. (4)). To ensure a fair comparison with 462 ETF, we also evaluate performance using ETF as prototypes instead of an orthonormal basis. For 463 fully-supervised learning, we utilize all labels in the training datasets for both SupCon and CLOP. 464 In the semi-supervised setting, we employ 10% of the labeled data for both linear classifier and 465 CLOP training. For all experiments, we report both top-1 (Figure 6, 7) and top-5 (Appendix B) 466 classification accuracy using the supervised linear classifier. 467

CLOP Enables Smaller Batch Sizes. We trained models with batch sizes of 32, 64, 128, 256, 512, 468 1024, and 2048 on CIFAR-100 and ImageNet for 200 epochs and on Tiny-ImageNet for 100 epochs. 469 The learning rate was fixed at $(0.3 \times \text{batch size}/256)$ for optimal performance. The corresponding 470 classification accuracies are presented in Figure 6. CLOP consistently outperformed the baseline 471 methods across all batch sizes. As reported in the original papers Chen et al. (2020a); Khosla 472 et al. (2020), contrastive learning performs optimally when the batch size exceeds 1024, a finding 473 corroborated by our experiments. However, with the addition of CLOP, we observe significantly 474 less performance degradation at smaller batch sizes. Remarkably, CLOP achieved similar accuracy 475 with a batch size of 32 compared to the baseline SupCon with a batch size of 2048 for CIFAR-100.

476 CLOP Prevents Collapse with Large Learning Rates. We trained models with learning rates 477 ranging from 0.1 to 10 on CIFAR-100 and ImageNet for 200 epochs and Tiny-ImageNet for 100 478 epochs, using a batch size of 1024. The corresponding classification accuracies are presented in 479 Figure 7. Across both datasets, CLOP consistently outperforms the baseline methods. Moreover, 480 as demonstrated by Theorem 1, excessively large learning rates can lead to complete collapse, as 481 clearly observed in the baseline methods at a learning rate of 10 on both datasets. However, with the incorporation of CLOP into the loss function, we observe a significantly smaller performance 482 degradation on both datasets. 483

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486 Ablation Study on λ Tuning. To evaluate the sensi-487 tivity of the tuning parameter λ in CLOP, we trained 488 the model with SupCon loss across different λ val-489 ues, keeping the batch size fixed at 1024. The clas-490 sification accuracy on both CIFAR-100 and Tiny-ImageNet is reported in Table 1. We observe that 491 the performance remains stable for λ values ranging 492 from 0.1 to 1.5, with $\lambda = 1.0$ and $\lambda = 1.5$ yielding 493 the best overall performance. <u>191</u>

495Ablation Study on the Choice of Similarity Metric.496To evaluate the impact of different similarity functions497on Eq. (4), we trained the same ResNet-50 architecture498on CIFAR-100 using cosine similarity, Euclidean similarity, and Manhattan similarity. The results, presented500in Table 5, indicate that cosine similarity, which aligns501with \mathcal{L}_{CL} in Eq. (4), achieves the highest performance.

502 Ablation Study on the Choice of Augmentation 503 To evaluate the impact of augmentation strategies on CLOP, we trained the same ResNet-50 model on Tiny-504 ImageNet with a batch size of 1024. We selected three 505 commonly used augmentation methods: 1) RandAug-506 ment: Augmentation with three operations randomly 507 chosen from all image processing functions in PyTorch 508 (e.g., padding, resizing, cropping, rotation, color jitter, 509 Gaussian blur, inversion, contrast adjustment, equaliza-510 tion); 2) AutoAugment using the ImageNet policy pro-511 posed in Cubuk et al. (2018); 3) SimCLR Augmentation 512 Policy.

λ	CIFAR-100		Tiny-ImageNet		
	Top-1	Top-5	Top-1	Top-5	
0.1	0.745	0.935	0.616	0.868	
0.5	0.740	0.931	0.695	0.909	
1.0	0.754	0.938	0.696	0.900	
1.5	0.760	0.937	0.696	0.893	

Table 1: Accuracy of different λ values.

Similarity Metric	Top-1	Top-5	
Cosine	0.754	0.938	
Euclidean	0.749	0.933	
Manhattan	0.715	0.899	

Table 2: Accuracy of different similaritymetric.

Augmentation	Top-1	Top-5	
RandAug	0.696	0.9	
AutoAug-Imagenet	0.546	0.776	
SimCLR	0.499	0.77	

Table 3: Accuracy of different augmentation strategies.

6 CONCLUSION

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In this paper, we conducted a comprehensive study on dimensional collapse in contrastive learning. Our contributions are threefold. First, we derived a theoretical upper bound on the learning rate, which prevents the embedding mean from shifting towards the boundary of the embedding space, ultimately avoiding complete collapse. Second, we identified the connection between dimensional collapse and cosine similarity by explaining the tendency of embeddings to reside on a hyperplane rather than occupying the full embedding space. To avoid dimensional collapse, we proposed a novel semi-supervised loss function, CLOP, which promotes better separation of the embedding space by pulling a subset of labeled training data towards orthonormal prototypes.

Our experiments on CIFAR-100, Tiny-ImageNet, and ImageNet demonstrated the effectiveness of
 CLOP, showing significant improvements in stability across varying learning rates and batch sizes.
 Additionally, our results indicate that CLOP enables the model to perform exceptionally well even
 with small batch sizes (e.g., 32), making the method particularly suitable for edge devices with
 limited memory.

In future work, we aim to further explore the use of pseudo-labeling for self-supervised learning with CLOP, reducing dependence on labeled data and extending the method's applicability to a broader range of contrastive learning tasks.

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A RELATED WORK

Method	Affinity Metric	Aff. to Prob.	Divergence Function	Top-1	Top-5		
CPC-v2 Henaff (2020)	Cosine	Softmax	CrossEntropy	71.5	90.1		
MOCO-v2 Chen et al. (2020b)	Cosine	Softmax	CrossEntropy	71.1	-		
SimCLR Chen et al. (2020a)	Cosine	Softmax	CrossEntropy	69.3	89.0		
Inclusion/Removal of Terms within InfoNCE							
PCL Cui et al. (2021)	Cosine	Softmax	CrossEntropy	67.6	-		
LOOC Xiao et al. (2020)	Cosine	Softmax	CrossEntropy Variant	-	-		
DCL Yeh et al. (2022)	Cosine	Decoupled Sftmx	CrossEntropy	68.2	-		
RC Wang et al. (2022a)	Cosine	Softmax	CrossEntropy + L2	61.6	-		
Adjustments to the Similarity Function of InfoNCE							
Debiased Chuang et al. (2020)	Floor Cosine	Softmax	CrossEntropy	-	-		
GCL Koishekenov et al. (2023)	Arccosine	Softmax	CrossEntropy	-	-		
HCL Ge et al. (2023)	Cos. + Poincaré	Softmax	CrossEntropy	58.5	-		
Innovations							
InfoMin Tian et al. (2020b)	Cosine	Softmax	MinMax CrossEntropy	73.0	91.1		
VICref Bardes et al. (2021)	Euclidean	NA	Distance + Var + Cov	73.1	91.1		
BT Zbontar et al. (2021)	Dimensional Cos	. NA	L2	73.2	91.0		

Table 4: Overview of Novel Loss Functions and Baseline Results from 2020: Image Classification
Accuracy on ImageNet1K with Unsupervised Learning and Full Label Fine-Tuning. The accuracy
measurements are based on training a standard ResNet-50 with 24M parameters. The symbol '-'
indicates that the corresponding metric was not reported in the original paper.



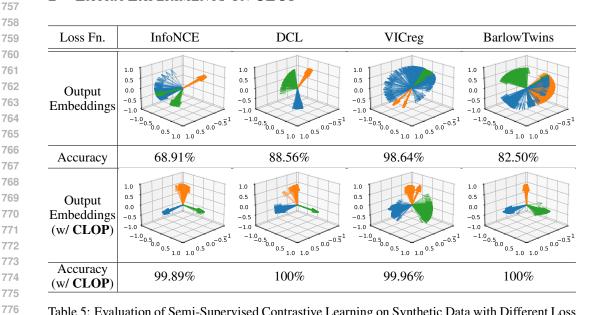


Table 5: Evaluation of Semi-Supervised Contrastive Learning on Synthetic Data with Different Loss Functions. A 3-layer Feedforward Neural Network (FFN) is trained on synthetic data with 10% labeled samples. Both the input and output embeddings reside in a 3-dimensional space, with the output embeddings visualized. The color of each point represents its ground truth label. Additionally, the K-Nearest Neighbors (KNN) classification accuracy (k = 5) is reported, where the model is trained on the labeled 10% of data and tested on the remaining unlabeled data.

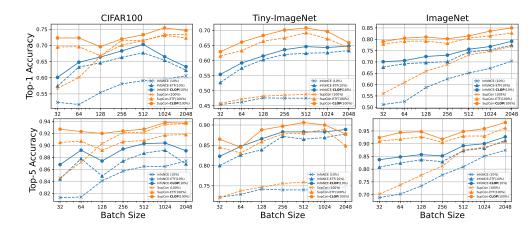


Figure 8: Top-1 classification accuracy across different batch sizes. The percentage of labels used for supervised training is indicated in the legend.

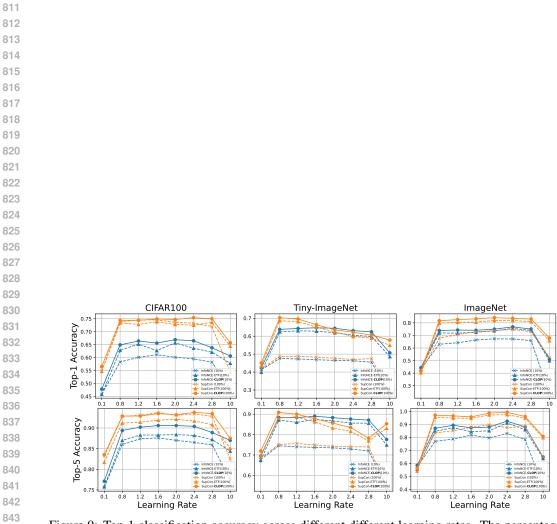


Figure 9: Top-1 classification accuracy across different different learning rates. The percentage of labels used for supervised training is indicated in the legend.

864 C PROOF OF THEOREM 1

Proof of Theorem 1. Consider \mathcal{L}_i as the i-th loss term of $\mathcal{L}_{InfoNCE}$, defined by the following expression:

$$\mathcal{L}_i := -\log \mathbb{P}_i$$

where \mathbb{P}_i denotes the probability that i-th embedding choose its positive pair as closest neighbor:

$$\mathbb{P}_i := \frac{\exp(\mathbf{z}_i^{\top} \mathbf{z}_{j(i)}/\tau)}{\exp(\mathbf{z}_i^{\top} \mathbf{z}_{j(i)}/\tau) + \sum_{a \notin \{i, j(i)\}} \exp(\mathbf{z}_i^{\top} \mathbf{z}_a/\tau)}$$

As detailed in Yeh et al. (2022), the gradient of \mathcal{L}_i with respect to \mathbf{z}_i , $\mathbf{z}_{j(i)}$, and \mathbf{z}_a can be derived as follows:

$$-\frac{\partial \mathcal{L}_i}{\partial \mathbf{z}_i} := (1 - \mathbb{P}_i) / \tau \left(\mathbf{z}_{j(i)} - \sum_{a \notin \{i, j(i)\}} \frac{\exp(\mathbf{z}_i^\top \mathbf{z}_a / \tau)}{\sum_{b \notin \{i, j(i)\}} \exp(\mathbf{z}_i^\top \mathbf{z}_b / \tau)} \mathbf{z}_a \right)$$

 $-rac{\partial \mathcal{L}_i}{\partial \mathbf{z}_{j(i)}} := rac{(1-\mathbb{P}_i)}{ au} \mathbf{z}_i$

$$-\frac{\partial \mathcal{L}_i}{\partial \mathbf{z}_a} := -\frac{(1-\mathbb{P}_i)}{\tau} \frac{\exp(\mathbf{z}_i^\top \mathbf{z}_a/\tau)}{\sum_{b \notin \{i,j(i)\}} \exp(\mathbf{z}_i^\top \mathbf{z}_b/\tau)} \mathbf{z}_i$$

In the standard setup of self-supervised learning, for any sample, there is one positive pair among I and the remainder are all negative pairs. By aggregating all the gradient respect to a single sample, we have the gradient of InfoNCE respect to z_i :

$$-\frac{\partial \mathcal{L}_{\text{InfoNCE}}}{\partial \mathbf{z}_{i}} := \frac{(1 - \mathbb{P}_{i}) + (1 - \mathbb{P}_{j(i)})}{\tau} \mathbf{z}_{j(i)} - \sum_{a \notin \{i, j(i)\}} \frac{(1 - \mathbb{P}_{i})}{\tau} \frac{\exp(\mathbf{z}_{i}^{\top} \mathbf{z}_{a}/\tau)}{\sum_{b \notin \{i, j(i)\}} \exp(\mathbf{z}_{i}^{\top} \mathbf{z}_{b}/\tau)} \mathbf{z}_{a} - \sum_{a \notin \{i, j(i)\}} \frac{(1 - \mathbb{P}_{a})}{\tau} \frac{\exp(\mathbf{z}_{i}^{\top} \mathbf{z}_{a}/\tau)}{\sum_{b \notin \{a, j(a)\}} \exp(\mathbf{z}_{i}^{\top} \mathbf{z}_{b}/\tau)} \mathbf{z}_{a}$$

Now, considering the first scenario, where all embeddings equal, that means that $\mathbf{z}_i = \mathbf{z}_{j(i)} = \mathbf{z}_a = \mathbf{z}^*$ for all $a \in I$, the loss terms \mathbb{P}_i , $\mathbb{P}_{j(i)}$, and \mathbb{P}_a converge to a constant \mathbb{P}^* , given by:

$$\mathbb{P}_i = \mathbb{P}_{j(i)} = \mathbb{P}_a = -\log \frac{1}{|I| - 1} := \mathbb{P}^*$$

Consequently, the gradient of $\mathcal{L}_{InfoNCE}$ with respect to \mathbf{z}_i under this assumption reduces to zero, aligning with our expectations:

$$-\frac{\partial \mathcal{L}_{\text{InfoNCE}}}{\partial \mathbf{z}_i} = \frac{2(1-\mathbb{P}^*)}{\tau} \mathbf{z}^* - 2(|I|-2)\frac{(1-\mathbb{P}^*)}{\tau}\frac{1}{|I|-2}\mathbf{z}^* = 0$$

We establish the existence of local minima in scenarios where all embeddings are identical. Now, we consider the second scenario where all embeddings generated reside within the same rank-1 subspace. Denoting z^* as their unit basis, we can represent each embedding z_i as:

$$\mathbf{z}_i = \alpha \mathbf{z}^*, \quad \alpha \in \{-1, 1\}, \quad \forall$$

⁹⁰⁷ The gradient of the loss function $\mathcal{L}_{\text{InfoNCE}}$ with respect to \mathbf{z}_i simplifies to:

$$-\frac{\partial \mathcal{L}}{\partial \mathbf{z}_i} = \beta \mathbf{z}_i$$

910 Here, β is a scalar that aggregates contributions from all relevant weights.

It is important to note that z^i represents the normalized output of the function f, with \tilde{z}_i denoting the original, unnormalized embedding. This implies the following relation:

$$-\frac{\partial \mathcal{L}}{\partial \tilde{\mathbf{z}}_i} = -\frac{\partial \mathcal{L}}{\partial \mathbf{z}_i} \frac{\partial \mathbf{z}_i}{\partial \tilde{\mathbf{z}}_i} = \frac{1}{\|\mathbf{z}_i\|_2} \left(\mathbb{I} - \frac{\mathbf{z}_i \mathbf{z}_i^{\top}}{\mathbf{z}_i^{\top} \mathbf{z}_i} \right) \beta \mathbf{z}_i = 0,$$

916 where \mathbb{I} represents the identity matrix.

918 D PROOF OF THEOREM 1

Proof. At each step of gradient descent, every point \mathbf{x}_i moves toward the negative of the mean of the other points with a step size η . Let the mean of all k points before the gradient descent step be $\boldsymbol{\mu}^{(0)} := \frac{1}{k} \sum_{i=1}^{k} \mathbf{x}_i^{(0)}$. The update rule for the *i*-th point is given by:

$$\mathbf{x}_{i}^{(1)} = \mathbf{x}_{i}^{(0)} - \eta \frac{1}{k-1} \left(n \boldsymbol{\mu}^{(0)} - \mathbf{x}_{i}^{(0)} \right) = \left(1 + \frac{\eta}{k-1} \right) \mathbf{x}_{i}^{(0)} - \eta \frac{k}{k-1} \boldsymbol{\mu}^{(0)}.$$

After the update, each point $\mathbf{x}_i^{(1)}$ is normalized to have unit norm, i.e., $\hat{\mathbf{x}}_i^{(1)} = \frac{\mathbf{x}_i^{(1)}}{\|\mathbf{x}_i^{(1)}\|}$. The expected norm of any updated vector is calculated as:

$$\mathbb{E}[\|\mathbf{x}_{i}^{(1)}\|^{2}] = \left(1 + \frac{\eta}{k-1}\right)^{2} \mathbb{E}\left[\|\mathbf{x}_{i}^{(0)}\|^{2}\right] + \eta^{2} \left(\frac{k}{k-1}\right)^{2} \mathbb{E}\left[\|\boldsymbol{\mu}^{(0)}\|^{2}\right] \\ - 2\eta \frac{k}{k-1} \left(1 + \frac{\eta}{k-1}\right) \mathbb{E}\left[\mathbf{x}_{i}^{(0)\top} \boldsymbol{\mu}^{(0)}\right].$$
(5)

Since $\mathbf{x}_i^{(0)}$ is uniformly distributed on the surface of an *m*-dimensional unit ball, its covariance is $\text{Cov}(\mathbf{x}_i^{(0)}) = \frac{1}{m} \mathbf{I}_m$. Therefore, the covariance of the mean is

$$\operatorname{Cov}(\boldsymbol{\mu}^{(0)}) = \operatorname{Cov}\left(\frac{1}{k}\sum_{i=1}^{k}\mathbf{x}_{i}^{(0)}\right) = \frac{1}{k^{2}}\sum_{i=1}^{k}\operatorname{Cov}(\mathbf{x}_{i}^{(0)}) = \frac{1}{km}\mathbf{I}_{m}$$

The second moment of $\mu^{(0)}$'s norm is the trace of its covariance matrix:

$$\mathbb{E}[\|\boldsymbol{\mu}^{(0)}\|^2] = \mathbb{E}[\boldsymbol{\mu}^{(0)\top}\boldsymbol{\mu}^{(0)}] = \operatorname{Tr}(\operatorname{Cov}(\boldsymbol{\mu}^{(0)})) = \frac{1}{km}\operatorname{Tr}(\mathbf{I}_m) = \frac{1}{k}.$$
(6)

Since $\mathbf{x}_i^{(0)}$ and $\mathbf{x}_j^{(0)}$ are independent for $i \neq j$, we know that $\mathbb{E}[\mathbf{x}_i^{(0)\top}\mathbf{x}_j^{(0)}] = 0$. Therefore,

$$\mathbb{E}[\mathbf{x}_{i}^{(0)\top}\boldsymbol{\mu}^{(0)}] = \mathbb{E}\left[\frac{1}{k}\|\mathbf{x}_{i}^{(0)}\|^{2} + \frac{1}{k}\sum_{j\neq i}\mathbf{x}_{i}^{(0)\top}\mathbf{x}_{j}^{(0)}\right] = \frac{1}{k}\mathbb{E}[\|\mathbf{x}_{i}^{(0)}\|^{2}].$$
(7)

Since $\mathbb{E}[\|\mathbf{x}_i^{(0)}\|^2] = 1$, substituting equations Eq. (6) and Eq. (7) into Eq. (5), we obtain

$$\begin{split} \mathbb{E}[\|\mathbf{x}_{i}^{(1)}\|^{2}] &= \left(1 + \frac{\eta}{k-1}\right)^{2} + \frac{k\eta^{2}}{(k-1)^{2}} - 2\eta \frac{k}{k-1} \left(1 + \frac{\eta}{k-1}\right) \frac{1}{k} \\ &= 1 + \frac{\eta}{k-1} - \frac{2\eta}{k} - 2\frac{\eta^{2}}{k(k-1)} + \frac{\eta^{2}k}{(k-1)^{2}}. \end{split}$$

Thus, the upper bound of the first-order expectation $\mathbb{E}[||\mathbf{x}_i^{(1)}||]$ can be denoted by B, where:

$$\mathbb{E}[\|\mathbf{x}_i^{(1)}\|] \le \sqrt{1 + \frac{\eta}{k-1} - \frac{2\eta}{k} - 2\frac{\eta^2}{k(k-1)} + \frac{\eta^2 k}{(k-1)^2}} := B$$

After the gradient descent step, the expectation of the new mean $\mu^{(1)}$ is bounded as follows:

$$\boldsymbol{\mu}^{(1)} = \frac{1}{k} \sum_{i=1}^{n} \hat{\mathbf{x}}_{i}^{(1)} \ge \frac{1}{kB} \sum_{i=1}^{n} \mathbf{x}_{i}^{(1)} = \frac{1-\eta}{B} \boldsymbol{\mu}^{(0)}.$$

To prevent complete collapse in $\hat{\mathbf{X}}^{(1)}$, the mean should not increase by more than $1 + \varepsilon$, where ε controls the tolerance for mean shift. By setting $\varepsilon = 0$, we can ensure that $\mu^{(1)}$ does not exceed $\mu^{(0)}$, thereby providing the safest bound for the learning rate. This implies that the learning rate η must satisfy $\frac{1-\eta}{B} \le 1 + \varepsilon$. This gives the condition:

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$$(1-\eta)^2 \le \left(1 + \frac{\eta}{k-1} - \frac{2\eta}{k} - 2\frac{\eta^2}{k(k-1)} + \frac{\eta^2 k}{(k-1)^2}\right) (1+\varepsilon)^2.$$

972 By setting $\varepsilon = 0$, we can simplify further to obtain the following inequality: 973

$$\left(-2 - \frac{1}{k-1} + \frac{2}{k}\right) + \eta \left(1 + 2\frac{1}{k(k-1)} - \frac{k}{(k-1)^2}\right) \le 0.$$

For k > 2, we have $1 + 2\frac{1}{k(k-1)} - \frac{k}{(k-1)^2} > 0$, leading to the bound:

$$\eta \leq \frac{2 + \frac{1}{k-1} - \frac{2}{k}}{1 + 2\frac{1}{k(k-1)} - \frac{k}{(k-1)^2}} = \frac{2k^3 - 5k^2 + 5k - 2}{k^3 - 3k^2 + 4k - 2} = 2 + O\left(\frac{1}{k}\right).$$

982 Since k is an integer, this bound is effectively O(1).

E PROOF OF THEOREM 2

Proof. Consider a list of k class embeddings in m-dimensional space, denoted as $\mathbf{X} := [\mathbf{x}_1, \dots, \mathbf{x}_k] \in \mathbb{R}^{m \times k}$, where $m \ge k$ and each class embedding has unit norm (i.e., $\|\mathbf{x}_i\|_2 = 1$ for all i). The loss function is defined as the sum of pairwise cosine similarities between the class embeddings (refer to Equation 3). We first assume that all class embeddings are linearly independent, implying that Rank $(\mathbf{X}) = k$. Our first goal is to show that there always exists another matrix $\mathbf{X}' \in \mathbb{R}^{m \times k}$ with Rank $(\mathbf{X}') = k - 1$, such that $\mathcal{L}(\mathbf{X}) > \mathcal{L}(\mathbf{X}')$.

To construct such a matrix \mathbf{X}' , we select a *class embedding* \mathbf{x}_k such that $\sum_{i \neq k} \mathbf{x}_i \neq 0$. The existence of such a *class embedding* \mathbf{x}_k can be easily established by contradiction. Suppose, for the sake of contradiction, that for all k, $\sum_{i \neq k} \mathbf{x}_i = 0$. This would imply that each \mathbf{x}_i must be zero, i.e., $\mathbf{x}_i = 0$ for all *i*, which contradicts the assumption that the Rank(\mathbf{X}) = *k*. Hence, such a *class embedding* \mathbf{x}_k must exist. Since the *class embeddings* are linearly independent, \mathbf{x}_k can be decomposed as a weighted sum of two unit-norm vectors: one orthogonal to all other *class embeddings*, and one lying in the subspace spanned by the remaining *class embeddings*. Specifically, we write:

$$\mathbf{x}_k = \eta \mathbf{x}_k^{\perp} + \sqrt{1 - \eta^2} \mathbf{x}_k^{\parallel}, \quad 0 < \eta \le 1,$$

where \mathbf{x}_k^{\perp} is orthogonal to all other *class embeddings* and \mathbf{x}_k^{\parallel} lies in the subspace spanned by the remaining *class embeddings*. The loss associated with the *k*-th *class embedding* is:

$$\mathcal{L}_k(\mathbf{X}) = \sum_{i \neq k} \mathbf{x}_i^\top \mathbf{x}_k = \sum_{i \neq k} \mathbf{x}_i^\top \left(\eta \mathbf{x}_k^\perp + \sqrt{1 - \eta^2} \mathbf{x}_k^\parallel \right).$$

7 Since $\mathbf{x}_i^{\top} \mathbf{x}_k^{\perp} = 0$ for all $i \neq k$, we have:

$$\mathcal{L}_k(\mathbf{X}) = \sqrt{1 - \eta^2} \sum_{i \neq k} \mathbf{x}_i^{\top} \mathbf{x}_k^{\parallel}$$

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Now, construct X' by replacing \mathbf{x}_k with \mathbf{x}_k^{\parallel} . The corresponding loss function becomes:

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$$\mathcal{L}_k(\mathbf{X}') = \sum_{i \neq k} \mathbf{x}_i^\top \mathbf{x}_k^\parallel$$
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It is important to note that we can always find $\sum_{i \neq k} \mathbf{x}_i^\top \mathbf{x}_k^{\parallel} < 0$. If this sum is not negative, we can simply invert the sign of \mathbf{x}_k^{\parallel} , ensuring the sum becomes negative. Since $0 < \eta \le 1$, it follows that $\sqrt{1-\eta^2} < 1$. Consequently, $\sqrt{1-\eta^2} \sum_{i\neq k} \mathbf{x}_i^\top \mathbf{x}_k^{\parallel} > \sum_{i\neq k} \mathbf{x}_i^\top \mathbf{x}_k^{\parallel}$. Therefore, we have $\mathcal{L}(\mathbf{X}) >$ $\mathcal{L}(\mathbf{X}')$, as required.

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