Towards the Generalization of Contrastive Self-Supervised Learning

Weiran Huang1∗ Mingyang Yi2,3∗ Xuyang Zhao4∗

1Huawei Noah’s Ark Lab
2University of Chinese Academy of Sciences
3Academy of Mathematics and Systems Science, Chinese Academy of Sciences
4Peking University

weiran.huang@outlook.com, yimingyang17@mails.ucas.edu.cn, 2101110088@pku.edu.cn

Abstract

Recently, self-supervised learning has attracted great attention, since it only requires unlabeled data for training. Contrastive learning is a popular approach for self-supervised learning and achieves promising empirical performance. However, the theoretical understanding of its generalization ability is still limited. To this end, we define a kind of \((\sigma, \delta)\)-measure to mathematically quantify the data augmentation, and then provide an upper bound of the downstream classification error based on the measure. We show that the generalization ability of contrastive self-supervised learning depends on three key factors: alignment of positive samples, divergence of class centers, and concentration of augmented data. The first two factors can be optimized by contrastive algorithms, while the third one is priorly determined by pre-defined data augmentation. With the above theoretical findings, we further study two canonical contrastive losses, InfoNCE and cross-correlation loss, and prove that both of them are able to obtain the embedding space satisfying the aforementioned factors. Finally, we conduct various experiments on the real-world dataset, and show that our theoretical inferences agree with the empirical observations.

1 Introduction

In recent years, contrastive Self-Supervised Learning (SSL) has attracted great attention for its fantastic data efficiency and generalization ability in both computer vision (He et al., 2020; Chen et al., 2020a,c; Grill et al., 2020; Chen and He, 2021; Zbontar et al., 2021) and natural language processing (Fang et al., 2020; Wu et al., 2020; Giorgi et al., 2020; Gao et al., 2021; Yan et al., 2021). In contrast to supervised learning, contrastive SSL learns the representation through a large number of unlabeled data and artificially defined self-supervision signals (i.e., regarding the augmented views of a data sample as positive samples). The model is updated by encouraging the embeddings of positive samples close to each other. To overcome the feature collapse issue, different losses (e.g., InfoNCE (Chen et al., 2020a) and cross-correlation (Zbontar et al., 2021)) and training tricks (e.g., stop gradient (Grill et al., 2020)) are proposed.

∗Equal contribution (alphabetical ordering).
Towards the Generalization of Contrastive Self-Supervised Learning

In spite of the empirical success of contrastive SSL methods in terms of their generalization ability on downstream tasks (evaluated via learning a linear classifier on the features to perform a downstream task), the theoretical understanding of it is still limited. Arora et al. (2019) propose a theoretical framework to show the provable downstream performance of contrastive SSL with the InfoNCE loss. However, their results rely on the assumption that positive samples are drawn from the same latent class, instead of the augmented views of a data point as in practice. Wang and Isola (2020) observe that alignment and uniformity of the learned embedding space can be used to explain the downstream performance, but they are empirical indicators and cannot theoretically guarantee the generalization. Furthermore, both of the above works avoid characterizing the role of data augmentation, which is the key to the success of contrastive SSL, since the only human knowledge is injected via data augmentation.

Besides the incomplete theoretical guarantees of generalization, there are also some interesting empirical observations of contrastive SSL that have not been unraveled theoretically yet. For example, why does the stronger data augmentation lead to the more clustered structure (Figure 2) as well as the better downstream performance? Why is aligning positive samples (augmented from the same data point) able to gather the samples from the same latent class into a cluster (Figure 2c)? Moreover, decorrelating components of representation like Barlow Twins (Zbontar et al., 2021) does not directly optimize the geometry of embedding space, but it still can result in the clustered structure. Why?

In this paper, we mainly focus on exploring the generalization ability of contrastive SSL provably, which can also provide insights for understanding the above interesting observations. We start with understanding and characterizing the role of data augmentation in contrastive SSL. Intuitively, samples from the same latent class are likely to have similar augmented views, which are mapped to the close locations in the embedding space. Since the augmented views of each sample are encouraged to be clustered in the embedding space by contrastive learning, different samples from the same latent class tend to be pulled closer. As an example, let’s consider two images of dogs with different backgrounds (Figure 1). If we augment them with operation “crop”, we may get two similar views (dog heads), whose representations (gray points in the embedding space) are close. As the augmented views of each dog image are enforced to be close in the embedding space due to the objective of contrastive learning, the representations of two dog images (green and blue points) will be pulled closer to their dog head views. Thus, aligning positive samples can obtain the clustered embedding space. Following the above intuition, we define the augmented distance between two samples as the minimum distance between their augmented views, and further introduce the $(\sigma, \delta)$-augmentation to measure the concentration of augmented data, i.e., for each latent class, the proportion of samples located in a ball with diameter $\delta$ (w.r.t. the augmented distance) is larger than $\sigma$.

With the mathematical description of data augmentation settled, we then provide an upper bound of downstream classification error. It reveals that the generalization of contrastive SSL depends on three key factors. The first one is the alignment of positive samples, which is the common objective that contrastive algorithms aim to optimize. The second one is the divergence of class centers, which prevents the collapse of representation. We find that a good alignment property can loosen the divergence condition, hence it characterizes the sufficient condition of generalization more precisely than the uniformity indicator of (Wang and Isola, 2020). The third factor is the concentration of augmented data, i.e., the model trained using the augmented data with smaller $\delta$ and larger $\sigma$ exhibits the better generalization ability. The first two factors, alignment and divergence, can be optimized by SSL algorithms, while the third factor is priorly decided by the pre-determined data augmentation. Therefore,
Choosing the appropriate data augmentations is critical to the generalization of contrastive SSL.

Furthermore, we apply our theoretical justification to two frequently-used contrastive losses, InfoNCE (Chen et al., 2020a; He et al., 2020) and cross-correlation loss (Zhontar et al., 2021). We show that both of them can be decomposed into two parts: one controls the alignment of positive samples, and the other preserves the divergence of class centers. We further prove that both pushing negative samples away and decorrelating components of representation can obtain the embedding space with distinguishable class centers. Thus, the generalization abilities of InfoNCE and cross-correlation loss are guaranteed.

Finally, we conduct various experiments on the real-world dataset to verify theoretical inferences on the relationship between the data augmentation and the generalization of contrastive self-supervised learning. The results show that the model trained using the augmented data with sharper concentration in terms of the proposed augmented distance indeed has better performance on downstream tasks.

The rest of this paper is organized as follows. In Section 2, we rigorously formulate the generalization problem of contrastive SSL. We then introduce the \((\sigma, \delta)\)-augmentation and explore which kind of embedding space can generalize to downstream tasks with theoretical guarantees in Section 3. In Section 4, we show how two canonical contrastive losses, InfoNCE and cross-correlation loss, are able to learn such embedding space. Finally, we verify our theoretical findings on the real-world dataset in Section 5. Due to space limitations, all proofs are deferred to the appendix.

## Related Work

### Self-Supervised Learning

There are three common approaches for self-supervised learning: generative based (Donahue et al., 2017; Dumoulin et al., 2017; Donahue and Simonyan, 2019), pretext based (Zhang et al., 2016; Pathak et al., 2016; Noroozi and Favaro, 2016; Gidaris et al., 2018; Lee et al., 2019; Teng and Huang, 2021) and contrastive based (Hjelm et al., 2018; Oord et al., 2018; Bachman et al., 2019; Tian et al., 2019; He et al., 2020; Chen et al., 2020a). These three approaches are quite different in technique, and we focus on studying contrastive self-supervised learning.

### Algorithm of Contrastive SSL

Early works such as MoCo (He et al., 2020; Chen et al., 2020c) and SimCLR (Chen et al., 2020a,b) use the InfoNCE loss to pull the positive samples close while enforcing them away from the negative samples in the embedding space. These methods require large batch sizes (Chen et al., 2020a), memory banks (He et al., 2020), or carefully designed negative sampling strategies (Hu et al., 2021). To obviate these, some recent works get rid of negative samples and prevent representation collapse by cross-correlation loss (Zhontar et al., 2021; Bardes et al., 2021) or training tricks (Grill et al., 2020; Chen and He, 2021). In this paper, we mainly study the effectiveness of InfoNCE and cross-correlation loss, and not enter the discussion of training tricks (e.g., stop gradient).

### Theory of Contrastive SSL

A number of recent works aim to theoretically explain the success of contrastive learning. One way to motivate contrastive SSL is to maximize the mutual information (MI) between positive samples (Oord et al., 2018; Bachman et al., 2019; Hjelm et al., 2018; Tian et al., 2019, 2020). However, Tschannen et al. (2019) find that optimizing the tighter bounds of MI does not imply better representations. Therefore, MI may not fully explain the success of contrastive SSL. Besides the MI perspective, Arora et al. (2019) directly analyze the generalization of InfoNCE loss based on the assumption that positive samples are drawn from the same latent classes, instead of the augmented views of a data point, which are practically used in contrastive algorithms. The behavior of InfoNCE loss is also studied from the perspective of alignment and uniformity properties of the embedding space, under the condition of infinite negative samples (Wang and Isola, 2020), sparse coding model (Wen and Li, 2021), or impractical “expansion” assumption (Wei et al., 2020). Most existing theoretical works focus on the InfoNCE loss only, and avoid characterizing the important role of data augmentation.

## 2 Problem Formulation

Given a number of unlabeled training data i.i.d. drawn from an unknown distribution, each sample belongs to one of \(K\) latent classes \(C_1, C_2, \ldots, C_K\). Based on a set \(A\) consisting of transformations, the set of potential positive samples generated from a data point \(x\) is denoted as \(A(x)\). We assume that \(x \in A(x)\) for any \(x\), and samples from different latent classes never transfer to the same augmented sample, i.e., \(\cap_{k=1}^{K} A(C_k) = \emptyset\). Notation \(\|\cdot\|\) without subscripts stands for \(\ell_2\)-norm or Frobenius norm for vectors and matrices.

The goal of contrastive SSL is to learn an encoder \(f\), such that positive samples are closely aligned, while the samples from different latent classes are far away from each other. To prevent the collapse of representation, a class of methods (e.g., SimCLR, MoCo) use the InfoNCE loss to push away negative pairs, i.e.,

\[
\ell_{\text{InfoNCE}} = - \mathbb{E}_{x, x' \sim A(x)} \log \frac{e^{f(x_1)^\top f(x_2)}}{e^{f(x_1)^\top f(x_1)} + e^{f(x_1)^\top f(x')}}.
\]
where \( x, x' \) are two random data points. Some other methods (e.g., Barlow Twins) use the cross-correlation loss to decorrelate the components of representation, i.e.,

\[
\mathcal{L}_{\text{Cross-Corr}} = \frac{d}{i=1} (1 - C_{ij})^{2} + \lambda \frac{d}{i<j} C_{ij}^{2},
\]

where \( C_{ij} = \mathbb{E}_{x, x'} \mathbb{E}_{x_{1}, x_{2} \in A(x)} [f_{i}(x_{1}) f_{j}(x_{2})] \), \( d \) is the dimension of encoder \( f \), and encoder \( f \) is normalized as \( \mathbb{E}_{x} \mathbb{E}_{x' \in A(x)} [f_{i}(x')]^{2} = 1 \) for each dimension.

The standard evaluation of an SSL method is to train a linear classifier over the self-supervised learned representation and regard its performance as the indicator. In order to simplify the theoretical analysis, we instead consider a non-parametric classifier – nearest neighbor (NN) classifier:

\[
G_{f}(x) = \arg \min_{k \in [K]} \| f(x) - \mu_{k} \|, 
\]

where \( \mu_{k} := \mathbb{E}_{x \in C_{k}} \mathbb{E}_{x' \in A(x)} [f(x')] \) is the center of class \( C_{k} \). In fact, the NN classifier can be regarded as a special linear classifier, namely,

\[
G_{f}(x) = \arg \max_{k \in [K]} (W f(x) + b_{k}),
\]

by setting the \( k \)-th row of \( W \) to be \( \mu_{k} \) and \( b_{k} = -\frac{1}{2} \| \mu_{k} \|^{2} \). Therefore, the directly learned linear classifier used in practice should have better performance than the NN classifier. In this paper, we use error rate to quantify the performance of \( G_{f} \), formulated as

\[
\text{Err}(G_{f}) = \sum_{k=1}^{K} \mathbb{P}[G_{f}(x) \neq k, \forall x \in C_{k}].
\]

In the sequel, we will show that contrastive SSL is able to achieve a small error rate \( \text{Err}(G_{f}) \).

## 3 Generalization of Contrastive SSL

Based on the NN classifier, if the samples are well clustered by latent classes in the embedding space, the error rate should be small. Thus, one expects to have a small intra-class distance \( \mathbb{E}_{x_{1}, x_{2} \in C_{k}} \| f(x_{1}) - f(x_{2}) \|^{2} \). However, contrastive algorithms only control the alignment of positive samples \( \mathbb{E}_{x_{1}, x_{2} \in A(x)} \| f(x_{1}) - f(x_{2}) \|^{2} \).

To bridge the gap between these two distances, we show that the concentration of augmented data plays an important role.

Motivated by Figure 1 introduced in Section 1, for a given data augmentation set \( A \), we first define the augmented distance between two samples as the minimum distance between their augmented views, i.e.,

\[
d_{A}(x_{1}, x_{2}) = \min_{x'_{1} \in A(x_{1}), x'_{2} \in A(x_{2})} \| x'_{1} - x'_{2} \|.
\]

For the dog images in Figure 1, although they are quite different in the pixel level, they contain similar semantic meanings. Meanwhile, they have a small augmented distance. Thus, the semantic distance can be partially characterized by the augmented distance. Based on the augmented distance, we introduce the definition of \((\sigma, \delta)\)-augmentation to measure the intra-class concentration of augmented data.

### Definition 1 \((\sigma, \delta)\)-Augmentation

The data augmentation set \( A \) is called a \((\sigma, \delta)\)-augmentation, if for each class \( C_{k} \), there exists a subset \( C_{0}^{k} \subseteq C_{k} \) (called the main part of \( C_{k} \)) such that the following two conditions hold:

a) \( \mathbb{P}[x \in C_{0}^{k}] \geq \sigma \mathbb{P}[x \in C_{k}] \) where \( \sigma \in (0, 1] \),

b) \( \sup_{x_{1}, x_{2} \in C_{0}^{k}} d_{A}(x_{1}, x_{2}) \leq \delta \).

Larger \( \sigma \) and smaller \( \delta \) indicate that the augmented data are more concentrated in terms of the augmented distance. One can verify that for any \( A' \supseteq A \) with more augmentations, we have \( d_{A'}(x_{1}, x_{2}) \leq d_{A}(x_{1}, x_{2}) \) for any \( x_{1}, x_{2} \). Therefore, more data augmentations lead to sharper concentration as \( \delta \) gets smaller.

With the above definition, our analysis will focus on the samples in the main parts with good alignment, i.e., \( (C_{0}^{1} \cup \cdots \cup C_{0}^{K}) \cap S_{c} \), where \( S_{c} := \{ x \in \bigcup_{k=1}^{K} C_{k} : \forall x_{1}, x_{2} \in A(x), \| f(x_{1}) - f(x_{2}) \| \leq c \} \) is the set of samples with \( c \)-close representations among augmented data. Furthermore, we let \( R_{c} := \mathbb{P}[S_{c}] \), which should be small for the encoder with good alignment.

### Lemma 3.1

For a \((\sigma, \delta)\)-augmentation with main part \( C_{0}^{k} \) of each class \( C_{k} \), if all samples belonging to \((C_{0}^{1} \cup \cdots \cup C_{0}^{K}) \cap S_{c} \) can be correctly classified by a classifier \( G \), then its downstream error rate \( \text{Err}(G) \leq (1 - \sigma) + R_{c} \).

The above lemma presents a sufficient condition to guarantee the generalization ability on downstream tasks. Based on it, we further need to 1) explore when samples in \((C_{0}^{1} \cup \cdots \cup C_{0}^{K}) \cap S_{c} \) can be correctly classified by the NN classifier \( G_{f} \), and 2) upper bound \( R_{c} \). We will tackle the first one below, and leave the second one in Section 3.1.

For simplicity, we assume that encoder \( f \) is normalized by \( \| f \| = r \) and has \( L \)-Lipschitz continuity, i.e., for any \( x_{1}, x_{2}, \| f(x_{1}) - f(x_{2}) \| \leq L \| x_{1} - x_{2} \| \). Let \( p_{k} := \mathbb{P}[x \in C_{k}] \).

### Lemma 3.2

For a \((\sigma, \delta)\)-augmentation and each \( \ell \in [K] \), if \( \mu_{k} \perp \mu_{\ell} < r^{2} \left( 1 - \rho_{\ell}(\sigma, \delta, \varepsilon) - \sqrt{2 \rho_{\ell}(\sigma, \delta, \varepsilon)} - \frac{2 \varepsilon}{\sigma} \right) \) holds for all \( k \neq \ell \), then every sample \( x \in C_{0}^{1} \cap S_{c} \) can be correctly classified by the NN classifier \( G_{f} \), where \( \rho_{\ell}(\sigma, \delta, \varepsilon) = 2(1 - \sigma) + \frac{\Delta_{\mu}}{\rho_{\ell}} + \sigma \left( \frac{\Delta_{\mu}}{\rho_{\ell}} + \frac{\Delta_{\mu}}{\rho_{\ell}} \right) \) and \( \Delta_{\mu} = 1 - \min_{k \in [K]} \| \mu_{k} \|^{2}/r^{2} \).
Combining Lemma 3.1 and 3.2, we can directly obtain the generalization guarantee of contrastive SSL as follows.

**Theorem 1.** For a $(\sigma, \delta)$-augmentation used in SSL, if

$$\mu_\ell \mu_k < \nu^2 \left(1 - \rho_{\max}(\sigma, \delta, \varepsilon) - \sqrt{2\rho_{\max}(\sigma, \delta, \varepsilon)} - \frac{\Delta}{2}\right)$$

holds for any pair of $(\ell, k)$ with $\ell \neq k$, then the downstream error rate of NN classifier $G_f$ holds for any pair of $(\ell, k)$ with $\ell \neq k$, then the downstream error rate of NN classifier $G_f$

$$\text{Err}(G_f) \leq (1 - \sigma) + R_\varepsilon,$$  

where $\rho_{\max}(\sigma, \delta, \varepsilon) = 2(1 - \sigma) + \frac{\mu_2}{\mu_1} + \sigma \left(\frac{\mu_4}{\mu_2} + \frac{\sigma^2}{\mu_2}\right)$ and $\Delta = 1 - \min_{k \in [K]} \|\mu_k\|^2/\mu^2$.

To better understand the above theorem, let us first consider a special case that any two samples from the latent class at least own a same augmented view ($\sigma = 1, \delta = 0$), and the positive samples are perfectly aligned after contrastive learning ($\varepsilon = 0, R_\varepsilon = 0$). In this case, the samples from the same latent class are embedded to a single point on the hypersphere, and thus arbitrarily small positive angle $\langle \mu_k, \mu_k \rangle < 1$ is enough to distinguish them by the NN classifier. In fact, one can quickly verify that $\rho_{\max}(\sigma, \delta, \varepsilon) = \Delta = 0$ holds in the above case. According to Theorem 1, if $\mu_\ell \mu_k / r^2 < 1 - \rho_{\max}(\sigma, \delta, \varepsilon) - \sqrt{2\rho_{\max}(\sigma, \delta, \varepsilon)} - \frac{\Delta}{2} = 1$, then $\text{Err}(G_f) = 0$. The conditions of $\mu_\ell \mu_k$ get matched.

Theorem 1 implies three key factors to the success of contrastive SSL, which can provide insights for contrastive algorithm analysis. The first one is the alignment of positive samples, which is the common objective that contrastive algorithms aim to optimize. The good alignment enables the small $R_\varepsilon$, which directly decreases the upper bound of error rate (1). The second factor is the divergence of class centers, i.e., the distance between class centers should be large enough. The divergence condition is related to the alignment ($R_\varepsilon$) and data augmentation $(\sigma, \delta)$. Better alignment and sharper concentration indicates smaller $\rho_{\max}(\sigma, \delta, \varepsilon)$ in the divergence condition. Thus, a good alignment property or concentrated augmented data can loosen the divergence condition, which can also be seen from the above special case. The third factor is the concentration of augmented data. When $\delta$ is given, sharper concentration implies larger $\sigma$, which directly affects the upper bound of error rate (1). For example, stronger data augmentation can make the augmented data more concentrated, and thus the better downstream performance. The first two factors can be optimized by contrastive algorithms, and we will verify this argument via two concrete examples in Section 4. In contrast, the third factor is primarily decided by the pre-defined data augmentation and is unrelated to algorithms. Thus, data augmentation is critical to the generalization of contrastive SSL.

Compared with (Wang and Isola, 2020), both of the works have the same meaning of “alignment” since it is the objective that contrastive algorithms aim to optimize, but their “uniformity” is fundamentally different from our “divergence”. Uniformity requires “all data” uniformly distributed on the embedding hypersphere, while our divergence characterizes the cosine distance between “class centers”. We do not require the divergence to be as large as better, instead, the divergence condition can be loosened by better alignment and concentration property. Furthermore, uniformity indicator is valid only for InfoNCE, but divergence is more fundamental and does not rely on the loss. Moreover, alignment and uniformity are empirical performance predictors, while alignment and divergence have explicit theoretical guarantees for the generalization of contrastive SSL.

### 3.1 Upper Bound of $R_\varepsilon$

In this part, we will upper bound the term $R_\varepsilon$ in the error rate (1) via $\mathbb{E}_x \mathbb{E}_{z_1,z_2 \in A(x)} \|f(x_1) - f(x_2)\|^2$, which is the alignment objective of contrastive algorithms.

We separate the augmentation set $A$ as discrete transformations $\{A_\gamma(\cdot): \gamma \in [m]\}$ and continuous transformations $\{A_\theta(\cdot): \theta \in [0,1]^n\}$. For example, random crop or flip can be categorized into the discrete transformation, while the others like random color distortion or Gaussian blur can be regarded as the continuous transformation parameterized by the augmentation strength $\theta$. Without loss of generality, we assume that for any given $x$, its augmented data are uniformly random sampled, i.e., $\mathbb{P}[x' = A_\gamma(x)] = \frac{1}{m}$ and $\mathbb{P}[x' \in \{A_\theta(x): \theta \in \Theta\}] = \frac{\text{vol}(\Theta)}{2}$ for any $\Theta \subseteq [0,1]^n$, where $\text{vol}(\Theta)$ denotes the volume of $\Theta$. For the continuous transformation, we further assume that the transformation is $M$-Lipschitz continuous w.r.t. $\theta$, i.e., $\|A_{\theta_1}(x) - A_{\theta_2}(x)\| \leq M\|\theta_1 - \theta_2\|$ for any $x, \theta_1, \theta_2$. Based on the above setting, we have the following guarantee of $R_\varepsilon$.

**Theorem 2.** If encoder $f$ is $L$-Lipschitz continuous, then

$$R_\varepsilon^2 \leq \eta(\varepsilon)^2 \cdot \mathbb{E}_{x_1, x_2 \in A(x)} \|f(x_1) - f(x_2)\|^2,$$

where $\eta(\varepsilon) = \inf_{\theta \in (0,1)} \frac{\max\{1, \frac{\sigma^2}{2\sqrt{mL}}\}}{\eta(\varepsilon - \frac{\sqrt{2}}{\sqrt{mL}}) = O(\frac{1}{\varepsilon})}$.

With the above theorem, if the good alignment is satisfied, then $R_\varepsilon$ is guaranteed to be small. Thus, according to Theorem 1, a small downstream error rate (1) and a loosen divergence condition can be achieved.
4 Analysis of Contrastive Losses

The objective of contrastive algorithms can be written as

\[ \mathcal{L}(f) = \mathcal{L}_{\text{pos}}(f) + \mathcal{L}_{\text{reg}}(f). \]  

(2)

Here \( \mathcal{L}_{\text{pos}}(f) \) measures the alignment of positive samples, which takes the form of \( \mathbb{E}_{x, x' \in A(x)} \| f(x_1) - f(x_2) \|^2 \) usually. The second term \( \mathcal{L}_{\text{reg}}(f) \) is the regularizer for preventing the collapse of representation. The critical difference among algorithms lies in the choice of \( \mathcal{L}_{\text{reg}}(f) \), where an effective regularizer should make the angles between positive samples, which takes the form of

\[ \mathcal{L}(f) = \mathcal{L}_{\text{InfoNCE}}(f) + \mathcal{L}_{\text{reg}}(f). \]

4.1 InfoNCE Loss

We first study the InfoNCE loss as a warmup, which is widely used in contrastive learning:

\[ \mathcal{L}_{\text{InfoNCE}} = - \mathbb{E}_{x, x' \in A(x)} \mathbb{E}_{x'' \in A(x')} \log \frac{e^{f(x_1)^\top f(x_2)}}{e^{f(x_1)^\top f(x_2)} + e^{f(x_1)^\top f(x_-)}}. \]

Intuitively, minimizing the above objective leads to the embedding space with small discrepancy between positive samples (i.e., large \( f(x_1)^\top f(x_2) \)) and large distance between negative pairs (i.e., small \( f(x_1)^\top f(x_-) \)). We decompose the InfoNCE loss into the two parts as the form of (2):

\[ \mathcal{L}_{\text{InfoNCE}} = \mathbb{E}_{x, x' \in A(x)} \mathbb{E}_{x'' \in A(x')} \left[ -f(x_1)^\top f(x_2) + \log \left( e^{f(x_1)^\top f(x_2)} + e^{f(x_1)^\top f(x_-)} \right) \right] \]

\[ = \frac{1}{2} \mathbb{E}_{x, x' \in A(x)} \mathbb{E}_{x'' \in A(x')} \left[ \| f(x_1) - f(x_2) \|^2 - 1 \right] \]

\[ = \mathcal{L}_1(f) \]

\[ + \mathbb{E}_{x, x' \in A(x)} \mathbb{E}_{x'' \in A(x')} \left[ \log \left( e^{f(x_1)^\top f(x_2)} + e^{f(x_1)^\top f(x_-)} \right) \right], \]

\[ = \mathcal{L}_2(f), \]

where the second equality uses the normalization condition of \( \| f \| = 1 \). Regarding the constant factors, we can see that \( \mathcal{L}_1(f) \) is exactly the term \( \mathcal{L}_{\text{pos}}(f) \) introduced in (2), which imposes an upper bound to \( R_c \) by Theorem 2. Thus, the requirement of alignment is naturally full-filled. In the following theorem, we show that \( \mathcal{L}_2(f) \) is the regularizer preventing the collapse of representation.

Theorem 3. Assume that encoder \( f \) with norm 1 is \( L \)-Lipschitz continuous. If the augmented data used in SimCLR is \((\sigma, \delta)\)-augmented, then for any \( \varepsilon > 0 \) and \( k \neq \ell \),

\[ \mu_k \mu_\ell \leq \log \left( \exp \left( \frac{\mathcal{L}_2(f) + \tau(\varepsilon, \sigma, \delta)}{\mu_k \mu_\ell} \right) - \exp(1 - \varepsilon) \right), \]

where \( \tau(\varepsilon, \sigma, \delta) \) is the upper bound of the mean of intra-class variance in the embedding space, i.e., \( \mathbb{E}_{x \in C_k} \mathbb{E}_{x \in A(x)} \| f(x_1) - \mu_k \|. \)

The specific formulation of \( \tau(\varepsilon, \sigma, \delta) \) is deferred to the appendix. Here we remark that \( \tau(\varepsilon, \sigma, \delta) \) depends on both \( R_c \) and augmentation parameters \((\sigma, \delta)\). Better alignment (hence less \( R_c \)) and sharper concentration of augmented data implies smaller \( \tau(\varepsilon, \sigma, \delta) \). Therefore, with the good alignment property, the divergence \( \mu_k \mu_\ell \) is mainly controlled by \( \mathcal{L}_2(f) \). In summary, minimizing the InfoNCE loss leads to both small \( \mathcal{L}_1(f) \) and \( \mathcal{L}_2(f) \), which guarantee good alignment and divergence, respectively. Thus, according to Theorem 1 and Theorem 2, the generalization ability of encoder \( f \) on the downstream task is implied, i.e.,

\[ \text{Err}(G_f) \leq (1 - \sigma) + (\varepsilon) \sqrt{2 + 2\mathcal{L}_1(f)}, \]

when the upper bound of \( \mu_k \mu_\ell \) in Theorem 3 is smaller than the threshold in Theorem 1.

In addition, we find that the form of InfoNCE is critical to meet the requirement of divergence when proving Theorem 3. For example, if we reformulate the contrastive loss (3) in a linear form instead of LogExp such that

\[ L'(f) = \mathbb{E}_{x, x' \in A(x)} \mathbb{E}_{x'' \in A(x')} \left[ -f(x_1)^\top f(x_2) + \lambda f(x_1)^\top f(x_-) \right] \]

\[ = \mathcal{L}_1(f) + \lambda \mathcal{L}_2'(f), \]

where \( \mathcal{L}_2'(f) \) is the regularizer weighted by any \( \lambda > 0 \). Due to the independence between \( x \) and \( x' \), \( \mathcal{L}_2'(f) = \| \mathbb{E}_{x \in A(x)} f(x_1) \|^2 \). Therefore, minimizing \( \mathcal{L}_2'(f) \) only leads to the encoder \( f \) with zero mean in the embedding space. Unfortunately, the objective of zero mean with \( \| f \| = 1 \) can not obviate the dimensional collapse of the model (Hua et al., 2021). For example, the encoder \( f \) can map the input data from multi classes into two points with the opposite directions on the hypersphere. This justifies the observation of (Wang and Liu, 2021): the uniformity of encoder on the embedded hypersphere becomes worse when the temperature of the loss increases, where the loss degenerates to \( L'(f) \) with infinite temperature.

\footnote{It is also called simple contrastive loss in some literature.}
4.2 Cross-Correlation Loss

In contrast to most existing contrastive algorithms, Barlow Twins (Zhontar et al., 2021) does not directly optimize the geometry of embedding space, instead, it learns the model via decorrelating the components of representation. In this section, we deeply explore the loss of Barlow Twins, and show that such a loss can implicitly optimizes the alignment and divergence factors suggested by Theorem 1. Thus, the generalization on the downstream task is implied.

The loss of Barlow Twins can be formulated as

$$\mathcal{L}_{\text{Cross-Corr}} = \sum_{i=1}^{d} \left( 1 - \mathbb{E}_{x_1, x_2 \in A(x)} [f_i(x_1)f_i(x_2)] \right)^2$$

$$+ \lambda \sum_{i \neq j} \left( \mathbb{E}_{x_1, x_2 \in A(x)} [f_i(x_1)f_j(x_2)] \right)^2,$$

with the normalization of $\mathbb{E}_{x} \mathbb{E}_{x \in A(x)} [f_i(x_1)] = 0$ and $\mathbb{E}_{x} \mathbb{E}_{x \in A(x)} [f_i(x_1)^2] = 1$ for each $i \in [d]$, where $d$ is the output dimension of encoder $f$. Positive coefficient $\lambda$ balances the importance between diagonal and non-diagonal elements of cross-correlation matrix: when $\lambda = 1$, the above loss is exactly the difference between the cross-correlation matrix and identity matrix. Similar to Section 4.1, we first decompose the loss into two terms by defining

$$\mathcal{L}_1(f) := \sum_{i=1}^{d} \left( 1 - \mathbb{E}_{x_1, x_2 \in A(x)} [f_i(x_1)f_i(x_2)] \right)^2$$

and

$$\mathcal{L}_2(f) := \left\| \mathbb{E}_{x_1, x_2 \in A(x)} [f(x_1)f(x_2)^\top] - I_d \right\|^2.$$

In this way, the loss of Barlow Twins becomes

$$\mathcal{L}_{\text{Cross-Corr}} = (1 - \lambda) \mathcal{L}_1(f) + \lambda \mathcal{L}_2(f).$$

We first show that $\mathcal{L}_1(f)$ controls the alignment factor.

Lemma 4.1. For a given encoder $f$, the alignment $\mathcal{L}_{\text{pos}}(f)$ in (2) is upper bounded via $\mathcal{L}_1(f)$, such that

$$\mathcal{L}_{\text{pos}}(f) = \mathbb{E}_{x_1, x_2 \in A(x)} \|f(x_1) - f(x_2)\|^2 \leq 2\sqrt{d\mathcal{L}_1(f)},$$

where $d$ is the output dimension of encoder $f$.

The above lemma connects $\mathcal{L}_{\text{pos}}(f)$ with $\mathcal{L}_1(f)$, indicating that the diagonal elements of the cross-correlation matrix determine the alignment of positive samples.

Next, we connect the divergence $\mu_k^\top \mu_{k'}$ with the second loss term $\mathcal{L}_2(f)$, which is challenging since $\mathcal{L}_2(f)$ is originally proposed for reducing the redundancy between encoder’s output units. When a good alignment is satisfied, one can expect that $f(x_1) \approx f(x_2)$ for any $x_1, x_2 \in A(x)$ for any $x$. Thus, $\mathcal{L}_2(f)$ approximately equals to $\| \mathbb{E}_{x} \mathbb{E}_{x \in A(x)} [f(x_1)f(x_1)^\top] - I_d \|^2$ by replacing $f(x_2)$ with $f(x_1)$. On the other hand, we prove in the appendix that most samples are close to its class center, i.e., smallest $\mathbb{E}_{x \in Cl_i} \mathbb{E}_{x \in A(x)} [f(x_1)f(x_1)^\top] - I_d$. Thus, we can further approximate $\mathbb{E}_{x} \mathbb{E}_{x \in A(x)} [f(x_1)f(x_1)^\top]$ by the weighted class center $\sum_{k=1}^{K} p_k \mu_k \mu_k^\top$. Thus, we conclude that the second term of loss $\mathcal{L}_2(f)$ approximately captures the difference between $\sum_{k=1}^{K} p_k \mu_k \mu_k^\top$ and the identity matrix:

$$\mathbb{E} [f(x_1)f(x_2)^\top] \approx \mathbb{E} [f(x_1)f(x_1)^\top] \approx \sum_{k=1}^{K} p_k \mu_k \mu_k^\top$$

$$\Rightarrow \mathcal{L}_2(f) \approx \left\| \sum_{k=1}^{K} p_k \mu_k \mu_k^\top - I_d \right\|^2.$$

Notice that the form of $\mu_k \mu_k^\top$ is only one step away from our goal $\mu_{k'} \mu_{k'}^\top$. If they can be connected to each other, the relation between $\mathcal{L}_2(f)$ and the divergence is built up.

In fact, this can be done as follows:

$$\left\| \sum_{k=1}^{K} p_k \mu_k \mu_k^\top - I_d \right\|^2$$

$$= \text{Tr} \left( UU^\top UU^\top - 2UU^\top + I_d \right)$$

$$= \text{Tr} \left[ (U^\top U - I) (I) \right] + d - K \quad (4)$$

$$= \|U^\top U - I_k\|^2 + d - K$$

$$= \sum_{k=1}^{K} \sum_{l=1}^{K} (\sqrt{p_l} \mu_l \mu_k^\top - \delta_{lk})^2 + d - K$$

$$\geq \sum_{k=1}^{K} (\sqrt{p_k} \mu_k^\top \mu_k - \delta_{kk})^2 + d - K.$$

where $U = (\sqrt{p_1} \mu_1, \ldots, \sqrt{p_K} \mu_K)$ is in $\mathbb{R}^{d \times K}$ and $\delta_{kk}$ is the Kronecker delta. We remark that (4) is the critical step to connect $\mu_k \mu_k^\top$ and $\mu_{k'} \mu_{k'}^\top$ due to the cyclic property of trace operator. The appearance of constant term $d - K$ is due to the rank mismatch between $\sum_{k=1}^{K} p_k \mu_k \mu_k^\top$ and $I_d$.

We summarize the above idea into the following theorem.

Theorem 4. Assume that encoder $f$ with norm $\sqrt{d}$ is $L$-Lipschitz continuous. If the augmented data used in Barlow Twins is $(\sigma, \delta)$-augmented, then for any $k \neq l$, we have

$$\mu_k^\top \mu_l \leq \sqrt{\frac{2}{p_k p_l} \left( \mathcal{L}_2(f) + \tau'(\epsilon, \sigma, \delta) - \frac{d - K}{2} \right)},$$

where the term $\tau'(\epsilon, \sigma, \delta)$ is the upper bound of

$$\| \mathbb{E}_{x} \mathbb{E}_{x_1, x_2 \in A(x)} [f(x_1)f(x_2)^\top] - \sum_{k=1}^{K} p_k \mu_k \mu_k^\top \|^2.$$
The specific formulation of $\tau'(\varepsilon, \sigma, \delta)$ is deferred to the appendix. Here we remark that $\tau'(\varepsilon, \sigma, \delta)$ depends on both $R_e$ and augmentation parameters $(\sigma, \delta)$. Better alignment (hence the less $R_e$) and sharper concentration of augmented data implies smaller $\tau'(\varepsilon, \sigma, \delta)$. Therefore, with the good alignment property, the divergence $\mu_k \mu_t$ is mainly controlled by $\mathcal{L}_2(f)$.

In summary, decorrelating the components of representation leads to the small $\mathcal{L}_1(f)$ as well as the $\mathcal{L}_2(f)$. With Lemma 4.1 and Theorem 4, we can conclude that the good alignment and divergence are guaranteed. Thus, according to Theorem 1 and Theorem 2, the generalization ability of $f$ on the downstream task is implied, i.e.,

$$\text{Err}(G_f) \leq (1 - \sigma) + \sqrt{2} \eta(\varepsilon) d^2 \mathcal{L}_1(f)^{\frac{1}{2}},$$

when the upper bound of $\mu_k^T \mu_t$ in Theorem 4 is smaller than the threshold in Theorem 1.

5 Experiments

The most critical argument we made in this paper is that data augmentation is crucial to the generalization of contrastive SSL, i.e., sharper concentration of augmented data in terms of the proposed augmented distance implies better generalization. In this section, we verify this theoretical finding through a variety of experiments.

Setup. Our experiments are conducted on CIFAR-10 (Krizhevsky, 2009), which is a colorful image dataset with 50000 training samples and 10000 test samples from 10 categories. We consider 5 kinds of data augmentations applied on CIFAR-10: (a) random cropping; (b) random Gaussian blur; (c) color dropping (i.e., randomly converting images to grayscale); (d) color distortion; (e) random horizontal flipping. We use ResNet-18 (He et al., 2016) as the encoder. The contrastive algorithms we used are SimCLR and Barlow Twins. Following their original settings, we use a 2-layer MLP as the projection head for SimCLR and a 3-layer MLP for Barlow Twins. To evaluate the quality of the learned encoder, we follow the KNN evaluation protocol: we compute the cosine similarities in the embedding space between the test image and its top-$k$ nearest neighbors, and make the prediction via weighted voting (Wu et al., 2018).

Different Concentration Levels. To construct augmented data with different levels of concentration, we conduct two groups of experiments. For the first, we compose all of 5 kinds of data augmentations together, and successively drop one of the composed operations from (e) to (b) to conduct a total of 5 experiments.

### Table 1: Performance of SimCLR and Barlow Twins trained with different combinations of operations on CIFAR-10.

| Augmentations | SimCLR | Barlow Twins |
|---------------|--------|--------------|
| (a) (b) (c) (d) (e) | 89.92 ± 0.05 | 83.93 ± 0.57 |
| ✓ ✓ ✓ ✓ ✓ | ✓ ✓ ✓ ✓ ✓ | ✓ ✓ ✓ ✓ ✓ |
| ✓ ✓ ✓ ✓ × | 88.41 ± 0.11 | 83.37 ± 0.43 |
| ✓ ✓ ✓ × × | 83.62 ± 0.19 | 73.70 ± 0.99 |
| ✓ × × × × | 62.91 ± 0.25 | 49.56 ± 0.11 |
| × × × × × | 62.37 ± 0.09 | 48.54 ± 0.29 |

Accordingly, the concentration of augmented data goes from sharp to flat. For the second group, we only keep random cropping (a) and color distortion (d) but set the color distortion strength varies in $\{\frac{1}{8}, \frac{1}{4}, \frac{1}{2}, 1\}$. Clearly, color distortion with stronger strength exhibits sharper concentration. We train the model 3 runs with batch size of 512 and 800 epochs for each run, and observe their mean accuracy and deviation.

Correlation between $\text{Err}(G_f)$ and $(\sigma, \delta)$. To investigate the relation between the downstream performance and our proposed $(\sigma, \delta)$-augmentation, we apply the 5 operations in pairs to conduct a total of 10 experiments. We observe the correlation between $\text{Err}(G_f)$ and $(1 - \sigma)$ for different $\delta$, suggested by Theorem 1. Each model is trained by SimCLR with batch size of 512 and 200 epochs.

### Table 2: Performance of SimCLR and Barlow Twins trained with different color distortion strengths on CIFAR-10.

| Color Distortion Strength | SimCLR | Barlow Twins |
|---------------------------|--------|--------------|
| 1/8                       | 73.60 ± 0.11 | 61.13 ± 2.81 |
| 1/4                       | 76.25 ± 0.16 | 68.30 ± 0.15 |
| 1/2                       | 78.49 ± 0.09 | 72.76 ± 1.50 |
| 1                         | 82.64 ± 0.57 | 78.79 ± 0.54 |

Main Results. Both Table 1 and 2 show that the generalization ability of contrastive learned model is
significantly influenced by the concentration level of augmented data, under different algorithms. In particular, from the bottom to top in Table 1, the downstream performance monotonously increases with the number of operations. This verifies our theoretical inference that more operations lead to a sharper concentration and thus better generalization, which does not depend on the choice of algorithm. We also observe that color dropping (c) and distortion (d) have a great impact on the performance of both algorithms. This is because color dropping and distortion enable the augmented data to vary in a very wide range, which makes the proposed augmented distance between samples largely decrease. Thus, the augmented data become more concentrated (smaller \( \delta \)) and the generalization gets better. As an intuitive example, if the right dog image in Figure 1 is replaced by a Husky image, then only with cropping, we will get two dog heads with similar shapes but different colors, which still have a large augmented distance. Instead, if color dropping/distortion is further applied, they will be similar both in shape and color. Therefore, \( \delta \) will get smaller and the performance will be better. In fact, given cropping and color distortion as the operations, we indeed observe in Table 2 that the downstream performance increases with stronger color distortions. These verify our argument that sharper concentration of augmented data implies better generalization.

More precisely, Figure 3 shows the relation between KNN error \( \text{Err}(G_f) \) and \((\sigma, \delta)\)-augmentation under different operation pairs. We observe that \( \text{Err}(G_f) \) is highly correlated to the value of \((1 - \sigma)\) when \( \delta \) is fixed, which matches (1) of Theorem 1. For example, if we fix one operation as random cropping \((a)\), both \( \text{Err}(G_f) \) and \((1 - \sigma)\) have the same order that \((a,d) < (a,c) < (a,e) < (a,b)\). Furthermore, both of them indicate that the combination of \((a)\) and \((d)\) is the most effective pair. In addition, we observe that the choice of \( \delta \) is not sensitive to the variation tendency of \((1 - \sigma)\) but affects their absolute values. This matches our Theorem 1 that, when the divergence condition is satisfied, a larger \( \delta \) implies a larger \( \sigma \), leading to a tighter upper bound of (1).

6 Future Work

In this paper, we theoretically study the generalization guarantees of contrastive SSL. One future work can be relaxing the assumption that \( \cap_{k=1}^K A(C_k) = \emptyset \), corresponding to the situation that the data augmentation is too strong. Another possible direction is to refine the solution by taking the sample size into account, to justify the phenomenon that batch size is sensitive to the performance of SimCLR but not sensitive for Barlow Twins. A more challenging direction can be studying the out-of-distribution generalization of contrastive SSL based on our framework, where the upstream data and downstream data have different distributions.

References

Sanjeev Arora, Hrishikesh Khandepurkar, Mikhail Khodak, Orestis Plevrakis, and Nikunj Saunshi. A theoretical analysis of contrastive unsupervised representation learning. arXiv preprint arXiv:1902.09229, 2019.

Philip Bachman, R Devon Hjelm, and William Buchwalter. Learning representations by maximizing mutual information across views. In Advances in Neural Information Processing Systems, pages 15535–15545, 2019.

Adrien Bardes, Jean Ponce, and Yann LeCun. Vicreg: Variance-invariance-covariance regularization for self-supervised learning. arXiv preprint arXiv:2105.04906, 2021.

Ting Chen, Simon Kornblith, Mohammad Norouzi, and Geoffrey Hinton. A simple framework for contrastive learning of visual representations. arXiv preprint arXiv:2002.05709, 2020a.

Ting Chen, Simon Kornblith, Kevin Swersky, Mohammad Norouzi, and Geoffrey Hinton. Big self-supervised models are strong semi-supervised learners. arXiv preprint arXiv:2006.10029, 2020b.

Xinlei Chen and Kaiming He. Exploring simple siamese representation learning. In Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition, pages 15750–15758, 2021.

Xinlei Chen, Haoqi Fan, Ross Girshick, and Kaiming He. Improved baselines with momentum contrastive learning. arXiv preprint arXiv:2003.04297, 2020c.

Jeff Donahue and Karen Simonyan. Large scale adversarial representation learning. In Advances in Neural Information Processing Systems, pages 7543–7553, 2019.
Towards the Generalization of Contrastive Self-Supervised Learning

Jeff Donahue, Philipp Krähenbühl, and Trevor Darrell. Adversarial feature learning. In *International Conference on Learning Representations (ICLR)*, 2017.

Vincent Dumoulin, Ishmael Belghazi, Ben Poole, Olivier Mastropietro, Alex Lamb, Martin Arjovsky, and Aaron Courville. Adversarially learned inference. In *International Conference on Learning Representations (ICLR)*, 2017.

Hongchao Fang, Sicheng Wang, Meng Zhou, Jiayuan Ding, and Pengtao Xie. Cert: Contrastive self-supervised learning for language understanding. *arXiv preprint arXiv:2005.12766*, 2020.

Tianyu Gao, Xingcheng Yao, and Danqi Chen. Simese: Simple contrastive learning of sentence embeddings. *arXiv preprint arXiv:2104.08821*, 2021.

Spyros Gidaris, Praveer Singh, and Nikos Komodakis. Unsupervised representation learning by predicting image rotations. *arXiv preprint arXiv:1803.07728*, 2018.

John M Giorgi, Osvald Nitski, Gary D Bader, and Bo Wang. Declutr: Deep contrastive learning for unsupervised textual representations. *arXiv preprint arXiv:2006.03659*, 2020.

Jean-Bastien Grill, Florian Strub, Florent Altché, Corentin Tallec, Pierre H Richemond, Elena Buchatskaya, Carl Doersch, Bernardo Avila Pires, Zhaohan Daniel Guo, Mohammad Gheshlaghi Azar, et al. Bootstrap your own latent: A new approach to self-supervised learning. *arXiv preprint arXiv:2006.07733*, 2020.

Kaiming He, Xiangyu Zhang, Shaoqing Ren, and Jian Sun. Deep residual learning for image recognition. In *Proceedings of the IEEE conference on computer vision and pattern recognition*, pages 770–778, 2016.

Kaiming He, Haoqi Fan, Yuxin Wu, Saining Xie, and Ross Girshick. Momentum contrast for unsupervised visual representation learning. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pages 9729–9738, 2020.

R Devon Hjelm, Alex Fedorov, Samuel Lavoie-Marchildon, Karan Grewal, Phil Bachman, Adam Trischler, and Yoshua Bengio. Learning deep representations by mutual information estimation and maximization. *arXiv preprint arXiv:1808.06670*, 2018.

Qianjiang Hu, Xiao Wang, Wei Hu, and Guo-Jun Qi. Adco: Adversarial contrast for efficient learning of unsupervised representations from self-trained negative adversaries. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pages 1074–1083, 2021.

Tianyu Hua, Wenhao Wang, Zihui Xue, Sucheng Ren, Yue Wang, and Hang Zhao. On feature decorrelation in self-supervised learning. In *Proceedings of the IEEE/CVF International Conference on Computer Vision*, pages 9598–9608, 2021.

Alex Krizhevsky. Learning multiple layers of features from tiny images. *University of Toronto*, 2009.

Jason D Lee, Qi Lei, Nikunj Saunshi, and Jiacheng Zhuo. Predicting what you already know helps: Provable self-supervised learning. *arXiv preprint arXiv:2008.01064*, 2020.

Mehdi Noroozi and Paolo Favaro. Unsupervised learning of visual representations by solving jigsaw puzzles. In *European Conference on Computer Vision*, pages 69–84. Springer, 2016.

Aaron van den Oord, Yazhe Li, and Oriol Vinyals. Representation learning with contrastive predictive coding. *arXiv preprint arXiv:1807.03748*, 2018.

Christos H Papadimitriou and Kenneth Steiglitz. *Combinatorial optimization: algorithms and complexity*. Courier Corporation, 1998.

Deepak Pathak, Philipp Krahenbühl, Jeff Donahue, Trevor Darrell, and Alexei A Efros. Context encoders: Feature learning by inpainting. In *Proceedings of the IEEE conference on computer vision and pattern recognition*, pages 2536–2544, 2016.

Jiaye Teng and Weiran Huang. Can pretext-based self-supervised learning be boosted by downstream data? A theoretical analysis. *arXiv preprint arXiv:2103.03568*, 2021.

Yonglong Tian, Dilip Krishnan, and Phillip Isola. Contrastive multiview coding. *arXiv preprint arXiv:1906.05849*, 2019.

Yonglong Tian, Chen Sun, Ben Poole, Dilip Krishnan, Cordelia Schmid, and Phillip Isola. What makes for good views for contrastive learning? *arXiv preprint arXiv:2005.10243*, 2020.

Michael Tschannen, Josip Djolonga, Paul K Rubenstein, Sylvain Gelly, and Mario Lucic. On mutual information maximization for representation learning. *arXiv preprint arXiv:1907.13625*, 2019.

Feng Wang and Huaping Liu. Understanding the behaviour of contrastive loss. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pages 2495–2504, 2021.

Tongzhou Wang and Phillip Isola. Understanding contrastive representation learning through alignment and uniformity on the hypersphere. In *International Conference on Machine Learning*, pages 9929–9939. PMLR, 2020.

Colin Wei, Kendrick Shen, Ying Sun, and Tengyu Ma. Theoretical analysis of self-training with
Towards the Generalization of Contrastive Self-Supervised Learning

deep networks on unlabeled data. *arXiv preprint arXiv:2010.03622*, 2020.

Zixin Wen and Yuanzhi Li. Toward understanding the feature learning process of self-supervised contrastive learning. *arXiv preprint arXiv:2105.15134*, 2021.

Zhirong Wu, Yuanjun Xiong, Stella X Yu, and Dahua Lin. Unsupervised feature learning via non-parametric instance discrimination. In *Proceedings of the IEEE conference on computer vision and pattern recognition*, pages 3733–3742, 2018.

Zhuofeng Wu, Sinong Wang, Jiatao Gu, Madian Khabba, Fei Sun, and Hao Ma. Clear: Contrastive learning for sentence representation. *arXiv preprint arXiv:2012.15466*, 2020.

Yuanmeng Yan, Rumei Li, Sirui Wang, Fuzheng Zhang, Wei Wu, and Weiran Xu. Consert: A contrastive framework for self-supervised sentence representation transfer. *arXiv preprint arXiv:2105.11741*, 2021.

Jure Zbontar, Li Jing, Ishan Misra, Yann LeCun, and Stéphane Deny. Barlow twins: Self-supervised learning via redundancy reduction. *arXiv preprint arXiv:2103.03230*, 2021.

Richard Zhang, Phillip Isola, and Alexei A Efros. Colorful image colorization. In *European conference on computer vision*, pages 649–666. Springer, 2016.
Appendix

We list all the proofs of lemmas and theorems in the appendix, which are organized by sections.

A Proofs for Section 3

Lemma 3.1. For a $(\sigma, \delta)$-augmentation with main part $C^0_k$ of each class $C_k$, if all samples belonging to $(C^0_1 \cup \cdots \cup C^0_K) \cap S_{\varepsilon}$ can be correctly classified by a classifier $G$, then its downstream error rate $\text{Err}(G) \leq (1 - \sigma) + R_{\varepsilon}$.

Proof. Since every sample $x \in (C^0_1 \cup \cdots \cup C^0_K) \cap S_{\varepsilon}$ can be correctly classified by $G$, then the error rate

$$\text{Err}(G) = \sum_{k=1}^{K} \mathbb{P}[G(x) \neq k, \forall x \in C_k]$$

$$\leq \mathbb{P}[ (C^0_1 \cup \cdots \cup C^0_K) \cap S_{\varepsilon} ]$$

$$= \mathbb{P}[ C^0_1 \cup \cdots \cup C^0_K \cup S_{\varepsilon} ]$$

$$\leq (1 - \sigma) + \mathbb{P} [ \tilde{S}_{\varepsilon} ]$$

$$= (1 - \sigma) + R_{\varepsilon}.$$

This finishes the proof. \ 

Lemma 3.2. For a $(\sigma, \delta)$-augmentation and each $\ell \in [K]$, if $\mu_k^T \mu_k < r^2 \left( 1 - \rho_\ell(\sigma, \delta, \varepsilon) - \sqrt{2\rho_\ell(\sigma, \delta, \varepsilon) - \frac{\Delta_2}{2}} \right)$ holds for all $k \neq \ell$, then every sample $x \in C^0_1 \cap S_{\varepsilon}$ can be correctly classified by the NN classifier $G_f$, where $\rho_\ell(\sigma, \delta, \varepsilon) = 2(1 - \sigma) + \frac{R_{\varepsilon}}{\rho_1} + \sigma \left( \frac{\Delta_1}{2} + \frac{\Delta_2}{4} \right)$ and $\Delta_2 = 1 - \min_{k \in [K]} \|\mu_k\|^2 / r^2$.

Proof. Without loss of generality, we consider $\ell = 1$. To show that every sample $x_0 \in C^0_1 \cap S_{\varepsilon}$ can be correctly classified by $G_f$, we need to prove that for all $k \neq 1$, $\|f(x_0) - \mu_1\| < \|f(x_0) - \mu_k\|$. It is equivalent to prove

$$f(x_0)^T \mu_1 - f(x_0)^T \mu_k - \left( \frac{1}{2} \|\mu_1\|^2 - \frac{1}{2} \|\mu_k\|^2 \right) > 0. \quad (5)$$

Let $\hat{f}(x) := \mathbb{E}_{x' \in A(x)}[f(x')]$. Then $\|\hat{f}(x)\| = \|\mathbb{E}_{x' \in A(x)}[f(x')]\| \leq \mathbb{E}_{x' \in A(x)}[\|f(x')\|] = r$.

On the one hand,

$$f(x_0)^T \mu_1 = \frac{1}{p_1} f(x_0)^T \mathbb{E}_x [\hat{f}(x)](x \in C_1)$$

$$= \frac{1}{p_1} f(x_0)^T \mathbb{E}_x [\hat{f}(x)] (x \in C_1 \cap C^0_1 \cap S_{\varepsilon}) + \frac{1}{p_1} f(x_0)^T \mathbb{E}_x [\hat{f}(x)](x \in C_1 \cap C^0_1 \cap S_{\varepsilon})$$

$$= \frac{p_1}{p_1} f(x_0)^T \mathbb{E}_x [\hat{f}(x)](x \in C_1 \cap C^0_1 \cap S_{\varepsilon}) + \frac{1}{p_1} \mathbb{E}_x [\hat{f}(x)](x \in C_1 \cap C^0_1 \cap S_{\varepsilon})$$

$$\geq \frac{p_1}{p_1} f(x_0)^T \mathbb{E}_x [\hat{f}(x)](x \in C_1 \cap S_{\varepsilon}) \frac{1}{p_1} = \mathbb{P} [C_1 \mid C^0_1 \cap S_{\varepsilon}], \quad (6)$$

where $\mathbb{I}(\cdot)$ is the indicator function. Note that

$$\mathbb{P}[C_1 \mid C^0_1 \cap S_{\varepsilon}] = \mathbb{P}[(C_1 \setminus C^0_1) \cup (C^0_1 \cap S_{\varepsilon})] \leq (1 - \sigma)p_1 + R_{\varepsilon}, \quad (7)$$

and

$$\mathbb{P}[C^0_1 \cap S_{\varepsilon}] = \mathbb{P}[C_1] - \mathbb{P}[C_1 \setminus C^0_1 \cap S_{\varepsilon}] \geq p_1 - ((1 - \sigma)p_1 + R_{\varepsilon}) = \sigma p_1 - R_{\varepsilon}. \quad (8)$$
Towards the Generalization of Contrastive Self-Supervised Learning

Plugging to Eq (6), we have

\[
    f(x_0)^\top \mu_1 \geq \frac{\mathbb{E}[C_1^0 \cap S_2]}{p_1} f(x_0)^\top \frac{\mathbb{E}}{x \in C_1^0 \cap S_r} [\tilde{f}(x)] - \frac{r^2}{p_1} \mathbb{E}[C_1 \setminus C_1^0 \cap S_r]
    \geq \left( \sigma - \frac{R_c}{p_1} \right) f(x_0)^\top \frac{\mathbb{E}}{x \in C_1^0 \cap S_r} [\tilde{f}(x)] - r^2 \left( 1 - \sigma + \frac{R_c}{p_1} \right).
\]

(9)

Notice that \( x_0 \in C_1^0 \cap S_r \). For any \( x \in C_1^0 \cap S_r \), we have \( d_A(x_0, x) \leq \delta \). Let \( (x_0^*, x^*) = \arg \min_{x_0^*, x^* \in A(x_0), x^* \in A(x)} \| x_0^* - x^* \| \). We have \( \| x_0^* - x^* \| \leq \delta \). Since \( f \) is \( L \)-Lipschitz continuous, we have \( \| f(x_0^*) - f(x^*) \| \leq L \cdot \| x_0^* - x^* \| \leq L \delta \). Since \( x \in S_r \), for any \( x^* \in A(x) \), \( \| f(x^*) - f(x^*) \| \leq \varepsilon \). Similarly, since \( x_0 \in S_r \) and \( x_0, x_0^* \in A(x_0) \), we have \( \| f(x_0) - f(x_0^*) \| \leq \varepsilon \).

The first term of Eq (9) can be bounded by

\[
    f(x_0)^\top \frac{\mathbb{E}}{x \in C_1^0 \cap S_r} [\tilde{f}(x)] = \frac{\mathbb{E}}{x \in C_1^0 \cap S_r, x^* \in A(x)} [f(x_0)^\top f(x^*)]
    \geq \frac{\mathbb{E}}{x \in C_1^0 \cap S_r, x^* \in A(x)} [f(x_0)^\top (f(x^*) - f(x_0) + f(x_0))]
    = r^2 + \frac{\mathbb{E}}{x \in C_1^0 \cap S_r, x^* \in A(x)} [f(x_0)^\top (f(x^*) - f(x_0))]
    \geq r^2 - \| \tilde{f} \| \leq \varepsilon
    = r^2 - r(L \delta + 2 \varepsilon).
\]

Therefore, Eq (9) turns to

\[
    f(x_0)^\top \mu_1 \geq \left( \sigma - \frac{R_c}{p_1} \right) f(x_0)^\top \frac{\mathbb{E}}{x \in C_1^0 \cap S_r} [\tilde{f}(x)] - r^2 \left( 1 - \sigma + \frac{R_c}{p_1} \right)
    \geq \left( \sigma - \frac{R_c}{p_1} \right) \left( r^2 - r(L \delta + 2 \varepsilon) \right) - r^2 \left( 1 - \sigma + \frac{R_c}{p_1} \right)
    = r^2 \left( 2 \sigma - 1 - \frac{R_c}{p_1} - \left( \sigma - \frac{R_c}{p_1} \right) \left( \frac{L \delta}{r} + \frac{2 \varepsilon}{r} \right) \right)
    = r^2 \left( 2(1 - \sigma - \frac{R_c}{p_1}) - \left( \sigma - \frac{R_c}{p_1} \right) \left( \frac{L \delta}{r} + \frac{2 \varepsilon}{r} \right) \right)
    = r^2 \left( 1 - 2(1 - \sigma) - \frac{R_c}{p_1} \left( \sigma - \frac{R_c}{p_1} \right) \left( \frac{L \delta}{r} + \frac{2 \varepsilon}{r} \right) \right)
    = r^2(1 - \rho_1(\sigma, \delta, \varepsilon)).
\]

(10)

On the other hand,

\[
    f(x_0)^\top \mu_k = (f(x_0) - \mu_1)^\top \mu_k + \mu_1^\top \mu_k
    \leq \| f(x_0) - \mu_1 \| \cdot \| \mu_k \| + \mu_1^\top \mu_k
    \leq r \sqrt{\| f(x_0) \|^2 - 2 f(x_0)^\top \mu_1 + \| \mu_1 \|^2} + \mu_1^\top \mu_k
    \leq r \sqrt{2r^2 - 2 f(x_0)^\top \mu_1 + \mu_1^\top \mu_k}
    \leq \sqrt{2 \rho_1(\sigma, \delta, \varepsilon) r^2} + \mu_1^\top \mu_k.
\]

(11)

Note that \( \Delta_\mu = 1 - \min_k \| \mu_k \|^2 / r^2 \), the LHS of Eq (5) is

\[
    f(x_0)^\top \mu_1 - f(x_0)^\top \mu_k - \frac{1}{2} \| \mu_1 \|^2 - \frac{1}{2} \| \mu_k \|^2 \geq f(x_0)^\top \mu_1 - f(x_0)^\top \mu_k - \frac{1}{2} \Delta_\mu
    \geq r^2(1 - \rho_1(\sigma, \delta, \varepsilon)) - \sqrt{2 \rho_1(\sigma, \delta, \varepsilon) r^2} - \mu_1^\top \mu_k - \frac{1}{2} \Delta_{\mu}.
\]
Towards the Generalization of Contrastive Self-Supervised Learning

\[ r^2 \left( 1 - \rho_1(\sigma, \delta, \varepsilon) - \sqrt{2\rho_1(\sigma, \delta, \varepsilon)} - \frac{1}{2} \Delta_\mu \right) - \mu_1^T \mu_k > 0, \]

where the second inequality is due to (10) and (11). This finishes the proof. \(\square\)

**Theorem 1.** For a \((\sigma, \delta)\)-augmentation used in SSL, if

\[ \mu_1^T \mu_k < r^2 \left( 1 - \rho_{\text{max}}(\sigma, \delta, \varepsilon) - \sqrt{2\rho_{\text{max}}(\sigma, \delta, \varepsilon)} - \frac{\Delta_\mu}{2} \right) \]

holds for any pair of \((\ell, k)\) with \(\ell \neq k\), then the downstream error rate of NN classifier \(G_f\)

\[ \text{Err}(G_f) \leq (1 - \sigma) + R_\varepsilon, \quad (1) \]

where \(\rho_{\text{max}}(\sigma, \delta, \varepsilon) = 2(1 - \sigma) + \frac{R_\varepsilon}{\min \rho_\varepsilon} + \sigma \left( \frac{L_\varepsilon^2}{\varepsilon} + \frac{2\varepsilon}{\min \rho_\varepsilon} \right) \) and \(\Delta_\mu = 1 - \min_{k \in [K]} \| \mu_k \|^2 / r^2\).

**Proof.** Since the augmentation \(A\) is \((\sigma, \delta)\)-augmented, there exists a main part \(C_k^0\) for each class \(C_k\) such that \(P[C_k^0] \geq \sigma p_k\) and \(\sup_{x_1, x_2 \in C_k^0} d_A(x_1, x_2) \leq \delta\). Since for any \(\ell \neq k\), we have

\[ \mu_1^T \mu_k < r^2 \left( 1 - \rho_{\text{max}}(\sigma, \delta, \varepsilon) - \sqrt{2\rho_{\text{max}}(\sigma, \delta, \varepsilon)} - \frac{\Delta_\mu}{2} \right) \leq r^2 \left( 1 - \rho_{\ell}(\sigma, \delta, \varepsilon) - \sqrt{2\rho_{\ell}(\sigma, \delta, \varepsilon)} - \frac{\Delta_\mu}{2} \right) \]

According to Lemma 3.2, every sample \(x \in C_k^0 \cap S_k\) can be correctly classified by \(G_f\). Therefore, every sample \(x \in (C_1^0 \cap \cdots \cap C_K^0) \cap S_k\) can be correctly classified by \(G_f\). According to Lemma 3.1, the error rate \(\text{Err}(G_f) \leq 1 - \sigma + R_\varepsilon\). \(\square\)

**Theorem 2.** If encoder \(f\) is \(L\)-Lipschitz continuous, then

\[ R_\varepsilon^2 \leq \eta(\varepsilon)^2 \cdot \mathbb{E}_{x_1, x_2 \in A(x)} \| f(x_1) - f(x_2) \|^2, \]

where \(\eta(\varepsilon) = \inf_{h \in (0, \frac{x}{2\sqrt{n}L\sigma^2})} \frac{4\max\{1, m^2h^{2n}\}}{h^{2n}(\varepsilon - 2\sqrt{n}LM\varepsilon)} = O\left( \frac{1}{\varepsilon} \right) \).

**Proof.** The parameter space \([0, 1]^n\) of \(\Theta\) can be separated to cubes \(\Theta_1, \ldots, \Theta_{m'}\) where \(m' = 1/h^n\) and each cube’s edge length is \(h \in (0, \frac{x}{2\sqrt{n}L\sigma^2})\). Then for any given \(x\), we have

\[
\begin{aligned}
\mathbb{E}_{x_1, x_2 \in A(x)} \| f(x_1) - f(x_2) \| &= \frac{1}{4m^2} \sum_{\gamma=1}^{m} \sum_{\beta=1}^{m} \| f(A_\gamma(x)) - f(A_\beta(x)) \| \\
&+ \frac{1}{2mn} \sum_{\gamma=1}^{m} \sum_{j=1}^{m'} \int_{\Theta_j} \frac{1}{h^n} \| f(A_\gamma(x)) - f(A_\theta(x)) \| d\theta \\
&+ \frac{1}{4m^2} \sum_{i=1}^{m} \sum_{j=1}^{m'} \int_{\Theta_i} \int_{\Theta_j} \frac{1}{h^{2n}} \| f(A_\gamma(x)) - f(A_\theta(x)) \| d\theta_2 d\theta_1 .
\end{aligned}
\]

By Cauchy-Schwarz inequality,

\[ \forall \theta, \| f(A_\gamma(x)) - f(A_\theta(x)) \| \leq \| f(A_\gamma(x)) - f(A_\theta(x)) \| + \| f(A_\theta(x)) - f(A_\gamma(x)) \|. \]

Then for any given \(\theta\),

\[
\begin{aligned}
\sup_{\theta'} \| f(A_\gamma(x)) - f(A_\theta(x)) \| &\leq \| f(A_\gamma(x)) - f(A_\theta(x)) \| + \sup_{\theta'} \| f(A_\theta(x)) - f(A_\theta(x)) \| \\
&\leq \| f(A_\gamma(x)) - f(A_\theta(x)) \| + \sup_{\theta_1, \theta_2} \| f(A_\theta_1(x)) - f(A_\theta_2(x)) \|. 
\end{aligned}
\]
Therefore, for any $\gamma \in [m], j \in [m']$, we have

$$\sup_{\theta' \in \Theta} \|f(A_{\gamma}(x)) - f(A_{\theta'}(x))\| = \int_{\Theta} \int_{\Theta} \frac{1}{2\pi} \sup_{\theta' \in \Theta} \|f(A_{\gamma}(x)) - f(A_{\theta'}(x))\| d\theta_2 d\theta_1$$

$$\leq \int_{\Theta} \int_{\Theta} \frac{1}{2\pi} \|f(A_{\gamma}(x)) - f(A_{\theta_2}(x))\| d\theta_2 d\theta_1 + \sup_{\theta_1, \theta_2 \in \Theta} \|f(A_{\theta_1}(x)) - f(A_{\theta_2}(x))\|$$

$$\leq \int_{\Theta} \int_{\Theta} \frac{1}{2\pi} \|f(A_{\gamma}(x)) - f(A_{\theta_2}(x))\| d\theta_2 d\theta_1 + \sqrt{\lambda}h$$

$$= \int_{\Theta} \int_{\Theta} \frac{1}{2\pi} \|f(A_{\gamma}(x)) - f(A_{\theta_2}(x))\| d\theta_2 d\theta_1 + \sqrt{\lambda}LMh.$$
Towards the Generalization of Contrastive Self-Supervised Learning

\[ \leq \max \left\{ \frac{4m^2 \Lambda_1}{2mm' \Lambda_2} \right\} + 2\sqrt{n}LMh \]

\[ \leq \max \{4m^2, 2mm', 4m'^2\} (\Lambda_1 + \Lambda_2 + \Lambda_3) + 2\sqrt{n}LMh \]

\[ = \max \{4m^2, 2mm', 4m'^2\} \mathbb{E}_{x_1, x_2 \in A(x)} \|f(x_1) - f(x_2)\| + 2\sqrt{n}LMh. \]

Thus, the following set \( S \) is a subset of \( S_\varepsilon \):

\[ S = \left\{ x : \mathbb{E}_{x_1, x_2 \in A(x)} \|f(x_1) - f(x_2)\| \leq \frac{\varepsilon - 2\sqrt{n}LMh}{\max \{4m^2, 2mm', 4m'^2\}} \right\} \subseteq S_\varepsilon. \]

Then by Markov’s inequality, we have

\[ R_\varepsilon = \mathbb{P} \left[ S \right] \leq \mathbb{P} \left[ S_0 \right] \leq \frac{\mathbb{E}_x \mathbb{E}_{x_1, x_2 \in A(x)} \|f(x_1) - f(x_2)\|}{\varepsilon - 2\sqrt{n}LMh} \]

\[ = \frac{\max \{4m^2, 2mm', 4m'^2\}}{h^{2n}(\varepsilon - 2\sqrt{n}LMh)} \mathbb{E}_{x_1, x_2 \in A(x)} \|f(x_1) - f(x_2)\| \]

\[ = 4 \max \{1, m^2 h^{2n}\} \mathbb{E}_{x_1, x_2 \in A(x)} \|f(x_1) - f(x_2)\|. \]

The above inequality holds for all \( h \in (0, \frac{\varepsilon}{2\sqrt{n}LM}) \), thus

\[ R_\varepsilon \leq \inf_{0 < h < \frac{\varepsilon}{2\sqrt{n}LM}} 4 \max \{1, m^2 h^{2n}\} \mathbb{E}_{x_1, x_2 \in A(x)} \|f(x_1) - f(x_2)\| = \eta(\varepsilon) \cdot \mathbb{E}_{x_1, x_2 \in A(x)} \|f(x_1) - f(x_2)\|. \]

Therefore, \( R_\varepsilon^2 \leq \eta(\varepsilon)^2 \cdot (\mathbb{E}_x \mathbb{E}_{x_1, x_2 \in A(x)} \|f(x_1) - f(x_2)\|)^2 \leq \eta(\varepsilon)^2 \cdot \mathbb{E}_x \mathbb{E}_{x_1, x_2 \in A(x)} \|f(x_1) - f(x_2)\|^2. \]

**B Proofs for Section 4**

Before providing our proofs, we give the following useful lemma, which upper bounds the first and second order moment of intra-difference within each class \( C_k \) via \( \varepsilon \) and \( R_\varepsilon \).

**Lemma B.1.** Suppose that \( \|f(x)\| = r \) for every \( x \). For each \( k \in [K], \)

\[ \mathbb{E}_{x \in C_k} \|f(x_1) - \mu_k\| \leq 2r \varepsilon + \frac{4r R_\varepsilon}{p_k} + \tau_1(\sigma, \delta), \]

and

\[ \mathbb{E}_{x \in C_k \quad x_1 \in A(x)} \|f(x_1) - \mu_k\|^2 \leq (2\varepsilon + L\delta)^2 + 4r \left( 1 - \sigma + \frac{R_\varepsilon}{p_k} \right) \left( r + 2\varepsilon + L\delta \right) + 4r^2 \left( 1 - \sigma + \frac{R_\varepsilon}{p_k} \right)^2. \]

where \( \tau_1(\sigma, \delta) := L\sigma\delta + 4r(1 - \sigma). \)

**Proof.** For each \( k \in [K], \)

\[ \mathbb{E}_{x \in C_k \quad x \in A(x)} \|f(x_1) - \mu_k\| \]

\[ = \frac{1}{p_k} \mathbb{E} \mathbb{E} [I(x \in C_k) \|f(x_1) - \mu_k\|] = \frac{1}{p_k} \mathbb{E} \mathbb{E} [I(x \in C_k') \|f(x_1) - \mu_k\|] + \frac{1}{p_k} \mathbb{E} \mathbb{E} [I(x \in C_k \setminus C_k') \|f(x_1) - \mu_k\|] \]
Towards the Generalization of Contrastive Self-Supervised Learning

\[
\begin{align*}
&\leq \frac{1}{p_k} E_{x, x_1 \in A(x)} \left[ \| (x \in C_k^0 \cap S_\varepsilon) \|f(x_1) - \mu_k\| \right] + \frac{2r P[C_k \setminus C_k^0 \cap S_\varepsilon]}{p_k} \\
&\leq \frac{1}{p_k} E_{x, x_1 \in A(x)} \left[ \| (x \in C_k^0 \cap S_\varepsilon) \|f(x_1) - \mu_k\| \right] + 2r \left( 1 - \sigma + \frac{R_\varepsilon}{p_k} \right) \quad \text{(using Eq (7))} \\
&\leq \frac{P[C_k^0 \cap S_\varepsilon]}{p_k} E_{x \in C_k^0 \cap S_\varepsilon, x_1 \in A(x)} \|f(x_1) - \mu_k\| + 2r \left( 1 - \sigma + \frac{R_\varepsilon}{p_k} \right) \\
&\leq \sigma E_{x \in C_k^0 \cap S_\varepsilon} \sup_{x_1 \in A(x)} \|f(x_1) - \mu_k\| + 2r \left( 1 - \sigma + \frac{R_\varepsilon}{p_k} \right) \quad \text{(12)}
\end{align*}
\]

where

\[
\begin{align*}
&\frac{1}{p_k} E_{x, x_1 \in A(x)} \|f(x_1) - \mu_k\| \\
&= \frac{1}{p_k} E_{x, x_2 \in A(x')} \|f(x_1) - E_{x' \in C_k \cap S_\varepsilon} f(x_2)\| \\
&= \frac{1}{p_k} E_{x, x_2 \in A(x')} \left[ \|f(x_1) - \frac{P[C_k^0 \cap S_\varepsilon]}{p_k} E_{x' \in C_k^0 \cap S_\varepsilon} E_{x_2 \in A(x')} f(x_2)\| + \frac{P[C_k \setminus C_k^0 \cap S_\varepsilon]}{p_k} \left( f(x_1) - E_{x' \in C_k \setminus C_k^0 \cap S_\varepsilon} f(x_2) \right) \right] \\
&\leq \frac{P[C_k^0 \cap S_\varepsilon]}{p_k} E_{x, x_2 \in A(x')} \|f(x_1) - \mu_k\| + \frac{P[C_k \setminus C_k^0 \cap S_\varepsilon]}{p_k} \cdot 2r \\
&\leq \sigma \sup_{x, x_1 \in C_k^0 \cap S_\varepsilon} \sup_{x_1 \in A(x)} \|f(x_1) - f(x_2)\| + 2r \left( 1 - \sigma + \frac{R_\varepsilon}{p_k} \right). \quad \text{(13)}
\end{align*}
\]

For any \(x, x' \in C_k^0 \cap S_\varepsilon\), we have \(d_A(x, x') \leq \delta\). Let \((x_1^*, x_2^*) = \arg\min_{x_1 \in A(x), x_2 \in A(x')} \|x_1 - x_2\|\). We have \(\|x_1^* - x_2^*\| \leq \delta\). Since \(f\) is \(L\)-Lipschitz continuous, we have \(\|f(x_1^*) - f(x_2^*)\| \leq L \cdot \|x_1^* - x_2^*\| \leq L \delta\). Since \(x \in S_\varepsilon\), for any \(x_1 \in A(x), \|f(x_1) - f(x_2)\| \leq \varepsilon\). Similarly, since \(x' \in S_\varepsilon\), for any \(x_2 \in A(x')\), we have \(\|f(x_2) - f(x_2^*)\| \leq \varepsilon\). Therefore, for any \(x, x' \in C_k^0 \cap S_\varepsilon\) and \(x_1 \in A(x), x_2 \in A(x')\),

\[
\|f(x_1) - f(x_2)\| \leq \|f(x_1) - f(x_1^*)\| + \|f(x_1^*) - f(x_2^*)\| + \|f(x_2^*) - f(x_2)\| \leq 2 \varepsilon + L \delta.
\]

Plugging into Eq (12) and (13), we obtain

\[
\begin{align*}
&\sigma \sup_{x, x_1 \in C_k^0 \cap S_\varepsilon} \sup_{x_1 \in A(x)} \|f(x_1) - f(x_2)\| + 2r \left( 1 - \sigma + \frac{R_\varepsilon}{p_k} \right).
\end{align*}
\]

Similar to Eq (12) and (13), we have

\[
\begin{align*}
&\frac{1}{p_k} E_{x, x_1 \in A(x)} \|f(x_1) - \mu_k\|^2 \\
&= \frac{1}{p_k} E_{x, x_2 \in A(x')} \left[ \|f(x_1) - \frac{P[C_k \setminus C_k^0 \cap S_\varepsilon]}{p_k} E_{x' \in C_k \setminus C_k^0 \cap S_\varepsilon} f(x_2)\|^2 + \frac{P[C_k \setminus C_k^0 \cap S_\varepsilon]}{p_k} \|f(x_1) - f(x_2)\|^2 \right] \\
&\leq \sigma \sup_{x, x_1 \in C_k^0 \cap S_\varepsilon} \sup_{x_1 \in A(x)} \|f(x_1) - f(x_2)\|^2 + 4r^2 \left( 1 - \sigma + \frac{R_\varepsilon}{p_k} \right).
\end{align*}
\]

and

\[
\begin{align*}
&\frac{1}{p_k} E_{x, x_1 \in A(x)} \|f(x_1) - \mu_k\|^2 \\
&= \frac{1}{p_k} E_{x, x_2 \in A(x')} \left[ \|f(x_1) - \frac{P[C_k \setminus C_k^0 \cap S_\varepsilon]}{p_k} E_{x' \in C_k \setminus C_k^0 \cap S_\varepsilon} f(x_2)\|^2 \right] \\
&= \frac{1}{p_k} E_{x, x_2 \in A(x')} \|f(x_1) - \mu_k\|^2 + 4r^2 \left( 1 - \sigma + \frac{R_\varepsilon}{p_k} \right).
\end{align*}
\]
Towards the Generalization of Contrastive Self-Supervised Learning

\[ + \frac{\mathbb{P}[C_k \setminus C_k^0 \cap S_e]}{p_k} \left( f(x_1) - \mathbb{E}_{x' \in C_k \setminus C_k^0 \cap S_e} \mathbb{E}_{x \in A(x')} f(x_2) \right) \]  
\[ \leq \mathbb{E}_{x' \in C_k^0 \cap S_e} \mathbb{E}_{x \in A(x')} \left( \sigma \left\| f(x_1) - \mathbb{E}_{x' \in C_k^0 \cap S_e} f(x_2) \right\| + 2r \left( 1 - \sigma + \frac{R_e}{p_k} \right) \right)^2 \]  
\[ \leq \left( \sigma(2\varepsilon + L\delta) + 2r \left( 1 - \sigma + \frac{R_e}{p_k} \right) \right)^2. \]

Therefore,

\[ \mathbb{E}_{x \in C_k} \mathbb{E}_{x_1 \in A(x)} \left\| f(x_1) - \mu_k \right\|^2 \leq \sigma^2(2\varepsilon + L\delta)^2 + 4r \left( 1 - \sigma + \frac{R_e}{p_k} \right) \left[ r + \sigma^2(2\varepsilon + L\delta) \right] + 4\sigma r^2 \left( 1 - \sigma + \frac{R_e}{p_k} \right)^2 \]
\[ \leq (2\varepsilon + L\delta)^2 + 4r \left( 1 - \sigma + \frac{R_e}{p_k} \right) \left[ r + 2\varepsilon + L\delta \right] + 4\sigma^2 \left( 1 - \sigma + \frac{R_e}{p_k} \right)^2. \]

This finishes the proof.

Now we are ready to give our proofs.

B.1 InfoNCE Loss

**Theorem 3.** Assume that encoder \( f \) with norm 1 is \( L \)-Lipschitz continuous. If the augmented data used in SimCLR is \((\sigma, \delta)\)-augmented, then for any \( \varepsilon > 0 \) and \( k \neq \ell \),

\[ \mu_k \mu_\ell \leq \log \left( \exp \left( \frac{\mathcal{L}_2(f) + \tau(\varepsilon, \sigma, \delta)}{p_k p_\ell} \right) - \exp(1 - \varepsilon) \right), \]

where \( \tau(\varepsilon, \sigma, \delta) \) is the upper bound of the mean of intra-class variance in the embedding space, i.e.,

\[ \mathbb{E}_{x \in C_k} \mathbb{E}_{x_1 \in A(x)} \left\| f(x_1) - \mu_k \right\|. \]

**Proof.** Given \( x \in S_e \), for any \( x_1, x_2 \in A(x) \), we have

\[ \log \left( e^{f(x_1) \top} f(x_2) + e^{f(x_1) \top} f(x^-) \right) = \log \left( e^{f(x_1) \top} f(x_2) e^{f(x_1) \top} (f(x_2) - f(x_1)) + e^{f(x_1) \top} f(x^-) \right) \]
\[ \geq \log \left( e_{\|f(x_1)\|} e^{-\|f(x_1)\| \varepsilon} e^{f(x_1) \top} f(x^-) \right) \]
\[ = \log \left( e^{1-\varepsilon} + e^{f(x_1) \top} f(x^-) \right). \]

Therefore, we have

\[ \mathcal{L}_2(f) = \mathbb{E}_{x, x' : x, x' \in A(x)} \mathbb{E}_{x^- \in A(x')} \left[ \log \left( e^{f(x_1) \top} f(x_2) + e^{f(x_1) \top} f(x^-) \right) \right] \]
\[ = \mathbb{E}_{x, x' : x, x' \in A(x)} \left[ \mathbb{I}(x \in S_e) + \mathbb{I}(x \in \bar{S}_e) \right] \log \left( e^{f(x_1) \top} f(x_2) + e^{f(x_1) \top} f(x^-) \right) \]
\[ \geq \sum_{k=1}^K \sum_{\ell=1}^K \mathbb{E}_{x, x'} \left[ \mathbb{I}(x \in S_e \cap C_k) \mathbb{I}(x' \in C_\ell) \mathbb{E}_{x_1 \in A(x)} \log \left( e^{1-\varepsilon} + e^{f(x_1) \top} \mu_\ell \right) \right] + \mathbb{E}_{x} \left[ \mathbb{I}(x \in \bar{S}_e) \log \left( e^{-1} + e^{-1} \right) \right] \]
\[ = \left( \sum_{k=1}^K \sum_{\ell=1}^K \mathbb{E}_{x, x'} \left[ \mathbb{I}(x \in C_k) \mathbb{I}(x' \in C_\ell) \log \left( e^{1-\varepsilon} + e^{f(x_1) \top} \mu_\ell \right) + \Delta_1 \right] \right) - (1 - \log 2) R_e \]
\[ = \sum_{k=1}^K \sum_{\ell=1}^K \left[ p_k p_\ell \log \left( e^{1-\varepsilon} + e^{f(x_1) \top} \mu_\ell \right) \right] - (1 - \log 2) R_e + \Delta_1 \]
Towards the Generalization of Contrastive Self-Supervised Learning

\[ \geq p_k p_\ell \log \left( e^{1 - \varepsilon} + e^{\mu_k^T \mu_\ell} \right) + \sum_{k=1}^{K} p_k^2 \log \left( e^{1 - \varepsilon} + e^{\|\mu_k\|^2} \right) - (1 - \log 2) R_{\varepsilon} + \Delta_1 \]

\[ \geq p_k p_\ell \log \left( e^{1 - \varepsilon} + e^{\mu_k^T \mu_\ell} \right) + \frac{1 - \varepsilon}{K} \sum_{k=1}^{K} p_k^2 - (1 - \log 2) R_{\varepsilon} + \Delta_1 \]

\[ \geq p_k p_\ell \log \left( e^{1 - \varepsilon} + e^{\mu_k^T \mu_\ell} \right) + \frac{1 - \varepsilon}{K} - (1 - \log 2) R_{\varepsilon} + \Delta_1, \]  

where \( \Delta_1 \) is defined as

\[ \Delta_1 := \sum_{k=1}^{K} \sum_{\ell=1}^{K} \mathbb{E}_{x, x'} \left[ \mathbb{I}(x \in S_{\varepsilon} \cap C_k) \mathbb{I}(x' \in C_\ell) \mathbb{E}_{x_1 \in A(x)} \mathbb{E}_{x^- \in A(x')} \log \left( e^{1 - \varepsilon} + e^{f(x_1)^T f(x^-)} \right) \right] \]

\[ - \sum_{k=1}^{K} \sum_{\ell=1}^{K} \mathbb{E}_{x, x'} \left[ \mathbb{I}(x \in C_k) \mathbb{I}(x' \in C_\ell) \log \left( e^{1 - \varepsilon} + e^{\mu_k^T \mu_\ell} \right) \right] \]

\[ = - \sum_{k=1}^{K} \sum_{\ell=1}^{K} \mathbb{E}_{x, x'} \left[ \left( \mathbb{I}(x \in C_k) - \mathbb{I}(x \in S_{\varepsilon} \cap C_k) \right) \mathbb{I}(x' \in C_\ell) \mathbb{E}_{x_1 \in A(x)} \mathbb{E}_{x^- \in A(x')} \log \left( e^{1 - \varepsilon} + e^{f(x_1)^T f(x^-)} \right) \right] \]

Then,

\[ |\Delta_1| \leq \log(2e) \sum_{k=1}^{K} \sum_{\ell=1}^{K} \mathbb{E}_{x, x'} \left[ \left( \mathbb{I}(x \in C_k) - \mathbb{I}(x \in S_{\varepsilon} \cap C_k) \right) \mathbb{I}(x' \in C_\ell) \right] \]

\[ + \sum_{k=1}^{K} \sum_{\ell=1}^{K} \mathbb{E}_{x, x'} \left[ \mathbb{I}(x \in C_k) \mathbb{I}(x' \in C_\ell) \mathbb{E}_{x_1 \in A(x)} \mathbb{E}_{x^- \in A(x')} \log \left( e^{1 - \varepsilon} + e^{f(x_1)^T f(x^-)} \right) - \log \left( e^{1 - \varepsilon} + e^{\mu_k^T \mu_\ell} \right) \right] \]

\[ \leq (1 + \log 2) R_{\varepsilon} + \sum_{k=1}^{K} \sum_{\ell=1}^{K} \mathbb{E}_{x, x'} \left[ \mathbb{I}(x \in C_k) \mathbb{I}(x' \in C_\ell) \mathbb{E}_{x_1 \in A(x)} \mathbb{E}_{x^- \in A(x')} \log \left( e^{1 - \varepsilon} + e^{f(x_1)^T f(x^-)} \right) - \log \left( e^{1 - \varepsilon} + e^{\mu_k^T \mu_\ell} \right) \right] \]

\[ \leq (1 + \log 2) R_{\varepsilon} + \sum_{k=1}^{K} \sum_{\ell=1}^{K} \mathbb{E}_{x, x'} \left[ \mathbb{I}(x \in C_k) \mathbb{I}(x' \in C_\ell) \mathbb{E}_{x_1 \in A(x)} \mathbb{E}_{x^- \in A(x')} \left( e^{\xi} + e^{\mu_k^T \mu_\ell} \right) \right] \]

\[ \leq (1 + \log 2) R_{\varepsilon} + \sum_{k=1}^{K} \sum_{\ell=1}^{K} \mathbb{E}_{x, x'} \left[ \mathbb{I}(x \in C_k) \mathbb{I}(x' \in C_\ell) \mathbb{E}_{x_1 \in A(x)} \mathbb{E}_{x^- \in A(x')} \left( |f(x_1)^T f(x^-) - \mu_k^T \mu_\ell| \right) \right] \]

\[ \leq (1 + \log 2) R_{\varepsilon} + \sum_{k=1}^{K} \sum_{\ell=1}^{K} \mathbb{E}_{x, x'} \left[ \mathbb{I}(x \in C_k) \mathbb{I}(x' \in C_\ell) \mathbb{E}_{x_1 \in A(x)} \mathbb{E}_{x^- \in A(x')} \left( |(f(x_1) - \mu_k)^T (f(x^-) - \mu_\ell)| \right) \right] \]

\[ + \|f(x_1) - \mu_k\| \cdot \|\mu_\ell\| + \|\mu_k\| \cdot \|f(x^-) - \mu_\ell\| \]

\[ \leq (1 + \log 2) R_{\varepsilon} + \sum_{k=1}^{K} \sum_{\ell=1}^{K} \mathbb{E}_{x, x'} \left[ \mathbb{I}(x \in C_k) \mathbb{I}(x' \in C_\ell) \mathbb{E}_{x_1 \in A(x)} \mathbb{E}_{x^- \in A(x')} \left( |(f(x_1) - \mu_k)^T (f(x^-) - \mu_\ell)| \right) \right] \]
\[
+ 2 \sum_{k=1}^{K} \mathbb{E} \left[ \mathbb{I}(x \in C_k) \sum_{x_i \in A(x)} \|f(x_1) - \mu_k\| \right] \\
\leq (1 + \log 2) R_e + \left( \sum_{k=1}^{K} p_k \mathbb{E} \mathbb{E} \|f(x_1) - \mu_k\| \right)^2 + 2 \sum_{k=1}^{K} p_k \mathbb{E} \mathbb{E} \|f(x_1) - \mu_k\| \\
\leq (1 + \log 2) R_e + \left( \sum_{k=1}^{K} \left( 2 \sigma \varepsilon + \frac{4}{p_k} R_e + \tau_1(\sigma, \delta) \right) \right)^2 + 2 \sum_{k=1}^{K} \left( 2 \sigma \varepsilon + \frac{4}{p_k} R_e + \tau_1(\sigma, \delta) \right) \\
\leq (1 + \log 2) R_e + \left( 2 \sigma \varepsilon + 4 K R_e + \tau_1(\sigma, \delta) \right)^2 + 2 \sigma \varepsilon + 4 K R_e + \tau_1(\sigma, \delta),
\]

which is a small. Then Eq (14) turns to

\[
p_k p_\ell \log \left( e^{1 - \varepsilon + \mu_k^T \mu_\ell} \right) \leq \mathcal{L}_2(f) - \frac{1 - \varepsilon}{K} + (1 - \log 2) R_e + |\Delta_1| \\
\leq \mathcal{L}_2(f) + \left( 2 \sigma \varepsilon + 4 K R_e + \tau_1(\sigma, \delta) \right)^2 + (2 \sigma + \frac{1}{K}) \varepsilon + (4 K + 2) R_e + \tau_1(\sigma, \delta) - \frac{1}{K},
\]

Let

\[
\tau(\varepsilon, \sigma, \delta) := \left( 2 \sigma \varepsilon + 4 K R_e + \tau_1(\sigma, \delta) \right)^2 + (2 \sigma + \frac{1}{K}) \varepsilon + (4 K + 2) R_e + \tau_1(\sigma, \delta) - \frac{1}{K},
\]

and we obtain

\[
\mu_k^T \mu_\ell \leq \log \left( \exp \left\{ \frac{\mathcal{L}_2(f) + \tau(\varepsilon, \sigma, \delta)}{p_k p_\ell} \right\} - \exp(1 - \varepsilon) \right). \tag{15}
\]

This finishes the proof. \qed

### B.2 Cross-Correlation Loss

**Lemma 4.1.** For a given encoder \( f \), the alignment \( \mathcal{L}_{pos}(f) \) in (2) is upper bounded via \( \mathcal{L}_1(f) \), such that

\[
\mathcal{L}_{pos}(f) = \mathbb{E} \mathbb{E} \|f(x_1) - f(x_2)\|^2 \leq 2 \sqrt{d \mathcal{L}_1(f)},
\]

where \( d \) is the output dimension of encoder \( f \).

**Proof.** Since \( \mathbb{E} \mathbb{E} f_i(x_1)^2 = 1 \), for each coordinate component \( i \), we have

\[
1 - \mathbb{E} \mathbb{E} \left[ f_i(x_1) f_i(x_2) \right] = \frac{1}{2} \mathbb{E} \mathbb{E} \left[ f_i(x_1)^2 + f_i(x_2)^2 \right] - \mathbb{E} \mathbb{E} \left[ f_i(x_1) f_i(x_2) \right] \\
= \frac{1}{2} \mathbb{E} \mathbb{E} \left[ f_i(x_1) - f_i(x_2) \right]^2.
\]

Then

\[
\mathbb{E} \mathbb{E} \|f(x_1) - f(x_2)\|^2 = \sum_{i=1}^{d} \mathbb{E} \mathbb{E} \left[ f_i(x_1) - f_i(x_2) \right]^2 \\
= 2 \sum_{i=1}^{d} \left( 1 - \mathbb{E} \mathbb{E} \left[ f_i(x_1) f_i(x_2) \right] \right) \\
\leq 2 \left( \sum_{i=1}^{d} \left( 1 - \mathbb{E} \mathbb{E} \left( f_i(x_1) f_i(x_2) \right) \right)^2 \right)^{\frac{1}{2}} \\
= 2d^2 \mathcal{L}_1(f)^2,
\]

where the inequality holds due to Cauchy inequality. \qed
Lemma B.2. Assume that encoder $f$ with norm $\sqrt{d}$ is $L$-Lipschitz continuous. If the augmented data used in Barlow Twins is $(\sigma, \delta)$-augmented, then for any $\varepsilon > 0$,

$$\left\| \mathbb{E}_{x_1, x_2 \in A(x)} \left[ f(x_1)f(x_2)^\top \right] - \sum_{k=1}^{K} p_k \mu_k \mu_k^\top \right\| \leq \tau'(\varepsilon, \sigma, \delta),$$

where

$$\tau'(\varepsilon, \sigma, \delta) := 4d \left( 1 - \sigma + \frac{2\varepsilon + L\delta}{2\sqrt{d}} \right)^2 + 4(1-\sigma)d + 8dKR_{\varepsilon} \left( \frac{3}{2} - \sigma + \frac{2\varepsilon + L\delta}{2\sqrt{d}} \right) + 4dR_{\varepsilon}^2 \left( \sum_{k=1}^{K} \frac{1}{p_k} \right) + \sqrt{2d^2 L_1(f)^{\frac{1}{2}}}.$$

Proof. We first decompose the LHS as

$$\mathbb{E}_{x_1, x_2 \in A(x)} \left[ f(x_1)f(x_2)^\top \right] - \sum_{k=1}^{K} p_k \mu_k \mu_k^\top$$

$$= \sum_{k=1}^{K} p_k \mathbb{E}_{x \in C_k, x_1, x_2 \in A(x)} \left[ f(x_1)f(x_2)^\top \right] - \sum_{k=1}^{K} p_k \mu_k \mu_k^\top$$

$$= \sum_{k=1}^{K} p_k \mathbb{E}_{x \in C_k, x_1 \in A(x)} \left[ f(x_1)f(x_1)^\top \right] - \sum_{k=1}^{K} p_k \mu_k \mu_k^\top + \sum_{k=1}^{K} p_k \mathbb{E}_{x \in C_k, x_1, x_2 \in A(x)} \left[ f(x_1)(f(x_2)^\top - f(x_1)^\top) \right]$$

$$= \sum_{k=1}^{K} p_k \mathbb{E}_{x \in C_k, x_1 \in A(x)} \left[ (f(x_1) - \mu_k)(f(x_1) - \mu_k)^\top \right] + \mathbb{E}_{x \in A(x)} \mathbb{E}_{x \neq x_1, x_2 \in A(x)} \left[ f(x_1)(f(x_2)^\top - f(x_1)^\top) \right].$$

Then its norm is

$$\left\| \mathbb{E}_{x_1, x_2 \in A(x)} \left[ f(x_1)f(x_2)^\top \right] - \sum_{k=1}^{K} p_k \mu_k \mu_k^\top \right\|$$

$$\leq \sum_{k=1}^{K} p_k \mathbb{E}_{x \in C_k, x_1 \in A(x)} \left[ \|f(x_1) - \mu_k\|^2 \right] + \mathbb{E}_{x \in A(x)} \mathbb{E}_{x \neq x_1, x_2 \in A(x)} \left[ \|f(x_1)f(x_2)^\top - f(x_1)^\top\| \right]$$

$$\leq \sum_{k=1}^{K} p_k \mathbb{E}_{x \in C_k, x_1 \in A(x)} \left[ \|f(x_1) - \mu_k\|^2 \right] + \mathbb{E}_{x \in A(x)} \mathbb{E}_{x \neq x_1, x_2 \in A(x)} \left[ \|f(x_1)f(x_2) - f(x_1)\| \right]$$

$$\leq \sum_{k=1}^{K} p_k \mathbb{E}_{x \in C_k, x_1 \in A(x)} \left[ \|f(x_1) - \mu_k\|^2 \right] + \mathbb{E}_{x \in A(x)} \mathbb{E}_{x \neq x_1, x_2 \in A(x)} \left[ \|f(x_1)f(x_2) - f(x_1)\|^2 \right] \frac{1}{2}$$

(Cauchy–Schwarz inequality)

$$\leq \sum_{k=1}^{K} p_k \mathbb{E}_{x \in C_k, x_1 \in A(x)} \left[ \|f(x_1) - \mu_k\|^2 \right] + \sqrt{d} \left( 2\sqrt{dL_1(f)} \right)^{\frac{1}{2}}$$

(Lemma 4.1)

$$\leq (2\varepsilon + L\delta)^2 + 4r(1-\sigma)(r + 2\varepsilon + L\delta) + 4r^2(1-\sigma)^2 + K R_{\varepsilon} [4r(r + 2\varepsilon + L\delta) + 8r^2(1-\sigma)] + 4r^2 R_{\varepsilon}^2 \left( \sum_{k=1}^{K} \frac{1}{p_k} \right) + \sqrt{2d^2 L_1(f)^{\frac{1}{2}}}$$

(Lemma B.1)

$$= 4r^2 \left( 1 - \sigma + \frac{2\varepsilon + L\delta}{2r} \right)^2 + 4(1-\sigma)d + 8dKR_{\varepsilon} \left( \frac{3}{2} - \sigma + \frac{2\varepsilon + L\delta}{2\sqrt{d}} \right) + 4dR_{\varepsilon}^2 \left( \sum_{k=1}^{K} \frac{1}{p_k} \right) + \sqrt{2d^2 L_1(f)^{\frac{1}{2}}}$$

$$= \tau'(\varepsilon, \sigma, \delta).$$

This finishes the proof.
Theorem 4. Assume that encoder \( f \) with norm \( \sqrt{d} \) is \( L \)-Lipschitz continuous. If the augmented data used in Barlow Twins is \((\sigma, \delta)\)-augmented, then for any \( k \neq \ell \), we have

\[
\mu_k^\top \mu_\ell \leq \sqrt{\frac{2}{p_k p_\ell}} \left( \mathcal{L}_2(f) + \tau'(\varepsilon, \sigma, \delta) - \frac{d - K}{2} \right),
\]

where the term \( \tau'(\varepsilon, \sigma, \delta) \) is the upper bound of \( \| E_x \mathbb{E}_{x_1, x_2 \in A(x)} [f(x_1) f(x_2)^\top] - \sum_{k=1}^K p_k \mu_k \mu_k^\top \|_2^2 \).

Proof. Let \( U = (\sqrt{p_1} \mu_1, \ldots, \sqrt{p_K} \mu_K) \in \mathbb{R}^{d \times K} \).

\[
\left\| \sum_{k=1}^K p_k \mu_k \mu_k^\top - I_d \right\|^2 \\
= \| U U^\top - I_d \|^2 \\
= \text{Tr}(U U^\top U U^\top - 2U U^\top + I_d) \\
= \text{Tr}(U U^\top U U^\top U - 2U U^\top + I_K) + d - K \\
= \| U U^\top U - I_K \|^2 + d - K \\
= \sum_{k=1}^K \sum_{\ell=1}^K (\sqrt{p_k p_\ell} \mu_k \mu_\ell - \delta_{k\ell})^2 + d - K \\
\geq p_k p_\ell (\mu_k^\top \mu_\ell)^2 + d - K.
\]

where \( \delta_{k\ell} \) is the Dirichlet function.

Therefore,

\[
\left( \mu_k^\top \mu_\ell \right)^2 \\
\leq \left\| \sum_{k=1}^K p_k \mu_k \mu_k^\top - I_d \right\|^2 - (d - K) \\
= \left\| \mathbb{E}_x \mathbb{E}_{x_1, x_2 \in A(x)} [f(x_1) f(x_2)^\top] - I_d + \sum_{k=1}^K p_k \mu_k \mu_k^\top - \mathbb{E}_x \mathbb{E}_{x_1, x_2 \in A(x)} [f(x_1) f(x_2)^\top] \right\|^2 - (d - K)
\]

\[
\leq \frac{2 \left\| \mathbb{E}_x \mathbb{E}_{x_1, x_2 \in A(x)} [f(x_1) f(x_2)^\top] - I_d \right\|^2 + 2 \left\| \sum_{k=1}^K p_k \mu_k \mu_k^\top - \mathbb{E}_x \mathbb{E}_{x_1, x_2 \in A(x)} [f(x_1) f(x_2)^\top] \right\|^2 - (d - K)}{p_k p_\ell} \\
\leq \frac{2 \mathcal{L}_2(f) + 2\tau'(\varepsilon, \sigma, \delta) - (d - K)}{p_k p_\ell} \\
= \frac{2}{p_k p_\ell} \left( \mathcal{L}_2(f) + \tau'(\varepsilon, \sigma, \delta) - \frac{d - K}{2} \right).
\]

This finishes the proof. \( \square \)