
Debiased Contrastive Learning

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Abstract

A prominent technique for self-supervised representation learning has been to contrast semantically similar and dissimilar pairs of samples. Without access to labels, dissimilar (negative) points are typically taken to be randomly sampled datapoints, implicitly accepting that these points may, in reality, actually have the same label. Perhaps unsurprisingly, we observe that sampling negative examples from truly different labels improves performance, in a synthetic setting where labels are available. Motivated by this observation, we develop a debiased contrastive objective that corrects for the sampling of same-label datapoints, even without knowledge of the true labels. Empirically, the proposed objective consistently outperforms the state-of-the-art for representation learning in vision, language, and reinforcement learning benchmarks. Theoretically, we establish generalization bounds for the downstream classification task.

1 Introduction

Learning good representations without supervision has been a long-standing goal of machine learning. One such approach is *self-supervised learning*, where auxiliary learning objectives leverage labels that can be observed without a human labeler. For instance, in computer vision, representations can be learned from colorization [45], predicting transformations [10, 32], or generative modeling [24, 14, 3]. Remarkable success has also been achieved in the language domain [30, 25, 8].

Recently, self-supervised representation learning algorithms that use a contrastive loss have outperformed even supervised learning [15, 28, 19, 18, 2]. The key idea of *contrastive learning* is to contrast semantically similar (positive) and dissimilar (negative) pairs of data points, encouraging the representations f of similar pairs (x, x^+) to be close, and those of dissimilar pairs (x, x^-) to be more orthogonal [33, 2]:

$$\mathbb{E}_{x, x^+, \{x_i^-\}_{i=1}^N} \left[-\log \frac{e^{f(x)^T f(x^+)}}{e^{f(x)^T f(x^+)} + \sum_{i=1}^N e^{f(x)^T f(x_i^-)}} \right]. \quad (1)$$

In practice, the expectation is replaced by the empirical estimate. For each training data point x , it is common to use one positive example, e.g., derived from perturbations, and N negative examples x_i^- . Since true labels or true semantic similarity are typically not available, negative counterparts x_i^- are commonly drawn uniformly from the training data. But, this means it is possible that x_i^- is actually similar to x , as illustrated in Figure 1. This phenomenon, which we refer to as *sampling bias*, can empirically lead to significant performance drop. Figure 2 compares the accuracy for learning with this bias, and for drawing x_i^- from data with truly different labels than x ; we refer to this method as *unbiased* (further details in Section 5.1).

However, the ideal unbiased objective is unachievable in practice since it requires knowing the labels, i.e., *supervised* learning. This dilemma poses the question whether it is possible to reduce the gap

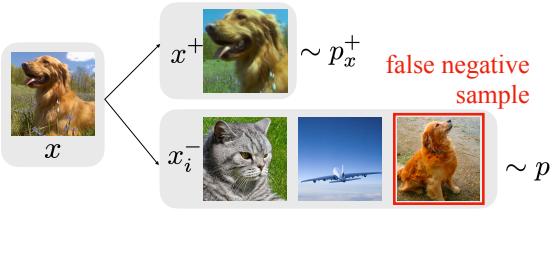


Figure 1: **“Sampling bias”**: The common practice of drawing negative examples x_i^- from the data distribution $p(x)$ may result in x_i^- that are actually similar to x .

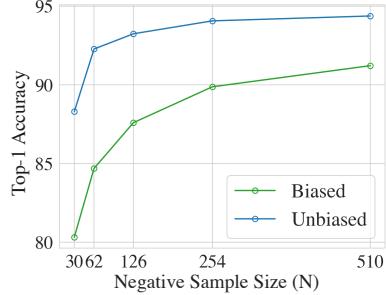


Figure 2: **Sampling bias leads to performance drop**: Results on CIFAR-10 for drawing x_i^- from $p(x)$ (biased) and from data with different labels, i.e., truly semantically different data (unbiased).

between the ideal objective and standard contrastive learning, without supervision. In this work, we demonstrate that this is indeed possible, while still assuming only access to unlabeled training data and positive examples. In particular, we develop a correction for the sampling bias that yields a new, modified loss that we call *debiased contrastive loss*. The key idea underlying our approach is to indirectly approximate the distribution of negative examples. The new objective is easily compatible with any algorithm that optimizes the standard contrastive loss. Empirically, our approach improves over the state of the art in vision, language and reinforcement learning benchmarks.

Our theoretical analysis relates the debiased contrastive loss to supervised learning: optimizing the debiased contrastive loss corresponds to minimizing an upper bound on a supervised loss. This leads to a generalization bound for the supervised task, when training with the debiased contrastive loss.

In short, this work makes the following contributions:

- We develop a new, *debiased contrastive objective* that corrects for the sampling bias of negative examples, while only assuming access to positive examples and the unlabeled data;
- We evaluate our approach via experiments in vision, language, and reinforcement learning;
- We provide a theoretical analysis of the debiased contrastive representation with generalization guarantees for a resulting classifier.

2 Related Work

Contrastive Representation Learning. The contrastive loss has recently become a prominent tool in unsupervised representation learning, leading to state-of-the-art results. The main difference between different approaches to contrastive learning lies in their strategy for obtaining positive pairs. Examples in computer vision include random cropping and flipping [33], or different views of the same scene [40]. Chen et al. [2] extensively study various data augmentation methods. For language, Logeswaran and Lee [28] treat the context sentences as positive samples to efficiently learn sentence representations. Srinivas et al. [37] improve the sample efficiency of reinforcement learning with representations learned via the contrastive loss. Computational efficiency has been improved by maintaining a dictionary of negative examples [18, 4]. Concurrently, Wang and Isola [42] analyze the asymptotic contrastive loss and propose new metrics to measure the representation quality. All of these works sample negative examples from $p(x)$.

Arora et al. [1] theoretically analyze the effect of contrastive representation learning on a downstream, “average” classification task and provide a generalization bound for the standard objective. They too point out the sampling bias as a problem, but do not propose any models to address it.

Positive-unlabeled Learning. Since we approximate the contrastive loss with only unlabeled data from $p(x)$ and positive examples, our work is also related to *Positive-Unlabeled* (PU) learning, i.e., learning from only positive (P) and unlabeled (U) data. Common applications of PU learning are retrieval or outlier detection [13, 12, 11]. Our approach is related to *unbiased PU learning*, where the unlabeled data is used as negative examples, but down-weighted appropriately [26, 12, 11].

While these works focus on zero-one losses, we here address the contrastive loss, where existing PU estimators are not directly applicable.

3 Setup and Sampling Bias in Contrastive Learning

Contrastive learning assumes access to semantically similar pairs of data points (x, x^+) , where x is drawn from a data distribution $p(x)$ over \mathcal{X} . The goal is to learn an embedding $f : \mathcal{X} \rightarrow \mathbb{R}^d$ that maps an observation x to a point on a hypersphere with radius $1/t$, where t is the temperature scaling hyperparameter. Without loss of generality, we set $t = 1$ for all theoretical results.

Similar to [1], we assume an underlying set of discrete latent classes \mathcal{C} that represent semantic content, i.e., similar pairs (x, x^+) have the same latent class. Denoting the distribution over classes by $\rho(c)$, we obtain the joint distribution $p_{x,c}(x, c) = p(x|c)\rho(c)$. Let $h : \mathcal{X} \rightarrow \mathcal{C}$ be the function assigning the latent class labels. Then $p_x^+(x') = p(x'|h(x') = h(x))$ is the probability of observing x' as a positive example for x and $p_x^-(x') = p(x'|h(x') \neq h(x))$ the probability of a negative example. We assume that the class probabilities $\rho(c) = \tau^+$ are uniform, and let $\tau^- = 1 - \tau^+$ be the probability of observing any different class.

Note that to remain unsupervised in practice, our method and other contrastive losses only sample from the data distribution and a “surrogate” positive distribution, mimicked by data augmentations or context sentences [2, 28].

3.1 Sampling Bias

Intuitively, the contrastive loss will provide most informative representations for downstream classification tasks if the positive and negative pairs correspond to the desired latent classes. Hence, the ideal loss to optimize would be

$$L_{\text{Unbiased}}^N(f) = \mathbb{E}_{\substack{x \sim p, x^+ \sim p_x^+ \\ x_i^- \sim p_x^-}} \left[-\log \frac{e^{f(x)^T f(x^+)}}{e^{f(x)^T f(x^+)} + \frac{Q}{N} \sum_{i=1}^N e^{f(x)^T f(x_i^-)}} \right], \quad (2)$$

which we will refer to as the *unbiased loss*. Here, we introduce a weighting parameter Q for the analysis. When the number N of negative examples is finite, we set $Q = N$, in agreement with the standard contrastive loss. In practice, however, $p_x^-(x_i^-) = p(x_i^-|h(x_i^-) \neq h(x))$ is not accessible. The standard approach is thus to sample negative examples x_i^- from the (unlabeled) $p(x)$ instead. We refer to the resulting loss as the *biased loss* L_{Biased}^N . When drawn from $p(x)$, the sample x_i^- will come from the same class as x with probability τ^+ .

Lemma 1 shows that in the limit, the standard loss L_{Biased}^N upper bounds the ideal, unbiased loss.

Lemma 1. *For any embedding f and finite N , we have*

$$L_{\text{Biased}}^N(f) \geq L_{\text{Unbiased}}^N(f) + \mathbb{E}_{x \sim p} \left[0 \wedge \log \frac{\mathbb{E}_{x^+ \sim p_x^+} \exp f(x)^\top f(x^+)}{\mathbb{E}_{x^- \sim p_x^-} \exp f(x)^\top f(x^-)} \right] - e^{3/2} \sqrt{\frac{\pi}{2N}}. \quad (3)$$

where $a \wedge b$ denotes the minimum of two real numbers a and b .

Recent works often use large N , e.g., $N = 65536$ in [18], making the last term negligible. While, in general, minimizing an upper bound on a target objective is a reasonable idea, two issues arise here: (1) the smaller the unbiased loss, the larger is the second term, widening the gap; and (2) the empirical results in Figure 2 and Section 5 show that minimizing the upper bound L_{Biased}^N and minimizing the ideal loss L_{Unbiased}^N can result in very different learned representations.

4 Debiased Contrastive Loss

Next, we derive a loss that is closer to the ideal L_{Unbiased}^N , while only having access to positive samples and samples from p . Figure 2 shows that the resulting embeddings are closer to those learned with L_{Unbiased}^N . We begin by decomposing the data distribution as

$$p(x') = \tau^+ p_x^+(x') + \tau^- p_x^-(x').$$

An immediate approach would be to replace p_x^- in L_{Unbiased}^N with $p_x^-(x') = (p(x') - \tau^+ p_x^+(x'))/\tau^-$ and then use the empirical counterparts for p and p_x^+ . The resulting objective can be estimated with samples from only p and p_x^+ , but is computationally expensive for large N :

$$\frac{1}{(\tau^-)^N} \sum_{k=0}^N \binom{N}{k} (-\tau^+)^k \mathbb{E}_{\substack{x \sim p, x^+ \sim p_x^+ \\ \{x_i^-\}_{i=1}^k \sim p_x^- \\ \{x_i^-\}_{i=k+1}^N \sim p}} \left[-\log \frac{e^{f(x)^T f(x^+)}}{e^{f(x)^T f(x^+)} + \sum_{i=1}^N e^{f(x)^T f(x_i^-)}} \right], \quad (4)$$

where $\{x_i^-\}_{i=k}^j = \emptyset$ if $k > j$. It also demands at least N positive samples. To obtain a more practical form, we consider the asymptotic form as the number N of negative examples goes to infinity.

Lemma 2. *For fixed Q and $N \rightarrow \infty$, it holds that*

$$\mathbb{E}_{\substack{x \sim p, x^+ \sim p_x^+ \\ \{x_i^-\}_{i=1}^N \sim p_x^-}} \left[-\log \frac{e^{f(x)^T f(x^+)}}{e^{f(x)^T f(x^+)} + \frac{Q}{N} \sum_{i=1}^N e^{f(x)^T f(x_i^-)}} \right] \quad (5)$$

$$\longrightarrow \mathbb{E}_{\substack{x \sim p \\ x^+ \sim p_x^+}} \left[-\log \frac{e^{f(x)^T f(x^+)}}{e^{f(x)^T f(x^+)} + \frac{Q}{\tau^-} (\mathbb{E}_{x^- \sim p} [e^{f(x)^T f(x^-)}] - \tau^+ \mathbb{E}_{v \sim p_x^+} [e^{f(x)^T f(v)}])} \right]. \quad (6)$$

The limiting objective (6), which we denote by $\tilde{L}_{\text{Debiased}}^Q$, still samples examples x^- from p , but corrects for that with additional positive samples v . This essentially reweights positive and negative terms in the denominator.

The empirical estimate of $\tilde{L}_{\text{Debiased}}^Q$ is much easier to compute than the straightforward objective (5). With N samples $\{u_i\}_{i=1}^N$ from p and M samples $\{v_i\}_{i=1}^M$ from p_x^+ , we estimate the expectation of the second term in the denominator as

$$g(x, \{u_i\}_{i=1}^N, \{v_i\}_{i=1}^M) = \max \left\{ \frac{1}{\tau^-} \left(\frac{1}{N} \sum_{i=1}^N e^{f(x)^T f(u_i)} - \tau^+ \frac{1}{M} \sum_{i=1}^M e^{f(x)^T f(v_i)} \right), e^{-1/t} \right\}. \quad (7)$$

We constrain the estimator g to be greater than its theoretical minimum $e^{-1/t} \leq \mathbb{E}_{x^- \sim p_x^-} e^{f(x)^T f(x^-)}$ to prevent calculating the logarithm of a negative number. The resulting population loss with fixed N and M per data point is

$$L_{\text{Debiased}}^{N,M}(f) = \mathbb{E}_{\substack{x \sim p; x^+ \sim p_x^+ \\ \{u_i\}_{i=1}^N \sim p_x^- \\ \{v_i\}_{i=1}^M \sim p_x^+}} \left[-\log \frac{e^{f(x)^T f(x^+)}}{e^{f(x)^T f(x^+)} + Ng(x, \{u_i\}_{i=1}^N, \{v_i\}_{i=1}^M)} \right], \quad (8)$$

where, for simplicity, we set Q to the finite N . The class prior τ^+ can be estimated from data [21, 6] or treated as a hyperparameter. Theorem 3 bounds the error due to finite N and M as decreasing with rate $\mathcal{O}(N^{-1/2} + M^{-1/2})$.

Theorem 3. *For any embedding f and finite N and M , we have*

$$\left| \tilde{L}_{\text{Debiased}}^N(f) - L_{\text{Debiased}}^{N,M}(f) \right| \leq \frac{e^{3/2}}{\tau^-} \sqrt{\frac{\pi}{2N}} + \frac{e^{3/2} \tau^+}{\tau^-} \sqrt{\frac{\pi}{2M}}. \quad (9)$$

Empirically, the experiments in Section 5 also show that larger N and M consistently lead to better performance. In the implementations, we use a full empirical estimate for $L_{\text{Debiased}}^{N,M}$ that averages the loss over T points x , for finite N and M .

5 Experiments

In this section, we evaluate our new objective L_{Debiased}^N empirically, and compare it to the standard loss L_{Biased}^N and the ideal loss L_{Unbiased}^N . In summary, we observe the following: (1) the new loss outperforms state of the art contrastive learning on vision, language and reinforcement learning benchmarks; (2) the learned embeddings are closer to those of the ideal, unbiased objective; (3) both larger N and large M improve the performance; even one more positive example than the standard $M = 1$ can help noticeably. Detailed experimental settings can be found in the appendix. The code is available at <https://github.com/chingyaoc/DCL>.

```

1 # pos: exponential for positive example
2 # neg: sum of exponentials for negative examples
3 # N : number of negative examples
4 # t : temperature scaling
5 # tau_plus: class probability
6
7 standard_loss = -log(pos / (pos + neg))
8 Ng = max((-N * tau_plus * pos + neg) / (1-tau_plus), N * e**(-1/t))
9 debiased_loss = -log(pos / (pos + Ng))

```

Figure 3: **Pseudocode for debiased objective with $M = 1$.** The implementation only requires a small modification of the code. We can simply extend the code to debiased objective with $M > 1$ by changing the pos in line 8 with an average of exponentials for M positive samples.

5.1 CIFAR10 and STL10

First, for CIFAR10 [27] and STL10 [7], we implement SimCLR [2] with ResNet-50 [17] as the encoder architecture and use the Adam optimizer [23] with learning rate 0.001. Following [2], we set the temperature to $t = 0.5$ and the dimension of the latent vector to 128. All the models are trained for 400 epochs and evaluated by training a linear classifier after fixing the learned embedding. Detailed experimental settings can be found in Appendix B.

To understand the effect of the sampling bias, we additionally consider an estimate of the ideal L_{Unbiased}^N , which is a *supervised* version of the standard loss, where negative examples x_i^- are drawn from the true p_{x^-} , i.e., using known classes. Since STL10 is not fully labeled, we only use the unbiased objective on CIFAR10.

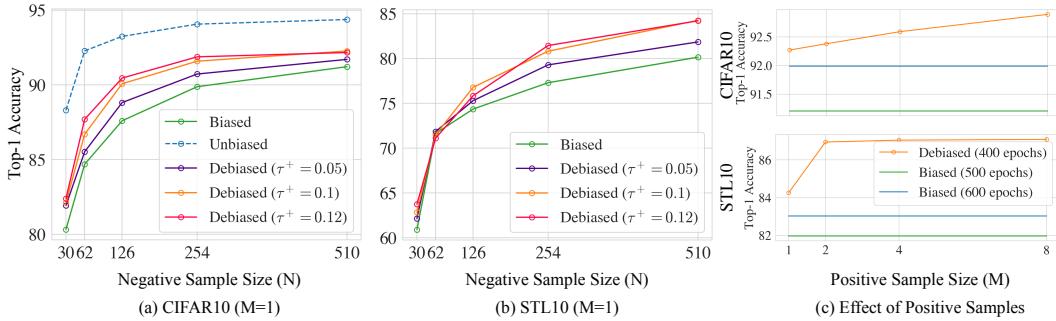


Figure 4: **Classification accuracy on CIFAR10 and STL10.** (a,b) Biased and Debiased ($M = 1$) SimCLR with different negative sample size N where $N = 2(\text{BatchSize} - 1)$. (c) Comparison with biased SimCLR with 50% more training epochs (600 epochs) while fixing the training epoch for Debiased ($M \geq 1$) SimCLR to 400 epochs.

Debiased Objective with $M = 1$. For a fair comparison, i.e., no possible advantage from additional samples, we first examine our debiased objective with positive sample size $M = 1$ by setting $v_1 = x^+$. Then, our approach uses exactly the same data batch as the biased baseline. The debiased objective can be easily implemented by a slight modification of the code as Figure 3 shows. The results with different τ^+ are shown in Figure 4(a,b). Increasing τ^+ in Objective (7) leads to more correction, and gradually improves the performance in both benchmarks for different N . Remarkably, with only a slight modification to the loss, we improve the accuracy of SimCLR on STL10 by 4.26%. The performance of the debiased objective also improves by increasing the negative sample size N .

Debiased Objective with $M \geq 1$. By Theorem 3, a larger positive sample size M leads to a better estimate of the loss. To probe its effect, we increase M for all x (e.g., M times data augmentation) while fixing $N = 256$ and $\tau^+ = 0.1$. Since increasing M requires additional computation, we compare our debiased objective with biased SimCLR trained for 50% more epochs (600 epochs). The results for $M = 1, 2, 4, 8$ are shown in Figure 4(c), and indicate that the performance of the debiased objective can indeed be further improved by increasing the number of positive samples. Surprisingly,

with only one additional positive sample, the top-1 accuracy on STL10 can be significantly improved. We can also see that the debiased objective ($M > 1$) even outperforms a biased baseline trained with 50% more epochs.

Figure 5 shows t-SNE visualizations of the representations learned by the biased and debiased objectives ($N = 256$) on CIFAR10. The debiased contrastive loss leads to better class separation than the contrastive loss, and the result is closer to that of the ideal, unbiased loss.

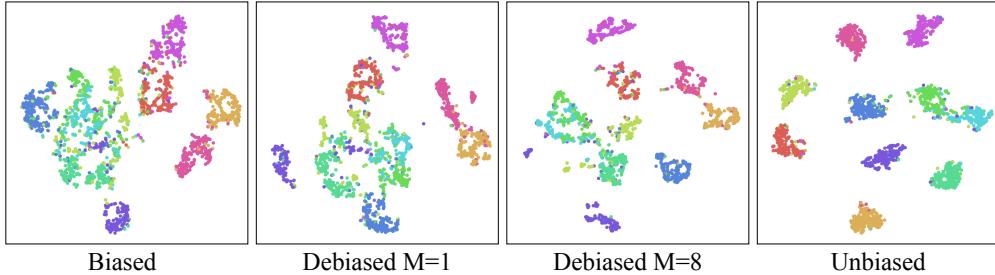


Figure 5: **t-SNE visualization of learned representations on CIFAR10.** Classes are indicated by colors. The debiased objective ($\tau^+ = 0.1$) leads to better data clustering than the (standard) biased loss; its effect is closer to the supervised unbiased objective.

5.2 ImageNet-100

Following [40], we test our approach on ImageNet-100, a randomly chosen subset of 100 classes of Imagenet. Compared to CIFAR10, ImageNet-100 has more classes and hence smaller class probabilities τ^+ . We use contrastive multiview coding (CMC) [40] as our contrastive learning baseline, and $M = 1$ for a fair comparison. The results in Table 1 show that, although τ^+ is small, our debiased objective still improves over the biased baseline.

Objective	Top-1	Top-5
Biased (CMC)	73.58	92.06
Debiased ($\tau^+ = 0.005$)	73.86	91.86
Debiased ($\tau^+ = 0.01$)	74.6	92.08

Table 1: **ImageNet-100** Top-1 and Top-5 classification results.

5.3 Sentence Embeddings

Next, we test the debiased objective for learning sentence embeddings. We use the BookCorpus dataset [25] and examine six classification tasks: movie review sentiment (MR) [35], product reviews (CR) [20], subjectivity classification (SUBJ) [34], opinion polarity (MPQA) [43], question type classification (TREC) [41], and paraphrase identification (MSRP) [9]. Our experimental settings follow those for quick-thought (QT) vectors in [28]. In contrast to vision tasks, positive pairs here are chosen as neighboring sentences, which can form a different positive distribution from data augmentation. The minibatch of QT is constructed with a contiguous set of sentences, hence we can use the preceding and succeeding sentences as positive samples ($M = 2$). We retrain each model 3 times and show the average in Table 2. The debiased objective improves over the baseline in 4 out of 6 downstream tasks, verifying that our objective also works for a different modality.

Objective	MR	CR	SUBJ	MPQA	TREC	MSRP	
						(Acc)	(F1)
Biased (QT)	76.8	81.3	86.6	93.4	89.8	73.6	81.8
Debiased ($\tau^+ = 0.005$)	76.5	81.5	86.6	93.6	89.1	74.2	82.3
Debiased ($\tau^+ = 0.01$)	76.2	82.9	86.9	93.7	89.1	74.7	82.7

Table 2: **Classification accuracy on downstream tasks.** We compare sentence representations on six classification tasks. 10-fold cross validation is used in testing the performance for binary classification tasks (MR, CR, SUBJ, MPQA).

5.4 Reinforcement Learning

Lastly, we consider reinforcement learning. We follow the experimental settings of Contrastive Unsupervised Representations for Reinforcement Learning (CURL) [37] to perform image-based policy control on top of the learned contrastive representations. Similar to vision tasks, the positive pairs are two different augmentations of the same image. We again set $M = 1$ for a fair comparison. Methods are tested at 100k environment steps on the DeepMind control suite [39], which consists of several continuous control tasks. We retrain each model 3 times and show the mean and standard deviation in Table 3. Our method consistently outperforms the state-of-the-art baseline (CURL) in different control tasks, indicating that correcting the sampling bias also improves the performance and data efficiency of reinforcement learning. In several tasks, the debiased approach also has smaller variance. With more positive examples ($M = 2$), we obtain further improvements.

Objective	Finger Spin	Cartpole Swingup	Reacher Easy	Cheetah Run	Walker Walk	Ball in Cup Catch
Biased (CURL)	310 \pm 33	850 \pm 20	918 \pm 96	266 \pm 41	623 \pm 120	928 \pm 47
<i>Debiased Objective with $M = 1$</i>						
Debiased ($\tau^+ = 0.01$)	324 \pm 34	843 \pm 30	927\pm99	310\pm12	626\pm82	937 \pm 9
Debiased ($\tau^+ = 0.05$)	308 \pm 57	866\pm7	916 \pm 114	284 \pm 20	613 \pm 22	945 \pm 13
Debiased ($\tau^+ = 0.1$)	364\pm36	860 \pm 4	868 \pm 177	302 \pm 29	594 \pm 33	951\pm11
<i>Debiased Objective with $M = 2$</i>						
Debiased ($\tau^+ = 0.01$)	330 \pm 10	858 \pm 10	754 \pm 179	286 \pm 20	746\pm93	949 \pm 5
Debiased ($\tau^+ = 0.1$)	381\pm24	864 \pm 6	904 \pm 117	303 \pm 5	671 \pm 75	957\pm5

Table 3: **Scores achieved by biased and debiased objectives.** Our debiased objective outperforms the biased baseline (CURL) in all the environments, and often has smaller variance.

5.5 Discussion

Class Distribution: Our theoretical results assume that the class distribution ρ is close to uniform. In reality, this is often not the case, e.g., in our experiments, CIFAR10 and Imagenet-100 are the only two datasets with perfectly balanced class distributions. Nevertheless, our debiased objective still improves over the baselines even when the classes are not well balanced, indicating that the objective is robust to violations of the class balance assumption.

Positive Distribution: Even if we approximate the true positive distribution with a surrogate positive distribution, our debiased objective still consistently improves over the baselines. It is an interesting avenue of future work to adopt our debiased objective to a semi-supervised learning setting [44] where true positive samples are accessible.

6 Theoretical Analysis: Generalization Implications for Classification Tasks

Next, we relate the debiased contrastive objective to a supervised loss, and show how our contrastive learning approach leads to a generalization bound for a downstream supervised learning task.

We consider a supervised classification task \mathcal{T} with K classes $\{c_1, \dots, c_K\} \subseteq \mathcal{C}$. After contrastive representation learning, we fix the representations $f(x)$ and then train a linear classifier $q(x) = Wf(x)$ on task \mathcal{T} with the standard multiclass softmax cross entropy loss $L_{\text{Softmax}}(\mathcal{T}, q)$. Hence, we define the supervised loss for the representation f as

$$L_{\text{Sup}}(\mathcal{T}, f) = \inf_{W \in \mathbb{R}^{K \times d}} L_{\text{Softmax}}(\mathcal{T}, Wf). \quad (10)$$

In line with the approach of [1] we analyze the supervised loss of a mean classifier [36], where for each class c , the rows of W are set to the mean of the representations $\mu_c = \mathbb{E}_{x \sim p(\cdot|c)}[f(x)]$. We will use $L_{\text{Sup}}^\mu(\mathcal{T}, f)$ as shorthand for its loss. Note that $L_{\text{Sup}}^\mu(\mathcal{T}, f)$ is always an upper bound on $L_{\text{Sup}}(\mathcal{T}, f)$. To allow for uncertainty about the task \mathcal{T} , we will bound the average supervised loss for a uniform distribution \mathcal{D} over K -way classification tasks with classes in \mathcal{C} .

$$L_{\text{Sup}}(f) = \mathbb{E}_{\mathcal{T} \sim \mathcal{D}} L_{\text{Sup}}(\mathcal{T}, f). \quad (11)$$

We begin by showing that the asymptotic unbiased contrastive loss is an upper bound on the supervised loss of the mean classifier.

Lemma 4. *For any embedding f , whenever $N \geq K - 1$ we have*

$$L_{\text{Sup}}(f) \leq L_{\text{Sup}}^{\mu}(f) \leq \tilde{L}_{\text{Debiased}}^N(f).$$

Lemma 4 uses the asymptotic version of the debiased loss. Together with Theorem 3 and a concentration of measure result, it leads to a generalization bound for debiased contrastive learning, as we show next.

Generalization Bound. In practice, we use an empirical estimate $\hat{L}_{\text{Debiased}}^{N,M}$, i.e., an average over T data points x , with M positive and N negative samples for each x . Our algorithm learns an empirical risk minimizer $\hat{f} \in \arg \min_{f \in \mathcal{F}} \hat{L}_{\text{Debiased}}^{N,M}(f)$ from a function class \mathcal{F} . The generalization depends on the *empirical Rademacher complexity* $\mathcal{R}_{\mathcal{S}}(\mathcal{F})$ of \mathcal{F} with respect to our data sample $\mathcal{S} = \{x_j, x_j^+, \{u_{i,j}\}_{i=1}^N, \{v_{i,j}\}_{i=1}^M\}_{j=1}^T$. Let $f|_{\mathcal{S}} = (f_k(x_j), f_k(x_j^+), \{f_k(u_{i,j})\}_{i=1}^N, \{f_k(v_{i,j})\}_{i=1}^M)_{j \in [T], k \in [d]} \in \mathbb{R}^{(N+M+2)dT}$ be the restriction of f onto \mathcal{S} , using $[T] = \{1, \dots, T\}$. Then $\mathcal{R}_{\mathcal{S}}(\mathcal{F})$ is defined as

$$\mathcal{R}_{\mathcal{S}}(\mathcal{F}) := \mathbb{E}_{\sigma} \sup_{f \in \mathcal{F}} \langle \sigma, f|_{\mathcal{S}} \rangle \quad (12)$$

where $\sigma \sim \{\pm 1\}^{(N+M+1)dT}$ are Rademacher random variables. Combining Theorem 3 and Lemma 4 with a concentration of measure argument yields the final generalization bound for debiased contrastive learning.

Theorem 5. *With probability at least $1 - \delta$, for all $f \in \mathcal{F}$ and $N \geq K - 1$,*

$$L_{\text{Sup}}(\hat{f}) \leq L_{\text{Debiased}}^{N,M}(f) + \mathcal{O} \left(\frac{1}{\tau^-} \sqrt{\frac{1}{N}} + \frac{\tau^+}{\tau^-} \sqrt{\frac{1}{M}} + \frac{\lambda \mathcal{R}_{\mathcal{S}}(\mathcal{F})}{T} + B \sqrt{\frac{\log \frac{1}{\delta}}{T}} \right) \quad (13)$$

where $\lambda = \sqrt{\frac{1}{(\tau^-)^2} \left(\frac{M}{N} + 1 \right) + (\tau^+)^2 \left(\frac{N}{M} + 1 \right)}$ and $B = \log N \left(\frac{1}{\tau^-} + \tau^+ \right)$.

The bound states that if the function class \mathcal{F} is sufficiently rich to contain some embedding for which $L_{\text{Debiased}}^{N,M}$ is small, then the representation encoder \hat{f} , learned from a large enough dataset, will perform well on the downstream classification task. The bound also highlights the role of the positive and unlabeled sample sizes M and N in the objective function, in line with the observation that a larger number of negative/positive examples in the objective leads to better results [18, 2]. The last two terms in the bound grow slowly with N , but the effect of this on the generalization error is small if the dataset size T is much larger than N and M , as is commonly the case. The dependence on N and T in Theorem 5 is roughly equivalent to the result in [1], but the two bounds are not directly comparable since the proof strategies differ.

7 Conclusion

In this work, we propose *debiased contrastive learning*, a new unsupervised contrastive representation learning framework that corrects for the bias introduced by the common practice of sampling negative (dissimilar) examples for a point from the overall data distribution. Our debiased objective consistently improves the state-of-the-art baselines in various benchmarks in vision, language and reinforcement learning. The proposed framework is accompanied by generalization guarantees for the downstream classification task. Interesting directions of future work include (1) trying the debiased objective in semi-supervised learning or few shot learning, and (2) studying the effect of how positive (similar) examples are drawn, e.g., analyzing different data augmentation techniques.

Broader Impact

Unsupervised representation learning can improve learning when only small amounts of labeled data are available. This is the case in many applications of societal interest, such as medical data analysis [5, 31], the sciences [22], or drug discovery and repurposing [38]. Improving representation learning, as we do here, can potentially benefit all these applications.

However, biases in the data can naturally lead to biases in the learned representation [29]. These biases can, for example, lead to worse performance for smaller classes or groups. For instance, the majority groups are sampled more frequently than the minority ones [16]. In this respect, our method may suffer from similar biases as standard contrastive learning, and it is an interesting avenue of future research to thoroughly test and evaluate this.

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A Proofs of Theoretical Results

A.1 Proof of Lemma 1

The first result we give shows the relation between the unbiased, and conventional (sample biased) objective.

Lemma 1. *For any embedding f and finite N , we have*

$$L_{\text{Biased}}^N(f) \geq L_{\text{Unbiased}}^N(f) + \mathbb{E}_{x \sim p} \left[0 \wedge \log \frac{\mathbb{E}_{x^+ \sim p_x^+} \exp f(x)^\top f(x^+)}{\mathbb{E}_{x^- \sim p_x^-} \exp f(x)^\top f(x^-)} \right] - e^{3/2} \sqrt{\frac{\pi}{2N}}.$$

where $a \wedge b$ denotes the minimum of two real numbers a and b .

Proof. We use the notation $h(x, \bar{x}) = \exp^{f(x)^\top f(\bar{x})}$ for the critic. We will use Theorem 3 to prove this lemma. Setting $\tau^+ = 0$, Theorem 3 states that

$$\begin{aligned} & \mathbb{E}_{\substack{x \sim p \\ x^+ \sim p_x^+}} \left[-\log \frac{h(x, x^+)}{h(x, x^+) + N \mathbb{E}_{x^- \sim p} h(x, x^-)} \right] \\ & - \mathbb{E}_{\substack{x \sim p \\ x^+ \sim p_x^+ \\ \{x_i^-\}_{i=1}^N \sim p^N}} \left[-\log \frac{h(x, x^+)}{h(x, x^+) + \sum_{i=1}^N h(x, x_i^-)} \right] \leq e^{3/2} \sqrt{\frac{\pi}{2N}}. \end{aligned}$$

Equipped with this inequality, the biased objective can be decomposed into the sum of the debiased objective and a second term as follows:

$$\begin{aligned} & L_{\text{Biased}}^N(f) \\ &= \mathbb{E}_{\substack{x \sim p \\ x^+ \sim p_x^+ \\ \{x_i^-\}_{i=1}^N \sim p^N}} \left[-\log \frac{h(x, x^+)}{h(x, x^+) + \sum_{i=1}^N h(x, x_i^-)} \right] \\ &\geq \mathbb{E}_{\substack{x \sim p \\ x^+ \sim p_x^+}} \left[-\log \frac{h(x, x^+)}{h(x, x^+) + N \mathbb{E}_{x^- \sim p_x^-} h(x, x^-)} \right] - e^{3/2} \sqrt{\frac{\pi}{2N}} \\ &= \mathbb{E}_{\substack{x \sim p \\ x^+ \sim p_x^+}} \left[-\log \frac{h(x, x^+)}{h(x, x^+) + N \mathbb{E}_{x^- \sim p_x^-} h(x, x^-)} \right] \\ &\quad + \mathbb{E}_{\substack{x \sim p \\ x^+ \sim p_x^+}} \left[\log \frac{h(x, x^+) + N \mathbb{E}_{x^- \sim p_x^-} h(x, x^-)}{h(x, x^+) + N \mathbb{E}_{x^- \sim p_x^-} h(x, x^-)} \right] - e^{3/2} \sqrt{\frac{\pi}{2N}} \\ &= L_{\text{Debiased}}^N(f) + \mathbb{E}_{\substack{x \sim p \\ x^+ \sim p_x^+}} \left[\log \frac{h(x, x^+) + N \mathbb{E}_{x^- \sim p_x^-} h(x, x^-)}{h(x, x^+) + N \mathbb{E}_{x^- \sim p_x^-} h(x, x^-)} \right] - e^{3/2} \sqrt{\frac{\pi}{2N}} \\ &= L_{\text{Debiased}}^N(f) + \mathbb{E}_{\substack{x \sim p \\ x^+ \sim p_x^+}} \underbrace{\left[\log \frac{h(x, x^+) + \tau^- N \mathbb{E}_{x^- \sim p_x^-} h(x, x^-) + \tau^+ N \mathbb{E}_{x^- \sim p_x^+} h(x, x^-)}{h(x, x^+) + \tau^- N \mathbb{E}_{x^- \sim p_x^-} h(x, x^-) + \tau^+ N \mathbb{E}_{x^- \sim p_x^+} h(x, x^-)} \right]}_{g(x, x^+)} - e^{3/2} \sqrt{\frac{\pi}{2N}}. \end{aligned}$$

If $\mathbb{E}_{x^- \sim p_x^-} h(x, x^-) \geq \mathbb{E}_{x^- \sim p_x^+} h(x, x^-)$, then $g(x, x^+)$ can be lower bounded by $\log 1 = 0$. Otherwise, if $\mathbb{E}_{x^- \sim p_x^+} h(x, x^-) \leq \mathbb{E}_{x^- \sim p_x^-} h(x, x^-)$, we can use the elementary fact that $\frac{a+c}{b+c} \geq \frac{a}{b}$ for $a \leq b$ and $a, b, c \geq 0$. Combining these two cases, we conclude that

$$L_{\text{Biased}}^N(f) \geq L_{\text{Unbiased}}^N(f) + \mathbb{E}_{x \sim p} \left[0 \wedge \log \frac{\mathbb{E}_{x^+ \sim p_x^+} \exp f(x)^\top f(x^+)}{\mathbb{E}_{x^- \sim p_x^-} \exp f(x)^\top f(x^-)} \right] - e^{3/2} \sqrt{\frac{\pi}{2N}},$$

where we replaced the dummy variable x^- in the numerator by x^+ . \square

A.2 Proof of Lemma 2

The next result is a consequence of the dominated convergence theorem.

Lemma 2. For fixed Q and $N \rightarrow \infty$, it holds that

$$\begin{aligned} & \mathbb{E}_{\substack{x \sim p, x^+ \sim p_x^+ \\ \{x_i^-\}_{i=1}^N \sim p_x^-}} \left[-\log \frac{e^{f(x)^T f(x^+)}}{e^{f(x)^T f(x^+)} + \frac{Q}{N} \sum_{i=1}^N e^{f(x)^T f(x_i^-)}} \right] \\ & \longrightarrow \mathbb{E}_{\substack{x \sim p \\ x^+ \sim p_x^+}} \left[-\log \frac{e^{f(x)^T f(x^+)}}{e^{f(x)^T f(x^+)} + \frac{Q}{\tau^-} (\mathbb{E}_{x^- \sim p} [e^{f(x)^T f(x^-)}] - \tau^+ \mathbb{E}_{v \sim p_x^+} [e^{f(x)^T f(v)}])} \right]. \end{aligned}$$

Proof. Since the contrastive loss is bounded, applying the Dominated Convergence Theorem completes the proof:

$$\begin{aligned} & \lim_{N \rightarrow \infty} \mathbb{E} \left[-\log \frac{e^{f(x)^T f(x^+)}}{e^{f(x)^T f(x^+)} + \frac{Q}{N} \sum_{i=1}^N e^{f(x)^T f(x_i^-)}} \right] \\ & = \mathbb{E} \left[\lim_{N \rightarrow \infty} -\log \frac{e^{f(x)^T f(x^+)}}{e^{f(x)^T f(x^+)} + \frac{Q}{N} \sum_{i=1}^N e^{f(x)^T f(x_i^-)}} \right] \quad (\text{Dominated Convergence Theorem}) \\ & = \mathbb{E} \left[-\log \frac{e^{f(x)^T f(x^+)}}{e^{f(x)^T f(x^+)} + Q \mathbb{E}_{x^- \sim p_x^-} e^{f(x)^T f(x^-)}} \right]. \end{aligned}$$

Since $p_x^-(x') = (p(x') - \tau^+ p_x^+(x'))/\tau^-$ and by the linearity of the expectation, we have

$$\mathbb{E}_{x^- \sim p_x^-} e^{f(x)^T f(x^-)} = \tau^- (\mathbb{E}_{x^- \sim p} [e^{f(x)^T f(x^-)}] - \tau^+ \mathbb{E}_{x^- \sim p_x^+} [e^{f(x)^T f(x^-)}]),$$

which completes the proof. \square

A.3 Proof of Theorem 3

In order to prove Theorem 3, which shows that the empirical estimate of the asymptotic debiased objective is a good estimate, we first seek a bound on the tail probability that the difference between the integrands of the asymptotic and non-asymptotic objective functions is large. That is, we wish to bound the probability that the following quantity is greater than ε :

$$\Delta = \left| -\log \frac{h(x, x^+)}{h(x, x^+) + Q g(x, \{u_i\}_{i=1}^N, \{v_i\}_{i=1}^M)} + \log \frac{h(x, x^+)}{h(x, x^+) + Q \mathbb{E}_{x^- \sim p_x^-} h(x, x^-)} \right|,$$

where we again write $h(x, \bar{x}) = \exp^{f(x)^\top f(\bar{x})}$. Note that implicitly, Δ depends on x, x^+ and the collections $\{u_i\}_{i=1}^N$ and $\{v_i\}_{i=1}^M$. We achieve control over the tail via the following lemma.

Lemma A.2. Let x and x^+ in \mathcal{X} be fixed. Further, let $\{u_i\}_{i=1}^N$ and $\{v_i\}_{i=1}^M$ be collections of i.i.d. random variables sampled from p and p_x^+ respectively. Then for all $\varepsilon > 0$,

$$\mathbb{P}(\Delta \geq \varepsilon) \leq 2 \exp \left(-\frac{N \varepsilon^2 (\tau^-)^2}{2e^3} \right) + 2 \exp \left(-\frac{M \varepsilon^2 (\tau^-/\tau^+)^2}{2e^3} \right).$$

We delay the proof until after we prove Theorem 3, which we are ready to prove with this fact in hand.

Theorem 3. For any embedding f and finite N and M , we have

$$\left| \tilde{L}_{\text{Debiased}}^N(f) - L_{\text{Debiased}}^{N,M}(f) \right| \leq \frac{\varepsilon^{3/2}}{\tau^-} \sqrt{\frac{\pi}{2N}} + \frac{\varepsilon^{3/2} \tau^+}{\tau^-} \sqrt{\frac{\pi}{2M}}.$$

Proof. By Jensen's inequality, we may push the absolute value inside the expectation to see that $|\tilde{L}_{\text{Unbiased}}^N(f) - L_{\text{Debiased}}^{N,M}(f)| \leq \mathbb{E} \Delta$. All that remains is to exploit the exponential tail bound of Lemma A.2.

To do this we write the expectation of Δ for fixed x, x^+ as the integral of its tail probability,

$$\begin{aligned}\mathbb{E} \Delta &= \mathbb{E}_{x,x^+} [\mathbb{E}[\Delta|x, x^+]] = \mathbb{E}_{x,x^+} \left[\int_0^\infty \mathbb{P}(\Delta \geq \varepsilon|x, x^+) d\varepsilon \right] \\ &\leq \int_0^\infty 2 \exp \left(-\frac{N\varepsilon^2(\tau^-)^2}{2e^3} \right) d\varepsilon + \int_0^\infty 2 \exp \left(-\frac{M\varepsilon^2(\tau^-/\tau^+)^2}{2e^3} \right) d\varepsilon.\end{aligned}$$

The outer expectation disappears since the tail probably bound of Theorem A.2 holds uniformly for all fixed x, x^+ . Both integrals can be computed analytically using the classical identity

$$\int_0^\infty e^{-cz^2} dz = \frac{1}{2} \sqrt{\frac{\pi}{c}}.$$

Applying the identity to each integral we finally obtain the claimed bound,

$$\sqrt{\frac{2e^3\pi}{(\tau^-)^2 N}} + \sqrt{\frac{2e^3\pi}{(\tau^-/\tau^+)^2 M}} = \frac{e^{3/2}}{\tau^-} \sqrt{\frac{2\pi}{N}} + \frac{e^{3/2}\tau^+}{\tau^-} \sqrt{\frac{2\pi}{M}}.$$

□

We still owe the reader a proof of Lemma A.2, which we give now.

Proof of Lemma A.2. We first decompose the probability as

$$\begin{aligned}&\mathbb{P}\left(\left| -\log \frac{h(x, x^+)}{h(x, x^+) + Qg(x, \{u_i\}_{i=1}^N, \{v_i\}_{i=1}^M)} + \log \frac{h(x, x^+)}{h(x, x^+) + Q\mathbb{E}_{x^- \sim p_x^-} h(x, x^-)} \right| \geq \varepsilon\right) \\ &= \mathbb{P}\left(\left| \log \{h(x, x^+) + Qg(x, \{u_i\}_{i=1}^N, \{v_i\}_{i=1}^M)\} - \log \{h(x, x^+) + Q\mathbb{E}_{x^- \sim p_x^-} h(x, x^-)\} \right| \geq \varepsilon\right) \\ &= \mathbb{P}\left(\log \{h(x, x^+) + Qg(x, \{u_i\}_{i=1}^N, \{v_i\}_{i=1}^M)\} - \log \{h(x, x^+) + Q\mathbb{E}_{x^- \sim p_x^-} h(x, x^-)\} \geq \varepsilon\right) \\ &\quad + \mathbb{P}\left(-\log \{h(x, x^+) + Qg(x, \{u_i\}_{i=1}^N, \{v_i\}_{i=1}^M)\} + \log \{h(x, x^+) + Q\mathbb{E}_{x^- \sim p_x^-} h(x, x^-)\} \geq \varepsilon\right)\end{aligned}$$

where the final equality holds simply because $|X| \geq \varepsilon$ if and only if $X \geq \varepsilon$ or $-X \geq \varepsilon$. The first term can be bounded as

$$\begin{aligned}&\mathbb{P}\left(\log \{h(x, x^+) + Qg(x, \{u_i\}_{i=1}^N, \{v_i\}_{i=1}^M)\} - \log \{h(x, x^+) + Q\mathbb{E}_{x^- \sim p_x^-} h(x, x^-)\} \geq \varepsilon\right) \\ &= \mathbb{P}\left(\log \frac{h(x, x^+) + Qg(x, \{u_i\}_{i=1}^N, \{v_i\}_{i=1}^M)}{h(x, x^+) + Q\mathbb{E}_{x^- \sim p_x^-} h(x, x^-)} \geq \varepsilon\right) \\ &\leq \mathbb{P}\left(\frac{Qg(x, \{u_i\}_{i=1}^N, \{v_i\}_{i=1}^M) - Q\mathbb{E}_{x^- \sim p_x^-} h(x, x^-)}{h(x, x^+) + Q\mathbb{E}_{x^- \sim p_x^-} h(x, x^-)} \geq \varepsilon\right) \\ &= \mathbb{P}\left(g(x, \{u_i\}_{i=1}^N, \{v_i\}_{i=1}^M) - \mathbb{E}_{x^- \sim p_x^-} h(x, x^-) \geq \varepsilon \left\{ \frac{1}{Q} h(x, x^+) + \mathbb{E}_{x^- \sim p_x^-} h(x, x^-) \right\}\right) \\ &\leq \mathbb{P}\left(g(x, \{u_i\}_{i=1}^N, \{v_i\}_{i=1}^M) - \mathbb{E}_{x^- \sim p_x^-} h(x, x^-) \geq \varepsilon e^{-1}\right).\end{aligned}\tag{14}$$

The first inequality follows by applying the fact that $\log x \leq x - 1$ for $x > 0$. The second inequality holds since $\frac{1}{Q} h(x, x^+) + \mathbb{E}_{x^- \sim p_x^-} h(x, x^-) \geq 1/e$. Next, we move on to bounding the second term,

which proceeds similarly, using the same two bounds.

$$\begin{aligned}
& \mathbb{P} \left\{ -\log (h(x, x^+) + Qg(x, \{u_i\}_{i=1}^N, \{v_i\}_{i=1}^M)) + \log \{h(x, x^+) + Q\mathbb{E}_{x^- \sim p_x^-} h(x, x^-)\} \geq \varepsilon \right\} \\
&= \mathbb{P} \left(\log \frac{h(x, x^+) + Q\mathbb{E}_{x^- \sim p_x^-} h(x, x^-)}{h(x, x^+) + Qg(x, \{u_i\}_{i=1}^N, \{v_i\}_{i=1}^M)} \geq \varepsilon \right) \\
&\leq \mathbb{P} \left(\frac{Q\mathbb{E}_{x^- \sim p_x^-} h(x, x^-) - Qg(x, \{u_i\}_{i=1}^N, \{v_i\}_{i=1}^M)}{h(x, x^+) + Qg(x, \{u_i\}_{i=1}^N, \{v_i\}_{i=1}^M)} \geq \varepsilon \right) \\
&= \mathbb{P} \left(\mathbb{E}_{x^- \sim p_x^-} h(x, x^-) - g(x, \{u_i\}_{i=1}^N, \{v_i\}_{i=1}^M) \geq \varepsilon \left\{ \frac{1}{Q} h(x, x^+) + g(x, \{u_i\}_{i=1}^N, \{v_i\}_{i=1}^M) \right\} \right) \\
&\leq \mathbb{P} \left(\mathbb{E}_{x^- \sim p_x^-} h(x, x^-) - g(x, \{u_i\}_{i=1}^N, \{v_i\}_{i=1}^M) \geq \varepsilon e^{-1} \right). \tag{15}
\end{aligned}$$

Combining equation (14) and equation (15), we have

$$\mathbb{P}(\Delta \geq \varepsilon) \leq \mathbb{P} \left(|g(x, \{u_i\}_{i=1}^N, \{v_i\}_{i=1}^M) - \mathbb{E}_{x^- \sim p_x^-} h(x, x^-)| \geq \varepsilon e^{-1} \right).$$

We then proceed to bound the right hand tail probability. We are bounding the tail of a difference of the form $|\max(a, b) - c|$ where $c \geq b$. Notice that $|\max(a, b) - c| \leq |a - c|$. If $a > b$ then this relation is obvious, while if $a \leq b$ we have $|\max(a, b) - c| = |b - c| = c - b \leq c - a \leq |a - c|$. Using this elementary observation, we can decompose the random variable whose tail we wish to control as follows:

$$\begin{aligned}
& |g(x, \{u_i\}_{i=1}^N, \{v_i\}_{i=1}^M) - \mathbb{E}_{x^- \sim p_x^-} h(x, x^-)| \\
&\leq \frac{1}{\tau^-} \left| \frac{1}{N} \sum_{i=1}^N \mathbb{E}_{x \sim p} h(x, u_i) - \mathbb{E}_{x^- \sim p} h(x, x^-) \right| + \frac{\tau^+}{\tau^-} \left| \frac{1}{M} \sum_{i=1}^M \mathbb{E}_{x \sim p} h(x, v_i) - \mathbb{E}_{x^- \sim p_x^+} h(x, x^-) \right|
\end{aligned}$$

Using this observation, we find that

$$\begin{aligned}
& \mathbb{P} \left(|g(x, \{u_i\}_{i=1}^N, \{v_i\}_{i=1}^M) - \mathbb{E}_{x^- \sim p_x^-} h(x, x^-)| \geq \varepsilon e^{-1} \right) \\
&\leq \mathbb{P} \left(\left| \frac{1}{\tau^-} \left(\frac{1}{N} \sum_{i=1}^N e^{f(x)^T f(u_i)} - \tau^+ \frac{1}{M} \sum_{i=1}^M e^{f(x)^T f(v_i)} \right) - \mathbb{E}_{x^- \sim p_x^-} h(x, x^-) \right| \geq \varepsilon e^{-1} \right) \\
&\leq \mathbf{I}(\varepsilon) + \mathbf{II}(\varepsilon).
\end{aligned}$$

where

$$\begin{aligned}
\mathbf{I}(\varepsilon) &= \mathbb{P} \left(\left| \frac{1}{\tau^-} \left(\frac{1}{N} \sum_{i=1}^N h(x, u_i) - \mathbb{E}_{x^- \sim p} h(x, x^-) \right) \right| \geq \frac{\varepsilon e^{-1}}{2} \right) \\
\mathbf{II}(\varepsilon) &= \mathbb{P} \left(\left| \frac{\tau^+}{\tau^-} \left(\frac{1}{M} \sum_{i=1}^M h(x, v_i) - \mathbb{E}_{x^- \sim p_x^+} h(x, x^-) \right) \right| \geq \frac{\varepsilon e^{-1}}{2} \right).
\end{aligned}$$

Hoeffding's inequality states that if X, X_1, \dots, X_N are i.i.d random variables bounded in the range $[a, b]$, then

$$\mathbb{P} \left(\left| \frac{1}{n} \sum_{i=1}^N X_i - \mathbb{E} X \right| \geq \varepsilon \right) \leq 2 \exp \left(-\frac{2N\varepsilon^2}{b-a} \right).$$

In our particular case, $e^{-1} \leq h(x, \bar{x}) \leq e$, yielding the following bound on the tails of both terms:

$$\mathbf{I}(\varepsilon) \leq 2 \exp \left(-\frac{N\varepsilon^2(\tau^-)^2}{2e^3} \right) \quad \text{and} \quad \mathbf{II}(\varepsilon) \leq 2 \exp \left(-\frac{M\varepsilon^2(\tau^-/\tau^+)^2}{2e^3} \right).$$

□

A.4 Proof of Lemma 4

Lemma 4. For any embedding f , whenever $N \geq K - 1$ we have

$$L_{\text{Sup}}(f) \leq L_{\text{Sup}}^\mu(f) \leq \tilde{L}_{\text{Debiased}}^N(f).$$

Proof. We first show that $N = K - 1$ gives the smallest loss:

$$\begin{aligned} \tilde{L}_{\text{Unbiased}}^N(f) &= \mathbb{E}_{\substack{x \sim p \\ x^+ \sim p_x^+}} \left[-\log \frac{e^{f(x)^T f(x^+)}}{e^{f(x)^T f(x^+)} + N \mathbb{E}_{x^- \sim p_x^-} e^{f(x)^T f(x^-)}} \right] \\ &\geq \mathbb{E}_{\substack{x \sim p \\ x^+ \sim p_x^+}} \left[-\log \frac{e^{f(x)^T f(x^+)}}{e^{f(x)^T f(x^+)} + (K-1) \mathbb{E}_{x^- \sim p_x^-} e^{f(x)^T f(x^-)}} \right] \\ &= L_{\text{Unbiased}}^{K-1}(f) \end{aligned}$$

To show that $L_{\text{Unbiased}}^{K-1}(f)$ is an upper bound on the supervised loss $L_{\text{Sup}}(f)$, we additionally introduce a task specific class distribution $\rho_{\mathcal{T}}$ which is a uniform distribution over all the possible K -way classification tasks with classes in \mathcal{C} . That is, we consider all the possible task with K distinct classes $\{c_1, \dots, c_K\} \subseteq \mathcal{C}$.

$$\begin{aligned} L_{\text{Unbiased}}^{K-1}(f) &= \mathbb{E}_{\substack{x \sim p \\ x^+ \sim p_x^+}} \left[-\log \frac{e^{f(x)^T f(x^+)}}{e^{f(x)^T f(x^+)} + (K-1) \mathbb{E}_{x^- \sim p_x^-} e^{f(x)^T f(x^-)}} \right] \\ &= \mathbb{E}_{\mathcal{T} \sim \mathcal{D}} \mathbb{E}_{\substack{c \sim \rho_{\mathcal{T}}; x \sim p(\cdot|c) \\ x^+ \sim p(\cdot|c)}} \left[-\log \frac{e^{f(x)^T f(x^+)}}{e^{f(x)^T f(x^+)} + (K-1) \mathbb{E}_{\mathcal{T} \sim \mathcal{D}} \mathbb{E}_{\rho_{\mathcal{T}}(c^- \sim |c^- \neq h(x))} \mathbb{E}_{x^- \sim p(\cdot|c^-)} e^{f(x)^T f(x^-)}} \right] \\ &\geq \mathbb{E}_{\mathcal{T} \sim \mathcal{D}} \mathbb{E}_{\substack{c \sim \rho_{\mathcal{T}}; x \sim p(\cdot|c) \\ x^+ \sim p_x^+, \mathcal{T}}} \left[-\log \frac{e^{f(x)^T \mathbb{E}_{x^+ \sim p(\cdot|c)} f(x^+)}}{e^{f(x)^T \mathbb{E}_{x^+ \sim p_x^+, \mathcal{T}} f(x^+)} + (K-1) \mathbb{E}_{\mathcal{T} \sim \mathcal{D}} \mathbb{E}_{\rho_{\mathcal{T}}(c^- \sim |c^- \neq h(x))} \mathbb{E}_{x^- \sim p(\cdot|c^-)} e^{f(x)^T f(x^-)}} \right] \\ &\geq \mathbb{E}_{\mathcal{T} \sim \mathcal{D}} \mathbb{E}_{\substack{c \sim \rho_{\mathcal{T}}; x \sim p(\cdot|c) \\ x^+ \sim p(\cdot|c)}} \left[-\log \frac{e^{f(x)^T \mathbb{E}_{x^+ \sim p(\cdot|c)} f(x^+)}}{e^{f(x)^T \mathbb{E}_{x^+ \sim p(\cdot|c)} f(x^+)} + (K-1) \mathbb{E}_{\rho_{\mathcal{T}}(c^- \sim |c^- \neq h(x))} \mathbb{E}_{x^- \sim p(\cdot|c^-)} e^{f(x)^T f(x^-)}} \right] \\ &= \mathbb{E}_{\mathcal{T} \sim \mathcal{D}} \mathbb{E}_{\substack{c \sim \rho_{\mathcal{T}}; x \sim p(\cdot|c) \\ x^+ \sim p(\cdot|c)}} \left[-\log \frac{e^{f(x)^T \mathbb{E}_{x^+ \sim p(\cdot|c)} f(x^+)}}{e^{f(x)^T \mathbb{E}_{x^+ \sim p(\cdot|c)} f(x^+)} + (K-1) \mathbb{E}_{\rho_{\mathcal{T}}(c^- \sim |c^- \neq h(x))} \mathbb{E}_{x^- \sim p(\cdot|c^-)} e^{f(x)^T f(x^-)}} \right] \\ &\geq \mathbb{E}_{\mathcal{T} \sim \mathcal{D}} \mathbb{E}_{\substack{c \sim \rho_{\mathcal{T}}; x \sim p(\cdot|c) \\ x^+ \sim p(\cdot|c)}} \left[-\log \frac{e^{f(x)^T \mathbb{E}_{x^+ \sim p(\cdot|c)} f(x^+)}}{e^{f(x)^T \mathbb{E}_{x^+ \sim p(\cdot|c)} f(x^+)} + (K-1) \mathbb{E}_{\rho_{\mathcal{T}}(c^- \sim |c^- \neq h(x))} e^{f(x)^T \mathbb{E}_{x^- \sim p(\cdot|c^-)} f(x^-)}} \right] \\ &= \mathbb{E}_{\mathcal{T} \sim \mathcal{D}} \mathbb{E}_{\substack{c \sim \rho_{\mathcal{T}}; x \sim p(\cdot|c) \\ x^+ \sim p(\cdot|c)}} \left[-\log \frac{\exp(f(x)^T \mu_c)}{\exp(f(x)^T \mu_c) + \sum_{c^- \in \mathcal{T}, c^- \neq c} \exp(f(x)^T \mu_{c^-})} \right] \\ &= \mathbb{E}_{\mathcal{T} \sim \mathcal{D}} L_{\text{Sup}}^\mu(\mathcal{T}, f) \\ &= \bar{L}_{\text{Sup}}^\mu(f) \end{aligned}$$

where the three inequalities follow from Jensen's inequality. The first and third inequality shift the expectations $\mathbb{E}_{x^+ \sim p_x^+, \mathcal{T}}$ and $\mathbb{E}_{x^- \sim p(\cdot|c^-)}$, respectively, via the convexity of the functions and the second moves the expectation $\mathbb{E}_{\mathcal{T} \sim \mathcal{D}}$ out using concavity. Note that $\bar{L}_{\text{Sup}}(f) \leq \bar{L}_{\text{Sup}}^\mu(f)$ holds trivially. \square

A.5 Proof of Theorem 5

We wish to derive a data dependent bound on the downstream supervised generalization error of the debiased contrastive objective. Recall that a sample $(x, x^+, \{u_i\}_{i=1}^N, \{v_i\}_{i=1}^M)$ yields loss

$$-\log \left\{ \frac{e^{f(x)^\top f(x^+)}}{e^{f(x)^\top f(x^+)} + N g(x, \{u_i\}_{i=1}^N, \{v_i\}_{i=1}^M)} \right\} = \log \left\{ 1 + N \frac{g(x, \{u_i\}_{i=1}^N, \{v_i\}_{i=1}^M)}{e^{f(x)^\top f(x^+)}} \right\}$$

which is equal to $\ell \left(\left\{ f(x)^\top (f(u_i) - f(x^+)) \right\}_{i=1}^N, \left\{ f(x)^\top (f(v_i) - f(x^+)) \right\}_{i=1}^M \right)$, where we define

$$\ell(\{a_i\}_{i=1}^N, \{b_i\}_{i=1}^M) = \log \left\{ 1 + N \max \left(\frac{1}{\tau^-} \frac{1}{N} \sum_{i=1}^N a_i - \tau^+ \frac{1}{M} \sum_{i=1}^M b_i, e^{-1} \right) \right\}.$$

To derive our bound, we will exploit a concentration of measure result due to [1]. They consider an objective of the form

$$L_{un}(f) = \mathbb{E} \left[\ell \left(\left\{ f(x)^\top (f(x_i) - f(x^+)) \right\}_{i=1}^k \right) \right],$$

where $(x, x^+, x_1^-, \dots, x_k^-)$ are sampled from any fixed distribution on \mathcal{X}^{k+2} (they were particularly focused on the case where $x_i^- \sim p$, but the proof holds for arbitrary distributions). Let \mathcal{F} be a class of representation functions $\mathcal{X} \rightarrow \mathbb{R}^d$ such that $\|f(\cdot)\| \leq R$ for $R > 0$. The corresponding empirical risk minimizer is

$$\hat{f} \in \arg \min_{f \in \mathcal{F}} \frac{1}{T} \sum_{j=1}^T \ell \left(\left\{ f(x_j)^\top (f(x_{ji}) - f(x^+)) \right\}_{i=1}^k \right)$$

over a training set $\mathcal{S} = \{(x_j, x_j^+, x_{j1}^-, \dots, x_{jk}^-)\}_{j=1}^T$ of i.i.d. samples. Their result bounds the loss of the empirical risk minimizer as follows.

Lemma A.3. [1] *Let $\ell : \mathbb{R}^k \rightarrow \mathbb{R}$ be η -Lipschitz and bounded by B . Then with probability at least $1 - \delta$ over the training set $\mathcal{S} = \{(x_j, x_j^+, x_{j1}^-, \dots, x_{jk}^-)\}_{j=1}^T$, for all $f \in \mathcal{F}$*

$$L_{un}(\hat{f}) \leq L_{un}(f) + \mathcal{O} \left(\frac{\eta R \sqrt{k} \mathcal{R}_{\mathcal{S}}(\mathcal{F})}{T} + B \sqrt{\frac{\log \frac{1}{\delta}}{T}} \right)$$

where

$$\mathcal{R}_{\mathcal{S}}(\mathcal{F}) = \mathbb{E}_{\sigma \sim \{\pm 1\}^{(k+2)dT}} \left[\sup_{f \in \mathcal{F}} \langle \sigma, f|_{\mathcal{S}} \rangle \right],$$

and $f|_{\mathcal{S}} = \left(f_t(x_j), f_t(x_j^+), f_t(x_{j1}^-), \dots, f_t(x_{jk}^-) \right)_{\substack{j \in [T] \\ t \in [d]}}$.

In our context, we have $k = N + M$ and $R = e$. So, it remains to obtain constants η and B such that $\ell(\{a_i\}_{i=1}^N, \{b_i\}_{i=1}^M)$ is η -Lipschitz, and bounded by B . Note that since we consider normalized embeddings f , we have $\|f(\cdot)\| \leq 1$ and therefore only need to consider the domain where $e^{-1} \leq a_i, b_i \leq e$.

Lemma A.4. *Suppose that $e^{-1} \leq a_i, b_i \leq e$. The function $\ell(\{a_i\}_{i=1}^N, \{b_i\}_{i=1}^M)$ is η -Lipschitz, and bounded by B for*

$$\eta = e \cdot \sqrt{\frac{1}{(\tau^-)^2 N} + \frac{(\tau^+)^2}{M}}, \quad B = \mathcal{O} \left(\log N \left(\frac{1}{\tau^-} + \tau^+ \right) \right).$$

Proof. First, it is easily observed that ℓ is upper bounded by plugging in $a_i = e$ and $b_i = e^{-1}$, yielding a bound of

$$\log \left\{ 1 + N \max \left(\frac{1}{\tau^-} e - \tau^+ e^{-1}, e^{-1} \right) \right\} = \mathcal{O} \left(\log N \left(\frac{1}{\tau^-} + \tau^+ \right) \right).$$

To bound the Lipschitz constant we view ℓ as a composition $\ell(\{a_i\}_{i=1}^N, \{b_i\}_{i=1}^M) = \phi(g(\ell(\{a_i\}_{i=1}^N, \{b_i\}_{i=1}^M))$ where¹,

$$\begin{aligned}\phi(z) &= \log \left(1 + N \max(z, e^{-1}) \right) \\ g(\{a_i\}_{i=1}^N, \{b_i\}_{i=1}^M) &= \frac{1}{\tau^-} \frac{1}{N} \sum_{i=1}^N a_i - \tau^+ \frac{1}{M} \sum_{i=1}^M b_i.\end{aligned}$$

If $z < e^{-1}$ then $\partial_z \phi(z) = 0$, while if $z \geq e^{-1}$ then $\partial_z \phi(z) = \frac{N}{1+Nz} \leq \frac{N}{1+Ne^{-1}} \leq e$. We therefore conclude that ϕ is e -Lipschitz. Meanwhile, $\partial_{a_i} g = \frac{1}{\tau^- N}$ and $\partial_{b_i} g = \frac{\tau^+}{M}$. The Lipschitz constant of g is bounded by the Frobenius norm of the Jacobian of g , which equals

$$\sqrt{\sum_{i=1}^N \frac{1}{(\tau^- N)^2} + \sum_{j=1}^M \frac{(\tau^+)^2}{M^2}} = \sqrt{\frac{1}{(\tau^-)^2 N} + \frac{(\tau^+)^2}{M}}.$$

□

Now we have control on the bound on ℓ and its Lipschitz constant, we are ready to prove Theorem 5 by combining several of our previous results with Lemma A.3.

Theorem 5. *With probability at least $1 - \delta$, for all $f \in \mathcal{F}$ and $N \geq K - 1$,*

$$L_{\text{Sup}}(\hat{f}) \leq L_{\text{Sup}}^\mu(f) \leq L_{\text{Debiased}}^{N,M}(f) + \mathcal{O} \left(\frac{1}{\tau^-} \sqrt{\frac{1}{N}} + \frac{\tau^+}{\tau^-} \sqrt{\frac{1}{M}} + \frac{\lambda \mathcal{R}_{\mathcal{S}}(\mathcal{F})}{T} + B \sqrt{\frac{\log \frac{1}{\delta}}{T}} \right)$$

where $\lambda = \sqrt{\frac{1}{\tau^{-2}} \left(\frac{M}{N} + 1 \right) + \tau^{+2} \left(\frac{N}{M} + 1 \right)}$ and $B = \log N \left(\frac{1}{\tau^-} + \tau^+ \right)$.

Proof. By Lemma 4 and Theorem 3 we have

$$L_{\text{sup}}(\hat{f}) \leq \tilde{L}_{\text{Unbiased}}^N(\hat{f}) \leq L_{\text{Debiased}}^{N,M}(\hat{f}) + \frac{e^{3/2}}{\tau^-} \sqrt{\frac{\pi}{2N}} + \frac{e^{3/2} \tau^+}{\tau^-} \sqrt{\frac{\pi}{2M}}.$$

Combining Lemma A.3 and Lemma A.4, with probability at least $1 - \delta$, for all $f \in \mathcal{F}$, we have

$$L_{\text{Debiased}}^{N,M}(\hat{f}) \leq L_{\text{Debiased}}^{N,M}(f) + \mathcal{O} \left(\frac{\lambda \mathcal{R}_{\mathcal{S}}(\mathcal{F})}{T} + B \sqrt{\frac{\log \frac{1}{\delta}}{T}} \right),$$

where $\lambda = \eta \sqrt{k} = \sqrt{\frac{1}{\tau^{-2}} \left(\frac{M}{N} + 1 \right) + \tau^{+2} \left(\frac{N}{M} + 1 \right)}$ and $B = \log N \left(\frac{1}{\tau^-} + \tau^+ \right)$. □

A.6 Derivation of Equation (4)

In Section 4, we mentioned that the obvious way to approximate the unbiased objective is to replace p_x^- with $p_x^-(x') = (p(x') - \tau^+ p_x^+(x'))/\tau^-$ and then use the empirical counterparts for p and p_x^+ , and that this yields an objective that is a sum of $N + 1$ expectations. To give the derivation of this claim, let

$$\ell(x, x^+, \{x_i^-\}_{i=1}^N, f) = -\log \frac{e^{f(x)^T f(x^+)}}{e^{f(x)^T f(x^+)} + \sum_{i=1}^N e^{f(x)^T f(x_i^-)}}.$$

¹Note the definition of g is slightly modified in this context.

We plug in the decomposition as follows:

$$\begin{aligned}
& \mathbb{E}_{\substack{x \sim p, x^+ \sim p_x^+ \\ \{x_i^-\}_{i=1}^N \sim p_x^-}} [\ell(x, x^+, \{x_i^-\}_{i=1}^N, f)] \\
&= \int p(x) p_x^+(x^+) \prod_{i=1}^N p_x^-(x_i^-) \ell(x, x^+, \{x_i^-\}_{i=1}^N, f) dx dx^+ \prod_{i=1}^N dx_i^- \\
&= \int p(x) p_x^+(x^+) \prod_{i=1}^N \frac{p(x_i^-) - \tau^+ p_x^+(x_i^-)}{\tau^-} \ell(x, x^+, \{x_i^-\}_{i=1}^N, f) dx dx^+ \prod_{i=1}^N dx_i^- \\
&= \frac{1}{(\tau^-)^N} \int p(x) p_x^+(x^+) \prod_{i=1}^N \left(p(x_i^-) - \tau^+ p_x^+(x_i^-) \right) \ell(x, x^+, \{x_i^-\}_{i=1}^N, f) dx dx^+ \prod_{i=1}^N dx_i^-.
\end{aligned}$$

By the Binomial Theorem, the product inside the integral can be separated into $N + 1$ groups corresponding to how many x_i^- are sampled from p .

$$\begin{aligned}
(1) \quad & \prod_{i=1}^N p(x_i^-) \\
(2) \quad & \binom{N}{1} (-\tau^+) p_x^+(x_1^-) \prod_{i=2}^N p(x_i^-) \\
(3) \quad & \binom{N}{2} \prod_{j=1}^2 (-\tau^+) p_x^+(x_j^-) \prod_{i=3}^N p(x_i^-) \\
& \dots \\
(k+1) \quad & \binom{N}{k} \prod_{j=1}^k (-\tau^+) p_x^+(x_j^-) \prod_{i=k+1}^N p(x_i^-) \\
& \dots \\
(N+1) \quad & \prod_{i=1}^N (-\tau^+) p_x^+(x_i^-)
\end{aligned}$$

In particular, the objective becomes

$$\frac{1}{(\tau^-)^N} \sum_{k=0}^N \binom{N}{k} (-\tau^+)^k \mathbb{E}_{\substack{x \sim p, x^+ \sim p_x^+ \\ \{x_i^-\}_{i=1}^k \sim p_x^- \\ \{x_i^-\}_{i=k+1}^N \sim p}} \left[-\log \frac{e^{f(x)^T f(x^+)}}{e^{f(x)^T f(x^+)} + \sum_{i=1}^N e^{f(x)^T f(x_i^-)}} \right],$$

where $\{x_i^-\}_{i=k}^j = \emptyset$ if $k > j$. Note that this is exactly the *Inclusion–exclusion principle*. The numerical value of this objective is extremely small when N is large. We tried various approaches to optimize this objective, but none of them worked.

B Experimental Details

CIFAR10 and STL10 We adopt PyTorch to implement SimCLR [2] with ResNet-50 [17] as the encoder architecture and use the Adam optimizer [23] with learning rate 0.001 and weight decay $1e - 6$. We set the temperature t to 0.5 and the dimension of the latent vector to 128. All the models are trained for 400 epochs. The data augmentation uses the following PyTorch code:

The models are evaluated by training a linear classifier with cross entropy loss after fixing the learned embedding. We again use the Adam optimizer with learning rate 0.001 and weight decay $1e - 6$.

Imagenet-100 We adopt the official code² for contrastive multiview coding (CMC) [40]. To implement the debiased objective, we only modify the “NCE/NCECriterion.py” file and adopt the rest

²<https://github.com/HobbitLong/CMC/>

```

1 train_transform = transforms.Compose([
2     transforms.RandomResizedCrop(32),
3     transforms.RandomHorizontalFlip(p=0.5),
4     transforms.RandomApply([transforms.ColorJitter(0.4, 0.4, 0.4, 0.1)], p
5 =0.8),
6     transforms.RandomGrayscale(p=0.2),
7     GaussianBlur(kernel_size=int(0.1 * 32)),
8     transforms.ToTensor(),
9     transforms.Normalize([0.4914, 0.4822, 0.4465], [0.2023, 0.1994, 0.2010])
10])

```

Figure 6: PyTorch code for SimCLR data augmentation.

of the code without change. The temperature of CMC is set to 0.07, which often makes the estimator $\frac{1}{\tau^-} \left(\frac{1}{N} \sum_{i=1}^N e^{f(x)^T f(u_i)} - \tau^+ \frac{1}{M} \sum_{i=1}^M e^{f(x)^T f(v_i)} \right)$ less than $e^{-1/t}$. To retain the learning signal, whenever the estimator is less than $e^{-1/t}$, we optimize the biased loss instead. This improves the convergence and stability of our method.

Sentence Embedding We adopt the official code³ for quick-thought (QT) vectors [28]. To implement the debiased objective, we only modify the “src/s2v-model.py” file and adopt the rest of the code without changes. Since the official BookCorpus [25] dataset is missing, we use the inofficial version⁴ for the experiments. The feature vector of QT is not normalized, therefore, we simply constrain the estimator described in equation (7) to be greater than zero.

Reinforcement Learning We adopt the official code⁵ of Contrastive unsupervised representations for reinforcement learning (CURL) [37]. To implement the debiased objective, we only modify the “curl-sac.py” file and adopt the rest of the code without changes. We again constrain the estimator described in equation (7) to be greater than zero since the feature vector of CURL is not normalized.

³<https://github.com/lajanugen/S2V>

⁴<https://github.com/soskek/bookcorpus>

⁵<https://github.com/MishaLaskin/curl>