

---

# Debiased Contrastive Learning

---

Ching-Yao Chuang, Joshua Robinson, Lin Yen-Chen

Antonio Torralba, Stefanie Jegelka

CSAIL, Massachusetts Institute of Technology

Cambridge, MA 02139, USA

{cychuang, joshrob, yenchenl, torralba, stefje}@mit.edu

## 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  $x^-$  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

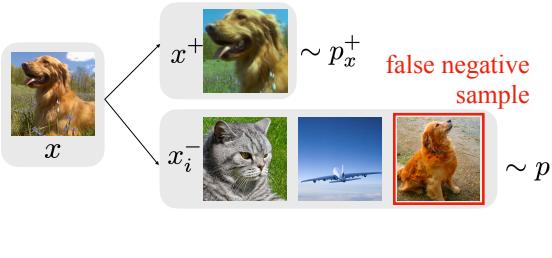


Figure 1: “Sampling bias”: The common practice of drawing negative examples  $x_i^-$  from the data distribution  $p(x)$  may result in  $x_i^-$  that are actually similar to  $x$ .

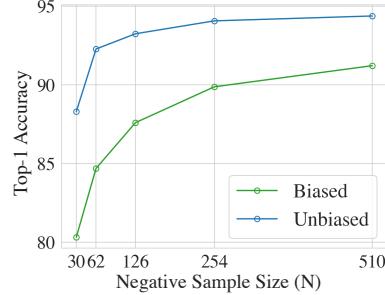


Figure 2: Sampling bias leads to performance drop: Results on CIFAR-10 for drawing  $x_i^-$  from  $p(x)$  (biased) and from data with different labels, i.e., truly semantically different data (unbiased).

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*  $L_{\text{Biased}}^N$ . When drawn from  $p(x)$ , the sample  $x_i^-$  will come from the same class as  $x$  with probability  $\tau^+$ .

Lemma 1 shows that in the limit, the standard loss  $L_{\text{Biased}}^N$  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  $L_{\text{Biased}}^N$  and minimizing the ideal loss  $L_{\text{Unbiased}}^N$  can result in very different learned representations.

### 4 Debiased Contrastive Loss

Next, we derive a loss that is closer to the ideal  $L_{\text{Unbiased}}^N$ , while only having access to positive samples and samples from  $p$ . Figure 2 shows that the resulting embeddings are closer to those learned with  $L_{\text{Unbiased}}^N$ . 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  $L_{\text{Unbiased}}^N$  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  $\tau^+$  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  $L_{\text{Debiased}}^N$  empirically, and compare it to the standard loss  $L_{\text{Biased}}^N$  and the ideal loss  $L_{\text{Unbiased}}^N$ . 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  $L_{\text{Unbiased}}^N$ , 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.

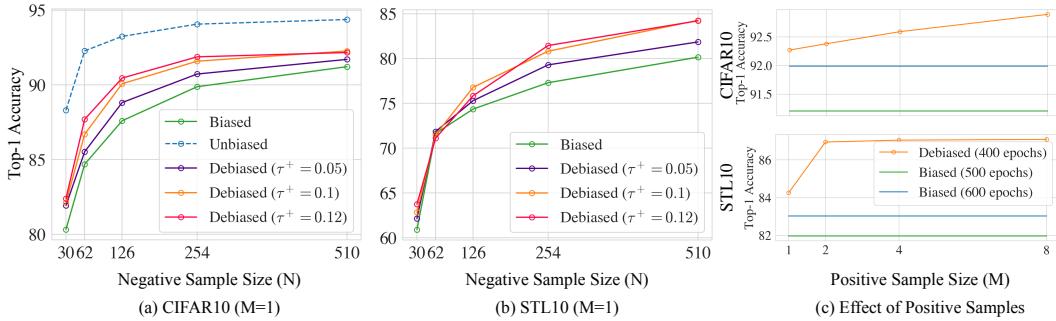


Figure 4: **Classification accuracy on CIFAR10 and STL10.** (a,b) Biased and Debiased ( $M = 1$ ) SimCLR with different negative sample size  $N$  where  $N = 2(\text{BatchSize} - 1)$ . (c) Comparison with biased SimCLR with 50% more training epochs (600 epochs) while fixing the training epoch for Debiased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

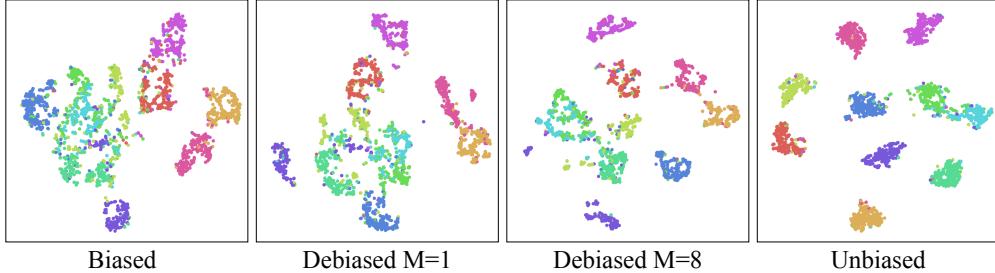


Figure 5: **t-SNE visualization of learned representations on CIFAR10.** Classes are indicated by colors. The debiased objective ( $\tau^+ = 0.1$ ) leads to better data clustering than the (standard) biased loss; its effect is closer to the supervised unbiased objective.

## 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  $\tau^+$ . 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  $\tau^+$  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 ( $\tau^+ = 0.01$ )	<b>74.6</b>	<b>92.08</b>

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)	<b>76.8</b>	81.3	86.6	93.4	<b>89.8</b>	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	<b>82.9</b>	<b>86.9</b>	<b>93.7</b>	89.1	<b>74.7</b>	<b>82.7</b>

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±33	850±20	918±96	266±41	623±120	928±47
<i>Debiased Objective with <math>M = 1</math></i>						
Debiased ( $\tau^+ = 0.01$ )	324±34	843±30	<b>927±99</b>	<b>310±12</b>	<b>626±82</b>	937±9
Debiased ( $\tau^+ = 0.05$ )	308±57	<b>866±7</b>	916±114	284±20	613±22	945±13
Debiased ( $\tau^+ = 0.1$ )	<b>364±36</b>	860±4	868±177	302±29	594±33	<b>951±11</b>
<i>Debiased Objective with <math>M = 2</math></i>						
Debiased ( $\tau^+ = 0.01$ )	330±10	858±10	754±179	286±20	<b>746±93</b>	949±5
Debiased ( $\tau^+ = 0.1$ )	<b>381±24</b>	864±6	904±117	303±5	671±75	<b>957±5</b>

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  $\rho$  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.

**Acknowledgements** This work was supported by MIT-IBM Watson AI Lab, an NSF TRIPODS+X grant (number: 1839258), NSF BIDGATA award 1741341 and the MIT-MSR Trustworthy and Robust AI Collaboration. We thank Wei Fang, Tongzhou Wang, Wei-Chiu Ma, and Behrooz Tahmasebi for helpful discussions and suggestions.

## References

- [1] Sanjeev Arora, Hrishikesh Khandeparkar, Mikhail Khodak, Orestis Plevrakis, and Nikunj Saunshi. A theoretical analysis of contrastive unsupervised representation learning. *International Conference on Machine Learning*, 2019.
- [2] Ting Chen, Simon Kornblith, Mohammad Norouzi, and Geoffrey Hinton. A simple framework for contrastive learning of visual representations. *arXiv preprint arXiv:2002.05709*, 2020.
- [3] Xi Chen, Yan Duan, Rein Houthooft, John Schulman, Ilya Sutskever, and Pieter Abbeel. Infogan: Interpretable representation learning by information maximizing generative adversarial nets. In *Advances in neural information processing systems*, pages 2172–2180, 2016.
- [4] Xinlei Chen, Haoqi Fan, Ross Girshick, and Kaiming He. Improved baselines with momentum contrastive learning. *arXiv preprint arXiv:2003.04297*, 2020.
- [5] Youngduck Choi, Chill Yi-I Chiu, and David Sontag. Learning low-dimensional representations of medical concepts. *AMIA Summits on Translational Science Proceedings*, 2016:41, 2016.
- [6] Marthinus Christoffel, Gang Niu, and Masashi Sugiyama. Class-prior estimation for learning from positive and unlabeled data. In *Asian Conference on Machine Learning*, pages 221–236, 2016.
- [7] Adam Coates, Andrew Ng, and Honglak Lee. An analysis of single-layer networks in unsupervised feature learning. In *Proceedings of the fourteenth international conference on artificial intelligence and statistics*, pages 215–223, 2011.
- [8] Jacob Devlin, Ming-Wei Chang, Kenton Lee, and Kristina Toutanova. Bert: Pre-training of deep bidirectional transformers for language understanding. In *Proceedings of the 2019 Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies, Volume 1 (Long and Short Papers)*, pages 4171–4186, 2019.
- [9] Bill Dolan, Chris Quirk, and Chris Brockett. Unsupervised construction of large paraphrase corpora: Exploiting massively parallel news sources. In *Proceedings of the 20th international conference on Computational Linguistics*, page 350. Association for Computational Linguistics, 2004.
- [10] Alexey Dosovitskiy, Jost Tobias Springenberg, Martin Riedmiller, and Thomas Brox. Discriminative unsupervised feature learning with convolutional neural networks. In *Advances in neural information processing systems*, pages 766–774, 2014.
- [11] Marthinus Du Plessis, Gang Niu, and Masashi Sugiyama. Convex formulation for learning from positive and unlabeled data. In *International Conference on Machine Learning*, pages 1386–1394, 2015.
- [12] Marthinus C Du Plessis, Gang Niu, and Masashi Sugiyama. Analysis of learning from positive and unlabeled data. In *Advances in neural information processing systems*, pages 703–711, 2014.
- [13] Charles Elkan and Keith Noto. Learning classifiers from only positive and unlabeled data. In *Proceedings of the 14th ACM SIGKDD international conference on Knowledge discovery and data mining*, pages 213–220, 2008.

- [14] Ian Goodfellow, Jean Pouget-Abadie, Mehdi Mirza, Bing Xu, David Warde-Farley, Sherjil Ozair, Aaron Courville, and Yoshua Bengio. Generative adversarial nets. In *Advances in neural information processing systems*, pages 2672–2680, 2014.
- [15] Raia Hadsell, Sumit Chopra, and Yann LeCun. Dimensionality reduction by learning an invariant mapping. In *2006 IEEE Computer Society Conference on Computer Vision and Pattern Recognition (CVPR’06)*, volume 2, pages 1735–1742. IEEE, 2006.
- [16] Tatsunori Hashimoto, Megha Srivastava, Hongseok Namkoong, and Percy Liang. Fairness without demographics in repeated loss minimization. In *International Conference on Machine Learning*, pages 1929–1938, 2018.
- [17] 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.
- [18] Kaiming He, Haoqi Fan, Yuxin Wu, Saining Xie, and Ross Girshick. Momentum contrast for unsupervised visual representation learning. *Proceedings of the IEEE conference on computer vision and pattern recognition*, 2020.
- [19] Olivier J Hénaff, Aravind Srinivas, Jeffrey De Fauw, Ali Razavi, Carl Doersch, SM Eslami, and Aaron van den Oord. Data-efficient image recognition with contrastive predictive coding. *arXiv preprint arXiv:1905.09272*, 2019.
- [20] Minqing Hu and Bing Liu. Mining and summarizing customer reviews. In *Proceedings of the tenth ACM SIGKDD international conference on Knowledge discovery and data mining*, pages 168–177, 2004.
- [21] Shantanu Jain, Martha White, and Predrag Radivojac. Estimating the class prior and posterior from noisy positives and unlabeled data. In *Advances in neural information processing systems*, pages 2693–2701, 2016.
- [22] Edward Kim, Zach Jensen, Alexander van Grootel, Kevin Huang, Matthew Staib, Sheshera Mysore, Haw-Shiuan Chang, Emma Strubell, Andrew McCallum, Stefanie Jegelka, et al. Inorganic materials synthesis planning with literature-trained neural networks. *Journal of Chemical Information and Modeling*, 60(3):1194–1201, 2020.
- [23] Diederik P Kingma and Jimmy Ba. Adam: A method for stochastic optimization. *International Conference on Learning Representations*, 2015.
- [24] Diederik P Kingma and Max Welling. Auto-encoding variational bayes. *International Conference on Learning Representations*, 2014.
- [25] Ryan Kiros, Yukun Zhu, Russ R Salakhutdinov, Richard Zemel, Raquel Urtasun, Antonio Torralba, and Sanja Fidler. Skip-thought vectors. In *Advances in neural information processing systems*, pages 3294–3302, 2015.
- [26] Ryuichi Kiryo, Gang Niu, Marthinus C du Plessis, and Masashi Sugiyama. Positive-unlabeled learning with non-negative risk estimator. In *Advances in neural information processing systems*, pages 1675–1685, 2017.
- [27] Alex Krizhevsky et al. Learning multiple layers of features from tiny images. 2009.
- [28] Lajanugen Logeswaran and Honglak Lee. An efficient framework for learning sentence representations. *International Conference on Learning Representations*, 2018.
- [29] Ninareh Mehrabi, Fred Morstatter, Nripsuta Saxena, Kristina Lerman, and Aram Galstyan. A survey on bias and fairness in machine learning. *arXiv preprint arXiv:1908.09635*, 2019.
- [30] Tomas Mikolov, Ilya Sutskever, Kai Chen, Greg S Corrado, and Jeff Dean. Distributed representations of words and phrases and their compositionality. In *Advances in neural information processing systems*, pages 3111–3119, 2013.
- [31] Riccardo Miotto, Fei Wang, Shuang Wang, Xiaoqian Jiang, and Joel T Dudley. Deep learning for healthcare: review, opportunities and challenges. *Briefings in bioinformatics*, 19(6):1236–1246, 2018.
- [32] 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.
- [33] Aaron van den Oord, Yazhe Li, and Oriol Vinyals. Representation learning with contrastive predictive coding. *arXiv preprint arXiv:1807.03748*, 2018.

- [34] Bo Pang and Lillian Lee. A sentimental education: Sentiment analysis using subjectivity summarization based on minimum cuts. In *Proceedings of the 42nd annual meeting on Association for Computational Linguistics*, page 271. Association for Computational Linguistics, 2004.
- [35] Bo Pang and Lillian Lee. Seeing stars: Exploiting class relationships for sentiment categorization with respect to rating scales. In *Proceedings of the 43rd annual meeting on association for computational linguistics*, pages 115–124. Association for Computational Linguistics, 2005.
- [36] Jake Snell, Kevin Swersky, and Richard Zemel. Prototypical networks for few-shot learning. In *Advances in neural information processing systems*, pages 4077–4087, 2017.
- [37] Aravind Srinivas, Michael Laskin, and Pieter Abbeel. Curl: Contrastive unsupervised representations for reinforcement learning. *arXiv preprint arXiv:2004.04136*, 2020.
- [38] Jonathan M Stokes, Kevin Yang, Kyle Swanson, Wengong Jin, Andres Cubillos-Ruiz, Nina M Donghia, Craig R MacNair, Shawn French, Lindsey A Carfrae, Zohar Bloom-Ackerman, et al. A deep learning approach to antibiotic discovery. *Cell*, 180(4):688–702, 2020.
- [39] Yuval Tassa, Yotam Doron, Alistair Muldal, Tom Erez, Yazhe Li, Diego de Las Casas, David Budden, Abbas Abdolmaleki, Josh Merel, Andrew Lefrancq, et al. Deepmind control suite. *arXiv preprint arXiv:1801.00690*, 2018.
- [40] Yonglong Tian, Dilip Krishnan, and Phillip Isola. Contrastive multiview coding. *arXiv preprint arXiv:1906.05849*, 2019.
- [41] Ellen M Voorhees. Overview of trec 2002.
- [42] Tongzhou Wang and Phillip Isola. Understanding contrastive representation learning through alignment and uniformity on the hypersphere. *arXiv preprint arXiv:2005.10242*, 2020.
- [43] Janyce Wiebe, Theresa Wilson, and Claire Cardie. Annotating expressions of opinions and emotions in language. *Language resources and evaluation*, 39(2-3):165–210, 2005.
- [44] Xiaohua Zhai, Avital Oliver, Alexander Kolesnikov, and Lucas Beyer. S4l: Self-supervised semi-supervised learning. In *Proceedings of the IEEE international conference on computer vision*, pages 1476–1485, 2019.
- [45] Richard Zhang, Phillip Isola, and Alexei A Efros. Colorful image colorization. In *European conference on computer vision*, pages 649–666. Springer, 2016.