CONDITIONAL NEGATIVE SAMPLING FOR CONTRASTIVE LEARNING OF VISUAL REPRESENTATIONS

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ABSTRACT

Recent methods for learning unsupervised visual representations, dubbed contrastive learning, optimize the noise-contrastive estimation (NCE) bound on mutual information between two views of an image. NCE uses randomly sampled negative examples to normalize the objective. In this paper, we show that choosing difficult negatives, or those more similar to the current instance, can yield stronger representations. To do this, we introduce a family of mutual information estimators that sample negatives conditionally – in a “ring” around each positive. We prove that these estimators lower-bound mutual information, with higher bias but lower variance than NCE. Experimentally, we find our approach, applied on top of existing models (IR, CMC, and MoCo) improves accuracy by 2-5% points in each case, measured by linear evaluation on four standard image datasets. Moreover, we find continued benefits when transferring features to a variety of new image distributions from the Meta-Dataset collection and to a variety of downstream tasks such as object detection, instance segmentation, and keypoint detection.

1 INTRODUCTION

Supervised learning algorithms have given rise to human-level performance in several visual tasks (Russakovsky et al., 2015; Redmon et al., 2016; He et al., 2017), relying heavily on large image datasets paired with semantic annotations. These annotations vary in difficulty and cost, spanning from simple class labels (Deng et al., 2009) to more granular descriptions like bounding boxes (Everingham et al., 2010; Lin et al., 2014) and key points (Lin et al., 2014). As it is impractical to scale high quality annotations to the size that modern deep learning demands, this reliance on supervision poses a barrier to widespread adoption. In response, we have seen the growth of unsupervised approaches to learning representations, or embeddings, that are general and can be re-used for many tasks at once. In natural language processing, this approach has been highly successful, resulting in the popular GPT (Radford et al., 2018; 2019; Brown et al., 2020) and BERT (Devlin et al., 2018; Liu et al., 2019) models. While supervised pretraining is still dominant in computer vision, recent approaches using “contrastive” objectives, have sparked great interest from the research community (Wu et al., 2018; Oord et al., 2018; Hjelm et al., 2018; Zhuang et al., 2019; Henaff et al., 2019; Misra & Maaten, 2020; He et al., 2019; Chen et al., 2020a,b; Grill et al., 2020). In the last two years, contrastive methods have already achieved remarkable results, quickly closing the gap to supervised methods (He et al., 2016; 2019; Chen et al., 2020a; Grill et al., 2020).

Recent contrastive algorithms were developed as estimators of mutual information (Oord et al., 2018; Hjelm et al., 2018; Bachman et al., 2019), building on the intuition that a good low-dimensional “representation” would be one that linearizes the useful information embedded within a high-dimensional data point. In the visual domain, these estimators optimize an encoder by maximizing the similarity of encodings for two augmentations (i.e. transformations) of the same image. Doing so is trivial unless this similarity function is normalized. This is done by using “negative examples”, contrasting an image (e.g. of a cat) with a set of possible other images (e.g. of dogs, tables, cars, etc.). We hypothesize that the manner in which we choose these negatives greatly effects the quality of the representations. For instance, differentiating a cat from other breeds of cats is visually more difficult than differentiating a cat from other classes. The encoder may thus have to focus on more granular, semantic information (e.g. fur patterns) that may be useful for downstream visual...
tasks (e.g., object classification). While research in contrastive learning has explored architectures, augmentations, and pretext tasks, there has been little attention given to how one chooses negative samples beyond the common tactic of uniformly sampling from the training dataset.

While choosing more difficult negatives seems promising, there are several unanswered theoretical and practical questions. Naively choosing difficult negatives may yield an objective that no longer bounds mutual information. Since such bounds are the basis for many contrastive objectives, and have been used for choosing good augmentations (Tian et al., 2020) and other innovations, it is desirable to use harder negatives without losing this property. Moreover, even if choosing difficult negatives is theoretically justified, we do not know if it will yield representations better for downstream tasks. In this paper, we present a new family of estimators that supports sampling negatives from a particular class of conditional distributions. We then prove that this family remains a lower bound of mutual information. Moreover, we show that while they are a looser bound than the well-known noise contrastive estimator, estimators in this family have lower variance. We propose a particular method, the Ring model, within this family for choosing negatives that are close, but not too close, to the positive example. We then apply Ring to representation learning, where it is straightforward to adjust state-of-the-art contrastive objectives (e.g., MoCo, CMC) to sample harder negatives. We find that Ring negatives improve transfer performance across datasets and across underlying objectives, making this an easy and useful addition to contrastive learning methods.

2 Background

Recent contrastive learning has focused heavily on exemplar-based objectives, where examples, or instances, are compared to one another to learn a representation. Many of these exemplar-based losses (Hjelm et al., 2018; Wu et al., 2018; Bachman et al., 2019; Zhuang et al., 2019; Tian et al., 2019; Chen et al., 2020a) are equivalent to noise contrastive estimation, or NCE (Gutmann & Hyvärinen, 2010; Oord et al., 2018; Poole et al., 2019), which is a popular lower bound on the mutual information, denoted by $I$, between two random variables. This connection is well-known and stated in several works (Chen et al., 2020a; Tschannen et al., 2019; Tian et al., 2020, as well as explicitly motivating several algorithms (e.g., Deep InfoMax (Hjelm et al., 2018; Bachman et al., 2019)), and choices of image views (Tian et al., 2020). To review, recall the NCE objective:

$$I(U; V) \geq \mathcal{L}_{\text{NCE}}(u_i, v_i) = \mathbb{E}_{u_i, v_i \sim p(u, v)} \mathbb{E}_{v_1, v_2 \sim p(v)} \left[ \log \frac{e^{f_\theta(u_i, v_i)}}{\frac{1}{k+1} \sum_{j \in \{i, 1, \ldots, k\}} e^{f_\theta(u_i, v_j)}} \right]$$

(1)

where $u, v$ are realizations of two random variables of interest, $U$ and $V$. We call $v_{1:k} = \{v_1, \ldots, v_k\}$ “negative examples” that normalize the numerator with respect to other possible realizations of $V$. A proof of the inequality in Eq. 1 can be found in Poole et al. (2019).

Now, suppose $U$ and $V$ are derived from the same random variable $X$, and we are given a dataset $D = \{x_i\}_{i=1}^n$ of $n$ values that $X$ can take, sampled from a distribution $p(x)$. Define $T$ as a family of functions where each member $t : X \rightarrow X$ maps one realization of $X$ to another. We call a transformed input $t(x)$ a “view” of $x$. In vision, $t \in T$ is user-specified to be a composition of cropping, adding color jitter, gaussian blurring, among many others (Wu et al., 2018; Bachman et al., 2019; Chen et al., 2020a). The choice of view family is a primary determinant of how successful a contrastive algorithm is (Tian et al., 2020, 2019; Chen et al., 2020a). Finally, let $p(t)$ denote a distribution over $T$ from which we can sample, a common choice being uniform over $T$.

Next, introduce an encoder $g_\theta : X \rightarrow \mathbb{R}^d$ that maps an instance to a representation. Then, a general contrastive objective for the $i$-th example in $D$ is:

$$\mathcal{L}(x_i) = \mathbb{E}_{t, t', t_1, k \sim p(t)} \mathbb{E}_{x_1, k \sim p(x)} \left[ \log \frac{e^{g_\theta(t(x_i))^T g_\theta(t'(x_i))/\tau}}{\frac{1}{k+1} \sum_{j \in \{i, 1, \ldots, k\}} e^{g_\theta(t(x_j))^T g_\theta(t'(x_j))/\tau}} \right]$$

(2)

where $\tau$ is a temperature used to scale the dot product. The equivalence to NCE is immediate given $f_\theta(u, v) = g_\theta(u)^T g_\theta(v)/\tau$. We can interpret maximizing Eq. 2 as choosing an embedding that pulls two views of the same instance together while pushing two views of distinct instances apart. As a result, the learned representation is invariant to the transformations in $T$. The output of $g_\theta$ is $L_2$ normalized to prevent trivial solutions. That is, it is optimal to uniformly disperse representations across the surface of the hypersphere. A drawback to NCE, and consequently to this
class of contrastive objectives, is that the number of negative examples $k$ must be large to faithfully approximate the true partition function. However, the size of $k$ in Eq. 2 is limited by compute and memory when optimizing. Thus, recent innovations have focused on tackling this challenge.

Instance Discrimination (Wu et al., 2018), or IR, introduces a memory bank $M$ to cache embeddings of each $x_i \in D$. Since every epoch we observe each instance once, the memory bank will save the embedding of the view of $x_i$ observed last epoch in its $i$-th entry. Then, the objective is:

$$
\mathcal{L}_{IR}(x_i; M) = \mathbb{E}_{t \sim p(t)} \mathbb{E}_{j \sim U(1,n)} \left[ \log \frac{e^{g(t(x_i))^T M[i]/\tau}}{ \frac{1}{k+1} \sum_{j \in \{i,j_{1:k}\}} e^{g(t(x_i))^T M[j]/\tau}} \right],
$$

where $M[i]$ represents fetching the $i$-th entry in $M$, and $j_{1:k} \sim U(1,n)$ indicates uniformly sampling $k$ integers from 1 to $n$, or equivalently entries from $M$. Observe that sampling uniformly $k$ times from $M$ is equivalent to $x_{1:k} \sim p(x)$. Representations stored in the memory bank are removed from the automatic differentiation tape, but in return, we can choose a large $k$. Several later approaches (Zhuang et al. 2019; Tian et al. 2019; IScen et al. 2019; Srinivas et al. 2020) build on the IR framework. In particular, Contrastive Multiview Coding (Tian et al., 2019), or CMC, decomposes an image into luminance and AB-color channels. Then, CMC is the sum of two IR losses where the memory banks for each “modality” are swapped, encouraging the representation of the luminance of an image to be “close” to the representation of the AB-color of that image, and vice versa.

Momentum Contrast (He et al., 2019; Chen et al., 2020b), or MoCo, observed that the representations stored in the memory bank grow stale, since possibly thousands of optimization steps pass before updating an entry twice. This is problematic as stale entries could bias gradients. So, MoCo makes two important changes to the IR framework. First, it replaces the memory bank with a first-in-first-out (FIFO) queue $Q$ of size $k$. During each minibatch, representations are cached into the queue while the most stale ones are removed. Since elements in a minibatch are chosen i.i.d. from $p(x)$, using the queue as negatives is equivalent to drawing $x_{1:k} \sim p(x)$ i.i.d. Second, MoCo introduces a second (momentum) encoder $g_{\theta'}$. Now, the primary encoder $g_\theta$ is used to embed one view of instance $x_i$, whereas the momentum encoder is used to embed the other. Again, gradients are not propagated to $g_{\theta'}$. Instead, its parameters are deterministically set by $\theta' = m\theta + (1 - m)\theta$ where $m$ is a “momentum” coefficient. In summary, the MoCo objective is

$$
\mathcal{L}_{MoCo}(x_i; Q) = \mathbb{E}_{t \sim p(t)} \mathbb{E}_{j \sim U(1,n)} \left[ \log \frac{e^{g(t(x_i))^T g_{\theta'}(t'(x_i))/\tau}}{ \frac{1}{k+1} \sum_{j \in \{i,j_{1:k}\}} e^{g(t(x_i))^T Q[j]/\tau}} \right],
$$

again equivalent to NCE under a slightly different implementation.

3 Conditional Noise Contrastive Estimation

In NCE, the negative examples are sampled i.i.d. from the marginal distribution. Indeed, the existing proof that NCE lower bounds mutual information (Poole et al., 2019) assumes this to be true. However, choosing negatives in this manner may not be the best choice for learning a good representation. For instance, prior work in metric learning has shown the effectiveness of hard negative mining in optimizing triplet losses (Wu et al., 2017; Yuan et al., 2017; Schroff et al., 2015). In this work, we similarly wish to exploit choosing negatives conditional on the current instance but to do so in a manner that preserves the relationship of contrastive algorithms to mutual information.

We consider the general case of two random variables $U$ and $V$ according to a distribution $p(u, v)$, although the application to the contrastive setting is straightforward. To start, suppose we define a new distribution $q(v|v^*)$ conditional on a specific realization $v^*$ of $V$. Ideally, we would like for $q(v|v^*)$ to belong to any distribution family but not all choices of $q$ preserve a bound. We provide a counterexample in the Appendix. This does not, however, imply that we can only sample negatives from the marginal $p(v)$ (Poole et al., 2019; Oord et al., 2018). One of our theoretical contributions is to formally define a family of conditional distributions $Q$ such that for any $q \in Q$, we can draw negative examples from it, instead of $p$, in the NCE estimator while maintaining a lower bound on $\mathcal{I}(U; V)$. We call our new lower bound on mutual information the Conditional Noise Contrastive Estimator, or CNCE. The next Theorem shows CNCE to bound $\mathcal{I}(U; V)$.

**Theorem 3.1.** Define $U$ and $V_i$ by $p(u, v_1)$ and let $V_1, \ldots, V_k$ be i.i.d. Fix any $f: (U, V_j) \rightarrow \mathbb{R}$ and put $c = \mathbb{E}_{p(v_1)}[e^{f(u, v_1)}]$. Pick $B \subset \mathbb{R}$ strictly lower-bounded by $c$. Assume $p(S_B) > 0$ for
If \( v \) is truly similar to the fixed point \( u \), then

\[
\text{Bias}_p(Z) \leq \text{Bias}_{\tilde{q}}(Z) \text{ and } \text{Var}_p(Z) \geq \text{Var}_{\tilde{q}}(Z).
\]

That is, sampling \( v \) instead of \( q \) achieves a higher bias for lower variance.

Theorem 3.2. Define \( U \) and \( V_1 \) by \( u, v_1 \sim p(u, v_1) \). Fix \( q \) as stated in Theorem 3.1. Define

\[
Z(v_{2:k}) = \sum_{i=1}^{k} \frac{e^{f(u,v_i)}}{e^{f(u,v_j)}},
\]

By Theorem 3.1, \( E_{p(v_{2:k})}[Z] \) and \( E_{q(v_{2:k})}[Z] \) are estimators for the mutual information between \( U \) and \( V_1 \). Suppose that \( S_B \) is chosen to ensure \( \text{Var}_{\tilde{q}}(Z) \leq \text{Var}_{\tilde{q}}(Z) \), where \( \tilde{q}(A) = \frac{p(A | S_B)}{p(S_B)} \). Then \( \text{Bias}_p(Z) \leq \text{Bias}_{\tilde{q}}(Z) \) and \( \text{Var}_p(Z) \geq \text{Var}_{\tilde{q}}(Z) \).

The proof is in Sec. A.2. Given a good similarity function \( f \), the elements inside \( S_B \) contain values of \( v \) truly similar to the fixed point \( u \) as measured by \( f \). Thus, the elements outside of \( S_B \) occupy a larger range of \( f \), and thereby are more varied, satisfying the assumption. Thm. 3.2 provides one answer to our question of looseness. In stochastic optimization, a lower variance objective may lead to better local optima. For representation learning, using CNCE to sample more difficult negatives may (1) encourage the representation to distinguish fine-grained features useful in transfer tasks, and (2) provide less noisy gradients. Thm. 3.2 also raises a warning: for a bad similarity function \( f \), such as a randomly initialized neural network, we may not get the benefits of lower variance. We will explore the consequences of this for representation learning in the next section.

4 RING DISCRIMINATION

We have shown that the CNCE objective provides a lower variance bound on the mutual information between two random variables. Now, we wish to apply CNCE to contrastive learning where the two random variables are derived from two views of a complex random variable \( X \). To do so, we must...
specify a concrete proposal for the support set $S_B$. Suppose we take the $i$-th example $x_i \in D$, and choose a percentile $w_t \in [0, 100]$. Given the dataset $D$, we consider each $x$ as a negative example if and only if the normalized distance, $g_0(t(x_i))^T g_0(t'(x))$, is above the $w_t$-th percentile of all $x \in D$ for fixed transforms $t, t' \sim p(t)$. That is, we construct $q(x|t(x_i))$ such that we remove examples from the dataset whose representation dot product with the representation of $t(x_i)$ is “too low”. (Note that $w_t = 0$ recovers Eq. [2].) Under this formulation, $w_t$ uniquely specifies a set of distances $B$ (recall Thm. [3.1]) no lower than a threshold. For a smaller enough choice of $w_t$, this threshold will be greater than expected distance with respect to $p$. In effect, the pre-image set $S_B$ contains all $x \in D$ whose distance to $t(x_i)$ in representation space is above the $w_t$-th percentile.

However, picking the closest examples to $t(x_i)$ as its negative examples may be inappropriate, as these examples might be better suited as positive views rather than negatives [Zhuang et al., 2019; Xie et al., 2020]. As an extreme case, if the same image is included in the dataset twice, we would not like to select it as a negative example for itself. Furthermore, choosing negatives “too close” to the current instance may result in representations that pick up on fine-grain details only, ignoring larger semantic concepts. For instance, we may find representations that can distinguish two cats based on fur but are unable to classify animals from cars. This suggests removing a set from $S_B$ of instances we consider “too close” to the current example. In practice, this translates to picking two percentiles $w_t < w_u \in [0, 100]$. Now, we consider each example $x$ as a negative example for $x_i$ if and only if $g_0(t(x_i))^T g_0(t'(x))$ is within the $w_t$-th to $w_u$-th percentiles of all $x \in D$. We are free to define the support set $S_B$ in this manner as Thm. [3.1] does not require $S_B$ to contain all elements with high similarity to $t(x_i)$. Intuitively, we construct a conditional distribution for negative examples that are (1) not too easy since their representations are fairly similar to that of $t(x_i)$ and (2) not too hard since we remove the “closest” instances to $x_i$ from $S_B$. We call this algorithm Ring Discrimination, or Ring, inspired by the shape of negative set (see Fig. [1]).

Ring can be easily added to popular contrastive algorithms. For IR and CMC, this amounts to simply sampling entries in the memory bank that fall within the $w_t$-th to $w_u$-th percentile of all distances to the current instance view (in representation space). Similarly, for MoCo, we sample from a subset of the queue (chosen to be in the $w_t$-th to $w_u$-th percentile), preserving the FIFO ordering.

**Algorithm 1: MoCoRing**

```python
# g, g_k: encoder networks
# m: momentum: t: temperature
# omega_u: upper threshold
# omega_l: lower threshold
# all: total number of negatives
# sorted: sorted by distance
# t: t set from farthest to closest neg
# all: total number of negatives
# sorted: sorted by distance
# t: t set from farthest to closest neg
# all: total number of negatives
# sorted: sorted by distance

Algorithm 1: MoCoRing

```

Annealing Policy. Naively using Ring can collapse to a poor representation, as hinted by Thm. [3.2]. Early in training, when the representations are still disorganized, choosing negatives that are close in representation may detrimentally exclude those examples that are “actually” close. This could lock in poor local minima. To avoid this possibility we propose to use Ring with an annealing policy that reduces the size of $S_B$ throughout training. To do this, early in training we choose $w_t$ to be small. Over many epochs, we slowly anneal $w_t$ to approach $w_u$ thereby selecting more difficult negatives. We explored several annealing policies and found a linear schedule to be well-performing and simple (see Appendix). In our experiments, we found annealing thresholds to be crucial: being too aggressive with negatives early in training resulted in convergence to poor optima.

5 Experiments

We explore our method applied to IR, CMC, and MoCo in four commonly used visual datasets. As in prior work [Wu et al., 2018; Zhuang et al., 2019; He et al., 2019; Misra & Maaten, 2020; Henaff et al., 2019; Kolesnikov et al., 2019; Donahue & Simonyan, 2019; Bachman et al., 2019; Tran et al., 2019; Chen et al., 2020a], we evaluate each method by linear classification on frozen embeddings. That is, we optimize a contrastive objective on a pretraining dataset to learn a representation; then,
using a transfer dataset, we fit logistic regression on representations only. A better representation would contain more “object-centric” information, thereby achieving a higher classification score.

**Training Details.** We resize input images to be 256 by 256 pixels, and normalize them using dataset mean and standard deviation. The temperature \( \tau \) is set to 0.07. We use a composition of a 224 by 224-pixel random crop, random color jittering, random horizontal flip, and random grayscale conversion as our augmentation family \( T \). We use a ResNet-18 encoder with a output dimension of 128. For CMC, we use two ResNet-18 encoders, doubling the number of parameters. For linear classification, we treat the pre-pool output (size \( 512 \times 7 \times 7 \)) after the last convolutional layer as the input to the logistic regression. Note that this setup is equivalent to using a linear projection head (Chen et al., 2020a;b). In pretraining, we use SGD with learning rate 0.03, momentum 0.9 and weight decay 1e-4 for 300 epochs and batch size 256 (128 for CMC). We drop the learning rate twice by a factor of 10 on epochs 200 and 250. In transfer, we use SGD with learning rate 0.01, momentum 0.9, and no weight decay for 100 epochs without dropping learning rate. Future work can explore orthogonal factors such as choice of architecture or pretext task.

### Table 1: Comparison of contrastive algorithms on three image domains.

| Model          | Transfer Acc | Model          | Transfer Acc | Model          | Transfer Acc | Model          | Transfer Acc |
|----------------|--------------|----------------|--------------|----------------|--------------|----------------|--------------|
| IR             | 81.2         | IR             | 60.4         | IR             | 61.4         | IR             | 43.2         |
| IRing          | 83.9 (2.7)   | IRing          | 62.3 (1.9)   | IRing          | 64.3 (2.9)   | IRing          | 48.4 (5.2)   |
| CMC            | 85.6         | CMC            | 56.0         | CMC            | 63.8         | CMC            | 48.2         |
| CMCRing        | 87.6 (2.0)   | CMCRing        | 56.0 (1.0)   | CMCRing        | 64.4 (2.6)   | CMCRing        | 50.4 (2.2)   |
| MoCo           | 83.1         | MoCo           | 59.1         | MoCo           | 63.8         | MoCo           | 52.8         |
| MoCoRing       | 86.1 (3.0)   | MoCoRing       | 61.5 (2.4)   | MoCoRing       | 65.2 (1.4)   | MoCoRing       | 54.6 (1.8)   |
| LA             | 83.9         | LA             | 61.4         | LA             | 65.0         | LA             | 48.0         |

(a) CIFAR10       (b) CIFAR100      (c) STL10       (d) ImageNet

The results for CIFAR10, CIFAR100, STL10, and ImageNet are in Table 1. Overall, IR, CMC, and MoCo all benefit from using more difficult negatives as shown by 2-5% absolute points of improvement across the four datasets. While we find different contrastive objectives to perform best in each dataset, the improvements from Ring are consistent: the Ring variant outperforms the base for every model and every dataset. We also include as a baseline Local Aggregation, or LA (Zhuang et al., 2019), a popular contrastive algorithm (see Sec. 5) that implicitly uses hard negatives without annealing. We find our methods to outperform LA by up to 4% absolute.

### Table 2: Lesioning the effects of annealing and choice of \( w_u \).

| Model          | Acc. | Model          | Acc. | Model          | Acc. | Model          | Acc. |
|----------------|------|----------------|------|----------------|------|----------------|------|
| IR             | 81.2 | IR             | 43.2 | IR             | 48.4 | IR             | 47.3 |
| IRing (No Anneal) | 81.4 | IRing (No Anneal) | 41.3 | IRing (No Anneal) | 47.3 |

(a) CIFAR10  (b) ImageNet

**Lesions: Annealing and Upper Boundary.** Having found good performance with Ring Discrimination, we want to assess the importance of the individual components that comprise Ring. We focus on the annealing policy and the exclusion of very close negatives from \( S_B \). Concretely, we measure the transfer accuracy of (1) IRing without annealing and (2) IRing with an upper percentile \( w_u \) set to 100, thereby excluding no close negatives. That is, \( S_B \) contains all examples in the dataset with representation similarity greater than the \( w_u \)-th percentile (a “ball” instead of a “ring”). Table 2 compares these lesions to IR and full IRing on CIFAR10 and ImageNet classification transfer. We observe that both lesions result in worse transfer accuracy, with proper annealing being especially important, confirming the suspicions raised by Thm. 3.2.

**Transferring Features.** Thus far we have only evaluated the learned representations on unseen examples from the training distribution. As the goal of unsupervised learning is to capture general representations, we are also interested in their performance on new, unseen distributions. To gauge this, we use the same linear classification paradigm on a suite of image datasets from the “Meta Dataset” collection (Triantafillou et al., 2019) that have been used before in contrastive literature (Chen et al., 2020a). All representations were trained on CIFAR10. For each transfer dataset, we compute mean and variance from a training split to normalize input images, which we found important for generalization to new visual domains.
We find in Table 3 that the Ring models are competitive with the non-Ring analogues, with increases in transfer accuracies of 0.5 to 2% absolute. Most notable are the TrafficSign and VGGFlower datasets in which Ring models surpass others by a larger margin. We also observe that IRing largely outperforms LA. This suggests the features learned with more difficult negatives are not only useful for the training distribution but may also be transferrable to many visual datasets.

**More Downstream Tasks.** Object classification is a popular transfer task, but we want our learned representations to capture holistic knowledge about the contents of an image. We must thus evaluate performance on transfer tasks such as detection and segmentation that require different kinds of visual information. We study four additional downstream tasks: object detection on COCO (Lin *et al.*, 2014) and Pascal VOC’07 (Everingham *et al.*, 2010), instance segmentation on COCO, and keypoint detection on COCO. In all cases, we employ embeddings trained on ImageNet with a ResNet-18 encoder. We base these experiments after those found in He *et al.* (2019) with the same hyperparameters. However, we use a smaller backbone (ResNet-18 versus ResNet-50) and we freeze its parameters instead of finetuning them. We adapt code from Detectron2 (Wu *et al.*, 2019).

| Model | Aircraft | CU/Birds | DTD | Fungi | MNIST | FashionMNIST | TrafficSign | VGGFlower | MSCOCO |
|-------|----------|----------|------|-------|-------|--------------|------------|-----------|--------|
| IR    | 40.9     | 17.9     | 39.2 | 2.7   | 96.9  | 91.7         | 97.1       | 68.1      | 52.4   |
| IRing | 40.6 (+0.3) | 17.9 (+0.0) | 39.5 (+0.3) | 3.4 (+0.7) | 97.6 (+0.9) | 91.6 (+0.1) | 98.8 (+1.7) | 68.5 (+0.4) | 52.5 (+0.1) |
| MoCo  | 41.5     | 18.0     | 39.7 | 3.1   | 96.9  | 90.9         | 97.3       | 64.5      | 52.0   |
| MoCoRing | 41.6 (+0.1) | 18.6 (+0.6) | 39.5 (+0.2) | 3.6 (+0.5) | 97.9 (+1.0) | 91.3 (+0.4) | 99.3 (+2.0) | 69.1 (+4.6) | 52.6 (+0.6) |
| CMC   | 40.1     | 15.8     | 38.3 | 4.3   | 97.5  | 91.5         | 94.6       | 67.1      | 51.4   |
| CMCRing | 40.8 (+0.7) | 16.8 (+1.0) | 40.6 (+2.3) | 4.2 (+0.1) | 97.9 (+0.4) | 92.1 (+0.6) | 97.1 (+2.5) | 69.1 (+2.0) | 52.1 (+0.7) |
| LA    | 41.3     | 17.8     | 39.0 | 2.3   | 97.2  | 92.3         | 98.2       | 66.9      | 52.3   |

Table 3: Transferring CIFAR10 embeddings to various image distributions.

We find in Table 4 that IRing outperforms IR by around 2.3 points in COCO object detection, 2.5 points in COCO Inst. Segmentation, 2.6 points in COCO keypoint detection, and 2.1 points in VOC object detection. Similarly, MoCoRing finds consistent improvements of 1-3 points over MoCo on the four tasks. Future work can investigate orthogonal directions of using larger encoders (e.g. ResNet-50) and finetuning ResNet parameters for these individual tasks.

| Arch. | Mask R-CNN, 1x, FPN, 1x schedule | R-CNN, R18-FPN | Faster R-CNN, R18-C4 |
|-------|---------------------------------|----------------|---------------------|
| Model | AP50 | AP75 | AP50 | AP75 | AP50 | AP75 | AP50 | AP75 | AP50 | AP75 |
| IR    | 10.6 | 19.0 | 6.6 | 8.5 | 17.4 | 7.4 | 34.6 | 63.0 | 32.9 | 5.5 | 14.5 |
| IRing | 10.9 | 22.9 | 8.7 | 11.0 | 20.9 | 9.6 | 37.2 | 66.1 | 35.7 | 7.6 | 20.3 |
| MoCo  | 6.0 | 14.3 | 4.0 | 10.8 | 21.4 | 9.7 | 37.6 | 66.5 | 36.9 | 7.3 | 17.9 |
| MoCoRing | 9.4 | 20.3 | 7.6 | 12.0 | 22.9 | 10.8 | 38.7 | 67.7 | 37.9 | 8.0 | 22.1 |
| LA    | 10.2 | 22.0 | 8.1 | 10.0 | 20.3 | 9.0 | 36.3 | 65.3 | 35.1 | 7.6 | 20.0 |

Table 4: Evaluation of ImageNet representations using four visual transfer tasks.

**6 Related Work**

Several of the ideas in Ring Discrimination relate to existing work. Below, we explore these connections, and at the same time, place our work in a fast-paced and growing field.

**Hard negative mining.** While it has not been deeply explored in modern contrastive learning, negative mining has a rich line of research in the metric learning community. Deep metric learning utilizes triplet objectives of the form $L_{triplet} = d(g_\theta(x_i), g_\theta(x_+)) - d(g_\theta(x_i), g_\theta(x_-) + \alpha)$ where $d$ is a distance function (e.g. L2 distance), $x_+$ and $x_-$ are a positive and negative example, respectively, relative to $x_i$, the current instance, and $\alpha \in \mathbb{R}^+$ is a margin. In this context, several approaches pick semi-hard negatives: [Schroff *et al.*, 2015] treats the furthest (in L2 distance) example in the same minibatch as $x_i$ as its negative, whereas [Oh Song *et al.*, 2016] weight each example in the minibatch by its distance to $g_\theta(x_i)$, thereby being a continuous version of [Schroff *et al.*, 2015]. More sophisticated negative sampling strategies developed over time. In [Wu *et al.*, 2017], the authors pick negatives from a fixed normal distribution that is shown to approximate L2 normalized embeddings in high dimensions. The authors show that weighting by this distribution samples more diverse negatives. Similarly, HDC [Yuan *et al.*, 2017] simulates a triplet loss using many levels...
of “hardness” in negatives, again improving the diversity. Although triplet objectives paved the way for modern NCE-based objectives, the focus on negative mining has largely been overlooked. Ring Discrimination, being inspired by the deep metric learning literature, reminds that negative sampling is still an effective way of learning stronger representations in the new NCE framework. As such, an important contribution was to do so while retaining the theoretical properties of NCE, namely in relation to mutual information. This, to the best of our knowledge, is novel as negative mining in metric learning literature was not characterized in terms of information theory.

That being said, there are some cases of negative mining in contrastive literature. In CPC (Oord et al., 2018), the authors explore using negatives from the same speaker versus from mixed speakers in audio applications, the former of which can be interpreted as being more difficult. A recent paper, InterCLR (Xie et al., 2020), also finds that using “semi-hard negatives” is beneficial to contrastive learning whereas negatives that are too difficult or too easy produce worse representations. Where InterCLR uses a margin-based approach to sample negatives, we explore a wider family of negative distributions and show analysis that annealing offers a simple and easy solution to choosing between easy and hard negatives. Further, as InterCLR’s negative sampling procedure is a special case of CNCE, we provide theory ground these approaches in information theory. Finally, a separate line of work in contrastive learning explores using neighboring examples (in embedding space) as “positive” views of the instance \( \{x_j\} \) such that we consider \( x_j = t(x_i) \) for the current instance \( x_i \). While this does not deal with negatives explicitly, it shares similarities to our approach by employing other examples in the contrastive objective to learn better representations. In the Appendix, we discuss how one of these algorithms, LA (Zhuang et al., 2019), implicitly uses hard negatives and expand the Ring family with ideas inspired by it.

Contrastive learning. We focused primarily on comparing Ring Discrimination to three recent and highly performing contrastive algorithms, but the field contains much more. The basic idea of learning representations to be invariant under a family of transformations is an old one, having been explored with self-organizing maps (Becker & Hinton, 1992) and dimensionality reduction (Hadsell et al., 2006). Before IR, the idea of instance discrimination was studied (Dosovitskiy et al., 2014, Wang & Gupta, 2015) among many pretext objectives such as position prediction (Doersch et al., 2015), color prediction (Zhang et al., 2016), multi-task objectives (Doersch & Zisserman, 2017), rotation prediction (Gidaris et al., 2018; Chen et al., 2019), and many other “pretext” objectives (Pathak et al., 2017). As we have mentioned, one of the primary challenges to instance discrimination is making such a large softmax objective tractable. Moving from a parametric (Dosovitskiy et al., 2014) to a nonparametric softmax reduced issues with vanishing gradients, shifting the challenge to efficient negative sampling. The memory bank approach (Wu et al., 2018) is a simple and memory-efficient solution, quickly being adopted by the research community (Zhuang et al., 2019, Tian et al., 2019, He et al., 2019, Chen et al., 2020a, Misra & Maaten, 2020). With enough computational resources, it is now also possible to reuse examples in a large minibatch and negatives of one another (Ye et al., 2019, Ji et al., 2019, Chen et al., 2020a). In our work, we focus on hard negative mining in the context of a memory bank or queue due to its computational efficiency. However, the same principles should be applicable to batch-based methods (e.g. SimCLR): assuming a large enough batch size, for each example, we only use a subset of the minibatch as negatives as in Ring. Finally, more recent work (Grill et al., 2020) removes negatives altogether, which is speculated to implicitly use negative samples via batch normalization (Ioffe & Szegedy, 2015). We leave a more thorough understanding of negatives in BYOL to future work.

7 Conclusion

In this work, we presented a family of mutual information estimators that approximate the partition function using samples from a class of conditional distributions. We proved several theoretical statements about this family, showing a bound on mutual information and a tradeoff between bias and variance. Then, we applied these estimators as objectives in contrastive representation learning. In doing so, we found that our representations outperform existing approaches consistently across a spectrum of contrastive objectives, data distributions, and transfer tasks. Overall, we hope our work to encourage more exploration of negative sampling in the recent growth of research in contrastive learning. Future work can investigate better annealing protocols to ensure diversity.
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A Proofs

A.1 Counterexample Against Unrestricted \( q \).

Pick some \( x^* \sim p(x) \) and take \( f \) to be a continuous function whose range spans \([0, 1]\). For any \( \epsilon > 0 \), pick \( q \) to be a distribution such that for every \( x \sim q \) with non-zero probability, we have \( f(x, x^*) < \epsilon \).

Then, by varying \( \epsilon \) closer to 0, we can bring our bound on mutual information to infinity, regardless of the true value, thus ceasing to be a bound. As such, we cannot use an unrestricted family of conditional distributions and preserve a bound.

A.2 Proof of Theorem 3.2

Proof. We separately show the statements regarding bias and variance.

First, as \( Z(v_{2:k}) \) with \( v_{2:k} \sim p(v_{2:k}) \) (or NCE) is unbiased, and \( \mathbb{E}_{q(v_{2:k})}[Z] \) (or CNCE) lower bounds \( \mathbb{E}_{q[v_{2:k}]}[Z] \) (Thm. 3.1), the first statement follows immediately for any choice of \( k \).

Second, by the law of total variance,

\[
\mathbb{E}_{p}[\mathbb{V}_{p}[Z|1_S]] + \mathbb{V}_{p}(\mathbb{E}_{p}[Z|1_S]) = \mathbb{V}_{p}[Z]
\]

Since both summands are non-negative and the variance on the right is the desired upper-bound, it suffices to show that

\[
p(S_B) \cdot \mathbb{V}_{q(v_{2:k})}[Z] \leq \mathbb{E}_{p}[\mathbb{V}_{p}[Z|1_S]].
\]

This follows immediately from the observation that by definition of \( q(\cdot) \) as the conditional distribution \( p(\cdot|S_B) \), the expectation on the right is precisely

\[
p(S_B) \cdot \mathbb{V}_{q(v_{2:k})}[Z] + (1 - p(S_B)) \cdot \mathbb{V}_{\tilde{q}(v_{2:k})}[Z],
\]

where \( \tilde{q} \) is the conditional distribution \( p(\cdot|\sim S_B) \). \( \square \)

B A Toy Example

Interestingly, Thm. 3.1 shows CNCE to lower bound NCE. To confirm this experimentally, we reproduce the toy setting from Tschannen et al. (2019). Pick two random variables \( Z \) and \( \epsilon \) distributed such that \( z_i \sim \mathcal{N}(0, \Sigma_Z) \) and \( \epsilon_i \sim \mathcal{N}(0, \Sigma_\epsilon) \) where \( \Sigma_Z = \begin{pmatrix} 1 & -0.5 \\ -0.5 & 1 \end{pmatrix} \) and \( \Sigma_\epsilon = \begin{pmatrix} 1 & 0.9 \\ 0.9 & 1 \end{pmatrix} \).

Then, let \((X, Y) = Z + \epsilon \). That is, let \( X \) be the first dimension of the sum and \( Y \) the second.

The mutual information between \( X \) and \( Y \) can be analytically computed as

\[
\frac{1}{2} \log(1 - \frac{\Sigma[1,2][2,1]}{\Sigma[1,1][2,2]})
\]

since \((X, Y)\) is jointly Gaussian with covariance \( \Sigma = \Sigma_Z + \Sigma_\epsilon \). For this toy experiment, let \( w_\ell \)

| True  | NCE | CNCE |
|-------|-----|------|
| \( \omega \) | 10  | 25   | 50   | 75   | 90   | 95   |
| Mean  | 0.02041 | 0.01345 | 0.01241 | 0.00220 | 7.29e-5 | 1.67e-5 | 5.87e-6 | 1.97e-6 |
| Stdev | 0.001 | 3e-4 | 1e-4 | 9e-6 | 2e-6 | 1e-6 | 4e-6 |

Table 5: Looseness of CNCE as \( w_\ell \) increases.

be a percentage from 0 to 100. Now, we define \( S_B \) as all examples whose dot product with the embedding of the current transformed instance is in the top \( w_\ell \) percentage of all examples in the dataset. We can tractably compute this using a memory bank. As \( w_\ell \) increases from 10 to 95, \( q(x|t(x_i)) \) has smaller support meaning that negative samples are more difficult to separate from the current instance \( x_i \). Table 5 compares the estimated mutual information between \( X \) and \( Y \) from each estimator to the ground truth over 5 runs. The encoders are 5-layer MLPs with 10 hidden dimensions and ReLU nonlinearities. To build the dataset, we sample 2000 points and optimize the NCE objective with Adam with a learning rate of 0.03, batch size 128, and no weight decay for 100 epochs. Given a percentage for CNCE, we compute distances between all elements in the memory bank and the representation the current image — we only sample 100 negatives from the top \( p \) percent. We conduct the experiment with 5 different random seeds.
C Bias and Variance Experiment Details

For IR, we explore $k = 16, 32, 64, 128, 256, 512, 1024, 4096$. For MoCo, we only evaluate $k = 256, 512, 1024, 4096$ as the queue cannot be smaller than the batch size. All hyperparameter choices are as detailed in the main experiments. To find the nearest neighbor of the training example, we store all embeddings in a memory bank (separate from the one possibly used in training).

D Detectron2 Experiments

We make heavy usage of the Detectron2 code found at https://github.com/facebookresearch/detectron2. In particular, the script https://github.com/facebookresearch/detectron2/blob/master/tools/convert-torchvision-to-d2.py allows us to convert a trained ResNet18 model from torchvision to the format needed for Detectron2. The repository has default configuration files for all experiments. We change the following fields to support using a frozen ResNet18:

- **Input:** Format: RGB
- **Model:**
  - **Backbone:** Freeze at: 5
  - **Pixel mean:**
    - 123.675
    - 103.53
    - 116.28
  - **Pixel std:**
    - 58.395
    - 57.12
    - 57.375
  - **ResNets:**
    - Depth: 18
    - Res2_out_channels: 64
    - Stride in 1x1: False
  - **Weights:** <Path_to_converted_torchvision_weights>

We acknowledge that ResNet50 and larger are the commonly used backbones, so our results will not be state-of-the-art. However, the ordering in performance between algorithms is still meaningful and our primary interest. Future work can explore larger architectures.

E Additional Experiments

We discuss a few observations surrounding Ring Discrimination and in particular, annealing.

**Hard negative mining is not always productive.** We can attribute this to the poor quality of embeddings early in training: using hard negatives can (1) simply be too difficult for the encoder to discriminate, or (2) focus the embedding on smaller, perhaps spurious, differences between the instance and the hard negatives, rather than prioritizing higher level semantic information (e.g. object identity). As a demonstration of this phenomena, Fig. 2 shows several training runs of IRing on CIFAR10 with varying thresholds $\omega_\ell$ initialized at every 50 epochs of an IR model for a total of 200 epochs. In the legend, a smaller percentage indicates drawing negatives more similar to the embedding of the current instance as measured by dot products. (IRing (100%) and IR are identical.) The y-axis plots the accuracy of classification where for each test example, we predict the label of its $L_2$ nearest neighbor in the training split (Wu et al., 2018; Zhuang et al., 2019). Fig. 2 shows that (1) using smaller thresholds at the beginning of training results in lower test accuracies; (2) in the middle of training (epoch 50), the performance is equivalent for all models; and (3) in later training stages (epoch 100), using more difficult negatives is better. Notice the ordering of the lines in Fig. 2: $10\% < 25\% < 50\% < 100\%$ early in training while the inequalities are flipped at epoch 100.
Exploring annealing policies. Given that our experiments show annealing is important, there is a question of “how to anneal”. In our experiments, we opted for a simple linear policy: slowly reducing $w_{u}$ from 100% to 10% in 100 epochs and maintaining it constant at 10% for the remaining epochs. Here, we briefly compare this to three other policies: a step function; an adaptive policy that lowers the threshold every epoch if the performance on a validation set increases, otherwise decreasing the threshold; and a similar adaptive policy that updates every step based on negative training loss. Fig. 2b compares the nearest neighbor test accuracies over 200 epochs of training IRing on CIFAR10 whereas Fig. 2c plots the threshold $w_{u}$. We find that all the policies converge to roughly the same test accuracy, although linear and step policies appear to converge more quickly. From Fig 2, we observe that the adaptive methods naturally push the threshold down to 10% (the lowest allowed threshold) around step 150, confirming our intuition that a smaller threshold later in training is desirable. Future work could explore more sophisticated policies.

F RELATED WORK: RING AND LOCAL AGGREGATION

Of the many algorithms listed above, we focus on Local Aggregation (Zhuang et al. 2019), or LA, which we conjecture to already be (implicitly) mining hard negatives. While IR seeks to uniformly distribute embeddings, uniformity may not be optimal in all cases. For instance, images of the same class should intuitively be closer together than other images. The LA objective captures this intuition using a “close neighbor set” $C_{i}$ and “background neighbor set” $B_{i}$ conditioned on the current transformed instance $t(x_{i})$. The background neighbor set contains the indices of elements in the dataset whose embeddings are closest to $g_{θ}(t(x_{i}))$ in L2 distance. The close neighbor set contains elements same cluster as $t(x_{i})$ using Kmeans assignments. Although not originally formulated in this manner, we can view the background neighbor set as being sampled from a variational distribution $q(B_{i}|t(x_{i}))$ with the lower threshold $w_{u}$ set to 0 i.e. the ring is fully enclosed. Now, writing LA in the notation of Eq.2 its objective is

$$L_{LA}(x_{i}; M) = E_{t \sim p(t)} E_{B_{i} \sim q(B_{i}|t(x_{i}))} \left[ \log \frac{1}{|C_{i}|} \sum_{j \in C_{i}} e^{g_{θ}(t(x_{i}))^{T} M[j]/\tau} \right]$$

Although Ring Discrimination and LA both mine hard negatives, LA additionally uses instances in the same KMeans cluster as positive views of $x_{i}$. Borrowing ideas from LA, we can explore several extensions of Ring Discrimination. First, by “Cave” Discrimination (including IRCave ad

| Model         | Top1  |
|---------------|-------|
| LA            | 83.9  |
| IRCave        | 84.0  |
| CMCCave       | 87.2  |
| IRing (+C_{i})| 84.3  |
| CMCRing (+C_{i}) | 87.8  |

Table 6: Variants of Ring

CMCCave), we denote drawing negative samples from a CNCE distribution $q$ with a support restricted to the examples in the same KMeans clustering as the current instance (Note that such a
definition falls under Theorem 3.1 as a particular choice for the restricted set $S_B$). Second, Ring ($+C_i$) instead, includes members of the KMeans clustering as positive views of $x_i$, like in LA — here, negative samples are drawn as in regular Ring. Note that LA and IRing ($+C_i$) differ only by the lower threshold $w_{\ell}$, which is zero in the former and nonzero in the latter. Table 6 shows promising results on CIFAR10 as these variations produce strong representations. This suggests that choosing good views and good negatives together can build even better contrastive algorithms.