Multi-label Contrastive Predictive Coding

Jiaming Song  
Stanford University  
tsong@cs.stanford.edu

Stefano Ermon  
Stanford University  
ermon@cs.stanford.edu

Abstract

Variational mutual information (MI) estimators are widely used in unsupervised representation learning methods such as contrastive predictive coding (CPC). A lower bound on MI can be obtained from a multi-class classification problem, where a critic attempts to distinguish a positive sample drawn from the underlying joint distribution from \((m-1)\) negative samples drawn from a suitable proposal distribution. Using this approach, MI estimates are bounded above by \(\log m\), and could thus severely underestimate unless \(m\) is very large. To overcome this limitation, we introduce a novel estimator based on a multi-label classification problem, where the critic needs to jointly identify multiple positive samples at the same time. We show that using the same amount of negative samples, multi-label CPC is able to exceed the \(\log m\) bound, while still being a valid lower bound of mutual information. We demonstrate that the proposed approach is able to lead to better mutual information estimation, gain empirical improvements in unsupervised representation learning, and beat a state-of-the-art knowledge distillation method over 10 out of 13 tasks.

1 Introduction

Learning efficient representations from data with minimal supervision is a critical problem in machine learning with significant practical impact [35, 12, 36, 39, 6]. Representations obtained using large amounts of unlabeled data can boost performance on downstream tasks where labeled data is scarce. This paradigm is already successful in a variety of domains; for example, representations trained on large amounts of unlabeled images can be used to improve performance on detection and segmentation [49, 17, 9].

In the context of learning visual representations, contrastive objectives based on variational mutual information (MI) estimation are among the most successful ones [44, 3, 13, 38, 42]. One such approach, named Contrastive Predictive Coding (CPC, [44]), obtains a lower bound to MI via a multi-class classification problem. In CPC, a critic is generally trained to distinguish a pair of representations from two augmentations of the same image (positive), apart from \((m-1)\) pairs of representations from different images (negative). The representation network is then trained to increase the MI estimates given by the critic. This brings together the two representations from the positive pair and pushes apart the two representations from the negative pairs.

It has been empirically observed that factors leading to better MI estimates, such as training for more iterations and increasing the complexity of the critic [9, 10], can generally result in improvements over downstream tasks. In the context of CPC, increasing the number of negative samples per positive sample (i.e. increasing \(m\)) also helps with downstream performance [48, 17, 9, 42]. This can be explained from a mutual information estimation perspective that CPC estimates are upper bounded by \(\log m\), so increasing \(m\) could reduce bias when the actual mutual information is much higher [33]. However, due to constraints over compute, memory and data, there is a limit to how many negative samples we can obtain per positive sample.
In this paper, we propose generalizations to CPC that can increase the \( \log m \) bound without additional computational costs, thus decreasing bias. We first generalize CPC through \( \log m \) re-weighting the influence of positive and negative samples in the underlying the classification problem. This increases the \( \log m \) bound and leads to bias reduction, yet the re-weighted CPC objective is no longer guaranteed to be a lower bound to mutual information.

To this end, we introduce multi-label CPC (ML-CPC) which poses mutual information estimation as a multi-label classification problem. Instead of identifying one positive sample for each classification task (as in CPC), the critic now simultaneously identifies multiple positive samples that come from the same batch. We prove for ML-CPC that under certain choices of the weights, we can increase the \( \log m \) bound and reduce bias, while guaranteeing that the new objective is still lower bounded by mutual information.

Re-weighted ML-CPC encompasses a range of mutual information lower bound estimators with different bias-variance trade-offs, which can be chosen with minimal impact on the computational costs. We demonstrate the effectiveness of re-weighted ML-CPC over CPC empirically on several tasks, including mutual information estimation, knowledge distillation and unsupervised representation learning. In particular, ML-CPC is able to beat the current state-of-the-art of knowledge distillation [42] on 10 out of 13 distillation tasks for CIFAR-100.

2 Background

In representation learning, we are interested in learning a (possibly stochastic) network \( h : \mathcal{X} \to \mathcal{Y} \) that maps some data \( x \in \mathcal{X} \) to a compact representation \( h(x) \in \mathcal{Y} \). For ease of notation, we denote \( p(x) \) as the data distribution, \( p(x, y) \) as the joint distribution for data and representations (denoted as \( y \)), \( p(y) \) as the marginal distribution of the representations, and \( X, Y \) as the random variables associated with data and representations. The InfoMax principle [30, 4], [3], [38] for learning representations considers variational maximization of the mutual information \( I(X; Y) \):

\[
I(X; Y) := \mathbb{E}_{(x,y) \sim p(x,y)} \left[ \log \frac{p(x,y)}{p(x)p(y)} \right]
\]

A variety of mutual information estimators with different bias-variance trade-offs have been proposed for representation learning [37, 43, 3, 38]. Contrastive predictive coding (CPC, also known as InfoNCE [44]), poses the MI estimation problem as an \( m \)-class classification problem. Here, the goal is to distinguish a positive pair \((x, y) \sim p(x, y)\) from \((m - 1)\) negative pairs \((x, \overline{y}) \sim p(x)p(y)\). If the optimal classifier is able to distinguish positive and negative pairs easily, it means \( x \) and \( y \) are tied to each other, indicating high mutual information.

For a batch of \( n \) positive pairs \( \{(x_i, y_i)\}_{i=1}^n \), the CPC objective is defined as:

\[
L(g) := \mathbb{E} \left[ \frac{1}{n} \sum_{i=1}^n \log \frac{m \cdot g(x_i, y_i)}{g(x_i, y_i) + \sum_{j=1}^{n-1} g(x_i, \overline{y}_j)} \right]
\]

for some positive critic function \( g : \mathcal{X} \times \mathcal{Y} \to \mathbb{R}_+ \), where the expectation is taken over \( n \) positive pairs \((x_i, y_i) \sim p(x, y)\) and \( n(m - 1) \) negative pairs \((x_i, \overline{y}_j) \sim p(x)p(y)\). For all \( m, n \) and \( g \), the CPC objective \( L(g) \) is a variational lower bound to the mutual information \( I(X; Y) \). Therefore, one can train \( g \) and \( h \) to maximize \( L(g) \) (recall that \( L \) depends on \( h \) via \( y = h(x) \)), resulting in higher lower bounds to \( I(X; Y) \) and more informative representation maps.

When \( m \) grows to infinity, the optimal critic function has the form [38]:

\[
g^*(x, y) = p(y|x) \cdot c(x)
\]

where \( c : \mathcal{X} \to \mathbb{R} \) is any positive function that only depends on \( x \). For this choice of \( g^* \), a positive sample \((x, y)\) and infinite negative samples

\[
\lim_{m \to \infty} \mathbb{E}_{(\overline{y})_{i=1}^n \sim p^n(y)} \left[ \frac{m \cdot g^*(x, y)}{g^*(x, y) + \sum_{i=1}^{n-1} g^*(x, \overline{y}_i)} \right] = \frac{p(x, y)}{p(x)p(y)}
\]

\[1\]We suppress the dependencies on \( n \) and \( m \) in \( L(g) \) (and in subsequent objectives) for conciseness.

\[2\]We prove this in Proposition 3, Appendix A as a more general case than the proof in [38].
which recovers the density ratio between \( p(x, y) \) and \( p(x)p(y) \), so \( \lim_{m \to \infty} L(g^*) = I(X; Y) \).

For finite \( m \), however, since \( g(x_i, y_i) \) appears in both the numerator and denominator of Equation 2 and \( g \) is positive, the density ratio estimates can be no larger than \( m \), and the value of \( L(g) \) is thus upper bounded by \( \log m \) \([44]\). While this is acceptable for certain low dimensional scenarios, this can lead to high-bias if the true mutual information is much larger than any \( m \) that is computationally feasible. This can be problematic in high dimensions because MI can scale linearly with dimension. For example, if \( X \) and \( Y \) are 1000-dimensional random variables where the marginal distribution for each dimension is standard Gaussian, and for each dimension \( d \), \( X_d \) and \( Y_d \) has a correlation of 0.2, then the mutual information \( I(X; Y) \) is around 20.5, which means that \( m \) has to be greater than \( 4 \times 10^8 \) in order for CPC estimates to approach this value. In comparison, state-of-the-art image representation learning methods use a \( m \) that is around 65536 and representation dimensions between 128 to 2048 \([43][17][9]\) due to batch size and memory limitations, as one would need a sizeable batch of positive samples in order to apply batch normalization \([23]\).

3 Methods

3.1 Re-weighted Contrastive Predictive Coding

Under the computational limitations imposed by \( m \) (i.e., we cannot obtain too many negative samples per positive sample), we wish to develop generalizations to CPC that reduce the bias while still being lower bounds to mutual information. We do not consider other types of estimators such as MINE \([3]\) or NWJ \([57]\) because they would exhibit high variance on the order of \( O(e^{I(X; Y)}) \) \([41]\), and thus are much less stable to optimize.

One possible approach is to decrease the weights of the positive sample when calculating the sum in the denominator; this leads to the following objective, called \( \alpha \)-CPC:

\[
L_\alpha(g) := E \left[ \frac{1}{n} \sum_{i=1}^{n} \log \frac{m \cdot g(x_i, y_i)}{\alpha g(x_i, y_i) + \sum_{j=1}^{m-1} g(x_i, y_{i,j})} \right]
\]

(5)

where the positive sample is weighted by \( \alpha \) and negative samples are weighted by \( \frac{m-\alpha}{\alpha} \). The purpose of adding weights to negative samples is to make sure the the weights sum to \( m \), like in the original case where each sample has weight 1 and there are \( m \) samples in total. Clearly, the original CPC objective is a special case when \( \alpha = 1 \).

On the one hand, \( L_\alpha(g) \) is now upper bounded by \( \log \frac{m}{\alpha} \), which is larger than \( \log m \) when \( \alpha \in (0,1) \). Thus, \( \alpha \)-CPC has the potential to reduce bias when \( \log m \) is much smaller than \( I(X; Y) \). On the other hand, when we set a smaller \( \alpha \), the variance of the estimator becomes larger, and the task becomes more difficult to optimize \([20][21]\). Therefore, selecting an appropriate \( \alpha \) to balance bias-variance trade-off is helpful for optimization in practice.

However, it is now possible for \( L_\alpha(g) \) to be larger than \( I(X; Y) \) as the number of classes \( m \) grows to infinity, so optimizing \( L_\alpha(g) \) does not necessarily recover a lower bound to mutual information. We illustrate this via the following example (more details in Appendix C).

**Example 1.** Let \( X, Y \) be two binary r.v.s such that \( \Pr(X = 1, Y = 1) = \Pr(X = 0, Y = 0) = 0.5 \).

Then \( I(X; Y) = \log 2 \approx 0.69 \). However, when \( \alpha = 0.5 \) and \( n = m = 3 \), we can analytically compute \( L_\alpha(g) \approx 0.72 \geq I(X; Y) \) for \( g(x, y) = 1 \) if \( x = y \) and near 0 otherwise.

3.2 Multi-label Contrastive Predictive Coding

While \( \alpha \)-CPC could be useful empirically, we lack a principled way to select proper values of \( \alpha \) as \( L_\alpha(g) \) may no longer be a lower bound to mutual information. In the following sections, we propose an approach that allows us to achieve both, i.e., for all \( \alpha \) in a certain range (that only depends on \( n \) and \( m \)), we can achieve an upper bound of \( \log \frac{m}{\alpha} \) while ensuring that the objective is still a lower bound on mutual information. This allows us to select different values of \( \alpha \) to reflect different preferences over bias-variance trade-offs, all while keeping the computational cost identical.

We consider solving a “\( nm \)-class, \( n \)-label” classification problem, where given \( n \) positive samples and \( n(m - 1) \) negative samples \( y_{j,e} \sim p(y) \), we wish to jointly identify the top-\( n \) samples that are
We perform a similar analysis in Appendix A to show that evaluating the gradients of the objectives which results in the following objective called $\alpha$

where the expectation is taken over the $n$ positive samples $(x_i, y_i) \sim p(x, y)$ for $i \in [n]$ and the $n(m - 1)$ negative samples $y_{j,k} \sim p(y)$ for $j \in [n], k \in [m - 1]$. We call this multi-label contrastive predictive coding (ML-CPC), since the classifier now needs to predict $n$ positive labels from $nm$ options at the same time, instead of 1 positive label from $m$ options as in traditional CPC.

**Distinctions from CPC** Despite its similarity compared to CPC (both are based on classification), we note that the multi-label perspective is fundamentally different from the CPC paradigm in three aspects, and cannot be treated as simply increasing the number of negative samples.

1. The MC-CPC objective value depends on the batch size $n$, whereas the CPC objective does not.
2. In CPC the positive pair and negative pairs are share a same element (similar to $\alpha$), whereas in ML-CPC the negative pairs no longer have such restrictions; this could be useful for smaller datasets $D$ when the number of possible negative pairs increases from $O(|D|)$ to $O(|D|^2)$.
3. The optimal critic for ML-CPC when $m \to \infty$ satisfies $g^* = c \cdot p(x_j) / (p(x_j) p(y))$, where $c$ is a positive constant; this is a subset of the set of optimal critics for CPC since $c$ cannot depend on $x$. This removes certain undesirable solutions in CPC where the optimal critic satisfies $g(x_i, y_j) < g(x_j, y_{j,k})$ when $c(x_i) < c(x_j)$; if we use the critic based on some notion of similarity between the representations [43], this would mean that representations from some negative pairs could be closer than that of certain positive pairs even in optimal CPC solutions.

**Computational cost of ML-CPC** To compute CPC with a batch size of $n$, one would need $nm$ critic evaluations and compute $n$ sums in the denominator, each over a different set of $m$ evaluations. To compute ML-CPC, one needs $nm$ critic evaluations, and compute 1 sum over all $nm$ evaluations. Therefore, ML-CPC has almost the same computational cost compared to CPC which is $O(nm)$. We perform a similar analysis in Appendix A to show that evaluating the gradients of the objectives also has similar costs, so ML-CPC is computationally as efficient as CPC.

### 3.3 Re-weighted Multi-label Contrastive Predictive Coding

Similar to $\alpha$-CPC, we can modify the multi-label objective $J(g)$ by re-weighting the critic predictions, which results in the following objective called $\alpha$-ML-CPC:

$$ J_\alpha(g) := \mathbb{E} \left[ \frac{1}{n} \sum_{i=1}^{n} \log \frac{\alpha \sum_{j=1}^{n} g(x_i, y_j)}{\sum_{j=1}^{n} \sum_{k=1}^{m-1} g(x_i, y_{j,k})} \right] $$

For $\alpha \in (0, 1)$, we down-weight the positive critic outputs by $\alpha$ and up-weight the negative critic outputs by $\frac{\alpha}{m-1}$ (similar to $\alpha$-CPC). Setting a smaller $\alpha$ has the potential to reduce bias, since the upper bound of $\log m$ is changed to $\log \frac{m}{\alpha}$, which is larger when $\alpha \in (0, 1)$. In contrast to $\alpha$-CPC, $J_\alpha(g)$ is now guaranteed to be a lower bound to mutual information for a wide range of $\alpha$, as we show in the following theorem.

**Theorem 1.** \( \forall n \geq 1, m \geq 2, \text{define } \alpha_{m,n} = \frac{m}{n(m-1)+1} \). If $\alpha \in [\alpha_{m,n}, 1]$, then $\forall g : \mathcal{X} \times \mathcal{Y} \to \mathbb{R}_+$,

$$ J_\alpha(g) \leq I(X; Y) $$

**Proof.** In Appendix A

The above theorem shows that for an appropriate range of $\alpha$ values, the objective $J_\alpha(g)$ is still guaranteed to be a variational lower bound to mutual information, like the original CPC objective. Selecting $\alpha$ within this range results in estimators with different bias-variance trade-offs. Here, a smaller $\alpha$ could lead to low-bias high-variance estimates; this achieves a similar effect to increasing the number of classes $m$ to nearly $m/\alpha$, but without the actual additional computational costs that comes with obtaining more negative samples in CPC.
Illustrative example

We consider the case of $X, Y$ being binary and equal random variables in Example 1, where $I(X; Y) = \log 2 \approx 0.69$, the optimal critic $g$ is known, and both $L_\alpha(g)$ and $J_\alpha(g)$ can be computed in closed-form for any $\alpha$ and $g$ in $O(m)$ time (details in Appendix C). We plot the CPC (Eq.(5)) and ML-CPC (Eq.(7)) objectives with different choices of $\alpha$ and $m$ in Figure 1. The estimates of ML-CPC when $\alpha \geq \alpha_{m,n}$ are lower bounds to the ground truth MI, which indeed aligns with our theory.

Furthermore, in Figure 2 we illustrate the bias-variance trade-offs for CPC and $\alpha_{m,n}$-ML-CPC as we vary the number of classes $m$ (for simplicity, we choose $n = m$). Despite having slightly higher variance in the estimates, $\alpha_{m,n}$-ML-CPC has significantly less bias than CPC, which suggests that it is helpful in cases where lower bias is preferable than lower variance. In practice, the user could select different values of $\alpha$ to indicate the desired trade-off, all without having to change the number of negative samples and increase computational costs.

We include the pseudo-code and a PyTorch implementation to $\alpha$-ML-CPC in Appendix B.

4 Related Work

Contrastive methods for representation learning

The general principle of contrastive methods for representation learning encourages representations to be closer between “positive” pairs and further between “negative” pairs, and have been applied to learning representations in various domains such as images [18, 48, 17, 9], words [35, 12], graphs [45] and videos [16]. Commonly used objectives include the logistic loss [35], margin triplet loss [40], the noise contrastive estimation loss [15] and other objectives based on variational lower bounds of mutual information, such as MINE [3] and CPC [44]. CPC-based approaches have gained much recent interest due to its superior performance in downstream tasks compared to other losses such as the logistic and margin loss [9].

Variational mutual information estimators

Estimating mutual information from samples is challenging [34]. Most variational approaches to mutual information estimation are based on the Fenchel dual representation of $f$-divergences [37], where a critic function is trained to learn the density ratio $p(x, y)/(p(x)p(y))$. These approaches mostly vary in terms of how the critics are modeled and optimized [2, 38], and exhibit different bias-variance trade-offs from these choices.

CPC would tend to underestimate the density ratio (since it is capped at $m$) and generally requires $O(e^{I(X; Y)})$ samples to achieve low bias; MINE [3] (based on the Donsker-Varadhan inequality [14]) is a biased estimator and requires $O(e^{I(X; Y)})$ samples to achieve low variance [41]. Poole et al. [38] proposed an estimator that interpolates between two types of estimators, allowing for certain bias-variance trade-offs; this is relevant to our proposed re-weighted CPC in the sense that positive samples are down-weighted, but an additional baseline model is required during training. Through ML-CPC, we introduce a family of unbiased mutual information lower bound estimators, and reflect a wide range of bias-variance trade-offs without the need of more negative samples.
Re-weighted softmax loss  Generalizations to the softmax loss have been proposed in which different weights are assigned to different classes or samples [31, 32, 46], which are commonly used with regularization [7]. When the dataset has extremely imbalanced classes, higher weights are given to classes with less frequency [20, 21, 47] or classes with less effective samples [11]. Cao et al. [8] investigate re-weighting approaches that encourages large margins to the decision boundary for minority classes; such a context is also studied for detection [29] and segmentation [24] where class imbalance exists. Our work introduce re-weighting approaches to the context of unsupervised representation learning (where class labels do not exist), where we aim for flexible bias-variance trade-offs in contrastive mutual information estimators.

5 Experiments

We evaluate our proposed methods on mutual information estimation, knowledge distillation and unsupervised representation learning. To ensure fair comparisons are made, we only make adjustments to the training objective, and keep the remaining experimental setup identical to that of the baselines. We describe details to the experimental setup in Appendix C and include code to the experiments in the supplementary material.

5.1 Mutual Information Estimation

Setup  We first consider mutual information estimation between two correlated Gaussians of 20 dimensions, following the setup in [38, 41] where the ground truth mutual information is known and increases by 2 every 4k iterations, for a total of 20k iterations. We evaluate CPC and ML-CPC with different choices of $\alpha$ (ranging from 1.0 to 0.0001) under two types of critic, named joint [3] and separable [44]. We use $m = n = 128$ in our experiments.

Results  We illustrates the estimates and the ground truth MI in Figure 3. Both CPC and ML-CPC estimates are bounded by $\log m$ when $\alpha = 1$, which is no longer the case when we set smaller values of $\alpha$; however, as we decrease $\alpha$, CPC estimates are no longer guaranteed to be lower bounds to mutual information, whereas ML-CPC estimates still provide lower bound estimates in general. Moreover, a reduction in $\alpha$ for ML-CPC reduces bias at the cost of increasing variance, as the problem becomes more difficult with re-weighting. The time to compute 200 updates on a Nvidia 1080 Ti GPU with the a PyTorch implementation is 1.15 ± 0.06 seconds with CPC and 1.14 ± 0.04 seconds with ML-CPC, so the computational costs are indeed near identical.

5.2 Knowledge Distillation

Setup  We apply re-weighted CPC and ML-CPC to knowledge distillation (KD, [19]), in which one neural network model (teacher) transfers its knowledge to another model (student, typically smaller) so that the student’s performance is higher than training from labels alone. Contrastive representation
distillation (CRD, [42]) is a state-of-the-art method that regularizes the student model so that its features have higher mutual information with that of the teacher; CRD is implemented via a type of noise contrastive estimation objective [13]. We replace this objective with CPC and ML-CPC, using different choices of $\alpha$ that are fixed throughout training, and keeping the remaining hyperparameters identical the CRD ones in [42]. Two baselines are considered: the original KD objective in [19] and the state-of-the-art CRD objective in [42], since other baselines [27, 1, 22, 25] are shown to have inferior performance in general.

**Results**

Following the procedure in [42], we evaluate over 13 different student-teacher pairs on CIFAR-100 [28]. The student and teacher have the same type of architecture in 7 cases and different types in 6 cases. We report top-1 test accuracy in Table 1 (same type) and Table 2 (different types), where each case is the mean evaluation from 3 random seeds. While CPC and ML-CPC are generally inferior to that of CRD when $\alpha = 1.0$ (this aligns with the observation in [42]), they outperform CRD in 10 out of 13 cases when a smaller $\alpha$ is selected.

To demonstrate the effect of improved performance of smaller $\alpha$, we evaluate average top-1 accuracies with $\alpha \in \{0.01, 0.05, 0.1, 0.2, 0.5, 1.0\}$ in Figure 4. Both CPC and ML-CPC are generally inferior to CRD when $\alpha = 1.0$ or 0.5, but as we select smaller values of $\alpha$, they become superior to CRD and reaches the highest values at around 0.01 to 0.05, with ML-CPC being slightly better. Moreover, $n = 64$, $m = 16384$ so $\alpha_{m,n} \approx 0.015$, which achieves the lowest bias while ensuring ML-CPC to be a lower bound to MI. Thus this observation aligns with our claims on $\alpha_{m,n}$ in Theorem 1.

### Table 1: Top-1 test accuracy (%) of students networks on CIFAR100 where the student and teacher networks are of the same type. (↑) and (↓) denotes superior and inferior performance relative to CRD. Each result is the mean of 3 random runs. $L_{\alpha}$ and $J_{\alpha}$ denote $\alpha$-CPC and $\alpha$-ML-CPC.

| Teacher | Student | WRN-40-2 | WRN-40-2 | resnet56 | resnet110 | resnet110 | resnet32x4 | vgg13 | vgg8 |
|---------|---------|---------|---------|---------|---------|---------|---------|-------|-------|
| KD      | CRD     | 74.92   | 73.54   | 70.66   | 70.67   | 73.08   | 73.33   | 72.98 |
| $L_{1.0}$ | $L_{0.1}$ | 75.42   | 74.16   | 71.32   | 71.39   | 73.57   | 75.50   | 73.60 |
| $J_{1.0}$  |       | 75.39   | 74.18   | 71.28   | 71.28   | 73.58   | 75.32   | 73.67 |
| $J_{0.05}$ |       | 75.64   | 74.27   | 71.33   | 71.24   | 73.57   | 75.50   | 74.01 |
| $J_{0.01}$ |       | **75.83** | **74.24** | **71.50** | **71.27** | **73.90** | **75.37** | **73.95** |

### Table 2: Top-1 test accuracy (%) of students networks on CIFAR100 where the student and teacher networks are from different types. (↑) and (↓) denotes superior and inferior performance relative to CRD. Each result is the mean of 3 random runs. $L_{\alpha}$ and $J_{\alpha}$ denote $\alpha$-CPC and $\alpha$-ML-CPC.

| Teacher | Student | vgg13 | MobileNetV2 | MobileNetV2 | vgg8 | resnet32x4 | resnet32x4 | WRN-40-2 | WRN-40-2 |
|---------|---------|-------|------------|------------|------|------------|------------|----------|----------|
| KD      | CRD     | 74.64 | 79.34      | 79.34      | 79.42 | 79.42      | 79.42      | 75.61    | 75.61    |
| $L_{1.0}$ | $L_{0.1}$ | 67.37 | 67.35      | 73.81      | 74.07  | 74.45      | 74.83      | 67.05    | 67.05    |
| $J_{1.0}$  |       | 69.73 | 69.11      | 74.30      | 75.11  | 75.65      | 76.05      | 75.72    | 75.72    |
| $J_{0.05}$ |       | 69.24 | 69.02      | 73.66      | 75.00  | 75.93      | 75.72      | 76.12    | 76.12    |
| $J_{0.01}$ |       | 68.92 | 68.80      | 73.65      | 75.39  | 75.88      | 75.70      | 76.03    | 76.03    |

To demonstrate the effect of improved performance of smaller $\alpha$, we evaluate average top-1 accuracies with $\alpha \in \{0.01, 0.05, 0.1, 0.2, 0.5, 1.0\}$ in Figure 4. Both CPC and ML-CPC are generally inferior to CRD when $\alpha = 1.0$ or 0.5, but as we select smaller values of $\alpha$, they become superior to CRD and reach the highest values at around 0.01 to 0.05, with ML-CPC being slightly better. Moreover, $n = 64$, $m = 16384$ so $\alpha_{m,n} \approx 0.015$, which achieves the lowest bias while ensuring ML-CPC to be a lower bound to MI. Thus this observation aligns with our claims on $\alpha_{m,n}$ in Theorem 1.
Table 3: Top-1 accuracy of unsupervised representation learning under the linear evaluation protocol.

| Epochs | 200      | 500      | 1000     |
|--------|----------|----------|----------|
| $J_{1,0} \rightarrow J_{1,0}$ | 83.28 (%) | 89.31 (%) | 91.20 (%) |
| $J_{2,0} \rightarrow J_{0,5}$ | 84.31 (%) | 89.47 (%) | 91.43 (%) |
| $J_{5,0} \rightarrow J_{0,2}$ | 85.52 (%) | 89.85 (%) | 91.50 (%) |
| $J_{10,0} \rightarrow J_{0,1}$ | **86.16 (%)** | 89.49 (%) | **91.86 (%)** |

5.3 Representation Learning

**Setup** Finally, we consider ML-CPC for unsupervised representation learning as a replacement to CPC. We follow the experiment procedures in MoCo-v2 [10] (which used the CPC objective), where negative samples are obtained from a key encoder that updates more slowly than the representation network. We use the “linear evaluation protocol” where the learned representations are evaluated via the test top-1 accuracy when a linear classifier is trained to predict labels from representations. Different from knowledge distillation, we do not have labels and fixed teacher representations, so the problem becomes much more difficult and using small values of $\alpha$ alone will lead to high variance in initial estimates which could hinder the final performance. To this end, we use a curriculum learning $\alpha$ approach where we select $\alpha$ values from high to low throughout training: higher $\alpha$ has higher bias, lower variance and easier to learn, whereas lower $\alpha$ has lower bias, higher variance and harder to learn. For ML-CPC, we consider 4 types of geometrically decreasing schedules for $\alpha$; fixed at 1.0; from 2.0 to 0.5; from 5.0 to 2.0; and from 10.0 to 0.1; so $\alpha = 1.0$ for all cases when we reached half of the training epochs. We use the same values for other hyperparameters as those used in the MoCo-v2 CPC baseline (more details in Appendix C).

**Results** We show the top-1 accuracy of the learned representations under the linear evaluation protocol in Table 4. While the original ML-CPC objective (denoted as $J_{1,0} \rightarrow J_{1,0}$) already outperforms the CPC baseline in most cases, we observe that using a curriculum from easy to hard objective has the potential to further improve performance of the representations. Notably, the $J_{10,0} \rightarrow J_{0,1}$ schedule improve the performance on both datasets by almost 2.5 percent with trained for 200 epochs. This demonstrates that the curriculum learning approach (specific to ML-CPC with re-weighting schedules) could be useful to unsupervised representation learning in general.

6 Conclusion

In this paper, we proposed multi-label contrastive predictive coding for representation learning, which provides a generalization to contrastive predictive coding via multi-label classification. Reweighted ML-CPC is able to enjoy less bias while being a lower bound to mutual information. We demonstrate the effectiveness of ML-CPC on mutual information, knowledge distillation and unsupervised representation learning. It would be interesting to further apply this method to other application domains, investigate alternative methods to control the re-weighting procedure (such as using angular margins [31]), and develop more principled approaches towards curriculum learning for unsupervised representation learning.
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A Proofs

A.1 Preliminary Lemma and Propositions

To prove the main results, we need the following Lemma and Propositions 1 and 2. The Lemma is a special case to the dual representation of $f$-divergences discussed in [37].

**Lemma 1** (Nguyen et al. [37]). $\forall P, Q \in \mathcal{P}(X)$ such that $P \ll Q$, 

$$D_{\text{KL}}(P||Q) = \sup_{T \in L^{\infty}(Q)} E_P[T] - E_Q[e^{T-1}]$$

(9)

**Proposition 1.** $\forall n \geq 1, m \geq 2$, and for any collection of positive random variables $\{X_i\}_{i=1}^n$, $\{X_{i,j}\}_{j=1}^m$, such that $\forall i \in [n]$, $X_i, X_{i,1}, X_{i,2}, \ldots, X_{i,m-1}$ are exchangeable, then $\forall \alpha \in (0, \frac{2m}{m+1})$,

$$E \left[ \frac{1}{n} \sum_{i=1}^{n} \frac{mX_i}{\alpha X_i + \frac{m-\alpha}{m} \sum_{j=1}^{m-1} X_{i,j}} \right] \leq \frac{1}{\alpha}$$

(10)

**Proof.** First, for $\alpha \in (0, \frac{2m}{m+1})$ we have:

$$nE \left[ \frac{1}{n} \sum_{i=1}^{n} \frac{mX_i}{\alpha X_i + \frac{m-\alpha}{m} \sum_{j=1}^{m-1} X_{i,j}} \right]$$

(11)

$$= E \left[ \sum_{i=1}^{n} \frac{m \sum_{j=1}^{m-1} X_{i,j}}{(\sum_{j=1}^{m-1} X_{i,j}) - \alpha m \sum_{j=1}^{m-1} X_{i,j}} \right]$$

(12)

$$= E \left[ \sum_{i=1}^{n} \frac{m \sum_{j=1}^{m-1} X_{i,j}}{\sum_{j=1}^{m-1} X_{i,j}} \right]$$

(13)

$$= \frac{m}{m-\alpha} E \left[ \sum_{i=1}^{n} \left( \frac{X_i}{\sum_{j=1}^{m-1} X_{i,j}} \right)^{p+1} \right] \left( 1 - \frac{m-1}{m - \alpha} \right)^p$$

(Taylor expansion)

(14)

$$= \frac{m}{m-\alpha} \sum_{i=1}^{n} \sum_{p=0}^{\infty} E \left[ \left( \frac{X_i}{\sum_{j=1}^{m-1} X_{i,j}} \right)^{p+1} \right] \left( 1 - \frac{m-1}{m - \alpha} \right)^p$$

(15)

where we simplify the notation with $\Sigma_i := X_i + \sum_{j=1}^{m-1} X_{i,j}$. Furthermore, we note that the Taylor series converges because $(1 - \frac{m-1}{m - \alpha}) \in (-1, 1)$.

Since the random variables are exchangeable, switching the ordering of $X_i, X_{i,1}, \ldots, X_{i,m-1}$ does not affect the joint distribution, and the summing function is permutation invariant. Therefore, for all $i \in [n], p \geq 0$

$$E \left( \frac{X_i}{\Sigma_i} \right)^{p+1} = \frac{1}{m} E \left( \frac{X_i}{\sum_{j=1}^{m-1} X_{i,j}} \right)^{p+1}$$

(16)

$$\leq \frac{1}{m} E \left( \frac{X_i}{\Sigma_i} + \sum_{j=1}^{m-1} \frac{X_{i,j}}{\Sigma_i} \right)^{p+1} = \frac{1}{m}$$

(17)

where the last inequality comes from the fact that $(X_i + \sum_{j=1}^{m-1} X_{i,j}) / \Sigma_i = 1$ and all the random variables are positive. Continuing from Eq. (15), we have:

$$nE \left[ \frac{1}{n} \sum_{i=1}^{n} \frac{mX_i}{\alpha X_i + \frac{m-\alpha}{m} \sum_{j=1}^{m-1} X_{i,j}} \right]$$

(18)

$$\leq \frac{n}{m-\alpha} \sum_{p=0}^{\infty} \frac{1}{m} \left(1 - \frac{m-1}{m - \alpha} \right)^p = \frac{m-1}{m - \alpha} \frac{n}{m - \alpha} = \frac{n}{\alpha}$$

(19)

Dividing both sides by $n$ completes the proof for $\alpha \in (0, \frac{2m}{m+1})$. 

\[\square\]
Proposition 2. ∀n ≥ 1, m ≥ 2, and for any collection of positive random variables \( \{X_i\}_{i=1}^{m} \) such that ∀i ∈ [n], \( X_i, X_i, X_i, 1, X_i, 2, \ldots, X_i, m-1 \) are exchangeable, then ∀α ∈ [1, \( \frac{m}{\alpha} \)],

\[
\mathbb{E} \left[ \frac{1}{n} \sum_{i=1}^{n} \alpha X_i + \frac{m-\alpha}{m-1} \sum_{j=1}^{m-1} \frac{1}{X_{i,j}} \right] \leq 1
\]

(20)

Proof. The case for \( \alpha \in [1, \frac{2m}{m+1}] \) is apparent from Proposition 1. For \( \alpha \in (2m/(m+1), m/2] \), we have for all \( n \leq m-1 \):

\[
\mathbb{E} \left[ \frac{1}{n} \sum_{i=1}^{n} \alpha X_i + \frac{m-\alpha}{m-1} \sum_{j=1}^{m-1} \frac{1}{X_{i,j}} \right] \leq \mathbb{E} \left[ \frac{1}{n} \sum_{i=1}^{n} \alpha X_i + \frac{m}{m-1} \sum_{j=1}^{m-1} \frac{1}{X_{i,j}} \right] \leq \mathbb{E} \left[ \frac{1}{n} \sum_{i=1}^{n} \alpha X_i + \frac{tX_{i,j}}{mX_{i,j} + \frac{t}{2} \sum_{k=j}^{m-1} \frac{1}{X_{i,k}}} \right]
\]

(21)

(22)

(23)

where we define \( \overline{X_{i,k}} = \frac{X_{i,k}}{m-k} \) when \( k > (m-1) \) and use the concavity of the inverse function (or equivalently the HM-AM inequality) to establish Eq. (22). For any \( \alpha \in (2m/(m+1), m/2] \), we can choose \( t \) to be any integer from the interval \( \frac{m}{\alpha}, \frac{2m}{\alpha} \); we note that such an integer always exists because the the length of the interval is greater or equal to 1:

\[
\frac{2m}{\alpha} - \frac{m}{\alpha} = \frac{m}{\alpha} - 1 \geq 1
\]

Then we can apply the result in Proposition 1 for \( t \) samples and the new \( \alpha \) being \( \frac{t\alpha}{m} \); from our construction of \( t \), this satisfies the condition in Proposition 1 that:

\[
1 \leq \frac{t\alpha}{m} \leq \frac{2t}{t+1}
\]

Therefore we can apply Proposition 1 to a valid choice of \( t \) to obtain

\[
\mathbb{E} \left[ \frac{1}{n} \sum_{i=1}^{n} \alpha X_i + \frac{m-\alpha}{m-1} \sum_{j=1}^{m-1} \frac{1}{X_{i,j}} \right] \leq \mathbb{E} \left[ \frac{1}{n} \sum_{i=1}^{n} \alpha X_i + \frac{tX_{i,j}}{mX_{i,j} + \frac{t}{2} \sum_{k=j}^{m-1} \frac{1}{X_{i,k}}} \right] \leq \frac{m}{t\alpha} \leq 1
\]

which proves the result. \( \square \)

A.2 Proof that CPC is a lower bound to MI in general

Proposition 3. ∀n ≥ 1, m ≥ 2, then ∀g : \( X \times Y \rightarrow \mathbb{R}_+ \),

\[
L(g) \leq I(X; Y)
\]

(24)

Proof. We note that the proof here is more general than the one introduced in Poole et al. \[38\], where they assumed a specific form of negative sampling (where \( n = m \)).

\[
L(g) := \mathbb{E} \left[ \frac{1}{n} \sum_{i=1}^{n} \log \frac{m \cdot g(x_i, y_i)}{g(x_i, y_i) + \sum_{j=1}^{m-1} g(x_i, y_{i,j})} \right]
\]

(25)

\[
\leq \frac{1}{n} \sum_{i=1}^{n} (D_{KL}(p(x, y)\|p(x)p(y))) \leq 1 + \mathbb{E} \left[ \frac{1}{n} \sum_{i=1}^{n} \log \frac{m \cdot g(x_i, y_i)}{g(x_i, y_i) + \sum_{j=1}^{m-1} g(x_i, y_{i,j})} \right]
\]

(26)

\[
= I(X; Y) - 1 + \mathbb{E} \left[ \frac{1}{n} \sum_{i=1}^{n} \log \frac{m \cdot g(x_i, y_i)}{g(x_i, y_i) + \sum_{j=1}^{m-1} g(x_i, y_{i,j})} \right]
\]

(27)
where the inequality in Eq. (26) comes from Lemma 1. Then, we note that since \((x_i, y_i) \sim p(x)p(y)\), so \(g(x_i, y_i)\) and \(g(x_i, y_{i,j})\) are exchangeable random variables, so we can apply Proposition 2 with \(\alpha = 1\), such that:

\[
\mathbb{E}_{(x_i, y_i) \sim p(x)p(y)} \left[ \frac{1}{n} \sum_{i=1}^{n} \log \frac{m \cdot g(x_i, y_i)}{g(x_i, y_i) + \sum_{j=1}^{m-1} g(x_i, y_{i,j})} \right] \leq 1
\] (28)

Therefore, we can combine this with Eq. (27):

\[
L(g) \leq I(X;Y) - 1 + 1 = I(X;Y)
\] (29)

which proves the statement.

\[\square\]

### A.3 Proof of Theorem 1

**Theorem 1.** \(\forall n \geq 1, m \geq 2\), define \(\alpha_{m,n} = \frac{m}{n(m-1)+1}\). If \(\alpha \in [\alpha_{m,n}, 1]\), then \(\forall g : \mathcal{X} \times \mathcal{Y} \to \mathbb{R}_+\),

\[
J_\alpha(g) \leq I(X;Y)
\] (8)

**Proof.** First, we have

\[
J_\alpha(g) := \mathbb{E} \left[ \frac{1}{n} \sum_{i=1}^{n} \log \frac{nm \cdot g(x_i, y_i)}{\alpha \sum_{j=1}^{n} g(x_i, y_j) + \frac{m-\alpha}{m-1} \sum_{j=1}^{n} \sum_{k=1}^{m-1} g(x_j, y_{j,k})} \right]
\] (30)

\[
= \mathbb{E} \left[ \frac{1}{n} \sum_{i=1}^{n} \log (nm \cdot g(x_i, y_i)) - \log \left( \alpha \sum_{j=1}^{n} g(x_j, y_j) + \frac{m-\alpha}{m-1} \sum_{j=1}^{n} \sum_{k=1}^{m-1} g(x_j, y_{j,k}) \right) \right]
\] (31)

\[
= \mathbb{E} \left[ \frac{1}{n} \sum_{i=1}^{n} \log (nm \cdot g(x_i, y_i)) - \log \left( n \alpha g(x_i, y_i) + \frac{m-\alpha}{m-1} \sum_{j=1}^{n} \sum_{k=1}^{m-1} g(x_j, y_{j,k}) \right) \right]
\] (32)

\[
\leq I(X;Y) - 1 + \mathbb{E}_{(x_i, y_i) \sim p(x)p(y)} \left[ \frac{1}{n} \sum_{i=1}^{n} \log (nm \cdot g(x_i, y_i)) - n \alpha g(x_i, y_i) + \frac{m-\alpha}{m-1} \sum_{j=1}^{n} \sum_{k=1}^{m-1} g(x_j, y_{j,k}) \right]
\] (33)

where we use Jensen’s inequality over \(\log\) in Eq. (31) and Lemma 1 in Eq. (33).

Since \((x_i, y_i) \sim p(x)p(y)\), so \(g(x_i, y_i)\) and all the \(g(x_j, y_{j,k})\) are \((n(m-1) + 1)\) exchangeable random variables, and

\(m \geq 2, \alpha \in \left[ \frac{m}{n(m-1)+1}, 1 \right] \Rightarrow \frac{n(m-1)+1}{m} \alpha \in \left[ 1, \frac{n(m-1)+1}{2} \right], \)

we can apply Proposition 2 to the \((n(m-1) + 1)\) exchangeable variables:

\[
\mathbb{E}_{(x_i, y_i) \sim p(x)p(y)} \left[ \frac{1}{n} \sum_{i=1}^{n} \log (nm \cdot g(x_i, y_i)) - n \alpha g(x_i, y_i) + \frac{m-\alpha}{m-1} \sum_{j=1}^{n} \sum_{k=1}^{m-1} g(x_j, y_{j,k}) \right]
\]

\[
= \mathbb{E}_{(x_i, y_i) \sim p(x)p(y)} \left[ \frac{1}{n} \sum_{i=1}^{n} \frac{(n(m-1)+1) \cdot g(x_i, y_i)}{m} \right] \leq 1
\]

Combining the above to Eq. (33), we have that:

\[
J_\alpha(g) \leq I(X;Y)
\] (34)

for the given range of \(\alpha\). \[\square\]
A.4 Time complexity of gradient calculation in ML-CPC

Suppose $g$ is a neural network parametrized by $\theta$, then the gradient to the ML-CPC objective is

$$\nabla_\theta J(g) = E \left[ \frac{1}{n} \sum_{i=1}^{n} \nabla_\theta g_\theta(x_i, y_i) - \sum_{j=1}^{n} \nabla_\theta g_\theta(x_j, y_j) + \sum_{j=1}^{n} \sum_{k=1}^{m-1} \nabla_\theta g_\theta(x_j, y_{j,k}) \right]$$

(35)

Computing the gradient through the empirical estimate of $J(g)$ requires us to perform back-propagation through all $nm$ critic evaluations, which is identical to the amount of back-propagation passes needed for CPC. So the time complexity to compute the ML-CPC gradient is $O(nm)$.

B Pseudo-code and PyTorch implementation to ML-CPC

We include a PyTorch implementation to $\alpha$-ML-CPC as follows.

```python
def ml_cpc(logits, alpha):
    
    # We assume that logits are of shape (n, m),
    # and the predictions over positive are logits[:, 0].
    # Alternatively, one can use kl_div() to ensure that the loss is non-negative.
    
    n, m = logits.size(0), logits.size(1)
    beta = (m - alpha) / (m - 1)
    pos = logits.select(1, 0)
    neg = logits.narrow(1, 1, m)
    denom = torch.cat([pos + torch.log(torch.tensor(alpha)).float(),
                       neg + torch.log(torch.tensor(beta)).float()], dim=1)
    denom = denom.logsumexp(dim=1).logsumexp(dim=0)
    loss = denom - pos.sum()
    return loss / n
```

To ensure that the loss value is non-negative, one can alternatively use the kl_div() function that evaluates the KL divergence between the predicted label distribution with a ground truth label distribution. This is equivalent to the negative of the $\alpha$-ML-CPC objective shifted by a constant. We describe this idea in the following algorithm.

**Algorithm 1** Pseudo-code for $\alpha$-ML-CPC

1: **Input:** the critic $g$, input values $x_i, y_i, y_{j,k}$
2: **Output:** shifted negative objective value $J_\alpha(g)$ for optimization
3: Compute logit values $\ell_{i,i} = \log g(x_i, y_i) + \log \alpha$ and $\ell_{j,k} = \log g(x_j, y_{j,k}) + \log \frac{m-\alpha}{m-1}$.
4: Compute the normalization value $Z = \sum_i \exp(\ell_{i,i}) + \sum_{j,k} \exp(\ell_{j,k})$.
5: Compute the predicted probabilities $p'_{i,i} = \exp(\ell_{i,i})/Z$, $p'_{j,k} = \exp(\ell_{j,k})/Z$
6: Assign the ground truth probabilities $p_{i,i} = 1/n$, $p_{j,k} = 0$.
7: Compute the KL divergence between $p$ and $p'$.

C Experimental Details

C.1 Binary simulation experiments

Let $X, Y$ be two binary r.v.s such that $\Pr(X = 1, Y = 1) = p$, $\Pr(X = 0, Y = 0) = 1 - p$. We can simulate the case of a batch size of $n$ with $n-1$ negative samples. For the example of CPC, we have:

$$L(g) := E \left[ \frac{1}{n} \sum_{i=1}^{n} \log \frac{n \cdot g(x_i, y_i)}{\sum_{j=1}^{n} g(x_i, y_j)} \right]$$

(36)
180 and 210 epochs. We use $16384$

We sample each dimension of $\mathbf{x}_i$ in order to compute one term of the expectation. If we have $t$ pairs of $(1, 1)$ and $(n-t)$ pairs of $(0, 0)$, then for $g(1, 1) = g(0, 0) = 1$, $g(0, 1) = g(1, 0) = 0$ we have that:

$$\frac{1}{n} \sum_{i=1}^{n} \log \frac{n \cdot g(\mathbf{x}_i, \mathbf{y}_i)}{\sum_{j=1}^{n} g(\mathbf{x}_i, \mathbf{y}_j)} = \frac{1}{n} \left( t \log \frac{n}{t} + (n-t) \log \frac{n-t}{n-t} \right)$$  \hspace{1cm} (37)

Moreover the probability of such an arrangement can be computed from the Binomial distribution

$$\Pr(t \text{ pairs of } (1, 1)) = \binom{n}{t} p^t (1-p)^{n-t}$$  \hspace{1cm} (38)

Therefore, we can compute the expectation that is $L(g)$ in closed form by computing the sum for $t$ from 0 to $n$. We can apply a similar argument to computing the mean of ML-CPC values as well as the variance of the empirical estimates. This allows us to analytically compute the optimal value of the objective values, which allows us to perform direct comparisons over them.

### C.2 Mutual information estimation

The general procedure follows that in [38] and [41].

**Tasks** We sample each dimension of $(\mathbf{x}, \mathbf{y})$ independently from a correlated Gaussian with mean 0 and correlation of $\rho$, where $\mathcal{X} = \mathcal{Y} = \mathbb{R}^{20}$. The true mutual information is computed as: $I(\mathbf{x}, \mathbf{y}) = -\frac{d}{2} \log (1 - \rho^2)$ The initial mutual information is 2, and we increase the mutual information by 2 every $4k$ iterations.

**Architecture and training procedure** We consider two types of architectures — *joint* and *separable*. The *joint* architecture concatenates the inputs $\mathbf{x}$, $\mathbf{y}$, and then passes through a two layer MLP with 256 neurons in each layer with ReLU activations at each layer. The *separable architecture* learns two separate neural networks for $\mathbf{x}$ and $\mathbf{y}$ (denoted as $g(\mathbf{x})$ and $h(\mathbf{y})$) and predicts $g(\mathbf{x})^\top h(\mathbf{y})$: $g$ and $h$ are two neural networks, each is a two layer MLP with 256 neurons in each layer with ReLU activations at each layer; the output of $g$ and $h$ are 32 dimensions. For all the cases, we use with the Adam optimizer [26] with learning rate $1 \times 10^{-3}$ and $\beta_1 = 0.9$, $\beta_2 = 0.999$ and train for $20k$ iterations with a batch size of 128.

### C.3 Knowledge distillation

The general procedure follows that in [42], where we use the same training hyperparameters. Specifically, we train for 240 epochs with the SGD optimizer with a momentum of 0.9 and weight decay of $5 \times 10^{-4}$. We use a default initial learning rate of 0.1, and divide the learning rate by 10 at 150, 180 and 210 epochs. We use 16384 negative samples per positive sample and a temperature of 0.07 for the critic. We did not additionally include the knowledge distillation loss to reduce potential compounding effects over the representation learning performance.

### C.4 Unsupervised representation learning

The general procedure follows that of MoCo-v2 [17, 10], with some slight changes adapted to CIFAR-10. First, we use the standard ResNet50 adaptation of $3 \times 3$ kernels instead of $7 \times 7$ kernels used for the larger resolution ImageNet, with representation learning dimension of 2048. Next, we use a temperature of $\tau = 0.07$, a batch size of 256 and a learning rate of 0.3 for the representation learner, and a learning rate of 3 for the linear classifier; we observe that these hyperparameters combinations is able to achieve higher performance on the CPC objective for CIFAR-10, so we use these for all our other experiments. The remaining hyperparameters are identical to the ImageNet setup for MoCo-v2.

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3We note that this is smaller than what is used in [42], and it is possible to achieve additional (though not much) improvements by using more negative samples.