Abstract

Negative sampling is a limiting factor w.r.t. the generalization of metric-learned neural networks. We show that uniform negative sampling provides little information about the class boundaries and thus propose three novel techniques for efficient negative sampling: drawing negative samples from (1) the top-\(k\) most semantically similar classes, (2) the top-\(k\) most semantically similar samples and (3) interpolating between contrastive latent representations to create pseudo negatives. Our experiments on CIFAR-10, CIFAR-100 and Tiny-ImageNet-200 show that our proposed Semantically Conditioned Negative Sampling and Latent Mixup lead to consistent performance improvements. In the standard supervised learning setting, on average we increase test accuracy by 1.52% percentage points on CIFAR-10 across various network architectures. In the knowledge distillation setting, (1) the performance of student networks increase by 4.56% percentage points on Tiny-ImageNet-200 and 3.29% on CIFAR-100 over student networks trained with no teacher and (2) 1.23% and 1.72% respectively over a hard-to-beat baseline (Hinton et al., 2015).

1. Introduction

Training deep neural networks using contrastive learning has shown state of the art (SoTA) performance in domains such as computer vision (Oord et al., 2018; He et al., 2020; Chen et al., 2020; Henaff, 2020), speech recognition (Oord et al., 2018) and natural language processing (Mueller & Thyagarajan, 2016; Logeswaran & Lee, 2018; Fang & Xie, 2020). The generalization performance in contrastive learning heavily relies on techniques that enable training of large batch sizes, such as learning a lookup table (Xiao et al., 2017; Wu et al., 2018; He et al., 2020) to store lower-dimensional latent features of negative samples. However, training large models using contrastive learning can be inefficient when using uniformly sampled negatives (USNs) as the total number of potential negative sample pairs is \(O((N - N_+)N)\) where \(N\) is the number of training samples and \(N_+\) is the number of positive class samples. Hence, even a lookup table may poorly estimate negative sample latent features, even for a large number of USNs and training epochs.

A complementary approach to improve the learning efficiency of a contrastive learned neural network is to reduce the model size using model compression techniques such as knowledge distillation (KD; Buciluă et al., 2006). In neural networks, this is achieved by transferring the logits of a larger “teacher” network to learn a smaller “student” network (Hinton et al., 2015). There has been various KD methods proposed (Romero et al., 2014; Hinton et al., 2015; Zagoruyko & Komodakis, 2016a; Yim et al., 2017; Pasalis & Tefas, 2018; Tung & Mori, 2019; Peng et al., 2019). They involve minimizing KL divergence (KLD) between the student network and teacher network logits (Hinton et al., 2015), minimizing the squared error between the student and teacher network intermediate layers (Romero et al., 2014), metric learning approaches (Tung & Mori, 2019; Ahn et al., 2019; Tian et al., 2019; Park et al., 2019), attention transfer of convolution maps (Zagoruyko & Komodakis, 2016a) and activation boundary transfer (Heo et al., 2019).

In this paper, we propose three efficient negative sampling (NS) alternatives to uniform NS and show their efficacy in standard supervised learning and the aforementioned KD setting. Our NS techniques are also complementary to the aforementioned lookup tables used for retrieving negative latent features. All three techniques have a common factor in that they produce negatives that are semantically similar to the positive targets on both instance- and class-levels. We collectively refer to these sampling methods as Semantically Conditioned Negative Sampling (SCNS) as we replace a uniform prior over negative samples with a conditional probability distribution defined by the embeddings produced by a pretrained network. SCNS provides more informative negatives in contrast to USNs where many samples are easy
to classify and do not support the class boundaries. Additionally, it requires no additional parameters at training time and thus can be used with large training sets and models. The pretrained representations are used to estimate pairwise class-level and instance-level semantic similarities to define a top-$k$ NS probability distribution. This reduces the number of negative pairs from $O(N(N - N_+))$ to $O(Nk)$ where $k$ is the number of nearest neighbor negative samples for each sample. Below is a summary of our contributions.

1) Class and Instance Conditioned Negative Sampling: We define the NS distribution of each class by drawing negative samples proportional to the top-$k$ cosine similarity between pretrained word embeddings of the class labels. We also propose top-$k$ instance-level similarity for defining the NS distribution by performing a forward pass with a pretrained network prior to training.

2) Contrastive Representation Mixup: In subsection 3.2, we propose Latent Mixup (LM), a variant of Mixup (Zhang et al., 2017) that operates on latent representations between teacher positive and negative representations to produce harder pseudo negative sample representations that lie closer to the class boundaries. This is also carried out for the student network representations and a distance (or divergence) is minimized between both mixed representations.

3) Theoretical Analysis of Conditioned Sampling: We reformulate the mutual information lower bound to account for semantic similarity of contrastive pairs and describe the sample efficiency of SCNS compared to uniform sampling.

2. Related Research

Before describing our proposed methods, we review related work on the two most related aspects: efficient NS and KD.

Efficient Negative Sampling Efficient NS has been explored in the literature, predominantly for triplet learning. Semi-hard NS has been used to sample negative pairs yet are still further in Euclidean distance than the anchor-positive pair (Schroff et al., 2015). Oh Song et al. (2016) combine contrastive and triplet losses to mine negative structured embedding samples, drawing negative samples proportional to a Gaussian distribution of negative sample distances to the anchor sample Harwood et al. (2017). Suh et al. (2019) select hard negatives from the class-to-sample distances and then search on the instance-level within the selected class to retrieve negative samples. Wu et al. (2017) proposed a distance weighted sampling that selects more stable and informative samples when compared to uniform sampling and show that data selection is at least as important as the choice of loss function. Zhuang et al. (2019) define two neighborhoods using $k$-means clustering, close neighbors and dissimilar samples are background neighbors. Wu et al. (2020) use ball discrimination to discriminate between hard and easy negative unsupervised representations where positive pairs are different views of the same image. Tran et al. (2019) use the prior probability of observing a class to draw negative samples and then further sample instances within the chosen class based on the inner product with the anchor of the triplet, showing improvements over semi-hard NS without the use of informative priors.

Knowledge Distillation The original KD objective minimizes the Kullbeck-Leibler divergence between student network and teacher network logits (Hinton et al., 2015). Romero et al. (2014) instead restrict the student network hidden representation to behave similarly to the teacher network hidden representations by minimizing the squared error between corresponding layers of the two networks. The main restriction in this method is that both networks have to be the same depth and of similar architectures. Attention Transfer (AT) (Zagoruyko & Komodakis, 2016a) performs KD by forcing the student network to mimic the attention maps over convolutional layers of the pretrained teacher network. Passalis & Tefas (2018) use Gaussian and Cosine-based kernel density estimators (KDEs) to maximize the similarity between the student and teacher probability distributions. They find consistent improvements over Hinton et al. (2015) and Hint layers used in Fitnet (Romero et al., 2014). Similarity-Preserving (SP) (Tung & Mori, 2019) KD ensures that the activation patterns of the student network are similar to that in the teacher network for semantically similar input pairs. Peng et al. (2019) propose Correlation Congruence (CC) to maximize multiple cross-correlations between samples of the same class. Ahn et al. (2019) provide an information-theoretic view of KD by maximizing the mutual information between student and teacher networks through variational information maximization (Barber & Agakov, 2003). Moreover, Park et al. (2019) argue that the distance between relation structures created from multiple samples of the student and teacher networks should be minimized. They propose Relational KD (RKD), which involves the use of both distance-wise and angle-wise distillation losses that penalize structural discrepancies between multiple instance outputs from both networks. Contrastive Representation Distillation (Tian et al., 2019) uses a CL objective to maximize a lower bound on the mutual to capture higher order dependencies between positive and negative samples, adapting their loss from Hjelm et al. (2018).

3. Methodology

We begin by defining a dataset as $D := \{(x_i, y_i)\}_{i=1}^N$, which consists of $N$ samples of an input vector $x \in \mathbb{R}^n$ and a corresponding target $y \in \{0, 1\}^C$ where sample $s_i := (x_i, y_i)$ and $C$ is the number of classes. In the CL setting $x = (x_s, x_{+}, x_{-1}, \ldots, x_{-M})$ where $X_+ := (x_s, x_{+})$ and $X_- := (x_s, x_{-1}, \ldots, x_{-M})$ for $M$ negative pairs.
We denote a neural network as \( f_\theta(x) \) which has parameters \( \theta := (\theta_1, \theta_2, \ldots, \theta_L) \) where \( \theta_l := \{ w_l, b_l \} \), \( w_l \in \mathbb{R}^{d_l \times d_{l+1}} \), \( b_l \in \mathbb{R}^{d_{l+1}} \) and \( d_l \) denotes the dimensionality of the \( l \)-th layer. The input to each subsequent layer is denoted as \( h_l \in \mathbb{R}^{d_l} \) where \( x := h_0 \) and the corresponding output activation is denoted as \( z_l = g(h_l) \). For brevity, we refer to \( z = g(h_L) \) as the unnormalized output where \( g : \mathbb{R}^{d_L} \to \mathbb{R}^p \) and \( z \in \mathbb{R}^p \). However, when using a metric loss, \( g : \mathbb{R}^{d_L} \to \mathbb{R}^{d_L} \) and therefore \( z \in \mathbb{R}^{d_L} \). In the former case, the cross-entropy loss is used for supervised learning and defined as \( \ell_{CE}(D) := \frac{1}{N} \sum_{i=1}^{N} \sum_{c=1}^{V} -y_{ic} \log \hat{y}_{ic} \), where \( \hat{y}_i = \sigma(f_\theta(x_i)/\tau) \), \( \hat{y}_i \in \mathbb{R}^p \) and \( \tau \in (0, +\infty) \) is the temperature of the softmax \( \sigma \).

We also consider the KD setting where a student network \( f_\theta^S \) learns from a pretrained teacher network \( f_\theta^T \) with pretrained and frozen parameters \( \omega \). The last hidden layer representation of \( f_\theta^S \) is given as \( z^S := f_\theta^S(x) \) and similarly \( z^T := f_\theta^T(x) \). The Kullback-Leibler Divergence (KLD), \( D_{KLD} \), between \( z^S \) and \( z^T \) is defined in Equation 1

\[
D_{KLD}(\mathbb{Y}^T|\mathbb{Y}^S) = \mathbb{H}(\mathbb{Y}^T) - \mathbb{Y}^T \log(\mathbb{Y}^S) \\
\mathbb{Y}^S = \sigma(z^S/\tau), \quad \mathbb{Y}^T = \sigma(z^T/\tau) \tag{1}
\]

where \( \mathbb{H}(\mathbb{Y}^T) \) is the entropy of the teacher distribution \( \mathbb{Y}^T \). Following Hinton et al. (2015), the weighted sum of cross-entropy loss and KLD loss shown in Equation 2 is used as our main KD baseline, where \( \alpha \in [0, 1] \).

\[
\ell_{KD} = (1 - \alpha)\ell_{CE}(\mathbb{Y}^S, \mathbb{Y}^T) + \alpha \tau D_{KLD}(\mathbb{Y}^S, \mathbb{Y}^T) \tag{2}
\]

To carry out KD using the KLD loss, the outputs of the pretrained teacher \( f_\theta^T \) are stored after performing a single forward pass over mini-batches \( B \subset D \) in our training set. These outputs are then retrieved for each mini-batch update of the smaller student network \( f_\theta^S \). Given this background, the next two subsections will describe our three main approaches to improving NS in contrastive learning.

### 3.1. Semantically Conditioned Negative Sampling

Here, we describe two of our three approaches for improving NS efficiency that both involve using \( f_\theta^T \) to define a NS distribution. The first involves a cross-modal teacher network (i.e pretrained word embeddings for image classification) to define a class-level NS distribution and in the second \( f_\theta^T \) is a pretrained image classifier that defines an instance-level NS distribution.

#### 3.1.1. Class-Level Negative Sampling

Our first method assumes that word embedding similarity between class labels highly correlates with image embedding similarity (Leong & Mihalcea, 2011; Frome et al., 2013). Pretrained word embedding similarities are used to improve the sample efficiency of NS in contrastive learning and replace uniform NS that is typically used. The cosine similarity is measured between the pretrained word embeddings \( (z_{w_i}^T, z_{w_j}^T) \) where \( (w_i, w_j) \) are the class labels in the vocabulary \( V \) and \( |V| = C \). This is carried out for all pairs to construct an all pair cosine similarity matrix \( Z_V \in \mathbb{R}^{|V| \times |V|} \) that is then row-normalized with the softmax function \( \sigma \) as \( \mathbf{P}_V := \sigma(Z_V/\tau) \). Here, setting \( \tau \) high leads to harder negative samples being chosen from the most similar classes. \( \mathbf{P} \) represents the conditional probability matrix used to define \( X_\sim \) by drawing samples as Equation 3 where \( D_w \)

\[
x_\sim \sim \mathcal{D}_w \propto \mathbf{P}_w \tag{3}
\]

represents all samples \( (x_1^w, \ldots, x_M^w) \) for a given class associated with \( w \). This is repeated \( M \) times when using CL.

#### Hard k-Nearest Class-Level Negative Samples

Instead of sampling over a possible \( M = |V| - 1 \) number of negative samples, we can define the top-\( k \) most similar hard negative samples. The top-\( k \) cosine similarities from other labels in \( V \) are selected by applying Equation 4 where \( z_{w_i}^T \in \mathbb{R}^{d_w} \) and \( z_{w_i} := f_\theta^T(w_i) \) of the class label \( w_i \).

\[
\text{topk}_w(z_{w_i}^T) = \arg \max_{k \neq i} \left[ \cos(z_{w_i}^T, z_{w_k}^T) \right] \tag{4}
\]

The \( k \)-nearest neighbor (\( k \)-NN) similarity scores are then stored in \( Z^k_V \in \mathbb{R}^{|V| \times k} \) with a corresponding matrix \( I^k_V \in \mathbb{R}^{|V| \times |V|} \) that stores the \( k \)-NN class indices \( Z^k_V \) retrieved by applying Equation 4. We focus on only sampling from the top-\( k \) classes and therefore define the normalized top-\( k \) class distribution matrix as \( \mathbf{P}^k_V := \sigma(Z^k_V/\tau) \). A row vector of \( \mathbf{P}^k_v \) is denoted as \( \mathbf{P}^k_w \) consisting of the \( k \) truncated conditional probabilities corresponding to the \( k \) nearest class labels of \( w \) in \( V \). We then sample as in Equation 3 instead with top-\( k \) negative samples \( D^k_w \subset D_w \) and \( |D^k_w| = k|D_w| \).

**Figure 1.** CIFAR-100 subset of word embedding class similarities
Figure (1) shows a submatrix of \( P_Y \) as a heatmap corresponding to a subset of CIFAR-100 class labels on the x and y-axis. We see that “willow-tree” has a high similarity score with “maple-tree”, “oak-tree”, “palm-tree” and “pine-tree”. Therefore, samples from these class labels will be sampled more frequently as hard yet more informative negative samples. Similarly, (“man”, “woman”) and (“tractor”, “pickup-truck”) would be sampled at a higher rate than the remaining terms.

### 3.1.2. INSTANCE-LEVEL CONDITIONED SAMPLING

Class-level SCNS (or Class-SCNS) may not be granular enough as the conditional probability assigned to a class is the same for all samples within that class. In instance-level SCNS we define the top-\( k \) nearest samples for each \( x \in \mathcal{D} \). A top-\( k \) instance similarity matrix produced by \( f^S_{th} \) is iteratively constructed \( \forall x \in \mathcal{D} \) and the outputs are stored in \( Z^k \in \mathbb{R}^{N \times k} \). As before, we define \( P^k_x \) and sample \( z \sim \mathcal{D}^k \propto P^k_x \). Unlike Class-SCNS, \( f^S_{th} \) is trained on the same modality (e.g. images) as \( f^S_{th} \) and \( P^k_x \) is now a SCNS matrix for each \( x \in \mathcal{D} \) and not per class label \( w \in \mathcal{V} \).

For image classification, we choose \( f^T_{th} \) to be a pretrained CNN. We use the final hidden representation \( z^T_{th} \) to be a pretrained CNN. The conditional probability that the representation of a negative sample \( x_- \) matches in the circular queue is given by Equation 6.

\[
q_i = \frac{e^{v_i^T z^S_i / \tau}}{\sum_{m=1}^{N_u} e^{u_m^T z^S_i / \tau} + \sum_{n=1}^{N_q} e^{u_n^T z^S_i / \tau}}
\]

The gradient \( \nabla z^S \mathbb{E}_{z^S} [\log p_i] \) is defined in the backward pass as Equation 7.

\[
\frac{\partial \ell}{\partial z^S} = \frac{1}{\tau} \left[ \left( 1 - p_i v - \sum_{j=1}^{N_y} \sum_{j \neq y} p_j v_j - \sum_{k=1}^{N_t} q_k u_k \right) \right]
\]

where \( y \) is the column of \( V \) corresponding to the \( y \)-th target \( y \in \mathbb{N}_+ \) and \( y^T \) in the KD setting. This lookup table can be used complementary to SCNS and we use it in our experiments. It is also easier to compare to prior CL approaches (Tian et al., 2019) as they too use a lookup table.

### 3.1.3. CONDITIONED SAMPLES WITH A LOOKUP TABLE

To further reduce training time we can combine SCNS with a lookup table (Xiao et al., 2017) that stores negative sample features and updates during training. For \( \forall \mathcal{X}_+ \in \mathcal{B} \), the dot product is computed between \( z^S \) and the \( i \)-th column of the \( L_2 \) row normalized lookup table \( V \in \mathbb{R}^{d_i \times N_v} \). If the \( i \)-th target \( y_i \) is predicted then the update \( v_i \leftarrow \gamma v_i + (1 - \gamma) z^S \) is performed in the backward pass. A high \( \gamma \in [0, 1] \) results in a smaller update \( v_i \in \mathbb{R}^{d_i} \) in the lookup table. For \( \mathcal{X}_- \), a circular queue \( Q \in \mathbb{R}^{d_i \times N_q} \) is used where \( N_q \) is the queue size and the dot product \( Q^T z^S \) is computed. The current features are put into the queue and older features are removed from the queue during training. Equation 5 shows the conditional probability \( p_i \) corresponding to the target \( y_i \) where \( u_n \in \mathbb{R}^{d_i} \) is stored as the \( n \)-th row of \( Q \).

\[
p_i = \frac{e^{v_i^T z^S_i / \tau}}{\sum_{m=1}^{N_v} e^{u_m^T z^S_i / \tau} + \sum_{n=1}^{N_q} e^{u_n^T z^S_i / \tau}}
\]
Mixup (Zhang et al., 2017) is a simple regularization technique that performs a linear interpolation of inputs. Our proposed LM instead mixes the latent representations between positive and negative pairs given by the student and teacher networks as opposed to mixing the raw images. The motivation for this is that \( f_\theta^S \) learns more about the geometry of the embedding space induced by \( f_\theta^T \) and interpolating on a lower-dimensional manifold than the original input can lead to smoother interpolations. The interpolation function \( \kappa(z_i, z_j) \) in Equation 8 outputs a contrastive mixture \( \tilde{z} \) from \( z_i \in \mathbb{R}^d, z_j \in \mathbb{R}^d \) and the mixture coefficient \( \nu \in [0,1] \) is drawn from the beta distribution \( \nu \sim \text{Beta}(\beta, \beta) \) where \( \beta \in [0, \infty] \) and \( \beta \to 0 \) approaches the empirical risk.

\[
\kappa(z_i, z_j) = \nu z_i + (1 - \nu) z_j \tag{8}
\]

Both student and teacher LM representations and teacher targets are then computed as,

\[
\begin{align*}
\tilde{z}_{ij}^S &= \kappa(z_i^S, z_j^S), \quad \tilde{z}_{ij}^T = \kappa(z_i^T, z_j^T) \\
\tilde{y}_{ij}^T &= \sigma(W^T \tilde{z}_{ij}^T / \tau), \quad \tilde{y}_{ij}^T = \sigma(\kappa(y_i^T, y_j^T) / \tau) \tag{9}
\end{align*}
\]

where \( \tilde{y}_{ij}^T \) is a synthetic bimodal mixup target. Henceforth, we will denote mixup teacher targets as \( \tilde{y}_{ij}^T \) and LM representations as \( \tilde{z}^S \) and \( \tilde{z}^T \). The objective can then be described by the KLD as Equation 11 where \( H(\cdot) \) is the entropy of the predicted teacher distribution over classes \( \tilde{y}^T \).

From Equation 13, we see that \( I(x_+, x_+) \geq \log(M) - \ell \) (Oord et al., 2018) and the larger the number of negative samples, \( M \), the tighter the MI bound. However, we argue that if a pretrained \( f_\theta^T \) has training error close to 0, then \( \log(M) \) should be replaced with a term that accounts for the geometry of the embedding space as not all negative samples are equally important for reducing \( \ell \). Therefore, we express how top-\( k \) samples from SCNS tightens the lower bound estimate on MI when compared to using USNs. Given that we are not restricted to a distance, divergence or similarity between vectors, we refer to a general alignment function \( A \) that outputs an alignment score \( a \in [0,1] \).

Given \( x_+ \), the expected alignment score for the top-\( k \) negative samples is \( a_{x_+}^k := \mathbb{E}_{x_- \sim \mathcal{D}_k} [A(z_+, x_-)] \) and for negative samples outside of the top-\( k \) samples, \( a_{x_-}^r := \mathbb{E}_{x_- \sim \mathcal{D}_r} [A(z_+, x_-)] \) where \( \mathcal{D}_k \subseteq \mathcal{D}, \mathcal{D}_r \notin \mathcal{D}_k, r = N - N_y - k \), and \( N_y \) is the number of samples of class \( y \). The alignment weight (AW) \( \Omega_{x_+} := 1 - \frac{a_{x_+}^k}{a_{x_+}^r + a_{x_+}^r} \) is then used to represent the difference in ‘closeness’ between the top-\( k \) negative samples and the remaining negative samples.

**Lemma 1.** Given \( \Omega := \sum_{i=1}^{M} \Omega_{x_i} \), we can reformulate the MI lower bound when using SCNS as Equation 14.

\[
I(X, Y) \geq \ell + \log(2\Omega) \tag{14}
\]

**Proof.** We substitute \( \log(2\Omega) \) for \( \log(M) \) in Equation 13 as \( a_{x_+}^r \approx a_{x_+}^r \) in uniform sampling as \( M \to \infty \).
This lower bound favors top-k negative samples that have alignment with the positive class boundary and are relatively close compared to the negative samples outside of the top-k. It is dependent on the loss of $f^*$ where $\ell \approx 0$ results in an accurate alignment estimation for all embedding pairs.

**Lemma 2.** In the worst case, when all $M$ negatives are equidistant to $x_*$, forming a ring on the $L_2$ embedding hypersphere, SCNS is equivalent to uniform sampling.

**Proof.** This holds as $\log(2\Omega) \approx \log(M)$ when the centroids of both sets $a_k^* = a_i^*$ and $\Omega = M/2$. Therefore, in the worst case SCNS is equivalent to uniform sampling. □

The above case can be due to degenerative representations used in the top-k SCNS similarity computation (i.e. $\epsilon_{ir}$ not close to 0) or a characteristic of the training data itself. Then, the relation between $M$ USNs and top-k SCNS can be formed as follows. Let $\Omega_{D_{k^*}}$ be the AW of USNs for $x$ and $\Omega_{D_k}$ be the AW for the top-k negative samples. When $|D_{k^*}^x| \approx |D_k^x|$ we have,

$$I(X, Y) \geq \ell + \log(2\Omega_{D_k^x}) \geq \ell + \log(2\Omega_{D_k}) \quad (15)$$

given the non-uniform prior over negative samples as defined in SCNS. For some $k \leq N$, $2(\Omega_k - \Omega_{D_\ell}) = 0$ is met when a subset of $D_{k^*}^x$ negative samples have $\bar{x} \approx \bar{z}_x$ where $\bar{x}$ denotes the aforementioned subset and $\bar{z}_x$ is the centroid of the top-k negative samples.

**Number of Uniform Draws To Observe Top-k SCNS**

We can now describe the expected number of USNs draws required to observe the top-k samples at least once for a given $x_*$. Let $C_i$ denote the number of negative samples observed until the $i$-th new negative sample among the top-k samples is observed and $N$ is the total number of samples until all top-k negative samples are observed. Since $C = \sum_{i=1}^{k} C_i$, $E[C] = E[\sum_{i=1}^{k} C_i] = \sum_{i=1}^{k} E[C_i]$ where $C_i$ follows a geometric distribution with parameter $(k + 1 - i)/M$. Therefore, $E[C_i] = M/(k + 1 - i)$ and thus the expected number of draws is given by Equation 16.

$$E[C] = M \sum_{i=1}^{k} (k + 1 - i)^{-1} = M \sum_{i=1}^{k} i^{-1} \quad (16)$$

We reformulate this for mini-batch training where consecutive batches of size $b$ for $x_*$ are drawn with replacement. This is a special case of the Coupon Collector’s Problem ((CCP) Von Schelling, 1954).

**Theorem 3.** The batch variant of the CCP formulates the probability of the expected number of batches of size $b$ to observe top-k SCNS samples at least once as Equation 17.

$$\sum_{j=0}^{\infty} P(K > ib) = \sum_{j=0}^{M-1} (-1)^{M-j+1} \binom{M}{j} \frac{1}{1 - (\frac{b}{M})^j} \quad (17)$$

**Proof.** See Appendix E for the proof.

As $M$ grows more mini-batches are required to observe the top-k hard negative samples. Thus, $b$ has to be larger for uniform sampling to cover the informative negative samples, coinciding with the MI formulation in Equation 15. Further justifications are found in Appendix D and Appendix E.

### 4. Experiments

We now discuss the experimental results and note that additional details on hardware, datasets, model architectures and settings are found in Appendix A, B and C.

**Standard Supervised Learning** We first test our three NS approaches in the standard supervised learning setting on CIFAR-10. Several ResNet-based architectures (He et al., 2016; Zagoruyko & Komodakis, 2016b; Xie et al., 2017) are trained with (1) cross entropy between LM representations and the cross-entropy between student predictions and targets (Cross-Entropy + LM) and CL (InfoNCE + LM), (2) only using CL with the LM representations of each contrastive pair (InfoNCE-LM) and (3) Class-SCNS (InfoNCE + Class-SCNS) and Instance-SCNS (InfoNCE + Instance-SCNS) with the InfoNCE loss.

| Methods                     | resnet20 | resnet32 | resnet110 | wide-16-1 | wide-40-1 | resnext32x4 |
|-----------------------------|---------|---------|-----------|-----------|-----------|-------------|
| Cross-Entropy               | 91.44   | 92.49   | 93.38     | 94.06     | 94.47     | 95.38       |
| Cross-Entropy + LM (17)     | 92.74   | 92.75   | 93.53     | 94.28     | 94.54     | 95.47       |
| InfoNCE                     | 91.68   | 92.90   | 94.04     | 94.39     | 95.23     | 95.77       |
| -LM (β=0.01)                | 91.72   | 92.90   | 94.09     | 94.48     | 95.55     | 95.87       |
| -LM (β=0.05)                | 91.90   | 93.08   | 94.24     | 94.67     | 95.81     | 95.89       |
| -LM (β=0.1)                 | 91.97   | 93.17   | 94.42     | 94.81     | 95.95     | 96.01       |
| -LM (β=0.2)                 | 92.17   | 93.12   | 94.63     | 94.99     | 96.00     | 96.07       |
| -LM (β=0.3)                 | 92.38   | 93.31   | 94.85     | 95.11     | 96.09     | 96.22       |
| -LM (β=0.5)                 | 92.96†† | 93.56   | 95.02     | 95.29††   | 95.13     | 96.08       |
| -Class-SCNS (β=1)           | 92.04   | 93.08   | 94.61     | 93.97     | 95.52     | 95.82       |
| -Class-SCNS (β=2)           | 92.44†  | 93.10   | 94.83     | 94.42     | 96.08††   | 96.09       |
| -Class-SCNS (β=5)           | 91.98†  | 93.02   | 94.43     | 93.88     | 95.23     | 95.77       |
| -Instance-SCNS (β=0.01)     | 92.01   | 93.27   | 94.34     | 93.49     | 95.28     | 95.19       |
| -Instance-SCNS (β=0.1)      | 92.12   | 93.29   | 94.09     | 93.54     | 95.32     | 95.41       |
| -Instance-SCNS (β=0.2)      | 92.20†† | 93.25   | 94.83     | 94.14     | 95.66     | 95.99       |
| -Instance-SCNS (β=0.5)      | 92.42†  | 93.39   | 95.11††   | 94.56     | 95.91     | 96.08       |
| -Instance-SCNS (β=1/5000)   | 92.38†† | 93.55†† | 95.02††   | 93.86††   | 95.72††   | 96.27††     |

**Table 1.** Test accuracy (%) of student networks on CIFAR-10.
ResNet architectures leads to increases in test accuracy.

**Knowledge Distillation** We now discuss results of the KD experiments on CIFAR-100 (Krizhevsky et al., 2009). Figure 2 shows the test accuracies for each KD method where the student-teacher pair is different for each row and the colours correspond to [0-1] row normalized test accuracies to visualize the relative percentage increase or decrease between each KD method. We find that combining LM with InfoNCE + Instance-SCNS with a lookup table outperforms only using LM or instance-level SCNS with a lookup table. Moreover, ‘InfoNCE-LM + Class-SCNS’ outperforms all other KD methods for all but one student-teacher pairing (PKT found to have the highest test accuracy for ‘resnet14-wrn-16-1’ student-teacher pair). However, the original KLD distillation loss remains a very strong baseline that is competitive with CL and even outperforms our proposed non-contrastive baselines. We find a 0.24 point increase in the 0-1 normalized average score (‘Kullback Leibler Distillation’ = 0.75 and ‘InfoNCE-LM + Class-SCSN’=0.99). We also find w.r.t. the student-teacher network capacity gap, increasing the capacity of the teacher network does not necessarily lead to improved student network performance if the gap is large. The performance difference between ‘resnet14-wrn-16-1’ and ‘resnet14-wrn-40-1’ is relatively small and ‘resnet14-wrn-40-1’ has higher accuracy than ‘resnet14-wrn-16-1’ in only 7/16 different loss functions. However, in 3/4 of the CL cases (4 rightmost columns of Figure 2) the larger teacher network in ‘resnet14-wrn-40-1’ has significantly improved accuracy. Figure 4 shows the convergence time comparing InfoNCE when using USNs and SCNS for the resnet32-wrn-16-1 student-teacher pair.

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1The naming conventions of baselines, including our own KD baselines are described in Appendix B.
Table 2. Test accuracy (%) of student networks on Tiny-ImageNet-200

| Teacher Network | Student Network | resnet110 | resnet101 | wrn-16-1 | wrn-16-4 | wrn-40-1 | wrn-40-4 |
|----------------|----------------|----------|----------|----------|----------|----------|----------|
| Teacher (Cross-Entropy) | 61.94 | 63.17 | 65.80 | 71.04 | 70.31 | 71.58 |
| Student (Cross-Entropy) | 61.55 | 62.94 | 68.59 | 70.95 | 70.25 | 71.26 |
| Teacher + KL Distillation (Hinton et al., 2015) | 61.78 | 63.03 | 65.33 | 70.88 | 70.33 | 71.19 |
| Contrastive-CKA (Linear) | 61.83 | 63.18 | 65.43 | 70.92 | 70.32 | 71.24 |

Table 3. An ablation of efficient NS techniques on CIFAR-100.

| Class-SCNS (β = 100) | 60.93 | 63.20 | 65.46 | 69.31 | 69.64 | 70.41 |
|------------------------|-------|-------|-------|-------|-------|-------|
| Class-SCNS (β = 1/10) | 70.88 | 64.83 | 69.73 | 71.09 | 69.62 | 72.83 |
| Class-SCNS (β = 1) | 71.32 | 69.61 | 68.40 | 75.42 | 72.20 | 72.89 |
| Class-SCNS (β = 10) | 71.03 | 62.14 | 66.73 | 72.02 | 71.02 | 72.08 |
| Class-SCNS (β = 100) | 69.35 | 61.51 | 66.05 | 70.99 | 69.81 | 71.76 |

almost all student-teacher network combinations, Instance-SCNS, Class-SCNS samples and both with Contrastive LM regularization have led to performance improvements over all previously proposed KD methods. However, the original KDL distillation loss (Hinton et al., 2015) remains a very strong baseline. We also find that increasing the capacity of the teacher network for the same sized student network can result in the same or poorer performance if the original student-teacher network capacity difference is large. For example, if we compare ‘resnet14-wrn-16-1’ to ‘resnet14-wrn-40-1’ we can see there is little difference in performance across the different KD methods. However, increasing the student network size closer to the teacher network leads to improved performance e.g ‘resnet32-wrn-16-1’ consistently improves over ‘resnet14-wrn-16-1’.

Table 3 shows the ablation of all three proposed methods on CIFAR-100. The most consistent gain in performance is found when using Instance-SCNS as it achieves the best performance for 4 out of 6 student networks. Class-SCNS performs the best for resnet20 student networks, which have relatively larger capacity compared to resnet8 and resnet14.

Distilling Transfer Learned Representations To test how SCNS performs in the transfer learning setting, we learn a student network from teacher network that takes inputs and outputs of different sizes. We use pretrained ImageNet models and fine-tune them on Tiny-ImageNet-200 by replacing the last 1000 dimensional linear layer with a 200 dimensional layer. The pretrained models are fine-tuned by resizing Tiny-ImageNet-200 images from 64x64 to 256x256 without any additional data augmentation. These models are used as the teacher networks that take in 256x256 images while the student network takes the original 64x64 input. This KD setup is slightly different as the teacher network is fine-tuned using transfer learning from the original ImageNet dataset, not from random initialization.

Table 2 shows each KD technique along with our proposed techniques from row ‘Contrastive-PC’ to the last row. In
5. Conclusion

We proposed (1) semantically conditional negative sampling, a method that use pretrained networks to define a negative sampling distribution and (2) latent mixup, a simple strategy to form hard negative samples. We found that when used in a contrastive learning setting, both proposals consistently outperform previous knowledge distillation methods and improve contrastive learned models in the standard supervised learning setup.

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A. Hardware Details
All experiments were run on a Titan RTX P8 24G memory graphics processing unit.

B. Network Architectures
The below CNN architectures are used for standard supervised learning experiments on CIFAR10 and for KD experiments on CIFAR100 and Tiny-ImageNet-200.

- Wide Residual Network (WRN; Zagoruyko & Komodakis, 2016b). WRN-d-w represents wide resnet with depth d and width factor w.
- ResNet (He et al., 2016). We use resnet-d to represent cifar-style resnet with 3 groups of basic blocks, each with 16, 32, and 64 channels respectively. In our experiments, resnet8x4 and resnet32x4 indicate a 4 times wider network (namely, with 64, 128, and 256 channels for each of the block).
- ResNet (He et al., 2016). ResNet-d represents ImageNet-style ResNet with Bottleneck blocks and more channels.
- ResNeXt (Xie et al., 2017). ResNeXt ImageNet-style ResNet with Bottleneck blocks and more channels.
- VGG (Simonyan & Zisserman, 2014). The pretrained VGG network are adapted from its original ImageNet counterpart.
- DenseNet (Huang et al., 2017). We use a pretrained ImageNet DenseNet-121 and fine-tune on Tiny-ImageNet-200 with upscale images (64x64 to 256x256).

C. Experiment Details
C.1. Conditional Negative Sampling Details
Before running experiments for supervised learning and knowledge distillation, we must first define the negative sampling distribution on the instance-level or class-level. For class-level SCNS we use cross-modal transfer by using word embeddings for the class labels. We use skipgram word vectors (Mikolov et al., 2013) that are pretrained on GoogleNews and can be retrieved from [https://code.google.com/archive/p/word2vec/](https://code.google.com/archive/p/word2vec/). For class labels that are phrases, we average the pretrained word embeddings of each constituent embedding prior to computing cosine similarity. We find best results for our proposed method with the temperature $\tau = 5$ when constructing $P$. This ensures that the distribution is not too flat and encourages tighter coupling of neighbours.

For instance-level SCNS, pair similarity is defined by a pretrained network of the same type that is used for training in the supervised learning setting. For knowledge distillation, the teacher network is used to define the pair similarity.

C.2. Dataset and Model Details
For all models used in the standard supervised learning and KD settings, we use the cross-entropy loss optimized using Stochastic Gradient Descent (SGD) with a decay rate (different setting for each task). Additionally, hyperparameter tuning of $\beta$ and $k$ is tested on a randomly sampled 5% of the predefined training data of all three datasets.

CIFAR-10 For CIFAR-10, the learning rate is set to 0.01, momentum=0.9 and weight decay=0.0005. The images are randomly cropped and horizontally flipped and normalized along the input channels (as two tuple arguments (0.4914, 0.4822, 0.4465), (0.2023, 0.1994, 0.2010) in the transforms.Normalize method in the torchvision library). The batch size is 128 for training.

CIFAR-100 For CIFAR-100 a dataset with 50k training images (500 samples per 100 classes) and 10k test images, the learning rate is set to 0.05 with a decay rate 0.1 at every 25 epochs after 100 epochs until the last 200 epoch. The batch size is set to 64.

Tiny-ImageNet-200 For Tiny-ImageNet-200, we train for 100 epochs and decay the learning rate every 20 epochs. The batch size is also set to 64. The student is trained by a combination of cross-entropy classification objective and a KD objective as $\ell = \ell_{CE} + \alpha \ell_{KD}$.

Baseline KD Settings The abbreviations refer to correspond to the KD method names listed in Table 4.

The main KD influence factor $\alpha$ is set based on either the original paper settings or a set using a grid search over...
Knowledge Distillation (KD; Hinton et al., 2015) - Fitnets
Similarity-Preserving Relational Knowledge Distillation
A gift from knowledge distillation: Fast optimization, network minimization and transfer learning (FSP; Yim et al., 2017)
Attention Transfer
Correlation Congruence
Learning deep representations with Paraphrasing complex network: Network compression via Variational information distillation

Our Proposed KD Baseline Method Settings

| Abbreviation | KD Method |
|--------------|-----------|
| KLD          | Knowledge Distillation (KD; Hinton et al., 2015) - Kullbeck Leibler Divergence |
| Fitnets      | Fitnets: Hints for thin deep nets (Romero et al., 2014) |
| AT           | Attention Transfer (AT; Zagoruyko & Komodakis, 2016a) |
| SP           | Similarity-Preserving Knowledge Distillation (SP; Tung & Mori, 2019) |
| CC           | Correlation Congruence (CC; Peng et al., 2019) |
| VID          | Variational information distillation for knowledge transfer (VID; Ahn et al., 2019) |
| RKD          | Relational Knowledge Distillation (RKD; Park et al., 2019) |
| PKT          | Learning deep representations with probabilistic knowledge transfer (PKT; Passalis & Tefas, 2018) |
| FT           | Paraphrasing complex network: Network compression via factor transfer (FT; Kim et al., 2018) |
| FSP          | A gift from knowledge distillation: Fast optimization, network minimization and transfer learning (FSP; Yim et al., 2017) |

Table 4. Abbreviations for Knowledge Distillation Baselines

1. Fitnets (Romero et al., 2014): $\alpha = 80$
2. AT (Zagoruyko & Komodakis, 2016a): $\alpha = 600$
3. SP (Tung & Mori, 2019): $\alpha = 2000$
4. CC (Peng et al., 2019): $\alpha = 0.05$
5. VID (Ahn et al., 2019): $\alpha = 0.8$
6. RKD (Park et al., 2019): $\alpha_1 = 25$ for distance and $\alpha_2 = 50$ for angle. For this loss, we combine both terms following the original paper.
7. PKT Probabilistic Knowledge Transfer (Passalis & Tefas, 2018) (Passalis & Tefas, 2018): $\alpha = 10000$
8. AB (Heo et al., 2019): $\alpha = 0.2$, distillation happens in a separate pre-training stage where only distillation objective applies.
9. FT (Kim et al., 2018): $\alpha = 500$
10. FSP (Yim et al., 2017): $\alpha = 0$, distillation happens in a separate pre-training stage where only distillation objective applies.
11. NST (Huang & Wang, 2017): $\alpha = 50$
12. CRD Contrastive Representation Distillation (Tian et al., 2019): $\alpha = 0.8$, in general $\alpha \in [0.5, 1.5]$ works well.
13. Kullbeck-Leibler Divergence Distillation (KLD) (Hinton et al., 2015): $\alpha = 0.9$ and $\tau = 4$.

Our Proposed SCNS-Based KD Settings

1. InfoNCE Loss with Instance-level SCNS: $\alpha = 0.9$
2. InfoNCE-LM: This is the InfoNCE loss between latent mixup representations as in Equation 9.
3. InfoNCE+Class SCNS: This represents SCNS with an InfoNCE loss, $\alpha = 0.65$
4. InfoNCE-LM + Class-SCNS: This represents SCNS with an InfoNCE loss with an second InfoNCE loss for latent mixup representations, $\alpha = 0.65$

Preprocessing Details

For experiments with the CKA objective we group mini-batches by their targets as CKA operates on cross-correlations between samples of the same class. Therefore, random shuffling is carried out on the mini-batch level but not on the instance level. For all other objectives, standard random shuffling of the training data is performed.

C.3. Metric Learning Distillation Objectives

In our work we also propose two correlation and kernel-based loss functions that can be used for both standard pointwise-based KD and metric-learned KD. These are used as alternatives from those described in the related research, which we describe below.

Metric-based Centered Kernel Alignment

The CKA function measures the closeness of two set of points that can be represented as matrices. Thus far it has only been used for analysing representation similarity in neural networks (Kornblith et al., 2019) but not for optimizing a neural network. We propose to distil the knowledge of the teacher...
network by minimizing the alignment between student and teacher representations using CKA as a baseline.

For two arbitrary matrices \( \mathbf{Z}_i \in \mathbb{R}^{M \times d_k} \) and \( \mathbf{Z}_j \in \mathbb{R}^{M \times d_k} \), each consisting of a set of neural network representations, the centered alignment (CA) can be expressed as

\[
CA(\mathbf{Z}_i, \mathbf{Z}_j) = \frac{\langle \text{vec}(\mathbf{Z}_i^\top \mathbf{Z}_j), \text{vec}(\mathbf{Z}_j^\top \mathbf{Z}_j) \rangle}{\|\mathbf{Z}_i\|_F \|\mathbf{Z}_j\|_F}
\]

(18)

where \( \| \cdot \|_F \) is the Frobenius norm. We can replace the dot product in numerator with a kernel function \( K(\cdot, \cdot) \) to compute the CKA. The kernel function is smooth and differentiable, hence we use it as a loss function for KD-based metric learning to maximize the similarity between the positive class latent representations given by \((z^S_+, z^T_+)\) and negative class latent representations \((z^S_-, z^T_-)\). Equation 19 shows the formulation of CKA where a kernel is used instead of the dot product.

\[
CKA(\mathbf{Z}_i, \mathbf{Z}_j) = K(\mathbf{Z}_i, \mathbf{Z}_j) - \mathbb{E}_Z[K(\mathbf{Z}_i, \mathbf{Z}_j)] - \mathbb{E}_{Z_i,Z_j}[K(\mathbf{Z}_i, \mathbf{Z}_j)]
\]

(19)

In our experiments, a linear kernel and a radial basis function \( K(\mathbf{Z}_i, \mathbf{Z}_j) = \exp(-\|\text{vec}(\mathbf{Z}_i) - \text{vec}(\mathbf{Z}_j)\|_2^2/2S^2) \) were used where \( S^2 \) is the sample variance. To account for intra-variations and inter-variations between student and teacher representations the CKA loss is used as apart of a triplet loss that maximizes the kernel similarity between the positive pair of the student anchor and student positive sample and also the student anchor with the teacher anchor. This is shown as \( \ell^+_{\text{CKA}} \) in Equation 20, where \( z_* \) represents the anchor sample. The same is computed for the negative pair, denoted by \( \ell^-_{\text{CKA}} \). Both losses are combined as one where \( \zeta \) controls the tradeoff between positive pair losses and negative pair losses and \( m \) is the margin.

\[
\ell^+_{\text{CKA}} = \text{CKA}(z^S_+, z^S_+) + \text{CKA}(z^S_-, z^T_-),
\ell^-_{\text{CKA}} = \text{CKA}(z^S_-, z^S_+) + \text{CKA}(z^S_+, z^T_-),
\ell_{\text{CKA}} = \max(0, \zeta \ell^+_{\text{CKA}} - (1 - \zeta) \ell^-_{\text{CKA}} + m)
\]

(20)

Concretely, this will force all positive class representations to have high a CKA score within and across the samples for the student and teacher representations, and similarly for the negative pair of the triplet.

**Pearson Correlation Representation Distillation** An alternative to maximizing the mutual information between \( z^S \) and \( z^T \) (Belghazi et al., 2018) is instead to maximize the linear interactions using a PC-based loss as a strong baseline. The objective to be maximized is expressed as Equation 21

\[
\ell^+_{\text{PC}} = \rho_{\text{PC}}(z^S_+, z^T_+) + \rho_{\text{PC}}(z^S_-, z^T_-),
\ell^-_{\text{PC}} = \rho_{\text{PC}}(z^S_-, z^T_+) + \rho_{\text{PC}}(z^S_+, z^T_-),
\ell_{\text{PC}} = \max(0, \zeta \ell^+_{\text{PC}} - (1 - \zeta) \ell^-_{\text{PC}} + m)
\]

(21)

where \( \rho_{\text{PC}} \in [-1, 1] \) computes the correlation coefficient. When using the \( \ell_{\text{PC}} \) loss with contrastive learning (“Contrastive-PC”) we take the average loss as \( \frac{1}{N} \sum_{i=1}^{N-1} \rho_{\text{PC}}(z^S_i, z^S_i) \) and similarly for the remaining losses that use negative sample representations.

**D. Connection Between Mutual Information & Conditional Negative Sampling**

In this section we describe contrastive learning with our proposed conditional negative sampling in terms of mutual information (MI). Let \( p(y) \) be the probability of observing the class label \( y \) and \( p(x, y) \) denote the probability density function of the corresponding joint distribution. Then, the MI is defined as Equation 22

\[
I(X; Y) = \sum_y \int_x p(x, y) \log \frac{p(x, y)}{p(x)p(y)} dx
\]

(22)

and can be further expressed in terms of the entropy \( \mathbb{H}(X) \) and conditional entropy \( \mathbb{H}(X|Y) \) as shown in Equation 23.

\[
I(X; Y) = \sum_y \int_x p(x, y) \log \frac{p(x|y)}{p(x)} dx
= - \int_x p(x) \log p(x) - (- \int_y \sum_{y} \log p(x, y)p(x|y))
= \mathbb{H}(X) - \mathbb{H}(X|Y)
\]

(23)

Then \( I(X; Y) \) can be formulated as the KL divergence between \( p(x, y) \) and the product of marginals \( p(x) \) and \( p(y) \),

\[
I(X; Y) = D_{KL}(p(x, y)||p(x)p(y)) = \mathbb{E}_{p(x,y)} \left[ \frac{p(x,y)}{p(x)p(y)} \right]
\]

(24)

Hence, if the classifier can accurately distinguish between samples drawn from the joint \( p(x, y) \) and those drawn from the product of marginals \( p(x)p(y) \), then \( X \) and \( Y \) have a high MI. However, estimating MI between high-dimensional continuous variables is difficult and therefore easier to approximate by maximizing a lower bound on MI. This is known as the InfoMax principle (Liniker, 1988). In the below subsections, we describe how this MI lower bound is maximized using the InfoNCE loss (Oord et al., 2018).
D.1. Estimating Mutual Information with InfoNCE

The InfoNCE loss maximizes the MI between \( z_i \) and \( z_j \) (which is bounded by the MI between \( z_i \) and \( z_j \)). The optimal value for \( f(z_j, z_i) \) is given by \( p(z_j|z_i)/p(z_j) \). Inserting this back into Equation 4 and splitting \( X \) into the positive sample and the negative examples \( X_n \) results in:

\[
\ell = -\mathbb{E}_{X} \log \left[ \frac{p(x_i|x_j)}{p(x_i)} + \sum_{x_i \in X_n} \frac{p(x_i|x_j)}{p(x_i)} \right] = \mathbb{E}_{X} \log \left[ 1 + \frac{p(x_j)}{p(x_j|x_i)} + \sum_{x_i \in X_n} \frac{p(x_i|x_j)}{p(x_i)} \right] \approx \mathbb{E}_{X} \log \left[ 1 + \frac{p(x_j)}{p(x_j|x_i)}(M-1) \mathbb{E}_{x_i} \frac{p(x_i|x_j)}{p(x_i)} \right] = \mathbb{E}_{X} \log \left[ 1 + \frac{p(x_j)}{p(x_j|x_i)}(M-1) \right] \geq \mathbb{E}_{X} \log \left[ \frac{p(x_j)}{p(x_j|x_i)} M \right] = -I(x_i, x_j) + \log(M)
\]

Therefore, \( I(z_j, z_i) \geq \log(N) - \ell \) which holds for any \( f \), where higher \( \ell \) leads to a looser MI bound. This MI bound becomes tighter as the number of negative sample pairs \( M \) increases and in turn is likely to reduce \( \ell \). In our work we argue that the \( \log(M) \) term be replaced with a term that accounts for the geometry of the embedding space as not all negative sample pairs are equally important for reducing \( \ell \). Therefore, the next subsection describes our formulation of the MI bound that incorporates the notion of semantic similarity between embeddings of the sample pairs in order to choose an informative \( M \) sample to tight the bound.

D.2. Mutual Information Lower Bounds for Semantically Conditioned Negative Sampling

We formalize the connection between SCNS and maximizing MI between representations in the contrastive learning and formulate an expression that describes how SCNS tightens the lower bound estimate on MI. We begin by defining ‘closeness’ between representations \( \{z_s, z_+, z_-\} \in \mathcal{Z} \) of samples \( \{x_s, x_+, x_-\} \in \mathcal{X} \). Given that we are not restricted to a distance, divergence or similarity between vectors, we refer to a general measure as an alignment function \( A \) that outputs an alignment score \( a \in [0, 1] \).

Given an anchor sample \( x_s \), the expected alignment score for the top-\( k \) negative samples is \( a^k_{x^+} := \mathbb{E}_{x^+ \sim D^k_x} [A(z_s, z_+)] \) and for the negative samples outside of the top-\( k \) samples it is \( a^k_{x^-} := \mathbb{E}_{x^- \sim D^k_x} [A(z_s, z_-)] \) where \( D^k_x \subseteq D, D^k_x \not\subseteq D^k_x \), \( r = N - N_y - k \), and \( N_y \) is the number of samples of class \( y \).

From the above, \( \alpha \approx 1 \) corresponds to negative samples that lie very close to \( x_s \). We can then use the alignment weight (AW) \( \Omega_z := 1 - a^k_x/(a^k_x + a^k_{x^-}) \) to represent the difference in ‘closeness’ between the top-\( k \) negative samples and the remaining negative samples. This is visualized as the difference in alignment between the centroids in the embedding space shown in Figure 5.

We can then replace \( M \) negative samples as \( \Omega := \sum_{i=1}^{M} \Omega_{x_i} \) and substitute \( \log(M) \) with \( \log(2\Omega) \) in Equation 25. When the centroids of both negative sample sets are close (i.e \( a^k_x = a^k_{x^-} \)) then \( \Omega = M/2 \). Hence \( \log(2\Omega) \approx \log(M) \) when the negative samples are centered in the same region, in which case uniform sampling provides the same guarantees as SCNS. The new MI lower bound is then Equation 26.

\[
I(X, Y) \geq \ell + \log(2\Omega) \tag{26}
\]

Intuitively, this bound favors top-\( k \) negative samples that are close to the positive class boundary but are also relatively close compared to the remaining negative samples. This is dependent on how the embedding space is constructed from the pretrained network and which \( A \) is chosen. Hence, this is clearly an estimation on the true MI lower bound.

We can now define the relation between \( M \) uniformly sampled negatives (USNs) and top-\( k \) SCNSs. Let \( \Omega_{D^k_x} \) be the AW of USNs for \( x_s \) and \( \Omega_{D^k_x} \) is the AW for the top-\( k \) negative samples. When \( |D^k_x| \approx |D^k_x| \) (i.e both negative sample sets lie on a ring on the hypersphere around \( x_s \)),

\[
I(X, Y) \leq \ell + \log(2\Omega_{D^k_x}) \leq \ell + \log(2\Omega_D) \tag{27}
\]

given the non-uniform prior over negative samples as defined in SCNS. For some \( k \ll N, 2(\Omega_k - \Omega_D) = 0 \) is met.
when a subset of $D^d_i$ negative samples have $z_{x_1}^d \approx z_{x_2}^k$ where
the subscript $\hat{x}$ denotes the aforementioned subset and $z_x^k$ is
the centroid of the top-$k$ negative samples

**E. Uniform vs SCNS Sample Complexity**

In this section, we aim to identify the relationship between
uniform sampling and SCNS by formulating how many draws are required to cover the the top-$k$ samples. We begin by the simpler case of single draws with a uniform
distribution and extend it to batches of negative samples of
size $b$ are drawn uniformly. We then repeat this with draws of
unequal probability in subsection E.2, as is the case for
SCNS.

**E.1. Number of Samples Until Observing Top-$k$ SCNS Samples Under a Uniform Distribution**

We now describe the expected number of i.i.d drawn negative
samples from $M$ to observe the top-$k$ samples at least once
for a given $x$. Let $N_i$ denote the number of negative
samples observed until you see the $i$-th new negative sample
among the top-$k$ samples and $N$ is the number of samples
until all top-$k$ negative samples are observed. Since
$N = \sum_{i=1}^k N_i$,

$$E[N] = E\left[ \sum_{i=1}^k N_i \right] = \sum_{i=1}^k E[N_i]$$

(28)

where $N_i$ follows a geometric distribution with parameter
$(k + 1 - i)/M$. Therefore $E[N_i] = \frac{M}{k+1-i}$ and $E[N] =
M \sum_{i=1}^k (k + 1 - i)^{-1} = M \sum_{i=1}^k i^{-1}$.

**E.1.1. Number Of Batches To Cover All Samples**

In subsection E.1, we formulate the expected number of negative
samples required to cover the top-$k$ negative samples at least once
for a single consecutive draws. However, in practice mini-batch training is carried out and therefore it
is necessary to reformulate this for consecutive mini-batch draws of size $b$ for a given $x$ with replacement. This is a special case of the Coupon Collector’s Problem.

$$\sum_{j=0}^{\infty} P(K > ib) = \sum_{i=0}^{\infty} \left(1 - \frac{M!}{M^b} \binom{M}{ib}\right)$$

$$= \sum_{i=0}^{\infty} \left(1 - \frac{1}{M^b} \sum_{j=0}^{M-1} (-1)^{M-j} \binom{M}{j} \frac{ib}{j} \right)$$

$$= \sum_{j=0}^{M-1} \sum_{j=0}^{M-1} (-1)^{M-j+1} \binom{M}{j} \frac{ib}{j}$$

$$= \sum_{j=0}^{M-1} (-1)^{M-j+1} \binom{M}{j} \frac{1}{1 - \left(\frac{b}{M}\right)^j}$$

(29)

Hence, as $M$ grows more mini-batch updates are needed
until the top-$k$ hard negative samples are observed. Thus,
$b$ is required to be larger which is typically required in the
MI formulation of NCE. To define the difference between
USNs and SCNS we also need to define the CCP for unequal
probabilities as defined by $P_{x_*$ for $x_*$. We first make a distribu-
tional assumption. Here, we assume that the distances (or
alignment) for $x$ to its $N$ negative samples follows a power
law distribution. This is well-established for text (Bollegala
et al., 2010; Piantadosi, 2014) and we also observe a power
law trend when computing the cosine similarities between
all pairs with $f^T$.

**E.2. Number of Samples Until Observing Top-$k$ SCNS Samples Under an SCNS Distribution**

In this subsection, we formulate the expected number of negative
samples required for non-uniform sampling distribu-
tions, namely our proposed SCNS distribution provided
by the teacher network.

**Maximum-Minimum Identity Approach** The number of draws required to observe all top-$k$ NS is $C = \max\{C_1, \ldots, C_N\}$ where $N_i$ has a conditional probability $p_i$ of being sampled as defined in SCNS. Since the minimum of $N_i$ and $N_j$ is the number of negative samples needed to obtain either the $i$-th top-$k$ sample or the $j$-th top-$k$ sample, it follows that for $i \neq j$, $\min(N_i, N_j)$ has probability $p_i + p_j$ and the same is true for the minimum of any finite number of these random variables. The Maximum-
Minimums Identity (Ross, 2014) is then used to compute the
expected number of draws:

$$E[N] = E\left[ \max_{i=1, \ldots, M} N_i \right] = \sum_i E[N_i] - \sum_{i<j} E[\min(N_i, N_j)]$$

$$\quad + \sum_{i<j<k} E[\min(N_i, N_j, N_k)] - \ldots$$

$$\quad + (-1)^{M+1} E[\min(N_1, N_2, \ldots, N_M)]$$

(30)

We can then express the above in terms of the individual
probabilities associated with drawing $M$ negative samples conditioned on a given $x_*$ as,

$$E[N] = \sum_i 1_{p_i} - \sum_{i<j} 1_{p_i + p_j} +$$

$$\sum_{i<j<k} \frac{1}{p_i + p_j + p_k} + (-1)^{M+1} \frac{1}{p_1 + \ldots + p_M}$$

(31)

Since $\int_0^{\infty} e^{-px} dx = \frac{e^{-px}}{p} \bigg|_{x=0}^{x=\infty} = \frac{1}{p}$, integrating gives
which case we first assume that the number of negative samples to draw
is proportionally larger in \( N \). However, our original goal is
to only sample from the most probably top-\( k \) samples, in
which case \( \mathbb{E}[Z] \) is lower.

**F. Additional Results**

Figure 6 is a boxplot of how the performance changes for
different KD methods as the student-teacher capacity gap
varies. The purpose of this is to identify how much the
performance increases are due to larger capacity as opposed
to the particular KD method used.

![Figure 6. Tiny-ImageNet Boxplot Test Accuracy for Knowledge Distillation Approaches](image)

**Figure 7** and **Figure 8** (below the references section) show
the KD results with the unscaled (i.e no \([0, 1]\) normalization)
color codings and **Figure 9** and **Figure 10** shows the
corresponding \([0, 1]\) row-normalized results to highlight
the relative differences between each KD method. We note
the last ‘Average Score’ row displays the average performance
over all student-teacher architecture pairs for each
KD method.

Figures 11(a) to 11(f) shows the Tiny-ImageNet-200 embed-
dding similarity of classes and Figures 11(g) to 11(k) shows
the embedding similarity for CIFAR-100.

\[
1 - \prod_{i=1}^{N} (1 - e^{-p_i x}) = \sum_{i} e^{-p_i x} = \sum_{i<j} e^{-p_i p_j x} + \ldots + (-1)^{N+1} e^{-(p_1 + \ldots + p_N)x} \tag{32}
\]

Hence, we get a concise equivalent expression (Flajolet et al., 1992):

\[
\mathbb{E}[X_-] = \int_{0}^{+\infty} \left( 1 - \prod_{i=1}^{N} (1 - e^{-p_i x}) \right) dx \tag{33}
\]

The probability of sampling the \( i \)-th top-\( k \) negative sample
is \( p_i \geq 0 \) such that \( p_1 + \ldots + p_N = 1 \). To determine \( \mathbb{E}[N] \),
we first assume that the number of negative samples to draw
t at \( X_-(t) \), follows a Poisson distribution with parameter
\( \lambda = 1 \). Let \( I_i \) be the inter-arrival time between the \((i - 1)\)-th
and the \( i \)-th negative sample draw; \( I_i \) has exponential
distribution with parameter \( \lambda = 1 \). Let \( Z_i \) be the time in
which the \( i \)-negative sample arrives for the first (hence
\( Z_i \sim \text{exp}(p_i) \)) and let \( Z = \max\{Z_1, \ldots, Z_N\} \) be the time
in which we have observed all samples at least once. Note
that \( Z = \sum_{i=0}^{N} I_i \) and \( \mathbb{E}[X] = \mathbb{E}[Z] \), indeed:

\[
\mathbb{E}[Z] = \mathbb{E}[\mathbb{E}[Z|N]] = \sum_{k} \mathbb{E}\left[ \sum_{i=1}^{k} I_i|N = k \right] P(N = k) \\
= \sum_{k} \left[ \sum_{i=1}^{k} I_i \right] P(X = k) = \sum_{k} \sum_{i=1}^{k} \mathbb{E}[I_i] P(N = k) \\
= \sum_{k} k P(N = k) = \mathbb{E}(N) \tag{34}
\]

It follows that it suffices to calculate \( \mathbb{E}[Z] \) to get \( \mathbb{E}[N] \).
Since \( Z = \max\{Z_1, \ldots, Z_N\} \), we have \( F_Z(t) = P(Z \leq t) = \prod_{i=1}^{N} F_{Z_i}(t) = \prod_{i=1}^{N} (1 - e^{-p_i t}) \) and then

\[
\mathbb{E}[Z] = \sum_{0}^{+\infty} P(Z > t) dt = \sum_{0}^{+\infty} \left( 1 - \prod_{i=1}^{N} (1 - e^{-p_i t}) \right) dt \tag{35}
\]

From the above expression, we clearly see that when \( p_i \) is
defined by a non-uniform distribution, the number of draws
is proportionally larger in \( N \). However, our original goal is
to only sample from the most probably top-\( k \) samples, in
which case \( \mathbb{E}[Z] \) is lower.
Figure 7. CIFAR-100 Test Accuracy for KD Approaches

Figure 8. Tiny-Imagenet 200 Test Accuracy for KD Approaches
### Figure 9. CIFAR-100 Normalized Test Accuracy for Knowledge Distillation Approaches

| Model         | Siamese PC | Linear CKA | Factor Transfer | Hint | Attention Transfer | Bilinear | Unitary | Entropy Preserving (EP) | Cross-entropy (CE) | Variational Distribution | VCD | MDL | Correlation | Probabilistic Knowledge Transfer | Contrastive PC | MMAD_Latent | MMAD_Latent + Class-SOS | MMAD_Latent + Class-SOS |
|---------------|------------|------------|----------------|------|--------------------|----------|---------|-------------------------|-------------------|--------------------------|-----|-----|------------|-----------------------------|----------------|----------------|--------------------------|--------------------------|
| resnet20-xresnet34  | 0.35      | 0.34      | 0.25          | 0.43 | 0.34               | 0.37     | 0.84   | 0.56                     | 0.24              | 0.21                     | 0.40 | 0.28 | 0.00       | 0.90                        | 0.80            | 1.00          |
| resnet9-xresnet18  | 0.71      | 0.59      | 0.00          | 0.34 | 0.38               | 0.77     | 0.79   | 0.57                     | 0.60              | 0.40                     | 0.71 | 0.68 | 0.55       | 0.98                        | 0.84            | 1.00          |
| resnet14-xresnet6  | 0.77      | 0.85      | 0.00          | 0.72 | 0.85               | 0.82     | 0.68   | 0.59                     | 0.08              | 0.08                     | 0.86 | 1.00 | 0.83       | 0.89                        | 0.94            | 0.94          |
| resnet20-xresnet6  | 0.49      | 0.49      | 0.00          | 0.55 | 0.68               | 0.78     | 0.83   | 0.59                     | 0.45              | 0.26                     | 0.48 | 0.74 | 0.50       | 0.95                        | 0.87            | 1.00          |
| resnet18-xresnet6  | 0.42      | 0.35      | 0.00          | 0.33 | 0.39               | 0.58     | 0.55   | 0.28                     | 0.23              | 0.02                     | 0.38 | 0.52 | 0.37       | 0.92                        | 0.69            | 1.00          |
| resnet32-xresnet6  | 0.60      | 0.68      | 0.11          | 0.27 | 0.67               | 0.82     | 0.65   | 0.52                     | 0.57              | 0.00                     | 0.66 | 0.83 | 0.64       | 0.89                        | 0.78            | 1.00          |
| Average Score    | 0.56      | 0.55      | 0.06          | 0.44 | 0.55               | 0.69     | 0.75   | 0.54                     | 0.45              | 0.16                     | 0.58 | 0.68 | 0.48       | 0.92                        | 0.82            | 0.99          |

### Figure 10. Tiny-Imagenet 200 Test Accuracy for Knowledge Distillation Approaches

| Model         | Siamese PC | Linear CKA | Factor Transfer | Hint | Attention Transfer | Bilinear | Unitary | Entropy Preserving (EP) | Cross-entropy (CE) | Variational Distribution | VCD | MDL | Correlation | Probabilistic Knowledge Transfer | Contrastive PC | MMAD_Latent | MMAD_Latent + Class-SOS | MMAD_Latent + Class-SOS |
|---------------|------------|------------|----------------|------|--------------------|----------|---------|-------------------------|-------------------|--------------------------|-----|-----|------------|-----------------------------|----------------|----------------|--------------------------|--------------------------|
| resnet56-xresnet15  | 0.27      | 0.14      | 0.90          | 0.40 | 0.52               | 0.76     | 0.54   | 0.93                     | 0.64              | 0.00                     | 0.58 | 0.17 | 0.91       | 0.89                        | 0.93            | 0.98          | 1.00                     |
| resnet4-xresnet18  | 0.32      | 0.36      | 0.31          | 0.57 | 0.44               | 0.45     | 0.34   | 1.00                     | 0.59              | 0.00                     | 0.47 | 0.39 | 0.83       | 0.77                        | 0.94            | 0.86          | 1.00                     |
| resnet20-xresnet6  | 0.26      | 0.25      | 0.28          | 0.42 | 0.33               | 0.55     | 0.00   | 0.73                     | 0.44              | 0.48                     | 0.27 | 0.36 | 0.80       | 0.57                        | 0.66            | 0.93          | 1.00                     |
| resnet18-xresnet6  | 0.23      | 0.37      | 0.19          | 0.27 | 0.36               | 0.66     | 0.04   | 0.92                     | 0.47              | 0.22                     | 0.40 | 0.00 | 0.84       | 0.77                        | 0.81            | 0.94          | 1.00                     |
| resnet32-xresnet15  | 1.00      | 0.60      | 0.59          | 0.63 | 0.00               | 0.84     | 0.54   | 1.00                     | 0.67              | 0.58                     | 0.71 | 0.64 | 0.88       | 0.87                        | 0.94            | 0.92          | 0.95                     |
| resnet32-xresnet18  | 0.72      | 0.65      | 0.68          | 0.71 | 0.30               | 0.90     | 0.64   | 0.84                     | 0.81              | 0.72                     | 0.40 | 0.00 | 0.94       | 0.90                        | 1.00            | 0.96          | 0.98                     |
| resnet18-xresnet6  | 0.23      | 0.24      | 0.00          | 0.34 | 0.31               | 0.08     | 0.69   | 0.35                     | 0.35              | 0.45                     | 0.28 | 0.71 | 0.60       | 0.56                        | 0.59            | 0.92          | 1.00                     |
| resnet14-xresnet6  | 0.73      | 0.69      | 0.61          | 0.97 | 0.70               | 0.66     | 0.57   | 0.73                     | 0.76              | 0.74                     | 0.67 | 0.00 | 0.86       | 0.78                        | 0.86            | 0.96          | 1.00                     |
| resnet14-xresnet34  | 0.00      | 0.41      | 0.19          | 0.25 | 0.16               | 0.44     | 0.00   | 0.56                     | 0.35              | 0.01                     | 0.50 | 0.06 | 0.60       | 0.38                        | 0.63            | 0.70          | 1.00                     |
| resnet120-xresnet6  | 0.39      | 0.41      | 0.24          | 0.26 | 0.38               | 0.50     | 0.30   | 1.00                     | 0.44              | 0.00                     | 0.43 | 0.24 | 0.71       | 0.70                        | 0.74            | 0.76          | 0.82                     |
| Average Score    | 0.41      | 0.41      | 0.51          | 0.39 | 0.61               | 0.30     | 0.84   | 0.55                     | 0.31              | 0.49                     | 0.21 | 0.81 | 0.72       | 0.81                        | 0.89            | 0.97          | 0.97                     |
