Unsupervised Feature Learning by Cross-Level Instance-Group Discrimination

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Abstract

Unsupervised feature learning has made great strides with contrastive learning based on instance discrimination and invariant mapping, as benchmarked on curated class-balanced datasets. However, natural data could be highly correlated and long-tail distributed. Natural between-instance similarity conflicts with the presumed instance distinction, causing unstable training and poor performance.

Our idea is to discover and integrate between-instance similarity into contrastive learning, not directly by instance grouping, but by cross-level discrimination (CLD) between instances and local instance groups. While invariant mapping of each instance is imposed by attraction within its augmented views, between-instance similarity could emerge from common repulsion against instance groups.

Our batch-wise and cross-view comparisons also greatly improve the positive/negative sample ratio of contrastive learning and achieve better invariant mapping. To effect both grouping and discrimination objectives, we impose them on features separately derived from a shared representation. In addition, we propose normalized projection heads and unsupervised hyper-parameter tuning for the first time.

Our extensive experimentation demonstrates that CLD is a lean and powerful add-on to existing methods such as NPID, MoCo, InfoMin, and BYOL on highly correlated, long-tail, or balanced datasets. It not only achieves new state-of-the-art on self-supervision, semi-supervision, and transfer learning benchmarks, but also beats MoCo v2 and SimCLR on every reported performance attained with a much larger compute. CLD effectively brings unsupervised learning closer to natural data and real-world applications. Our code is publicly available at: https://github.com/frank-xwang/CLD-UnsupervisedLearning.

1. Introduction

Representation learning aims to extract latent or semantic information from raw data. Typically, a model is first trained on a large-scale annotated dataset [37] and then tuned on a small-scale dataset for a downstream task [27]. As the model gets bigger and deeper [28, 31], more annotated data are needed; supervised pre-training is no longer viable.

Self-supervised learning [15, 47, 70, 44, 16, 42] gets around labeling with a pre-text task which does not require annotations and yet would be better accomplished with semantics. For example, to predict the color of an object from its grayscale image does not require labeling; however, doing it well would require a sense of what the object is. The biggest drawback is that pre-text tasks are domain-specific and hand-designed, and they are not directly related to downstream semantic classification.

Unsupervised contrastive learning has emerged as a direct winning alternative [58, 71, 63, 7, 26]. The training objective and the downstream classification are aligned on discrimination, albeit at different levels of granularities: training is to discriminate known individual instances, whereas testing is to discriminate unknown groups of instances.

Contrastive learning approaches have made great strides with two ideas: invariant mapping [25] and instance discrimination [58]. That is, the learned representation should be 1) stable for certain transformed versions of an instance, and 2) distinctive for different instances. Both aspects can be formulated without labels, and the feature learned appears to automatically capture semantic similarity, as benchmarked by downstream classification on standard datasets such as CIFAR100 and ImageNet [7]. However, these datasets are curated with distinctive and class-balanced instances, whereas natural data could be highly correlated within the class (e.g., repeats) and long-tail distributed across classes.

Natural between-instance similarity demands instance grouping not instance discrimination, where all the instances are presumed different. Consequently, feature learning by instance discrimination is unstable and under-performing without instance grouping, whereas instance grouping based on the feature learned without instance discrimination is easily trapped into degeneracy. Ad-hoc tricks [4, 5] and mutual information maximization with a uniform class distribution prior [34] have been used to prevent feature degeneracy.

We propose to discover and integrate between-instance similarity into contrastive learning, not directly by instance grouping, e.g., by imposing group-level discrimination as
While the feature for the groupings is still to be developed. (LA) [71], but by imposing cross-level discrimination (CLD) between-instance repulsion (Fig. 1a). An chicken-and-egg challenge is to discover such groupings for feature learning while the feature for the groupings is still to be developed.

Our key insight is that grouping could result from not just attraction, but also common repulsion. While invariant mapping without instance discrimination). CLD delivers a significant performance boost not only on highly correlated, long-tail, and balanced datasets, but also on all the self-supervision, semi-supervision, and transfer learning benchmarks under fair comparison settings [58, 26, 69].

Our work makes three major contributions. 1) We extend unsupervised feature learning to natural data with high correlation and long-tail distributions. 2) We propose cross-level discrimination between instances and local groups, to discover and integrate between-instance similarity into contrastive learning. We also propose normalized projection heads and unsupervised hyper-parameter tuning. 3) Our experimentation demonstrates that adding CLD to existing methods has an negligible overhead and yet delivers a significant boost. It achieves new SOTA on all the benchmarks, and beats MoCo v2 [8] and SimCLR [7] on every reported performance attained with a much larger compute.

2. Related Works

Unsupervised representation learning [15, 47, 70, 44, 16, 38, 33, 21, 68] aims to learn features transferable to downstream tasks. Our work is closely related to contrastive learning and unsupervised feature learning with grouping. Contrastive learning maps positive samples closer and negative samples apart in the feature space [58, 42, 53, 26, 8, 7].
Positive samples come from augmented views of each instance, whereas negative ones come from different instances. The key distinction among existing methods lies in how these samples are obtained and maintained during learning.

**Batch methods** [7] draw samples from the current mini-batch with the same encoder, updated end-to-end with backpropagation. **Memory-bank methods** [58, 42] draw samples from a memory bank that stores the prototypes of all the instances computed previously. **Hybrid methods** [26, 8] encode positive samples by a momentum-updated encoder and maintain negative samples in a queue.

Instance discrimination methods presume distinctive instances. Their performance drops on natural data that are highly correlated or long-tail distributed, e.g., consecutive frames in a video, or different views of the same instance. Note that our setting is completely unsupervised and different from learning representation across views [1, 55, 53]: We have mixed data without any object or view labels.

**Feature learning with grouping** exploits natural organization of data [59, 60, 5, 71]. Unlike self-supervised learning [47, 44, 21], it does not require domain knowledge [4].

Earlier works restrict learning to linear feature transformations. DisCluster [11, 14] and DisKmeans [62] iteratively apply K-means to generate cluster labels and then use linear discriminant analysis (LDA) to select the most discriminative subspace. [61] applies LDA along with spectral clustering [57], [43] uses linear regression as a regularization term to handle out-of-sample data in spectral clustering.

Nonlinear feature transformations have also been studied. [52] applies a deep sparse autoencoder to a normalized graph similarity matrix and performs K-means on the latent representation. [56] implements t-SNE embedding with a deep neural network. Deep Embedded Clustering [59] simultaneously learns cluster centroids and feature mapping such that centroid-based soft assignments in the embedding matches a desirable target distribution.

Recent works jointly optimize the feature and the cluster assignment. **DeepCluster** [4, 5] gets pseudo-class labels from global clustering and applies supervised learning to iteratively fine-tune the model, whereas our CLD incorporates local clustering into contrastive metric learning. **Local Aggregation (LA)** [71] identifies a local neighbourhood of each instance through clustering, and restricts instance-level discrimination within individual neighbourhoods, whereas CLD looks beyond local neighbourhoods and conducts cross-level instance-group discrimination. PCL [39] is a concurrent work that compares instance features with group centroids which are obtained through global clustering per epoch, whereas our CLD uses local clustering per batch and compares instance-group features within the batch. Global clusters not only takes more time to compute during training, but conceptually also do not align with classes in downstream tasks. Empirically, PCL gains much over MoCo but not over MoCo v2 [39]. SegSort [32] extends representation learning from classification to segmentation. It learns a feature per pixel, and assumes that all the pixels in the same region form a cluster in the feature space. SegSort uses one common feature and contrasts each pixel with cluster centroids in the feature from the same-view, whereas our CLD uses two separate features and contrasts each image with cluster centroids in the feature from a different view.

**Discussions.** While clustering on a fixed feature is well studied [19], clustering with an adapting feature is a tricky model selection problem: 1) Clustering could fall into trivial solutions where most samples are assigned to a single cluster, trapping feature learning into degeneracy [4]. 2) Without any external supervision, it is unclear how to ensure that the learned feature captures latent semantics.

Our work combines contrastive learning and grouping in a single framework, by expanding discrimination between instances to that between instances and local groups. Discrimination prevents feature learning from degeneracy, while grouping improves stability and helps instance-level discrimination see beyond the finest granularity. With these two aspects integrated, our CLD significantly improves the learned representation for downstream classification.

3. Learning with Cross-Level Discrimination

Given $n$ images, we regard instance $x_i$ as a view obtained by a certain transformation (e.g. cropping) of the $i$-th image. Let $x_i$ and $x'_i$ denote two different views of the $i$-th instance. **Contrastive learning** [25, 58, 26, 53, 45, 7] aims to learn a mapping function $f$ such that in the $f(x)$ feature space, instance $x_i$ is 1) close to positive sample $x'_i$ (invariant mapping), and 2) far from negative sample $x_j$ (with $j \neq i$) of any other instances (instance discrimination).

We model $f$ by a convolutional neural network (CNN) with parameters $\theta$, mapping $x$ onto a $d$-dimensional hypersphere such that $\|f(x)\| = 1$. Let $f, f^+, f^-$ denote the feature for an instance and its positive / negative samples respectively. We optimize $\theta$ by minimizing loss $C$ over all $n$ instances so that $f$ attracts $f^+$ and repels $f^-.$

**instance-centric contrastive loss:**

$$C(f_i, f^+_i, f^-_i) = - \log \frac{\exp \frac{<f_i, f^+_i>}{T}}{\exp \frac{<f_i, f^+_i>}{T} + \sum_{j \neq i} \exp \frac{<f_i, f^-_j>}{T}}$$

(1)

Temperature $T$ is a hyperparameter regulating what distance is close. $C$ is the noise contrastive estimation (NCE) [24] of softmax instance classification loss [58], and it can be viewed as maximizing a lower bound of mutual information (MI) between samples of the same instances [46, 25, 45].

**Implementation of** $(f_i, f^+_i, f^-_i)$ **during training.** For sample $x_i$, the self feature is $f_i = f(x_i)$, whereas positive feature $f^+_i$ and negative feature $f^-_i$ come from a memory bank $v$ that holds the representative feature for $\{x_i\}^n_{i=1}$. It
is computed as the average feature of all the augmented versions of \( x_i \) seen so far [58, 7]. It could also be encoded by a parametric model as in MoCo [26]. Existing methods apply \( C \) at the instance level, between instance feature \( f_I \) and its average \( v: C (f_I(x_i), v_i, v_{\neq i}) \) (Fig. 2 instance branch).

**Pros and cons of instance-level contrastive learning.** Contrastive learning has greatly closed the gap with supervised classification [58, 45, 26, 7]. However, there are 4 caveats.

1. It focuses on within-instance similarity by data augmentation, oblivious of between-instance similarity.
2. It focuses on discrimination at the finest instance level, oblivious of natural groups which often underlie downstream tasks’ discrimination at a coarser semantic level.
3. It presumes distinctive instances, whereas non-curated data could contain repeats, redundant observations of the same instance, and long-tail distributed instances across classes in the downstream task. For feature \( f_i \), its negative features \( \{ f_{i,j} \} \) would thus contain highly correlated samples which \( f_i \) should ideally attract rather than repel.
4. Each instance has a high positive/negative imbalance ratio (1 vs. rest); the more negatives, the larger the signal-to-noise ratio [49], and the better the performance [30, 53]. However, the model also leans towards more instance discrimination than invariant mapping, reducing robustness.

**Feature grouping.** To overcome these caveats, we step beyond individual instances and discover how they might be related. We acknowledge the natural grouping of instances by finding local clusters within a batch of samples. Which specific clustering method to use is not as critical; we apply spherical K-means to the unit-length feature vectors.

Local clustering could be rather noisy, especially at the early stage of learning. Instead of imposing group-level discrimination, we validate local groupings across views and impose consistent discrimination between individual instances and their cross-view local groups.

**Group branch.** Grouping and discrimination are opposite in nature. To effect both objectives, we fork two branches (just one FC layer each) from feature \( f_I \): fine-grained instance branch \( f_I \) and coarse-grained group branch \( f_G \) (Fig. 2). We first extract \( f_G \) at the instance level in a batch, then compute \( k \) local cluster centroids \( \{ M_1, \ldots, M_k \} \) and assign each instance to its nearest centroid. Clustering assignment \( \Gamma(i) = j \) means that instance \( i \) is assigned to centroid \( j \).

**Cross-level discrimination.** Natural groups identified in the group branch allows the expansion of positive samples from augmented versions of an individual instance to like-kind other instances. We also expand negative samples from other instances to groups of their like-kind instances. We apply local (i.e., batch-wise) contrastive loss across views between instance feature \( f_G(x_i) \) and group centroids \( M \), i.e., \( C (f_G(x'_i), M_{\Gamma(i)}, M_{\neq \Gamma(i)}) \) and vice versa for \( f_G(x_j) \) (Fig. 2). Intuitively, if local clustering \( \Gamma \) separates \( \{ x_i \} \) well, when \( x_i \) is replaced by its alternative view \( x'_i \), it should still be close to \( x_i \)'s centroid \( M_{\Gamma(i)} \) and far from other centroids \( M_{\neq \Gamma(i)} \). That is, instances and their local clusters should retain their grouping relationships across views.

Comparisons across levels, instances, views are beneficial:

1. For instances clustered in the same group, instance feature \( f_G(x_i) \) and \( f_G(x_j) \) would be attracted to the same group centroid \( M \) or \( M' \) and are thus drawn closer.
2. For similar instances \( x_i \) and \( x_j \) not in the same cluster, they likely repel common group centroids, thereby pulling instance features \( f_G(x_i) \) and \( f_G(x_j) \) closer.
3. CLD discriminates at instance and group levels, more in line with coarser discrimination at downstream tasks.
4. Comparisons between \( f_C \) and \( M \) not only avoid direct repulsion between similar instances, but also greatly improves the positive/negative ratio for invariant mapping. For example, the ratio on ImageNet is \( \frac{1}{4096} \) for NPID [58]’s set-wise NCE vs. \( \frac{1}{128} \) for CLD’s batch-wise NCE.
5. Cross-view comparisons between $x_i$ and $x'_i$ focus the model more on invariant mapping.

**Probabilistic interpretation of CLD.** Our CLD objective can be understood as minimizing the cross entropy between hard clustering assignment $p_{ij}$ (as ground-truth) based on $f_G(x_i)$ and soft assignment $q_{ij}$ predicted from $f_G(x'_i)$ in a different view. Since $p_{ij} = 1$ only when $j = \Gamma(i)$, we have a loss that validates local groupings across different views:

$$-E_p[\log q] = \sum_i C(f_G(x'_i), M_{\Gamma(i)}, M_{\neq \Gamma(i)}; T_G). \quad (2)$$

**Total contrastive learning loss.** We add CLD to instance discrimination (with temperatures $T_i$, $T_G$, weight $\lambda$) in symmetrical terms over views $x_i$ and $x'_i$:

$$L(f; T_i, T_G, \lambda) = \sum_i C(f_i(x_i), v_i, v_{\neq i}; T_i) + C(f_i(x'_i), v_i, v_{\neq i}; T_i)$$

$$+ \lambda \sum_i C(f_G(x'_i), M_{\Gamma(i)}), M_{\neq \Gamma(i)}; T_G) + C(f_G(x_i), M_{\Gamma(i)}; M_{\neq \Gamma(i)}; T_G).$$

We analyze why two feature branches are better than one branch, where $f_1 = f_G$ and $M$ is simply the group centroids of $f_1(x_i)$ or $v$. In that case, while the instance discrimination term would repel $x_i$ against any other instances $\{x_j\}$, the CLD term would make $x_i$ attract some other instances $\{x_j\}$ in the same group of $x_i$ through their group centroid. Minimizing the two terms would lead to opposite effects no matter what the local clustering is. Basing instance feature $f_1$ and group feature $f_G$ as separate branches off feature $f$ would force $f$ to be discriminative enough for the instance branch yet loosely similar enough for the group branch.

**Normalized projection head.** Existing methods derive instance feature $f_1(x)$ by mapping the latent feature $f(x)$ onto a unit hypersphere with first a projection head and then normalization. NPID [58] and MoCo [26] use one FC layer as a linear projection head. MoCo v2 [8], SimCLR [7], and BYOL [23] use a multi-layer perceptron (MLP) head; it is better for large datasets and worse for small datasets.

We propose to normalize both the FC layer weights $W$ and the shared feature vector $f$ so that projecting $f$ onto $W$ simply calculates their cosine similarity. The $t$-th component of normalized feature $N(x_i)$ (where $N = f_1$ or $N = f_G$) is:

$$N_t(x_i) = \frac{W_t^T f(x_i)}{\|W_t\| \cdot \|f(x_i)\|}.$$ \quad (3)

Normalized linear (NormLinear) or MLP (NormMLP) projection heads bring additional gains to CLD. Empirically, they help reduce feature variance from data augmentation.

### 4. Experiments

We use ResNet-50 for ImageNet data and ResNet-18 otherwise. We compare linear classification accuracies on ImageNet, and follow NPID on using kNN accuracies ($k = 200$) for all the small-scale benchmarks. The kNN accuracies are higher and more fitting for metric learning. Results marked by † are obtained with released code.

We consider 3 types of datasets. 1) **High-correlation:** Kitchen-HC is constructed by extracting objects in their bounding boxes from the multi-view RGB-D Kitchen dataset [20]. It has 11 categories with highly correlated samples and 20.8K / 4K / 14.4K instances in train / validation / test sets. 2) **Long-tail:** CIFAR10-LT, CIFAR100-LT and ImageNet-LT [40]. 3) **Major benchmarks:** CIFAR [36], STL10 [10], ImageNet-100 [53], ImageNet [13]. Following [65], we train models on 5K samples in the train set and 100K samples in the unlabeled set, and test on the test set of STL10.

#### 4.1. Benchmarking Results

**Results on high-correlation data.** Having highly correlated instances breaks the instance discrimination presumption and causes slow or unstable training. Accuracies in Fig. 3 and feature visualization in Fig. 4 indeed show that CLD is much better and fast converging towards a more distinctive feature representation. At Epoch 10, CLD outperforms by 40% (23% vs. 63%). CLD outperforms NPID by 9.4%, when the number of groups used in local clustering is closer to the number of semantic classes in the downstream classification. Likewise, MoCo + CLD outperforms its counterpart MoCo by 5.5%.

**Results on long-tailed data.** Table 1 shows that CLD outperforms baselines by a large margin on CIFAR10-LT and

![Figure 3: Left: CLD is more accurate and fast converging than NPID on Kitchen-HC, esp. when the number of groups is closer to the number of classes 11. The average top-1 kNN accuracy of 5 runs is reported. Right: CLD outperforms NPID or MoCo on high correlation dataset Kitchen-HC.](image1)

![Figure 4: CLD has earlier and better separation between classes (indicated by the dot color) than NPID in the t-SNE visualization of instance feature $f_i(x_i)$ on Kitchen-HC.](image2)
Table 1: CLD outperforms unsupervised baselines on long-tailed datasets, approaching supervised cross-entropy (CE) and OLTR [40]. The kNN (linear) classifiers are used for CIFAR (ImageNet-LT). CLD is significantly better than supervised CE on many-shot (100+), medium-shot ([20, 100]), few-shot (20–), and gets close to OLTR.

| kNN accuracies | STL10 | CIFAR10 | CIFAR100 | ImageNet100 |
|----------------|-------|---------|----------|-------------|
| DeepCluster    | -     | 67.6    | -        | -           |
| Exemplar [17]  | 79.3  | 76.5    | -        | -           |
| Inv. Spread [63]| 81.6  | 83.6    | -        | -           |
| CMC [53]       | -     | -       | 79.2     | -           |
| NPID [58]      | 79.1  | 80.8    | 51.6     | 75.3        |
| MoCo [26]      | 83.6  | 86.7    | 57.5     | 79.7        |
| MoCo + CLD     | +4.5  | +5.9    | +5.9     | +3.6        |
| BYOL [23]      | 80.8  | 82.1    | 53.1     | 76.6        |
| BYOL + CLD     | +3.5  | +5.4    | +5.0     | +4.9        |
| BYOL + CLD     | -     | -       | 75.8     | -           |
| BYOL + CLD     | -     | -       | 81.1     | -           |
| CLD + NPID     | +4.7  | +4.7    | +4.7     | +4.7        |

Table 2: On self-supervised learning on small/medium-sized benchmarks: STL10, CIFAR10, CIFAR100 and ImageNet100, CLD delivers consistent gains as an add-on to various methods which use either standard contrastive loss (e.g. MoCo [26]) or without negative pairs (e.g. BYOL [23]). On ImageNet-100, we use our re-implemented code for baselines as they are better than those in CMC [53]. All baselines and their CLD add-on’s are optimized with the same training recipe for fair comparisons. For small- and medium-sized datasets, the nonlinear multi-layer perceptron (MLP) head performs worse than a linear projection head.

CIFAR100-LT. On ImageNet-LT, CLD outperforms NPID by 4.5% per top-5 accuracy, with the largest relative gain (24%) on few-shot classes. Our unsupervised CLD even significantly outperforms supervised plain Cross-Entropy (CE) by 8-14% and is catching up closely with supervised long-tail classifier OLTR (33.3% vs. 35.6%).

Results on major benchmarks. Table 2 shows that CLD outperforms SOTA on STL10, CIFAR10, CIFAR100 and ImageNet-100. On ImageNet, Table 3 shows that CLD consistently outperforms baselines under fair comparison settings: 200 training epochs, standard augmentations [58], and comparable model sizes. Adding CLD to InfoMin instead of MoCo produces 7.7% gain, by using an MLP projection head over feature \( f(x) \), a cosine learning scheduler, extra data augmentation [8, 7, 54], and a JigSaw branch as in PIRL [42]. Fig. A.11 shows CLD retrievals less distracted by textures.

Results on semi-supervised learning. Table 4 shows that CLD utilizes annotations far more efficiently, outperforming SOTA (InfoMin) by 6.1% with only 1% labeled samples. Baselines and CLD follow OpenSelfSup benchmarks [69] for fair comparisons. Baseline results are copied from [69].

Transfer learning for object detection. We test the feature transferability by fine-tuning an ImageNet trained model for Pascal VOC object detection [18]. Table 5 shows that CLD not only outperforms its supervised learning counterpart by more than 6% (3%) in terms of AP in VOC07(VOC07+12), but also surpasses current SOTA of MoCo and MoCo v2.

4.2. Further Analysis

Why CLD performs better on long-tailed data? CLD groups similar samples and uses coarse-grained group prototypes instead of instance prototypes. There are two consequences. 1) The positive to negative sample ratio is greatly increased from the instance branch to our group branch. For example, while each instance is compared against 4,096 negatives (as in MoCo), it is only compared against \( k \) negative centroids in our group branch, where \( k \leq 256 \) – our batch size. The importance of positives increases from \( \frac{1}{4096} \) to \( \frac{1}{k} \). CLD thus achieves better invariant mapping for all the classes, head or tail. However, the increased ratio is more important for tail classes, as they don’t have so many instances to rely on as head classes. 2) The imbalance between head and tail classes in the negatives is also reduced in our group branch. While the distribution of instances in a random mini-batch is long-tailed, it would be more flattened across classes after clustering. The tail-class negatives would be better represented in the NCE loss. Fig. 6 shows that indeed
CLD has clearer class separation than MoCo.

**How many groups shall CLD use?** The ideal number of groups depends on the level of instance correlation, the number of classes, and the batch size. Table 7 shows that for CIFAR100, CLD is best when the number of groups is close to the number of classes, although CLD already outperforms MoCo at 10 groups. For ImageNet, the instance correlation is low: since the number of classes of 1,000 is larger than the batch size that our 8 GPUs can afford, we just choose the largest number of groups possible. We expect continuous gain with more groups and larger batches afforded by more GPUs. Nevertheless, our model wins with its merit of the CLD idea instead of a large compute.

**Similarity among positives / negatives?** We measure fea-
Table 6: The feature quality of $f_I$ and $f_G$ evaluated by retrieval, normalized mutual information and kNN.

| CIFAR10 | retrieval | NMI | kNN | # groups | top-1 |
|---------|-----------|-----|-----|----------|-------|
| NPID $f_I$ | 75.1 | 57.7 | 80.8 | baseline | 53.1 |
| CLD $f_I$ | 78.6 | 65.3 | 86.7 | 10 | 55.2 |
| CLD $f_G$ | 75.6 | 69.0 | 81.4 | 20 | 55.4 |

Table 7: #groups vs. accuracy on CIFAR100 for CLD.

| CIFAR100 | retrieval | NMI | kNN | # groups | top-1 |
|----------|-----------|-----|-----|----------|-------|
| NPID $f_I$ | 48.7 | 36.1 | 51.6 | 80 | 57.4 |
| CLD $f_I$ | 50.2 | 43.8 | 57.5 | 100 | 57.7 |
| CLD $f_G$ | 48.8 | 49.4 | 51.8 | 128 | 58.1 |

Figure 7: CLD has more (dis)similar instances in positive (negative) pairs than baseline MoCo, creating a larger similarity gap. Columns 1-3 are the histograms of cosine similarities between positive and negative pairs and their differences for the linear projection layer for $f_I(x_i)$ (Row 1) and $f(x_i)$ (Row 2) on ImageNet100.

Mutual information characterization? We use kNN classification accuracy, Normalized Mutual Information (NMI), and retrieval accuracy $R$ to compare features. NMI($f, Y$) = $I(C|f) / H(Y)$ reflects global MI between feature $f$ and downstream classification labels $Y$, where $C$ is cluster labels predicted from k-Means clustering of $f$ ($k$ assuming the number of classes), $H(\cdot)$ is entropy, and $I(C|f; Y)$ is the MI between $Y$ and $C$ [51]. The top-1 retrieval accuracy $R(f, Y)$ reflects instance-level mutual information.

Table 6 shows that $f_I$ is more accurate than $f_G$ at retrievals and downstream classification. While $f_G$ has higher NMI, its kNN accuracy is worse than $f_I$. That is, maximizing global MI would not deliver better downstream classification; maximizing instance-level MI is also important.

Unsupervised hyper-parameter tuning? Unsupervised learning is meant to draw inference from unlabeled data. However, its hyper-parameters such as our weight $\lambda$ and temperature $T$ are often selected by labeled data in the downstream task. Self-supervised feature learning benchmarks pass as a supervised shallow feature learner with a few hyper-parameters. We explore unsupervised hyper-parameter selection based entirely on the unlabeled data.

We study how the supervised linear accuracy at the downstream can be indicated by unsupervised metrics such as NMI and $R$ between feature $f(x)$ and $f' = f(x')$. Fig. 8 shows that the linear accuracy is well indicated by $R(f, f')$ for $\lambda$ and by NMI($f, f'$) for temperatures, but neither alone is sufficient. Their product NMI($f, f'$) · $R(f, f')$ turns out to be a promising unsupervised evaluation metric.

5. Summary

We extend unsupervised learning to natural data with correlation and long-tail distributions by integrating local clustering into contrastive learning. It discovers between-instance similarity not by direct attraction and repulsion at the instance or group level, but cross-level between instances and groups. Their batch-wise and cross-view comparisons greatly improve the positive/negative sample ratio for achieving more invariant mapping. We also propose normalized projection heads and unsupervised hyper-parameter tuning.

Our extensive experimentation and analysis shows that CLD is a lean and powerful add-on to existing SOTA methods, delivering a significant performance boost on all the benchmarks and beating MoCo v2 and SimCLR on every reported performance with a much smaller compute.

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6. Supplementary Materials

We provide further details on Kitchen-HC construction, implementation details, and various choices and experiments we have explored to validate our approach.

6.1. Kitchen-HC Dataset Construction

The original multi-view RGB-D kitchen dataset [20] is comprised of densely sampled views of several kitchen counter-top scenes with annotations in both 2D and 3D. The viewpoints of the scenes are densely sampled and objects in the scenes are annotated with bounding boxes and in the 3D point cloud. Kitchen-HC is constructed from multi-view RGB-D dataset Kitchen by extracting objects in their 2D bounding boxes. The customized Kitchen-HC dataset has 11 categories with highly correlated samples (from different viewing angles) and 20.8K / 4K / 14.4K instances for training / validation / testing. Fig. A.9 shows sample images in the original RGB-D Kitchen dataset from which our Kitchen-HC data are constructed (See samples used in Fig. 1).

![Figure A.9: Samples of multi-view RGB-D dataset Kitchen [20]. Instances of the same category captured from different perspectives are highly correlated. The high-correlation dataset Kitchen-HC is constructed from Kitchen by extracting objects in their bounding boxes.](image)

6.2. Implementation Details

We use SGD as our optimizer, with weight decay 0.0001 and momentum 0.9. We follow MoCo and NPID [58, 26] and use only standard data augmentation methods for experiments on NPID+CLD and MoCo+CLD: random cropping, resizing, horizontal flipping, color and grayscale transformation, unless otherwise noticed.

1. **ImageNet-[100 [53], ILSVRC-2012 [13], Long-tail [40]]**. For ILSVRC-2012 and ImageNet-LT, we use mini-batch size 256, initial learning rate 0.03, on 8 RTX 2080Ti GPUs. For ImageNet-100, we use batch size 512 and a larger initial learning rate of 0.8 on 8 GPUs, and apply the same setting to baselines and our methods. Training images are randomly cropped and resized to 224 × 224. For experiments on MoCov2+CLD with an MLP projection head, we extend the original augmentation in [26] by including the blur augmentation and apply cosine learning rate scheduler to further improve the performance on recognition as in [8]. BYOL+CLD is implemented based on OpenSelfSup [69] benchmark. For experiments on InfoMin+CLD and BYOL+CLD, we follow the same training recipe with InfoMin and BYOL [54, 23] for fair comparisons.

2. **CIFAR-10, 100, 10-LT, 100-LT, Kitchen-HC**. As [58], we use mini-batch size 256, initial learning rate 0.03 on 1 GPU for CIFAR [36] and Kitchen-HC. The number of epochs is 200 for CIFAR and 80 for Kitchen-HC. Training images are randomly cropped and resized to 32 × 32.

3. **STL-10 [10]**. Following [63], we use mini-batch size 256, initial learning rate 0.03, on 2 GPUs. Baseline models and baselines with CLD are trained on "train+unlabelled" split (105k samples), and tested on "test" split (5k samples). Training images are randomly cropped and resized to 96 × 96.

4. **Transfer learning on object detection**. We use Faster R-CNN with a backbone of R50-C4, with tuned synchronized batch normalization layers [48] as the detector. As in [26], the detector is fine-tuned for 24k iterations for the experiment on Pascal VOC trainval07+12 and 9k iterations for the experiment on Pascal VOC trainval07. The image scale is [480, 800] pixels during training and 800 at inference. NPID+CLD and MoCo+CLD use the same hyper-parameters as in MoCo [26]. The VOC-style evaluation metric AP50 at IoU threshold is 50% and COCO-style evaluation metric AP are used.

5. **Semi-supervised learning**. To make fair comparisons with baseline methods, we use OpenSelfSup [69] benchmark to implement baseline results and ours. We follow [67] and fine-tune the pre-trained model on two subsets for semi-supervised learning experiments, i.e. 1% and 10% of the labeled ImageNet-1k training datasets in a class-balanced way. The necks or heads are removed and only the backbone CNN is evaluated by appending a linear classification head.

We apply greedy search on a list of hyper-parameter settings with the base learning rate from {0.001, 0.01, 0.1} and the learning rate multiplier for the head from {1, 10, 100}. We choose the optimal hyper-parameter...
setting for each method. Empirically, all baselines and their alternatives with CLD obtain the best performance with a learning rate of 0.01 and a learning rate multiplier for the head of 100. We train the network for 20 epochs using SGD with weight decay 0.0001 and a momentum of 0.9, and a mini-batch of 256 on 4 GPUs. The learning rate is decayed by 5 times at epoch 12 and 16 respectively.

### 6.3. Which Clustering Method to Use?

We have tried two popular clustering methods: k-Means clustering and spectral clustering, both implemented in Pytorch for fast performance on GPUs.

**k-Means clustering** \([3, 35]\) aims to partition \(n\) representations into \(k\) groups, each representation belongs to the cluster with the nearest cluster centroid, serving as a prototype of the cluster. We use spherical k-Means clustering which minimizes: \(\sum (1 - \cos(f_i, u_{c(i)}))\) over all assignments \(c\) of objects \(i\) to cluster ids \(c(i)\) \(\in\) \(\{1, ..., k\}\) and over all prototypes \(u_1, ..., u_k\) in the same feature space as the feature vector \(f_i\) representing the objects. We use binary cluster assignment, where the cluster membership \(m_{ij} = 1\) if item \(i\) is assigned to cluster \(j\) and 0 otherwise. The following k-means objective can be solved using the standard Expectation-Maximization algorithm \([12]\):

\[
\Phi(M, \{u_1, ..., u_k\}) = \sum_{i,j} m_{ij}(1 - \cos(f_i, u_{c(i)})) = \sum_{i,j} m_{ij}(1 - \frac{f_i \cdot u_{c(i)}}{||f_i|| \cdot ||u_{c(i)}||}).
\]

### 4. Are Separate Feature and Group Branches Necessary?

Intuitively, instance grouping and instance discrimination are at odds with each other. Our solution is to formulate the feature learning on a common representation, forking off two branches where we can impose grouping and discrimination separately. Table A.9 shows that projecting the representation to different spaces and jointly optimize the two losses increase top-1 kNN accuracy by 1.5% and 1.8% on CIFAR-10 and CIFAR-100 respectively.

### 6.5. How Effective Is Cross-Augmentation Comparisons?

Instance-level discrimination presumes each instance is its own class and any other instance is a negative. The groups needed for any group-level discrimination have to be built upon local clustering results extracted from the current feature in training, which are fluid and unreliable.

Our solution is to seek the most certainty among all the uncertainties: We presume stable grouping between one instance and its augmented version, and our cross-level discrimination compares the former with the groups derived from the latter. We roll the three processes: instance grouping, invariant mapping, and instance-group discrimination all into one CLD loss.

Table A.9 shows that our cross-augmentation comparison increases the top-1 accuracy by more than 2% on recognition task. It demands the feature not only to be invariant to data augmentation, but also to be respectful of natural grouping between individual instances, often aligning better with downstream semantic classification.

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Table A.8: Top-1 kNN accuracies on Kitchen-HC under different group numbers for different clustering methods.

| group  | spectral | k-Means |
|--------|----------|---------|
| 10     | 77.1%    | 78.9%   |
| 64     | 74.5%    | 76.3%   |
| 128    | 72.6%    | 73.4%   |
| 256    | 70.5%    | 70.8%   |

Table A.9: Ablation study on various components of our method, i.e. adding the cross-level discrimination, projecting the representation to two different spaces, and using cross-augmentation comparison between \(x_i\) and \(x_i'\). kNN top-1 accuracy is reported here.

| NPID+CLD Subspace Cross-augmentation | CIFAR-10 | CIFAR-100 |
|-------------------------------------|----------|-----------|
| x                                  | 80.8%    | 51.6%     |
| ✓ share                            | 82.7%    | 53.3%     |
| ✓ separate                         | 84.2%    | 55.0%     |
| ✓ separate                         | 86.5%    | 57.5%     |
6.6. How Sensitive Are Hyper-parameters Weight $\lambda$ and Temperature $T$?

$\lambda$ controls the relative importance of CLD with respect to instance-level discrimination, and helps strike a balance between the caveats of noisy initial grouping and the benefits it brings with coarse-grained repulsion between instances and local groups. Table A.10 shows that, at a fixed group number, $\lambda = 0.25$ achieves optimal performance, and a larger $\lambda$ generally leads to worse performance and even decreases top-1 accuracy by 3.1% at $\lambda = 3$.

| $\lambda$ | NPID+CLD | MoCo+CLD |
|-----------|----------|----------|
|           | top-1 (%) | top-5 (%) | top-1 (%) | top-5 (%) |
| 0         | 75.3     | 92.4     | 77.6     | 93.8     |
| 0.1       | 78.8     | 94.4     | 80.3     | 95.0     |
| 0.25      | 79.7     | 95.1     | 81.7     | 95.7     |
| 0.5       | 78.9     | 94.4     | 80.5     | 95.2     |
| 1         | 78.8     | 94.5     | 80.1     | 94.8     |
| 3         | 76.6     | 93.2     | 78.4     | 94.1     |

Table A.10: Top-1 and top-5 linear classification accuracies (%) on ImageNet-100 with different $\lambda$’s. The backbone network is ResNet-50.

$T$ is known to critical for discriminative learning and can be sometimes tricky to choose. Table A.11 shows that the best performance is achieved at $T = 0.2$ for both CIFAR and ImageNet-100. With local grouping built into our CLD method, we find the sensitivity of $T$ is greatly reduced.

| $T(T_1 = T_2)$ | CIFAR-100 | ImageNet-100 |
|----------------|-----------|--------------|
| 0.07           | 57.9%     | 79.3%        |
| 0.1            | 57.8%     | 79.6%        |
| 0.2            | 58.1%     | 81.7%        |
| 0.3            | 58.1%     | 80.7%        |
| 0.4            | 57.6%     | 79.4%        |
| 0.5            | 57.2%     | 79.0%        |

Table A.11: Linear (ImageNet-100) and kNN (CIFAR-100) evaluations for models trained with different choices of temperature $T$, $T_1 = T_2$ for simplicity.

6.7. Is A Larger Memory Bank Always Better for Discriminative Learning?

A larger memory bank includes more negatives and is known to deliver a better discriminator. However, we cannot simply adjust the memory bank size according to NMI or retrieval accuracy in order to deliver the best performance on downstream classification.

Fig. A.10 compares NMI and retrieval accuracies under different negative prototype sizes. If there are too many negatives, the model would focus on repelling negative instances, ignoring the commonality between instances; if there are too few negatives, the model would be subject to random fluctuations from batch to batch, affecting optimization and convergence. However, neither the number of negatives (i.e. infoNCE-k) to obtain the best retrieval accuracy nor the number of negatives to achieve the best NMI score can deliver the best downstream classification task. To deliver optimal performance at downstream classification task, there is a trade-off between local mutual information (evaluated by retrieval task) and global mutual information (evaluated by Normalized Mutual Information).

6.8. Sample Retrievals

Fig. A.11 shows our near-perfect sample retrievals on ImageNet-100 using $f_I(x)$ in our NPID + CLD model. On the contrary, NPID seems to be much more sensitive to textural appearance (e.g., Rows 1,4,6,7), first retrieve those with similar textures or colors. CLD is able to retrieve semantically similar samples. Our conjecture is that by gathering similar textures into groups, CLD can actually find more informative feature that contrasts between groups. For example, the 5th query image is a Chocolate sauce, which has similar texture with Grouper fish. NPID incorrectly retrieves many images from the Grouper Fish class, but CLD successfully captures the semantic information of the query image, and retrieves instances with the same semantic information.
Figure A.11: Comparisons of top retrieves by NPID (Columns 2-9) and NPID+CLD (Columns 10-17) according to $f_I$ for the query images (Column 1) from the ImageNet validation set. The results are sorted by NPID’s performance: Retrievals with the same category as the query are outlined in green and otherwise in red. NPID seems to be much more sensitive to textural appearance (e.g., Rows 1, 4, 5, 7), first retrieve those with similar textures or colors. Integrated with CLD, NPID+CLD is able to retrieve semantically similar samples. (Zoom in for details)