# GRADIENT-OPTIMIZED CONTRASTIVE LEARNING

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# ABSTRACT

Contrastive learning is a crucial technique in representation learning, producing robust embeddings by distinguishing between similar and dissimilar pairs. In this paper, we introduce a novel framework, *Gradient-Optimized Contrastive Learning (GOAL)*, which enhances network training by optimizing gradient updates during backpropagation as a bilevel optimization problem. Our approach offers three key insights that set it apart from existing methods: (1) Contrastive learning can be seen as an approximation of a one-class support vector machine (OC-SVM) using multiple neural tangent kernels (NTKs) in the network's parameter space; (2) Hard triplet samples are vital for defining support vectors and outliers in OC-SVMs within NTK spaces, with their difficulty measured using Lagrangian multipliers; (3) Contrastive losses like InfoNCE provide efficient yet dense approximations of sparse Lagrangian multipliers by implicitly leveraging gradients. To address the computational complexity of GOAL, we propose a novel contrastive loss function, *Sparse InfoNCE (SINCE)*, which improves the Lagrangian multiplier approximation by incorporating hard triplet sampling into InfoNCE. Our experimental results demonstrate the effectiveness and efficiency of SINCE in tasks such as image classification and point cloud completion. Demo code is attached in the supplementary file.

#### **028** 1 INTRODUCTION

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> Contrastive learning [\(Chopra et al., 2005;](#page-10-0) [Hadsell et al., 2006\)](#page-11-0) has become one of the dominant methods in representation learning. Typically, contrastive learning constructs positive pairs and negative pairs by creating two augmented views of the same image. The goal is to bring the embeddings of positive pairs closer and push those of negative pairs apart in the latent space, often optimized using a loss function such as InfoNCE [\(Van den Oord et al., 2018;](#page-13-0) [Chen et al., 2020a\)](#page-10-1).

**035 036 037 038 039 040 041 042 043 044 Motivation.** To better understand contrastive learning, we start by analyzing the impacts of positive and negative samples on the gradients during backpropagation in training. We discover that recent contrastive losses often result in bounded positive weights for linear combinations of triplet gradient features in stochastic gradient descent (SGD). For instance, [Tian](#page-13-1) [\(2022\)](#page-13-1) recently proposed a family of  $(\phi, \psi)$ -contrastive losses defined as  $\ell_{\phi, \psi} = \sum_x \phi \left( \sum_x - \psi \left( f(x, x^+, x^-; \omega) \right) \right)$ , where the scalar functions  $\phi$  and  $\psi$  are increasing monotonically and differentiable. The function  $f(x, x^+, x^-; \omega) =$  $\frac{1}{2}[\|h(x;\omega)-h(x^+;\omega)\|^2 - \|h(x;\omega)-h(x^-;\omega)\|^2]$  measures the distance difference between the positive and negative pairs. We list some examples in Table [1](#page-1-0) where  $\alpha_x$ − denotes the weights for feature combination during learning. As we see, all the  $\alpha_x$ −'s are positive and the summation over negative samples for each loss is no greater than one.

**045 046 047 048 049 050 051 052 053** This behavior raises concerns about the effectiveness and robustness of the gradients in contrastive learning because useful (hard) negative samples can be easily buried among many non-useful (easy) negative samples, leading to similar weights for generating gradients. Such concerns have recently garnered increased attention. For instance, [Wang & Liu](#page-13-2) [\(2021\)](#page-13-2) claimed that "A well-designed contrastive loss should have some extent of tolerance to the closeness of semantically similar samples," and thus proposed an explicitly hard negative sampling method by *filtering out uninformative* negative samples. [Chuang et al.](#page-10-2) [\(2020\)](#page-10-2) proposed a *debiased* contrastive learning method that corrects for the sampling of same-label datapoints by thresholding in the contrastive loss. Motivated by these works, in this paper we aim to address the following question:

*How should we optimize the gradients in contrastive learning, effectively and efficiently?*



<span id="page-1-0"></span>Table 1: Some examples of  $(\phi, \psi)$ -contrastive losses with corresponding analytical expressions.

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**065 066 067 068 069 070 071 072 073 074 075 076 077 078 079 080** Approach. In contrast to the literature, we propose a novel framework, namely *Gradient-Optimized Contrastive Learning (GOAL)*, to learn to optimize gradients in backpropagation. Specifically, we formulate the lower-level optimization problem as a one-class support vector machine (OC-SVM) [\(Schölkopf et al., 1999\)](#page-12-0) in a neural tangent kernel (NTK) [\(Jacot et al., 2018\)](#page-11-1) space to determine the weights (*i.e.,* Lagrangian multipliers) for the upper-level summation loss over the triplets. We hypothesize that these weights may be taken as sub-optimal solutions to the dual of these kernel machines that explicitly learn to maximize the triplet separation in each NTK space. This interpretation is motivated by the strong connections between the dual form of OC-SVM and the linear combination weights for the gradients ( $e.g., \alpha_{x-}$  in Table [1\)](#page-1-0) in contrastive learning. Our analysis also implies that truly hard negative samples (in the context of triplets, rather than pairs as in traditional methods) should be defined as the support vectors and outliers of OC-SVMs in the NTK spaces, rather than in the spatial domain of images or the output space of the network. To address the computational issue in GOAL due to the nature of bilevel optimization for largescale learning, we further propose a new contrastive loss, namely, *Sparse InfoNCE (SINCE)*, for better approximations of Lagrangian multipliers based on InfoNCE with hard triplet sampling. We demonstrate its effectiveness and efficiency in the tasks of image classification and point cloud completion, with significant improvements.

Contributions. In summary, our key contributions are as follows:

- We propose a new contrastive learning framework, GOAL, based on bilevel optimization that learns to optimize gradients in backpropagation for training networks. Our approach provides novel insights to understand contrastive learning from a perspective of sparse kernel machines.
- We propose a new contrastive loss, SINCE, to mitigate the computational issue in bilevel optimization by approximating the Lagrangian multipliers using InfoNCE with hard triplet sampling.
- We demonstrate superior performance in both image classification and point cloud completion, showcasing the effectiveness and efficiency of our approach.

2 RELATED WORK

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**093 094 095 096 097 098 099 100 101 102 103 104 105 106 107** Contrastive Learning. Learning representations from unlabeled data in a contrastive way has been one of the most competitive research fields [\(Van den Oord et al., 2018;](#page-13-0) [Hjelm et al., 2018;](#page-11-2) [Wu et al.,](#page-14-0) [2018;](#page-14-0) [Tian et al., 2020a;](#page-13-5) [Sohn, 2016;](#page-13-4) [Chen et al., 2020a;](#page-10-1) [Jaiswal et al., 2020;](#page-11-3) [Li et al., 2020b;](#page-11-4) [He](#page-11-5) [et al., 2020;](#page-11-5) [Chen et al., 2020c](#page-10-4)[;b;](#page-10-5) [Bachman et al., 2019;](#page-10-6) [Misra & Maaten, 2020;](#page-12-1) [Caron et al., 2020\)](#page-10-7) where contrastive loss optimizes data representations by aligning the two views of the same image (*i.e.,* positive pairs) while pushing different images (*i.e.,* negative pairs) away. A large number of works in contrastive learning are about how to augment the data. Empirically, positive pairs could be different modalities of a signal [\(Arandjelovic & Zisserman, 2018;](#page-10-8) [Tian et al., 2020a;](#page-13-5) [Tschannen et al.,](#page-13-6) [2020\)](#page-13-6) or different augmented samples of the same image *e.g.,* color distortion and random crop [\(Chen](#page-10-1) [et al., 2020a;](#page-10-1)[c;](#page-10-4) [Grill et al., 2020\)](#page-11-6). [Tian et al.](#page-13-7) [\(2020b\)](#page-13-7) suggested generating positive pairs with the "InfoMin principle" so that the generated positive pairs maintain the minimal information necessary for downstream tasks. [Selvaraju et al.](#page-12-2) [\(2021\)](#page-12-2); [Peng et al.](#page-12-3) [\(2022\)](#page-12-3); [Mishra et al.](#page-12-4) [\(2021\)](#page-12-4); [Li et al.](#page-11-7) [\(2022\)](#page-11-7) proposed selecting meaningful but not fully overlapped contrastive crops with guidance such as attention maps or object-scene relations. [Shen et al.](#page-12-5) [\(2020\)](#page-12-5) empirically demonstrated that introducing extra convex combinations of data as positive augmentation improves representation learning. Similar mixing data strategies could be found in [\(Lee et al., 2020;](#page-11-8) [Kim et al., 2020;](#page-11-9) [Verma et al., 2021;](#page-13-8) [Li](#page-11-10) [et al., 2020a;](#page-11-10) [Ren et al., 2022\)](#page-12-6). In addition to exploring positive augmentation, some recent work

**108 109 110 111 112 113 114 115 116 117** also focuses on negative data selection in contrastive learning. Typically, negative samples are drawn uniformly from the training data. Based on the argument that not all negatives are true negatives, [Chuang et al.](#page-10-2) [\(2020\)](#page-10-2); [Robinson et al.](#page-12-7) [\(2020\)](#page-12-7) developed debiased contrastive losses to assign higher weights to "harder" negative samples. [Wang & Liu](#page-13-2) [\(2021\)](#page-13-2) proposed an explicit way to select hard negative samples that are similar to the positives. To provide more meaningful negative samples, [Kalantidis et al.](#page-11-11) [\(2020\)](#page-11-11) studied the Mixup [\(Zhang et al., 2017\)](#page-14-1) strategy in latent space to generate hard negatives. [Hu et al.](#page-11-12) [\(2021\)](#page-11-12) proposed learning a set of negative adversaries directly. [Ge et al.](#page-10-9) [\(2021\)](#page-10-9) generated negative samples by texture synthesis or selecting non-semantic patches from existing images. [Yue et al.](#page-14-2) [\(2024\)](#page-14-2) studied hard negative samples in the hyperbolic space and proposed a new contrastive loss by considering both Euclidean and hyperbolic spaces.

**118 119 120 121 122 123 124 125 126 127 128** Sparse Kernel Machines. A sparse kernel machine is a type of statistical learning algorithm that focuses on using a subset of training data to make predictions. This approach is beneficial in scenarios where the dataset is large, as it helps reduce computational complexity and improve efficiency. OC-SVMs [\(Schölkopf et al., 1999;](#page-12-0) [Tax & Duin, 1999;](#page-13-9) [Sain, 1996;](#page-12-8) [Schölkopf et al., 2001;](#page-12-9) [Tax & Duin,](#page-13-10) [2004;](#page-13-10) [Tax, 2002\)](#page-13-11), a classical one-class learning algorithm, are frequently used in outlier or novelty detection [\(Pimentel et al., 2014;](#page-12-10) [Chandola, 2007;](#page-10-10) [Ratsch et al., 2002\)](#page-12-11) to detect if a test sample belongs to the same distribution of training data. For instance, Tax  $\&$  Duin [\(1999\)](#page-13-9) proposed minimizing the volume of a hypersphere that contains as many as possible of the "normal" training data, which has been shown to be equivalent to [\(Schölkopf et al., 2001\)](#page-12-9) for certain kernels. Some good surveys are provided in [\(Subrahmanya & Shin, 2009;](#page-13-12) [Li et al., 2020c\)](#page-11-13). Particularly, max-margin based contrastive learning [\(Chen et al., 2021;](#page-10-11) [Shah et al., 2022\)](#page-12-12) have been studied as well.

**129 130 131 132 133 134 135 136 137 138 139 140** Point Cloud Completion. In computer vision, this refers to an important and challenging task of inferring the complete 3D shape of an object or scene from incomplete raw 3D point clouds. Recently, many deep learning approaches have been developed for this task. For instance, PCN [\(Yuan et al.,](#page-14-3) [2018\)](#page-14-3), the first deep neural network for point cloud completion, extracts global features directly from point clouds and then generates points using the folding operations from FoldingNet [\(Yang et al.,](#page-14-4) [2018\)](#page-14-4). [Zhang et al.](#page-14-5) [\(2020\)](#page-14-5) proposed extracting multiscale features from different network layers to capture local structures and improve performance. Attention mechanisms such as Transformer [\(Vaswani et al., 2017\)](#page-13-13) excel at capturing long-term interactions. Accordingly, SnowflakeNet [\(Xiang](#page-14-6) [et al., 2021\)](#page-14-6), PointTr [\(Yu et al., 2021\)](#page-14-7), and SeedFormer [\(Zhou et al., 2022\)](#page-14-8) accentuate the decoder component by incorporating Transformer designs. PointAttN [\(Wang et al., 2022\)](#page-13-14) is conceived entirely on Transformer foundations. In particular, [Lin et al.](#page-12-13) [\(2023\)](#page-12-13) proposed an InfoCD loss by introducing contrastive learning into point cloud completion, achieving the state-of-the-art performance.

# 3 GOAL: GRADIENT-OPTIMIZED CONTRASTIVE LEARNING

## 3.1 PRELIMINARY

**155 156 157** **Learning with InfoNCE.** We denote  $x \in \mathcal{X}, x^+ \in \mathcal{X}^+, x^- \in \mathcal{X}^-$  as an archor sample and its positive and negative samples, respectively. We further denote  $h(x; \omega) : \mathcal{X} \times \Omega \to \mathbb{R}^d$  as a differentiable function that is implemented by a neural network and parametrized by  $\omega \in \Omega$ , and

<span id="page-2-0"></span>
$$
f_{\tau,\tau'}(x, x^+, x^-; \omega) = \frac{1}{\tau} d(x^+, x; \omega) - \frac{1}{\tau'} d(x^-, x; \omega)
$$
 (1)

**151 152 153 154** as a distance measure for the triplet  $(x, x^+, x^-)$  with some form of pairwise distance measure d, where  $\tau, \tau' \geq 0$  denote two predefined scalars. Note that the smaller  $f_{\tau,\tau'}(x, x^+, x^-; \omega)$  is, the better the separation between the positive and negative pairs. By defining  $d(\cdot, x; \omega) = ||h(\cdot; \omega) - h(x; \omega)||_2^2$ in Equation [\(1\)](#page-2-0), the InfoNCE loss in [\(Van den Oord et al., 2018\)](#page-13-0) can be written as follows:

<span id="page-2-1"></span>
$$
\ell(\omega) = \mathbb{E}_x \Big[ \ell_\tau(x; \omega) \Big] = \mathbb{E}_x \left[ \log \sum_{x^-} \exp \left\{ f_{\tau, \tau}(x, x^+, x^-; \omega) \right\} \right],\tag{2}
$$

**158 159** where only one positive sample is considered and  $E$  denotes the expectation operator. Now based on this equation, we can compute the gradients in backpropagation during training as

$$
\nabla \ell_{\tau}(x;\omega) = \sum_{x^{-}} \alpha_{x^{-}} \nabla f_{\tau,\tau}(x, x^{+}, x^{-}; \omega), \text{ where } \alpha_{x^{-}} = \frac{\exp\{f_{\tau,\tau}(x, x^{+}, x^{-}; \omega)\}}{\sum_{x^{-}} \exp\{f_{\tau,\tau}(x, x^{+}, x^{-}; \omega)\}}.
$$
 (3)

**162 163 164 165** Clearly, it holds that  $0 \le \alpha_{x-} \le 1$ ,  $\sum_{x-} \alpha_{x-} = 1$ . Therefore,  $\nabla \ell_{\tau}(x;\omega)$  computes the mean of the gradients  $\nabla f_{\tau,\tau}(x, x^+, \overline{x^-}; \omega)$  from all positive and negative samples *w.r.t.* x, and  $\nabla \ell_{\tau}(\omega)$  =  $\mathbb{E}_x[\nabla \ell_\tau(x;\omega)]$  computes the mean of  $\nabla \ell_\tau(x;\omega)$  over x. All the expressions of  $\alpha_{x-}$ 's in Table [1](#page-1-0) are computed in a similar way given different objectives.

**167** 3.2 OUR BILEVEL MODEL

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**169 170 171 172 173 174 175 176 177 178 179 180 181** In Figure [1,](#page-3-0) we illustrate a geometric view of SGD based on a *local linear approximation* of the loss landscape at each parameter update. The loss landscape is parameterized by the network parameter  $\omega$ , and at each update  $\omega_t$ , a neural tangent space is constructed by taking triplets {(x, x+, x−)} as input to generate *triplet gradient features*  $\nabla f_{\tau,\tau'}(x, x^+, x^-; \omega_t)$ , and then the gradient  $\Delta \omega_t$  is computed by a linear combination of such triplet features, *i.e.*,  $\Delta \omega_t =$  $\sum_{(x,x^+,x^-)} \alpha^{(t)}_{(x,x^+,x^-)} \nabla f_{\tau,\tau'}(x,x^+,x^-;\omega_t),$ where  $\alpha_{i}^{(t)}$  $\binom{t}{(x,x^+,x^-)}$  stands for a sample weight at the t-th iteration in SGD.

<span id="page-3-0"></span>

Figure 1: Illustration of local linear approximation of a contrastive loss landscape during training with SGD. The gradient  $\Delta\omega$  is often a linear combination of triplet gradient features in the tangent space, and we show that such increments may be interpreted as approximations of linear OC-SVMs.

**182 183 184 185 186 187** Motivation: Sample weights for gradients and network weights may be fully coupled. When the calculation of each  $\alpha_{(r)}^{(t)}$  $(x)$ <sub>(x,x+,x-)</sub> relies on the triplet features  $\nabla f_{\tau,\tau'}(x, x^+, x^-; \omega_t)$ , it becomes evident that  $\alpha_{\ell,r}^{(t)}$  $\binom{t}{(x,x^+,x^-)}$  is a function of  $\omega_t$ . Consequently, training can be iteratively performed by optimizing  $\omega$  towards a specific objective. Indeed, all the contrastive losses in Table [1](#page-1-0) are designed in such a way that each  $\alpha_{(x,x^+,x^-)}$  explicitly depends on  $\omega$ , as shown in Equation [\(3\)](#page-2-1). Now the question is:

What if 
$$
\alpha_{(x,x^+,x^-)}
$$
 does not have an explicit form of  $\omega$ ?

**190 191 192 193 194 195** To answer this question, we propose using bilevel optimization [\(Colson et al., 2007\)](#page-10-12), where one problem is embedded (nested) within another, to model the dependency between the sample weights for gradients and network weights. In this structure, the *upper-level (UL)* problem is influenced by the *optimal* parameters from the *lower-level (LL)* problem, whereas the LL problem is influenced by the *non-optimal* parameters from the UL problem. In our model, we use the UL problem to update network weights, and the LL problem to learn optimal gradients for SGD.

**196 197 198 199 200 201 202 203 204** Upper-level Objective. At the early age of contrastive learning, the losses such as [\(Chopra et al.,](#page-10-0) [2005;](#page-10-0) [Schroff et al., 2015\)](#page-12-14) always favor sparse samples for learning. For instance, the triplet loss [\(Schroff et al., 2015\)](#page-12-14) is defined as  $\ell_{triplet}(x, x^+, x^-; \omega) = \max\left\{0, f_{1,1}(x, x^+, x^-; \omega) + \epsilon\right\}$ , where  $\epsilon > 0$  is a predefined parameter to control the minimum offset between distances of similar and dissimilar pairs. In fact, triplet loss is a variant of the hinge loss commonly used in SVMs. Regarding gradient calculation, the triplet loss assigns a combination weight of either 0 or 1 to the gradient of each triplet, which differs from modern contrastive losses such as InfoNCE. Considering these, we propose the following UL objective that involves the optimal solution  $\{\alpha_{ijk}^*\}$  from the LL problem to model the sample weights for gradients explicitly:

<span id="page-3-1"></span>
$$
\min_{\omega} \sum_{i,j,k} \alpha_{ijk}^* f_{\tau,\tau'}(x_i, x_{ij}^+, x_{ik}^-; \omega), \tag{4}
$$

where i, j, k denote the i-th anchor, its j-th positive and k-th negative samples, respectively. In this way, we can control the gradients based on these sample weights in SGD.

**211 212 213 214 215** Lower-level Objective. Recall that at the t-th iteration in SGD, the gradient  $\Delta \omega_t$  can be represented as a linear combination of triplet gradient features  $\nabla f_{\tau,\tau'}(x, x^+, x^-; \omega_t)$  with weights  $\alpha_{\tau}^{(t)}$  $\binom{t}{(x,x^+,x^-)}$ . This reminds us of the classic representer theorem [\(Dinuzzo & Schölkopf, 2012\)](#page-10-13) for kernel methods, and motivates us to learn  $\Delta\omega_t$  based on local linear approximation, namely,  $f_{\tau,\tau'}(x, x^+, x^-; \omega_t - \Delta\omega_t) \approx$  $f_{\tau,\tau'}(x, x^+, x^-; \omega_t) - \Delta \omega_t^T \nabla f_{\tau,\tau'}(x, x^+, x^-; \omega_t)$  where  $(\cdot)^T$  denotes the matrix transpose operator. We expect that after the update, the value of  $f_{\tau,\tau'}(x, x^+, x^-; \omega_t - \Delta \omega_t)$  could be no bigger than a

**216 217 218** threshold  $\rho_t$ . Motivated by one-class support vector machine (OC-SVM) in [\(Schölkopf et al., 1999\)](#page-12-0), we propose the following regularized OC-SVM as our LL objective:

<span id="page-4-0"></span>
$$
\min_{\nu_t, \rho_t, \{\xi_{ijk}^{(t)}\}} \frac{1}{2} \|\Delta \omega_t\|^2 + \rho_t + C \sum_{i,j,k} \xi_{ijk}^{(t)},
$$
\n(5)

$$
\text{s.t. } f_{\tau,\tau'}(x_i, x_{ij}^+, x_{ik}^-; \omega_t) - \Delta \omega_t^T \nabla f_{\tau,\tau'}(x_i, x_{ij}^+, x_{ik}^-; \omega_t) \le \rho_t + \xi_{ijk}^{(t)}, \xi_{ijk}^{(t)} \ge 0, \forall i, \forall j, \forall k, \forall t,
$$

with a predefined constant  $C \geq 0$  and a set of slack variables  $\{\xi_{ijk}^{(t)}\}$ .

Bilevel Formulation. As we discussed before, the sample weights for gradients,  $\alpha$ , and the network weights,  $\omega$ , are coupled, and one can be optimized alternatively by fixing the other (a widely used technique for solving bilevel optimization [\(Xiao et al., 2024\)](#page-14-9)). Therefore, by incorporating our UL objective in Equation [\(4\)](#page-3-1) and the dual form of our LL objective in Equation [\(5\)](#page-4-0), we propose the following bilevel optimization problem for contrastive learning:

$$
\omega^* \in \arg\min_{\omega} \sum_{i,j,k} \alpha^*_{ijk} f_{\tau,\tau'}(x_i, x_{ij}^+, x_{ik}^-; \omega), \tag{6}
$$

<span id="page-4-1"></span>
$$
\text{s.t. } \{\alpha_{ijk}^*\} \in \underset{\{\alpha_{ijk}\}}{\text{arg min}} \left\{ \frac{1}{2} \sum_{jk,j'k'} \alpha_{ijk} \kappa_{\omega^*} \left( \mathcal{X}_{ijk}, \mathcal{X}_{ij'k'} \right) \alpha_{ij'k'} - \sum_{j,k} \alpha_{ijk} f_{\tau, \tau'} \left( x_i, x_{ij}^+, x_{ik}^-, \omega^* \right) \right\}
$$
\n
$$
\text{s.t. } \sum_{j,k} \alpha_{ijk} = 1, 0 \le \alpha_{ijk} \le C, \forall i, \forall j, \forall k,
$$

**238 239 240 241 242 243** where for simplicity,  $\mathcal{X}_{ijk} = \{x_i, x_{ij}^+, x_{ik}^-\}, \mathcal{X}_{ij'k'} = \{x_i, x_{ij'}^+, x_{ik'}^-\}$  stand for two triplets, respectively, and  $\kappa_{\omega^*}(\mathcal{X}_{ijk}, \mathcal{X}_{ij'k'}) = \nabla f_{\tau,\tau'}(x_i, x_{ij}^+, x_{ik}^-; \omega^*)^T \nabla f_{\tau,\tau'}(x_i, x_{ij'}^+, x_{ik'}^-; \omega^*)$  defines a neural tangent kernel (NTK) in the network parameter space. Our bilevel formulation also indicates that hard triplet samples are essential for defining support vectors and outliers in OC-SVMs within NTK spaces, with their degree of difficulty measured using Lagrangian multipliers  $\{\alpha_{ijk}\}\$ as sample weights.

**244 Alternating Optimization.** To solve Equation [\(6\)](#page-4-1), we simply learn  $\{\alpha_{ijk}^*\}$  and  $\omega^*$  as follows:

**245** Step 1: Randomly sample triplets from the training dataset;

**246** Step 2: Compute the solution  $\{\alpha_{ijk}^*\}$  of the dual form of the OC-SVM in the LL problem;

- **247 248** Step 3: Update  $\omega$  using SGD as the UL solution  $\omega^*$  based on the solution  $\{\alpha^*_{ijk}\}$ ;
- **249** Step 4: Repeat Step 1-3 until the UL objective converges.

#### <span id="page-4-2"></span>3.3 ANALYSIS

 $Δ<sub>ω</sub>$ 

Lemma 1 (Contrastive Learning as NTK Regression). *Suppose that contrastive learning updates*  $t$ he model parameter  $\omega$  as  $\omega_{t+1} = \omega_t - \eta_t\nabla\ell(\omega_t) = \omega_t - \eta_t\sum_{i,j,k}\alpha_{ijk}^{(t)}\nabla f_{\tau,\tau'}(x_i,x_{ij}^+,x_{ik}^-;\omega_t)$  to minimize some contrastive loss  $\ell(\omega)$ , where  $\alpha_{ijk}^{(t)} \geq 0$  denotes the sample weight for each training triplet  $(x_i, x_{ij}^+, x_{ik}^-)$  at the  $t$ -th iteration and function  $f$  is differentiable (everywhere). Assuming that *the learning rates,*  $\{\eta_t\}$ *, satisfy*  $\lim_{t\to\infty} \eta_t = 0$ ,  $\sum_{t=0}^{\infty} \eta_t = \infty$ ,  $\sum_{t=0}^{\infty} \eta_t^2 < \infty$ *, then given a test triplet*  $(\tilde{x}, \tilde{x}^+, \tilde{x}^-)$ *, it holds that at the* T-th iteration,

$$
f_{\tau,\tau'}(\tilde{x},\tilde{x}^+,\tilde{x}^-;\omega_T) \le A - \sum_{t=0}^{T-1} \eta_t \left[ \sum_{i,j,k} \alpha_{ijk}^{(t)} \kappa_{\omega_t} \left( (x_i, x_{ij}^+, x_{ik}^-), (\tilde{x}, \tilde{x}^+, \tilde{x}^-) \right) \right],
$$
 (7)

.

where  $A = \sup \left( f_{\tau,\tau'}(\tilde{x}, \tilde{x}^+, \tilde{x}^-; \omega_0) + O\left( \sum_{t=0}^{T-1} \eta_t^2 \right) \right)$ , provided that  $f_{\tau,\tau'}(\tilde{x}, \tilde{x}^+, \tilde{x}^-; \omega_0)$  for any triplet  $(\tilde{x}, \tilde{x}^+, \tilde{x}^-)$  is bounded.

#### *Proof.* Based on local linear approximation and the assumptions in the lemma, we have

$$
f_{\tau,\tau'}(\tilde{x},\tilde{x}^+,\tilde{x}^-;\omega_{t+1}) - f_{\tau,\tau'}(\tilde{x},\tilde{x}^+,\tilde{x}^-;\omega_t) = O(\eta_t^2) - \sum_{i,j,k} \alpha_{ijk}^{(t)} \kappa_{\omega_t} ((x_i,x_{ij}^+,x_{ik}^-),(\tilde{x},\tilde{x}^+,\tilde{x}^-))
$$

Now by summing up over t from 0 to  $T - 1$  recursively, we can complete our proof.  $\Box$  **270 271 272 273** In practice, a loss function with a neural network as  $f$  can be taken as a differentiable function and  $\eta_t = O(\frac{1}{t})$  can easily satisfy the assumption. This lemma also indicates that contrastive learning can be viewed as an approximation of an OC-SVM with multiple NTKs in the network parameter space.

Relation to Max-Margin Contrastive Learning. To make sure that the distance from the positive sample,  $d(x^+, x; \omega)$ , is as small as possible compared with that from a negative sample,  $d(x^-, x; \omega)$ , we need to minimize  $f_{\tau,\tau'}(\tilde{x}, \tilde{x}^+, \tilde{x}^-; \omega_T)$ . Based on Lemma [1,](#page-4-2) we have a direct result as follows:

$$
\min f_{\tau,\tau'}(\tilde{x}, \tilde{x}^+, \tilde{x}^-; \omega_T) \equiv \sum_{t=0}^{T-1} \eta_t \left[ \max \left\{ \sum_{i,j,k} \alpha_{ijk}^{(t)} \kappa_{\omega_t} \left( (x_i, x_{ij}^+, x_{ik}^-), (\tilde{x}, \tilde{x}^+, \tilde{x}^-) \right) \right\} \right], \quad (8)
$$

where the RHS can be viewed as a maximum margin, learned within multiple NTK spaces at each iteration where each anchor  $x_i$  introduce a kernel. That is, minimizing the distance between a positive pair and a negative pair is equivalent to maximizing a (weighted) margin with multiple NTKs.

Different from the literature of max-margin contrastive learning, such as [\(Shah et al., 2022\)](#page-12-12), we aim to understand the behavior of contrastive learning from a geometric view of local linear approximations of the loss landscape, and accordingly learn to optimize gradients in backpropagation. To the best of our knowledge, we are the *first* to conduct such a study, leading us to different:

- *Reproducing Kernel Hilbert Space (RKHS):* Due to the gradient, our RKHS is the network parameter space, while a much smaller network output space is used in [\(Shah et al., 2022\)](#page-12-12).
- *Kernel Methods:* We introduce OC-SVMs to learn optimal gradients with no labels, while [\(Shah](#page-12-12) [et al., 2022\)](#page-12-12) uses binary SVMs to select hard negative samples.
- *Theorems:* Our theorem reveals a strong connection between contrastive learning and (max-margin) kernel methods with multiple NTKs, which is missing in the current literature.

## 4 SINCE: SPARSE INFONCE LOSS FOR EFFICIENT SOLUTIONS

Similar to [\(Shah et al., 2022\)](#page-12-12), tackling our bilevel optimization problem directly in deep learning proves to be highly challenging in practice. The vast RKHS, with its millions of dimensions, poses significant computational and storage difficulties on hardware like GPUs. To mitigate this issue, we introduce a novel contrastive loss, SINCE, designed to approximate the solutions of our GOAL.

**301 302 303 Motivation.** In fact, since the LL problem in Equation [\(6\)](#page-4-1) is a convex problem, we can use projected gradient descent (PGD) to compute the dual solution,  $\alpha^* = {\alpha^*_{ijk}}$ , as follows:

$$
\boldsymbol{\alpha}_{t'+1} = \text{Proj}_{\Delta}\Big(\boldsymbol{\alpha}_{t'} - \lambda_{t'}\left(\mathbf{K}_{\omega^*}(x_i)\boldsymbol{\alpha}_{t'} - \mathbf{f}_t(x_i)\right)\Big) = \text{Proj}_{\Delta}\Big(\lambda_{t'}\mathbf{f}_t(x_i) + (\mathbf{I} - \lambda_{t'}\mathbf{K}_{\omega^*}(x_i))\boldsymbol{\alpha}_{t'}\Big),\tag{9}
$$

**307 308 309 310 311 312** where at the t' iteration,  $\mathbf{K}_{\omega^*}(x_i) = [\kappa_{\omega^*}(\mathcal{X}_{ijk}, \mathcal{X}_{ij'k'})]$  stands for the NTK matrix for the anchor  $x_i, \forall i$ ,  $\mathbf{f}_t(x_i) = [f_{\tau, \tau'}(x_i, x_{ij}^+, x_{ik}^-; \omega_t)]$  for a vector, I for an identity matrix,  $\lambda_{t'} \geq 0$  for a proper learning rate, and Proj<sub>∧</sub> for the projection-onto-simplex operator that can be conducted efficiently, *e.g.,* [Chen & Ye](#page-10-14) [\(2011\)](#page-10-14). However, in our case with very high dimensional RKHS, it is not practical to use many iterations to compute  $\alpha^*$ . To address these issues, based on [Chen & Ye](#page-10-14) [\(2011\)](#page-10-14) we alternatively use the one-step approximation of Equation [\(9\)](#page-5-0) with  $\alpha_0 = 0$  as shown below:

<span id="page-5-1"></span><span id="page-5-0"></span>
$$
\boldsymbol{\alpha}^* \approx \boldsymbol{\alpha}_1 = \text{Proj}_{\Delta}\big(\lambda_0 \mathbf{f}_t(x_i)\big) = \max\Big\{\mathbf{0}, \lambda_0 \mathbf{f}_t(x_i) - \mu_t \mathbf{1}\Big\},\tag{10}
$$

**315 316** where  $\mu_t$  is a scalar that is determined by the vector  $\lambda_0 f_t(x_i)$  and 1 is a vector of ones. In summary, *the solution of the OC-SVM can be approximated based on entry-wise rescaling followed by thresholding.*

**317 318 319 320** Loss Formulation: InfoNCE with Thresholding. Based on our analysis above, we propose a strategy of *thresholding first and then normalization* for InfoNCE to approximate the OC-SVM solutions. This is equivalent to preserving "harder" triplets with larger  $f$  values and removing "easier" ones, leading to a binary mask for each  $f_t(x_i)$ . Accordingly, we formally define our SINCE loss as

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$$
\ell_{SINCE} = \mathbb{E}_x \left[ \log \sum_{(x^+, x^-)} \exp \left\{ f_{\tau, \tau'}(x, x^+, x^-; \omega) \right\} \cdot 1_{\{ f_{\tau, \tau'}(x, x^+, x^-; \omega) \ge \mu_x \}} \right], \quad (11)
$$

Table 2: Test accuracy comparison with the linear probe protocol.

<span id="page-6-1"></span>

	CIFAR-10						$STL-10$					
	$#$ triplets						# triplets					
	20	40		60 80		100 16,256 20			40 60 80		100 16.256	
InfoNCE 28.56 28.99 23.46 36.91 36.92 57.75 27.48 28.93 35.58 33.70 35.09 50.65												
GOAL 30.22 34.62 38.79 45.13 49.41 - 31.91 42.70 45.38 44.17 46.66												
SINCE 30.28 36.37 25.42 38.14 41.29 58.84 28.87 30.02 37.67 36.67 37.73 52.65												

where  $\mu_x$  is a predefined threshold, and  $1_{\{.\}}$  is an indicator function returning 1 if the condition holds, otherwise, 0. Note that instead of using  $\mu_x$  in our experiments, which has an indeterminate range of values beforehand, we introduce another predefined parameter,  $\gamma \in [0, 1]$ , to control the ratio of triplets to be removed. This approach allows us to efficiently construct binary masks in Equation [\(11\)](#page-5-1).

**337 338 339 340 341 342** 5 EXPERIMENTS 5.1 IMAGE CLASSIFICATION Table 3: Performance improvements (%) using SINCE over InfoNCE, with all triplets. CIFAR-10 STL-10 ImageNet-100 SimCLR 1.09 2.00 2.46 We follow the representation learning and linear probe  $\begin{array}{|l|c|c|c|c|c|} \hline \text{MOCO} & 2.54 & 4.19 & 2.24 \ \hline \text{BYOL} & 2.69 & 3.36 & 2.53 \ \hline \end{array}$ 

**343** protocol [\(Oord et al., 2018;](#page-12-15) [He et al., 2016;](#page-11-14) [Yeh et al.,](#page-14-10)

**344 345** [2021\)](#page-14-10) for image classification to conduct comprehensive experiments on CIFAR-10 [\(Krizhevsky](#page-11-15) [et al., 2009\)](#page-11-15), STL-10 [\(Coates et al., 2011\)](#page-10-15), and ImageNet-100 [\(Chun-Hsiao Yeh, 2022\)](#page-10-16) datasets.

**346 347 348 349 350** Datasets. We take the labeled part for self-supervised pretraining without label leaking. We create a toy dataset CIFAR-10-toy by sampling 25% data from the original dataset for pretraining to mitigate the training overload, while for STL-10 we utilize its training data with no change. The downstream linear evaluation is made on the original test data in both CIFAR-10 and STL-10. We randomly sample an ImageNet-100 dataset from the ImageNet-1K dataset [\(Deng et al., 2009\)](#page-10-17).

**351 352 353 354 355 356 357 358** Baselines. We employ SimCLR [\(Chen et al.,](#page-10-1) [2020a\)](#page-10-1), MOCO [\(He et al., 2020\)](#page-11-5), and BYOL [\(Grill et al., 2020\)](#page-11-6) with ResNet-18 [\(He et al.,](#page-11-14) [2016\)](#page-11-14) as the backbone encoder for CIFAR-10 and STL-10, but with ResNet-50 for ImageNet-100. We compare our approach with InfoNCE loss to demonstrate its effectiveness of SINCE.

**359 360 361 362 363 364 365** Training Protocols. In our GOAL and SINCE, we utilize Euclidean distances in Equation [\(1\)](#page-2-0). We train our approach and baseline methods for 50 epochs with batch size 64, SGD optimizer with a momentum of 0.9, and weight decay of 10<sup>−</sup><sup>4</sup> . we conduct our experiments on an Intel(R) Xeon(R) Silver 4214 CPU@2.20GHz and a single Nvidia Quadro RTX 6000 with 24GB

<span id="page-6-2"></span><span id="page-6-0"></span>

Figure 2: Comparison on gradient feature weights from InfoNCE as  $p(x^{-})$ , and our GOAL as  $\alpha$ .

**366 367 368 369 370 371** memory. We apply CVXOPT [\(Vandenberghe, 2010\)](#page-13-15) to solve the LL problem in Equation [\(6\)](#page-4-1) for GOAL, which runs on the CPU. We implement our algorithm and baseline methods based on the work of [\(Peng et al., 2022\)](#page-12-3). Following the small-scale benchmark [\(Chen et al., 2020a;](#page-10-1) [Yeh et al.,](#page-14-10) [2021;](#page-14-10) [Peng et al., 2022\)](#page-12-3), we set both temperatures  $\tau$ ,  $\tau'$  to 0.07. We use a cosine-annealed learning rate of 0.5 for InfoNCE. The hyperparameter C in Equation [\(6\)](#page-4-1) is set to 0.15 for CIFAR-10 and 0.17 for STL-10 with slightly fine-tuning. For SINCE, we set  $\gamma = 0.1$  in all the experiments.

**372 373 374 375 376** Evaluation Protocols. Following the same setting as in [\(Peng et al., 2022\)](#page-12-3) we train a linear classifier for each method. Specifically, after self-supervised pretraining, we freeze the network except for the last fully connected layer. We train the last-layer classifier in a supervised way using the full dataset. The linear classifier is trained for 50 epochs with a learning rate of 10.0, a batch size of 512, and a momentum of 0.9 in SGD for all experiments. We report the best performance of each method.

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Results. We summarize our results from three aspects as follows:

<span id="page-7-0"></span>

Figure 3: On ShapeNet-Part using CP-Net: (a) L2-CD *vs.* point removal ratio (smaller is better); (b) An illustration of matched point pairs preserved with  $\gamma = 0.9$  for an airplance point cloud.

- *Sample Weight Comparison:* We illustrate a comparison of sample weights for gradients in InfoNCE and our GOAL for the same 127 triplets with the same  $x, x^+$  in Figure [2.](#page-6-0) The feature extraction network is pretrained with 60 samples in each mini-batch on STL-10. As we see, the extremely high values of  $p(x^{-})$  and  $\alpha$  co-occur quite frequently. For instance, the peak values around the 63rd triplet are 0.14 and 0.15 in InfoNCE and GOAL, respectively. Such observations are widely made when comparing the weights from both approaches. Therefore, the co-occurrences of large values in  $p(x^{-})$  and  $\alpha$  indicate that the triplets that decide the boundaries of SVMs are almost those that contribute most to the gradient update in contrastive learning. In other words, we observe that *InfoNCE can produce good estimators for the solutions of OC-SVMs in SGD iterations.*
- *InfoNCE* vs. *GOAL* vs. *SINCE:* Table [2](#page-6-1) lists our comparison results on CIFAR-10 and STL-10, where "-" indicates no results using all triples due to the hardware limit and running time. Although a smaller number of triplets would reduce the top-1 accuracy in the linear probe, our GOAL can significantly outperform both InfoNCE and SINCE in such cases. Using only 100 triplets per iteration, our GOAL can achieve performance that is close to both InfoNCE and SINCE with the full set of triplets. Besides, the performance of GOAL seems to be boosted more significantly than the other two with increasing number of triplets, which may benefit more for few-shot learning.
- *InfoNCE* vs. *SINCE for Self-Supervised Learning:* Table [3](#page-6-2) shows the performance improvements achieved by our SINCE method with various network backbones for self-supervised learning on several benchmark datasets. In our experiments, we did not observe a significant difference in running time between the methods, as the number of images was relatively small.

#### 5.2 3D POINT CLOUD COMPLETION

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**416 417 418 419 420** We demonstrate the effectiveness and efficiency of our SINCE loss by comparing with the recently proposed InfoCD [Lin et al.](#page-12-13) [\(2023\)](#page-12-13), which achieves the state-of-the-art for point cloud completion. To apply Equation [\(11\)](#page-5-1) to the formulation of InfoCD, without loss of generality, letting  $y_{ik}$ ,  $y_{ik'}$  be two points in the ground-truth point cloud and  $x_i = [x_{ij}]$  be the completed point cloud returned by some network with parameters  $\omega$ , we can define f in Equation [\(11\)](#page-5-1) as follows:

$$
f_{\tau,\tau'}(x_i, y_{ik}, y_{ik'}; \omega) = \frac{1}{\tau'} \min_j \|x_{ij} - y_{ik}\| - \frac{1}{\tau} \min_j \|x_{ij} - y_{ik'}\|.
$$
 (12)

**424 425 426** That is, for each ground-truth point, we search for the nearest neighbor in the point cloud returned by the completion network, and use the distance difference of an arbitrary pair as function  $f$ .

**427 428 429 430 431** Datasets & Backbone Networks. We conduct our experiments on the five benchmark datasets: PCN [\(Yuan et al., 2018\)](#page-14-3), MVP [\(Pan et al., 2021\)](#page-12-16), ShapeNet-55/34 [\(Yu et al., 2021\)](#page-14-7), ShapeNet-Part [\(Yi](#page-14-11) [et al., 2016\)](#page-14-11), and KITTI [\(Geiger et al., 2012\)](#page-11-16). We compare our method using **thirteen** different existing backbone networks: FoldingNet [\(Yang et al., 2018\)](#page-14-4), PMP-Net [\(Wen et al., 2021\)](#page-13-16), PoinTr [\(Yu](#page-14-7) [et al., 2021\)](#page-14-7), SnowflakeNet [\(Xiang et al., 2021\)](#page-14-6), CP-Net [\(Lin et al., 2022\)](#page-12-17), PointAttN [\(Wang et al.,](#page-13-14) [2022\)](#page-13-14), SeedFormer [\(Zhou et al., 2022\)](#page-14-8), PCN [\(Yuan et al., 2018\)](#page-14-3), PFNet [\(Huang et al., 2020\)](#page-11-17), TopNet

<span id="page-8-3"></span>



[\(Tchapmi et al., 2019\)](#page-13-17), MSN [\(Liu et al., 2020\)](#page-12-18), Cascaded [\(Wang et al., 2020\)](#page-13-18), and VRC [\(Pan et al.,](#page-12-16) [2021\)](#page-12-16), where we replace the CD loss with our SINCE wherever it occurs.

**Training & Evaluation Protocols.** We modify the public code<sup>[1](#page-8-0)</sup> by replacing the InfoCD loss with our SINCE loss. For fair comparison, we strictly follow the experimental settings in InfoCD [\(Lin et al.,](#page-12-13) [2023\)](#page-12-13), including the same hyperparameters such as learning rate and its scheduler, regularization parameter, number of epochs, random seed, and batch size and order. We run all the comparisons on a server with 10 NVIDIA RTX 2080Ti 11G GPUs. Following the literature, we evaluate the best performance of all the methods using vanilla CD (lower is better). We also use F1-Score@1% (higher is better) to evaluate the performance on ShapeNet-55/34. For KITTI, we utilize the metrics of Fidelity and Maximum Mean Discrepancy (MMD) for each method (lower is better for both metrics).

**448 449 450 451 452 453 454 455 456 457 458 459 460** Results. We first show our performance comparison on the ShapeNet-Part [\(Yi et al., 2016\)](#page-14-11) dataset using CP-Net [Lin et al.](#page-12-17) [\(2022\)](#page-12-17) as the backbone network. We illustrate our results in Figure [3.](#page-7-0) As we see in (a), it is clear that thresholding can significantly improve the performance of InfoCD that is equivalent to our SINCE with  $\gamma = 0$ , in all the tested cases. In (b), we visualize the top 10% pairs of matched points between a completed point cloud (left) and its ground truth (right) in terms of Euclidean distance, which. These points can already capture well the global structures of the point clouds, which may lead to a better regularizer in training. Here, we set  $\gamma = 0.9$  in all point cloud experiments without further tuning.

<span id="page-8-1"></span>

Figure 4: Training loss comparison on ShapeNet-Part using CP-Net.

**461 462 463 464** Figure [4](#page-8-1) illustrates the training loss curves of InfoCD and our SINCE with  $\gamma = 0.9$ , where we have normalized the binary masks for both for fair comparison. As we see, SINCE converges significantly faster than InfoCD with much lower losses, leading to better performance. As for running time, InfoCD takes  $454.0 \pm 7.5$  seconds per epoch, while SINCE takes  $480.0 \pm 4.9$  seconds per epoch.

**465 466 467 468 469** We also summarize detailed comparison results in Table [4,](#page-8-2) Table [5,](#page-8-3) Table 4: Average per-point L1-Table [6,](#page-9-0) Table [7,](#page-9-1) and Table [8,](#page-9-2) where SINCE outperforms InfoCD  $CD \times 1000$  on PCN. in all the cases, leading to new state-of-the-art results. Note that for KITTI, we follow [\(Xie et al., 2020\)](#page-14-12) to finetune the models on ShapeNetCars [\(Yuan et al., 2018\)](#page-14-3) and evaluate them on KITTI.

<span id="page-8-2"></span>

**473 474** In this paper, we aim to interpret deep contrastive learning from a geometric perspective by optimizing gradients in backpropagation.

**475 476 477 478 479 480 481** By drawing connections with OC-SVMs, we propose a new gradient-optimized contrastive learning (GOAL) approach based on bilevel optimization. In this approach, optimal gradients are learned through OC-SVMs as the lower-level problem, while the upper-level problem updates the network weights using SGD based on these optimal gradients. We also reveal a strong connection between contrastive learning and kernel methods with multiple NTKs. Furthermore, we introduce a new SINCE loss to address the computational challenges of GOAL for large-scale learning. We demonstrate the superior performance of our approach in the tasks of image classification and point cloud completion.

**482 483 484** Limitations. Thresholding in SINCE may introduce additional computational burdens in learning, and GOAL has not yet reached its full potential in real-world applications such as few-shot learning. We will investigate both aspects in future work.

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6 CONCLUSION

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<span id="page-8-0"></span><sup>1</sup><https://github.com/Zhang-VISLab/NeurIPS2023-InfoCD>

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	Table 6: Completion results on MVP in terms of L2-CD $\times 10^4$ () and EMD $\times 10^2$ ().										
	airplane Methods	$\emph{cal}$	$ch_{\rm 21}$ <b>Car</b>	$q u_{\rm IP}$ sofa	tabel	watercraft beq	$b_{\mathrm{en}_{\mathrm{C}\!,f}}$	$b_{\rm OoKsheff}$ $\mathfrak{b}_\mathfrak{u_S}$	$\mathit{Suit}_{\mathit{a}_T}$	$\label{eq:1} \textit{m}\textit{ot}_{\textit{Orbi}}{}_{\textit{Ke}}$ pistol	skateboard Avg.
CD	<b>PCN</b> InfoCD+PCN <b>SINCE+PCN</b> TopNet InfoCD+TopNet SINCE+TopNet MSN InfoCD+MSN <b>SINCE+MSN</b> Cascaded InfoCD+Cascaded 2.43 8.05 5.73 8.77 10.47 8.24 9.18 6.41 14.37 6.02 10.45 4.70 1.45 4.23 4.16 2.99 SINCE+Cascaded 2.32 7.94 5.62 8.64 10.35 8.16 9.07 6.28 14.25 5.90 10.42 4.58 1.32 4.10 4.04 2.87 VRC InfoCD+VRC <b>SINCE+VRC</b>		2.03 7.88 5.41 7.31	4.50 8.83 6.41 13.01 21.33 9.90 12.86 9.46 20.00 10.26 14.63 4.94 1.73 6.17 5.84 5.76 9.78 3.95 8.82 6.38 12.03 17.43 9.63 12.41 8.69 18.92 8.75 13.40 5.02 1.84 6.06 5.81 4.37 3.76 8.65 6.19 11.84 17.24 9.45 12.22 8.52 18.73 8.56 13.22 4.84 1.67 5.87 5.68 4.15 9.23 4.12 9.84 7.44 13.26 18.64 10.77 12.95 8.98 19.99 9.21 16.06 5.47 2.36 7.06 7.04 4.68 10.30 3.98 9.81 7.42 13.24 17.87 10.52 12.45 8.93 19.69 8.52 14.62 5.42 2.35 7.05 6.52 4.21 10.01 3.74 9.57 7.18 13.02 17.61 10.27 12.23 8.68 19.44 8.32 14.39 5.18 2.14 6.86 6.34 3.99 9.78 2.73 8.92 6.50 10.75 13.37 9.26 10.17 7.70 17.27 6.64 12.10 5.21 1.37 4.59 4.62 3.38 7.28 8.51 6.03 10.18 12.91 8.87 9.72 7.24 16.82 6.21 11.67 4.79 0.91 4.15 4.17 2.97 6.98 8.24 5.78 9.92 12.60 8.55 9.40 7.01 16.43 5.92 11.14 4.21 0.81 3.86 3.88 2.68 2.54 8.62 5.93 8.76 11.22 8.46 9.20 6.61 14.63 6.09 10.17 4.95 1.55 4.34 4.23 3.19 2.20 7.92 5.60 7.49 8.15 7.45 7.52 5.20 11.90 4.88 7.39 4.53 1.15 3.90 3.44 3.22 7.22 7.92 1.94 7.43 5.15 7.03 7.62 7.01 7.03 4.75 11.41 4.34 6.87 4.02 0.91 4.41 2.96 2.78 5.62							9.41 7.99 7.56 7.28 7.25 7.12 7.01 6.09 7.30 5.01 11.67 4.65 7.14 4.30 0.97 4.68 3.19 3.04 5.87
<b>EMD</b>	<b>PCN</b> InfoCD+PCN <b>SINCE+PCN</b> TopNet InfoCD+TopNet <b>SINCE+TopNet</b> MSN InfoCD+MSN <b>SINCE+MSN</b> Cascaded InfoCD+Cascaded 2.87 6.23 5.39 5.06 7.10 5.45 4.57 4.79 6.42 SINCE+Cascaded 2.52 6.05 5.17 5.01 7.02 5.32 4.41 4.63 6.21 3.31 5.02 5.47 3.42 4.10 4.11 2.75 4.85 VRC InfoCD+VRC <b>SINCE+VRC</b>		2.75 4.02 3.47 4.44 6.28 2.18 3.51 2.97 3.96 5.77 1.95 3.28 2.73 3.72 5.53 3.03 6.82 5.44 5.16 7.55	4.70 7.99 5.75 6.90 11.99 5.32 6.60 5.40 9.84 3.75 5.59 3.97 5.23 10.11 4.42 5.45 4.67 7.29 4.21 5.55 3.53 6.12 4.02 4.70 3.84 5.17 3.22 5.03 3.43 4.72 9.54 3.88 4.91 4.12 6.75 4.89 6.30 4.07 7.01 10.75 6.47 7.50 4.68 8.09 4.47 6.02 3.81 6.82 10.21 6.05 4.02 5.66 3.43 6.44 9.82 5.67 6.76 4.01 7.51 5.48 5.65 2.95 3.68 4.74 5.45 2.77 3.21 3.03 7.57 6.14 5.49 6.15 5.80 4.65 4.97 6.58 2.68 7.26 5.83 5.15 5.82 5.49 4.36 4.68 6.22 3.13 4.97 6.26 2.77 4.13 4.15 2.89 4.97 2.47 7.07 5.64 4.95 5.63 5.30 4.17 4.47 5.96 3.02 4.76 6.05 2.55 3.91 4.01 2.78 4.78		7.12 4.37 7.87 3.74 4.46 3.82 5.27 3.92 3.24 4.75 5.57 4.73 4.88 6.85	4.85 5.87	6.27 6.80 3.50 4.21 4.26 6.02 3.49 3.34 4.28 2.92 2.07 3.30 3.62 2.21 2.86 3.79 2.41 1.50 2.81 3.09 2.64 3.02 3.68 3.02 4.51 2.62 3.54 2.18 1.27 2.57 2.85 2.41 3.51 5.71 5.81 5.30 4.30 4.42 3.44 3.49 5.15 5.72 3.58 4.19 4.27 2.91 3.45 5.28 6.59 3.08 4.45 4.56 3.20	6.02 3.31 4.06 4.11 5.82 3.15		7.87 5.24 10.56 4.93 4.86 5.59 6.80 $3.65$ 5.00 3.02 5.57 4.39 4.16 3.29 4.63 6.18 5.72 5.35 3.94 3.38 3.15 5.18 5.01 5.27
	Table 7: Results on ShapeNet-34 using L2-CD $\times$ 1000 ( $\downarrow$ ) and F1 score ( $\uparrow$ ).										
	Methods	$CD-S$		34 seen categories CD-M CD-H Avg.		F1	$CD-S$		21 unseen categories CD-M CD-H Avg.		F1
	FoldingNet $InfoCD + FoldingNet$ <b>SINCE + FoldingNet</b> PoinTr $InfoCD + PointTr$ $SINCE + PointTr$		1.86 1.81 1.54 1.60 1.47 1.54	3.38 3.10 3.02	2.35 2.08 2.01	0.139 0.177 0.183	2.76 2.42 2.36	2.74 2.49 2.43	5.36 5.01 4.99	3.62 3.31 3.26	0.095 0.157 0.160
			1.05 0.76 0.47 0.69 0.41 0.65	1.88 1.35 1.28	1.23 0.84 0.78	0.421 0.529 0.534	1.04 0.61 0.61	1.67 1.06 1.02	3.44 2.55 2.51	2.05 1.41 1.37	0.384 0.493 0.496
	SeedFormer $InfoCD + SeedFormer$ <b>SINCE + SeedFormer</b>		0.48 0.70 0.43 0.63 0.41 0.62	1.30 1.21 1.20	0.83 0.75 0.74	0.452 0.581 0.583	0.61 0.54 0.52	1.08 1.01 1.02	2.37 2.18 2.12	1.35 1.24 1.21	0.402 0.449 0.452
	Table 8: Results on ShapeNet-55 using L2-CD $\times$ 1000 ( $\downarrow$ ) and F1 score ( $\uparrow$ ).										
	Methods		Table	Chair Plane	Car	Sofa	$CD-S$	CD-M CD-H Avg.			F1
	FoldingNet $InfoCD + FoldingNet$ <b>SINCE + FoldingNet</b>		2.81 2.53 2.14 2.37 2.06 2.28	1.43 1.03 1.01	1.98 1.55 1.43	2.48 2.04 2.02	2.67 2.17 2.14	2.66 2.50 2.45	4.05 3.46 3.38	3.12 2.71 2.65	0.082 0.137 0.141
	PoinTr $InfoCD + PointTr$ SINCE + PoinTr		0.81 0.95 0.83 0.69 0.62 0.78	0.44 0.33 0.32	0.91 0.80 0.74	0.79 0.67 0.62	0.58 0.47 0.40	0.88 0.73 0.67	1.79 1.50 1.43	1.09 0.90 0.83	0.464 0.524 0.529

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<span id="page-9-2"></span><span id="page-9-1"></span> $\text{SINCE} + \text{SeedFormer} \parallel 0.62 \quad 0.71 \quad 0.30 \quad 0.75 \quad 0.63 \mid 0.42 \quad 0.68 \quad 1.36 \quad 0.82 \mid 0.493$ 



<span id="page-10-17"></span><span id="page-10-16"></span><span id="page-10-15"></span><span id="page-10-14"></span><span id="page-10-13"></span><span id="page-10-12"></span><span id="page-10-11"></span><span id="page-10-10"></span><span id="page-10-9"></span><span id="page-10-8"></span><span id="page-10-7"></span><span id="page-10-6"></span><span id="page-10-5"></span><span id="page-10-4"></span><span id="page-10-3"></span><span id="page-10-2"></span><span id="page-10-1"></span><span id="page-10-0"></span>

<span id="page-11-1"></span>**621 622 623**

<span id="page-11-8"></span>**634 635 636**

<span id="page-11-16"></span>

- <span id="page-11-6"></span>**598 599 600 601** Jean-Bastien Grill, Florian Strub, Florent Altché, Corentin Tallec, Pierre Richemond, Elena Buchatskaya, Carl Doersch, Bernardo Avila Pires, Zhaohan Guo, Mohammad Gheshlaghi Azar, et al. Bootstrap your own latent-a new approach to self-supervised learning. *Advances in neural information processing systems*, 33:21271–21284, 2020.
- <span id="page-11-0"></span>**602 603 604** Raia Hadsell, Sumit Chopra, and Yann LeCun. Dimensionality reduction by learning an invariant mapping. In *2006 IEEE Computer Society Conference on Computer Vision and Pattern Recognition (CVPR'06)*, volume 2, pp. 1735–1742. IEEE, 2006.
- <span id="page-11-14"></span>**605 606 607 608** Kaiming He, Xiangyu Zhang, Shaoqing Ren, and Jian Sun. Deep residual learning for image recognition. In *Proceedings of the IEEE conference on computer vision and pattern recognition*, pp. 770–778, 2016.
- <span id="page-11-5"></span>**609 610 611** Kaiming He, Haoqi Fan, Yuxin Wu, Saining Xie, and Ross Girshick. Momentum contrast for unsupervised visual representation learning. In *Proceedings of the IEEE/CVF conference on computer vision and pattern recognition*, pp. 9729–9738, 2020.
- <span id="page-11-2"></span>**612 613 614** R Devon Hjelm, Alex Fedorov, Samuel Lavoie-Marchildon, Karan Grewal, Phil Bachman, Adam Trischler, and Yoshua Bengio. Learning deep representations by mutual information estimation and maximization. *arXiv preprint arXiv:1808.06670*, 2018.
- <span id="page-11-12"></span>**615 616 617 618** Qianjiang Hu, Xiao Wang, Wei Hu, and Guo-Jun Qi. Adco: Adversarial contrast for efficient learning of unsupervised representations from self-trained negative adversaries. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pp. 1074–1083, 2021.
- <span id="page-11-17"></span>**619 620** Zitian Huang, Yikuan Yu, Jiawen Xu, Feng Ni, and Xinyi Le. Pf-net: Point fractal network for 3d point cloud completion. In *CVPR*, 2020.
	- Arthur Jacot, Franck Gabriel, and Clément Hongler. Neural tangent kernel: Convergence and generalization in neural networks. *Advances in neural information processing systems*, 31, 2018.
- <span id="page-11-3"></span>**624 625** Ashish Jaiswal, Ashwin Ramesh Babu, Mohammad Zaki Zadeh, Debapriya Banerjee, and Fillia Makedon. A survey on contrastive self-supervised learning. *Technologies*, 9(1):2, 2020.
- <span id="page-11-11"></span>**626 627 628 629** Yannis Kalantidis, Mert Bulent Sariyildiz, Noe Pion, Philippe Weinzaepfel, and Diane Larlus. Hard negative mixing for contrastive learning. *Advances in Neural Information Processing Systems*, 33: 21798–21809, 2020.
- <span id="page-11-9"></span>**630 631** Sungnyun Kim, Gihun Lee, Sangmin Bae, and Se-Young Yun. Mixco: Mix-up contrastive learning for visual representation. *arXiv preprint arXiv:2010.06300*, 2020.
- <span id="page-11-15"></span>**632 633** Alex Krizhevsky, Geoffrey Hinton, et al. Learning multiple layers of features from tiny images. 2009.
	- Kibok Lee, Yian Zhu, Kihyuk Sohn, Chun-Liang Li, Jinwoo Shin, and Honglak Lee. i-mix: A domain-agnostic strategy for contrastive representation learning. *arXiv preprint arXiv:2010.08887*, 2020.
- <span id="page-11-10"></span>**637 638 639 640** Chunyuan Li, Xiujun Li, Lei Zhang, Baolin Peng, Mingyuan Zhou, and Jianfeng Gao. Self-supervised pre-training with hard examples improves visual representations. *arXiv preprint arXiv:2012.13493*, 2020a.
	- Junnan Li, Pan Zhou, Caiming Xiong, and Steven CH Hoi. Prototypical contrastive learning of unsupervised representations. *arXiv preprint arXiv:2005.04966*, 2020b.
- <span id="page-11-13"></span><span id="page-11-4"></span>**643 644 645** Xiaoping Li, Yadi Wang, and Rubén Ruiz. A survey on sparse learning models for feature selection. *IEEE transactions on cybernetics*, 52(3):1642–1660, 2020c.
- <span id="page-11-7"></span>**646 647** Zhaowen Li, Yousong Zhu, Fan Yang, Wei Li, Chaoyang Zhao, Yingying Chen, Zhiyang Chen, Jiahao Xie, Liwei Wu, Rui Zhao, et al. Univip: A unified framework for self-supervised visual pre-training. *arXiv preprint arXiv:2203.06965*, 2022.

<span id="page-12-17"></span>

- <span id="page-12-13"></span>**652 653 654** Fangzhou Lin, Yun Yue, Ziming Zhang, Songlin Hou, Kazunori Yamada, Vijaya B Kolachalama, and Venkatesh Saligrama. InfoCD: A contrastive chamfer distance loss for point cloud completion. In *Thirty-seventh Conference on Neural Information Processing Systems*, 2023.
- <span id="page-12-18"></span>**655 656 657** Minghua Liu, Lu Sheng, Sheng Yang, Jing Shao, and Shi-Min Hu. Morphing and sampling network for dense point cloud completion. In *Proceedings of the AAAI conference on artificial intelligence*, volume 34, pp. 11596–11603, 2020.
- <span id="page-12-4"></span>**658 659 660 661** Shlok Mishra, Anshul Shah, Ankan Bansal, Abhyuday Jagannatha, Abhishek Sharma, David Jacobs, and Dilip Krishnan. Object-aware cropping for self-supervised learning. *arXiv preprint arXiv:2112.00319*, 2021.
- <span id="page-12-1"></span>**662 663 664** Ishan Misra and Laurens van der Maaten. Self-supervised learning of pretext-invariant representations. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pp. 6707–6717, 2020.
- <span id="page-12-15"></span>**665 666** Aaron van den Oord, Yazhe Li, and Oriol Vinyals. Representation learning with contrastive predictive coding. *arXiv preprint arXiv:1807.03748*, 2018.
- <span id="page-12-16"></span>**667 668 669** Liang Pan, Xinyi Chen, Zhongang Cai, Junzhe Zhang, Haiyu Zhao, Shuai Yi, and Ziwei Liu. Variational relational point completion network. In *CVPR*, 2021.
- <span id="page-12-3"></span>**670 671** Xiangyu Peng, Kai Wang, Zheng Zhu, and Yang You. Crafting better contrastive views for siamese representation learning. *arXiv preprint arXiv:2202.03278*, 2022.
- <span id="page-12-10"></span>**672 673 674** Marco AF Pimentel, David A Clifton, Lei Clifton, and Lionel Tarassenko. A review of novelty detection. *Signal processing*, 99:215–249, 2014.
- <span id="page-12-11"></span>**675 676 677** Gunnar Ratsch, Sebastian Mika, Bernhard Scholkopf, and K-R Muller. Constructing boosting algorithms from svms: An application to one-class classification. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 24(9):1184–1199, 2002.
	- Sucheng Ren, Huiyu Wang, Zhengqi Gao, Shengfeng He, Alan Yuille, Yuyin Zhou, and Cihang Xie. A simple data mixing prior for improving self-supervised learning. In *CVPR*, 2022.
- <span id="page-12-7"></span>**681 682** Joshua Robinson, Ching-Yao Chuang, Suvrit Sra, and Stefanie Jegelka. Contrastive learning with hard negative samples. *arXiv preprint arXiv:2010.04592*, 2020.
- <span id="page-12-8"></span>**683 684** Stephan R Sain. The nature of statistical learning theory, 1996.

<span id="page-12-6"></span>**678 679 680**

- <span id="page-12-0"></span>**685 686** Bernhard Schölkopf, Robert C Williamson, Alex Smola, John Shawe-Taylor, and John Platt. Support vector method for novelty detection. *Advances in neural information processing systems*, 12, 1999.
- <span id="page-12-9"></span>**687 688 689** Bernhard Schölkopf, John C Platt, John Shawe-Taylor, Alex J Smola, and Robert C Williamson. Estimating the support of a high-dimensional distribution. *Neural computation*, 13(7):1443–1471, 2001.
- <span id="page-12-14"></span>**691 692 693** Florian Schroff, Dmitry Kalenichenko, and James Philbin. Facenet: A unified embedding for face recognition and clustering. In *Proceedings of the IEEE conference on computer vision and pattern recognition*, pp. 815–823, 2015.
- <span id="page-12-2"></span>**694 695 696** Ramprasaath R Selvaraju, Karan Desai, Justin Johnson, and Nikhil Naik. Casting your model: Learning to localize improves self-supervised representations. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pp. 11058–11067, 2021.
- <span id="page-12-12"></span>**697 698 699** Anshul Shah, Suvrit Sra, Rama Chellappa, and Anoop Cherian. Max-margin contrastive learning. In *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 36, pp. 8220–8230, 2022.
- <span id="page-12-5"></span>**700 701** Zhiqiang Shen, Zechun Liu, Zhuang Liu, Marios Savvides, Trevor Darrell, and Eric Xing. Unmix: Rethinking image mixtures for unsupervised visual representation learning. *arXiv preprint arXiv:2003.05438*, 2020.

<span id="page-13-18"></span><span id="page-13-17"></span><span id="page-13-16"></span><span id="page-13-15"></span><span id="page-13-14"></span><span id="page-13-13"></span><span id="page-13-12"></span><span id="page-13-11"></span><span id="page-13-10"></span><span id="page-13-9"></span><span id="page-13-8"></span><span id="page-13-7"></span><span id="page-13-6"></span><span id="page-13-5"></span><span id="page-13-4"></span><span id="page-13-3"></span><span id="page-13-2"></span><span id="page-13-1"></span><span id="page-13-0"></span>**702 703 704 705 706 707 708 709 710 711 712 713 714 715 716 717 718 719 720 721 722 723 724 725 726 727 728 729 730 731 732 733 734 735 736 737 738 739 740 741 742 743 744 745 746 747 748 749 750 751 752 753 754 755** Kihyuk Sohn. Improved deep metric learning with multi-class n-pair loss objective. *Advances in neural information processing systems*, 29, 2016. Niranjan Subrahmanya and Yung C Shin. Sparse multiple kernel learning for signal processing applications. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 32(5):788–798, 2009. David Martinus Johannes Tax. One-class classification: Concept learning in the absence of counterexamples. 2002. David MJ Tax and Robert PW Duin. Support vector domain description. *Pattern recognition letters*, 20(11-13):1191–1199, 1999. David MJ Tax and Robert PW Duin. Support vector data description. *Machine learning*, 54(1):45–66, 2004. Lyne P. Tchapmi, Vineet Kosaraju, Hamid Rezatofighi, Ian Reid, and Silvio Savarese. Topnet: Structural point cloud decoder. In *CVPR*, 2019. Yonglong Tian, Dilip Krishnan, and Phillip Isola. Contrastive multiview coding. In *European conference on computer vision*, pp. 776–794. Springer, 2020a. Yonglong Tian, Chen Sun, Ben Poole, Dilip Krishnan, Cordelia Schmid, and Phillip Isola. What makes for good views for contrastive learning? *Advances in Neural Information Processing Systems*, 33:6827–6839, 2020b. Yuandong Tian. Understanding deep contrastive learning via coordinate-wise optimization. In *Advances in Neural Information Processing Systems*, 2022. Yuandong Tian, Lantao Yu, Xinlei Chen, and Surya Ganguli. Understanding self-supervised learning with dual deep networks. *arXiv preprint arXiv:2010.00578*, 2020c. Michael Tschannen, Josip Djolonga, Marvin Ritter, Aravindh Mahendran, Neil Houlsby, Sylvain Gelly, and Mario Lucic. Self-supervised learning of video-induced visual invariances. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pp. 13806–13815, 2020. Aaron Van den Oord, Yazhe Li, and Oriol Vinyals. Representation learning with contrastive predictive coding. *arXiv e-prints*, pp. arXiv–1807, 2018. Lieven Vandenberghe. The cvxopt linear and quadratic cone program solvers. *Online: http://cvxopt. org/documentation/coneprog. pdf*, 2010. Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N Gomez, Łukasz Kaiser, and Illia Polosukhin. Attention is all you need. *Advances in neural information processing systems*, 30, 2017. Vikas Verma, Thang Luong, Kenji Kawaguchi, Hieu Pham, and Quoc Le. Towards domain-agnostic contrastive learning. In *International Conference on Machine Learning*, pp. 10530–10541. PMLR, 2021. Feng Wang and Huaping Liu. Understanding the behaviour of contrastive loss. In *Proceedings of the IEEE/CVF conference on computer vision and pattern recognition*, pp. 2495–2504, 2021. Jun Wang, Ying Cui, Dongyan Guo, Junxia Li, Qingshan Liu, and Chunhua Shen. Pointattn: You only need attention for point cloud completion. *arXiv preprint arXiv:2203.08485*, 2022. Xiaogang Wang, Marcelo H Ang Jr, and Gim Hee Lee. Cascaded refinement network for point cloud completion. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pp. 790–799, 2020. Xin Wen, Peng Xiang, Zhizhong Han, Yan-Pei Cao, Pengfei Wan, Wen Zheng, and Yu-Shen Liu. Pmp-net: Point cloud completion by learning multi-step point moving paths. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pp. 7443–7452, 2021.

<span id="page-14-12"></span><span id="page-14-11"></span><span id="page-14-10"></span><span id="page-14-9"></span><span id="page-14-8"></span><span id="page-14-7"></span><span id="page-14-6"></span><span id="page-14-5"></span><span id="page-14-4"></span><span id="page-14-3"></span><span id="page-14-2"></span><span id="page-14-1"></span><span id="page-14-0"></span>