Positive Unlabeled Contrastive Learning

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Abstract

Self-supervised pretraining on unlabeled data followed by supervised finetuning on labeled data is a popular paradigm for learning from limited labeled examples. In this paper, we investigate and extend this paradigm to the classical positive unlabeled (PU) setting - the weakly supervised task of learning a binary classifier only using a few labeled positive examples and a set of unlabeled samples. We propose a novel PU learning objective positive unlabeled Noise Contrastive Estimation (puNCE) that leverages the available explicit (from labeled samples) and implicit (from unlabeled samples) supervision to learn useful representations from positive unlabeled input data. The underlying idea is to assign each training sample an individual weight; labeled positives are given unit weight; unlabeled samples are duplicated, one copy is labeled positive and the other as negative with weights $\pi$ and $(1 - \pi)$ where $\pi$ denotes the class prior. Extensive experiments across vision and natural language tasks reveal that puNCE consistently improves over existing unsupervised and supervised contrastive baselines under limited supervision.

1 Introduction

Learning from limited amount of labeled data is a long-standing challenge in modern machine learning. Owing to its recent widespread success in both computer vision and natural language processing tasks (Chen et al., 2020c; Grill et al., 2020; Radford et al., 2021; Gao et al., 2021; Dai and Le, 2015; Radford et al., 2018) self supervised pretraining followed by supervised finetuning has become the de-facto approach to learn from limited supervision.

These approaches typically leverage unlabeled data in a task agnostic manner during pretraining and use the available label information during finetuning (Hinton et al., 2006; Bengio et al., 2006; Mikolov et al., 2013; Kiros et al., 2015; Devlin et al., 2018; Zbontar et al., 2021; Asrani et al., 2020). In this context, contrastive learning has emerged as one of the most promising approach to learn useful representations from unlabeled data by encouraging them to be invariant to distortions.

This paper investigates and extends contrastive representation learning to the Positive Unlabeled (PU) Learning (Denis, 1998) setting - the weakly supervised task of learning a binary classifier in

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Figure 2: **Learning from Positive Unlabeled data.** No negative examples are labeled i.e. a classifier needs to be trained from an incomplete set of positive and a set of unlabeled samples such that it can discriminate between samples from positive and negative classes.

Absence of any explicitly labeled negative examples i.e. using an incomplete set of positive and a set of unlabeled samples. PU learning also implies learning under distribution shift since it involves generalization to unseen negative class (Garg et al., 2021). This setting arises naturally in several real-world applications where obtaining negative samples is either too resource-intensive or improbable. For example, consider personalized recommendation systems (Naumov et al., 2019) where the training data is typically extracted from user feedback. Since explicit user feedback (e.g. user ratings) is hard to obtain, most practical recommendation systems rely on implicit user feedback (e.g. browsing history) (Kelly and Teevan, 2003) which usually indicates user’s positive preference (e.g. if a user browses a product frequently or watched a movie then the user-item pair is labeled positive) (Chen et al., 2021). This setup has also been motivated by applications like gene and protein identification (Elkan and Noto, 2008), anomaly detection (Blanchard et al., 2010) and matrix completion (Hsieh et al., 2015).

While self-supervised contrastive losses e.g. InfoNCE (Gutmann and Hyvärinen, 2010) have gained remarkable success in unsupervised representation learning; recent works (He et al., 2020; Kolesnikov et al., 2019) have pointed out that purely self-supervised approaches often produce inferior visual representation compared to fully supervised approaches. To address this issue, researchers (Khosla et al., 2020; Assran et al., 2020; Graf et al., 2021) proposed supervised variants of contrastive loss (SCL) that, by leveraging available supervision, is able to obtain equally (or even more) discriminative representations as fully supervised cross entropy objective. Motivated by these observations, our **goal is to design a contrastive loss leveraging the available weak supervision in an efficient manner to learn rich representation** $g_B(x)$ **from Positive Unlabeled dataset, which is able to discriminate between positive and negative classes.**

To this end, we propose **puNCE (positive unlabeled Noise Contrastive Estimation)** - a novel contrastive training objective that extends the standard self supervised infoNCE (Gutmann and Hyvärinen, 2010; Chen et al., 2020b) loss to the positive unlabeled setting; by incorporating available biased supervision. Unlike recent supervised variants of infoNCE (Khosla et al., 2020; Assran et al., 2020; Zhong et al., 2021) which can only leverage explicit (strong) supervision (e.g. in form of labeled data), puNCE is also able to leverage implicit (weak) supervision from the unlabeled data. The main idea is to use the fact that unlabeled data is distributed as a mixture of positive and negative marginals where the mixture proportion is given by class prior $\pi$ (Elkan and Noto, 2008; Niu et al., 2016; Du Plessis et al., 2014; Elkan, 2001). puNCE treats each unlabeled sample as a positive example and a negative example with appropriate probabilities and further uses the available explicit label information (i.e. set of positive labeled samples) to pull together multiple positive samples in the embedding space (Khosla et al., 2020). Our experiments across PU and binary semi-supervised settings suggest that in settings with limited supervision puNCE can be particularly effective and often produce stronger representations than both infoNCE and its supervised variants (Khosla et al., 2020; Assran et al., 2020). Our experiments on standard PU learning benchmarks reveal that even with small amount of weak supervision, puNCE can dramatically improve the quality of the resulting embedding compared to unsupervised contrastive training using infoNCE. For example, on PU CIFAR10 with
ResNet-18 puNCE achieves over 3% improvement compared to infoNCE while using 20% labeled data, and over 2% improvement when using only 5% labeled data. We further show that the resulting PU Learning approach i.e. contrastive training the encoder using puNCE, followed by freezing the encoder and training a linear layer on top using standard cost-sensitive PU loss (Elkan and Noto, 2008; Du Plessis et al., 2014; Kiryo et al., 2017) results in significant improvement in generalization performance compared to current state-of-the-art (Figure 1, Table 2). For example, on PU CIFAR-10 benchmark with only 1k positive labeled samples (i.e. rest 49k training samples unlabeled), our contrastive approach improves over existing PU learning approaches by 8.9% with a ResNet-18.

Our contributions can be summarized as follows:

- We investigate the limitation of general self-supervised pretraining and finetuning approach on the weakly supervised PU learning task. We observe that self supervised contrastive losses are unable to leverage available supervision and produce inferior representations compared to fully supervised approaches. The gains from existing supervised contrastive losses are also limited when amount of explicitly labeled data is small (Table 1).
- We propose a novel contrastive training objective - puNCE (positive unlabeled Noise Contrastive Estimation), that extends contrastive loss to the positive unlabeled setting by incorporating the available biased supervision via appropriately re-weighting the samples.
- We perform experiments on three settings with limited supervision - (a) Positive Unlabeled Classification, (b) Binary semi-supervised (PNU) classification and (c) Contrastive few shot finetuning of pretrained language model. Across all the setting, puNCE consistently outperforms supervised and unsupervised contrastive losses and is especially powerful when available supervision is scarce. On PU classification task, contrastive pretraining with puNCE results in large improvement over current state-of-the-art PU learning algorithms (Table 2).

2 Problem Setup.

2.1 Positive Unlabeled Learning.

Let \( x \in \mathbb{R}^d, d \in \mathbb{N} \) and \( y \in \{\pm 1\} \) be the input and output random variables respectively and \( p(x, y) \) be the true underlying joint density of \( (x, y) \). PU dataset \( \mathcal{X}_{PU} \) is composed of two independent sets of data, sampled uniformly at random from \( p(x, y) \): an incomplete set \( \mathcal{X}_P \) of \( n_p \) data-points with positive class and a set \( \mathcal{X}_U \) of \( n_u \) unlabeled samples:

\[
\mathcal{X}_P = \{x_i^p\}_{i=1}^{n_p} \sim p(x|y = 1); \quad \mathcal{X}_U = \{x_i^u\}_{i=1}^{n_u} \sim p(x); \quad \mathcal{X}_{PU} = \mathcal{X}_P \cup \mathcal{X}_U \tag{1}
\]

Since information about \( y \) is unavailable for all samples, it is convenient to define an indicator random variable \( s \) such that: \( s = 1 \) if \( x \) is labeled and \( 0 \) otherwise. Now viewing \( x, y, s \) as random variables allows us to assume that there is some true underlying distribution \( p(x, y, s) \) over triplets \((x, y, s)\) however, for each sample only \((x, s)\) is recorded. The definition of PU dataset (1) immediately implies the following two results:

\[
P(y = +1|s = 1) = 1, \quad p(s = 1|y = -1) = 0 \tag{2}
\]

**Assumption 1 (Known Class Prior).** Throughout the paper, we assume that the class prior \( \pi = p(y = +1) \) is either known or can be efficiently estimated from \( \mathcal{X}_{PU} \) via mixture proportion estimation algorithm (Christoffel et al., 2016; Ramaswamy et al., 2016; Ivanov, 2020; Garg et al., 2021).

Note that, this is a standard assumption made in PU Learning literature and is at the heart of most classical cost sensitive PU Learning algorithms (Elkan and Noto, 2008; Kiryo et al., 2017; Du Plessis et al., 2014; Chen et al., 2020a; Niu et al., 2016).

The PU Learning task is thus to train a classifier \( f : \mathbb{R}^d \rightarrow \mathbb{R} \) using only PU observations \((x, s)\) and knowledge of \( \pi \), such that \( f(x) \) is a close approximation of \( p(y = +1|x) \). Where, \( f \) is parameterized in terms of a linear layer \( v \in \mathbb{R}^k \) and feature extractor \( g_B(x) \in \mathbb{R}^{k \times d} \) i.e.

\[
f_{v,B} = v^T g_B(x) : \mathbb{R}^d \rightarrow \mathbb{R}, \quad g_B(x) \in \mathbb{R}^{k \times d}, \quad v \in \mathbb{R}^k \tag{3}
\]
2.2 Contrastive Representation Learning.

The main idea of contrastive learning (Sohn, 2016; Wu et al., 2018) is to contrast semantically similar and dissimilar samples - encouraging the representations of similar pairs to be close and that of the dissimilar pairs to be more orthogonal.

In particular, at iteration $t$, given a randomly sampled batch $D_t = \{x_i \sim p(x)\}_{i=1}^b$ of $b$ data points, the corresponding multi-viewed batch consists of $2b$ data points $\tilde{D}_t = \{x_i\}_{i=1}^{2b}$ where $x_{2i-1}$ and $x_{2i}$ are two views of $x_i \in D_t$ obtained via stochastic augmentations (Chen et al., 2020d; Tian et al., 2020). Within the multi-viewed batch, consider an arbitrary augmented data point indexed by $i \in \mathbb{I} \equiv \{1, \ldots, 2b\}$ and let $a(i)$ be the index of the corresponding augmented sample originating from the same source sample. Denote the embedding of sample $x_i$ as $z_i = g_B(x_i)$, then the self supervised contrastive loss InfoNCE (Gutmann and Hyvärinen, 2010; Oord et al., 2018) is given as:

$$L_{\text{InfoNCE}} = \sum_{i \in \mathbb{I}} \ell^{(i)}_{\text{InfoNCE}} = \sum_{i \in \mathbb{I}} -\log \frac{\exp (z_i \cdot z_{a(i)}/\tau)}{\sum_{k \in \mathbb{I}\setminus\{i\}} \exp (z_i \cdot z_k/\tau)}$$

(4)

In this context, $x_i$ is commonly referred to as the anchor, $x_{a(i)}$ is called positive and the other $2(b-1)$ samples are considered negatives. Simply put, InfoNCE loss pulls the anchor and the positive in the embedding space while pushing away anchor from negatives.

Projection Layer. Rather than directly using the output of the encoder $g_B(x)$ to contrast samples, it is common practice (Chen et al., 2020b; Zbontar et al., 2021; Grill et al., 2020; Khosla et al., 2020; Assran et al., 2020) to feed the representation through a projection network $h_{\theta_{proj}}$ to obtain a lower dimensional representation before comparing the representations i.e. instead of using $z_i = g_B(x_i)$, in practice we consider $z_i = h_{\theta_{proj}}(g_B(x_i))$. The projector is only used during optimization and discarded during downstream transfer task.

Contrastive learning with supervision. Supervised Contrastive Learning (SCL) (Khosla et al., 2020; Zhong et al., 2021; Graf et al., 2021; Assran et al., 2020) is a supervised variant of infoNCE that considers multiple positive pairs from other samples belonging to the same class as anchor in addition to the augmented view. In fully supervised setting, SCL can be computed as:

$$L_{\text{SCL}} = \sum_{i \in \mathbb{I}} \ell^{(i)}_{\text{SCL}} = -\sum_{i \in \mathbb{I}} \frac{1}{|Q(i)|} \sum_{j \in Q(i)} \log \frac{\exp (z_i \cdot z_j/\tau)}{\sum_{k \in \mathbb{I}\setminus\{i\}} \exp (z_i \cdot z_k/\tau)}$$

(5)

where, $Q(i) = \{t \in \mathbb{I}\setminus\{i\} : y_t = y_i\}$ denote the set of all samples in the current batch that belong to the same class as the anchor.

3 Positive Unlabeled NCE

We propose puNCE (positive unlabeled InfoNCE) that extends the self supervised InfoNCE loss to the PU learning setting. The main idea of puNCE is to consider an unlabeled sample as positive with probability $\pi$ and negative with probability $(1 - \pi)$. This follows from Bayes rule since we can write the marginal density of the unlabeled data as:

$$p(x) = \pi p(x|y=1) + (1 - \pi)p(x|y=-1)$$

(6)

In particular, consider a labeled anchor $x_i \in \mathcal{X}_P$, the puNCE risk corresponding to $x_i$ is computed by pulling together normalized embeddings of all the available labeled samples in multi-viewed batch $D_t$ as opposed to InfoNCE which only considers $x_{a(i)}$ as positive. This holds, since all labeled samples are guaranteed to come from the same latent class as $x_i$ (2). Given multi-view batch $\hat{D}_t$, let $P \equiv \{k \in \mathbb{I} : s_k = 1\}$ denote the set of indices of all labeled samples and $U \equiv \{k \in \mathbb{I} : s_k = 0\}$ indexes the unlabeled samples i.e. $U \equiv \mathbb{I}\setminus\mathbb{P}$. Then, puNCE empirical risk $\ell_P$ for the labeled samples is given as:

$$\ell_P = \sum_{i \in \mathbb{P}} \ell^{(i)}_{\text{puNCE}} = -\sum_{i \in \mathbb{P}} \frac{1}{|P| - 1} \sum_{j \in \mathbb{P}\setminus\{i\}} \log \frac{\exp (z_i \cdot z_j/\tau)}{\sum_{k \in \mathbb{P}\setminus\{i\}} \exp (z_i \cdot z_k/\tau)}$$

(7)

On the other hand, unlabeled anchor $x_i \in \mathcal{X}_U$, is treated as positive example with probability $\pi = p(y=1|s=0)$ and as negative example with probability $(1 - \pi)$. When considered positive
This simply says that, in essence puNCE assigns each training example an individual weight. In
the first term of (8) denotes the loss incurred by the positive contribution of the unlabeled samples and
the second term corresponds to the negative counterpart. Combining (7), (8) the puNCE empirical
risk can be computed as:

$$L_{puNCE} = \frac{1}{|D_t|} \sum_{i \in I} \ell_{puNCE} = \frac{1}{2b} \left[ \sum_{i \in P} \ell_{puNCE} + \sum_{i \in U} \ell_{puNCE} \right] = \frac{1}{2b} [\ell_P + \ell_U]$$

The first term of (8) denotes the loss incurred by the positive contribution of the unlabeled samples and
the second term corresponds to the negative counterpart. Combining (7), (8) the puNCE empirical
risk can be computed as:

$$
\ell_U = \sum_{i \in U} \ell_{puNCE} = -\sum_{i \in U} \left\{ \frac{\pi}{|P| + 1} \sum_{j \in \{P,a(i)\}} \log \frac{\exp (z_i \cdot z_j / \tau)}{\sum_{k \in \{I\} \setminus \{i\}} \exp (z_i \cdot z_k / \tau)} + (1 - \pi) \log \frac{\exp (z_i \cdot z_{a(i)} / \tau)}{\sum_{k \in \{I\} \setminus \{i\}} \exp (z_i \cdot z_k / \tau)} \right\}
$$

This simply says that, in essence puNCE assigns each training example an individual weight. In
particular, all the labeled samples are given unit weight and the unlabeled samples are duplicated;
one copy is labeled positive with weight \(\pi\) and the other copy is labeled negative with weight \((1 - \pi)\).

**Extension to binary semi-supervised learning.** PU Learning is closely related to semi-supervised
learning. In semi-supervised learning labeled samples from both the classes along with unlabeled
samples are available i.e. it contains three independent sets of samples: positive labeled, negative
labeled and unlabeled samples (referred to as positive negative unlabeled (PNU) learning). A natural
question to ask is if the idea of using implicit weak supervision from the unlabeled samples can also
help in the general binary semi-supervised learning setting i.e. when the training data is limited but
unbiased. Let \(P\), \(N\) and \(U\) denote the set of labeled positive, labeled negative and unlabeled samples.
respectively and \( Q(i) = \{ t \in \mathbb{I} \setminus \{ i \} : y_t = y_i \} \) denote the set of all samples in the current batch that belong to the same class as the anchor and \( P(i) = \{ P, a(i) \} \), \( N(i) = \{ N, a(i) \} \), \( \mathbb{I}(i) = \mathbb{I} \setminus i \). Then the puNCE loss in the PNU setting takes the following form:

\[
L_{puNCE}^{PNU} = -\frac{1}{2b} \left[ \sum_{i \in \mathbb{P}, j \in \mathbb{N}} \frac{1}{Q(i)} \log \left( \frac{\exp \left( z_i \cdot z_j / \tau \right)}{\sum_{k \in \mathbb{N} \setminus \{ i \}} \exp \left( z_i \cdot z_k / \tau \right)} \right) + \sum_{i \in \mathbb{U}} \left( \frac{\pi}{P(i)} \log \left( \frac{\exp \left( z_i \cdot z_j / \tau \right)}{\sum_{k \in \mathbb{I} \setminus \{ i \}} \exp \left( z_i \cdot z_k / \tau \right)} \right) + \frac{1 - \pi}{|P(i)|} \log \left( \frac{1}{\sum_{k \in \mathbb{I} \setminus \{ i \}} \exp \left( z_i \cdot z_k / \tau \right)} \right) \right) \right] \tag{10}
\]

**Supervised and Unsupervised Setting.** It is straightforward to see that in the fully supervised setting puNCE reduces to SCL and in the unsupervised setting it is equivalent to infoNCE.

## 4 Related Work

### PU Learning

Owing to its importance in several real world problems (e.g. recommendation), developing specialized learning algorithms for PU setting have received renewed impetus in the machine learning community. Most of the recent research in this area can be broadly categorized into two major class of algorithms - based on how they handle unlabeled samples. At a high level, the first class of algorithms (Liu et al., 2002, 2003; Bekker and Davis, 2020; Luo et al., 2021; Chen et al., 2020d) tries to identify potential (with high confidence) negative, positive or both samples from the unlabeled pool of data; then perform traditional supervised learning together with the available labeled P data. The second set of algorithms (Elkan and Noto, 2008; Du Plessis et al., 2014; Kiryo et al., 2017) instead rely on finding appropriate weights for the positive and unlabeled samples and then performing standard cost sensitive training (Elkan, 2001). Our approach is closely related to the second set of methods as we treat each unlabeled sample as a convex combination of positive and negative samples and weight them accordingly.

### Contrastive Loss

Self-supervised learning has demonstrated superior performances over supervised methods on various benchmarks. Joint-embedding methods (Chen et al., 2020b; Grill et al., 2020; Zbontar et al., 2021; Caron et al., 2021) are one the most promising approach for self-supervised representation learning where the embeddings are trained to be invariant to distortions. To prevent trivial solutions, a popular method is to apply pulsive force between embeddings from different images, known as contrastive learning. Contrastive loss is shown to be useful in various domains, including natural language processing (Gao et al., 2021), multimodal learning (Radford et al., 2021). Contrastive loss can also benefit supervised learning (Khosla et al., 2020).

## 5 Experiments

In this section we state our experimental setup, present our empirical findings and discuss insights about how puNCE benefits learning from weak supervision. We compare puNCE with other popular contrastive losses including losses that can leverage available supervision. We also perform several ablations on puNCE and downstream PU classification. To ensure reproducibility, all the experiments are run with deterministic cuDNN back-end and repeated 5 times with different random seeds and the confidence intervals are noted.

### Datasets

We evaluate puNCE on several common PU Learning image and text classification benchmarks consistent with recent literature (Garg et al., 2021; Chen et al., 2020d; Kiryo et al., 2017). In particular, for vision benchmarks we consider the following binary versions of MNIST and CIFAR10. (i) **CIFAR10** (Vehicle / Animal): Animal images (bird, cat, deer, dog, frog, horse) are treated as negative and Vehicle images (airplane, automobile, ship, truck) are treated as positive. (ii) **MNIST** (Odd / Even): Separate the odd digits (1, 3, 5, 7, 9) from the even digits (0, 2, 4, 6, 8). We perform text classification, on SST2 sentiment dataset (Socher et al., 2013) where the goal is to classify positive and negative reviews. We simulate PU settings from the binary data as follows: from the true positive samples in the training data we sample \( n_P \) samples uniformly at random and label them positive while we mark the remaining training samples as unlabeled. For example, PU
with parameters (abbreviated SupCon) (Khosla et al., 2020; Assran et al., 2020). Following the setup of prior work on other approaches like vPU (Chen et al., 2020a), SelfPU (Chen et al., 2020d).

Our baselines include: PN (Naumov et al., 2019; Elkan and Noto, 2008) - considering all the unlabeled samples as negative and performing binary classification using standard loss (e.g. CE), cost sensitive learning with limited supervision (Chen et al., 2020c; Assran et al., 2020) we adopt SCL to the PU setting in the following manner: At iteration $t$, given an augmented batch $\hat{D}_t$, on the labeled samples the contrastive loss is computed using SupCon loss while on the unlabeled samples in the augmented batch we compute the loss using standard infoNCE objective.

$$L_{SCL}^{PU} = -\frac{1}{2b} \left[ \sum_{i \in \mathcal{P}} \frac{1}{|\mathcal{P}| - 1} \sum_{j \in \mathcal{P} \setminus \{i\}} \log \frac{\exp \left( \frac{z_i \cdot z_j}{\tau} \right)}{\sum_{k \in \mathcal{I}(t)} \exp \left( \frac{z_i \cdot z_k}{\tau} \right) + \sum_{k \in \mathcal{U}} f^{\mu}(\mathbf{z}_k)} \right]$$

### PU Learning Baselines

We compare the downstream PU classification performance of puNCE against many related PU Learning algorithms at different levels of supervision ($n_p = 1k, 3k, 10k$). Our baselines include: PN (Naumov et al., 2019; Elkan and Noto, 2008) - considering all the unlabeled samples as negative and performing binary classification using standard loss (e.g. CE), cost sensitive approaches like PVU (Elkan, 2001), upU (Du Plessis et al., 2014), nnPU (Kiryo et al., 2017), and other approaches like vPU (Chen et al., 2020a), SelfPU (Chen et al., 2020d).

### 5.1 Contrastive Positive Unlabeled Learning

In this section we evaluate the performance of the proposed puNCE loss on downstream PU classification problem. As discussed before, our contrastive PU learning approach involves training...
encoder $g_B(\cdot)$ using contrastive loss, followed by training a linear layer on top using standard positive unlabeled loss (e.g. nnPU (Kiryo et al., 2017)). For non contrastive classic PU baselines both the encoder ($B$) and the linear layer ($v$) are jointly trained using the PU loss. Contrastive training is done using LARS optimizer (You et al., 2019), temperature set to 0.5. We used batch size 2048 for CIFAR10 experiments and 1024 for MNIST experiments. We used an initial learning rate of 0.01 with cosine annealing learning rate for 300 epochs on PU CIFAR10 and 200 epochs for PU MNIST.

**Fine Tune vs Linear Probe.**

After initializing the learner with the trained encoder parameters, we explore two popular transfer methods to transfer to the downstream Positive Unlabeled task - fine tuning (updating both $B$ and $v$), linear probing (updating $v$ while freezing the lower layers) using the PU training dataset.

In standard ID setting i.e. when finetuning and test data come from the same distribution, it is well known that finetuning results in better ID generalization performance than linear probing (He et al., 2020; Zhai et al., 2019). However, in the PU setting we observe that finetuning consistently under-performs linear probing. In fact, as the bias increases (i.e. for lower $n_P$), the gap becomes more significant (see Table 3). One possible way to explain this phenomenon is through feature distortion theorem (Kumar et al., 2022). Suppose, there exists an optimal $B_o$ and $v_o$ and suppose our representation quality is good such that our encoder parameters $B_o$ satisfies $\min_B ||B_o - U B_o|| \leq \epsilon$ over all rotation matrices $U \in \mathbb{R}^{k \times k}$ and $v$ is initialized randomly to $v_0$. Then we know that $v_0 v_0^T - B_0 B_0^T = v_f v_f^T - B_f B_f^T$ where $v_f, B_f$ denote the parameters post finetuning (Du et al., 2020). This suggest that since in PU setting the training data is biased, finetuning on it can result in significant feature distortion resulting in large error on data with large distribution shift. This is consistent with our observation, since as we reduce number of labeled samples i.e. we increase the bias and for small $n_P$, the distribution shift is large resulting in larger drop in performance.

**Fine tune loss.** We experiment with different cost sensitive PU losses to during linear probing. We notice that they perform similarly with nnPU performing marginally better (Figure 4b).

**Stability of PU Learning.** The classical cost-sensitive PU learning algorithms are notoriously unstable and tend to overfit the data. These methods need careful hyper parameter tuning and early stopping. Interestingly, we observe that when the model is initialized with parameters obtained from puNCE pretraining, the PU training becomes much more stable (Figure 4c) suggesting that puNCE pretraining is also inherently robust.

**Effect of Number of Labeled Samples.** To understand the benefit of increased supervision, we perform several experiments across different values of $n_P$. Our experiments (see Table 1 and Figure 4a) reveal that supervised approaches (SCL, puNCE) are consistently able to learn more powerful representation when supervision is available. The downstream performance of these approaches

### Table 3: Comparing different transfer methods on training ResNet18 on PU CIFAR 10 - Linear probing performs consistently better than fine-tuning.

| $n_P$ | LP | FT |
|------|--|--|
| 1k   | 97.59 ± 0.17 | 92.96 ± 0.19 (↓ 4.36) |
| 3k   | 97.87 ± 0.04  | 95.83 ± 0.15 (↓ 2.04) |
| 10k  | 97.95 ± 0.02  | 97.41 ± 0.09 (↓ 0.54) |
Table 4: Linear Evaluation of different contrastive losses under Semi-Supervised (PNU) setting - with 1%, 5% and 10% labeled training data. puNCE proves to be superior than infoNCE (Chen et al., 2020b) and semi-supervised SCL (Assran et al., 2020) especially in low supervision regime.

Table 5: Few shot learning test results for N=10,100,1000. puNCE achieves significant gains over previous SCL based approach (Gunel et al., 2020) and standard CE baseline.

improve with increased supervision. The results also suggest that puNCE can be particularly powerful when available supervision is small i.e. for smaller values of n_P and results in significant gains over both unsupervised and supervised contrastive approaches further emphasizing the importance of leveraging implicit supervision from unlabeled samples.

5.2 Contrastive Positive Negative Unlabeled learning

We further evaluate puNCE in the binary semi-supervised setting. Training data contains samples from both the classes and a set of unlabeled samples. In particular, we perform experiments when only 1%, 5% and 10% of the data is available (Figure 4). It is important to note that, unlike PU Learning settings, here we perform downstream tuning only over the labeled data. We see similar trends as in PU Learning experiments - puNCE improves over infoNCE by 4.13% and over SCL by 1.39% when using only 1% data on PU CIFAR10. With only 10% data puNCE is able to achieve similar accuracy as a fully supervised baseline (with cross entropy) improving over semi-supervised adaptation of SCL (Assran et al., 2020) by 0.18%.

5.3 PNU few shot learning.

Additionally, we also apply puNCE for pretrained language model finetuning (FT). In the few-shot learning setting, the goal is to FT a pretrained model on a downstream task using only a few labeled samples. FT with cross-entropy(CE) loss with only a few examples is highly unstable and can give very different results across different runs (Dodge et al., 2020; Zhang and Sabuncu, 2018). To mitigate this, recent works (Gunel et al., 2020; Chen et al., 2022) use contrastive loss in conjunction with CE i.e. $L = \lambda L_{CE} + (1 - \lambda) L_{CL}$. We closely follow the same setup, however, in addition to N labeled samples (N=10, 100, 1000), we also assume access to 500 unlabeled samples during finetuning. Note that for unlabeled samples, the CE term has no contribution. In this setting, we adopt a pretrained RoBERTa model for downstream SST2 binary sentiment classification and observe that puNCE results in 2.97% (N=10), 0.93%(N=100) and 0.47% improvement over the previous state-of-the-art that uses SCL.

6 Conclusions

In this work, we investigated the limitation of a general self-supervised pretraining and finetuning approach on weakly-supervised tasks. We proposed a novel contrastive training objective puNCE (positive unlabeled Noise Contrastive Estimation), that extends contrastive loss to the positive unlabeled setting by incorporating available biased supervision. Our method achieved state-of-the-art performances on several PU learning and semi-supervised settings across vision and natural language processing and is particularly powerful when available supervision is limited.
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A Appendix

A.1 Additional Experimental Details

A.1.1 Computing exact $\pi$

For our experiments we use the optimal $\pi$, i.e. probability of positive sample in unlabeled data exactly as follows: suppose $n_p$ positive samples are labeled and let $P^*$ and $N^*$ denote true number of positive and negatives. then we can readily use $\pi^* = \frac{P^* - n_p}{P^* + N^* - n_p}$.

A.1.2 Mixture Proportion Estimation

In real settings when we do not have knowledge about the dataset exact $\pi$ cannot be computed and needs to be estimated - referred to as the Mixture proportion estimation (MPE) problem. Formally speaking, mixture proportion estimation (MPE) refers to the task of estimating the weight of a component distribution in a mixture, given samples from the mixture (unlabeled data) and component (positive labeled data). We refer the reader to (Ramaswamy et al., 2016; Garg et al., 2021; Ivanov, 2020) for a detailed discussion on MPE algorithms.

A.1.3 MNIST Multi Layer Perceptron

```python
MLPContrastive(
    (backbone): Sequential(
        (0): Linear(in_features=784, out_features=5000, bias=True)
        (1): BatchNorm1d(5000, eps=1e-05, momentum=0.1, affine=True,
                        track_running_stats=True)
        (2): ReLU(inplace=True)
        (3): Linear(in_features=5000, out_features=5000, bias=True)
        (4): BatchNorm1d(5000, eps=1e-05, momentum=0.1, affine=True,
                        track_running_stats=True)
        (5): ReLU(inplace=True)
        (6): Linear(in_features=5000, out_features=50, bias=True)
        (7): BatchNorm1d(50, eps=1e-05, momentum=0.1, affine=True,
                        track_running_stats=True)
        (8): ReLU(inplace=True)
    )
    (projector): Sequential(
        (0): Linear(in_features=50, out_features=300, bias=True)
        (1): BatchNorm1d(300, eps=1e-05, momentum=0.1, affine=True,
                        track_running_stats=True)
        (2): ReLU(inplace=True)
        (3): Linear(in_features=300, out_features=50, bias=True)
    )
    (online_head): Linear(in_features=50, out_features=1, bias=True)
)
----------------
Num of Params = 29231151
```

A.1.4 All Convolution N/w

```python
AllConv(
    (backbone_cnn): Sequential(
        (0): Conv2d(3, 96, kernel_size=(3, 3), stride=(1, 1), padding=(1, 1))
        (1): BatchNorm2d(96, eps=1e-05, momentum=0.1, affine=True,
                        track_running_stats=True)
        (2): ReLU(inplace=True)
        (3): Conv2d(96, 96, kernel_size=(3, 3), stride=(1, 1), padding=(1, 1))
        (4): BatchNorm2d(96, eps=1e-05, momentum=0.1, affine=True,
                        track_running_stats=True)
        (5): ReLU(inplace=True)
    )
```

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(6): Conv2d(96, 96, kernel_size=(3, 3), stride=(2, 2), padding=(1, 1))
(7): BatchNorm2d(96, eps=1e-05, momentum=0.1, affine=True, track_running_stats=True)
(8): ReLU(inplace=True)
(9): Conv2d(96, 192, kernel_size=(3, 3), stride=(1, 1), padding=(1, 1))
(10): BatchNorm2d(192, eps=1e-05, momentum=0.1, affine=True, track_running_stats=True)
(11): ReLU(inplace=True)
(12): Conv2d(192, 192, kernel_size=(3, 3), stride=(1, 1), padding=(1, 1))
(13): BatchNorm2d(192, eps=1e-05, momentum=0.1, affine=True, track_running_stats=True)
(14): ReLU(inplace=True)
(15): Conv2d(192, 192, kernel_size=(3, 3), stride=(2, 2), padding=(1, 1))
(16): BatchNorm2d(192, eps=1e-05, momentum=0.1, affine=True, track_running_stats=True)
(17): ReLU(inplace=True)
(18): Conv2d(192, 192, kernel_size=(3, 3), stride=(1, 1), padding=(1, 1))
(19): BatchNorm2d(192, eps=1e-05, momentum=0.1, affine=True, track_running_stats=True)
(20): ReLU(inplace=True)
(21): Conv2d(192, 192, kernel_size=(1, 1), stride=(1, 1))
(22): BatchNorm2d(192, eps=1e-05, momentum=0.1, affine=True, track_running_stats=True)
(23): ReLU(inplace=True)
(24): Conv2d(192, 10, kernel_size=(1, 1), stride=(1, 1))
(25): BatchNorm2d(10, eps=1e-05, momentum=0.1, affine=True, track_running_stats=True)
(26): ReLU(inplace=True)
)
(backbone_lin): Sequential(
(0): Linear(in_features=640, out_features=1000, bias=True)
(1): ReLU(inplace=True)
(2): Linear(in_features=1000, out_features=1000, bias=True)
(3): ReLU(inplace=True)
)
(projector): Sequential(
(0): Linear(in_features=1000, out_features=1000, bias=True)
(1): BatchNorm1d(1000, eps=1e-05, momentum=0.1, affine=True, track_running_stats=True)
(2): ReLU(inplace=True)
(3): Linear(in_features=1000, out_features=1000, bias=True)
)
(online_head): Linear(in_features=1000, out_features=1, bias=True)
--------------------
Num of Params = 5019255

A.1.5 ResNet18

ResNet18Contrastive(
(backbone): Sequential(
(0): Conv2d(3, 64, kernel_size=(3, 3), stride=(1, 1), padding=(1, 1), bias=False)
(1): BatchNorm2d(64, eps=1e-05, momentum=0.1, affine=True, track_running_stats=True)
(2): ReLU(inplace=True)
(3): Sequential(
(0): BasicBlock(}

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(0): Conv2d(128, 256, kernel_size=(1, 1), stride=(2, 2), bias=False)
(1): BatchNorm2d(256, eps=1e-05, momentum=0.1, affine=True, track_running_stats=True)
)
(1): BasicBlock(
  (conv1): Conv2d(256, 256, kernel_size=(3, 3), stride=(1, 1), padding=(1, 1), bias=False)
  (bn1): BatchNorm2d(256, eps=1e-05, momentum=0.1, affine=True, track_running_stats=True)
  (relu): ReLU(inplace=True)
  (conv2): Conv2d(256, 256, kernel_size=(3, 3), stride=(1, 1), padding=(1, 1), bias=False)
  (bn2): BatchNorm2d(256, eps=1e-05, momentum=0.1, affine=True, track_running_stats=True)
)
)
(6): Sequential(
  (0): BasicBlock(
    (conv1): Conv2d(256, 512, kernel_size=(3, 3), stride=(2, 2), padding=(1, 1), bias=False)
    (bn1): BatchNorm2d(512, eps=1e-05, momentum=0.1, affine=True, track_running_stats=True)
    (relu): ReLU(inplace=True)
    (conv2): Conv2d(512, 512, kernel_size=(3, 3), stride=(1, 1), padding=(1, 1), bias=False)
    (bn2): BatchNorm2d(512, eps=1e-05, momentum=0.1, affine=True, track_running_stats=True)
    (downsample): Sequential(
      (0): Conv2d(256, 512, kernel_size=(1, 1), stride=(2, 2), bias=False)
        (1): BatchNorm2d(512, eps=1e-05, momentum=0.1, affine=True, track_running_stats=True)
    )
    (1): BasicBlock(
      (conv1): Conv2d(512, 512, kernel_size=(3, 3), stride=(1, 1), padding=(1, 1), bias=False)
      (bn1): BatchNorm2d(512, eps=1e-05, momentum=0.1, affine=True, track_running_stats=True)
      (relu): ReLU(inplace=True)
      (conv2): Conv2d(512, 512, kernel_size=(3, 3), stride=(1, 1), padding=(1, 1), bias=False)
      (bn2): BatchNorm2d(512, eps=1e-05, momentum=0.1, affine=True, track_running_stats=True)
    )
    (7): AdaptiveAvgPool2d(output_size=(1, 1))
  )
  (projector): Sequential(
    (0): Linear(in_features=512, out_features=256, bias=False)
    (1): BatchNorm1d(256, eps=1e-05, momentum=0.1, affine=True, track_running_stats=True)
    (2): ReLU(inplace=True)
    (3): Linear(in_features=256, out_features=128, bias=True)
  )
  (online_head): Linear(in_features=512, out_features=1, bias=True)
)

Num of Params = 11333825