Conditional Contrastive Learning: Removing Undesirable Information in Self-Supervised Representations

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Abstract

Self-supervised learning is a form of unsupervised learning that leverages rich information in data to learn representations. However, data sometimes contains certain information that may be undesirable for downstream tasks. For instance, gender information may lead to biased decisions on many gender-irrelevant tasks. In this paper, we develop conditional contrastive learning to remove undesirable information in self-supervised representations. To remove the effect of the undesirable variable, our proposed approach conditions on the undesirable variable (i.e., by fixing the variations of it) during the contrastive learning process. In particular, inspired by the contrastive objective InfoNCE, we introduce Conditional InfoNCE (C-InfoNCE), and its computationally efficient variant, Weak-Conditional InfoNCE (WeaC-InfoNCE), for conditional contrastive learning. We demonstrate empirically that our methods can successfully learn self-supervised representations for downstream tasks while removing a great level of information related to the undesirable variables. We study three scenarios, each with a different type of undesirable variables: task-irrelevant meta-information for self-supervised speech representation learning, sensitive attributes for fair representation learning, and domain specification for multi-domain visual representation learning.

1 Introduction

The prevalence of data has created many opportunities for machine learning systems to leverage information from it, especially for self-supervised learning (SSL). This unsupervised learning paradigm requires neither labels nor prior task knowledge to learn good representations. Nonetheless, the data may contain undesirable information that we should exclude. For example, protected attributes such as gender or ethnicity are present in many datasets [28]. Without careful intervention, a conventional SSL process will inevitably also learn from these attributes. As a result, the learned representations may lead to unfair decisions on the downstream tasks, which should not have taken these protected attributes into account [26]. Another case of undesirable information is the presence of meta-information in datasets. For example, in a speech recognition setting, speaker ID is often presented as meta-information, but speech representations, in general, should be independent of the concrete speaker identity. There are two reasons: the speaker’s information should not be leaked, and good representations of the speech signals should generalize well to new speakers. Hence, we should consider removing task-irrelevant meta-information in SSL. In the domain generalization setting, we may want to learn representations from multiple domains and expect the learned representations to generalize well across domains. This setup is related to Domain Adaptation [32], where the trained classifiers [47] or the learned features [45] are expected to be domain-invariant. From a practical perspective, we may want to remove the domain-specific information for better generalization when considering SSL data in new domains.

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One way to remove undesirable information in SSL is by adding a second objective to minimize the mutual information between the self-supervised representations and the underlying undesirable variable [38], or minimize the prediction ability from the representations to the variable [50]. However, these are not ideal due to the challenge of optimizing multiple objectives together and balancing the trade-off between the downstream performance and the undesirable variable’s effect [52]. In this work, to remove the undesirable information in SSL, we present a conditional SSL method that uses only a single objective. In particular, our SSL method removes the effect of variations of the undesirable variable by conditioning on its value. Intuitively, since the variations are fixed, the effect of the variable will not be accounted for in SSL.

For the conditional SSL, we present the conditional contrastive learning objectives given that the contrastive objectives [5, 43, 44] are most widely used in conventional SSL. One representative contrastive objective is InfoNCE [31], which aims to learn similar representations for correlated data pairs and dissimilar representations for unrelated data pairs. Inspired by InfoNCE, we develop the Conditional InfoNCE (C-InfoNCE) objective, which learns similar representations for conditionally-correlated data pairs and dissimilar representations for conditionally-unrelated data pairs. For example, if we choose the speaker ID and condition on speaker ID being # 1, the conditionally-correlated data pairs are representations of the same sequence from speaker # 1, and conditionally-unrelated data pairs are representations of different sequences from speaker # 1. In this example, both conditionally-correlated and unrelated data come from the speaker # 1, which in other words, the part of the information for speaker identification is fixed.

From an information-theoretical perspective, we show that learning representations using C-InfoNCE relates to conditional mutual information maximization within representations. In particular, conditional mutual information measures the shared information between representations when removing the effect of the conditioned variable, which in our case is the undesirable variable. Since recent theoretical studies show that mutual information maximization within representations can result in representations that perform well on the downstream tasks [2, 43], C-InfoNCE learned representations (using conditional mutual information maximization) might also enjoy competitive downstream performance with the additional benefit of removing undesirable information. However, C-InfoNCE requires the conditioned variable as input, resulting in extra computational cost compared to InfoNCE. To address this issue, we introduce a second objective, the Weak-Conditional InfoNCE (WeaC-InfoNCE), as a simplified form of C-InfoNCE, which does not require the conditioned variable as input like C-InfoNCE. We show that WeaC-InfoNCE is a lower bound of C-InfoNCE. Hence, learning representations using WeaC-InfoNCE also relates to the conditional mutual information maximization within representations.

To verify the effectiveness of our method, we conduct several experiments. First, we consider the speaker ID and sequence ID as the conditioned variables for self-supervised speech representation learning. The speaker and the sequence ID are the meta-information for human speech. We find removing this meta-information in the representations leads to better downstream performance on phoneme classification. Second, we consider age and gender as the conditioned variable for fair representation learning. We observe our methods can effectively remove a greater level of sensitive information compared to baseline methods. Finally, we consider the domain specification when performing self-supervised representation learning on data from multiple domains. We find removing the domain-specific information in learned representation leads to better downstream performance. To conclude, we find learning representations using either C-InfoNCE or WeaC-InfoNCE achieve competitive downstream task performance while successfully removing a significant level of the effect of the conditioned variable compared to conventional self-supervised representation baselines.

2 Method

In this section, we introduce conditional contrastive learning methods to remove undesirable information in self-supervised learning. In Subsection 2.1, we discuss the technical background - unconditional contrastive learning and the corresponding InfoNCE objective [31] under the conventional self-supervised learning setup. Next, Subsection 2.2 presents the Conditional InfoNCE (C-InfoNCE) objective, and in Subsection 2.3 we discuss the higher computational cost of C-InfoNCE (compared to InfoNCE) and then introduce the Weak-Conditional InfoNCE (WeaC-InfoNCE) as a more computationally efficient variant of C-InfoNCE.
We now discuss one idea to remove undesirable information from a variable from the self-supervised learning perspective.

We refer to the representation $Z$ (usually a two-layer fully connected neural network [5, 18]). At a high-level, InfoNCE is maximizing the mutual information (MI) between the input $(x, y)$ and the output $g(x)$. MI is the mutual information (MI) between $X$ and $Y$. A common choice of $f(x, y)$ is to consider the cosine similarity $f(x, y) = \cos\left(\frac{g(x), g(y)}{\tau}\right)$ with $\tau$ being the temperature hyper-parameter and $g(\cdot)$ being a shallow network (usually a two-layer fully connected neural network [5, 18]). At a high-level, InfoNCE is maximizing similarities for $(x_i, y_i) \sim P_{X,Y}$ and minimizing similarities for $(x_i, y_i) \sim P_X P_Y (i \neq j)$. As shown in Equation (1), InfoNCE is a lower bound of $\MI(X;Y)$, and Arora et al. [2], Tosh et al. [39], Tsai et al. [43] have shown that maximizing lower bounds of $\MI(X;Y)$ often leads to better representations for downstream tasks.

2.1 Unconditional Contrastive Learning

Unconditional contrastive learning [3, 5, 18] aims at learning similar representations for correlated data and dissimilar representations for unrelated data. Examples of the correlated data could be different crops [3] or distortions [5, 18] of the same image or the cross-modality pair (image-caption pair) [43] of a sample. Examples of the unrelated data include different images [5, 18] or an image and a caption from another image [43]. Below we briefly review a probabilistic interpretation of unconditional contrastive learning.

We refer to the representation $(x, y)$ from correlated data as $(x, y) \sim P_{X,Y}$, where $P_{X,Y}$ is the joint distribution on $X \times Y$. Similarly, we use $(x, y) \sim P_X P_Y$ to mean that the representations $(x, y)$ are from uncorrelated data, where $P_X P_Y$ is the product of marginal distributions. Poole et al. [35], Tschannen et al. [44] and Tsai et al. [42] have shown that the unconditional contrastive learning is essentially maximizing the divergence between $P_{X,Y}$ and $P_X P_Y$. For instance, a common contrastive approach, the InfoNCE [31] method, is maximizing $D_{KL}(P_{X,Y} \| P_X P_Y)$ as follows:

**Definition 2.1** (InfoNCE [31] for unconditional contrastive learning).

\[
\text{InfoNCE} := \sup_f \mathbb{E}_{(x,y) \sim P_{X,Y}} \left[ \log \frac{e^{f(x,y)}}{\sum_{n=1}^{\infty} e^{f(x_n,y_n)}} \right] \leq D_{KL}(P_{X,Y} \| P_X P_Y) = \MI(X;Y), \tag{1}
\]

where $\{(x_i, y_i)\}_{i=1}^{n}$ represents $n$ independent copies of $(x, y) \sim P_{X,Y}$, $f(x, y)$ is any critic function that considers the input $(x, y)$ and output a scalar, and $\MI(X;Y)$ is the mutual information (MI) between $X$ and $Y$. A common choice of $f(x, y)$ is to consider the cosine similarity $f(x, y) = \cos\left(\frac{g(x), g(y)}{\tau}\right)$ with $\tau$ being the temperature hyper-parameter and $g(\cdot)$ being a shallow network (usually a two-layer fully connected neural network [5, 18]). At a high-level, InfoNCE is maximizing similarities for $(x_i, y_i) \sim P_{X,Y}$ and minimizing similarities for $(x_i, y_i) \sim P_X P_Y (i \neq j)$. As shown in Equation (1), InfoNCE is a lower bound of $\MI(X;Y)$, and Arora et al. [2], Tosh et al. [39], Tsai et al. [43] have shown that maximizing lower bounds of $\MI(X;Y)$ often leads to better representations for downstream tasks.

2.2 Conditional Contrastive Learning

We now discuss one idea to remove undesirable information from a variable from the self-supervised representations: conditioning on it [7]. Intuitively, conditioning on a variable means fixing the variations of this variable, and hence its effect can be removed.

Our conditional contrastive learning hence aims at learning similar representations for conditionally-correlated data and dissimilar representations for conditionally-unrelated data. For instance, let us consider an example of conditional speech self-supervised learning, where we choose the speaker ID to be the conditioned variable and let the outcome of this variable be speaker # 1. Then, the conditionally-correlated data are two representations learned from the same sequence of speaker # 1, and the conditionally-unrelated data are two representations learned from different sequences of speaker # 1. In both cases, all sequences are from speaker # 1 because we condition on it. We update the representations by calculating the contrastive objective from the constructed data pairs. Then we condition on another speaker ID outcome, say speaker # 2, and construct new data pairs and update the representations using the new data pairs. In this example, the conditional contrastive learning method is learning representations by taking data pairs from the same speaker in each update step and different pairs across the update steps. We hope that such a paradigm can exclude the information about speakers’ identity in the representations (assuming the information regarding the
Speakers is undesirable information). Similar to the last section, below, we also provide a probabilistic interpretation of conditional contrastive learning.

We refer to the representation \((x, y)\) from the conditionally-correlated data as \((x, y) \sim P_{X,Y|z}\), where \(P_{X,Y|z}\) is the joint distribution on \(X \times Y\) conditioned on the undesirable variable \(Z = z\). And we refer to the representation \((x, y)\) from the conditionally-unrelated data pair as \((x, y) \sim P_{X|z}P_{Y|z}\), where \(P_{X|z}P_{Y|z}\) is the product of conditional marginal distributions. Recall that the unconditional contrastive learning aims to maximize the probability divergence between \(P_{XY}\) and \(P_{X}P_{Y}\), resulting in a connection with mutual information \(\text{MI}(X; Y)\). Similarly, the conditional contrastive learning aims to maximize the divergence between \(P_{XY|z}\) and \(P_{X|z}P_{Y|z}\) for all \(z \sim P_z\), leading to a connection with conditional mutual information \(\text{MI}(X; Y|Z)\):

**Definition 2.2 (Conditional Mutual Information).**

\[
\text{MI}(X; Y|Z) := \mathbb{E}_{Z \sim Z} [D_{KL}(P_{X,Y|Z=z} || P_{X|z}P_{Y|z})] = \int_Z D_{KL}(P_{X,Y|Z} || P_{X|Z}P_{Y|Z}) \, dP_Z = \int_Z p_Z(z) \int_{X,Y} p_{X,Y|Z}(x,y|z) \log \frac{p_{X,Y|Z}(x,y|z)}{p_{X|Z}p_{Y|Z}} \, dx \, dy \, dz. \tag{2}
\]

The conditional mutual information measures the expected mutual information of \(X\) and \(Y\) given \(Z\). In other words, it measures the averaged shared information between \(X\) and \(Y\) conditioning on \(Z\), and by conditioning on \(Z\), we fix its variations and exclude its effect.

Inspired by InfoNCE for unconditional contrastive learning, we present the Conditional InfoNCE (C-InfoNCE) objective for conditional contrastive learning:

**Proposition 2.3 (Conditional InfoNCE (C-InfoNCE) for conditional contrastive learning).**

\[
C - \text{InfoNCE} := \sup_f \mathbb{E}_{z \sim P_Z} \left[ \mathbb{E}_{(x_i,y_i) \sim P_{X,Y|z}} \left[ \log \frac{\sum_{i=1}^n e^{f(x_i,y_i,z)}}{n} \right] \right] \leq \text{MI}(X; Y|Z), \tag{3}
\]

where \(\{(x_i,y_i)\}_{i=1}^n\) represents \(n\) independent copies of \((x, y) \sim P_{X,Y|z}\) and \(f(x, y, z)\) takes in the input \((x, y, z)\) and outputs a scalar. We leave the derivations and proofs in Appendix. We design \(f(x, y, z)\) as the cosine similarity \(f(x, y, z) = \cos(g(x, z), g(y, z))/\tau\) with \(\tau\) being the temperature hyper-parameter and \(g(\cdot, \cdot)\) being a shallow network. As shown in Equation (3), C-InfoNCE is a lower bound of \(\text{MI}(X; Y|Z)\), and hence learning representation using C-InfoNCE results in conditional mutual information maximization within representations.

### 2.3 Weak-Conditional Contrastive Learning

Compared to InfoNCE (Equation (1)), a disadvantage of C-InfoNCE (Equation (3)) is the need to consider three variables (i.e., \(X, Y,\) and \(Z\)) instead of two (i.e., \(X\) and \(Y\)) in \(f(\cdot)\). In particular, introducing a third variable \(Z\) increases computational cost since the function \(f(\cdot)\) becomes more complex. To alleviate this problem, we introduce the following Weak-Conditional InfoNCE (WeaC-InfoNCE) objective to avoid having \(Z\) as an extra input variable:

**Proposition 2.4 (Weak-Conditional InfoNCE (WeaC-InfoNCE) for conditional contrastive learning).**

\[
\text{WeaC - InfoNCE} := \sup_f \mathbb{E}_{z \sim P_Z} \left[ \mathbb{E}_{(x_i,y_i) \sim P_{X,Y|z}} \left[ \log \frac{\sum_{i=1}^n e^{f(x_i,y_i)}}{n} \right] \right] \leq D_{KL} \left( P_{X,Y} \| \mathbb{E}_{P_Z} [P_{X|Z}P_{Y|Z}] \right) = \text{Weak} - \text{MI}(X; Y|Z) \leq \text{MI}(X; Y|Z), \tag{4}
\]

where \(f(x,y)\) takes in the input \((x, y)\) and outputs a scalar, instead of \(f(x, y, z)\) which takes in \((x, y, z)\) in C-InfoNCE. Same as InfoNCE, we consider \(f(x,y)\) in WeaC-InfoNCE as the cosine similarity \(f(x,y) = \cos(g(x), g(y))/\tau\) with \(\tau\) being the temperature hyper-parameter and \(g(\cdot)\) being a shallow network. WeaC - MI(\(X; Y|Z\)) represents the weak-conditional mutual information, which is the KL-divergence between \(P_{X,Y}\) and \(\mathbb{E}_{P_Z} [P_{X|Z}P_{Y|Z}]\). The notion of the weak-conditional mutual information comes from weak-conditional independence [5, 12, 13], which is defined as the case when \(P_{X,Y} = \mathbb{E}_{P_Z} [P_{X|Z}P_{Y|Z}]\).
We highlight the differences between the weak-conditional mutual information (i.e., Weak – MI (X; Y|Z)) and the standard conditional mutual information (i.e., MI (X; Y|Z)).

First, Weak – MI (X; Y|Z) measures $D_{KL} (P_{X,Y} \| P_{X|Z} P_{Y|Z})$ and MI (X; Y|Z) measures $\mathbb{E}_Z [D_{KL} (P_{X,Y|Z} \| P_{X|Z} P_{Y|Z})]$, where $D_{KL} (P_{X,Y} \| P_{X|Z} P_{Y|Z}) \leq \mathbb{E}_Z [D_{KL} (P_{X,Y|Z} \| P_{X|Z} P_{Y|Z})]$.

Hence, Weak – MI (X; Y|Z) is a lower bound on MI (X; Y|Z) and can be seen as a more “conservative” measurement of MI (X; Y|Z), capturing only part of information in MI (X; Y|Z). Second, MI (X; Y|Z) = 0 is a sufficient condition for Weak – MI (X; Y|Z) = 0, which suggests that conditional independence implies weak-conditional independence. See detailed derivations and proofs in Appendix.

To conclude, WeaC-InfoNCE (Equation (10)) objective is a surrogate for C-InfoNCE objective (Equation (3)), with the additional benefit of considering only two variables instead of three in $f(\cdot)$. Since WeaC-InfoNCE is also a lower bound on MI (X; Y|Z) (looser than C-InfoNCE), learning representations using WeaC-InfoNCE results in conditional mutual information maximization within representations, just like C-InfoNCE.

3 Experiments

We evaluate the proposed conditional contrastive learning on several tasks. In Section 3.1, we study self-supervised speech representation learning and consider the meta-information such as the speaker ID and sequence ID as the conditioned variable. We study whether removing the meta-information in the learned representations impacts downstream performance. In Section 3.2, we examine fair representation learning and consider the sensitive attributes, age and gender, as the conditioned variable. We hope to reduce the amount of sensitive information in our learned representations. In Section 3.3, we investigate multi-domain self-supervised learning and consider the domain specification (domain ID) as the conditioned variable. We aim to reduce domain-specific information in the representations so that they can transfer well across different domains.

In practice, the expectations in InfoNCE (Equation (1)), C-InfoNCE (Equation (3)), and WC-InfoNCE (Equation (10)) are replaced by the empirical mean of a batch of samples. For a fair comparison, when comparing InfoNCE, C-InfoNCE, and WC-InfoNCE, we will only alter the training objectives and leave the network design and the optimization procedure identical. The small difference is the design of the critic function $f(\cdot)$, and we ensure $g(\cdot)$ in $f(\cdot)$ has similar size across different objectives. We leave the details for the networks, the optimizers, the hyper-parameters, and more details for the datasets in Appendix.

3.1 Speech Representation Learning: Removing Effect from Meta-Information

For the first set of experiments, we consider learning self-supervised speech representations on Librispeech-100h dataset [33], which contains 100 hours of English speech from 251 speakers and 28,538 sequences. Following prior work [31, 36], we first pretrain the model using self-supervised objectives without downstream label access. Then, we fix the pretrained model, add an additional linear classifier on top of the pretrained representations, and fine-tune the linear classifier with labels. Note that the above steps are performed on the training set. For evaluation, we fix both the pretrained model and the linear classifier, and we report the top-1 accuracy metric on the evaluation set.

We consider the unconditional (conventional setup, InfoNCE [31] in Equation (1)) and the conditional (ours, C-InfoNCE in Equation (3) and WeaC-InfoNCE in Equation (10)) contrastive learning methods as the self-supervised objectives. And we select the meta-information, including the speaker and sequence ID, as the conditioned variable $Z$ in C-InfoNCE and WeaC-InfoNCE. Note that C-InfoNCE and WeaC-InfoNCE aim to remove the effect of the conditioned variable in the resulting representations. Hence, our goal is to see whether removing the meta-information will affect the representation’s performance on the downstream tasks, including Phoneme Classification and Speaker Classification.

We follow Oord et al. [31], Rivière et al. [36] for the experimental setup, where they consider InfoNCE as the objective. In particular, the correlatedly-paired representations $(x, y^+) \sim P_{X,Y}$ in InfoNCE are a pair of past and future states of a sequence. And unrelatedly-paired representations $(x, y^-) \sim P_X P_Y$ are two random states from different sequences. InfoNCE aims to learn similar correlatedly-paired representations and dissimilar unrelatedly-paired representations. Hence, this process is regarded as forward modeling, i.e., predicting the future states of a sequence from its
We consider two datasets: UCI German credit [10] and Adult [10] datasets. The German credit dataset includes 1,000 samples with 20 attributes, a binary age indicator variable as the sensitive attribute, and predicting credit approval as the downstream task. The Adult dataset includes 30,000 samples with 14 attributes and a sensitive attribute (gender). We train the meta-network with the pairs construction.

Table 1 shows results. First, we observe a performance improvement on phoneme classification by comparing C-InfoNCE and WeaC-InfoNCE with InfoNCE. Since C-InfoNCE and WeaC-InfoNCE aim to remove the meta-information (speaker and sequence ID) in the self-supervised representations, the improvement suggests that the meta-information should be irrelevant to the phoneme classification. Second, on speaker classification, we see an over 20% performance deterioration from 93.4% of InfoNCE to C-InfoNCE and WeaC-InfoNCE. This suggests that by conditioning on the speaker or sequence ID, the C-InfoNCE and WeaC-InfoNCE successfully remove a decent amount of speaker information. Note that the sequence ID implicitly contains speaker information because each sequence is from only one single speaker. Last, we compare C-InfoNCE and WeaC-InfoNCE and find that WeaC-InfoNCE performs in between InfoNCE and C-InfoNCE. The result suggests that C-InfoNCE is better at removing the effect from the conditioned variable than WeaC-InfoNCE. Yet, as discussed in Section 2.3, WeaC-InfoNCE is more computationally efficient than C-InfoNCE.

### 3.2 Fair Representation Learning: Removing Effect from Sensitive Attributes

For our second set of experiments, we consider removing sensitive information in self-supervised fair representation learning. We follow the setting in prior work [38], which learns the representations to maximally preserve information from data while removing the information from the sensitive attributes. In particular, let the input data be $X$, the learned representations be $Y$, and the sensitive attributes be $Z$. Song et al. [38] presents the pretraining stage as maximizing the conditional mutual information $\text{MI}(X; Y | Z)$ under the constraint $\text{MI}(Y; Z) < \epsilon$ (we set $\epsilon = 0.1$ in our experiments). Then, we fix the pretrained network and fine-tune the representations using logistic regression classifiers on top of the learned representations. The above steps are performed on the training set. For evaluation, the reported metrics are the demographic parity distance $\Delta_{DP}$ [26] and the representation quality based on the area under the ROC curve (AUC) on downstream tasks. Specifically, the demographic parity distance $\Delta_{DP}$ [26] is defined as the absolute expected difference in classifier outcomes between two sensitive groups (e.g., the male group and the female group from gender), and a lower $\Delta_{DP}$ suggests a fairer representation.

We consider two datasets: UCI German credit [10] and Adult [10] datasets. The German credit dataset contains 1,000 samples with 20 attributes, a binary age indicator variable as the sensitive attribute, and predicting credit approval as the downstream task. The Adult dataset includes
WeaC-InfoNCE) achieve at par or even better fairness and downstream performances compared to WeaC-InfoNCE belong to conditional learning objectives, which consider removing the sensitive attributes, would not sacrifice downstream performances. Second, we find that our methods (C-InfoNCE and L-MIFR) have lower fairness and lower downstream task performance than the conditional (L-MIFR, MIFR, C-InfoNCE, and WeaC-InfoNCE) self-supervised methods. For instance, on UCI Adult dataset, InfoNCE has lower fairness and lower downstream performance than the conditional (L-MIFR, MIFR, C-InfoNCE, and WeaC-InfoNCE) methods [38], to be the baselines. These two methods variationally lower-bound the mutual information: \( \text{MI}(X;Y) \). Different from InfoNCE, C-InfoNCE and WeaC-InfoNCE consider the conditionally-correlated pair (e.g., \( (x, y^+) \sim P_{X,Y|Z=z} \)) and the conditionally-unrelated pair (e.g., \( (x, y^-) \sim P_{X|Z=z}P_{Y|Z=z} \)) given the conditioned outcome \( z \sim P_Z \). For instance, let \( Z \) be gender, and we condition on the gender is female. Then the conditionally-correlated pair would be the data from a female and the learned representation from the same female. The conditionally-unrelated pair would be the data from a female and the learned representation from the data of another female. Lastly, we have the MIFR and the L-MIFR methods [38] to be the baselines. These two methods variationally lower-bound the conditional mutual information: \( \text{MI}(X;Y|Z) \geq \mathbb{E}_{q_{\phi}(X,Y,Z)} [\log q_{\theta}(X|Y,Z)] \), with \( q_{\phi} \) and \( p_{\theta} \) being two separate networks modeling different distributions. MIFR and L-MIFR consider the same objective but different optimization processes. To conclude, L-MIFR, MIFR, C-InfoNCE, and WeaC-InfoNCE belong to conditional learning objectives, which consider removing the sensitive information from the data representations.

Table 2 presents our results. First, we find the unconditional (InfoNCE) self-supervised method has lower fairness and lower downstream task performance than the conditional (L-MIFR, MIFR, C-InfoNCE, WeaC-InfoNCE) self-supervised methods. For instance, on UCI Adult dataset, InfoNCE has lower \( \Delta_{DP} \) (0.23 v.s. 0.06) and lower ROC AUC (0.62 v.s. 0.69) than C-InfoNCE. Note that both unconditional and conditional methods aim to preserve more information from the data in the representation, but the conditional methods additionally consider removing the effect from the sensitive attributes. The result suggests that the conditional methods can achieve better fairness and would not sacrifice downstream performances. Second, we find that our methods (C-InfoNCE and WeaC-InfoNCE) achieve at par or even better fairness and downstream performances compared to the strong baselines, L-MIFR and MIFR. The result suggests that our methods can be competitive for self-supervised fair representation learning.

### 3.3 Multi-domain Representation Learning: Removing Effect from Domain Specification

For the third set of experiments, we consider learning self-supervised representations from multiple domains. While more domains provide more information, we argue that domain-invariant information...
We now discuss the implementations of C-InfoNCE in Equation (3) and WeaC-InfoNCE with the domain specification being the conditioned variable we pre-train using a single dataset and the notion of multi-domain considers the pre-training using the mixture of the three selected datasets. The conditional contrastive learning considers the domain specification as the conditioned variable. We adopt the linear evaluation protocol [5, 18].

Table 3: Accuracy (%) for object detection and scene understanding using self-supervised representation learning with the presence of data from multiple domains. In the experiments, we regard a dataset as a domain with the selected datasets having similar scales but different purposes (object detection and scene understanding). The unconditional contrastive learning represents the setting in SimCLR [5], which utilizes the InfoNCE objective. The notion of uni-domain refers the setting that we pre-train using a single dataset and the notion of multi-domain considers the pre-training using the mixture of the three selected datasets. The conditional contrastive learning considers the domain specification as the conditioned variable. We adopt the linear evaluation protocol [5, 18].

| Objective | CIFAR-10 | Tiny ImageNet | SUN 397 |
|-----------|---------|---------------|---------|
| **Uni-Domain Unconditional Self-supervised Learning** | | | |
| InfoNCE [31] | 92.67±0.12 | 53.42±0.43 | 70.89±0.35 |
| **Multi-Domain Unconditional Self-supervised Learning** | | | |
| InfoNCE [31] | 91.13±0.11 | 50.38±0.32 | 68.23±0.45 |
| **Multi-Domain Conditional Self-supervised Learning (Z = Domain Specification)** | | | |
| C-InfoNCE (ours) | 93.54±0.21 | 57.46±0.23 | 74.62±0.26 |
| WeaC-InfoNCE (ours) | 94.23±0.31 | 57.01±0.19 | 74.23±0.31 |

The multiple-domain unconditional contrastive learning represents the same setting as the previous one except that we perform pretraining on the mixture of the three selected datasets. Hence, the unrelated-paired representations \((x, y^+)\sim P_X P_Y\) in InfoNCE are the learned representations from augmented variants of an image and the unrelated-paired representations \((x, y^-)\sim P_X P_Y\) are the representations of two random images in the dataset.

We now discuss the implementations of C-InfoNCE in Equation (3) and WeaC-InfoNCE in Equation (10), as well as various baseline methods. The results are presented in Table 3. First, the uni-domain unconditional contrastive learning is SimCLR [5] - a standard visual contrastive representation learning approach which considers InfoNCE [31] (Equation (1)) as its objective. Note that it performs pretraining on a single dataset and then evaluates on the same dataset. In particular, the correlated-paired representations \((x, y^+)\sim P_X Y\) in InfoNCE are always from the same dataset. We consider the same batch size across all settings for a fair comparison.

The multiple-domain unconditional contrastive learning represents the same setting as the previous one except that we perform pretraining on the mixture of the three selected datasets. Hence, the unrelated-paired representations \((x, y^-)\sim P_X P_Y\) can be the representations from different datasets (e.g., \(x\) from CIFAR-10 and \(y^-\) from Tiny ImageNet). Finally, the multiple-domain conditional contrastive learning considers C-InfoNCE and WeaC-InfoNCE as the pretraining objectives on the mixed datasets, with the domain specification being the conditioned variable \(Z\). Thus, in C-InfoNCE and WeaC-InfoNCE, the conditionally-correlated-paired representations \((x, y^+)\sim P_{X|Z=z} Y|Z=z\) and the conditionally-unrelated-paired representations \((x, y^-)\sim P_{X|Z=z} P_Y|Z=z\) are always from the same dataset. We consider the same batch size across all settings for a fair comparison.

Let us first consider CIFAR-10’s performance in Table 3. First, we see the performance drop from uni-domain unconditional contrastive learning (92.67) to multi-domain unconditional contrastive learning (91.13), where both methods use InfoNCE as the objective. Note that multi-domain unconditional one considers all data from the three datasets for the pretraining. In contrast, the uni-domain unconditional one only considers the data from a single dataset. The performance drop suggests that merely increasing the data in self-supervised learning may not result in better performance,
especially when the data come from multiple domains. Second, we see the performance improvement from the uni-modal and multi-modal unconditional methods (92.67 and 91.13) to the multi-domain conditional methods (93.54 and 94.23), where the conditional methods consider removing domain-specific information in the learned representations. The performance improvement suggests that the domain-specific information may be irrelevant to the downstream task. Third, we observe no obvious performance differences between C-InfoNCE and WeaC-InfoNCE. For instance, C-InfoNCE achieves worse performance than WeaC-InfoNCE on CIFAR-10 (93.54 v.s. 94.23), while it performs better on Tiny ImageNet (57.46 v.s. 57.01). Since WeaC-InfoNCE is computationally more efficient than C-InfoNCE, it may be a better choice for multi-domain self-supervised learning.

4 Related Work

Self-Supervised Learning Self-supervised learning takes pre-defined tasks from unlabeled samples for pretraining representations [19] and uses the learned representations for downstream tasks, such as visual object detection [6, 18], language understanding and Question Answering [9, 23], and automatic speech recognition [31, 36]. One major way of self-supervised learning is contrastive learning [5, 18, 31], which tries to construct pairs of related data (termed positive pairs) and pairs of unrelated samples (termed negative pairs) and learn a model that scores the positive and negative pairs differently [21]. Prior works [5, 31, 43] construct the correlated pairs and unrelated pairs from the unconditional joint and the product of marginal distributions. Meanwhile, the proposed C-InfoNCE and WeaC-InfoNCE consider the conditionally-correlated pairs and conditionally-unrelated pairs from the conditional joint and the product of conditional marginal distributions, respectively. Both distributions are conditioned on the same outcome of an undesirable variable.

Fair Representation Learning Fair representation learning [27] considers different measures to quantify algorithm’s fairness, including statistical parity [11], equality of opportunity [16], equalized odds [16], and individual fairness [11]. While most of the study focuses on a supervised setup [11, 16, 27], this paper studies the self-supervised setup where downstream tasks are unknown, but the learned representations still need to preserve fairness criterion [4, 26]. Song et al. [38] presents a suitable framework that maximizes the expressiveness of the representation while satisfying controllable levels of fairness using conditional mutual information. The difference between [38] and the proposed method is how we construct and maximize the lower bound of conditional mutual information.

Multi-Domain Learning Domain adaptation [34, 46] aims to solve a distribution shift [51] or domain change [15] between two domains that could degrade performance. Domain adaptation methods can achieve domain-invariant representations by minimizing the probability divergences [25, 37, 53] between source and target data domains. Our approach, on the other hand, reduces the effect of domain specifications to achieve domain-invariant representation by conditioning on the domain specifications (domain ID).

5 Conclusion and Discussions

In this paper, we developed conditional contrastive learning methods to remove the effect of an undesirable variable in self-supervised learning by conditioning on it. The proposed C-InfoNCE and WeaC-InfoNCE objectives lead to representations that perform better in downstream tasks and exclude a greater level of information of undesirable variables compared to baseline models in speech representation learning, fairness representation, and multi-domain visual representation learning. Nevertheless, we do recognize the limitations of the approach. First, it is not always easy to know which exact variables to condition when we want to remove certain undesirable information. Moreover, conditioning on the incorrect information may lead to suboptimal representations for downstream tasks. In terms of the potential broader impact of this work, the methods in the paper can bring a positive social impact by removing privacy-related information from representations. For example, in medical applications, our approach can be used to help protect patient information from being leaked out in learned representations. However, if the conditioned variable in a machine learning system also contains vital information useful for the downstream task, removing its effect may result in a performance drop and thus affect users of the system.
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12
A Theoretical Analysis

This section provides the theoretical analysis of Proposition 2.3 and Proposition 2.4 in the main text. The full set of assumptions of all theoretical results and complete proofs of all theoretical results are presented below.

A.1 Lemmas before Proof

We first present the following lemmas, which will be later used in the proof:

**Lemma A.1** (Nguyen et al. [30] with two variables). Let $\mathcal{X}$ and $\mathcal{Y}$ be the sample spaces for $X$ and $Y$, $f$ be any function: $(\mathcal{X} \times \mathcal{Y}) \to \mathbb{R}$, and $P$ and $Q$ be the probability measures on $\mathcal{X} \times \mathcal{Y}$. Then,

$$D_{\text{KL}} (P \parallel Q) = \sup_f \mathbb{E}_{(x,y) \sim P} [f(x,y)] - \mathbb{E}_{(x,y) \sim Q}[e^{f(x,y)}] + 1.$$

**Proof.** The second-order functional derivative of the objective is $-e^{f(x,y)} \cdot dQ$, which is always negative. The negative second-order functional derivative implies the objective has a supreme value. Then, take the first-order functional derivative and set it to zero:

$$dP - e^{f(x,y)} \cdot dQ = 0.$$

We then get the optimal $f^*(x, y) = \log \frac{dP}{dQ}$. Plug in $f^*(x, y)$ into the objective, we obtain

$$\mathbb{E}_P[f^*(x,y)] - \mathbb{E}_Q[e^{f^*(x,y)}] + 1 = \mathbb{E}_P[\log \frac{dP}{dQ}] = D_{\text{KL}} (P \parallel Q).$$

\qed

**Lemma A.2** (Nguyen et al. [30] with three variables). Let $\mathcal{X}$, $\mathcal{Y}$, and $\mathcal{Z}$ be the sample spaces for $X$, $Y$, and $Z$, $f$ be any function: $(\mathcal{X} \times \mathcal{Y} \times \mathcal{Z}) \to \mathbb{R}$, and $P$ and $Q$ be the probability measures on $\mathcal{X} \times \mathcal{Y} \times \mathcal{Z}$. Then,

$$D_{\text{KL}} (P \parallel Q) = \sup_f \mathbb{E}_{(x,y,z) \sim P} [f(x,y,z)] - \mathbb{E}_{(x,y,z) \sim Q}[e^{f(x,y,z)}] + 1.$$

**Proof.** The second-order functional derivative of the objective is $-e^{f(x,y,z)} \cdot dQ$, which is always negative. The negative second-order functional derivative implies the objective has a supreme value. Then, take the first-order functional derivative and set it to zero:

$$dP - e^{f(x,y,z)} \cdot dQ = 0.$$

We then get the optimal $f^*(x, y, z) = \log \frac{dP}{dQ}$. Plug in $f^*(x, y, z)$ into the objective, we obtain

$$\mathbb{E}_P[f^*(x,y,z)] - \mathbb{E}_Q[e^{f^*(x,y,z)}] + 1 = \mathbb{E}_P[\log \frac{dP}{dQ}] = D_{\text{KL}} (P \parallel Q).$$

\qed

A.1.1 Immediate results following Lemma A.1

**Lemma A.3.**

Weak $\text{MI} (X; Y | Z) = D_{\text{KL}} \left( P_{X,Y} \parallel \mathbb{E}_{P_Z} [P_{X|Z}P_{Y|Z}] \right) = \sup_f \mathbb{E}_{(x,y) \sim P_{X,Y}} [f(x,y)] - \mathbb{E}_{(x,y) \sim \mathbb{E}_{P_Z} [P_{X|Z}P_{Y|Z}]} [e^{f(x,y)}] + 1.$

**Proof.** Let $P$ be $P_{X,Y}$ and $Q$ be $\mathbb{E}_{P_Z} [P_{X|Z}P_{Y|Z}]$ in Lemma A.1. \qed

**Lemma A.4.** $\sup_f \mathbb{E}_{(x,y_1) \sim P, (x,y_2,\ldots) \sim Q^{\otimes (n-1)}} [\log \frac{e^{f(x,y_1)}}{\sum_{j=1}^n e^{f(x,y_j)}}] \leq D_{\text{KL}} (P \parallel Q).$
\begin{proof}
\forall f, we have

\begin{align*}
D_{\text{KL}}(\mathcal{P} \parallel \mathcal{Q}) &= E_{(x,y_2,n) \sim \mathcal{Q}^{\otimes (n-1)}} \left[ D_{\text{KL}}(\mathcal{P} \parallel \mathcal{Q}) \right] \\
& \geq E_{(x,y_2,n) \sim \mathcal{Q}^{\otimes (n-1)}} \left[ E_{(x,y_1) \sim \mathcal{P}} \left[ \log \frac{e^{f(x,y_1)}}{\frac{1}{n} \sum_{j=1}^{n} e^{f(x,y_j)}} \right] - E_{(x,y_1) \sim \mathcal{Q}} \left[ \frac{1}{n} \sum_{j=1}^{n} e^{f(x,y_j)} \right] + 1 \right] \\
& = E_{(x,y_2,n) \sim \mathcal{Q}^{\otimes (n-1)}} \left[ E_{(x,y_1) \sim \mathcal{P}} \left[ \log \frac{e^{f(x,y_1)}}{\frac{1}{n} \sum_{j=1}^{n} e^{f(x,y_j)}} \right] - 1 + 1 \right] \\
& = E_{(x,y_1) \sim \mathcal{P}, (x,y_2,n) \sim \mathcal{Q}^{\otimes (n-1)}} \left[ \log \frac{e^{f(x,y_1)}}{\frac{1}{n} \sum_{j=1}^{n} e^{f(x,y_j)}} \right].
\end{align*}

The first line comes from the fact that $D_{\text{KL}}(\mathcal{P} \parallel \mathcal{Q})$ is a constant. The second line comes from Lemma A.1. The third line comes from the fact that $(x, y_1)$ and $(x, y_2,n)$ are interchangeable when they are all sampled from $\mathcal{Q}$.

To conclude, since the inequality works for all $f$, and hence

\begin{align*}
\sup_{f} E_{(x,y_1) \sim \mathcal{P}, (x,y_2,n) \sim \mathcal{Q}^{\otimes (n-1)}} \left[ \log \frac{e^{f(x,y_1)}}{\frac{1}{n} \sum_{j=1}^{n} e^{f(x,y_j)}} \right] \leq D_{\text{KL}}(\mathcal{P} \parallel \mathcal{Q}).
\end{align*}

\end{proof}

Note that Lemma A.4 does not require $n \to \infty$, which is a much more practical setting compared to the analysis made only when $n \to \infty$. And a remark is that the equality holds in Lemma A.4 when $n \to \infty$.

A.1.2 Immediate results following Lemma A.2

Lemma A.5.

\[ \text{MI} (X; Y | Z) = E_{P_Z} \left[ D_{\text{KL}} (P_{X,Y,Z} \parallel P_{X,Z} P_{Y|Z}) \right] = D_{\text{KL}} (P_{X,Y,Z} \parallel P_{X,Z} P_{Y|Z}) = \sup_{f} E_{(x,y,z) \sim P_{X,Y,Z}} [f(x,y,z)] - E_{(x,y,z) \sim P_{X,Z} P_{Y|Z}} [e^{f(x,y,z)}] + 1. \]

\begin{proof}
Let $\mathcal{P}$ be $P_{X,Y,Z}$ and $\mathcal{Q}$ be $P_{Z} P_{X|Z} P_{Y|Z}$ in Lemma A.2.
\end{proof}

A.1.3 Showing Weak $- \text{MI} (X; Y | Z) \leq \text{MI} (X; Y | Z)$

Proposition A.6.

Weak $- \text{MI} (X; Y | Z) \leq \text{MI} (X; Y | Z)$.

\begin{proof}
According to Lemma A.3,

\begin{align*}
\text{Weak} - \text{MI} (X; Y | Z) &= \sup_{f} E_{(x,y) \sim P_{X,Y}} [f(x,y)] - E_{(x,y) \sim P_{X,Z} P_{Y|Z}} [e^{f(x,y)}] + 1 \\
& = \sup_{f} E_{(x,y,z) \sim P_{X,Y,Z}} [f(x,y)] - E_{(x,y,z) \sim P_{X,Z} P_{Y|Z}} [e^{f(x,y)}] + 1.
\end{align*}

Let $f_1^*(x,y)$ be the function when the equality for Weak $- \text{MI} (X; Y | Z)$ holds, and let $f_2^*(x,y,z) = f_1^*(x,y) (f_2^*(x,y,z) \neq f_2^*(x,y) \forall z \sim P_{Z})$:

\begin{align*}
\text{Weak} - \text{MI} (X; Y | Z) &= E_{(x,y,z) \sim P_{X,Y,Z}} [f_1^*(x,y)] - E_{(x,y,z) \sim P_{X,Z} P_{Y|Z}} [e^{f_1^*(x,y)}] + 1 \\
& = E_{(x,y,z) \sim P_{X,Y,Z}} [f_2^*(x,y,z)] - E_{(x,y,z) \sim P_{X,Z} P_{Y|Z}} [e^{f_2^*(x,y,z)}] + 1.
\end{align*}

Comparing the above equation to Lemma A.5,

\begin{align*}
\text{MI} (X; Y | Z) &= \sup_{f} E_{(x,y,z) \sim P_{X,Y,Z}} [f(x,y,z)] - E_{(x,y,z) \sim P_{X,Z} P_{Y|Z}} [e^{f(x,y,z)}] + 1,
\end{align*}

we conclude Weak $- \text{MI} (X; Y | Z) \leq \text{MI} (X; Y | Z)$.
\end{proof}
A.2 Proof of Proposition 2.3 in the Main Text

Proposition A.7 (Conditional InfoNCE (C-InfoNCE) for conditional contrastive learning, restating Proposition 2.3 in the main text),

\[
\text{C−InfoNCE} := \sup_f E_z \sim P_z \left[ \mathbb{E}_{(x, y) \sim P_{X,Y|z} \otimes n} \left[ \log \frac{e^{f(x, y, z)}}{\frac{1}{n} \sum_{j=1}^{n} e^{f(x, y, z)}} \right] \right] \\
\leq E_{P_z} \left[ D_{KL} \left( P_{X,Y|Z} \parallel P_{X|Z} P_{Y|Z} \right) \right] = \text{MI} (X; Y|Z),
\]

Proof. Given a \( z \sim P_Z \), we let \( P = P_{X,Y|Z=z} \) and \( Q = P_{X|Z=z} P_{Y|Z=z} \). Then,

\[
\mathbb{E}_{(x, y) \sim P, (x, y_2, n) \sim Q \otimes (n-1)} \left[ \log \frac{1}{n} \sum_{j=1}^{n} e^{f(x, y_j, z)} \right] = \mathbb{E}_{(x, y) \sim P_{X,Y|z} \otimes n} \left[ \log \frac{1}{n} \sum_{j=1}^{n} e^{f(x, y_j, z)} \right].
\]

The only variables in the above equation are \( X \) and \( Y \) with \( Z \) being fixed at \( z \), and hence the following can be obtained via Lemma A.4:

\[
\mathbb{E}_{(x, y) \sim P_{X,Y|z} \otimes n} \left[ \log \frac{1}{n} \sum_{j=1}^{n} e^{f(x, y_j, z)} \right] \leq D_{KL} (P \parallel Q) = D_{KL} (P_{X,Y|Z=z} \parallel P_{X|Z=z} P_{Y|Z=z}).
\]

The above inequality works for any function \( f(\cdot, \cdot, \cdot) \) and any \( z \sim P_Z \), and hence

\[
\sup_f E_z \sim P_z \left[ \mathbb{E}_{(x, y) \sim P_{X,Y|z} \otimes n} \left[ \log \frac{1}{n} \sum_{j=1}^{n} e^{f(x, y_j, z)} \right] \right] \leq E_{P_z} \left[ D_{KL} \left( P_{X,Y|Z} \parallel P_{X|Z} P_{Y|Z} \right) \right].
\]

A.3 Proof of Proposition 2.4 in the Main Text

Proposition A.8 (Weak-Conditional InfoNCE (WeaC-InfoNCE) for conditional contrastive learning, restating Proposition 2.4 in the main text),

\[
\text{WeaC−InfoNCE} := \sup_f E_z \sim P_z \left[ \mathbb{E}_{(x, y) \sim P_{X,Y|z} \otimes n} \left[ \log \frac{1}{n} \sum_{j=1}^{n} e^{f(x, y_j)} \right] \right] \\
\leq D_{KL} \left( P_{X,Y} \parallel E_{P_z} \left[ P_{X|Z} P_{Y|Z} \right] \right) = \text{Weak} \cdot \text{MI} (X; Y|Z) \leq \text{MI} (X; Y|Z).
\]

Proof. By defining \( P = P_{X,Y} \) and \( Q = E_{P_z} \left[ P_{X|Z} P_{Y|Z} \right] \), we have

\[
\mathbb{E}_{(x, y) \sim P, (x, y_2, n) \sim Q \otimes (n-1)} \left[ \log \frac{1}{n} \sum_{j=1}^{n} e^{f(x, y_j)} \right] = E_z \sim P_z \left[ \mathbb{E}_{(x, y) \sim P_{X,Y|z} \otimes n} \left[ \log \frac{1}{n} \sum_{j=1}^{n} e^{f(x, y_j)} \right] \right].
\]

Via Lemma A.4, we have

\[
\sup_f E_z \sim P_z \left[ \mathbb{E}_{(x, y) \sim P_{X,Y|z} \otimes n} \left[ \log \frac{1}{n} \sum_{j=1}^{n} e^{f(x, y_j)} \right] \right] \leq D_{KL} \left( P_{X,Y} \parallel E_{P_z} \left[ P_{X|Z} P_{Y|Z} \right] \right).
\]

Combing with Proposition A.6 that \( \text{Weak} \cdot \text{MI} (X; Y|Z) \leq \text{MI} (X; Y|Z) \), we conclude the proof.

A.4 Showing WeaC-InfoNCE is a lower bound of C-InfoNCE

Proposition A.9.

\[
\text{WeaC−InfoNCE} := \sup_f E_z \sim P_z \left[ \mathbb{E}_{(x, y) \sim P_{X,Y|z} \otimes n} \left[ \log \frac{1}{n} \sum_{j=1}^{n} e^{f(x, y_j)} \right] \right] \\
\leq \text{C−InfoNCE} := \sup_f E_z \sim P_z \left[ \mathbb{E}_{(x, y) \sim P_{X,Y|z} \otimes n} \left[ \log \frac{1}{n} \sum_{j=1}^{n} e^{f(x, y_j, z)} \right] \right].
\]
Proof. Let $f_1^*(x, y)$ be the function when the equality holds in WeaC-InfoNCE, and let $f_2^*(x, y, z) = f_1^*(x, y)$ ( $f_2^*(x, y, z)$ will not change $\forall z \sim P_Z$):

$$\text{WeaC - InfoNCE} := \mathbb{E}_{z \sim P_Z} \left[ \mathbb{E}_{(x_i, y_i) \sim P_{X,Y \mid z}} \log \frac{e^{f_1^*(x_i, y_i, z)}}{\sum_{j=1}^n e^{f_2^*(x_j, y_j, z)}} \right].$$

Since the equality holds with the supreme function in C-InfoNCE, and hence

$$\text{WeaC - InfoNCE} \leq C - \text{InfoNCE}.$$

\[\square\]

B Experimental setup

This section provides the experimental setup details of Section 3 in the main text, including hyperparameters, optimizers, code snippets, the total amount of computational resources, as well as more experimental results. Code, data, and instructions needed to reproduce the results are included in the released code under this anonymous link https://anonymous.4open.science/r/conditional_infonce-4232.

B.1 Speech Representation Learning

In this subsection, we provide experimental details of speech representation learning in Section 3.1 in the main text.

B.1.1 Dataset, Splits, and License

We use the Librispeech [33] dataset. The dataset is available at the link: https://www.openslr.org/12. It is a corpus of approximately 1,000 hours of English speech with a sampling rate of 16 kHz. There are three training splits, containing 100, 360, 500 hours of speech sequences, respectively. We use the 100 hour training split. There are also separate evaluation and test sets provided. The license of the dataset is Creative Commons Attribution 4.0 International. The dataset does not contain identifiable personality information.

B.1.2 Training Setups and Baseline Model

We use the 100-hour split from Librispeech to pretrain and fine-tune the models, and we use the predefined test set in the dataset to evaluate the models. We follow the baseline implemented in Rivière et al. [36], an implementation of InfoNCE on speech. In particular, given an input signal $x_{1:T}$ with $T$ being the time steps, we first pass it through an encoder $\phi_0$ parametrized by $\theta$ to produce a sequence of hidden representations $\{h_{1:T}\}$ where $h_t = \phi_0(x_t)$. Then, we obtain the contextual representation $c_t$ at time step $t$ with a sequential model $\psi_{\rho}$ parametrized by $\rho$: $c_t = \psi_{\rho}(h_1, \ldots, h_t)$, where $c_t$ contains context information before time step $t$.

For unsupervised pretraining, we select a multi-layer convolutional network as the encoder $\phi_0$, and we select a two-layer transformer with hidden dimension 256 as the sequential model $\psi_{\rho}$. Here, the positive pair is $(h_{t+k}, c_t)$ where $k$ is the number of time steps ahead, and the negative pairs are $(h_i, c_t)$, where $h_i$ hidden representations of a batch of random hidden representations assumed to be unrelated to $c_t$. The scoring function $f$ based on Equation (1) in the main text at step $t$ with $k$ steps ahead is $f_k = f_k(h, c_t) = \exp((h)^\top W_k c_t)$, where $W_k$ is a learnable linear transformation defined separately for each $k \in \{1, \ldots, K\}$ and $K$ is predetermined as 12 time steps. The loss will then be formulated as:

$$\ell^\text{InfoNCE}_t = -\frac{1}{K} \sum_{k=1}^K \frac{\exp(f_k(h_{t+k}, c_t))}{\sum_{h_i \in \mathcal{N}} \exp(f_k(h_i, c_t))} \right] \] \tag{5}$$

After the pretraining step, we then evaluate the network by the following: we first fix the pretrained model and add one additional linear classifier on top. We then fine-tune the linear classifier with
samples from the training split, but this time with labels. After fine-tuning, we fix both the pretrained model and the fine-tuned classifier and report the top-1 accuracy on the corresponding evaluation set (which in this case would be the “test-clean” split in Librispeech.)

B.1.3 C-InfoNCE and WeaC-InfoNCE

To implement the Conditional InfoNCE (C-InfoNCE) and the Weak-Conditional InfoNCE (WeaC-InfoNCE), for each update of the objective function, we sample a batch of sequences that comes from the same outcome of the conditioned variable $Z$ to calculate the loss function using C-InfoNCE or WeaC-InfoNCE. For instance, if we condition on speaker ID being Speaker 1, we first find all sequences that come from Speaker 1, and sample a batch of sequences from Speaker 1 to perform the calculation of C-InfoNCE or WeaC-InfoNCE. All positive and negative pairs would then be from Speaker 1. After we calculate C-InfoNCE or WeaC-InfoNCE and update the network parameters, we condition on a new outcome of speaker ID, say Speaker 2, and repeat the steps above. Which sequences are coming from which speakers are known as meta-data in the dataset, and the mapping from sequences to speakers is established at the beginning of training. For details, please refer to Line 361 to Line 408 in this file: https://github.com/facebookresearch/CPC_audio/blob/master/cpc/dataset.py.

In C-InfoNCE, we also need to include $z$, the speaker ID (or the sequence ID) in the network $f(\cdot)$. Since speaker or sequence IDs are indices, we convert the indices into an eight-dimension vector containing either 0 or 1 in each position for the speaker ID, or a sixteen-dimension vector for the sequence ID. Essentially, we convert the digital number of each speaker ID or sequence ID into its binary form and treat that as the $z$ vector. We then replace $f_k(h_{t+k}, c_t)$ with $f_k(h_{t+k}W_hz, c_tW_cz)$ in Equation 5, which results in the following formulation:

$$
\ell_{t}^{C{-}\text{InfoNCE}} = -\frac{1}{K} \sum_{k=1}^{K} \left[ \log \frac{\exp(f_k(h_{t+k}W_hz, c_tW_cz))}{\sum_{h_i \in \mathcal{N}} \exp(f_k(h_iW_hz, c_tW_cz))} \right]
$$

(6)

where $W_h$ and $W_c$ are two learnable linear transformations. For WC-InfoNCE, on the other hand, it follows the same loss function in Equation 5, as it does not require $z$ for $f(\cdot)$:

$$
\ell_{t}^{\text{WeaC{-}\text{InfoNCE}}} = -\frac{1}{K} \sum_{k=1}^{K} \left[ \log \frac{\exp(f_k(h_{t+k}, c_t))}{\sum_{h_i \in \mathcal{N}} \exp(f_k(h_i, c_t))} \right]
$$

(7)

B.1.4 Hyper-parameters and Optimization

We pretrain the network using the sequences in the 100–hour training set for 200 epochs. We set the batch size per GPU as 16, and sample 128 negative samples in each batch. We use the Adam optimizer [20], with a learning rate of $2e^{-4}$, $\beta_1 = 0.9$, $\beta_2 = 0.999$, and $\epsilon = 1e^{-8}$. We use a learning rate warm-up of 10. We fix all setups, including architecture, learning rate, and optimizer for InfoNCE, C-InfoNCE and WeaC-InfoNCE. For evaluation, we run 100 epochs using the pretrained model and the training sequences with labels; and we evaluate the fine-tuned model on the test split of Librispeech.

B.1.5 Computational Resource

The models are trained and evaluated on 4 RTX-2080Ti GPUs. 200 epochs of pretraining take 2 days.

B.2 Fair Representation Learning

In this subsection, we provide experimental details of fair representation learning in Section 3.2 in the main text.

B.2.1 Dataset, Splits, and License

We train our models on UCI German [10], UCI Adult [10] and Health Heritage [1] datasets, where we do not report the results for the third dataset in the main text.
WeaC-InfoNCE, we consider the same Lagrangian dual optimization process as L-MIFR, and we maximize $E_{p(x,y,z)} \left[ \log \frac{e^{f(x,y,z)}}{\sum_{j=1}^{n} e^{f(x,y,z_j)}} \right]$.

B.2.2 Training Setups and Baseline Methods

In the fair representation learning experiment, we first train models without labels by using contrastive self-supervised objectives: MIFR [38], L-MIFR [38], InfoNCE [31], C-InfoNCE and WeaC-InfoNCE. In this section, we first briefly review how MIFR and L-MIFR work.

For the optimization process for MIFR and L-MIFR, Song et al. [38] optimize $\max_\theta \max_\phi \mathbb{E}_{q_\phi(x,y,z)} \left[ \log p_\theta(x \mid y, z) \right]$, where $q_\phi$ and $p_\theta$ are two neural networks parameterized by $\phi \in \Phi$ and $\theta \in \Theta$. $q_\phi$ is used to approximate $P_{X \mid Y,Z}$ and $p_\theta$ is used to parameterize $P_X$. Furthermore, to ensure the optimization satisfies the constraint $MI(Y; Z) < \epsilon$, Song et al. [38] perform Lagrangian dual relaxation, where MIFR and L-MIFR consider different approaches to search for the Langrangian multipliers. The detailed discussion of this optimization is out of the scope in our paper, and readers can refer to the original paper for more clarification.

B.2.3 C-InfoNCE and WeaC-InfoNCE

The difference between the proposed C-InfoNCE/WeaC-InfoNCE and MIFR/L-MIFR from Song et al. [38] is the maximization of $MI(X; Y | Z)$. Unlike MIFR or L-MIFR Song et al. [38] which maximize $MI(X; Y | Z)$ by $E_{z \sim p_Z} \left( E_{(x_i,y_i) \sim P_{X,Y \mid z}} \left( \log \frac{e^{f(x_i,y_i)}}{\sum_{j=1}^{n} e^{f(x_j,y_j)}} \right) \right)$, C-InfoNCE maximizes $MI(X; Y | Z)$ by $E_{z \sim p_Z} \left( E_{(x_i,y_i) \sim P_{X,Y \mid z}} \left( \log \frac{e^{f(x_i,y_i)}}{\sum_{j=1}^{n} e^{f(x_j,y_j)}} \right) \right)$, and WeaC-InfoNCE maximizes $MI(X; Y | Z)$ by $E_{z \sim p_Z} \left( E_{(x_i,y_i) \sim P_{X,Y \mid z}} \left( \log \frac{e^{f(x_i,y_i)}}{\sum_{j=1}^{n} e^{f(x_j,y_j)}} \right) \right)$, respectively. In specific, for C-InfoNCE and WeaC-InfoNCE, we consider the same Lagrangian dual optimization process as L-MIFR, and we only change how we maximize $MI(X; Y | Z)$.

An implementation difference between C-InfoNCE and WeaC-InfoNCE is that the function $f(\cdot)$ in C-InfoNCE considers $Z$ as an input, while the function $f(\cdot)$ in WeaC-InfoNCE does not consider $Z$ as an input. Now, we discuss how we represent $Z$. For the UCI German dataset, $Z$ is a binary age indicator, and therefore $Z \in \{0, 1\}$. For the UCI Adult dataset, $Z$ is an indicator of male and female, and therefore $Z \in \{0, 1\}$. For the Health Heritage dataset, $Z$ is the Cartesian product of 9 age values and 2 genders, which in total we have 18 discrete values for $Z$. We use the binary representations for $Z$, and therefore $Z \in \{0, 1\}^5$ (a 5-dimensional vector).

1. https://www.kaggle.com/c/hhp
2. https://archive.ics.uci.edu/ml/datasets/statlog+(german+credit+data)
3. https://archive.ics.uci.edu/ml/datasets/health+heritage
4. https://archive.ics.uci.edu/ml/datasets/german+credit+data
5. https://archive.ics.uci.edu/ml/datasets/adult
B.2.4 Hyper-parameters and Optimization

We assume the model does not have access to labels during training; instead, it takes in the input and sensitive attributes. We follow Song et al. [38], where we consider maximizing the conditional mutual information given the fairness constraint. All neural networks for approximating distributions in MIFR and L-MIFR are two-layer neural networks. The \( f(\cdot) \)'s in C-InfoNCE and WeaC-InfoNCE are also two-layer networks. After pretraining, we use logistic regression classifiers over the representation \( Y \) for prediction tasks. We use \( \lambda_1 = \lambda_2 = 1.0 \) for optimization in MIFR, initialize \( \lambda_1 = \lambda_2 = 1.0 \) for L-MIFR and allow a range of \((0.01, 100)\), and fix \( \epsilon_1 = \epsilon_2 = 0.1 \) for all experimental settings. We use the Adam optimizer with learning rate \( 1e^{-3} \) and \( \beta_1 = 0.5 \) where the learning rate is multiplied by 0.98 every 1000 optimization iterations. For the Adult and the Health dataset, we optimize for 2000 epochs; we optimize for 10000 epochs for the German dataset.

B.2.5 Additional Results

Table 4 presents the new results for ROC-AUC on Health dataset. Note that we do not provide the \( \Delta_{DP} \) results since \( \Delta_{DP} \) is only defined for binary attributes, while the Health dataset considers 18 sensitive attributes. We find our methods (C-InfoNCE and WeaC-InfoNCE) work the best and C-InfoNCE outperforms WeaC-InfoNCE.

Next, on the UCI Adult dataset, we provide new results for other fairness criteria. Following Song et al. [38], we consider three fairness criteria: Demographic Parity, Equalized Odds, and Equalized Opportunity. Specifically, we consider these notions in terms of mutual information measurements constructed by the corresponding definition of each notion. For example, Demographic Parity requires that the representation \( Y \) and sensitive attribute \( Z \) are independent. From a mutual information perspective, that means \( Y \) and \( Z \) should have low mutual information, which is \( I_{DP} = \text{MI} (Y; Z) \). The second fairness criterion, the Equalized Odds, requires a classifier to predict labels equally well for all sensitive attribute values. In this case, the requirement is equivalent to \( Y \) and \( Z \) have low mutual information given the label, which is \( I_{EO} = \text{MI} (Y; Z|\text{label}) \). The third criteria, the Equalized Opportunity, considers \( y = 1 \) as a preferred label (a label that confers an advantage or benefit) and requires a classifier to predict the preferred label equally well for all sensitive attribute values. That is to say, we require that \( Y \) and \( Z \) have low mutual information given label \( = 1 \), which is \( I_{EOpp} = \text{MI} (Y; Z|\text{label} = 1) \). Readers can refer to [38] for more details.

From Table 5, C-InfoNCE achieves the lowest level of mutual information measurements on different fairness criteria, suggesting the representation learned through C-InfoNCE satisfies different fairness criteria better than other baselines when we measure different criteria using mutual information. We also notice that in both cases, WeaC-InfoNCE performs close to C-InfoNCE, achieving competitive downstream performance while preserving almost the same level of fairness as C-InfoNCE.

B.2.6 Computational Resource

We use one RTX-2080Ti GPU for training these datasets, and training 10,000 epochs on German, the longest among three datasets, takes six hours.

B.3 Multi-domain Visual Learning

In this subsection, we provide experimental details of multi-domain visual representation learning in Section 3.3 in the main text.

B.3.1 Dataset, Splits, and License

We train our models on CIFAR-10 [22], Tiny ImageNet [24] and SUN 397 [48]. CIFAR-10 [22] is an object detection dataset with 60,000 32 × 32 images in 10 classes. The test sets includes 10,000 images. Tiny ImageNet [24] is a scaled-down version of ImageNet dataset for object detection, with 100,000 64 × 64 images in 200 classes for training, and 10,000 test images for evaluation. SUN 397 dataset [48] is a scene understanding dataset with 108,753 images of 397 categories. We randomly partition the dataset into 76,128 images for training, 10,875 images for validation, and 21,750 images for testing. All three datasets are licensed under the Creative Commons Attribution 4.0 License.
Table 4: Results for the area under the ROC curve (ROC AUC, higher means better downstream performance) for fair representation learning on Health datasets. The conditioned variable (Z, the sensitive attributes) is the Cartesian product of two gender choices and nine age values. X are the input, and Y are the learned representations.

| Objective                                      | Health Heritage (ROC AUC (↑)) |
|------------------------------------------------|-------------------------------|
| Unconditional Self-supervised Learning         | max MI (X; Y) s.t. MI (Y; Z) < 0.1 |
| InfoNCE [31]                                   | 0.57                          |
| Conditional Self-supervised Learning (Z = Age × Gender) | max MI (X; Y|Z) s.t. MI (Y; Z) < 0.1 |
| L-MIFR [38]                                    | 0.63                          |
| MIFR [38]                                      | 0.56                          |
| C-InfoNCE (ours)                               | **0.66**                      |
| WeaC-InfoNCE (ours)                            | 0.65                          |

Table 5: Results for mutual information measurements of different fairness notions: Demographic Parity, Equalized Odds, and Equalized Opportunity (lower means better fairness) for fair representation learning on Adult datasets. The conditioned variable (Z, the sensitive attributes) is the gender attribute. X are the input, and Y are the learned representations.

| Objective                                      | I_{DP} = MI (Y; Z) (↓) | UCI Adult | I_{EO} (↓) | I_{EOpp} (↓) |
|------------------------------------------------|-------------------------|-----------|------------|-------------|
| Unconditional Self-supervised Learning         | max MI (X; Y) s.t. MI (Y; Z) < 0.1 |
| InfoNCE [31]                                   | 0.09                    | 0.10      | 0.07       |
| Conditional Self-supervised Learning (Z = Age or Gender) | max MI (X; Y|Z) s.t. MI (Y; Z) < 0.1 |
| L-MIFR [38]                                    | 0.08                    | 0.09      | 0.04       |
| MIFR [38]                                      | 0.13                    | 0.11      | 0.09       |
| C-InfoNCE (ours)                               | **0.06**                | **0.08**  | 0.04       |
| WeaC-InfoNCE (ours)                            | 0.07                    | **0.08**  | 0.04       |

B.3.2 Training Setups

We consider four different experimental settings: 1) uni-domain unconditional self-supervised learning using InfoNCE, 2) multi-domain unconditional self-supervised learning using InfoNCE, 3) multi-domain conditional self-supervised learning using C-InfoNCE, and 4) multi-domain conditional self-supervised learning using WeaC-InfoNCE. All the experiments are provided in https://anonymous.4open.science/r/conditional_infonce-4232.

Uni-domain Unconditional Self-supervised Learning using InfoNCE. This setting considers the exact same setup as SimCLR [5]. In particular, we perform pretraining on a single dataset and then evaluates the pretrained model on the same dataset. ResNet-50 [17] is chosen as the backbone model for performing the self-supervised pretraining. Note that we remove the last classifier layer in ResNet-50, and we consider 2048-2048-128 multi-layer perceptrons (MLPs) with ReLU non-linearity as the projection head in InfoNCE (g(·) in f(·) in InfoNCE).

After the pretraining, we consider the linear evaluation protocol [5], which fixes the pretrained encoder, removes the projection head, and adopts a linear classifier on top of the pretrained encoder. The linear classifier is fine-tuned with the downstream labels. Note that both the pretraining and the fine-tuning steps are performed on the training samples.

For evaluation, we fix the pretrained encoder as well as the linear classifier. We then report the evaluation accuracy on the test samples.
Multi-domain Unconditional Self-supervised Learning using InfoNCE. This setting is similar to the previous setting with two differences: 1) the composition of the data batch and 2) the network designs.

The composition of the data batch for input. Under the uni-domain setting, we consider the data only from a single dataset within a data batch. On the contrary, under the multi-domain setting, we consider the data from the three datasets within a data batch. Note that we ensure the same data batch size for both the uni-domain and the multi-domain setting. Particularly, for the uni-domain setting, we consider the data batch size 960. For the multi-domain setting, we consider the data batch size 320 for each dataset, resulting in 960 data batch size in total.

The network designs. We select the ResNet-50 as the feature encoder model. Nonetheless, under the multi-domain setting, images from different datasets can be of different sizes. Hence, for the few building blocks of the ResNet-50, we consider three separate blocks of $CONV − BN − RELU − MAXPOOL$ to handle various image sizes. The rest of the ResNet-50 model is shared for all three datasets.

Same as the uni-domain setting, the multi-domain setting considers the projection head on top of the multi-dataset 960-batched data after the feature encoder. The projection head is considering in the pretraining stage that uses InfoNCE. The fine-tuning stage considers different linear classifiers for different datasets.

Multi-domain Conditional Self-supervised Learning using C-InfoNCE. We also make the discussions based on the composition of the data batch and the network designs.

The composition of the data batch for input. The multi-domain conditional setting considers the domain specification (the dataset ID) as the conditioned variable, and hence each batch of the input data comes from the same conditioned value. In specific, the data within a data batch are always from the same dataset, not mixing the data from three datasets as in the multi-domain unconditional setting. In particular, we first sample the dataset ID (randomly choosing among CIFAR-10, Tiny ImageNet, and SUN 397), and then we sample 960 images from the selected dataset to form a data batch.

The network designs. We consider the same design of the feature encoder model as the design under the multi-domain unconditional setting.

The difference between the multi-domain unconditional setting and the multi-domain conditional setting using C-InfoNCE is the projection head. In particular, the function $f(\cdot)$ takes in representations $x, y$ as the input under multi-domain unconditional setting, while the function $f(\cdot)$ takes in representations $x, y$ as well as the conditional value $z$ as input under multi-domain conditional setting using C-InfoNCE. For the latter setting, we design $f(x, y, z) = \text{cosine similarity with temperature}(g(x, z), g(y, z))$ as cosine similarity with temperature $(g_z(x), g_z(y))$. $g_z(\cdot)$ represents the projection head considers for the conditioned value $z$ (in our case $Z$ is the dataset specification). Hence, we consider different projection heads for different datasets. The projection head is considering in the pretraining stage that uses InfoNCE. The fine-tuning stage considers different linear classifiers for different datasets.

Multi-domain Conditional Self-supervised Learning using WeaC-InfoNCE. We also make the discussions based on the composition of the data batch and the network designs.

The composition of the data batch for input. The composition of the data batch for input is exactly the same between multi-domain conditional setting using C-InfoNCE and WeaC-InfoNCE. The network designs. We consider the same design of the feature encoder model as the design under the multi-domain unconditional setting.

Different from the the multi-domain conditional setting using C-InfoNCE, we share the same projection head among datasets for WeaC-InfoNCE. The reason is that the function $f(\cdot)$ takes in only the representations $x, y$ as input for WeaC-InfoNCE. Hence, we design $f(x, y)$ as $f(x, y) = \text{cosine similarity with temperature}(g(x), g(y))$. $g(\cdot)$ represents the projection head that is shared among all datasets. The projection head is considering in the pretraining stage that uses InfoNCE. The fine-tuning stage considers different linear classifiers for different datasets.
We discuss briefly on how the two baselines, classifier-based and difference-based estimation work.

We use four RTX-2080Ti GPUs for pretraining, and the setting with the slowest speed, the multi-

500

We train the model for

epochs. We only tune one hyper-parameter, the temperature parameter \( \tau \) in the contrastive objectives by grid search, and the optimal value we found is 0.5.

### B.3.4 Computational Resource

We use four RTX-2080Ti GPUs for pretraining, and the setting with the slowest speed, the multi-

domain conditional training via C-InfoNCE, takes 2.5 days to train for 500 epochs.

### B.4 Conditional Mutual Information Estimation

In this section, we seek to understand if the proposed C-InfoNCE and WeaC-InfoNCE can estimate the conditional mutual information accordingly, as both of them are lower bounds of conditional mutual information. We compare the two with other different conditional mutual information estimators: classifier-based estimator [29] and difference-based estimator [29]. InfoNCE estimates \( \text{MI}(X;Z) \) but not the conditional mutual information, \( \text{MI}(X;Y|Z) \), thus we do not compare with it here. We base our implementation on prior work [29, 40].

#### B.4.1 Dataset, Splits, and License

Following [29], we generate two separate datasets based on two linear models, with three random variables \( X, Y \) and \( Z \), where \( X \) and \( Y \) is 1-dimensional while dimension \( z \) can scale. The two datasets are the following:

**Dataset I:** \( X \sim \mathcal{N}(0,1); Z \sim \mathcal{U}(-0.5,0.5)^d_z; \epsilon \sim \mathcal{N}(Z_1, \sigma_\epsilon^2); Y \sim X + \epsilon \)

**Dataset II:** \( X \sim \mathcal{N}(0,1); Z \sim \mathcal{N}(0,1)^d_z; U = w^TZ, \|w\|_1 = 1; \epsilon \sim \mathcal{N}(U, \sigma_\epsilon^2); Y \sim X + \epsilon \)

where \( \mathcal{U}(-0.5,0.5)^d_z \) means each coordinate of \( Z \) is drawn i.i.d. from a uniform distribution between \(-0.5 \) and \( 0.5 \). \( Z_1 \) is the first dimension of \( Z \). We set \( \sigma_\epsilon^2 = 0.1 \) (the same as [29]) and obtain unit norm random vector \( w \) from \( \mathcal{N}(0, I_{d_z}) \) and keep it constant. In Dataset I, \( Y \) only depends on \( Z_1 \), while in Dataset II the variables \( Y \) depends on all dimensions in \( Z \). For both setting we vary either the number of samples or dimension \( d_z \). For both these datasets, the sample size is varied as \( n \in \{5000, 10000, 20000, 50000\} \) keeping \( d_z \) fixed at 20. We also vary \( d_z \in \{1, 10, 20, 50, 100\} \), keeping sample size fixed at \( n = 20000 \). To split the dataset into the train set and the test set, the first two-thirds of the synthetic samples will be in the train set, and the rest will be in the test set. The dataset can be generated by the codebase we provide, and is open for public usage.

#### B.4.2 Training Setups and Baseline Models

We discuss briefly on how the two baselines, classifier-based and difference-based estimation work. Classifier-based estimation [29] is to train a classifier that could distinguish points from different distributions. To start with, recall the definition of conditional mutual information:

\[
\text{MI}(X;Y|Z) := \int_Z D_{KL}(P_{X,Y|Z} \| P_{X|Z} P_{Y|Z}) \, dP_Z = \int_Z D_{KL}(P_{X,Y|Z} \| P_{X,Z} P_{Y|Z}) \, dP_Z 
\]

Classifier-based method use \( \int_Z D_{KL}(P_{X,Y,Z} \| P_{X,Z} P_{Y|Z}) \, dP_Z \) to estimate conditional mutual information. To be specific, given \( n \) i.i.d samples \( \{(x_i, y_i, z_i)\}_{i=1}^n \), \( (x_i, y_i, z_i) \sim P_{X,Y,Z} \), Mukherjee et al. [29] use the generative model GAN [14] to model the conditional distribution \( P(Y|Z) \). For notation simplicity, we refer the GAN model as \( P^{\text{GAN}}(Y|Z) \). Given samples from the joint distribution, \( P_{X,Y,Z} \), and samples from \( P_{X,Z} P^{\text{GAN}}(Y|Z) \), classifier-based method labels the points drawn from \( P_{X,Y,Z} \) as \( label = 1 \) and the points from \( \hat{P}_{X,Z} P^{\text{GAN}}(Y|Z) \) as \( label = 0 \). Then, it trains a binary classifier for predicting the assigned binary label. Then the point-wise likelihood ratio \( \frac{p(x,y,z)}{p(x,z)p^{\text{GAN}}(y|z)} \) of each data point \((x_i, y_i, z_i)\) can be calculated by \( \frac{p_{Pr(label=1|(x_i, y_i, z_i))}}{1-p_{Pr(label=1|(x_i, y_i, z_i))}} \), where
Using the point-wise likelihood, we can obtain \( I(X;Y|Z) = \int_Z P_{KL}(P_{X,Y,Z} || P_X Z P_{Y|Z})dP_Z \) by plugging the point-wise likelihood into a lower bound of KL-divergence. Further discussions of this classifier-based estimation method is out of the scope of our discussion, and readers could refer to Mukherjee et al. [29] for more details.

Mukherjee et al. [29] further presents the difference-based method that represents the conditional mutual information as the difference between two mutual information quantities: \( I(X; Y|Z) = I(X; Y) - I(X; Z) \). Then, it considers the classifier-based estimation for both \( I(X; Y|Z) \) and \( I(X; Z) \).

### B.4.3 C-InfoNCE and WeaC-InfoNCE

On the other hand, the proposed C-InfoNCE and WeaC-InfoNCE are different. Given the formulations of C-InfoNCE and WeaC-InfoNCE:

\[
C - \text{InfoNCE} := \sup_{f} E_{x \sim P_{X}} \left[ \mathbb{E}_{(x_i, y_i) \sim P_{X,Y|Z}} \log \frac{e^{f(x_i, y_i)}}{\sum_{j=1}^{n} e^{f(x_j, y_j)}} \right] \leq \text{MI}(X; Y|Z), \tag{9}
\]

and

\[
\text{WeaC - InfoNCE} := \sup_{f} E_{x \sim P_{X}} \left[ \mathbb{E}_{(x_i, y_i) \sim P_{X,Y|Z}} \log \frac{e^{f(x_i, y_i)}}{\sum_{j=1}^{n} e^{f(x_j, y_j)}} \right] \leq \text{MI}(X; Y|Z) \tag{10}
\]

Given samples \((x, y, z)\) from the joint distribution \(P_{X,Y,Z}\), we want to sample from the conditional distribution \(P_{X,Y|Z}\) and from the product of conditional marginals \(P_{X|Z} P_{Y|Z}\). To be able to sample from \(P_{X,Y|Z}\) and \(P_{X|Z} P_{Y|Z}\), we first cluster the value of \(Z \in (-0.5, 0.5)\) to \(K\) clusters, \(\left\{ C_1, C_2, \ldots, C_k \right\}\) by performing K-mean clustering on it, with corresponding cluster centers \(\left\{ z_1, z_2, \ldots, z_K \right\}\). In our deployment, we set \(K = 10\). We can then sample the data points \((x, y, z) \sim P_{X,Y|Z=Z_m}\) by sampling from the set \(\left\{ (x, y, z) : z \in \text{cluster } C_m \right\}\). To sample from \(P_{X|Z=Z_m} P_{Y|Z=Z_m}\), we sample from the set \(\left\{ (x_i, y_i, z) : z \in \text{cluster } C_m \right\}\) where \(x_i\) and \(y_i\) come from different data points. For C-InfoNCE, we plug in the point \((x, y, z)\) into Equation 9 using \(f(x, y, z) = g_x(x) W_{xz} \cdot g_y(y) W_{yz}\) where \(W_{xz}\) and \(W_{yz}\) are learnable transformations, and \(g_x(\cdot)\) and \(g_y(\cdot)\) are two-layer fully connected neural networks with hidden dimension 64. For WeaC-InfoNCE, we plug in the point \((x, y, z)\) into Equation 10 using \(f(x, y) = g_x(x) \cdot g_y(y)\) as \(Z\) is not an input of WeaC-InfoNCE.

![Figure 1](image-url)

**Figure 1:** Conditional mutual information estimation on two datasets generated by two linear models. The proposed C-InfoNCE and WeaC-InfoNCE estimates conditional mutual information better than other baselines on both datasets and on two settings, either by fixing sample size \(n = 20,000\) and varying the dimension of the conditioned variable \(d_Z\), or fixing the dimension \(d_Z = 20\) and vary sample sizes.

### B.4.4 Hyper-parameters and Optimization

We use two-layer neural networks for the classifier in the classifier-based or difference-based methods and also for \(g(\cdot)\) in C-InfoNCE and WeaC-InfoNCE. The hidden dimension is 64. We use a batch size of 64 and an Adam optimizer with \(\beta_1 = 0.5\) and \(\beta_2 = 0.9\), with a learning rate of \(1e - 4\). We train for 100 epochs and use ReLU as the activation function.

### B.4.5 Results and Discussions

In Figure 1 we show the conditional mutual information estimation results. The proposed conditional methods can estimate mutual information better than classifier or difference-based methods under the
same dimension of $Z$ in sub-figure (a) and (c), and the estimations degrade less severely compared to other methods when we vary the dimension of $Z$ to as large as 200 (sub-figure (b) and (d)). We show that C-InfoNCE and WeaC-InfoNCE can be good tools for conditional mutual information estimation.

### B.4.6 Computational Resource

We use one RTX-2080Ti GPU for training on the two datasets, and training 20 epochs take less than one hour.