Rethinking Minimal Sufficient Representation in Contrastive Learning

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Abstract

Contrastive learning between different views of the data achieves outstanding success in the field of self-supervised representation learning and the learned representations are useful in broad downstream tasks. Since all supervision information for one view comes from the other view, contrastive learning approximately obtains the minimal sufficient representation which contains the shared information and eliminates the non-shared information between views. Considering the diversity of the downstream tasks, it cannot be guaranteed that all task-relevant information is shared between views. Therefore, we assume the non-shared task-relevant information cannot be ignored and theoretically prove that the minimal sufficient representation in contrastive learning is not sufficient for the downstream tasks, which causes performance degradation. This reveals a new problem that the contrastive learning models have the risk of over-fitting to the shared information between views. To alleviate this problem, we propose to increase the mutual information between the representation and input as regularization to approximately introduce more task-relevant information, since we cannot utilize any downstream task information during training. Extensive experiments verify the rationality of our analysis and the effectiveness of our method. It significantly improves the performance of several classic contrastive learning models in downstream tasks. Our code is available at https://github.com/Haoqing-Wang/InfoCL.

1. Introduction

Recently, contrastive learning [6–8, 18, 51] between different views of the data achieves outstanding success in the field of self-supervised representation learning. The learned representations are useful for broad downstream tasks in practice, such as classification, detection and segmentation [20]. In contrastive learning, the representation that contains all shared information between views is defined as sufficient representation, while the representation that contains only the shared and eliminates the non-shared information is defined as minimal sufficient representation [43]. Contrastive learning maximizes the mutual information between the representations of different views, thereby obtaining the sufficient representation. Furthermore, since all supervision information for one view comes from the other view [15], the non-shared information is often ignored, so that the minimal sufficient representation is approximately obtained.

Tian et al. [40] find that the optimal views for contrastive learning depend on the downstream tasks when the minimal sufficient representation is obtained. In other words, the optimal views for task $T_1$ may not be suitable for task $T_2$. The reason may be that some information relevant to $T_2$ is not shared between these views. In this work, we formalize this conjecture and assume that the non-shared task-relevant information cannot be ignored. Based on this assumption, we theoretically prove that the minimal sufficient representation contains less task-relevant information than other sufficient representations and has a non-ignorable gap with the optimal representation, which causes performance degradation. Concretely, we consider two types of the downstream task, i.e., classification and regression task, and prove that the lowest achievable error of the minimal sufficient representation is higher than other sufficient representations.

According to our analysis, when some task-relevant information is not shared between views, the learned representation in contrastive learning is not sufficient for the downstream tasks. This reveals that the contrastive learning
models have the risk of over-fitting to the shared information between views. To this end, we need to introduce more non-shared task-relevant information to the representations. Since we cannot utilize any downstream task information in the training stage, it is impossible to achieve this directly. As an alternative, we propose an objective term which increases the mutual information between the representation and input to approximately introduce more task-relevant information. This motivation is demonstrated in Fig. 1 using information diagrams. We consider two implementations to increase the mutual information. The first one reconstructs the input to make the representations containing the key information about the input [26,44]. The second one relies on the high-dimensional mutual information estimate [5,34].

Overall, we summarize our contributions as follows.

- To the best of our knowledge, this is the first work to theoretically reveal that contrastive learning has the risk of over-fitting to the shared information between views. We provide comprehensive analysis based on the internal mechanism of contrastive learning that the views provide supervision information to each other.

- To alleviate this problem, when the downstream task information is not available, we propose to increase the mutual information between the representation and input to approximately introduce more task-relevant information, as shown in Fig. 1.

- We verify the effectiveness of our method for SimCLR [7], BYOL [18] and Barlow Twins [51] in classification, detection and segmentation tasks. We also provide extensive analytical experiments to further understand our hypotheses, theoretical analysis and model.

2. Related works

Contrastive learning. Contrastive learning between different views of the data is a successful self-supervised representation learning framework. The views are constructed by exploiting the structure of the unlabeled data, such as local patches and the whole image [23], different augmentations of the same image [2,7,20,48], or video and text pairs [31,38]. Recently, Tian et al. [40] find that the optimal views for contrastive learning are task-dependent under the assumption of minimal sufficient representation. In other words, even if the given views are optimal for some downstream tasks, they may not be suitable for other tasks. In this work, we theoretically analyze this discovery and find that the contrastive learning models may over-fit to the shared information between views, and thus propose to increase the mutual information between representation and input to alleviate this problem. Some recent works [15,43] propose to learn the minimal sufficient representation. They assume that almost all the information relevant to downstream tasks is shared between views, which is an overly idealistic assumption and conflicts with the discovery in [40].

Information bottleneck theory. Based on the information bottleneck theory [36,41,42], a model extracts all task-relevant information in the first phase of learning (drift phase) to ensure sufficiency, and then compresses the task-irrelevant information in the second phase (diffusion phase). Our analysis shows that the learned representation in contrastive learning is not sufficient for the downstream tasks and can be seen as in the drift phase. We need to introduce more task-relevant information to achieve sufficiency.

3. Theoretical analysis and model

In this section, we first introduce the contrastive learning framework and theoretically analyze the disadvantages of minimal sufficient representation in contrastive learning, and then propose our method to approximately introduce more task-relevant information to the representations. Note that although the analysis is about the information content in the representations, its specific form is also very important. Therefore, our theoretical analysis is actually based on the premise that the information content in the representations is represented in the most appropriate form.

3.1. Contrastive learning

Contrastive learning is a general framework for unsupervised representation learning which maximizes the mutual information between the representations of two random variables \(v_1\) and \(v_2\) with the joint distribution \(p(v_1, v_2)\)

\[
\max_{f_1, f_2} I(z_1, z_2)
\]

where \(z_i = f_i(v_i), i = 1, 2\) are also random variables and \(f_i, i = 1, 2\) are encoding functions. In practice, \(v_1\) and \(v_2\) are usually two views of the data \(x\). When \(v_1\) and \(v_2\) have the same marginal distributions \((p(v_1) = p(v_2))\), the function \(f_1\) and \(f_2\) can be the same \((f_1 = f_2)\).
In contrastive learning, the variable $v_2$ provides supervision information for $v_1$ and plays the similar role as the label $y$ in the supervised learning, and vice versa [15]. This internal mechanism is illustrated in Fig. 2. Similar to the information bottleneck theory [1,42] in the supervised learning, we can define the sufficient representation and minimal sufficient representation of $v_1$ (or $v_2$) for $v_2$ (or $v_1$) in contrastive learning [40,43].

**Definition 1. (Sufficient Representation in Contrastive Learning)** The representation $z_1^{suf}$ of $v_1$ is sufficient for $v_2$ if and only if $I(z_1^{suf}, v_2) = I(v_1, v_2)$.

The sufficient representation $z_1^{suf}$ of $v_1$ keeps all the information about $v_2$ in $v_1$. In other words, $z_1^{suf}$ contains all the shared information between $v_1$ and $v_2$, i.e., $I(v_1, v_2|z_1^{suf}) = 0$. Symmetrically, the sufficient representation $z_2^{suf}$ of $v_2$ for $v_1$ satisfies $I(v_1, z_2^{suf}) = I(v_1, v_2)$.

**Definition 2. (Minimal Sufficient Representation in Contrastive Learning)** The sufficient representation $z_1^{min}$ of $v_1$ is minimal if and only if $I(z_1^{min}, v_1) \leq I(z_1^{suf}, v_1), \forall z_1^{suf}$ that is sufficient.

Among all sufficient representations, the minimal sufficient representation $z_1^{min}$ contains the least information about $v_1$. Further, it is usually assumed that $z_1^{min}$ only contains the shared information between views and eliminates other non-shared information, i.e., $I(z_1^{min}, v_1|v_2) = 0$.

Applying Data Processing Inequality [11] to the Markov chain $v_1 \rightarrow v_2 \rightarrow z_2$ and $z_2 \rightarrow v_1 \rightarrow z_1$, we have

$$I(v_1, v_2) \geq I(v_1, z_2) \geq I(z_1, z_2) \quad (2)$$

i.e., $I(v_1, v_2)$ is the upper bound of $I(z_1, z_2)$. Considering that $I(v_1, v_2)$ remains unchanged during the optimization process, contrastive learning optimizes the functions $f_1$ and $f_2$ so that $I(z_1, z_2)$ approximates $I(v_1, v_2)$. When these functions have enough capacity and are well learned based on sufficient data, we can assume $I(z_1, z_2) = I(v_1, v_2)$, which means the learned representations in contrastive learning are sufficient. They are also approximately minimal since all supervision information comes from the other view. Therefore, the shared information controls the properties of the representations.

The learned representations in contrastive learning are typically used in various downstream tasks, so we introduce a random variable $T$ to represent the information required for a downstream task which can be classification, regression or clustering task. Tian et al. [40] find that the optimal views for contrastive learning are task-dependent under the assumption of minimal sufficient representation. This discovery is intuitive since various downstream tasks need different information that is unknown during training.

It is difficult for the given views to share all the information required by these tasks. For example, when one view is a video stream and the other view is an audio stream, the shared information is sufficient for identity recognition task, but not for object tracking task. Some task-relevant information may not lie in the shared information between views, i.e., $I(v_1, T|v_2)$ cannot be ignored. Eliminating all non-shared information has the risk of damaging the performance of the representations in the downstream tasks.

### 3.2. Analysis on minimal sufficient representation

The minimal sufficient representation intuitively is not a good choice for downstream tasks, because it completely eliminates the non-shared information between views which may be important for some downstream tasks. We formalize this problem and theoretically prove that in contrastive learning, the minimal sufficient representation is expected to perform worse than other sufficient representations in the downstream tasks. All proofs for the below theorems are provided in Appendix.

Considering the symmetry between $v_1$ and $v_2$, without loss of generality, we take $v_2$ as the supervision signal for $v_1$ and take $v_1$ as the input of a task. It is generally believed that the more task-relevant information contained in the representations, the better performance can be obtained [11, 14]. Therefore, we examine the task-relevant information contained in the representations.

**Theorem 1. (Task-Relevant Information in Representations)** In contrastive learning, for a downstream task $T$, the minimal sufficient representation $z_1^{min}$ contains less task-relevant information from input $v_1$ than other sufficient representation $z_1^{suf}$, and $I(z_1^{min}, T)$ has a gap of $I(v_1, T|v_2)$ with the upper bound $I(v_1, T)$. Formally, we have

$$I(v_1, T) = I(z_1^{min}, T) + I(v_1, T|v_2) \geq I(z_1^{suf}, T) = I(z_1^{min}, T) + I(z_1^{suf}, T|v_2) \geq I(z_1^{min}, T)$$

(3)
Theorem 1 indicates that $z_{1}^{\text{su}}$ can have better performance in task $T$ than $z_{1}^{\text{min}}$ because it contains more task-relevant information. When non-shared task-relevant information $I(v_1, T|v_2)$ is significant, $z_{1}^{\text{min}}$ has poor performance because it loses a lot of useful information. See Fig. 3 for the demonstration using information diagrams. To make this observation more concrete, we examine two types of the downstream task: classification tasks and regression tasks, and provide theoretical analysis on the generalization error of the representations.

When the downstream task is a classification task and $T$ is a categorical variable, we consider the Bayes error rate $[16]$ which is the lowest achievable error for any classifier learned from the representations. Concretely, let $P_{e}$ be the Bayes error rate of arbitrary learned representation $z_1$ and $T$ be the prediction for $T$ based on $z_1$, have $P_{e} = 1 - \mathbb{E}_{p(z_1)}[\max_{v_i \in \mathbb{Y}} p(\hat{T} = t|z_1)]$ and $0 \leq P_{e} \leq 1 - 1/|T|$ where $|T|$ is the cardinality of $T$. According to the value range of $P_{e}$, we define a threshold function $\Gamma(x) = \min\{\max\{x, 0\}, 1 - 1/|T|\}$ to prevent overflow.

**Theorem 2.** (Bayes Error Rate of Representations) For arbitrary learned representation $z_1$, its Bayes error rate $P_{e} = \Gamma(\hat{P}_{e})$ with

$$P_{e} \leq 1 - \exp[-(H(T) - I(z_1, T|v_2) - I(z_1, v_2, T))] \tag{4}$$

Specifically, for sufficient representation $z_{1}^{\text{su}}$, its Bayes error rate $P_{\text{e}}^{\text{su}} = \Gamma(P_{\text{e}}^{\text{su}})$ with

$$P_{\text{e}}^{\text{su}} \leq 1 - \exp[-(H(T) - I(z_{1}^{\text{su}}, T|v_2) - I(v_1, v_2, T))] \tag{5}$$

for minimal sufficient representation $z_{1}^{\text{min}}$, its Bayes error rate $P_{\text{e}}^{\text{min}} = \Gamma(P_{\text{e}}^{\text{min}})$ with

$$P_{\text{e}}^{\text{min}} \leq 1 - \exp(-(H(T) - I(v_1, v_2, T))] \tag{6}$$

Since $I(z_{1}^{\text{su}}, T|v_2) \geq 0$, Theorem 2 indicates for classification task $T$, the upper bound of $P_{\text{e}}^{\text{min}}$ is larger than $P_{\text{e}}^{\text{su}}$. In other words, $z_{1}^{\text{min}}$ is expected to obtain a higher classification error rate in the task $T$ than $z_{1}^{\text{su}}$. According to the Eq. (5), considering that $H(T)$ and $I(v_1, v_2, T)$ are not related to the representations, increasing $I(z_{1}^{\text{su}}, T|v_2)$ can reduce the Bayes error rate in classification task $T$. When $I(z_{1}^{\text{su}}, T|v_2) = I(v_1, T|v_2)$, $z_{1}^{\text{su}}$ contains all the useful information for task $T$ in $v_1$.

When the downstream task is a regression task and $T$ is a continuous variable, let $\hat{T}$ be the prediction for $T$ based on arbitrary learned representation $z_1$, we consider the smallest achievable expected squared prediction error $R_{e} = \min_{\alpha} \mathbb{E}[(T - \hat{T}(z_1))^2] = \mathbb{E}[\epsilon^2]$ with $\epsilon(T, z_1) = T - \mathbb{E}[T|z_1]$.

**Theorem 3.** (Minimum Expected Squared Prediction Error of Representations) For arbitrary learned representation $z_1$, when the conditional distribution $p(\epsilon|z_1)$ is uniform, Laplacian or Gaussian distribution, the minimum expected squared prediction error $R_{e}$ satisfies

$$R_{e} = \alpha \cdot \exp[2 \cdot (H(T) - I(z_1, T|v_2) - I(z_1, v_2, T))] \tag{7}$$

Specifically, for sufficient representation $z_{1}^{\text{su}}$, its minimum expected squared prediction error $R_{e}^{\text{su}}$ satisfies

$$R_{e}^{\text{su}} = \alpha \cdot \exp[2 \cdot (H(T) - I(z_{1}^{\text{su}}, T|v_2) - I(v_1, v_2, T))] \tag{8}$$

for minimal sufficient representation $z_{1}^{\text{min}}$, its minimum expected squared prediction error $R_{e}^{\text{min}}$ satisfies

$$R_{e}^{\text{min}} = \alpha \cdot \exp[2 \cdot (H(T) - I(v_1, v_2, T))] \tag{9}$$

where the constant coefficient $\alpha$ depends on the conditional distribution $p(\epsilon|z_1)$.

The assumption about the estimation error $\epsilon$ in Theorem 3 is reasonable because $\epsilon$ is analogous to the ‘noise’ with the mean of 0, which is generally assumed to come from simple distributions (e.g., Gaussian distribution) in statistical learning theory. Similar to the classification tasks, Theorem 3 indicates that for regression tasks, $z_{1}^{\text{su}}$ can achieve lower expected squared prediction error than $z_{1}^{\text{min}}$ and increasing $I(z_{1}^{\text{su}}, T|v_2)$ can improve the performance.

Theorem 2 and Theorem 3 analyze the disadvantages of the minimal sufficient representation $z_{1}^{\text{min}}$ in classification tasks and regression tasks respectively. The essential reason is that $z_{1}^{\text{min}}$ has less task-relevant information than $z_{1}^{\text{su}}$ and has a non-ignorable gap $I(v_1, T|v_2)$ with the optimal representation, as shown in Theorem 1.

### 3.3. More non-shared task-relevant information

According to the above theoretical analysis, in contrastive learning, the minimal sufficient representation is not sufficient for downstream tasks due to the lack of some non-shared task-relevant information. Moreover, contrastive learning approximately learns the minimal sufficient representation, thereby having the risk of over-fitting to the shared information between views. To this end, we propose to extract more non-shared task-relevant information from $v_1$, i.e., increasing $I(z_1, T|v_2)$. However, we cannot utilize any downstream task information during training, so it is impossible to increase $I(z_1, T|v_2)$ directly. We consider increasing $I(z_1, v_1)$ as an alternative because the increased information from $v_1$ in $z_1$ may be relevant to some downstream tasks, and this motivation is demonstrated in Fig. 1. In addition, increasing $I(z_1, v_1)$ also helps to extract the shared information between views at the beginning of the optimization process. Concretely, considering the symmetry between $v_1$ and $v_2$, our optimization objective is

$$\max_{f_1, f_2} \sum_{i=1}^{2} \lambda_i I(z_i, v_i) \tag{10}$$

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which consists of the original optimization objective Eq. (1) in contrastive learning and the objective terms we proposed. The coefficients $\lambda_1$ and $\lambda_2$ are used to control the amount of increasing $I(z_i, v_i)$ and $I(z_2, v_2)$ respectively. For optimizing $I(z_1, z_2)$, we adopt the commonly used implementations in contrastive learning models [7, 17, 51]. For optimizing $I(z_i, v_i), i = 1, 2$, we consider two implementations.

**Implementation I** Since $I(z, v) = H(v) - H(v|z)$ and $H(v)$ is not related with $z$, we can equivalently decrease the conditional entropy $H(v|z)$ as $-E_{p(z, v)}[\ln p(v|z)]$. Concretely, we use the representation $z$ to reconstruct the original input $v$, as done in auto-encoder models [44]. Decreasing the entropy of reconstruction encourages the representation $z$ to contain more information about the original input $v$. However, the conditional distribution $p(v|z)$ is intractable in practice, so we use $q(v|z)$ as an approximation and get $E_{p(z, v)}[\ln q(v|z)]$, which is the lower bound of $E_{p(z, v)}[\ln p(v|z)]$. We can increase $E_{p(z, v)}[\ln q(v|z)]$ as an alternative objective. According to the type of input $v$ (e.g., images, text or audio), $q(v|z)$ can be an appropriate distribution with known probability density function, such as Bernoulli distribution, Gaussian distribution or Laplace distribution, and its parameters are the functions of $z$. For example, when $q(v|z)$ is the Gaussian distribution $\mathcal{N}(v; \mu(z), \sigma^2 I)$ with given variance $\sigma^2$ and deterministic mean function $\mu(\cdot)$ which is usually parameterized by neural networks, we have

$$E_{p(z, v)}[\ln q(v|z)] \propto -E_{p(z, v)}[\|v - \mu(z)\|_2^2] + c \quad (11)$$

where $c$ is a constant to representation $z$. The final optimization objective is

$$\max_{f_1, f_2, \mu} I(z_1, z_2) - \sum_{i=1}^{2} \lambda_i E_{p(z, v_i)}[\|v_i - \mu_i(z_i)\|_2^2] \quad (12)$$

**Implementation II** Although the above implementation is effective and preferred in practice, it needs to reconstruct the input, which is challenging for complex input and introduces more model parameters. To this end, we propose another representation-level implementation as an optional alternative. We investigate various lower bound estimates of mutual information, such as the bound of Barber and Agakov [4, 32], the bound of Nguyen, Wainwright and Jordan [5], and InfoNCE [34]. We choose the InfoNCE lower bound and the detailed discussion is provided in Appendix. Concretely, the InfoNCE lower bound is

$$\tilde{I}_{\text{NCE}}(z, v) = \mathbb{E} \left[ \frac{1}{N} \sum_{k=1}^{N} \ln \frac{p(z^{k}|v^{k})}{\frac{1}{N} \sum_{k=1}^{N} p(z^{k}|v^{k})} \right] \quad (13)$$

where $(z^{k}, v^{k}), k = 1, \cdots, N$ are $N$ copies of $(z, v)$ and the expectation is over $\Pi_{k} p(z^{k}, v^{k})$. In the implementation I, we map the input $v$ to the representation $z$ through a deterministic function $f$ with $z = f(v)$. Differently, here we need the expression of $p(z|v)$ to calculate the InfoNCE lower bound, which means the representation $z$ is no longer a deterministic output of input $v$, so we use the reparameterization trick [26] during training. For example, when we define $p(z|v)$ as the Gaussian distribution $\mathcal{N}(z; f(v), \sigma^2 I)$ with given variance $\sigma^2$ and the function $f$ is the same as in the implementation I, we have $z = f(v) + \epsilon \sigma, \epsilon \sim \mathcal{N}(0, I)$ and $\tilde{I}_{\text{NCE}}$ is equivalent to

$$\tilde{I}_{\text{NCE}}(z, v) = \mathbb{E} \left[ -\frac{1}{2} \sum_{k=1}^{N} \ln \sum_{l=1}^{N} \exp(-\rho \|z^{l} - f(v^{k})\|_2^2) \right] \quad (14)$$

where $\rho$ is a scale factor. In fact, it pushes the representations away from each other to increase $H(z)$, which can increase mutual information $I(z, v)$ since $I(z, v) = H(z) - H(z|v) = H(z) - \frac{1}{2}(\ln 2\pi + \ln \sigma^2 + 1)$ with $d$ being representation dimension. It also be denoted as uniformity property [47]. The final optimization objective is

$$\max_{f_1, f_2} I(z_1, z_2) + \sum_{i=1}^{2} \lambda_i \tilde{I}_{\text{NCE}}(z_i, v_i) \quad (15)$$

Since the objective term Eq. (14) is calculated at the representation-level, when we use the convolutional neural networks (e.g., ResNet [22]) to parameterize $f$, it can be applied to the output activation of multiple internal blocks.

**Discussion.** It is worth noting that increasing $I(z, v)$ does not conflict with the information bottleneck theory [42]. According to our analysis, the learned representations in contrastive learning are not sufficient for the downstream tasks. Therefore, we need to make the information in the representations more sufficient but not to compress it. On the other hand, we cannot introduce too much information from the input $v$ either, which may contain harmful noise. Here we use the coefficients $\lambda_1$ and $\lambda_2$ to control this.

4. Experiments

In this section, we first verify the effectiveness of increasing $I(z, v)$ on various datasets, and then provide some analytical experiments. We choose three classic contrastive learning models as our baselines: SimCLR [7], BYOL [18] and Barlow Twins [51]. We denote our first implementation Eq. (12) as "RC" for "ReConstruction" and the second implementation Eq. (15) as "LBE" for "Lower Bound Estimate". For all experiments, we use random cropping, flip and random color distortion as the data augmentation, as suggested by [7]. For "LBE", we set $\sigma = 0.1$ and $\rho = 0.05$.

4.1. Effectiveness of increasing $I(z, v)$

We consider different types of the downstream task, including classification, detection and segmentation tasks. The results of Barlow Twins are provided in Appendix.
We train the models on CIFAR10 \cite{krizhevsky2009cifar}, STL-10 \cite{deng2009stl} and ImageNet \cite{deng2009imagenet}. For CIFAR10 and STL-10, we use the ResNet18 \cite{he2016resnet} backbone and the models are trained for 200 epochs with batch size 256 using Adam optimizer with learning rate 3e-4. For ImageNet, we use the ResNet50 \cite{he2016resnet} backbone and the models are trained for 200 epochs with batch size 1024 using LARS optimizer \cite{you2017large}. We follow the linear evaluation protocol where a linear classifier is trained on top of the frozen backbone. The linear evaluation is conducted on the source dataset (CIFAR10, STL-10 or ImageNet) and other transfer datasets.

**Object detection and instance segmentation.** We conduct object detection on VOC07+12 \cite{everingham2010pascal} using Faster R-CNN \cite{ren2015faster}, and detection and instance segmentation on COCO \cite{caesar2017coco} using Mask R-CNN \cite{he2017mask}, following the setup in \cite{zhou2020object}. All methods use the R50-C4 \cite{he2016resnet} backbone that is initialized using the ResNet50 pre-trained on ImageNet. The results are shown in Table 2. Increasing $I(z,v)$ significantly improves the precision in object detection and instance segmentation tasks. These dense prediction tasks require some local semantic information from the input. Increasing $I(z,v)$ can make the representation $z$ contain more information from the input $v$ which may not be shared between views, thereby obtaining better precision.

![Image](image.png)
where $L$ be rewritten as a minimal sufficient representation. To this end, Federici al.
[15, 43] propose to eliminate the non-shared information. Some recent works
[16, 43] propose to eliminate the non-shared information between views in the representation to get the
minimal sufficient representation. To this end, Federici et al. [15] minimize the regularization term
\[ L_{MIB} = \frac{1}{2} [KL(p(z_1|v_1)||p(z_2|v_2)) + KL(p(z_2|v_2)||p(z_1|v_1))] \] (16)
where $KL(\cdot || \cdot)$ represents the Kullback-Leibler divergence. When $p(z_1|v_1)$ and $p(z_2|v_2)$ are modeled as
$\mathcal{N}(z_i; f_i(v_i), \sigma^2 I)$, $i = 1, 2$ with given variance $\sigma^2$, it can be rewritten as
$L_{MIB} = \mathbb{E}_{p(v_1, v_2)} [\|f_1(v_1) - f_2(v_2)\|^2]$. Idently, Tsai et al. [43] minimize the inverse predictive
loss $L_{IP} = \mathbb{E}_{p(v_1, v_2)} [\|f_1(v_1) - f_2(v_2)\|^2]$. The detailed derivation is provided in Appendix. We evaluate these
two regularization terms in the linear evaluation tasks and choose their coefficient with best accuracy on the source
dataset. The results are shown in Table 3 and the best result in each block is in bold. Although these two regularization
terms have the same form, $L_{MIB}$ uses stochastic encoders
which is equivalent to adding Gaussian noise, so we report the results of SimCLR with Gaussian noise, marked by $\dagger$.
As we can see, eliminating the non-shared information cannot change the accuracy in downstream classification tasks
much. This means that the sufficient representation learned in contrastive learning is approximately minimal and we
don’t need to further remove the non-shared information.

Changing the amount of increasing $I(z, v)$. Quantifying the mutual information between the high-dimensional variables is very difficult, and often leads to inaccurate calculation in practice [30, 37]. Therefore, we assume that the hyper-parameters $\lambda_1$ and $\lambda_2$ control the amount of increasing $I(z_1, v_1)$ and $I(z_2, v_2)$ respectively. Larger $\lambda_1$
is expected to increase $I(z_1, v_1)$ more, so as $\lambda_2$. We set $\lambda_1 = \lambda_2 = \lambda$ and evaluate the performance of different $\lambda$
from $\{0.001, 0.01, 0.1, 1, 10\}$. We choose SimCLR as the baseline and the results are shown in Fig. 4. We report the accuracy on the source dataset (CIFAR10 or STL-10) and the averaged accuracy on all transfer datasets with varying epochs.

Figure 4. Linear evaluation accuracy on the source dataset (CIFAR10 or STL-10) and the averaged accuracy on all transfer
datasets with varying hyper-parameter $\lambda$.

Figure 5. Linear evaluation accuracy on the source dataset (CIFAR10 or STL-10) and the averaged accuracy on all transfer
datasets with varying epochs.

### 4.2. Analytical experiments

We provide some analytical experiments to further understand our hypotheses, theoretical analysis and models.

Eliminating non-shared information. Some recent works [15, 43] propose to eliminate the non-shared information between views in the representation to get the minimal sufficient representation. To this end, Federici et al. [15] minimize the regularization term

\[ L_{MIB} = \frac{1}{2} [KL(p(z_1|v_1)||p(z_2|v_2)) + KL(p(z_2|v_2)||p(z_1|v_1))] \] (16)

where $KL(\cdot || \cdot)$ represents the Kullback-Leibler divergence. When $p(z_1|v_1)$ and $p(z_2|v_2)$ are modeled as
$\mathcal{N}(z_i; f_i(v_i), \sigma^2 I)$, $i = 1, 2$ with given variance $\sigma^2$, it can be rewritten as
$L_{MIB} = \mathbb{E}_{p(v_1, v_2)} [\|f_1(v_1) - f_2(v_2)\|^2]$. Idently, Tsai et al. [43] minimize the inverse predictive
loss $L_{IP} = \mathbb{E}_{p(v_1, v_2)} [\|f_1(v_1) - f_2(v_2)\|^2]$. The detailed derivation is provided in Appendix. We evaluate these
two regularization terms in the linear evaluation tasks and choose their coefficient with best accuracy on the source
dataset. The results are shown in Table 3 and the best result in each block is in bold. Although these two regularization
terms have the same form, $L_{MIB}$ uses stochastic encoders
which is equivalent to adding Gaussian noise, so we report the results of SimCLR with Gaussian noise, marked by $\dagger$.
As we can see, eliminating the non-shared information cannot change the accuracy in downstream classification tasks
much. This means that the sufficient representation learned in contrastive learning is approximately minimal and we
don’t need to further remove the non-shared information.

Changing the amount of increasing $I(z, v)$. Quantifying the mutual information between the high-dimensional variables is very difficult, and often leads to inaccurate calculation in practice [30, 37]. Therefore, we assume that the hyper-parameters $\lambda_1$ and $\lambda_2$ control the amount of increasing $I(z_1, v_1)$ and $I(z_2, v_2)$ respectively. Larger $\lambda_1$
is expected to increase $I(z_1, v_1)$ more, so as $\lambda_2$. We set $\lambda_1 = \lambda_2 = \lambda$ and evaluate the performance of different $\lambda$
from $\{0.001, 0.01, 0.1, 1, 10\}$. We choose SimCLR as the baseline and the results are shown in Fig. 4. We report the accuracy on the source dataset (CIFAR10 or STL-10) and the averaged accuracy on all transfer datasets with varying epochs.

Figure 4. Linear evaluation accuracy on the source dataset (CIFAR10 or STL-10) and the averaged accuracy on all transfer
datasets with varying hyper-parameter $\lambda$.

Table 3. Linear evaluation accuracy (%) on CIFAR10 and the transfer datasets. $\dagger$ represents adding Gaussian noise to the representations.
### Table 4. Linear evaluation accuracy (%) on the source dataset (CIFAR10 or CIFAR100) and the transfer datasets.

| Model          | CIFAR10  | DTD     | MNIST   | FaMNIST | CUBirds | VGGFlower | TrafficSigns |
|----------------|----------|---------|---------|---------|---------|-----------|--------------|
| Supervised     | 93.25    | 34.10   | 98.52   | 90.09   | 8.37    | 46.14     | 93.05        |
| Supervised+RC (ours) | 93.09    | 32.77   | 98.61   | 89.77   | 8.84    | 49.05     | 93.28        |
| Supervised+LBE (ours) | 93.18    | 34.79   | 98.68   | 90.40   | 9.72    | 53.15     | 94.47        |

| Model          | CIFAR100 | DTD     | MNIST   | FaMNIST | CUBirds | VGGFlower | TrafficSigns |
|----------------|----------|---------|---------|---------|---------|-----------|--------------|
| Supervised     | 71.92    | 36.06   | 98.48   | 88.97   | 11.51   | 64.21     | 96.54        |
| Supervised+RC (ours) | 72.02    | 34.79   | 98.59   | 89.35   | 10.94   | 65.34     | 96.67        |
| Supervised+LBE (ours) | 71.89    | 36.33   | 98.37   | 89.42   | 11.89   | 65.64     | 96.91        |

**Training with more epochs.** In the above experiments, we train all models for 200 epochs. Here we further show the behavior of the contrastive learning models and increasing \( I(z, v) \) when training with more epochs. We choose SimCLR as the baseline and train all models for 100, 200, 300, 400, 500 and 600 epochs. The results are shown in Fig. 5. With more training epochs, the learned representations in contrastive learning are more approximate to the minimal sufficient representation which mainly contain the shared information between views and ignore the non-shared information. For the classification tasks on the transfer datasets, the shared information between views is not sufficient. As shown in Fig. 5 (b) and (d), the accuracy on the transfer datasets decreases with more epochs and the learned representations over-fit to the shared information between views. Increasing \( I(z, v) \) can introduce non-shared information and obtain the significant improvement. For the classification tasks on the source datasets, the shared information between views is sufficient on CIFAR10 but not on STL-10. As shown in Fig. 5 (a) and (c), the accuracy on CIFAR10 increases with more epochs and increasing \( I(z, v) \) cannot make a difference. But the accuracy on STL-10 decreases with more epochs, and increasing \( I(z, v) \) can significantly improve the accuracy and does not decrease with more epochs. In fact, we use the unlabeled split for contrastive training on STL-10, so it is intuitive that the shared information between views is not sufficient for the classification tasks on the train and test split.

**Increasing \( I(z, x) \) in supervised learning.** According to the information bottleneck theory \([42]\), a model extracts the approximate minimal sufficient statistics of the input \( x \) with respect to the label \( y \) in supervised learning. In other words, the representation \( z \) only contains the information related to the label and eliminates other irrelevant information which is considered as noise. However, label-irrelevant information may be useful for some downstream tasks, so we evaluate the effect of increasing \( I(z, x) \) in supervised learning. We train the ResNet18 backbone using the cross-entropy classification loss on CIFAR10 and CIFAR100, and choose \( \lambda_1 = \lambda_2 = \lambda \) from \( \{0.001, 0.01, 0.1, 1, 10\} \). The linear evaluation results are shown in Table 4 and the best result in each block is in bold. As we can see, increasing \( I(z, x) \) improves the performance on the transfer datasets and achieves comparable results on the source dataset, which means it can effectively alleviate the over-fitting on the label information. This discovery helps to obtain more general representations in the field of supervised pre-training and we left it for the future work.

### 5. Limitations

Our work has the following limitations. 1) Based on our experimental observation, the assumption that non-shared task-relevant information cannot be ignored usually well holds for the cross-domain transfer tasks, but may not be satisfied for the tasks on the training dataset. 2) Increasing \( I(z, v) \) can also introduce noise (task-irrelevant) information which may increase the data demand in the downstream tasks, so one may need to adjust the coefficients \( \lambda_1 \) and \( \lambda_2 \) to achieve effective trade-off for the different downstream tasks. 3) Due to limited computing resources, we cannot reproduce the best results of SimCLR on ImageNet which need the batch size of 4096 and more training epochs.

### 6. Conclusions

In this work, we explore the relationship between the learned representations and downstream tasks in contrastive learning. Although some works propose to learn the minimal sufficient representation, we theoretically and empirically verify that the minimal sufficient representation is not sufficient for downstream tasks because it loses non-shared task-relevant information. We find that contrastive learning approximately obtains the minimal sufficient representation, which means it may over-fit to the shared information between views. To this end, we propose to increase the mutual information between the representation and input to approximately introduce more non-shared task-relevant information when the downstream tasks are unknown. For the future work, we can consider combining the reconstruction models \([3, 19]\) and contrastive learning for convolutional neural networks or vision transformers, since reconstruction can learn more sufficient information and contrast can make the representations more discriminative.
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