Abstract

Contrastive learning (CL) has achieved remarkable success in learning transferable representations. It has been identified that the temperature $\tau$ of CL loss plays an essential role in automatically concentrating on hard negative samples. However, recent work also indicates a uniformity-tolerance dilemma (UTD) connected to $\tau$, which will lead to unexpected performance degradation. We argue that it is the fixity of temperature that is inextricably linked to UTD and suboptimal embedding space. To tackle the challenge of UTD, we enrich the CL loss family by presenting a Model-Aware Contrastive Learning (MACL) strategy. In MACL, the temperature parameter is adaptive to the magnitude of alignment that reflects the basic confidence of the instance discrimination task. Lower alignment implies poor discrimination for the undertrained phase, then there is less possibility that the high similarity region contains latent positive samples (LPs). Thus, a small $\tau$ can impose larger penalties on hard negative samples to learn uniformly informative embeddings. Instead, a larger $\tau$ in the well-trained phase facilitates the exploration of semantic structures due to its increased tolerance for LPs.

Introduction

Modern representation learning has been greatly facilitated by deep neural networks (Bengio, Courville, and Vincent 2013; Liu et al. 2021; He et al. 2016). Self-supervised learning (SSL) is one of the most popular paradigms in the unsupervised scenario, which can learn transferable representations without depending on manual labeling (He et al. 2022; Chen and He 2021). Especially, SSL methods based on contrastive loss have highly boosted NLP, CV, and multimodal tasks (Grill et al. 2020; Fang et al. 2020; Radford et al. 2021). These contrastive learning (CL) frameworks generally map raw data on a hypersphere embedding space, whose embedding similarity can reflect semantic relationship (Wu et al. 2018; He et al. 2020). Among diverse contrastive losses, the Softmax-based InfoNCE loss is widely adopted in various CL algorithms (Van den Oord, Li, and Vinyals 2018; Tian, Krishnan, and Isola 2020), which attempts to attract positive samples to the anchor while pushing negative samples away.

InfoNCE loss is significant to the success of CL (Tian 2022; Wu et al. 2020). A hardness-aware property is pointed out, which enables InfoNCE loss automatically concentrate on optimizing hard negative samples (HNs, those having high similarities with the anchor) (Wang and Liu 2021; Zhang et al. 2022; Tian 2022). Particularly, the temperature parameter $\tau$ determines the penalty strength. Wang and Liu (2021) also shows that there exists a Uniformity-Tolerance Dilemma (UTD) that plagues CL performance. Specifically, as for the common instance discrimination task in CL, models are trained by maximizing the similarities of the anchor with its augmentations and minimizing the similarities of all the other different instances (Wu et al. 2018; Tian, Krishnan, and Isola 2020). Such CL strategy neglects the underlying semantic relationships. In this context, those HNs might contain latent positive samples (LPs), which have the same labels as the anchor. For example, the sample from an image...
of a cat will be heavily pushed away from the similar cat anchor though they are semantically consistent. Owing to the hardness-aware property, a smaller $\tau$ is conducive to the uniformity of the embedding space (Wang and Isola 2020), but goes against LPs due to excessive penalties on HNs. On the contrary, larger temperature parameters are beneficial for exploring potential semantic structures, while detrimental for learning informative separable features.

This work mainly focuses on addressing the uniformity-tolerance dilemma of InfoNCE, which is still an open problem in contrastive learning. We argue that a training-adaptive temperature is key to alleviating UTD. To further understand the training process, we evaluate the feature quality and confirm that the semantic sensitivity is empirically asymptotically along with training iterations. Such sensitivity reveals the capability of models for capturing underlying semantic structures. Specifically, its semantic sensitivity is underperforming for a poorly trained instance discrimination CL model. In this case, a smaller temperature parameter does help to improve alignment and uniformity of the hypersphere embedding space (Wang and Isola 2020). In contrast, the well-trained one is much better in terms of sensitivity, in which a larger temperature contributes to mining latent semantic relationships with more tolerance. Because the alignment of positive pairs (Wang and Isola 2020) exactly can reflect the prior expectation of the instance discrimination task but also needs no extra computations, we propose a model-aware temperature strategy based on alignment to solve the UTD problem. This strategy is illustrated in Fig. 1. On the other hand, theoretically, we identify the importance of negative sample size and temperature in a unified perspective of improving gradient reduction. With these explorations and Model-Aware Contrastive Learning (MACL) strategy, we construct a contrastive loss to enable CL model training with smaller negative sample size and learn high-quality representations. Overall, the main contributions are summarized as:

1) Recognizing that the semantic sensitivity of CL models varies with training, we propose a model-aware strategy for InfoNCE type loss in CL methods. The temperature parameter of MACL is adaptive to the feature alignment magnitude to automatically adjust the tolerance for hard negative samples to mitigate the UTD problem.

2) A rigorous analysis for gradient reduction related to negative sample size and temperature is provided. Moreover, we devise a novel contrastive loss, which can learn higher quality representations. Additionally, with the help of a redesigning anchor-wise weighting, the new contrastive loss facilitates training with fewer negative samples.

3) Experiments and analysis on some vision benchmarks with various InfoNCE type losses demonstrate that the proposed MACL strategy does help escape UTD and improve the learned embeddings.

Related Work
Self-supervised learning has achieved significant success, which can provide robust and semantically meaningful representations for downstream tasks (Liu et al. 2021, Radford et al. 2021, Zhbontar et al. 2021, He et al. 2017). Without any annotated information, various pretext tasks are exploited to train the models and improve the embedding space (Komodakis and Gidaris 2018, Noroozi and Favaro 2016, Pathak et al. 2016). More recently, the instance discrimination task combined with contrastive loss has achieved state-of-the-art among these pretext tasks, and even exhibited competitive performance to supervised methods (Chen et al. 2020, He et al. 2020).

Contrastive Self-Supervised Learning
Contrastive instance discrimination originates from (Wu et al. 2018), whose core idea is to learn instance-invariant representations. Instance discrimination treats instance-wise self-supervision as the extreme of the class-wise supervised scenario, i.e. each instance is viewed as a single class (Dosovitskiy et al. 2014). In effect, positive pairs are different augmentations or views of the same instance, while negative samples come from other distinct instances. The rational assumption behind is that maximizing similarities of the positive pairs and minimizing negative similarities can equip models with discrimination. To construct the negative sampling appropriately, Wu et al. (2018) proposes a memory bank to store vectors from instances. Moco family (He et al. 2020, Chen et al. 2020) adopts a queue structure and a momentum encoder for the consistency of negative samples. On the other hand, without additional parts for storing negative samples, some methods explore negative sampling within a large mini-batch, e.g., SimCLR (Chen et al. 2020a), CLIP (Radford et al. 2021).

Properties of Contrastive Loss
To understand the success of CL methods, recent work has attempted to explore important properties of contrastive loss from different perspectives. InfoNCE loss is constructed by CPC (Van den Oord, Li, and Vinyals 2018) and CMC (Tian, Krishnan, and Isola 2020) to maximize the mutual information of features from same instances. Similarly, Wu et al. (2020) shows that the CL loss maximizes a lower bound on the mutual information between different views. Besides, some work focus on the positive and negative pairwise similarity in InfoNCE. For example, Wang and Isola (2020) attributes the effectiveness of InfoNCE to the asymptotic alignment and uniformity properties of features on hypersphere in training. Following this, Wang and Lin (2021) has proven that the temperature parameter plays an essential role in controlling the penalty strength on negative samples, which is related to the hardness-aware property and a uniformity-tolerance dilemma. Tian (2022) also comes to a similar conclusion in a coordinate-wise optimization view. Furthermore, Zhang et al. (2022) extends the hardness-aware property anchor-wise and introduce an extra larger temperature for anchors to train with fewer negative samples. Also motivated by reducing the training batch size, DCL (Yeh et al. 2021) removes the positive similarity in the denominator of InfoNCE to eliminate a negative-positive-coupling effect. All the above studies exploit contrastive losses with fixed temperature parameters, which lead to performance degradation. Differently, our work mainly focuses
on alleviating UTD and designs a model-aware CL loss with an adaptive temperature strategy.

**Problem Definition**

**Contrastive Loss**

Let $X = \{x_1, \ldots, x_N\}$ denote the unlabeled training dataset. Also given encoders $f$ and $g$, instance $x_i$ is mapped to a query feature $f_i = f(x_i)$ and a corresponding key feature $g_i = g(x_i)$ on hypersphere, respectively. $g$ maybe a weight-shared network of $f$ or a momentum-updated encoder. Assume that the query (anchor) set and key set are denoted by $F = \{f_1, f_2, \ldots\}$ and $G = \{g_1, g_2, \ldots\}$, respectively. Then, the InfoNCE loss can be formulated as:

$$L_{f_i} = - \log \frac{\exp(f_i \cdot g_i / \tau)}{\sum_{j=1}^{K} \exp(f_i \cdot g_j / \tau)} + \sum_{j=1}^{K} \exp(f_i \cdot g_j / \tau),$$

where $\{f_i, g_i\}$ is the positive pair of the $i$-th instance, and $g_j$ denotes the negative sample from a distinct instance.

**Hardness-aware Property**

Previous work identifies the important hardness-aware property via gradient analysis. For convenience, suppose that $P_{i,j}$ indicates the probability of $x_i$ being recognized as $x_j$, which is described as follows:

$$P_{i,j} = \frac{\exp(f_i \cdot g_j / \tau)}{\sum_{r=1}^{K} \exp(f_i \cdot g_r / \tau)}.$$  

Then, the gradient with respect to the anchor $f_i$ can be formulated as follows:

$$\frac{\partial L_{f_i}}{\partial f_i} = - \frac{1}{\tau} \left( \sum_{j=1}^{K} P_{i,j} \right) \left( g_i - \sum_{j=1}^{K} \hat{P}_{i,j} \cdot g_j \right),$$

where $\hat{P}_{i,j} = P_{i,j} / \sum_{r=1}^{K} P_{i,r}$, and $\sum_{j=1}^{K} \hat{P}_{i,j} = 1$.

On the one hand, $P_{i,j}$ indicates an intra-anchor hardness-aware property. It implies that InfoNCE automatically puts larger penalty weights on the hard negative keys (Wang and Liu 2021). On the other hand, the sum item $\sum_{j=1}^{K} P_{i,j}$ is a gradient scaling factor and a variable for different anchors. As a result, an inter-anchor hardness-aware property is also identified (Zhang et al. 2022).

**Uniformity-Tolerance Dilemma**

The penalty weights distribution on negative sample $x_j$ is $\hat{P}_{i,j}$ formulated as:

$$\hat{P}_{i,j} = \frac{\exp(f_i \cdot g_j / \tau)}{\sum_{r=1}^{K} \exp(f_i \cdot g_r / \tau)}, \quad i \neq j$$

which is controlled by the temperature parameter (Wang and Liu 2021). (1) As $\tau$ decreases, the shape of $\hat{P}_{i,j}$ becomes sharper. This implies that a smaller temperature causes larger penalties on the high similarity region, which encourages the uniformity of embeddings but has less tolerance for LPs. (2) A larger temperature makes the shape of $\hat{P}_{i,j}$ flatter, then tends to give all negative samples the same magnitude of penalties. In this case, the optimization process is more tolerant to LPs while concentrating less on uniformity.

To measure the tolerance, Wang and Liu (2021) constructs a metric for local distribution of negative samples as follows:

$$T = \mathbb{E}_{x,y \sim i.i.d} \left[ \frac{1}{K} \sum_{i=1}^{K} \log \left( \frac{f(x) \cdot f(y)}{f(x) \cdot f_i + f_i \cdot f(y)} \right) \right],$$

where $l(x)$ denotes the supervised label of instance $x$. Indicator function $l(x) = 0$ for latent positive pairs, i.e., $l(x) = l(y)$, and has a value of 0 if $l(x) \neq l(y)$.

Besides, the adopted uniformity metric is formulated by Wang and Isola (2020) based on a gaussian kernel:

$$\mathcal{L}_{uniform} = \log \mathbb{E}_{x,y \sim i.i.d} \left[ e^{-\tau \| f(x) - f(y) \|_2^2} \right].$$

It has been proven that contrastive learning asymptotically optimizes two important properties in the training, i.e., alignment and uniformity (Wang and Isola 2020). The asymptotical uniformity loss enforces the negative features more separated around the anchor, while optimization for alignment loss in training encourages positive representations to be closer. The alignment loss is defined as follows:

$$\mathcal{L}_{align} = \mathbb{E}_{x \sim D} \| f(x) - g(x) \|_2^2.$$

**Model-Aware Contrastive Learning**

As we hope to improve both uniformity and tolerance for CL models, there exists a uniformity-tolerance dilemma (Wang and Liu 2021), which leads to suboptimal embedding space and performance degradation of downstream tasks. Considering that the fixity of temperature prevents InfoNCE from focusing both on uniformity and potentially semantic relationships, we exploit an adaptive strategy for contrastive learning to mitigate the challenge in this section.

**Empirically Asymptotical Semantic Sensitivity**

The uniformity-tolerance dilemma is rooted in the unsupervised instance discrimination task, in which the underlying semantic structures cannot be preserved in an explicit way. As mentioned above, strongly pushing all HNs away during the whole training process is harmful to learning an optimal embedding space. Wang and Liu (2021) utilizes tolerance as a measure to evaluate the local density. However, the tolerance formulated in Eq. (5) cannot comprehensively describe the semantic relationship. For example, mapping all the instances into the same feature on the hypersphere will maximize the tolerance, but the feature quantity is bad.

Intuitively, with a proper training strategy, the structure of embedding space can gradually reflect the semantic relationship, which is one of the main goals of representation learning. In another sense, the semantic sensitivity of a CL model is empirically asymptotical. To explore the semantic structures of learned representations, we construct a semantic sensitivity measure using the supervised similarity, which is formulated as:

$$S = \mathbb{E}_{x,y \sim i.i.d} \left[ e^{-H_{x,y} \cdot f(x) \cdot g(y)} \right],$$
where $H_{x,y} = 2 \left[ l(x) \cdot l(y) \right] - 1$ is the semantic similarity provided by supervised labels that are in a one-hot vector form. In this case, $H_{x,y} = 1$ if instances $x$ and $y$ belong to the same semantic class, and $H_{x,y} = -1$ when $l(x) \neq l(y)$. On the other hand, for the learned representations, we hope the similarities of latent positive pairs are larger, while that on negative pairs are small enough to facilitate the discrimination. The dot product operation on the hypersphere is equal to the cosine similarity, then $f(x) \cdot g(y) = \cos(f(x), g(y)) \in [-1, 1]$. Therefore, the semantic sensitivity formulated in Eq. (9) can measure the semantic structures captured by a CL model.

![Figure 2: Semantic sensitivity during training.](image)

**Figure 2:** Semantic sensitivity during training. The blue curve indicates the baseline with a fixed temperature $\tau = 0.07$. The green curve shows a Linearly varying strategy, i.e. $\tau = 0.07 + (1.4e - 4) \times \text{epoch}$. The setting on the red one is $\tau = 0.07 + (2.8e - 4) \times \text{epoch}$. These curves are trained on CIFAR10 with SimCLR (Chen et al. 2020a).

From Fig. 2 we have the following observations. The semantic sensitivity of a contrastive model is indeed empirically asymptotical during training, which also indicates that its confidence for capturing latent positive pairs is gradually improved. Nevertheless, as the analysis of UTD aforementioned, a fixed temperature leads to suboptimal representations. Thus, the CL models that are trained with linearly varying temperature parameters have higher semantic sensitivity along with training iterations. The accuracy metric results listed in Table 1 also show the correctness of the linearly changeable strategy. Moreover, the test performance on KNN classification with the linearly varying temperature is significantly much better than the fixed one, which also indicates its effectiveness for improving semantic structures.

| Strategy       | Fixed | Linear-1 | Linear-2 |
|----------------|-------|----------|----------|
| KNN (%)        | 78.70 | 85.46    | 87.06    |
| LE (%)         | 82.03 | 87.38    | 88.75    |

**Table 1:** Top-1 test accuracy of fixed and linearly varying temperature strategy, $k=200$ in KNN evaluation, and LE represents evaluation with training a linear classifier.

---

**Adaptive Temperature**

**Changeable Temperature** From the above analysis, contrastive loss with a changeable temperature can deal with UTD better for distinct penalty strengths on HNs along with training. More specifically, in the early stage, the CL model has less confidence to discriminate instances. As a result, there is a lower probability that the high similarity region contains LPs. In this case, a small temperature helps to put large penalties on HNs, which can improve the uniformity of the embedding space. In the later stage, the CL model has more confidence in recognizing semantically similar pairs. Then, excessively pushing away all the HNs that share similar representations is not beneficial for exploring semantic relations. Therefore, a larger temperature can be adopted to encourage tolerance.

**Adaptive to Alignment** Though the linearly varying temperature can alleviate UTD to some extent, it is still a heuristic approach by now. Because the semantic sensitivity of a CL model is not linearly varying or even a function of the training epoch, a more reasonable temperature adjustment strategy is needed to be investigated. What motivates us is the alignment property of the embedding space in training.

1) Alignment property is one of the most significant prior assumptions for instance discrimination task (Wu et al. 2018; Ye et al. 2019). Since there are no supervised labels available, it is impossible for SSL to explicitly construct semantic guidance. Instead, different views of the same instance are used for self-supervised training. Alignment implies the awareness of view-invariance of a CL model, which is the base for exploring semantically consistent samples.

2) Estimating the magnitude of alignment is not a computationally expensive operation. As shown in Eq. (1), the calculation of sample similarities is the required step for CL loss, in which the part of positive pairs can be directly exploited for alignment. Hence, no additional structures and computations are needed. Then the adaptive strategy is formulated as:

$$\tau_a = \tau_0 \times \alpha^A,$$

where $\alpha$ is the base value of the scaling factor, and $\alpha > 1$. On a hypersphere, $A = \mathbb{E} \left[ f_i \cdot g_i \right] = (2 - L_{\text{align}})/2$ is a measure for feature alignment when $\gamma = 2$, and $f_i \cdot g_i \in [-1, 1]$, then $\tau_a \in [\tau_0/\alpha, \tau_0\alpha]$. Besides, another alignment linearly adapted variant can be described as:

$$\tau_b = \tau_0 + \beta A \tau_0,$$

where $\beta$ is a scaling factor. We can have the following observations:

1) Eq. (9) and (10) show that our strategy enables the temperature parameter adaptive to the alignment magnitude of a CL model during training to escape UTD. Specifically, a smaller temperature works when the model is lacking training by aligning positive pairs and heavily penalizing those HNs. For the better-trained stage, the improved alignment indicates the CL model is more discriminative for samples. Naturally, larger temperature parameters can relax the penalty strength on the high similarity region, where is more possible to exist LPs now.
2) The proposed strategy is a fine-grained adjusting approach. As CL models are trained by sampling minibatches, \( A = \mathbb{E} [f_i \cdot g_i] \) can be estimated within a batch to promptly adjust the temperature. Compared with the linearly varying one that simply increases by iterations, this adaptive strategy is more online. For this reason, the proposed method is also named as Model-Aware Contrastive Learning (MACL) strategy.

Model-Aware Contrastive Loss

With MACL strategy, InfoNCE loss can be reformulated as:

\[
\mathcal{L}_{f_i}' = -\log \frac{\exp \left( f_i \cdot g_i / \sigma (\tau') \right)}{\sum_{j=1}^N \exp \left( f_i \cdot g_j / \sigma (\tau') \right)},
\]

where \( N = K + 1 \) denotes the size of the key set containing the positive key and all the negative keys. \( \tau' \) is the adaptive temperature parameter \( \tau_a \) or \( \tau_b \). \( \sigma(\cdot) \) is the stop gradient operation to maintain the basic assumptions of InfoNCE.

The improved InfoNCE loss can help to escape UTD. However, CL models are typically trained with a large number of negative samples to achieve great performance, which is not computing resource friendly. Some previous work tries to address this problem by modifying InfoNCE loss but each has its own opinion (Yeh et al. 2021; Zhang et al. 2022; Chen et al. [2021]). In this section, we provide a unified analysis of the issue in a gradient reduction view. Besides, we propose a new CL loss based on these analyses and MACL strategy, which can not only learn better representations but also help to train with fewer negative examples.

Gradient Reduction Caused by the Sum Item

The sum item \( W_i = \sum_{j=1}^K P_{i,j} \) in Eq. (3) also can be described as:

\[
W_i = 1 - \frac{\exp (f_i \cdot g_i / \tau)}{\exp (f_i \cdot g_i / \tau) + \sum_{j=1}^K \exp (f_i \cdot g_j / \tau)}.
\]

This item has small values for those easy positive pairs with high similarities, which will reduce the gradient in Eq. (2) (Yeh et al. [2021]). The gradient reduction problem will hinder the model learning, especially for low-precision floating-point training. Specifically, for an easy positive pair, a small \( K \) denotes the number of negative samples used in training, which also plays a significant role in scaling the gradient magnitude. Specifically, for an easy positive pair, a small \( K \) leads to a significant gradient reduction if the similarities of the negative pairs are lower. This is the rationale that the state-of-the-art CL models are often trained with a large number of negative samples.

From another aspect, \( W_i \) is a monotonic function of temperature. In particular, the shape of the sum item tends to become flat as temperature increases. We present an extreme example in Fig. 3, in which the similarities of the positive pair and negative pairs are set to 1 and -1, respectively. Furthermore, we have the following proposition:

Proposition 1 (Bound of gradient scaling factor w.r.t. \( K \))

Given the anchor feature \( f_i \) and temperature \( \tau_a \) or \( \tau_b \), if \( K \to +\infty \), then \( W_i \) approaches its upper bound 1. The limit is formulated as:

\[
\lim_{K \to +\infty} W_i = 1.
\]

Proposition 2 (Bound of gradient scaling factor w.r.t. \( \tau \))

Given \( f_i \) and key set \( G \), \( W_i \) monotonically changes with respect to \( \tau \). The monotonicity is determined by the similarity distribution of samples. If \( \tau \to +\infty \), then \( W_i \) approaches its bound \( K / (K + 1) \), formulated as:

\[
\lim_{\tau \to +\infty} W_i = \frac{K}{1 + K}.
\]

Proof of Proposition 1 and 2 is present in the supplementary material.

These results show that the gradient reduction problem can be addressed by increasing the number of negative keys or adopting an extra large temperature for \( W_i \). More specifically, sampling more negative keys can promote the accumulation of the exponential similarities then inhibit \( W_i \) too small. In another case, adopting a larger separate temperature makes \( W_i \) approach its bound then also improves the gradient reduction issue. This is the real reason why DCL (Yeh et al. [2021]), PlatNCE (Chen et al. [2021]), and dual temperature strategy (Zhang et al. [2022]) works.

Reweighting Contrastive Loss with a Constant

We design a new CL loss to address the gradient reduction issue but need no additional temperature parameter, which is formulated as follows:

\[
\mathcal{L}^M_{f_i} = -\log \left( \frac{1}{W_i} \right) \log \frac{\exp \left( f_i \cdot g_i / \sigma (\tau') \right)}{\sum_{j=1}^N \exp \left( f_i \cdot g_j / \sigma (\tau') \right)},
\]

(Zhang et al. [2022]) claims that reducing the inter-anchor hardness-awareness caused by \( W_i \) can boost the performance of CL, and an extra sufficiently large temperature is the key point. We identify the importance of temperature in Proposition 2. Therefore, we replace the \( W_i \) item in Eq. 5 with 1, which assigns to its upper bound directly. It is worth noting that the CL loss formulated in Eq. 15 reweights InfoNCE with a scalar but does not modify the computational graph, which is different from DCL (Yeh et al. [2021]).
Experiment

Implementation Setup

Pretraining We perform experiments on CIFAR10, CIFAR100 (Krizhevsky, Hinton et al. 2009), and STL10 (Coates, Ng, and Lee 2011). We adopt a Pytorch version SimCLR (Chen et al. 2020a) as the basic contrastive framework. Following Chen et al. (2020a), to extract appropriate features, a modified Resnet18 (He et al. 2016) is utilized as the backbone model. Specifically, we change the kernel size of the first convolution to $3 \times 3$ and remove the first max pooling module. For a fair comparison, we use four types of augmentations for pretraining: random cropping and resizing, random color jittering, random horizontal flip, and random gray scale conversion (Yeh et al. 2021; Wang and Liu 2021). The LARS optimizer in SimCLR is replaced by Adam with a fixed learning rate of $1e^{-3}$ and weight decay is $1e^{-6}$. We set the batch size to 256 and train the CL encoders for 200 epochs. The temperature $\tau_0$ is set to 0.1. $\alpha$ for $\tau_a$ and $\beta$ for $\tau_b$ are 2 and 0.5, respectively.

Evaluation Both linear evaluation (LE) and KNN ($k=200$) top-1 accuracy are reported. For linear evaluation, the trained CL models are evaluated by fine-tuning a linear classifier for 100 epochs on the top of frozen backbones. We utilize an SGD optimizer by setting the learning rate to 0.02, momentum to 0.9, and weight decay to 0. Besides, the metrics of semantic sensitivity, uniformity and alignment are also considered for models.

Baselines We compare our model-aware strategy with ordinary InfoNCE, DCL (Yeh et al. 2021), and Dual temperature strategy (Zhang et al. 2022). Info-a is the alignment-adaptive InfoNCE described in Eq. (11) using $\tau_a$. Besides, MACL-a and MACL-b are variants of Eq. (15) using $\tau_a$ and $\tau_b$, respectively. For a fair comparison, all the experiments are always implemented under the same setup except for specified variants.

Results and Analysis

Alignment-adaptive temperature strategy indeed alleviates uniformity-tolerance dilemma We report metric values for each model and visualize their magnitude in Fig. 4. As displayed in Fig. 4(a) and 4(b), the models trained using Info-a, MACL-a, and MACL-b outperform other counterparts in terms of semantic sensitivity and embedding uniformity. As these three CL losses are equipped with the proposed alignment-adaptive temperature strategy, uniformity or sensitivity are focused on in distinct training phases based on the model capability. Consequently, both underlying semantic structures and separable features are improved. The empirical results on CIFAR100 suggest that our strategy is superior for reducing UTD.

Model-aware loss leads to higher quality representations Alignment and uniformity of embedding space are proven to be optimization targets of contrastive learning and are adopted as metrics for representation quality (Wang and Isola 2020; Zhong et al. 2022). Fig. 4(b) and 4(c) illustrate that our Info-a, MACL-a, and MACL-b ensure the quality of the learned embedding space on CIFAR100. Besides, thanks to the reweighting method, representations learned with MACL-a and MACL-b exhibit higher quality compared with Info-a. KNN classification results in Fig. 4(d) corroborate above conclusions.

Model-aware strategy can boost the performance of contrastive learning To further validate the proposed strategy, we conduct experiments with variables on different datasets. We list the linear classification results to show downstream task performance. Due to space limitations, all of the corresponding KNN evaluation results are detailed in the supplementary material.

Table 2: Results of different epochs on CIFAR100.

| Epoch  | 100  | 200  | 300  | 400  | 500  |
|--------|------|------|------|------|------|
| InfoNCE| 55.04| 58.33| 60.58| 61.66| 62.59|
| DCL    | 57.68| 59.61| 61.16| 62.25| 63.14|
| Dual   | 57.46| 60.34| 61.18| 62.31| 63.20|
| Info-a | 57.37| 59.90| 62.27| 62.63| 63.13|
| MACL-a | 57.73| 61.81| 62.25| 62.72| 63.22|
| MACL-b | 57.84| 61.69| 62.27| 62.94| 63.71|

Varying Epochs on CIFAR100. Results exhibited in Table 2 verify the superiority of our MACL on CIFAR100 over different iterations. Info-a has a significant improvement compared with the original InfoNCE in both online and linear evaluation. Besides, MACL goes a step further and generates optimal results when trained for 500 epochs.

Table 3: Results of different minibatch sizes on CIFAR10.

| Batch size | 64   | 128  | 256  | 512  | 1024 |
|------------|------|------|------|------|------|
| InfoNCE    | 81.61| 82.77| 83.64| 83.74| 83.70|
| DCL        | 86.28| 86.04| 86.29| 85.78| 85.09|
| Dual       | 86.32| 86.40| 85.86| 85.72| 85.00|
| Info-a     | 85.68| 86.48| 87.23| 86.90| 86.63|
| MACL-a     | 86.73| 87.57| 87.37| 86.92| 86.55|
| MACL-b     | 87.11| 87.41| 87.27| 86.78| 86.00|

Varying Mini-batch Size on CIFAR10. As mentioned in the former part, addressing the gradient reduction problem and training with smaller negative sample size is another important goal. We experiment with a range of mini-batch sizes on CIFAR10 to evaluate the proposed CL loss. As shown in Table 3, these results show the efficacy of the proposed adaptive strategy and reweighting method. (1) MACL loss achieve the best performance over different mini-batch size. (2) These five improved approaches are less sensitive to mini-batch size compared with the original InfoNCE.

Varying $\tau_0$ on STL10. Experiments results on STL10 with a range of initial temperature $\tau_0$ are reported in Table 4. We have some conclusions. (1) The model trained with MACL-b
Figure 4: Metrics and performance of CL models trained with 6 different losses on CIFAR100. All of the higher values indicate better: (a) Semantic sensitivity metric of the learned representations. (b) Uniformity metric of the embedding space, and $U = -L_{\text{uniform}}$ for the plotting purpose. (c) Alignment metric of the embedding space, and $A = \mathbb{E}[f_i \cdot g_i]$. (d) KNN evaluation accuracy of trained encoders.

Table 4: Results under different $\tau (\tau_0)$ on STL10.

| Temperature | 0.07 | 0.1 | 0.15 | 0.2 | 0.3 |
|-------------|------|-----|------|-----|-----|
| InfoNCE     | 77.90| 81.00| 81.55| 81.26| 79.85|
| DCL         | 80.04| 80.30| 81.74| 80.95| 80.69|
| Dual        | 79.21| 80.94| 81.78| 80.96| 80.60|
| Info-a      | 80.83| 81.77| 81.66| 79.35| 76.58|
| MACL-a      | 81.36| 82.68| 81.38| 79.53| 79.53|
| MACL-b      | 81.21| 82.16| 82.90| 81.64| 81.16|

Table 5: Performance of MoCo under different queue sizes.

| Queue size | 256 | 512 | 1024 | 2048 | 4096 |
|------------|-----|-----|------|------|------|
| InfoNCE    | 60.30| 61.08| 61.24| 61.50| 62.03|
| DCL        | 60.78| 61.32| 61.55| 62.19| 62.34|
| Dual       | 60.49| 61.29| 61.17| 61.32| 61.98|
| Info-a     | 61.25| 61.66| 62.25| 62.97| 63.09|
| MACL-a     | 62.75| 62.41| 62.36| 62.43| 62.91|
| MACL-b     | 61.28| 61.68| 61.83| 62.16| 62.05|

MoCo framework can also be enhanced by model-aware strategy. MoCo family is another representative CL framework, which utilizes a queue structure to store negative features and updates them with a momentum encoder. Table 5 shows the LE accuracy under different queue sizes (detailed settings and KNN results are reported in the supplementary material). These results suggest: (1) MACL loss outperforms other counterparts though small queue sizes cannot provide keys of high quality (He et al. 2020). (2) Under larger queue size, Info-a leads to comparable or better performance. This corroborates the correctness of our judgment for gradient reduction and model-aware strategy.

Table 6: Results of different reweighting methods.

| Dataset      | CIFAR10 | CIFAR100 | STL10  |
|--------------|---------|----------|--------|
| MACL-a       | 87.37   | 61.81    | 82.68  |
| MACL-w       | 86.34   | 59.64    | 81.71  |

Inter-anchor hardness-aware property is inferior to the constant reweighting. Intuitively, inter-anchor hardness-awareness (Zhang et al. 2022) put more weight on those hard anchors, which may also be a facilitating property. We identify the impact by replacing $\text{sg} (1/W_i)$ with another reweighting method $\text{sg} \left( W'/W_i \right)$ denoted as MACL-w. $W'$ is described as:

$$W' = 2 - f_i \cdot g_i,$$

which alleviates the gradient reduction problem but retains the inter-anchor hardness-aware property. From the results in Table 6, however, we observe that MACL-w has no significant positive effect compared with MACL-a under the same settings. This implies that our constant reweighting is a better method.

Conclusion

In this work, we propose a Model-Aware Contrastive Learning (MACL) strategy to alleviate the uniformity-tolerance dilemma. Recognizing the empirically asymptotical semantic sensitivity in training, an alignment-adaptive temperature is designed to improve the learned embedding space. Besides, we offer some insights into the importance of large negative sample sizes and the temperature in contrastive learning by analyzing gradient reduction. A new contrastive loss is proposed based on these analyses and MACL strategy. Experiment results on different datasets verify the correctness of our MACL strategy. We also hope this work can inspire researchers to design novel loss and explore more interesting properties of contrastive learning.
References

Bengio, Y.; Courville, A.; and Vincent, P. 2013. Representation learning: A review and new perspectives. *IEEE transactions on pattern analysis and machine intelligence.*

Chen, J.; Gan, Z.; Li, X.; Guo, Q.; Chen, L.; Gao, S.; Chung, T.; Xu, Y.; Zeng, B.; Lu, W.; et al. 2021. Simpler, faster, stronger: Breaking the log-k curse on contrastive learners with flatness. *arXiv preprint arXiv:2107.01152.*

Chen, T.; Kornblith, S.; Norouzi, M.; and Hinton, G. 2020a. A simple framework for contrastive learning of visual representations. In *International conference on machine learning.*

Chen, X.; Fan, H.; Girshick, R.; and He, K. 2020b. Improved baselines with momentum contrastive learning. *arXiv preprint arXiv:2003.04297.*

Chen, X.; and He, K. 2021. Exploring simple siamese representation learning. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition.*

Coates, A.; Ng, A.; and Lee, H. 2011. An analysis of single-layer networks in unsupervised feature learning. In *Proceedings of the fourteenth international conference on artificial intelligence and statistics.*

Dosovitskiy, A.; Springenberg, J. T.; Riedmiller, M.; and Brox, T. 2014. Discriminative unsupervised feature learning with convolutional neural networks. *Advances in neural information processing systems.*

Fang, H.; Wang, S.; Zhou, M.; Ding, J.; and Xie, P. 2020. Cett: Contrastive self-supervised learning for language understanding. *arXiv preprint arXiv:2005.12766.*

Grill, J.-B.; Strub, F.; Altché, F.; Tallec, C.; Richemond, P.; Buchatskaya, E.; Doersch, C.; Avila Pires, B.; Guo, Z.; Gheshlaghi Azar, M.; et al. 2020. Bootstrap your own latent-a new approach to self-supervised learning. *Advances in Neural Information Processing Systems.*

He, K.; Chen, X.; Xie, S.; Li, Y.; Dollár, P.; and Girshick, R. 2022. Masked autoencoders are scalable vision learners. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition.*

He, K.; Fan, H.; Wu, Y.; Xie, S.; and Girshick, R. 2020. Momentum contrast for unsupervised visual representation learning. In *Proceedings of the IEEE/CVF conference on computer vision and pattern recognition.*

He, K.; Gkioxari, G.; Dollár, P.; and Girshick, R. 2017. Mask r-cnn. In *Proceedings of the IEEE international conference on computer vision.*

He, K.; Zhang, X.; Ren, S.; and Sun, J. 2016. Deep residual learning for image recognition. In *Proceedings of the IEEE conference on computer vision and pattern recognition.*

Komodakis, N.; and Gidaris, S. 2018. Unsupervised representation learning by predicting image rotations. In *International Conference on Learning Representations (ICLR).*

Krizhevsky, A.; Hinton, G.; et al. 2009. Learning multiple layers of features from tiny images.

Liu, Z.; Lin, Y.; Cao, Y.; Hu, H.; Wei, Y.; Zhang, Z.; Lin, S.; and Guo, B. 2021. Swin transformer: Hierarchical vision transformer using shifted windows. In *Proceedings of the IEEE/CVF International Conference on Computer Vision.*

Noroozi, M.; and Favaro, P. 2016. Unsupervised learning of visual representations by solving jigsaw puzzles. In *European conference on computer vision.*

Pathak, D.; Krahenbuhl, P.; Donahue, J.; Darrell, T.; and Efros, A. A. 2016. Context encoders: Feature learning by inpainting. In *Proceedings of the IEEE conference on computer vision and pattern recognition.*

Radford, A.; Kim, J. W.; Hallacy, C.; Ramesh, A.; Goh, G.; Agarwal, S.; Sastry, G.; Askell, A.; Mishkin, P.; Clark, J.; et al. 2021. Learning transferable visual models from natural language supervision. In *International Conference on Machine Learning.*

Tian, Y. 2022. Deep contrastive learning is provably (almost) principal component analysis. *arXiv preprint arXiv:2201.12680.*

Tian, Y.; Krishnan, D.; and Isola, P. 2020. Contrastive multiview coding. In *European conference on computer vision.*

Van den Oord, A.; Li, Y.; and Vinyals, O. 2018. Representation learning with contrastive predictive coding. *arXiv e-prints.*

Wang, F.; and Liu, H. 2021. Understanding the behaviour of contrastive loss. In *Proceedings of the IEEE/CVF conference on computer vision and pattern recognition.*

Wang, T.; and Isola, P. 2020. Understanding contrastive representation learning through alignment and uniformity on the hypersphere. In *International Conference on Machine Learning.*

Wu, M.; Zhuang, C.; Mosse, M.; Yamins, D.; and Goodman, N. 2020. On mutual information in contrastive learning for visual representations. *arXiv preprint arXiv:2005.13149.*

Wu, Z.; Xiong, Y.; Yu, S. X.; and Lin, D. 2018. Unsupervised Feature Learning via Non-Parametric Instance Discrimination. In *Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition (CVPR).*

Ye, M.; Zhang, X.; Yuen, P. C.; and Chang, S.-F. 2019. Unsupervised embedding learning via invariant and spreading instance feature. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition.*

Yeh, C.-H.; Hong, C.-Y.; Hsu, Y.-C.; Liu, T.-L.; Chen, Y.; and LeCun, Y. 2021. Decoupled Contrastive Learning. *arXiv preprint arXiv:2110.06848.*

Zbontar, J.; Jing, L.; Misra, I.; LeCun, Y.; and Deny, S. 2021. Barlow twins: Self-supervised learning via redundancy reduction. In *International Conference on Machine Learning.*

Zhang, C.; Zhang, K.; Pham, T. X.; Niu, A.; Qiao, Z.; Yoo, C. D.; and Kweon, I. S. 2022. Dual temperature helps contrastive learning without many negative samples: Towards understanding and simplifying moco. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition.*

Zhong, Y.; Tang, H.; Chen, J.; Peng, J.; and Wang, Y.-X. 2022. Is Self-Supervised Learning More Robust Than Supervised Learning? *arXiv preprint arXiv:2206.05239.*
Supplementary Material

Pseudocode of MACL

We show the pseudocode of MACL-a loss function for SimCLR and MoCo experiments in Algorithm 1 and 2, respectively. Besides, the code for MACL-b can be obtained with only a slight modification for temperature strategy.

Algorithm 1: Pseudocode of MACL-a loss function for SimCLR in a PyTorch-like style.

```python
# fx, gx: output features from encoders
# tau_init: initial temperature
# alpha: base value of scaling factor

def MACLa(fx, gx, tau_init, alpha):
    logits = fx @ gx.T
    A = (torch.trace(torch.softmax(logits) / fx.shape[0])).detach()
    tau = tau_init * alpha**A
    P = torch.softmax(logits / tau, dim=1)
    W = W1 / W0
    loss = -W.detach() * torch.log(P[:, 0])
    return loss.mean()
```

Algorithm 2: Pseudocode of MACL-a loss function for MoCo in a PyTorch-like style.

```python
# logits: dot product matrix of anchors and keys, the first column are value of positive pairs
# tau_init: initial temperature
# alpha: base value of scaling factor

def MACLa(logits, tau_init, alpha):
    s = logits.shape
    A = (torch.sum(logits[:, 0] / s[0])).detach()
    tau = tau_init * alpha**A
    P = torch.softmax(logits / torch.tensor(tau), dim=1)
    W = W1 / W0
    loss = -W.detach() * torch.log(P[:, 0])
    return loss.mean()
```

Proof of Propositions

We now recall Propositions [1] and [2].

**Proposition 1 (Bound of gradient scaling factor w.r.t. K)**  
Given the anchor feature \( f_i \), and temperature \( \tau \), if \( K \rightarrow +\infty \), then \( W_i \) approaches its upper bound 1. The limit is formulated as:
\[
\lim_{K \rightarrow +\infty} W_i = 1. \tag{17}
\]

**Proposition 2 (Bound of gradient scaling factor w.r.t. \( \tau \))**  
Given \( f_i \) and key set \( G \), \( W_i \) monotonically changes with respect to \( \tau \). The monotonicity is determined by the similarity distribution of samples. If \( \tau \rightarrow +\infty \), then \( W_i \) approaches its bound \( K/(K + 1) \), formulated as:
\[
\lim_{\tau \rightarrow +\infty} W_i = \frac{K}{1 + K}. \tag{18}
\]

For simplicity, let \( E_k = \exp(f_i \cdot g_k/\tau) \), \( s_k = f_i \cdot g_k \), \( E_{max} = \max(E_1, \ldots, E_p, \ldots, E_K), k \neq i \), and \( E_{min} = \min(E_1, \ldots, E_p, \ldots, E_K), k \neq i \).

**Proof 1 (Proof of Proposition 1)**  
Here
\[
W_i = 1 - \frac{E_i}{E_i + \sum_{j=1}^{K} E_j}, \tag{19}
\]
and the following inequality
\[
1 - \frac{E_i}{E_i + K \cdot E_{min}} \leq W_i \leq 1 - \frac{E_i}{E_i + K \cdot E_{max}}. \tag{20}
\]
Since we have the limit of the left part
\[
\lim_{K \rightarrow +\infty} (1 - \frac{E_i}{E_i + K \cdot E_{min}}) = 1 \tag{21}
\]
as well as the one of the right part
\[
\lim_{K \rightarrow +\infty} (1 - \frac{E_i}{E_i + K \cdot E_{max}}) = 1, \tag{22}
\]
thus the limit of \( W_i \) is
\[
\lim_{K \rightarrow +\infty} W_i = 1. \tag{23}
\]
Notice that \( E_k > 0 \) strictly, then for a given \( K \), \( W_i < 1 \). Thus, \( W_i \) has its upper bound of 1 w.r.t. \( K \).

**Proof 2 (Proof of Proposition 2)**  
For the temperature \( \tau \), we have
\[
\lim_{\tau \rightarrow +\infty} W_i = \lim_{\tau \rightarrow +\infty} \frac{\sum_{r=1}^{K} E_r}{\sum_{r=1}^{K} E_r + \sum_{j=1}^{K} E_j} \tag{24}
\]
\[
= \frac{\sum_{r=1}^{K} \lim_{\tau \rightarrow +\infty} E_r}{\lim_{\tau \rightarrow +\infty} E_i + \sum_{j=1}^{K} \lim_{\tau \rightarrow +\infty} E_j}. \tag{25}
\]
Since the similarity value on hypersphere is bounded, i.e., \( s_k = f_i \cdot g_k \in [-1, 1] \), so
\[
\lim_{\tau \rightarrow +\infty} E_k = 1. \tag{26}
\]

Hence, from Eq. 24 and 25
\[
\lim_{\tau \rightarrow +\infty} W_i = \frac{K}{1 + K}. \tag{27}
\]

The gradient of \( W_i \) with respect to \( \tau \) is derived as:
\[
\frac{\partial W_i}{\partial \tau} = \frac{1}{r^2} \cdot \frac{E_i}{(E_i + \sum_{j=1}^{K} E_j)^2} \cdot \sum_{j=1}^{K} (s_i - s_r) \cdot E_r. \tag{28}
\]
As \( E_k > 0 \), then we have
\[
\frac{\partial W_i}{\partial \tau} \propto \sum_{j=1}^{K} (s_i - s_r) \cdot E_r. \tag{29}
\]

For a batch of very poor embeddings, \( \partial W_i/\partial \tau \leq 0 \), then \( W_i \) is a monotonic decreasing function with respect to \( \tau \). In contrast, for a batch of good embeddings, \( W_i \) monotonically increases as \( \tau \) increases. So the similarity distribution of samples determine the monotonicity.

Naturally, Proposition 2 is a direct consequence of above conclusions. \( \square \)
About Experiments

Setup for MoCo

We adopt a Resnet50 ([He et al. 2016]) that has the same modification as the used SimCLR ([Chen et al. 2020a]) as query encoder. Besides, the utilized four types of augmentations are also the same as in SimCLR. We set the momentum of the key encoder to 0.99. Following MoCo v2, we used projection head in implementation ([He et al. 2020; Chen et al. 2020b]). We use Adam optimizer with learning rate 1e-3 and weight decay 1e-6. The settings for batch size, epochs, and temperature are also the same as SimCLR.

KNN accuracy

We report the KNN evaluation performance corresponding to LE results in experiments in this section. \( k=200 \) for all results.

Table 1: Performance under different epochs on CIFAR100.

| Epoch  | 100  | 200  | 300  | 400  | 500  |
|--------|------|------|------|------|------|
| InfoNCE| 46.32| 50.74| 54.10| 55.16| 56.27|
| DCL    | 50.91| 54.68| 56.74| 57.93| 59.17|
| Dual   | 50.61| 55.20| 57.21| 58.09| 59.19|
| Info-a | 50.89| 55.42| 57.67| 58.25| 59.67|
| MACL-a | 51.09| 55.70| 57.64| 58.78| 59.67|
| MACL-b | 50.94| 55.99| 57.50| 58.69| 59.87|

Table 2: KNN acc under different batchsizes on CIFAR10.

| Batch size | 64  | 128 | 256 | 512 | 1024 |
|------------|-----|-----|-----|-----|------|
| InfoNCE    | 77.35| 79.01| 80.28| 80.72| 81.32|
| DCL        | 84.59| 84.64| 83.86| 83.19| 82.47|
| Dual       | 84.40| 84.69| 83.87| 83.50| 82.53|
| Info-a     | 83.30| 85.11| 85.23| 84.92| 84.27|
| MACL-a     | 85.04| 85.67| 85.52| 84.96| 84.40|
| MACL-b     | 84.96| 84.85| 85.32| 84.90| 83.68|

Table 3: KNN accuracy with different \( \tau (\tau_0) \) on STL10.

| Temperature | 0.07 | 0.1  | 0.15 | 0.2  | 0.3  |
|-------------|------|------|------|------|------|
| InfoNCE     | 75.83| 77.53| 79.75| 78.79| 78.71|
| DCL         | 78.15| 78.41| 79.10| 78.91| 78.75|
| Dual        | 78.20| 78.74| 79.84| 78.51| 78.08|
| Info-a      | 79.81| 80.48| 79.94| 78.24| 76.83|
| MACL-a      | 80.94| 80.13| 79.06| 78.80| 77.01|
| MACL-b      | 80.80| 79.81| 79.70| 79.24| 78.03|

Table 4: KNN accuracy of MoCo under different queue sizes on CIFAR100.

| Queue size | 256 | 512 | 1024 | 2048 | 4096 |
|------------|-----|-----|------|------|------|
| InfoNCE    | 45.79| 47.46| 48.51| 49.28| 49.67|
| DCL        | 46.20| 47.71| 49.12| 50.05| 50.52|
| Dual       | 47.33| 48.56| 49.05| 49.23| 50.06|
| Info-a     | 49.21| 50.35| 50.22| 50.40| 51.23|
| MACL-a     | 50.99| 51.12| 51.09| 51.37| 50.73|
| MACL-b     | 48.49| 49.62| 49.78| 50.13| 50.03|

Table 5: Results of different reweighting methods

| Dataset  | CIFAR10 | CIFAR100 | STL10 |
|----------|---------|----------|-------|
| MACL-a   | 85.52   | 55.70    | 80.13 |
| MACL-w   | 84.90   | 54.87    | 80.53 |