## A. Gradient Analysis

## A.1. Contrastive Learning Methods

Derivation of the gradient for MoCo [17]. For simplicity, we denote $l\left(u_{1}^{o}\right)$ as the InfoNCE loss for the sample $u_{1}^{o}$ :

$$
\begin{equation*}
l\left(u_{1}^{o}\right)=-\log \frac{\exp \left(\cos \left(u_{1}^{o}, u_{2}^{m}\right) / \tau\right)}{\sum_{v^{m} \in \mathcal{V}_{\text {bank }}} \exp \left(\cos \left(u_{1}^{o}, v^{m}\right) / \tau\right)} \tag{16}
\end{equation*}
$$

Let $l\left(u_{1}^{o}\right)=-\log s_{u_{2}}, s_{u_{2}}=\frac{\exp \left(c_{u_{2}^{m}}\right)}{\sum_{v^{m} \in \mathcal{V}_{\text {bank }}} \exp \left(c_{v^{m}}\right)}, c_{v}=$ $\cos \left(u_{1}^{o}, v\right) / \tau$. According to the chain rule, we have

$$
\begin{align*}
\frac{\partial l\left(u_{1}^{o}\right)}{\partial u_{1}^{o}}= & \frac{\partial l\left(u_{1}^{o}\right)}{\partial s_{u_{2}}} \cdot \frac{\partial s_{u_{2}}}{\partial c_{u_{2}^{m}}} \cdot \frac{\partial c_{u_{2}^{m}}}{\partial u_{1}^{o}} \\
& +\sum_{v^{m} \in \mathcal{V}_{\text {bank }} \backslash u_{2}^{m}} \frac{\partial l\left(u_{1}^{o}\right)}{\partial s_{u_{2}}} \cdot \frac{\partial s_{u_{2}}}{\partial c_{v^{m}}} \cdot \frac{\partial c_{v^{m}}}{\partial u_{1}^{o}} \\
= & -\frac{1}{s_{u_{2}}} \cdot s_{u_{2}}\left(1-s_{u_{2}}\right) \cdot \frac{u_{2}^{m}}{\tau} \\
& -\sum_{v^{m} \in \mathcal{V}_{\text {bank }} \backslash u_{2}^{m}} \frac{1}{s_{u_{2}}} \cdot s_{u_{2}} s_{v} \cdot \frac{v^{m}}{\tau} \\
= & -\frac{u_{2}^{m}}{\tau}+\sum_{v^{m} \in \mathcal{V}_{\text {bank }}} s_{v} \frac{v^{m}}{\tau} \tag{17}
\end{align*}
$$

where $s_{v}=\frac{\exp \left(\cos \left(u_{1}^{o}, v^{m}\right) / \tau\right)}{\sum_{y^{m} \in \mathcal{V}_{\text {bank }}} \exp \left(\cos \left(u_{1}^{o}, y^{m}\right) / \tau\right)}$.
Denote $L$ as the averaged $l(\cdot)$ over a batch of N samples, its gradient w.r.t $u_{1}^{o}$ is

$$
\begin{equation*}
\frac{\partial L}{\partial u_{1}^{o}}=\frac{1}{N} \frac{\partial l\left(u_{1}^{o}\right)}{\partial u_{1}^{o}}=\frac{1}{\tau N}\left(-u_{2}^{m}+\sum_{v^{m} \in \mathcal{V}_{\text {bank }}} s_{v} v^{m}\right) . \tag{18}
\end{equation*}
$$

```
Algorithm 1 Pseudocode of MoCo in PyTorch style.
# u1, u2: normalized representations for two augmented
    views of shape [N, C]
# V_bank: the memory bank of shape [K, C]
# tau: the temperature coefficient
positive term
loss_pos = -(u1*u2.detach()).sum(-1) # [N, 1]
# negative term
weight = softmax(u1@V_bank.T/tau, dim=-1) # [N, K]
loss_neg = (weight@V_bank)*v1.sum(-1) # [N, 1]
# MoCo
loss =1/tau * (loss_pos + loss_neg).mean()
```

Derivation of the gradient for SimCLR [6]. For SimCLR, the InfoNCE loss $l\left(u_{1}^{o}\right)$ should be modified as

$$
\begin{equation*}
l\left(u_{1}^{o}\right)=-\log \frac{\exp \left(\cos \left(u_{1}^{o}, u_{2}^{s}\right) / \tau\right)}{\sum_{v^{s} \in \mathcal{V}_{\text {batch }} \backslash u_{1}^{o}} \exp \left(\cos \left(u_{1}^{o}, v^{s}\right) / \tau\right)} . \tag{19}
\end{equation*}
$$

Note that because the target branch is not detached from back-propagation, $u_{1}^{o}$ can receive gradients from $l\left(u_{2}^{s}\right)$ and $l\left(v^{s}\right)$. Accordingly, the gradient can be derived as

$$
\frac{\partial L}{\partial u_{1}^{o}}=\frac{1}{N}\left(\frac{\partial l\left(u_{1}^{o}\right)}{\partial u_{1}^{o}}+\frac{\partial l\left(u_{2}^{s}\right)}{\partial u_{1}^{o}}+\sum_{v^{s} \in \mathcal{V}_{\text {batch }} \backslash\left\{u_{1}^{o}, u_{2}^{s}\right\}} \frac{\partial l\left(v^{s}\right)}{\partial u_{1}^{o}}\right)
$$

$$
\begin{align*}
= & \frac{1}{\tau N}\left(-u_{2}^{s}+\sum_{\left.v^{s} \in \mathcal{V}_{\text {batch } \backslash u_{1}^{o}} s_{v} v^{s}\right)}\right. \\
& +\frac{1}{\tau N}\left(-u_{2}^{s}+t_{u_{2}} u_{2}^{s}\right)+\frac{1}{\tau N} \sum_{v^{s} \in \mathcal{V}_{\text {batch }} \backslash\left\{u_{1}^{o}, u_{2}^{s}\right\}} t_{v} v^{s} \\
= & \frac{1}{\tau N}\left(-u_{2}^{s}+\sum_{v^{s} \in \mathcal{V}_{\text {batch } \backslash u_{1}^{o}}} s_{v} v^{s}\right) \\
& +\frac{1}{\tau N}\left(-u_{2}^{s}+\sum_{\left.v^{s} \in \mathcal{V}_{\text {batch } \backslash u_{1}^{o}} t_{v} v^{s}\right),}\right. \tag{20}
\end{align*}
$$

where $t_{v}=\frac{\exp \left(\cos \left(v^{s}, u_{1}^{o}\right) / \tau\right)}{\sum_{y^{s} \in \mathcal{V}_{\text {batch }} \backslash v^{s}} \exp \left(\cos \left(v^{s}, y^{s}\right) / \tau\right)}$. If we stop the gradient from $l\left(u_{2}^{s}\right)$ and $l\left(v^{s}\right)$, Eq.(20) will reduce to

$$
\begin{equation*}
\frac{\partial L}{\partial u_{1}^{o}} \approx \frac{1}{\tau N}\left(-u_{2}^{s}+\sum_{v^{s} \in \mathcal{V}_{\mathrm{batch}} \backslash u_{1}^{o}} s_{v} v^{s}\right), \tag{21}
\end{equation*}
$$

which shares a similar structure with that of MoCo. We demonstrate empirically that this simplification does no harm to the performance as shown in Table 6.

```
Algorithm 2 Pseudocode of Simplified SimCLR in Py-
Torch style.
# ul, u2: normalized representations for two augmented
    views of shape [N, C]
# tau: the temperature coefficient
# positive term
loss_pos = -(u1*u2.detach()).sum(-1) # [N, 1]
# negative term
weight = softmax(u1@u2.T/tau, dim=-1) # [N, N]
loss_neg = (weight@u2).detach()*u1.sum(-1) # [N, 1]
# simplified SimCLR
loss = 1/tau * (loss_pos + loss_neg).mean()
```


## A.2. Asymmtric Network Methods

Derivation of the gradient for DirectPred [28]. DirectPred takes the negative cosine similarity loss between target sample and projected online sample:

$$
\begin{gather*}
l\left(u_{1}^{o}\right)=-\cos \left(\frac{W_{h} u_{1}^{o}}{\left\|W_{h} u_{1}^{o}\right\|_{2}}, u_{2}^{t}\right)  \tag{22}\\
W_{h}=U \Lambda_{h} U^{T}, \Lambda_{h}=\Lambda_{F}^{1 / 2}+\epsilon \lambda_{\max } I \tag{23}
\end{gather*}
$$

where $U$ and $\Lambda_{F}$ are the eigenvectors and eigenvalues of $F=\sum_{v^{o} \in \mathcal{V}_{\infty}} \rho_{v} v^{o} v^{o T}$, respectively. $\epsilon$ is a hyperparameter to boost small eigenvalues.

Denote $y_{1}=W_{h} u_{1}^{o}, y_{1}^{n}=\frac{y_{1}}{\left\|y_{1}\right\|_{2}}$, the gradient of $L$ can be derived as:

$$
\begin{aligned}
\frac{\partial L}{\partial u_{1}^{o}} & =\frac{1}{N}\left(\frac{\partial y_{1}}{\partial u_{1}^{o}} \cdot \frac{\partial y_{1}^{n}}{\partial y_{1}} \cdot \frac{\partial l}{\partial y_{1}^{n}}\right) \\
& =\frac{1}{N}\left(-W_{h}^{T} \cdot \frac{1}{\left\|y_{1}\right\|_{2}}\left(I-\frac{y_{1} y_{1}^{T}}{y_{1}^{T} y_{1}}\right) \cdot u_{2}^{t}\right) \\
& =\frac{1}{\left\|W_{h} u_{1}^{o}\right\|_{2} N}\left(-W_{h}^{T}\left(I-\frac{W_{h} u_{1}^{o} u_{1}^{o T} W_{h}^{T}}{u_{1}^{o T} W_{h}^{T} W_{h} u_{1}^{o}}\right) u_{2}^{t}\right)
\end{aligned}
$$

$$
\begin{equation*}
=\frac{1}{\left\|W_{h} u_{1}^{o}\right\|_{2} N}\left(-W_{h}^{T} u_{2}^{t}+\frac{u_{1}^{o T} W_{h}^{T} u_{2}^{t}}{u_{1}^{o T} W_{h}^{T} W_{h} u_{1}^{o}} W_{h}^{T} W_{h} u_{1}^{o}\right) \tag{24}
\end{equation*}
$$

Note that

$$
\begin{align*}
W_{h}^{T} W_{h} & =U \Lambda_{h}^{T} U^{T} U \Lambda_{h} U^{T} \\
& =U\left(\Lambda_{F}+2 \epsilon \lambda_{\max } \Lambda_{F}^{1 / 2}+\epsilon^{2} \lambda_{\max }^{2} I\right) U^{T} \\
& =F+2 \epsilon \lambda_{\max } F^{1 / 2}+\epsilon^{2} \lambda_{\max }^{2} I \tag{25}
\end{align*}
$$

Substituting Eq.(25) into Eq.(24) leads to

$$
\begin{align*}
\frac{\partial L}{\partial u_{1}^{o}}= & \frac{1}{\left\|W_{h} u_{1}^{o}\right\|_{2} N}\left(-W_{h}^{T} u_{2}^{t}\right. \\
& \left.+\tilde{\lambda}\left(F u_{1}^{o}+2 \epsilon \lambda_{\max } F^{1 / 2} u_{1}^{o}+\epsilon^{2} \lambda_{\max }^{2} u_{1}^{o}\right)\right) \tag{26}
\end{align*}
$$

where $\tilde{\lambda}=\frac{u_{1}^{o T} W_{h}^{T} u_{2}^{t}}{u_{1}^{o T}\left(F+2 \epsilon \lambda_{\text {max }} F^{1 / 2}+\epsilon^{2} \lambda_{\text {max }}^{2} I\right) u_{1}^{o}}$. For those three terms that are scaled by $\tilde{\lambda}$, we plot the value of their magnitude and the similarity of the first two terms in Figure 3(a). It's shown that the first two terms have highly similar direction so they are expected to have similar effect on the training. We have also verified that removing the $F^{1 / 2}$ term will not cause performance drop (see Table 6). Thus, the gradient can be simplified into

$$
\begin{equation*}
\frac{\partial L}{\partial u_{1}^{o}} \approx \frac{1}{\left\|W_{h} u_{1}^{o}\right\|_{2} N}\left(-W_{h}^{T} u_{2}^{t}+\lambda\left(F u_{1}^{o}+\epsilon^{2} \lambda_{\max }^{2} u_{1}^{o}\right)\right) \tag{27}
\end{equation*}
$$

where $\lambda=\frac{u_{1}^{o T} W_{h}^{T} u_{2}^{t}}{u_{1}^{o T}\left(F+\epsilon^{2} \lambda_{\text {max }}^{2} I\right) u_{1}^{o}}$.
When $u_{1}^{o}$ is $\ell_{2}$ normalized, we can further neglect the $\epsilon^{2} \lambda_{\text {max }}^{2} u_{1}^{o}$ term, because the gradient propagated to unnormalized $u_{1}^{o}$ is 0 . Hence, we simplify the gradient as

$$
\begin{align*}
\frac{\partial L}{\partial u_{1}^{o}} & \approx \frac{1}{\left\|W_{h} u_{1}^{o}\right\|_{2} N}\left(-W_{h}^{T} u_{2}^{t}+\lambda F u_{1}^{o}\right) \\
& =\frac{1}{\left\|W_{h} u_{1}^{o}\right\|_{2} N}\left(-W_{h}^{T} u_{2}^{t}+\lambda \sum_{v^{o} \in \mathcal{V}_{\infty}}\left(\rho_{v} u_{1}^{o T} v^{o}\right) v^{o}\right) \tag{28}
\end{align*}
$$

Note that $\lambda$ is a dynamic balance factor, but we find that its value tends to be quite stable (see Figure 3(b)), so it can also be substiuted by a constant scalar.

| Method | SimCLR [6] |  | DirectPred [28] |  |
| :---: | :---: | :---: | :---: | :---: |
| Gradient | Eq.(20) | Eq.(21) | Eq.(26) | Eq.(27) |
| Linear Eval | 67.5 | 67.6 | 70.2 | 70.2 |

Table 6. Simplification for the gradient of SimCLR and DirectPred. We use the 100 -epoch pre-training and lineal evaluation protocol described in Appendix B.

```
Algorithm 3 Pseudocode of Asymetric Networks.
# u1, u2: normalized representations for two augmented
# ul, ul: normalized repres
# F: the moving average of correlation matrix
# rho: the moving average coefficient
# eps: hyperparameter to boost small eigenvalues
# accumulate F
tmp_F = ((u1.T@u1 + u2.T@u2) / (2*N)).detach()
F = rho*F + (1-rho)*tmp_F # update moving average
# calculate Wh
U, lambda_F, V = torch.svd(F)
lambda_h = torch.sqrt(lambda_F) + eps*lambda_F.max()
Wh = U@ (torch.diag(lambda_h)@V) # [C, C]
# positive term
loss_pos = -(ul*(u2@Wh).detach()).sum(-1) # [N, 1]
# negative term
loss_neg = (u1*(u1@F).detach()).sum(-1) # [N, 1]
weight = 1/torch.linalg.norm(ul@Wh, dim=-1)
loss = (weight*(loss_pos + lambda * loss_neg)).mean()
```


(a) Dynamics of three terms in Eq. (26) (Appendix)

(c) Dynamics of the max and min value of $W_{\text {diag }}$ in Eq. (9)

(b) Dynamics of $\tilde{\lambda}$ in Eq. (26) (Appendix)

(d) Dynamics of similarity between the neglected and negative terms in Eq. (11)

Figure 3. Justifications for simplifications.

## A.3. Feature Decorrelation Methods

Derivation of the gradient for Barlow Twins [34]. Barlow Twins forces the cross-correlation matrix to be close to the identity matrix via the following loss function:

$$
\begin{equation*}
L=\sum_{i=1}^{C}\left(W_{i i}-1\right)^{2}+\lambda \sum_{i=1}^{C} \sum_{j \neq i} W_{i j}^{2} \tag{29}
\end{equation*}
$$

where $W=\frac{1}{N} \sum_{v_{1}^{o}, v_{2}^{s} \in \mathcal{V}_{\text {batch }}} v_{1}^{o} v_{2}^{s T}$ is the crosscorrelation matrix.

Denote $L_{1}=\sum_{i=1}^{C}\left(W_{i i}-1\right)^{2}, \quad L_{2}=$ $\lambda \sum_{i=1}^{C} \sum_{j \neq i} W_{i j}^{2}$. We use the operator $(\cdot)_{k}$ to represent the $k$-th element of a vector. For $L_{1}$, We have:

$$
\begin{equation*}
\frac{\partial L_{1}}{\partial\left(u_{1}^{o}\right)_{k}}=\frac{\partial L_{1}}{\partial W_{k k}} \cdot \frac{\partial W_{k k}}{\partial\left(u_{1}^{o}\right)_{k}}=2\left(W_{k k}-1\right) \cdot \frac{\left(u_{2}^{s}\right)_{k}}{N} \tag{30}
\end{equation*}
$$

For $L_{2}$, we have:

$$
\begin{align*}
& \frac{\partial L_{2}}{\partial\left(u_{1}^{o}\right)_{k}}=\lambda \sum_{j \neq k}^{C} 2 \frac{\partial L_{2}}{\partial W_{k j}} \cdot \frac{\partial W_{k j}}{\partial\left(u_{1}^{o}\right)_{k}}=\lambda \sum_{j \neq k}^{C} 2 W_{k j} \cdot \frac{\left(u_{2}^{s}\right)_{j}}{N} \\
& \quad=\frac{2 \lambda}{N}\left(-W_{k k}\left(u_{2}^{s}\right)_{k}+\sum_{j=1}^{C} W_{k j}\left(u_{2}^{s}\right)_{j}\right) \\
& \quad=\frac{2 \lambda}{N}\left(-W_{k k}\left(u_{2}^{s}\right)_{k}+\sum_{j=1}^{C} \frac{1}{N} \sum_{v_{1}^{o}, v_{2}^{s} \in \mathcal{V}_{\text {batch }}}\left(v_{1}^{o}\right)_{k}\left(v_{2}^{s}\right)_{j}\left(u_{2}^{s}\right)_{j}\right) \\
& \quad=\frac{2 \lambda}{N}\left(-W_{k k}\left(u_{2}^{s}\right)_{k}+\sum_{v_{1}^{o}, v_{2}^{s} \in \mathcal{V}_{\text {batch }}} \frac{1}{N}\left(v_{1}^{o}\right)_{k} \sum_{j=1}^{C}\left(v_{2}^{s}\right)_{j}\left(u_{2}^{s}\right)_{j}\right) \\
& \quad=\frac{2 \lambda}{N}\left(-W_{k k}\left(u_{2}^{s}\right)_{k}+\sum_{v_{1}^{o}, v_{2}^{s} \in \mathcal{V}_{\text {batch }}} \frac{u_{2}^{s T} v_{2}^{s}}{N}\left(v_{1}^{o}\right)_{k}\right) .(31) \tag{31}
\end{align*}
$$

Combining Eq.(30) and Eq.(31) together, we get:

$$
\begin{equation*}
\frac{\partial L}{\partial u_{1}^{o}}=\frac{2}{N}\left(-A u_{2}^{s}+\lambda \sum_{v_{1}^{o}, v_{2}^{s} \in \mathcal{V}_{\text {batch }}} \frac{u_{2}^{s T} v_{2}^{s}}{N} v_{1}^{o}\right) \tag{32}
\end{equation*}
$$

where $A=I-(1-\lambda) W_{\text {diag. }}$. Here $\left(W_{\text {diag }}\right)_{i j}=\delta_{i j} W_{i j}$ is the diagonal matrix of $W$, where $\delta_{i j}$ is the Kronecker delta.

```
Algorithm 4 Pseudocode of Barlow Twins in PyTorch style.
# u1, u2: representations for two augmented views of
    shape [N, C]
# lambda: the moving average coefficient
# correlation matrix
W_cor = ul.T@u2 / N # [C, C]
# positive term
pos = (1 - (1-lambda)*torch.diag(W_cor)) * u2
loss_pos = -(ul * pos.detach()).sum(-1) # [N, 1]
# negative term
weight = u2@u2.T / N
loss_neg = ((weight@ul).detach() * ul).sum(-1)
# Barlow Twins
loss = 2 * (loss_pos + lambda * loss_neg).mean()
```

Derivation of the gradient for VICReg [1]. The loss function of VICReg consists of three componets:

$$
\begin{gather*}
L_{1}=\frac{1}{N} \sum_{v_{1}^{o}, v_{2}^{s} \in \mathcal{V}_{\text {batch }}}\left\|v_{1}^{o}-v_{2}^{s}\right\|_{2}^{2},  \tag{33}\\
L_{2}=\frac{\lambda_{1}}{C} \sum_{i=1}^{C} \sum_{j \neq i}^{C} W_{i j}^{\prime 2},  \tag{34}\\
L_{3}=\frac{\lambda_{2}}{C} \sum_{i=1}^{C} \max \left(0, \gamma-\operatorname{std}\left(v_{1}^{o}\right)_{i}\right), \tag{35}
\end{gather*}
$$

where $W^{\prime}=\frac{1}{N-1} \sum_{v_{1}^{o} \in \mathcal{V}_{\text {batch }}}\left(v_{1}^{o}-\bar{v}_{1}^{o}\right)\left(v_{1}^{o}-\bar{v}_{1}^{o}\right)^{T}$.
For the invariance term $L_{1}$, we have:

$$
\begin{equation*}
\frac{\partial L_{1}}{\partial\left(u_{1}^{o}\right)_{k}}=\frac{2}{N}\left(u_{1}^{o}-u_{2}^{s}\right)_{k} . \tag{36}
\end{equation*}
$$

$$
\begin{align*}
& \text { Algorithm } 5 \text { Pseudocode of Simplified VICReg in PyTorch } \\
& \text { style. } \\
& \text { For the covariance term } L_{2} \text {, we have: } \\
& \frac{\partial L_{2}}{\partial\left(u_{1}^{o}\right)_{k}}=\frac{2 \lambda_{1}}{C} \sum_{j \neq k}^{C} \frac{\partial L_{2}}{\partial W_{k j}^{\prime}} \cdot \frac{\partial W_{k j}^{\prime}}{\partial\left(u_{1}^{o}\right)_{k}} \\
& =\frac{4 \lambda_{1}}{C} \sum_{j \neq k}^{C} W_{k j}^{\prime} \frac{\left(u_{1}^{o}-\bar{v}_{1}^{o}\right)_{j}}{N-1} \\
& =\frac{4 \lambda_{1}}{C(N-1)}\left(-W_{k k}^{\prime}\left(u_{1}^{o}-\bar{v}_{1}^{o}\right)_{k}+\sum_{j=1}^{C} W_{k j}^{\prime}\left(u_{1}^{o}-\bar{v}_{1}^{o}\right)_{j}\right) \\
& =\frac{4 \lambda_{1}}{C(N-1)}\left(-W_{k k}^{\prime}\left(u_{1}^{o}-\bar{v}_{1}^{o}\right)_{k}\right. \\
& \left.+\sum_{j=1}^{C} \sum_{v_{1}^{o} \in \mathcal{V}_{\text {batch }}} \frac{\left(u_{1}^{o}-\bar{v}_{1}^{o}\right)^{T}\left(v_{1}^{o}-\bar{v}_{1}^{o}\right)}{N-1}\left(v_{1}^{o}-\bar{v}_{1}^{o}\right)_{j}\right) \\
& =\frac{4 \lambda_{1} N}{C(N-1)^{2}}\left(-\frac{N-1}{N} W_{k k}^{\prime}\left(\tilde{u}_{1}^{o}\right)_{k}+\sum_{v_{1}^{o} \in \mathcal{V}_{\text {batch }}} \frac{\tilde{u}_{1}^{o T} \tilde{v}_{1}^{o}}{N}\left(\tilde{v}_{1}^{o}\right)_{j}\right) \\
& =\frac{2 \lambda}{N}\left(-\frac{N-1}{N} W_{k k}^{\prime}\left(\tilde{u}_{1}^{o}\right)_{k}+\sum_{v_{1}^{o} \in \mathcal{V}_{\text {batch }}} \frac{\tilde{u}_{1}^{o T} \tilde{v}_{1}^{o}}{N}\left(\tilde{v}_{1}^{o}\right)_{j}\right), \tag{37}
\end{align*}
$$

where $\lambda=\frac{2 \lambda_{1} N^{2}}{C(N-1)^{2}}$ and $\tilde{v}=v-\bar{v}$ is the de-centered sample.

For the variance term $L_{3}$, we have:

$$
\begin{align*}
\frac{\partial L_{3}}{\partial\left(u_{1}^{o}\right)_{k}} & =\frac{\lambda_{2}}{C} \frac{\partial \max \left(0, \gamma-\operatorname{std}\left(v_{1}^{o}\right)_{k}\right)}{\partial \operatorname{std}\left(v_{1}^{o}\right)_{k}} \cdot \frac{\partial \operatorname{std}\left(v_{1}^{o}\right)_{k}}{\partial\left(u_{1}^{o}\right)_{k}} \\
& =-\frac{\lambda_{2}}{C(N-1)} \mathbb{1}\left(\gamma-\operatorname{std}\left(v_{1}^{o}\right)_{k}>0\right) \frac{\left(\tilde{u}_{1}^{o}\right)_{k}}{\operatorname{std}\left(v_{1}^{o}\right)_{k}} \tag{38}
\end{align*}
$$

For final loss function $L=L_{1}+L_{2}+L_{3}$, its gradient w.r.t $u_{1}^{o}$ can be represented as:

$$
\begin{align*}
\frac{\partial L}{\partial u_{1}^{o}}= & \frac{2}{N}\left(u_{1}^{o}-u_{2}^{s}\right)-\frac{2 \lambda}{N}\left(\frac{N-1}{N} W_{\text {diag }}^{\prime} \tilde{u}_{1}^{o}-\sum_{v_{1}^{o} \in \mathcal{V}_{\text {batch }}} \frac{\tilde{u}_{1}^{o T} \tilde{v}_{1}^{o}}{N} \tilde{v}_{1}^{o}\right) \\
& -\frac{\lambda_{2}}{C(N-1)} \operatorname{diag}\left(\mathbb{1}\left(\gamma-\operatorname{std}\left(v_{1}^{o}\right)>0\right) \oslash \operatorname{std}\left(v_{1}^{o}\right)\right) \tilde{u}_{1}^{o} \\
= & \frac{2}{N}\left(-u_{2}^{s}+\lambda \sum_{v_{1}^{o} \in \mathcal{V}_{\text {batch }}} \frac{\tilde{u}_{1}^{o T} \tilde{v}_{1}^{o}}{N} \tilde{v}_{1}^{o}\right)+\frac{2 \lambda}{N}\left(\frac{1}{\lambda} u_{1}^{o}-B \tilde{u}_{1}^{o}\right), \tag{39}
\end{align*}
$$

where $B=\frac{N}{\lambda C(N-1)}\left(2 \lambda_{1} W_{\text {diag }}^{\prime}+\frac{\lambda_{2}}{2} \operatorname{diag}(\mathbb{1}(\gamma-\right.$ $\left.\left.\left.\operatorname{std}\left(v_{1}^{o}\right)>0\right) \oslash \operatorname{std}\left(v_{1}^{o}\right)\right)\right)$. Here $W_{\text {diag }}^{\prime}$ is the diagonal matrix of $W^{\prime}, \operatorname{diag}(x)$ is a matrix with diagonal filled with the vector $x, \mathbb{1}(\cdot)$ is the indicator function, and $\oslash$ denotes element-wise division.

## A.4. Pseudocode of UniGrad

```
Algorithm 6 Pseudocode of UniGrad in PyTorch style.
# u1, u2: normalized representations for two augmented
    views of shape [N, C]
# F: the moving average of correlation matrix
# rho: the moving average coefficient
# positive term
loss_pos = -(ul*u2.detach()).sum(-1) # [N, 1]
# negative term
tmp_F=((u1.T@u1 + u2.T@u2) / (2*N)).detach()
F = rho*F + (1-rho)*tmp_F # update moving average
loss_neg = (u1@F)*ul.sum(-1) # [N, 1]
# UniGrad
loss = (loss_pos + lambda * loss_neg).mean()
```


## B. Implementation Details

We provide the experimental settings used in this paper. For 100 epochs pre-training and linear evaluation, we mainly follow [8]; For 800 epochs pre-training, large batch size is adopted for faster training and hence we mainly follow [21].
Pre-training setting for 100 epochs. SGD is used as the optimizer. The weight decay is $1.0 \times 10^{-4}$ and the momentum is 0.9 . The learning rate is set according to linear scaling rule [16] as base_lr $\times$ batch_size/256, with base_lr $=0.05$. The learning rate has a cosine decay schedule for 100 epochs with 5 epochs linear warmup. The batch size is set to 1024 . We use $\operatorname{ResNet50~[18]~as~the~backbone.~}$ The projection MLP has three layers, with the hidden and output dimension set to 2048 . BN and ReLU are applied after the first two layers. If a momentum encoder is used, we follow BYOL [21] to increase the exponential moving average parameter from 0.996 to 1 with a cosine scheduler. We list these hyper-parameters in Table

Pre-training setting for 800 epochs. LARS [32] optimizer is used for 800 epochs pre-training with a batch size of 4096. The weight decay is $1.0 \times 10^{-6}$ and the momentum is 0.9 . The learning rate is set with base_lr $=0.3$ for the weights and base_lr $=0.05$ for the biases and batch normalization parameters. Cosine decay schedule is used after a linear warm-up of 10 epochs. We exclude the biases and batch normalization parameters from the LARS adaptation and weight decay. For the projector, We use a three-layer MLP with hidden and output dimension set to 8192. Other configurations keep the same as the pre-training setting for 100 epochs.
Linear evaluation. We follow the common practice to adopt linear evaluation as the performance metric. Such

| Hyper-parameter | Value |
| :--- | :--- |
| opitmizer | SGD |
| weight decay | $1.0 \times 10^{-4}$ |
| base lr | 0.05 |
| lr schedule | cosine |
| warmup | 5 epochs |
| batch size | 1024 |
| projector | 3 -layers MLP |
| init momentum | 0.996 |
| final momentum | 1.0 |
| momentum schedule | cosine |

Table 7. Hyper-parameters for 100 epochs pre-training. We use the same hyper-parameters for different loss functions.
practice trains a supervised linear classifier on top of the frozen features from pre-training. LARS [32] is used as the optimizer with weight decay as 0 and momentum as 0.9 . The base learning rate is 0.02 with 4096 batch size, and a cosine decay schedule is used for 90 epochs.

## C. Additional Results

## C.1. Projector Structure

The design of projector is another main factor that influences the final performance and also varies across different works. [17] applies linear projection to contrastive learning. SimCLR [6] finds that a 2-layer MLP can help boost the performance. SimSiam [8] further extends the projector depth to 3 . We explore the effects of different projector depths in Table 9. Here UniGrad with 100 epochs pre-training is used. The results show that increasing the depth of projector from 1 to 3 can greatly boost the linear evaluation accuracy. However, the improvement saturates when the projector becomes deeper.

Moreover, Barlow Twins [34] extends the dimension of projector from 2048 to 8192, showing notable improvement. We further study the effect of projector's width in Table 10. For simplicity, we change the output dimension together with the hidden dimension. UniGrad with 100 epochs pre-training is used. It's shown that increasing the projector width can steadily increase the performance, and does not seem to saturate even the dimension is increased to 16384.

## C.2. Semi-supervised Learning

We finetune the pretrained model on the $1 \%$ and $10 \%$ subset of ImageNet's training set, following the standard protocol in [6]. The results are reported in Table 11. Compared with previous methods, UniGrad is able to obtain comparable results with [29] and obtain $5 \%$ and $1 \%$ improvement from other methods on the $1 \%$ and $10 \%$ subset,

| Method | $\mathrm{VOCO}^{2}+12$ detection |  |  | COCO detection |  |  | COCO instance seg |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | $\mathrm{AP}_{\text {all }}$ | $\mathrm{AP}_{50}$ | $\mathrm{AP}_{75}$ | $\mathrm{AP}_{\text {all }}^{\text {box }}$ | $\mathrm{AP}_{50}^{\text {box }}$ | $\mathrm{AP}_{75}^{\text {box }}$ | $\mathrm{AP}_{\text {all }}^{\text {mask }}$ | $\mathrm{AP}_{50}^{\text {mask }}$ | $\mathrm{AP}_{75}^{\text {mask }}$ |
| Supervised | 54.7 | 84.5 | 60.8 | 38.9 | 59.6 | 42.7 | 35.4 | 56.5 | 38.1 |
| MoCov2 [7] | 56.4 | 81.6 | 62.4 | 39.8 | 59.8 | 43.6 | 36.1 | 56.9 | 38.7 |
| SimCLR [6] | 58.2 | 83.8 | 65.1 | 41.6 | 61.8 | 45.6 | 37.6 | 59.0 | 40.5 |
| DINO [5] | 57.2 | 83.5 | 63.7 | 41.4 | 62.2 | 45.3 | 37.5 | 58.8 | 40.2 |
| TWIST [29] | 58.1 | 84.2 | 65.4 | 41.9 | 62.6 | 45.7 | 37.9 | 59.7 | 40.6 |
| UniGrad | 57.8 | 84.0 | 64.9 | 42.0 | 62.6 | 45.7 | 37.9 | 59.7 | 40.7 |

Table 8. Transfer learning: object detection and instance segmentation. VOC benchmark uses Faster R-CNN with FPN. COCO benchmark uses Mask R-CNN with FPN. The supervised VOC results are run by us.

| Depth | 1 | 2 | 3 | 4 | 5 |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Linear Eval | 60.7 | 65.2 | 70.3 | 70.0 | 69.8 |

Table 9. Effect of projector depth.

| Width | 1024 | 2048 | 4096 | 8192 | 16384 |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Linear Eval | 68.3 | 70.3 | 70.5 | 70.9 | 71.2 |

Table 10. Effect of projector width.

| Method | $1 \%$ |  | $10 \%$ |  |
| :--- | :---: | :---: | :---: | :---: |
|  | Top 1 | Top 5 | Top 1 | Top 5 |
| Supervised | 25.4 | 48.4 | 56.4 | 80.4 |
| SimCLR [6] | 48.3 | 75.5 | 65.6 | 87.8 |
| BYOL [21] | 53.2 | 78.4 | 68.8 | 89.0 |
| Barlow Twins [34] | 55.0 | 79.2 | 69.7 | 89.3 |
| DINO [5] | 52.2 | 78.2 | 68.2 | 89.1 |
| TWIST [29] | 61.2 | 84.2 | 71.7 | 91.0 |
| UniGrad | 60.8 | 83.8 | 71.5 | 90.6 |

Table 11. Semi-supervised learning on ImageNet.
respectively.

## C.3. Transfer Learning

We also transfer the pretrained model to downstream stasks, including PASCAL VOC [14] object detection, COCO [25] object detection and instance segmentation. The model is finetuned in an end-to-end manner. Table 8 shows the final results. It can be seen that UniGrad delivers competitive transfer performance with other self-supervised learning methods, and surpasses the supervised baseline.

## D. Licenses of Assets

ImageNet [12] is subject to the ImageNet terms of access [11].

PASCAL VOC [14] uses images from Flickr, which is subject to the Flickr terms of use [15].

COCO [25]. The annotations are under the Creative Commons Attribution 4.0 License. The images are subject to the Flickr terms of use [15].

