An Investigation into Whitening Loss for Self-supervised Learning

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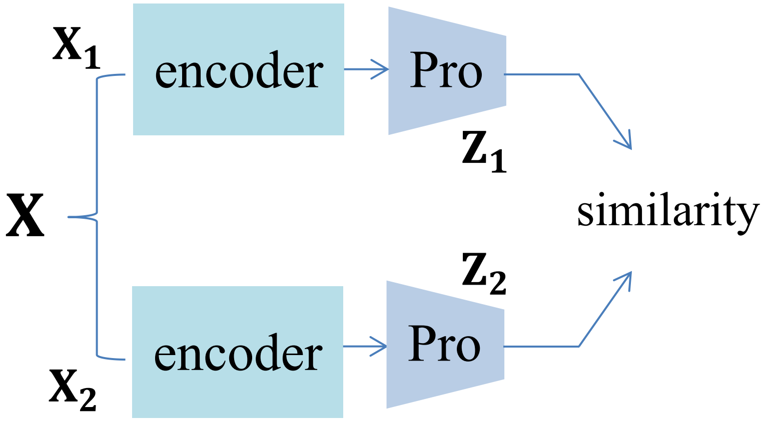
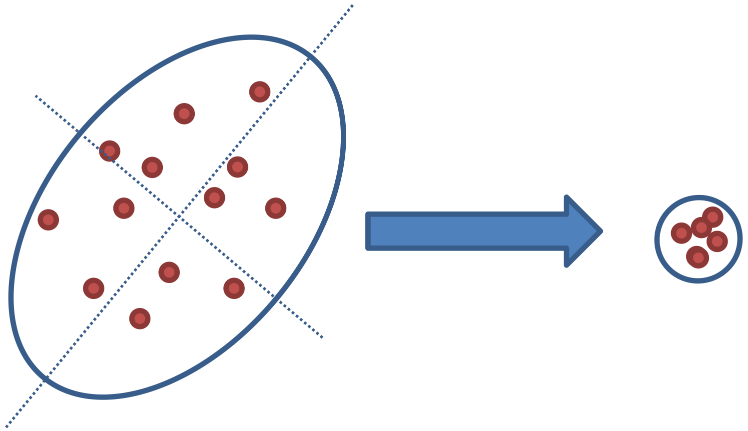
Siamese Network and Collapse

- Simaese Network

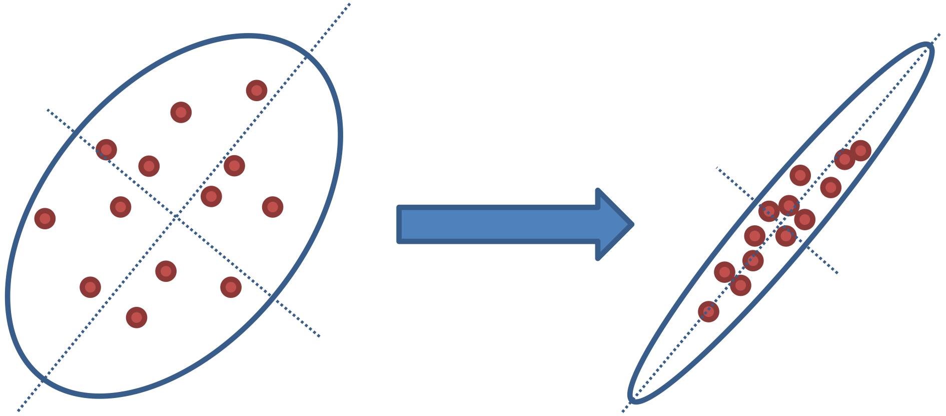


$$\mathcal{L}(\mathbf{x},\theta) = \mathbb{E}_{\mathbf{x}\sim\mathbb{D},\ \mathcal{T}_{1,2}\sim\mathbb{T}}\ \ell\big(f_\theta(\mathcal{T}_1(\mathbf{x})), f_\theta(\mathcal{T}_2(\mathbf{x}))\big)$$

- Complete Collapse

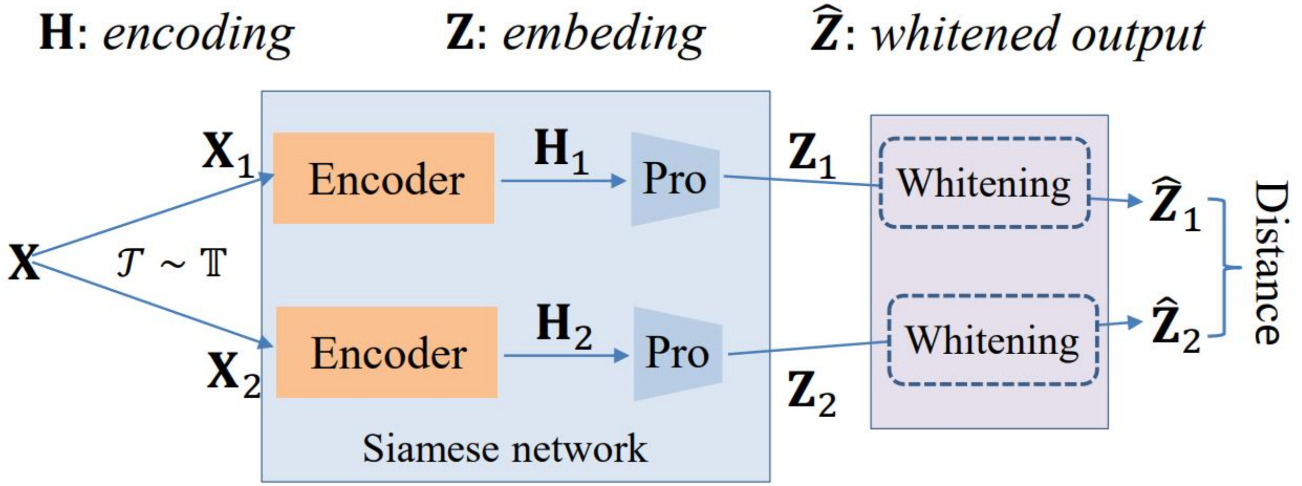


- Dimensional Collapse



Whitening loss

➢ Structure of whitening loss:



➢ Loss function:

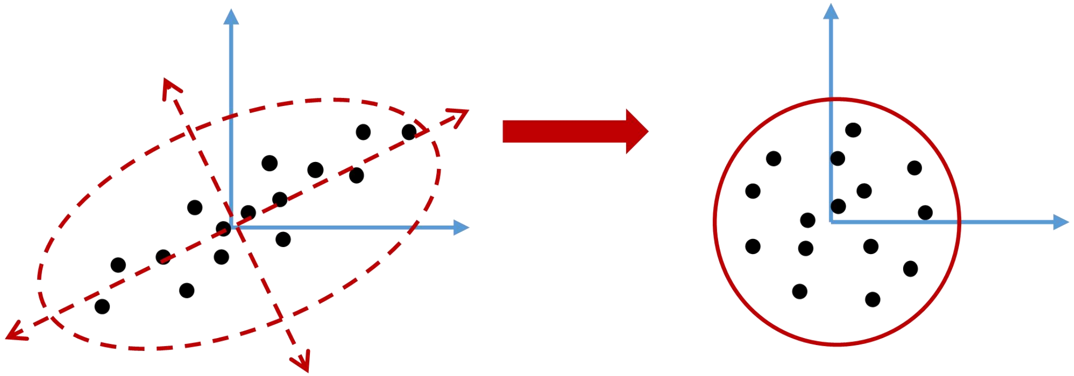
$$\min_{\theta} \mathcal{L}(\mathbf{x};\theta) = \mathbb{E}_{\mathbf{x}\sim\mathbb{D},\ \mathcal{T}_{1,2}\sim\mathbb{T}}\ \ell(\mathbf{z}_1, \mathbf{z}_2),$$
$$s.t.\ cov(\mathbf{z}_i, \mathbf{z}_i) = \mathbf{I},\ i \in \{1,2\}.$$

$$\min_{\theta} \mathcal{L}(\mathbf{X};\theta) = \mathbb{E}_{\mathbf{X}\sim\mathbb{D},\ \mathcal{T}_{1,2}\sim\mathbb{T}}\ \|\widehat{\mathbf{Z}}_1 - \widehat{\mathbf{Z}}_2\|_F^2$$
$$with\ \widehat{\mathbf{Z}}_i = \Phi(\mathbf{Z}_i),\ i \in \{1,2\},$$

Motivations of whitening loss

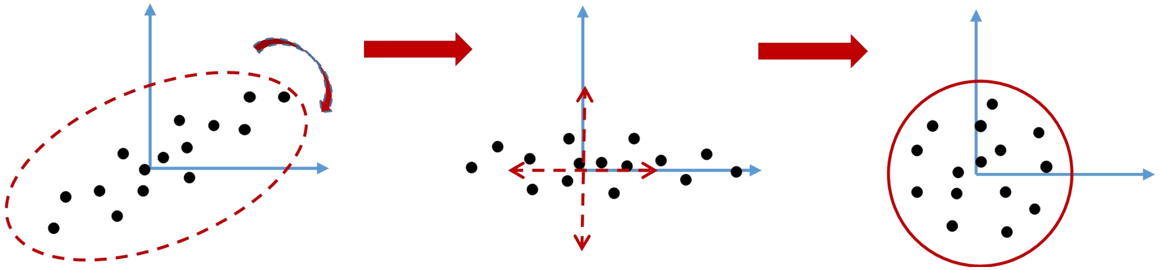
- Motivations of whitening loss:

1. Whitening operation can **remove the correlation among axes**
2. A whitened representation ensures the examples scattered in a **spherical distribution**



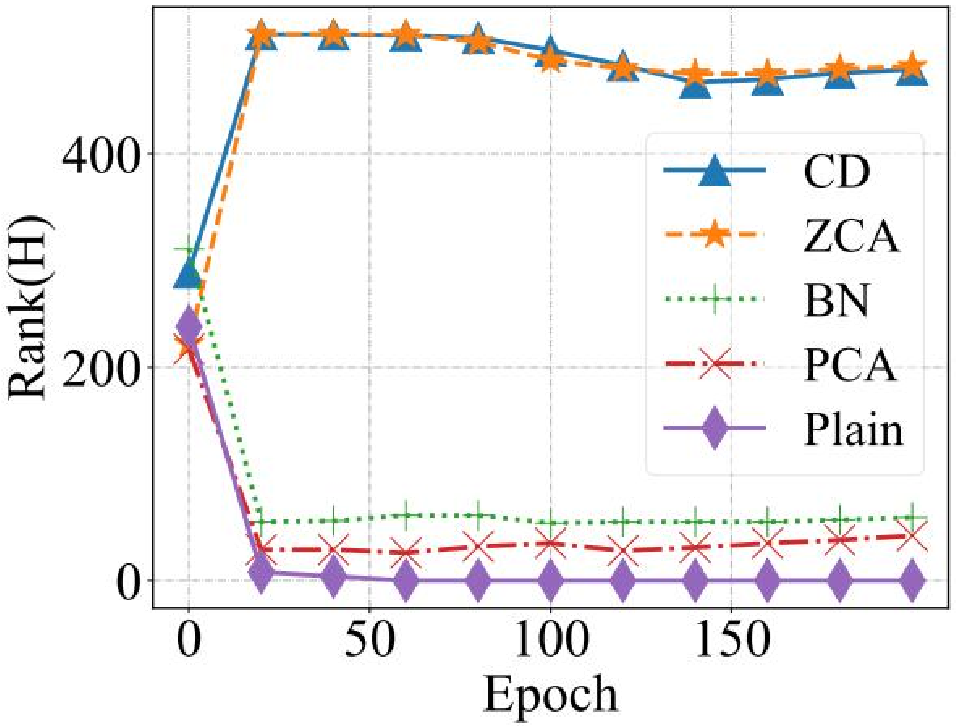
Are motivations of whitening loss correct?

➢ PCA Whitening (can also remove the correlation among axes)



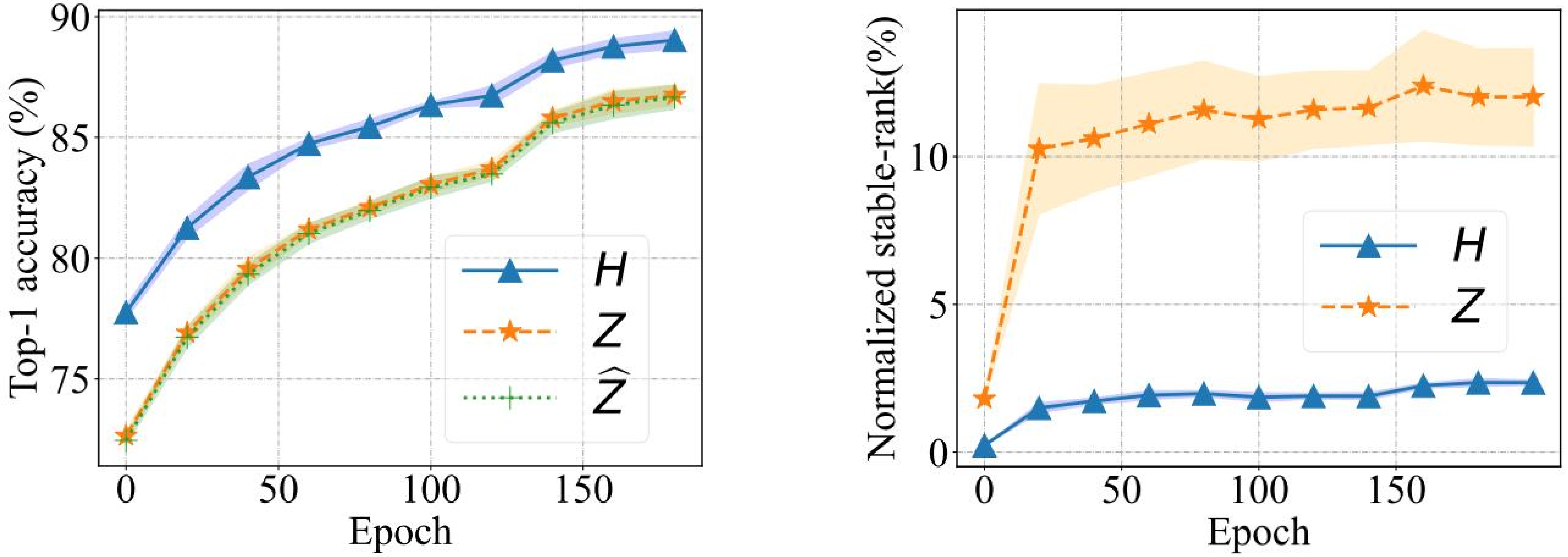
✓ A PCA whitened representation also ensures the examples scattered in a spherical distribution

➢ However, PCA Whitening Fails to Avoid Dimensional Collapse



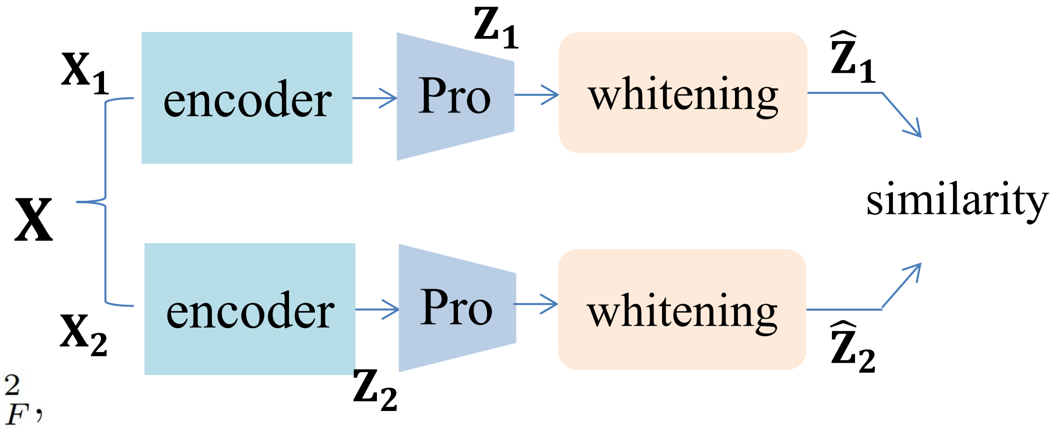
Are motivations of whitening loss correct?

➢Whitened Output is not a Good Representation.



The normalized stable-rank of $\widehat{Z}$ is always 100%

Analysing Decomposition of Whitening Loss

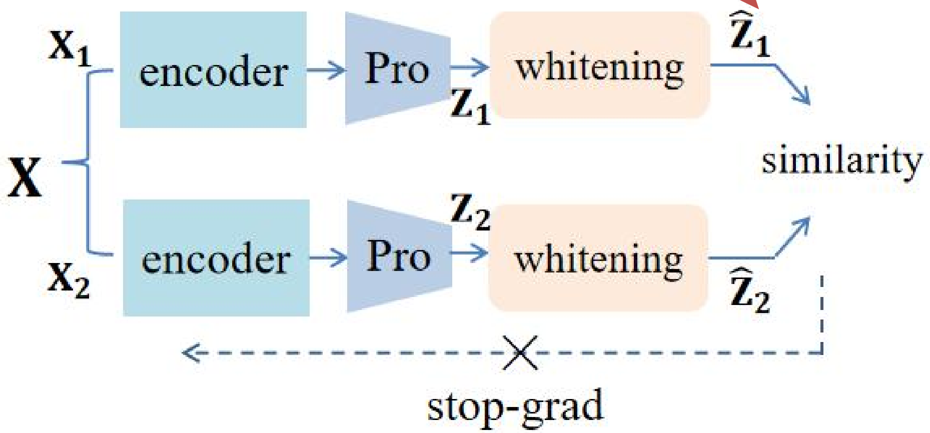


- Whitening loss:

$$\mathcal{L}(\mathbf{X}) = \frac{1}{m}\|\widehat{\mathbf{Z}}_1 - \widehat{\mathbf{Z}}_2\|_F^2.$$

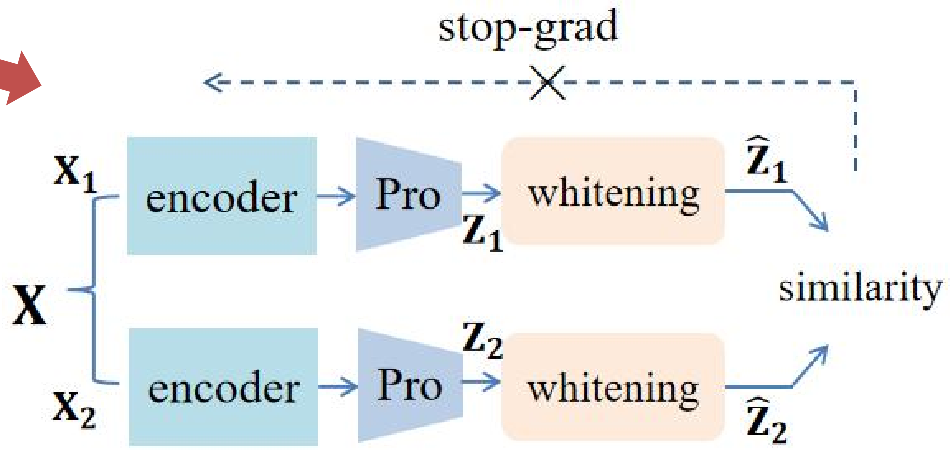
- A proxy loss:

$$\mathcal{L}'(\mathbf{X}) = \underbrace{\frac{1}{m}\|\widehat{\mathbf{Z}}_1 - (\widehat{\mathbf{Z}}_2)_{st}\|_F^2}_{\mathcal{L}'_1} + \underbrace{\frac{1}{m}\|(\widehat{\mathbf{Z}}_1)_{st} - \widehat{\mathbf{Z}}_2\|_F^2}_{\mathcal{L}'_2},$$



- We can prove

$$\frac{\partial \mathcal{L}}{\partial \theta} = \frac{\partial \mathcal{L}'}{\partial \theta}$$



Minimizing $\mathcal{L}'_1$ only require the embedding $\boldsymbol{Z}_1$ being full-rank, not whitened

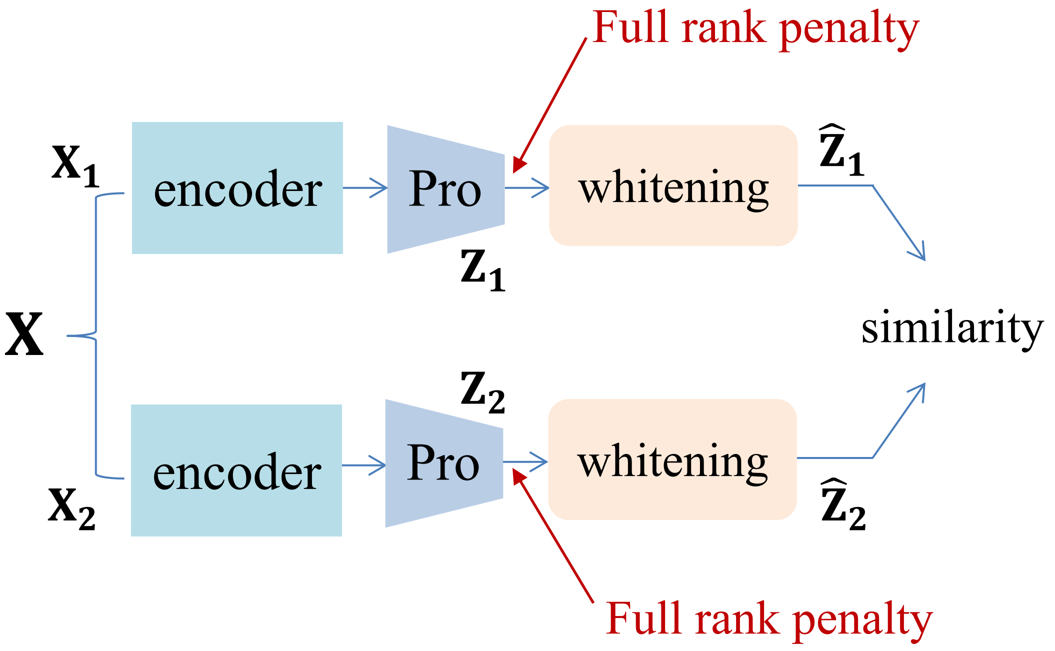
Connection to Soft Whitening

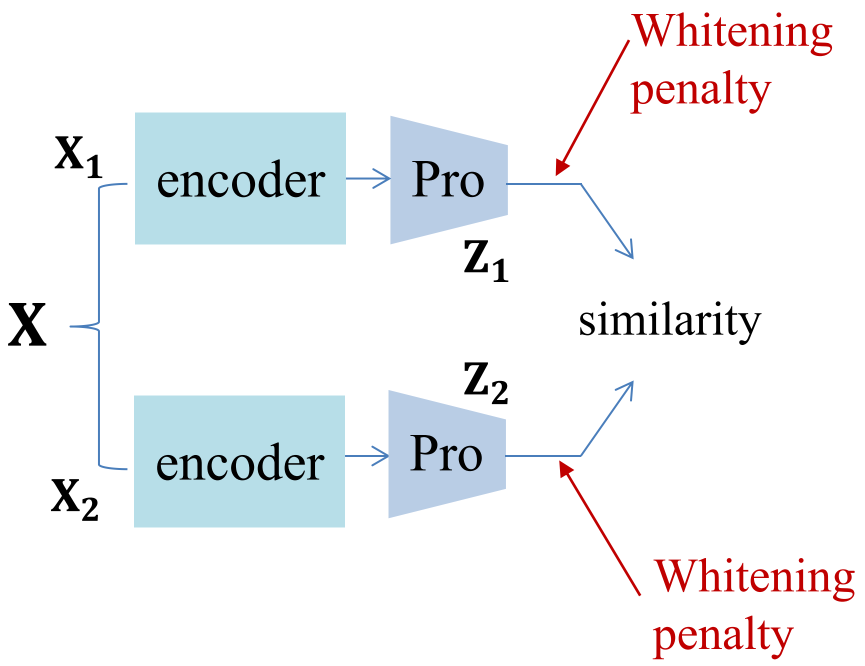
- Whitening loss:

$$\mathcal{L}(\mathbf{X}) = \frac{1}{m}\|\widehat{\mathbf{Z}}_1 - \widehat{\mathbf{Z}}_2\|_F^2.$$

- VICReg:

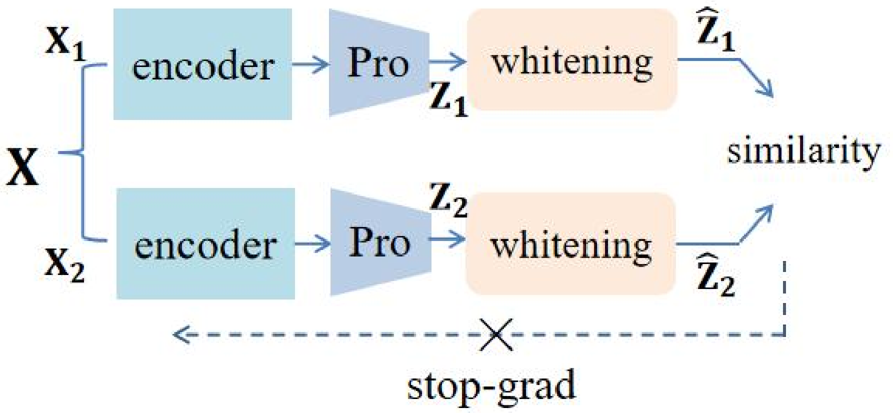
$$\mathcal{L}(\mathbf{X}) = \frac{1}{m}\|\mathbf{Z}_1 - \mathbf{Z}_2\|_F^2 + \alpha\sum_{i=1}^{2}(\|\frac{1}{m}\mathbf{Z}_i\mathbf{Z}_i^T - \lambda\mathbf{I}\|_F^2),$$

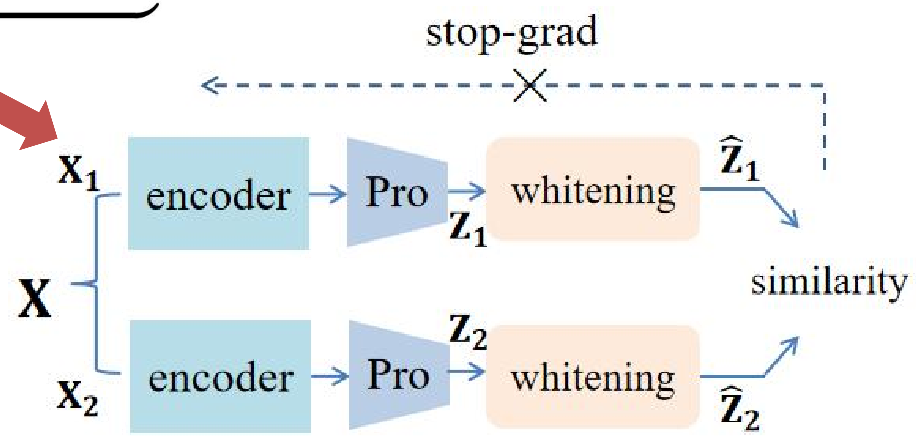


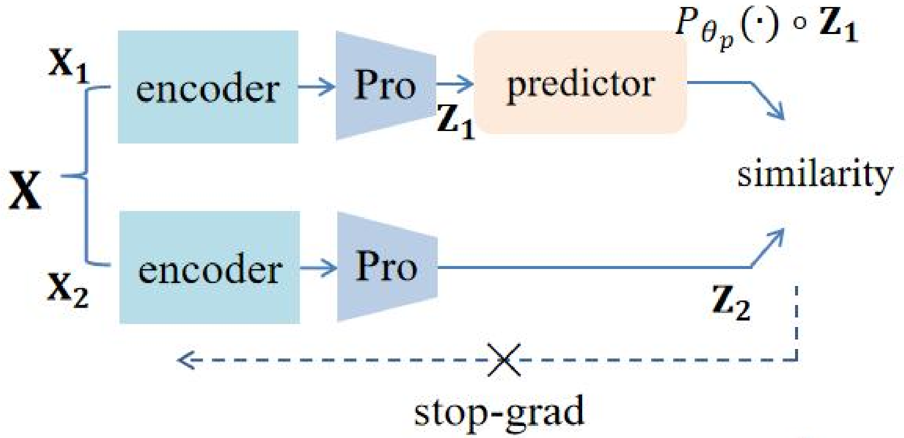


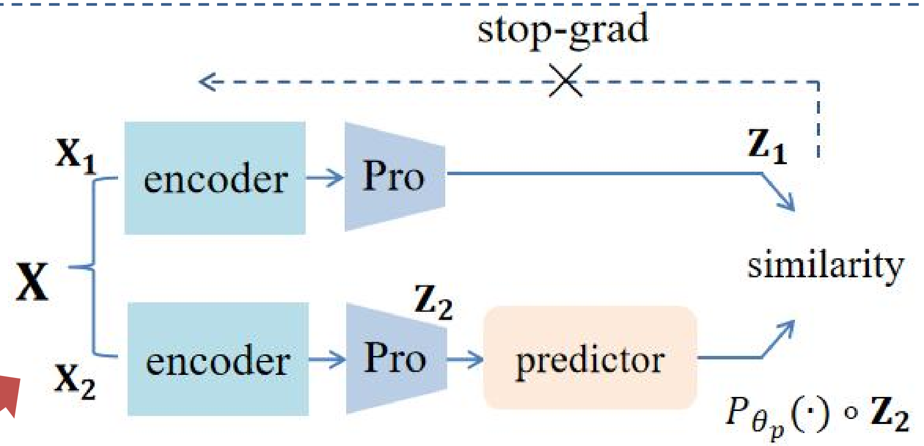
Connection to Asymmetirc Methods

- Whitening loss: $$\mathcal{L}^{'}(\mathbf{X}) = \underbrace{\frac{1}{m}\|\widehat{\mathbf{Z}}_1 - (\widehat{\mathbf{Z}}_2)_{st}\|_F^2}_{\mathcal{L}_1^{'}} + \underbrace{\frac{1}{m}\|(\widehat{\mathbf{Z}}_1)_{st} - \widehat{\mathbf{Z}}_2\|_F^2}_{\mathcal{L}_2^{'}},$$





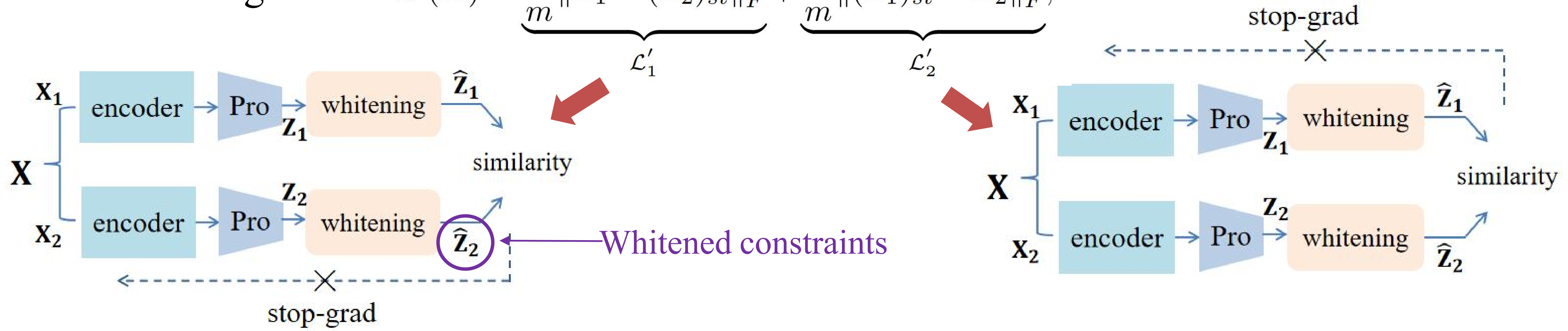


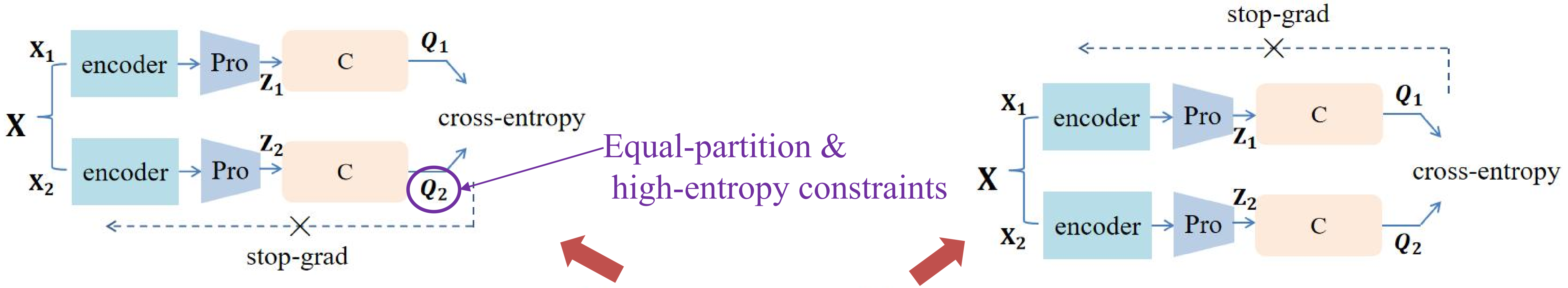


- SimSiam: $$\mathcal{L}(\mathbf{X}) = \frac{1}{m}\|P_{\theta_p}(\cdot) \circ \mathbf{Z}_1 - (\mathbf{Z}_2)_{st}\|_F^2 + \frac{1}{m}\|P_{\theta_p}(\cdot) \circ \mathbf{Z}_2 - (\mathbf{Z}_1)_{st}\|_F^2,$$

Connection to Other Non-contrastive Methods

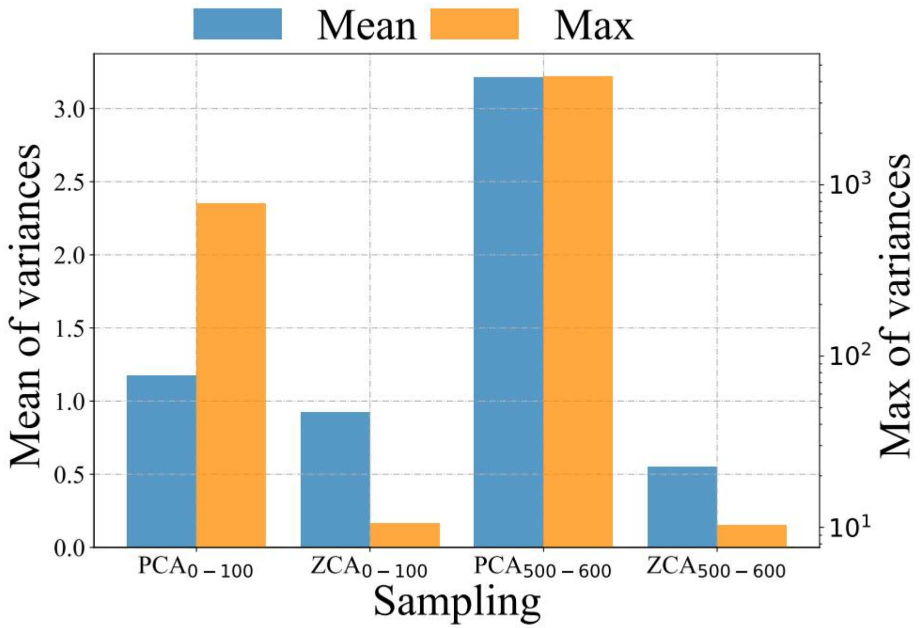
- Whitening loss: $$\mathcal{L}'(\mathbf{X}) = \underbrace{\frac{1}{m}\|\widehat{\mathbf{Z}}_1 - (\widehat{\mathbf{Z}}_2)_{st}\|_F^2}_{\mathcal{L}'_1} + \underbrace{\frac{1}{m}\|(\widehat{\mathbf{Z}}_1)_{st} - \widehat{\mathbf{Z}}_2\|_F^2}_{\mathcal{L}'_2},$$



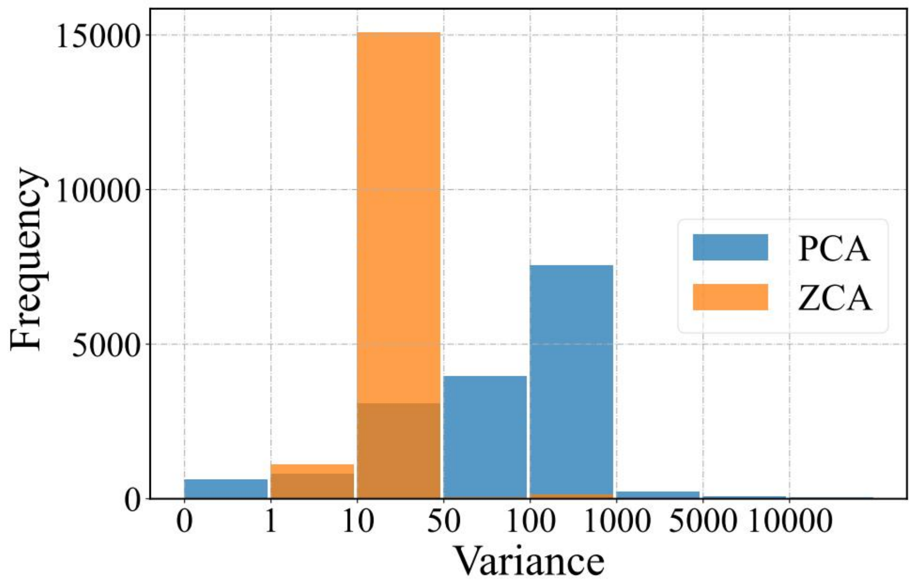


- SwAV: $$\mathcal{L}(\mathbf{X}) = \ell(\mathbf{C}^T\mathbf{Z}_1, (\mathbf{Q}_2)_{st}) + \ell(\mathbf{C}^T\mathbf{Z}_2, (\mathbf{Q}_1)_{st}).$$

Why PCA Whitening Fails to Avoid Dimensional Collapse?



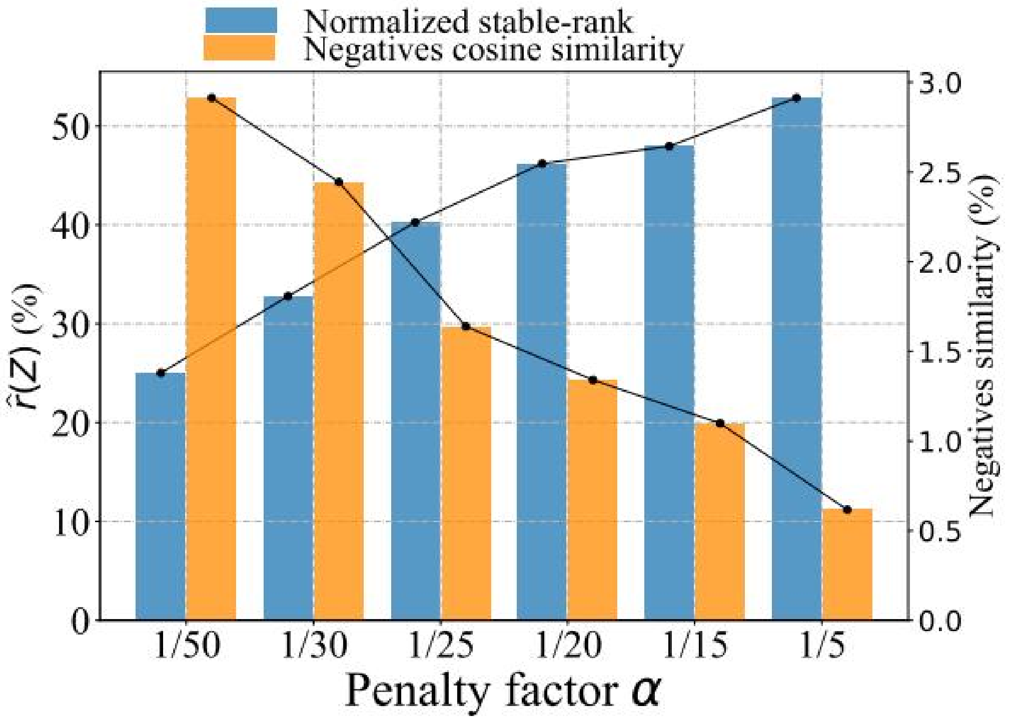
(a)



(b)

- PCA whitening: volatile sequence of whitened targets

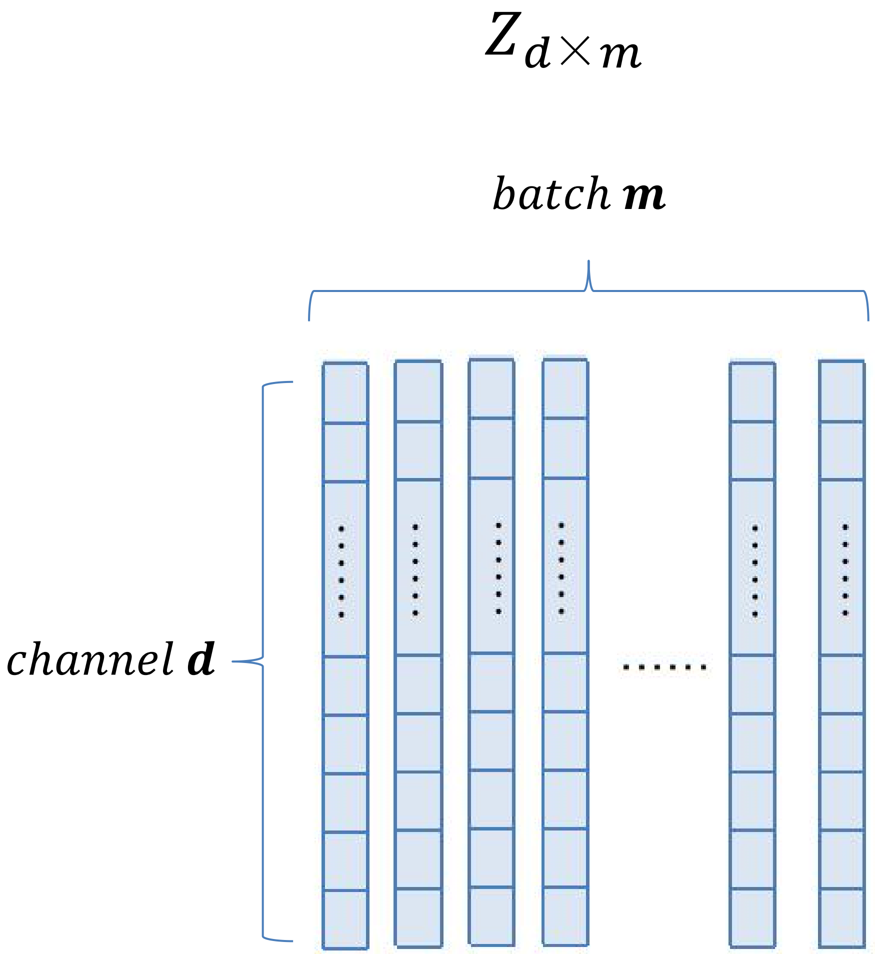
Why Whitened Output is not a Good Representation?



Similarity decreases when extent of whitening increases

- ➢ A whitened output leads to the state that can **break the potential manifold the examples in the same class belong to**

Channel Whitening (CW)



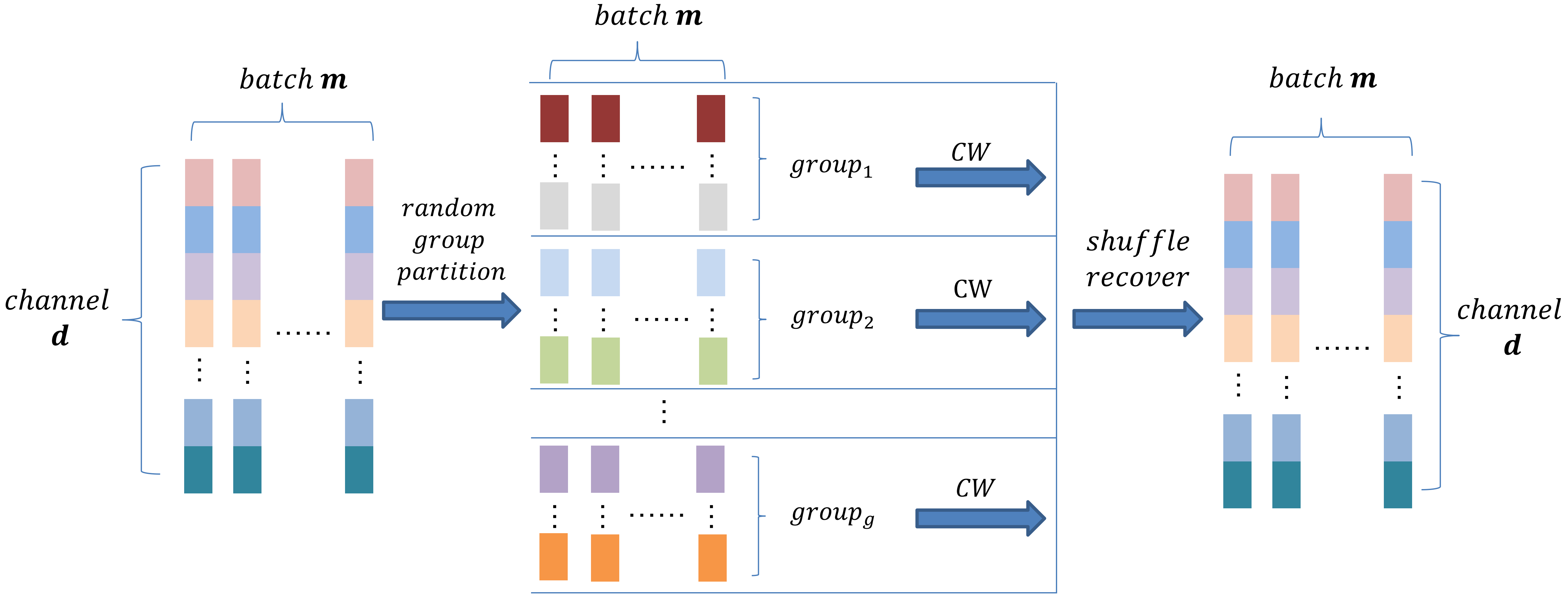
- Batch whitening (BW)
  - $centering: Z_B = Z \cdot (I - \frac{1}{m} 1 \cdot 1^T)$
  - $\Sigma = \frac{1}{m-1} Z_B \cdot {Z_B}^T$
  - $\widehat{Z} = \Phi \cdot Z_B$

requires **m > d** to avoid numerical instability.

- Channel whitening (CW)
  - $centering: Z_c = (I - \frac{1}{d} 1 \cdot 1^T) \cdot Z$
  - $\Sigma = \frac{1}{d-1} {Z_C}^T \cdot Z_C$
  - $\widehat{Z} = Z_C \cdot \Phi$

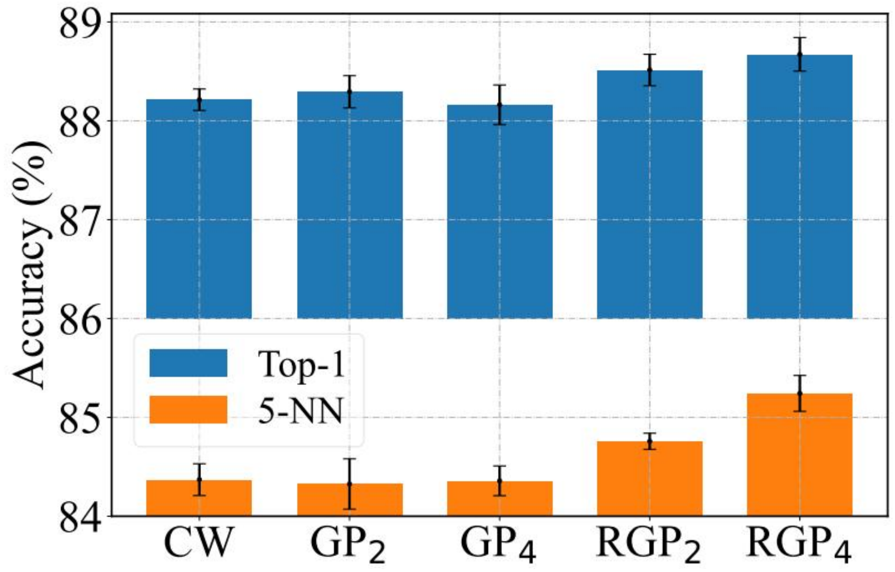
can obtain numerical stability **when the batch size is small**, since the condition that **d > m** can be obtained by design.

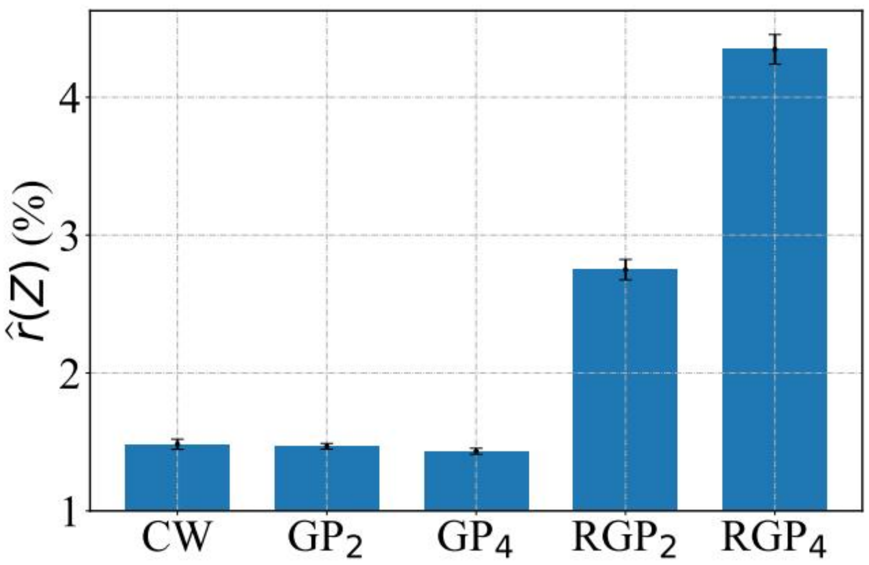
Random Group Partition (RGP)

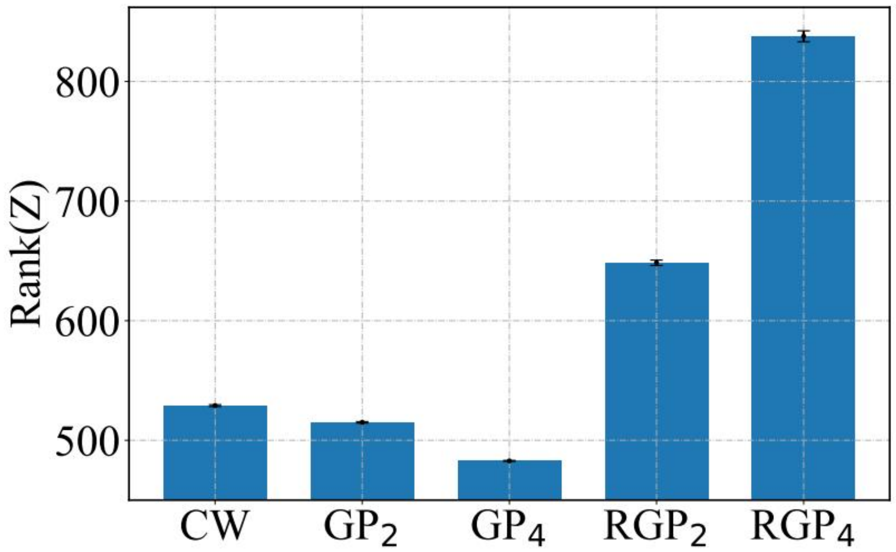


$$dimension\ of\ every\ group = \frac{d}{g}$$

Random Group Partition (RGP)







Method	CIFAR-10		CIFAR-100	
	linear	5-nn	linear	5-nn
CW 2	91.66	88.99	66.26	56.36
CW-GP 2	91.61	88.89	66.17	56.53
CW-RGP 2	**91.92**	**89.54**	**67.51**	**57.35**
CW 4	92.10	90.12	66.90	57.12
CW-GP 4	92.08	90.06	67.34	57.28
CW-RGP 4	**92.47**	**90.74**	**68.26**	**58.67**

Experiments for Empirical Study

➢ Experimental Setup for Comparison of Baselines

Table 1: Classification accuracy (top 1) of a linear classifier and a 5-nearest neighbors classifier for different loss functions and datasets with a ResNet-18 encoder.

Method	CIFAR-10		CIFAR-100		STL-10		Tiny-ImageNet	
	linear	5-nn	linear	5-nn	linear	5-nn	linear	5-nn
SimCLR [6]	91.80	88.42	66.83	56.56	90.51	85.68	48.84	32.86
BYOL [16]	91.73	89.45	66.60	56.82	91.99	88.64	**51.00**	**36.24**
SimSiam [8] (repro.)	90.51	86.82	66.04	55.79	88.91	84.84	48.29	34.21
Shuffled-DBN [21] (repro.)	90.45	88.15	66.07	56.97	89.20	84.51	48.60	32.14
Barlow Twins [45] (repro.)	88.51	86.53	65.78	55.76	88.36	83.71	47.44	32.65
VICReg [2] (repro.)	90.32	88.41	66.45	56.78	90.78	85.72	48.71	33.35
Zero-ICL [48] (repro.)	88.12	86.64	61.91	53.47	86.35	82.51	46.25	32.74
W-MSE 2 [12]	91.55	89.69	66.10	56.69	90.36	87.10	48.20	34.16
W-MSE 4 [12]	91.99	89.87	67.64	56.45	91.75	88.59	49.22	35.44
CW-RGP 2 (ours)	91.92	89.54	67.51	57.35	90.76	87.34	49.23	34.04
CW-RGP 4 (ours)	**92.47**	**90.74**	**68.26**	**58.67**	**92.04**	**88.95**	50.24	35.99

Experiments for Empirical Study

➢ Experimental Setup for Large-Scale Classification

Table 2: Comparisons on ImageNet linear classification. All are based on ResNet-50 encoder. The table is mostly inherited from [8].

Method	Batch size	100 eps	200 eps
SimCLR [6]	4096	66.5	68.3
MoCo v2 [7]	256	67.4	69.9
BYOL [16]	4096	66.5	70.6
SwAV [4]	4096	66.5	69.1
SimSiam [8]	256	68.1	70.0
W-MSE 4 [12]	4096	69.4	-
Zero-CL [48]	1024	68.9	-
BYOL [16] (repro.)	512	66.1	69.2
SwAV [4] (repro.)	512	65.8	67.9
W-MSE 4 [12] (repro.)	512	66.7	67.9
CW-RGP 4 (ours)	512	**69.7**	**71.0**

Experiments for Empirical Study

- Transfer to downstream tasks

Table 3: Transfer Learning. All competitive unsupervised methods are based on 200-epoch pre-training in ImageNet (IN). The table is mostly inherited from [8]. Our CW-RGP is performed with 3 random seeds, with mean and standard deviation reported.

Method	VOC 07+12 detection			COCO detection			COCO instance seg.		
	AP_{50}	AP	AP_{75}	AP_{50}	AP	AP_{75}	AP_{50}	AP	AP_{75}
Scratch	60.2	33.8	33.1	44.0	26.4	27.8	46.9	29.3	30.8
IN-supervised	81.3	53.5	58.8	58.2	38.2	41.2	54.7	33.3	35.2
SimCLR [6]	81.8	55.5	61.4	57.7	37.9	40.9	54.6	33.3	35.3
MoCo v2 [7]	**82.3**	57.0	63.3	58.8	39.2	42.5	55.5	34.3	36.6
BYOL [16]	81.4	55.3	61.1	57.8	37.9	40.9	54.3	33.2	35.0
SwAV [4]	81.5	55.4	61.4	57.6	37.6	40.3	54.2	33.1	35.1
SimSiam [8]	82.0	56.4	62.8	57.5	37.9	40.9	54.2	33.2	35.2
CW-RGP (ours)	$82.2_{\pm 0.07}$	$\mathbf{57.2}_{\pm 0.10}$	$\mathbf{63.8}_{\pm 0.11}$	$\mathbf{60.5}_{\pm 0.28}$	$\mathbf{40.7}_{\pm 0.14}$	$\mathbf{44.1}_{\pm 0.14}$	$\mathbf{57.3}_{\pm 0.16}$	$\mathbf{35.5}_{\pm 0.12}$	$\mathbf{37.9}_{\pm 0.14}$

- Take Away
  - An in-depth analysis in whitening loss
  - An effective SSL method: CW-RGP

Thank you

https://github.com/winci-ai/CW-RGP