An Investigation into Whitening Loss for Self-supervised Learning

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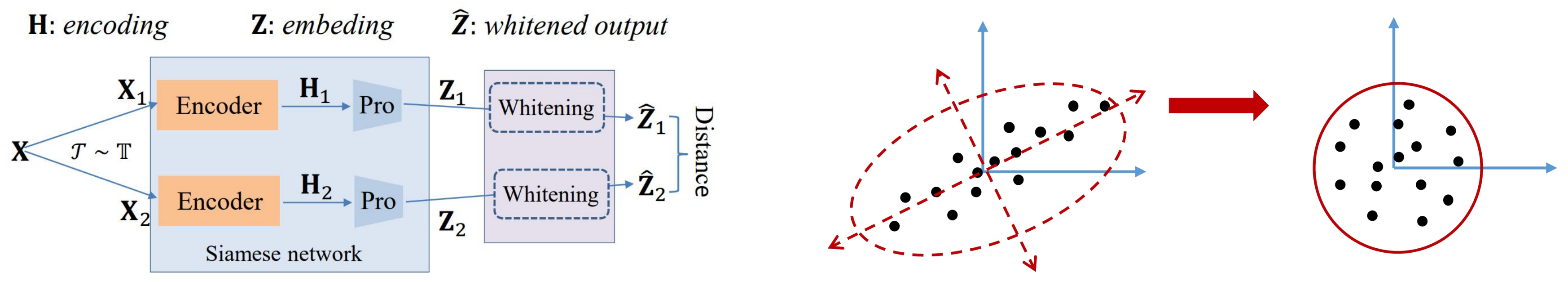
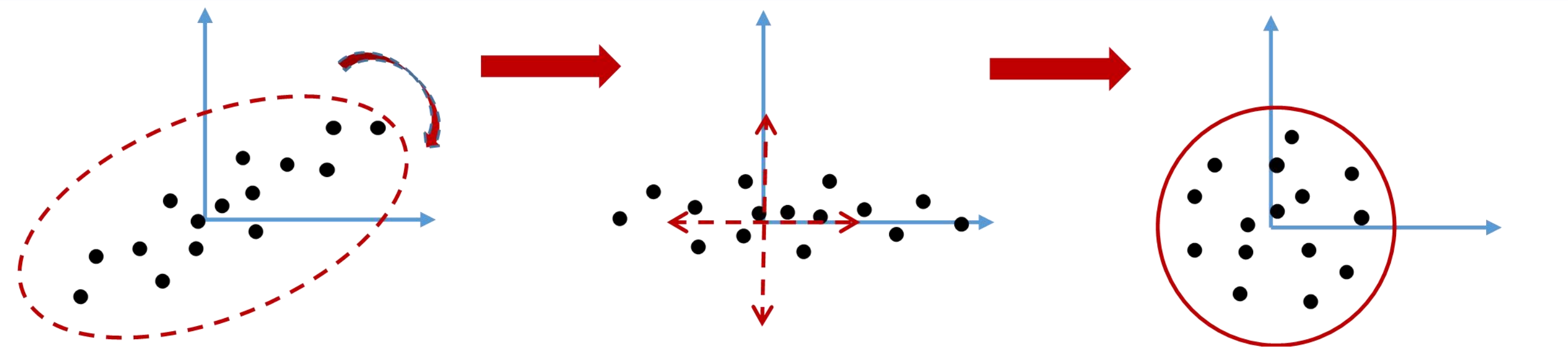
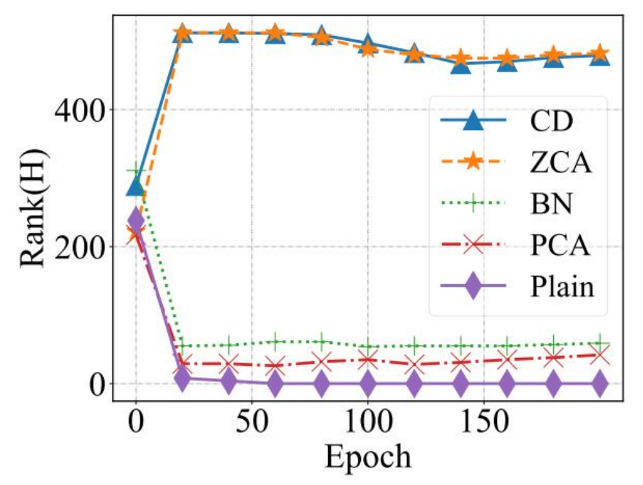
Empirical Investigation on Whitening Loss



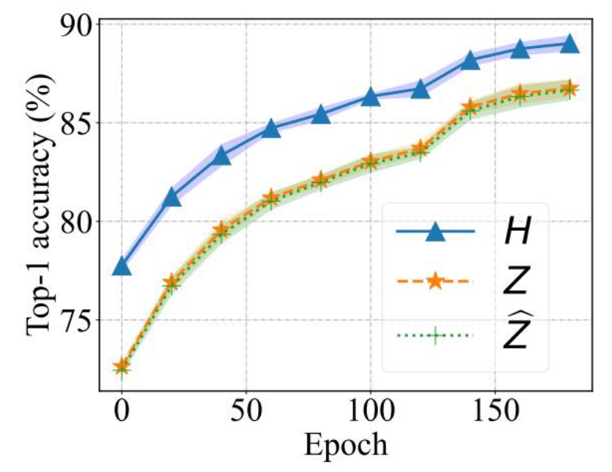
- Motivations of whitening loss for preventing collapse
  - whitening operation can remove the correlation among axes.
  - A whitened representation ensures the examples scattered in a spherical distribution.

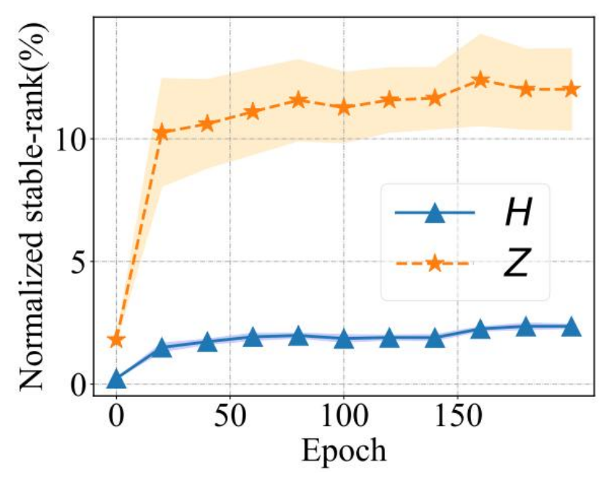
PCA Whitening Fails to Avoid Dimensional Collapse





Whitened Output is not a Good Representation

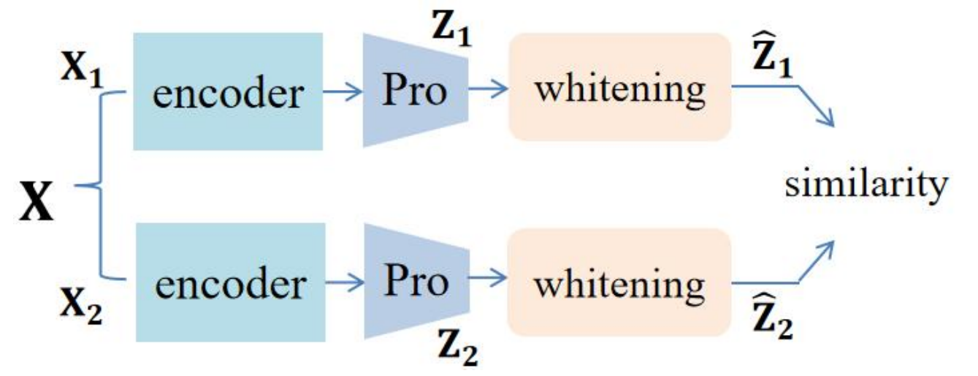




The normalized stable-rank of $\hat{Z}$ is always 100%

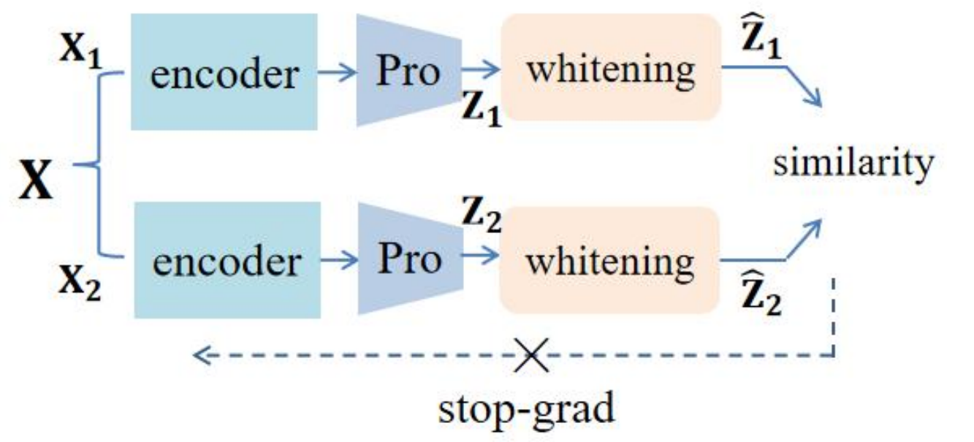
Analysing Decomposition of Whitening Loss

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



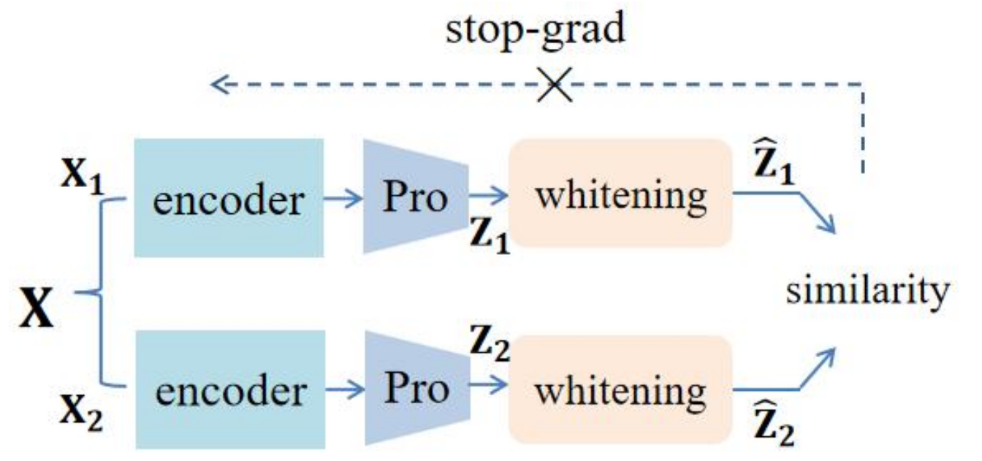
- A proxy loss:

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



We can prove that

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

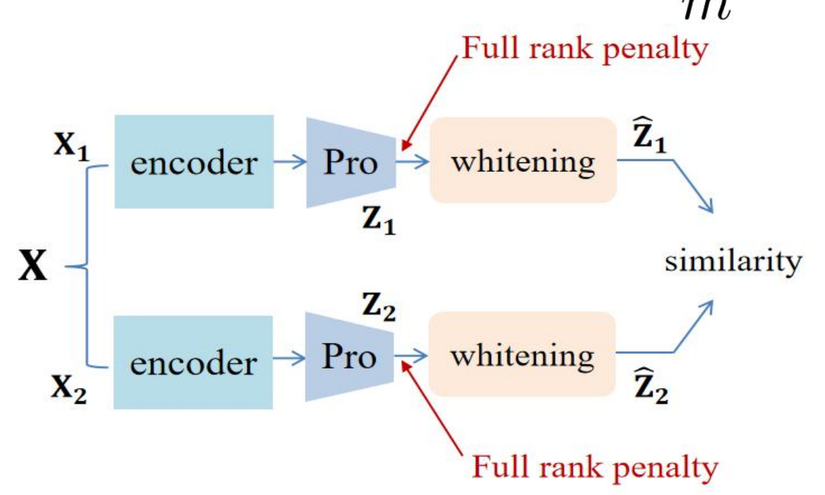


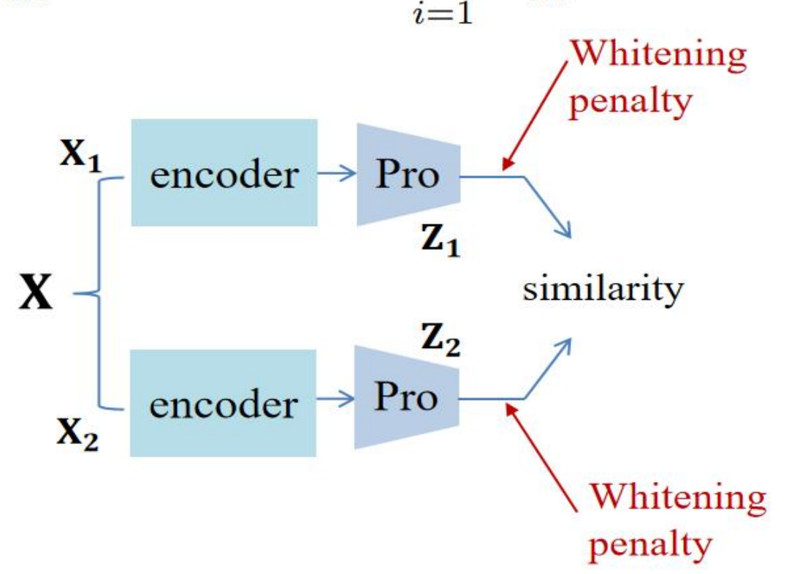
Minimizing $\mathcal{L}_1^{'}$only requires the embedding $\boldsymbol{Z}_1$ being full-rank, not whitened

Connection to Other Methods

- Connection to Soft whitening

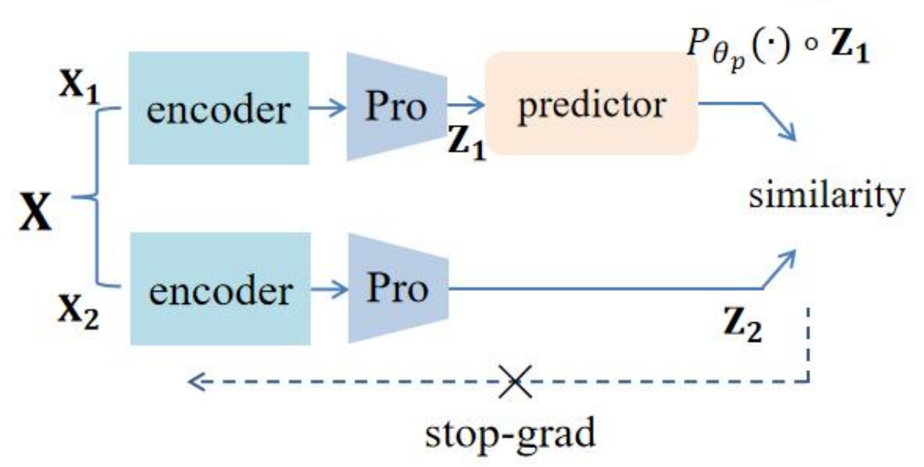
Whitening loss: $\mathcal{L}(\mathbf{X}) = \frac{1}{m}\|\widehat{\mathbf{Z}}_1 - \widehat{\mathbf{Z}}_2\|_F^2.$ VICReg: $\mathcal{L}(\mathbf{X}) = \frac{1}{m}\|\mathbf{Z}_1 - \mathbf{Z}_2\|_F^2 + \alpha\sum_{i=1}^{2}(\|\frac{1}{m}\mathbf{Z}_i\mathbf{Z}_i^T - \lambda\mathbf{I}\|_F^2),$

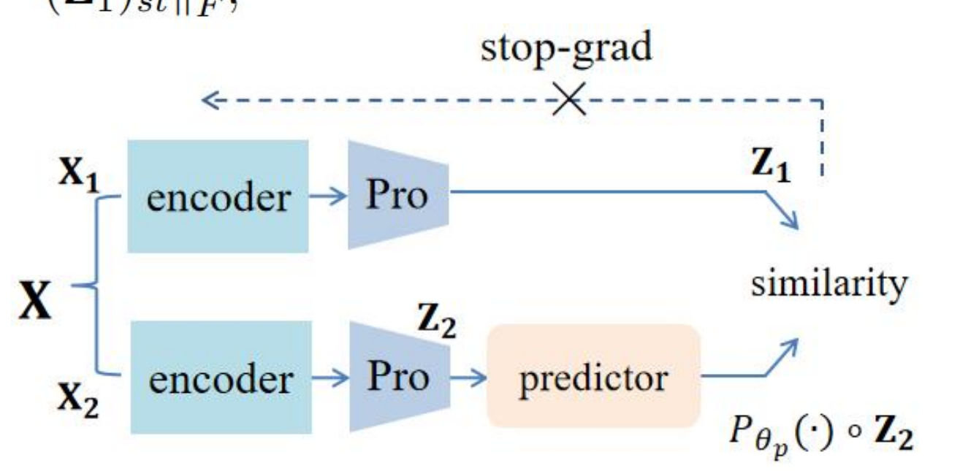




- Connection to Asymmetirc Methods

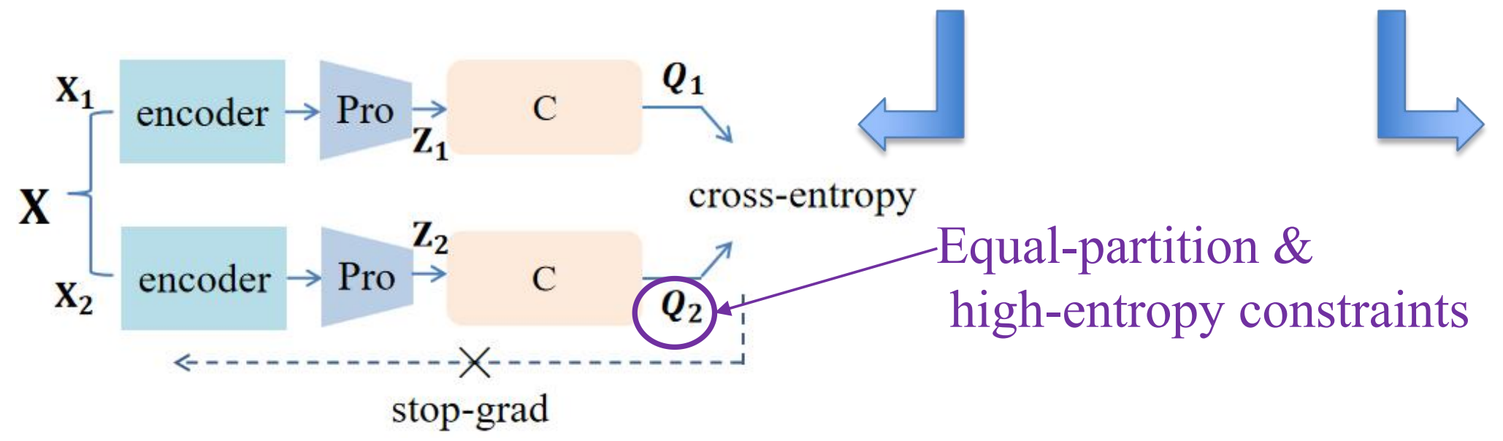
SimSiam: $\mathcal{L}(\mathbf{X}) = \frac{1}{m}\|P_{\theta_p}(\cdot)\circ\mathbf{Z}_1 - (\mathbf{Z}_2)_{st}\|_F^2 + \frac{1}{m}\|P_{\theta_p}(\cdot)\circ\mathbf{Z}_2 - (\mathbf{Z}_1)_{st}\|_F^2,$

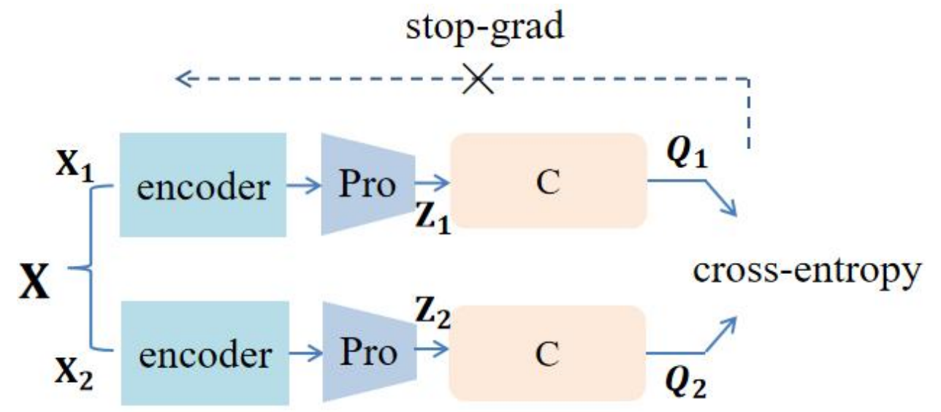




- Connection to Other Non-contrastive Methods

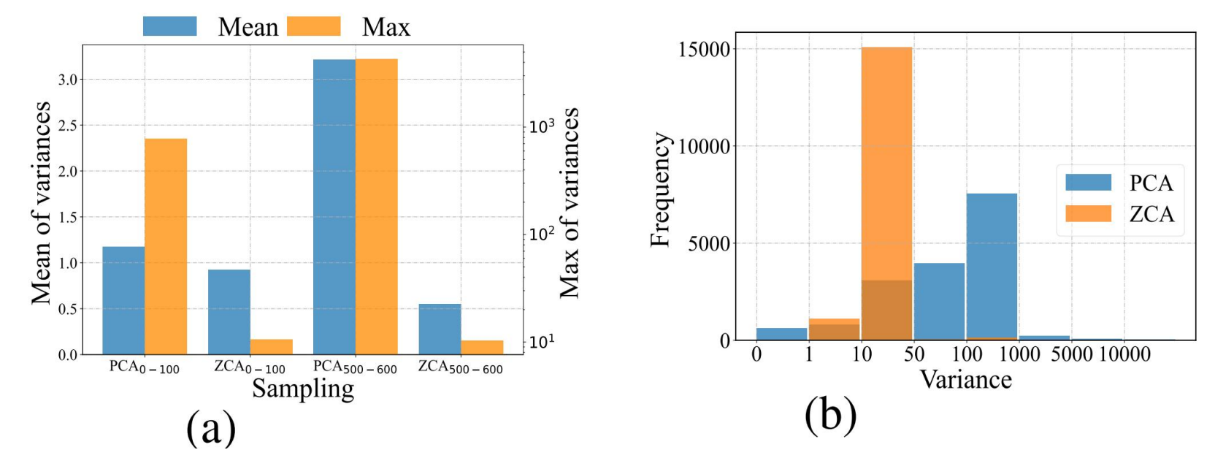
SwAV: $\mathcal{L}(\mathbf{X}) = \ell(\mathbf{C}^T\mathbf{Z}_1, (\mathbf{Q}_2)_{st}) + \ell(\mathbf{C}^T\mathbf{Z}_2, (\mathbf{Q}_1)_{st}).$



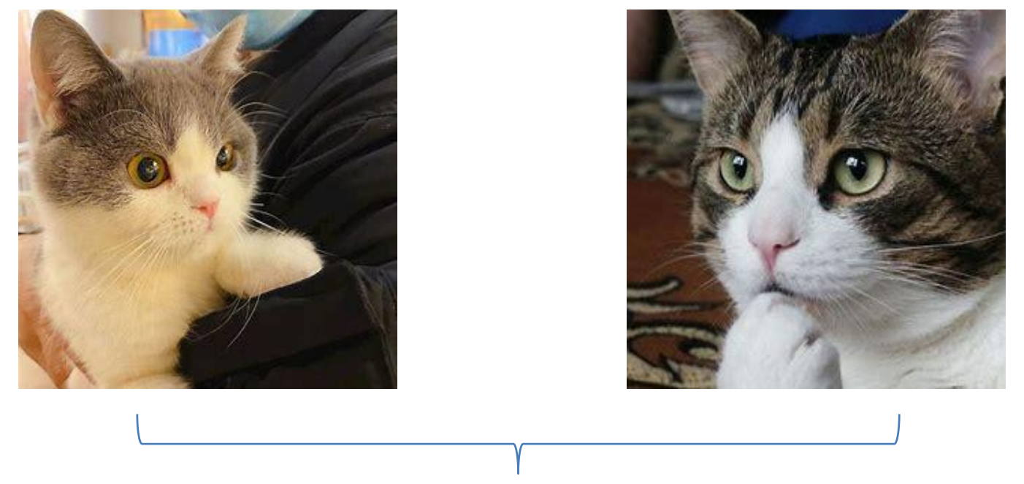


Explanation by the mechanism of decomposition

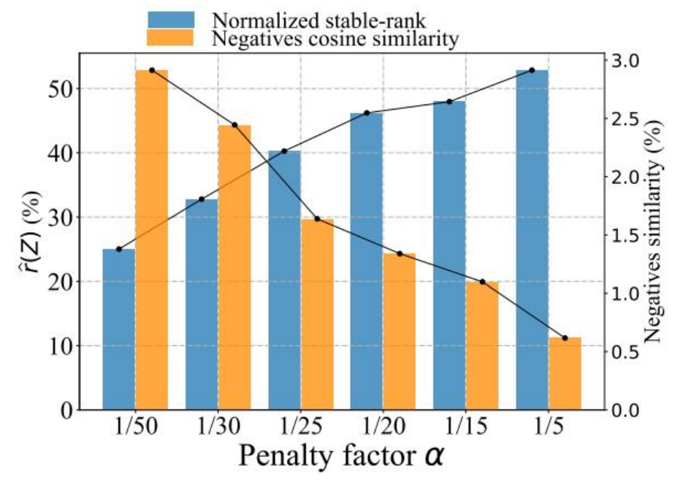
- PCA whitening: volatile sequence of whitened targets



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



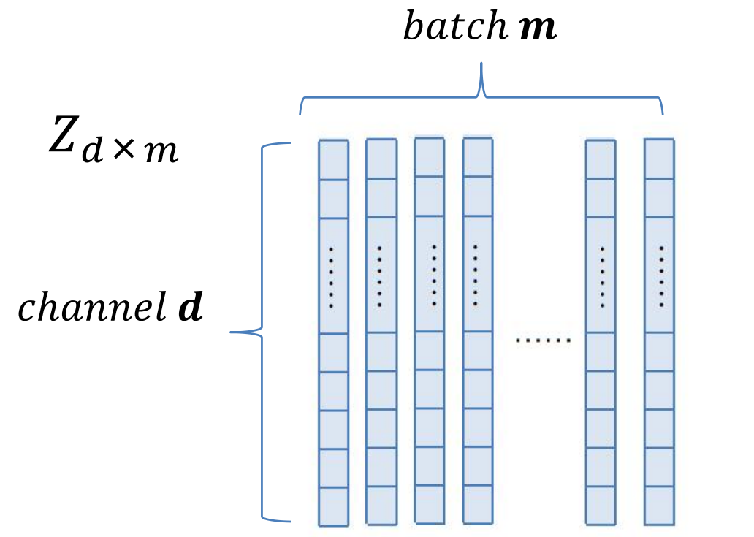
Similarity decreases when extent of whitening increases



Channel Whitening with Random Group Partition

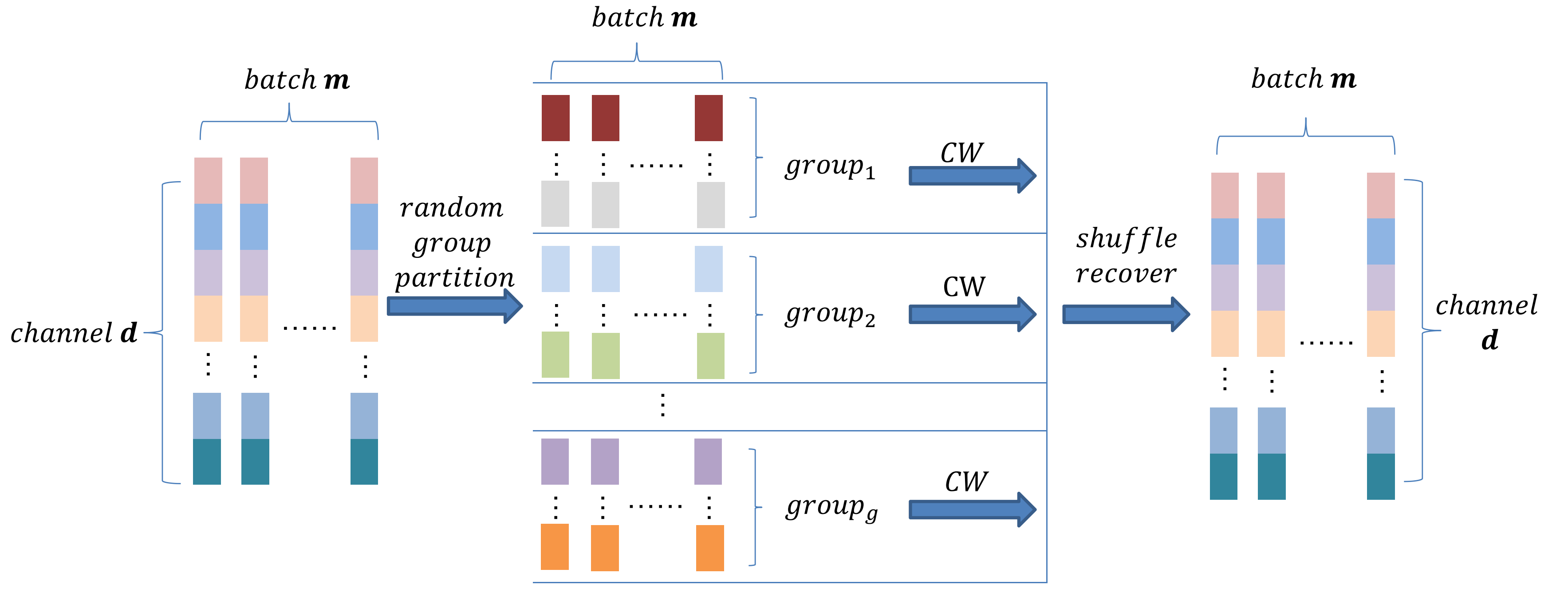
- Channel whitening (CW)
  - centering: $Z_c = (I - \frac{1}{d}1\cdot1^T)\cdot Z,$
  - $\Sigma = \frac{1}{d-1}{Z_C}^T\cdot Z_C, \quad \widehat{Z} = Z_C\cdot\Phi$

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 $= \frac{d}{g}$



Experiments for Empirical Study

- Evaluation for Classification

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

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**

- 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)	$82.2_{\pm0.07}$	$\mathbf{57.2}_{\pm0.10}$	$\mathbf{63.8}_{\pm0.11}$	$\mathbf{60.5}_{\pm0.28}$	$\mathbf{40.7}_{\pm0.14}$	$\mathbf{44.1}_{\pm0.14}$	$\mathbf{57.3}_{\pm0.16}$	$\mathbf{35.5}_{\pm0.12}$	$\mathbf{37.9}_{\pm0.14}$

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