

LSDL Lecture 04

Contrastive Learning

Ildus Sadrdinov, 07.10.24

Self-supervised pre-training

generative

generative
pre-text tasks

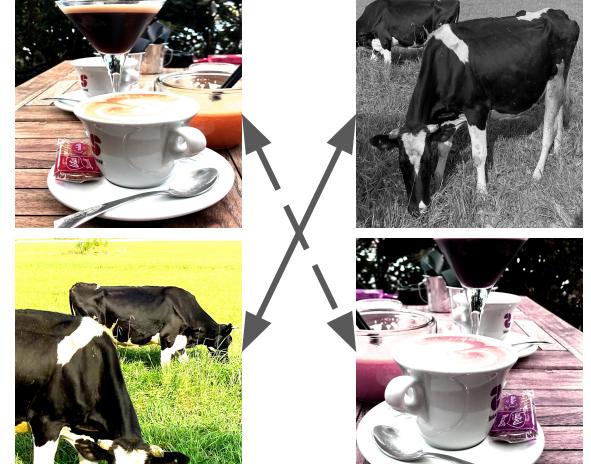


discriminative

discriminative
pre-text tasks



contrastive
tasks



Plan

- **Introduction to information theory**
 - Mutual information & InfoNCE
- **Contrastive learning with negative examples**
 - SimCLR, MoCo
- **Contrastive learning without negative examples**
 - BYOL, SimSiam
- **Contrastive learning inspired by clustering**
 - DeepCluster, SwAV
- **Bonus**
 - Dense Contrastive Learning
 - Supervised Contrastive Learning

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Information theory

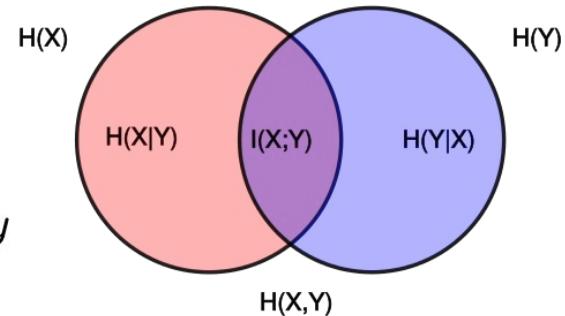
Is it possible to quantify information stored in a random variable?

- (Differential) Entropy: $H(X) = -\mathbb{E}_{p(X)} [\log p(X)] = - \int p(x) \log p(x) dx$
- Joint Entropy: $H(X, Y) = -\mathbb{E}_{p(X, Y)} [\log p(X, Y)] = - \int p(x, y) \log p(x, y) dx dy$
- Conditional Entropy: $H(Y|X) = -\mathbb{E}_{p(X, Y)} [\log p(Y|X)] = - \int p(x, y) \log \frac{p(x, y)}{p(x)} dx dy$

Information is measured in bits (if $\log = \log_2$) or in nats (if $\log = \ln$)

Mutual information

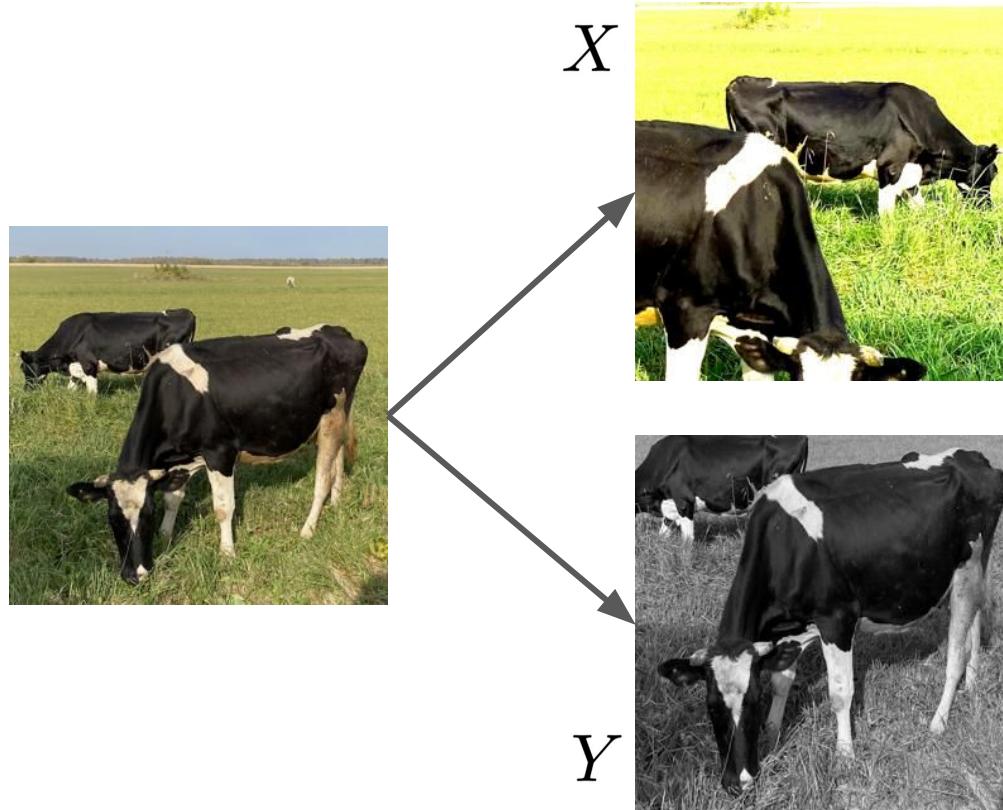
$$I(X;Y) = KL\left(P(X,Y) \middle\| P(X)P(Y)\right) = \int p(x,y) \log \frac{p(x,y)}{p(x)p(y)} dx dy$$



Properties:

- $I(X;Y) \geq 0$
- $I(X;Y) = I(Y;X)$
- $I(X;Y) \equiv H(X) - H(X | Y)$
 $\equiv H(Y) - H(Y | X)$
 $\equiv H(X) + H(Y) - H(X, Y)$
 $\equiv H(X, Y) - H(X | Y) - H(Y | X)$
- When $I(X;Y) = 0$?
- When $I(X;Y) \rightarrow \max$?

So what? (or the main idea of contrastive learning)



$$I\left(f_{\theta}(X), f_{\theta}(Y)\right) \rightarrow \max_{\theta}$$

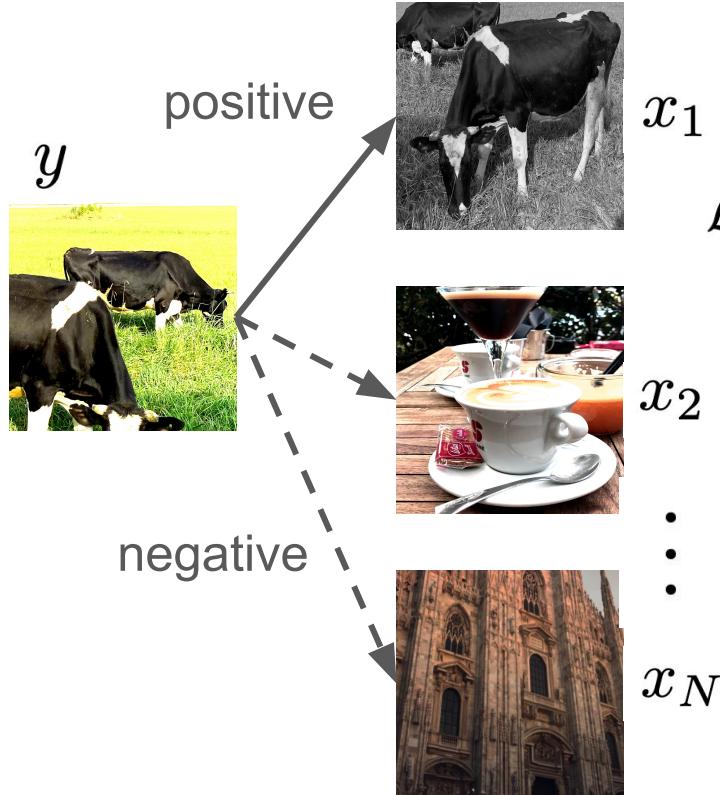
f_{θ} – our neural network with weights θ

Let's go training! Oh, wait...

$$I(X, Y) = \int p(x, y) \log \left(\frac{p(x, y)}{p(x)p(y)} \right) dx dy = \mathbb{E}_{p(x, y)} \left[\log \frac{p(x, y)}{p(x)p(y)} \right]$$

We do not know any of these PDFs! :(

InfoNCE loss and negative examples



$$\mathcal{L}_{NCE}(\theta) = \mathbb{E}_{p(x_{1:N}, y)} \left[-\log \frac{e^{f_\theta(x_1, y)}}{\sum_{n=1}^N e^{f_\theta(x_n, y)}} \right] \rightarrow \min_{\theta}$$

Noise Contrastive Estimation

InfoNCE is a lower bound for mutual information

$$I(X_1; Y) \geq \log N - \mathcal{L}_{NCE}$$

$$\mathcal{L}_{NCE}(\theta) = \mathbb{E}_{p(x_{1:N}, y)} \left[-\log \frac{e^{f_\theta(x_1, y)}}{\sum_{n=1}^N e^{f_\theta(x_n, y)}} \right]$$

Plan

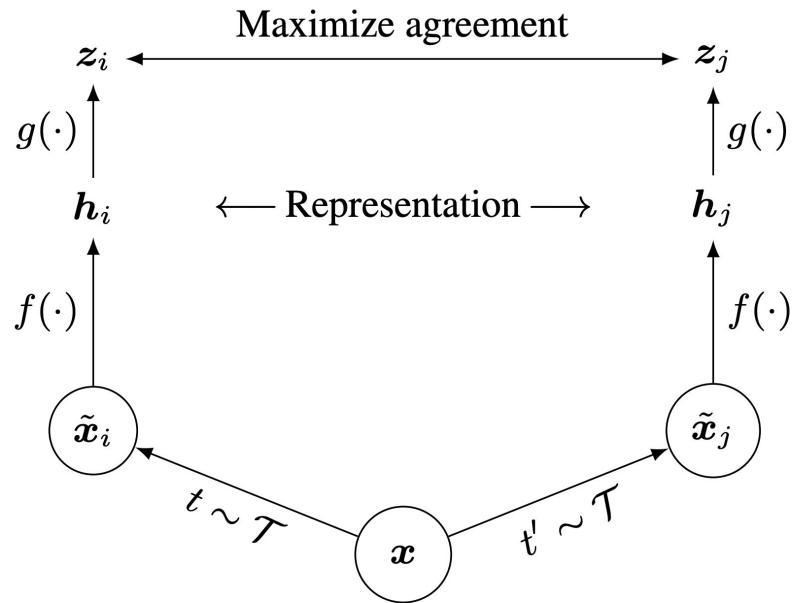
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SimCLR

A Simple Framework for Contrastive Learning of Visual Representations
Google Research

- Make a double batch of augmented images (each image has 2 view)
- Use each of two views both as an anchor (y) and a positive example (x_1)
- Very intense augmentations to make the task meaningful

SimCLR: scheme



$$\ell_{i,j} = -\log \frac{\exp(\text{sim}(z_i, z_j)/\tau)}{\sum_{k=1}^{2N} \mathbb{1}_{[k \neq i]} \exp(\text{sim}(z_i, z_k)/\tau)}$$
$$\mathcal{L} = \frac{1}{2N} \sum_{k=1}^N [\ell(2k-1, 2k) + \ell(2k, 2k-1)]$$

SimCLR: augmentations

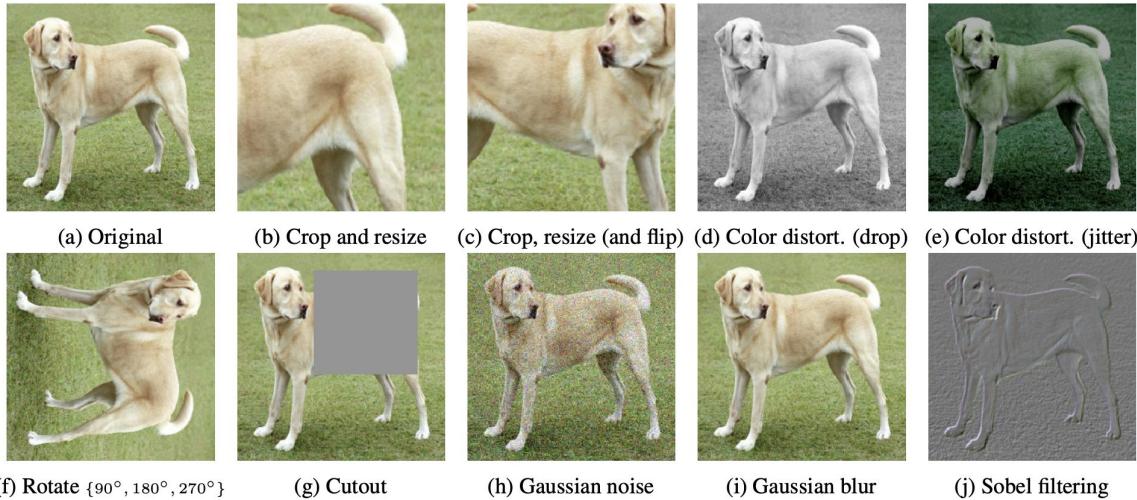


Figure 4. Illustrations of the studied data augmentation operators. Each augmentation can transform data stochastically with some internal parameters (e.g. rotation degree, noise level). Note that we *only* test these operators in ablation, the *augmentation policy used to train our models* only includes *random crop (with flip and resize), color distortion, and Gaussian blur*. (Original image cc-by: Von.grzanka)

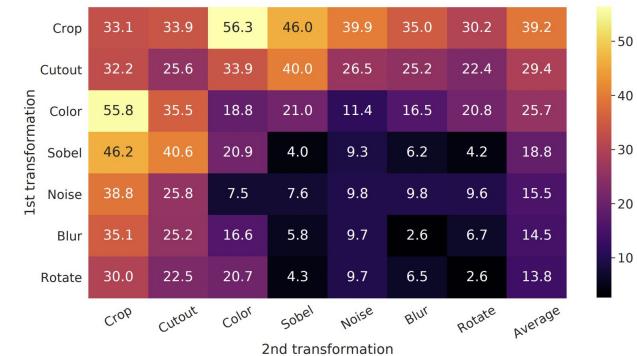
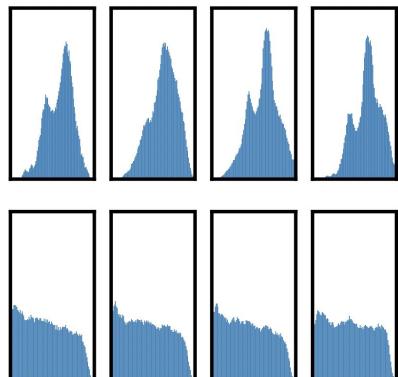
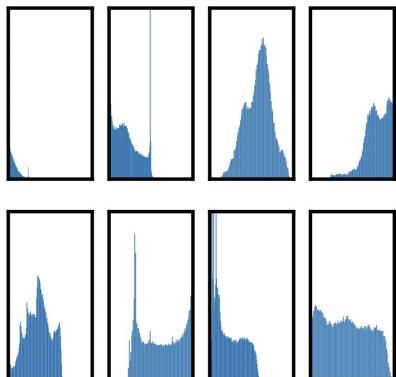


Figure 5. Linear evaluation (ImageNet top-1 accuracy) under individual or composition of data augmentations, applied only to one branch. For all columns but the last, diagonal entries correspond to single transformation, and off-diagonals correspond to composition of two transformations (applied sequentially). The last column reflects the average over the row.

SimCLR: augmentations



(a) Without color distortion.



(b) With color distortion.

Figure 6. Histograms of pixel intensities (over all channels) for different crops of two different images (i.e. two rows). The image for the first row is from Figure 4. All axes have the same range.

Methods	Color distortion strength					AutoAug
	1/8	1/4	1/2	1	1 (+Blur)	
SimCLR	59.6	61.0	62.6	63.2	64.5	61.1
Supervised	77.0	76.7	76.5	75.7	75.4	77.1

Table 1. Top-1 accuracy of unsupervised ResNet-50 using linear evaluation and supervised ResNet-50⁵, under varied color distortion strength (see Appendix A) and other data transformations. Strength 1 (+Blur) is our default data augmentation policy.

SimCLR: projection head

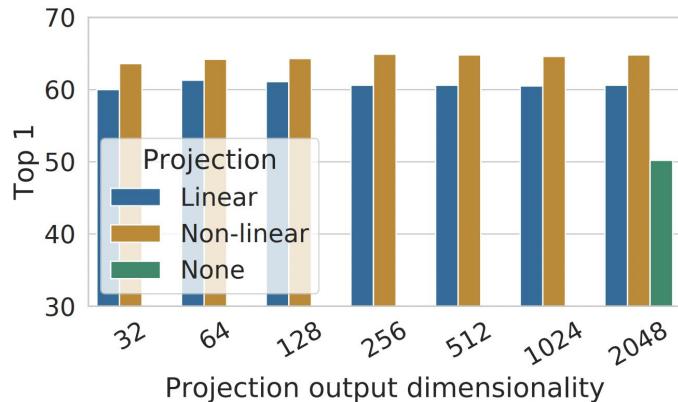


Figure 8. Linear evaluation of representations with different projection heads $g(\cdot)$ and various dimensions of $\mathbf{z} = g(\mathbf{h})$. The representation \mathbf{h} (before projection) is 2048-dimensional here.

What to predict?	Random guess	Representation \mathbf{h}	Representation $g(\mathbf{h})$
Color vs grayscale	80	99.3	97.4
Rotation	25	67.6	25.6
Orig. vs corrupted	50	99.5	59.6
Orig. vs Sobel filtered	50	96.6	56.3

Table 3. Accuracy of training additional MLPs on different representations to predict the transformation applied. Other than crop and color augmentation, we additionally and independently add rotation (one of $\{0^\circ, 90^\circ, 180^\circ, 270^\circ\}$), Gaussian noise, and Sobel filtering transformation during the pretraining for the last three rows. Both \mathbf{h} and $g(\mathbf{h})$ are of the same dimensionality, i.e. 2048.

SimCLR: model size and training time

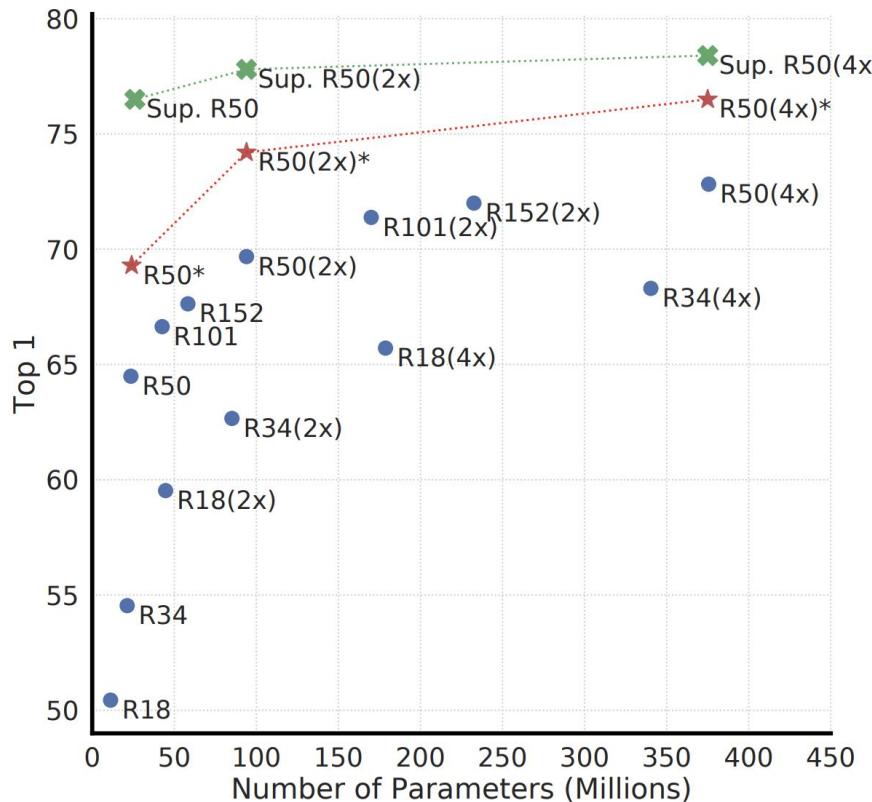


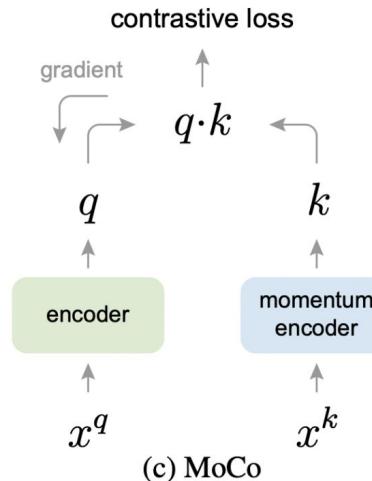
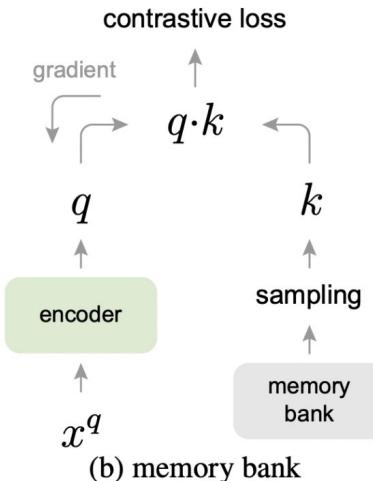
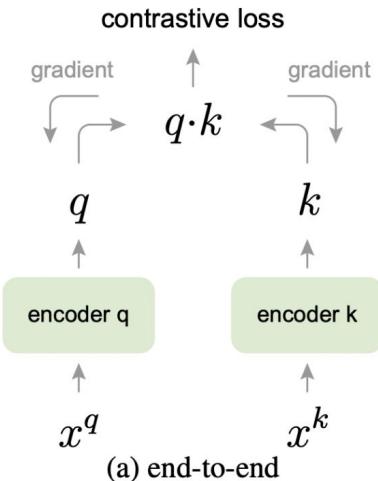
Figure 7. Linear evaluation of models with varied depth and width. Models in blue dots are ours trained for 100 epochs, models in red stars are ours trained for 1000 epochs, and models in green crosses are supervised ResNets trained for 90 epochs⁷ (He et al., 2016).

MoCo

Momentum Contrast, FAIR

- Momentum encoder makes contrastive learning asymmetric
- “Memory bank” to increase the number of negatives

$$\theta_k \leftarrow m\theta_k + (1 - m)\theta_q$$



[He et al., 2019](#)

MoCo: ablations

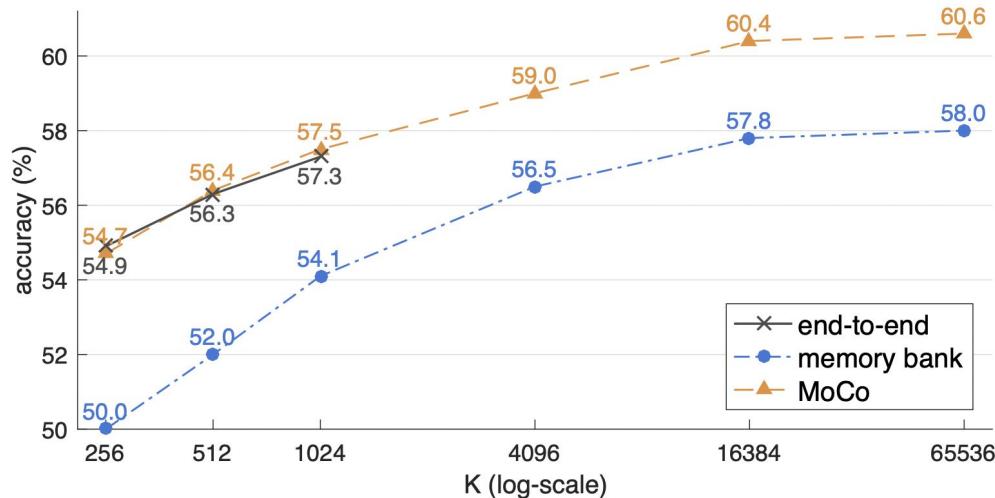


Figure 3. **Comparison of three contrastive loss mechanisms** under the ImageNet linear classification protocol. We adopt the same pretext task (Sec. 3.3) and only vary the contrastive loss mechanism (Figure 2). The number of negatives is K in memory bank and MoCo, and is $K-1$ in end-to-end (offset by one because the positive key is in the same mini-batch). The network is ResNet-50.

Ablation: momentum. The table below shows ResNet-50 accuracy with different MoCo momentum values (m in Eqn.(2)) used in pre-training ($K = 4096$ here) :

momentum m	0	0.9	0.99	0.999	0.9999
accuracy (%)	fail	55.2	57.8	59.0	58.9

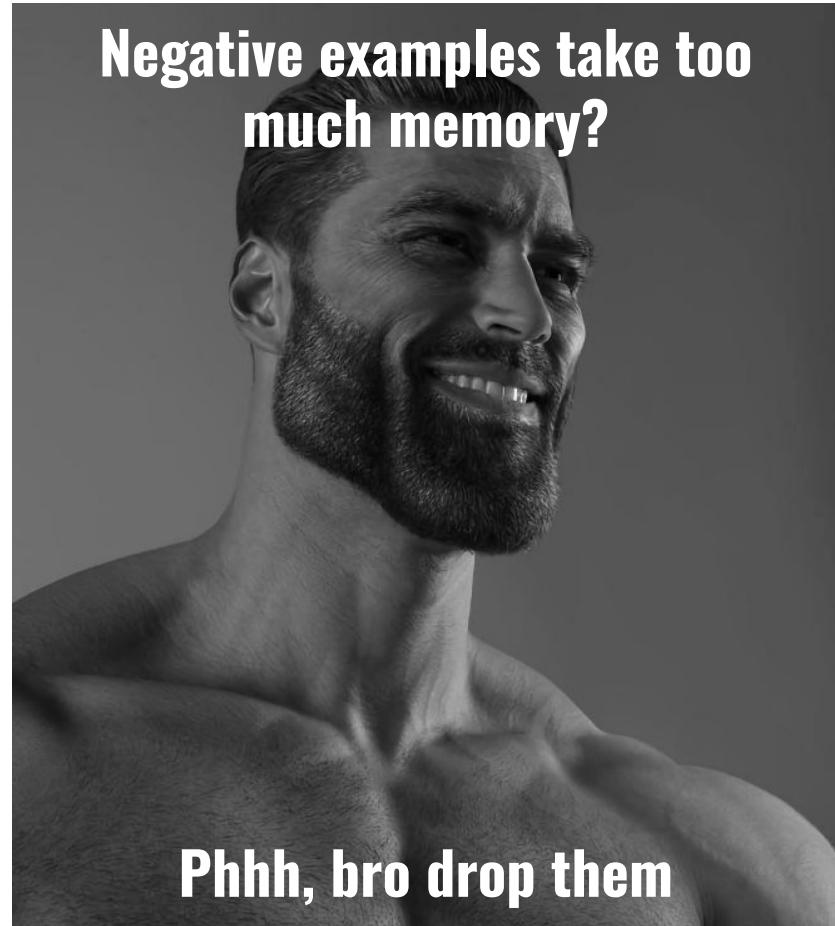
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BYOL

Bootstrap Your Own Latent, DeepMind

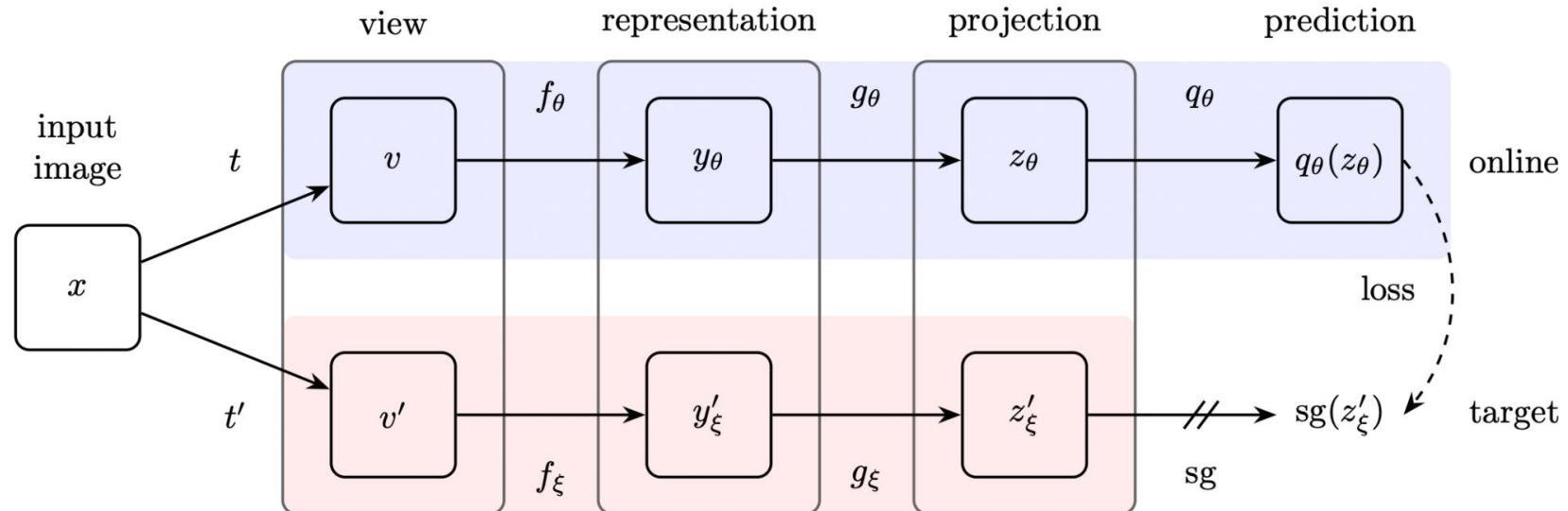
- Further development of momentum encoder from MoCo
- Contrastive learning **without negative examples**
- SOTA in pure contrastive methods



Negative examples take too
much memory?

Phhh, bro drop them

BYOL



$$\mathcal{L}_{\theta,\xi} \triangleq \|\overline{q_\theta}(z_\theta) - \overline{z}'_\xi\|_2^2 = 2 - 2 \cdot \frac{\langle q_\theta(z_\theta), z'_\xi \rangle}{\|q_\theta(z_\theta)\|_2 \cdot \|z'_\xi\|_2} \quad \begin{aligned} \theta &\leftarrow \text{optimizer}(\theta, \nabla_\theta \mathcal{L}_{\theta,\xi}^{\text{BYOL}}, \eta), \\ \xi &\leftarrow \tau \xi + (1 - \tau) \theta, \end{aligned}$$

BYOL: representation collapse

Why do we even need negative examples in contrastive learning?

$$\mathcal{L}_{\theta,\xi} \triangleq \left\| \overline{q_\theta}(z_\theta) - \overline{z}'_\xi \right\|_2^2$$

What if we take constant representations? We end up in a **global minimum** of the loss function with a **representation collapse!**

BYOL: representation collapse

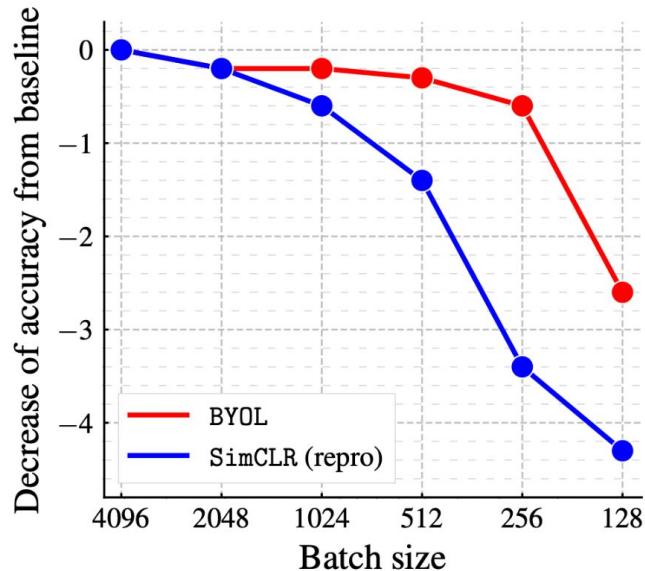
Why does BYOL not collapse in practice?

- Optimization steps are not in the direction of joint gradient $\nabla_{\theta,\xi} \mathcal{L}$

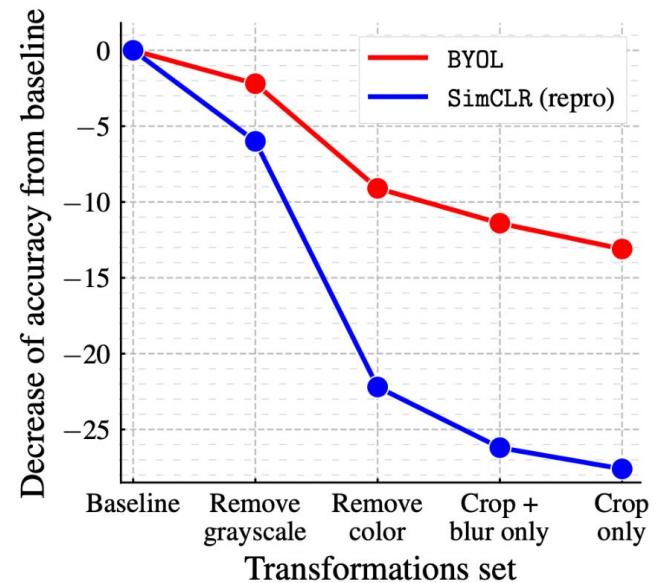
$$\begin{aligned}\theta &\leftarrow \text{optimizer}(\theta, \nabla_{\theta} \mathcal{L}_{\theta,\xi}^{\text{BYOL}}, \eta), \\ \xi &\leftarrow \tau \xi + (1 - \tau) \theta,\end{aligned}$$

- Collapsed global minimum is unstable
- Hyperparameters (EMA, weight decay) are important

BYOL: ablations



(a) Impact of batch size



(b) Impact of progressively removing transformations

Figure 3: Decrease in top-1 accuracy (in % points) of BYOL and our own reproduction of SimCLR at 300 epochs, under linear evaluation on ImageNet.

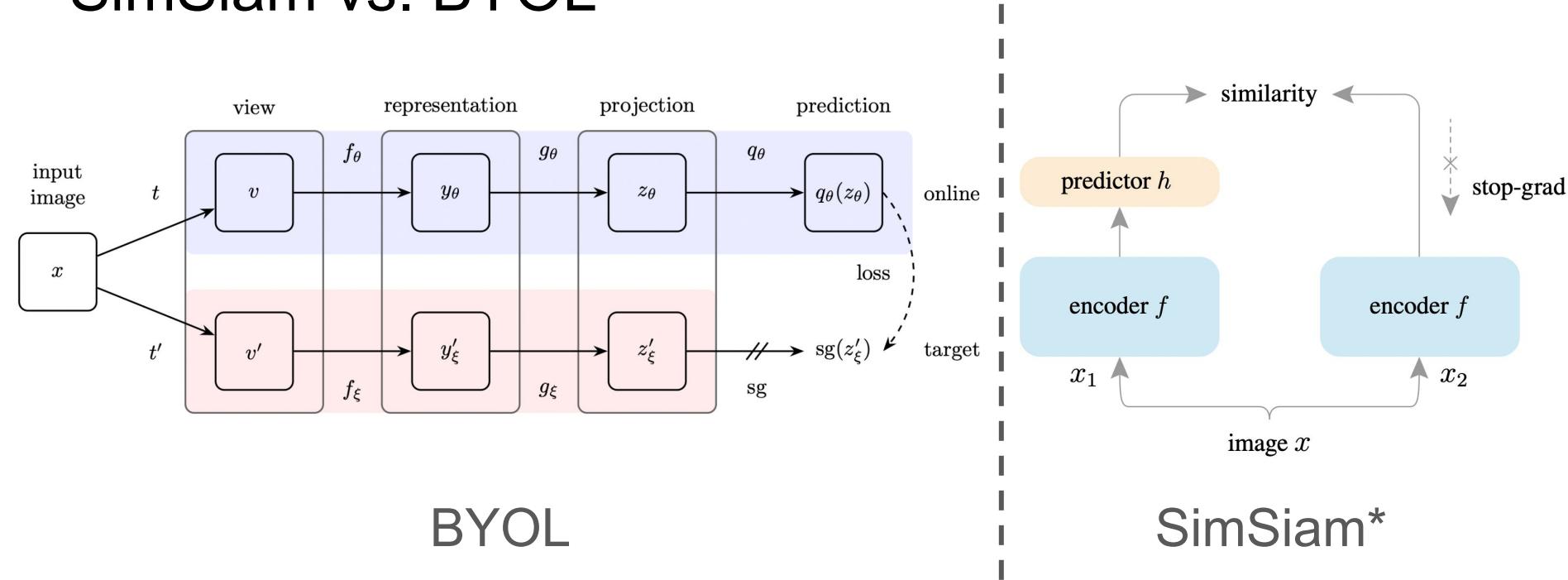
SimSiam

Simple Siamese networks, FAIR

- Momentum encoder is **unnecessary** for contrastive learning
- Overall performance worse than BYOL but still comparable to other methods



SimSiam vs. BYOL



*SimSiam encoder f includes both the convolutional part (BYOL's f_θ) and the MLP projection (BYOL's g_θ)

[Chen and He, 2020](#)

SimSiam: ablations

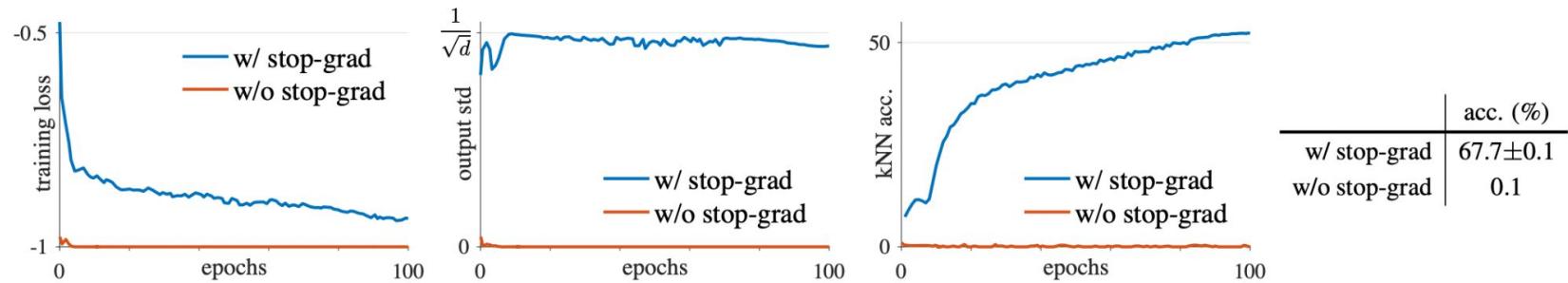


Figure 2. **SimSiam with vs. without stop-gradient.** **Left plot:** training loss. Without stop-gradient it degenerates immediately. **Middle plot:** the per-channel std of the ℓ_2 -normalized output, plotted as the averaged std over all channels. **Right plot:** validation accuracy of a kNN classifier [36] as a monitor of progress. **Table:** ImageNet linear evaluation (“w/ stop-grad” is mean \pm std over 5 trials).

	pred. MLP h	acc. (%)
baseline	lr with cosine decay	67.7
(a)	no pred. MLP	0.1
(b)	fixed random init.	1.5
(c)	lr not decayed	68.1

Table 1. **Effect of prediction MLP** (ImageNet linear evaluation accuracy with 100-epoch pre-training). In all these variants, we use the same schedule for the encoder f (lr with cosine decay).

[Chen and He, 2020](#)

SimSiam is EM algorithm???

$$\mathcal{L}(\theta, \eta) = \mathbb{E}_{x, \mathcal{T}} \left[\left\| \mathcal{F}_\theta(\mathcal{T}(x)) - \eta_x \right\|_2^2 \right]$$

$$\theta^t \quad \leftarrow \quad \arg \min_{\theta} \quad \mathcal{L}(\theta, \eta^{t-1})$$

$$\eta^t \quad \leftarrow \quad \arg \min_{\eta} \quad \mathcal{L}(\theta^t, \eta)$$

x – image

$\mathcal{T}(\cdot)$ – augmentation

$\mathcal{F}_\theta(\cdot)$ – encoder

η_x – representation of image x

SimSiam is EM algorithm???

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SimSiam is EM algorithm???

$$\mathcal{L}(\theta, \eta) = \mathbb{E}_{x, \mathcal{T}} \left[\left\| \mathcal{F}_\theta(\mathcal{T}(x)) - \eta_x \right\|_2^2 \right]$$

$$\eta_x^t \leftarrow \mathbb{E}_{\mathcal{T}} \left[\mathcal{F}_{\theta^t}(\mathcal{T}(x)) \right] \rightarrow \eta_x^t \leftarrow \mathcal{F}_{\theta^t}(\mathcal{T}'(x))$$

x – image

$\mathcal{T}(\cdot)$ – augmentation

$\mathcal{F}_\theta(\cdot)$ – encoder

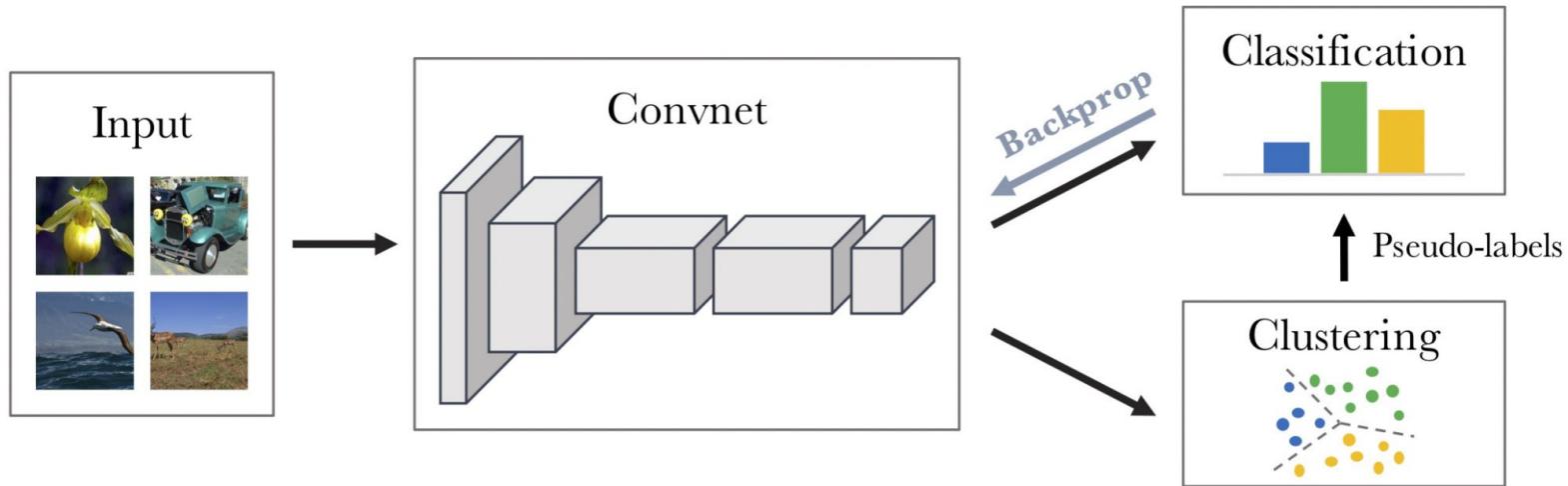
η_x – representation of image x

$$\theta^{t+1} \leftarrow \arg \min_{\theta} \mathbb{E}_{x, \mathcal{T}} \left[\left\| \mathcal{F}_\theta(\mathcal{T}(x)) - \mathcal{F}_{\theta^t}(\mathcal{T}'(x)) \right\|_2^2 \right]$$

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DeepCluster



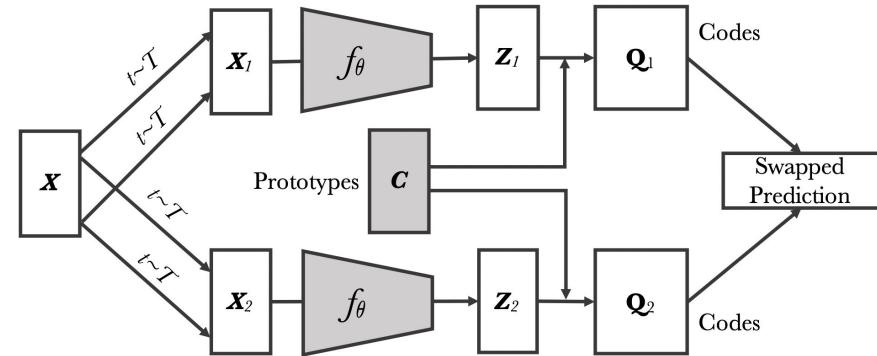
$$\min_{C \in \mathbb{R}^{d \times k}} \frac{1}{N} \sum_{n=1}^N \min_{y_n \in \{0,1\}^k} \|f_\theta(x_n) - Cy_n\|_2^2 \quad \text{such that} \quad y_n^\top \mathbf{1}_k = 1$$

[Caron et al., 2018](#)

SwAV

Swapping Assignments between Views, FAIR

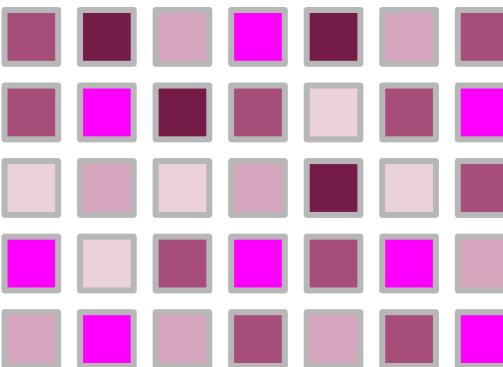
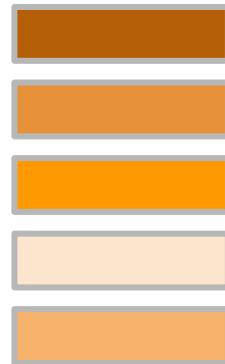
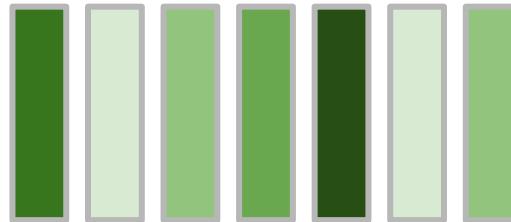
- Further development of DeepCluster
- Make cluster centroids learnable
- Do online clustering
- Swap cluster assignments between two augmented views of the image
(i.e. bring contrastive component to the clustering setup)



SwAV: scheme

Image representations

$$\mathbf{Z} = [\mathbf{z}_1, \dots, \mathbf{z}_B]$$



$$\mathbf{C} = [\mathbf{c}_1, \dots, \mathbf{c}_K]$$

Cluster prototypes (“centroids”)

$$\mathbf{Q} \in \mathbb{R}_+^{K \times B}$$

Cluster
assignments

[Caron et al., 2020](#)

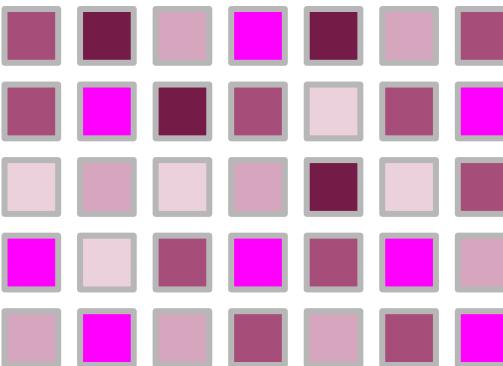
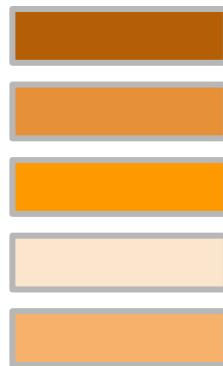
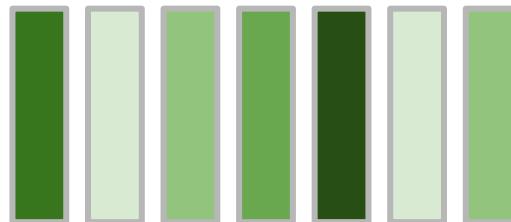
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Cluster prototypes (“centroids”)

Image representations

$$\mathbf{Z} = [\mathbf{z}_1, \dots, \mathbf{z}_B]$$



$$\mathbf{Q} \in \mathbb{R}_+^{K \times B}$$

Cluster assignments

$$\max_{\mathbf{Q} \in \mathcal{Q}} \text{Tr} (\mathbf{Q}^\top \mathbf{C}^\top \mathbf{Z}) + \varepsilon H(\mathbf{Q})$$

$$H(\mathbf{Q}) = - \sum_{ij} \mathbf{Q}_{ij} \log \mathbf{Q}_{ij}$$

$$\mathcal{Q} = \left\{ \mathbf{Q} \in \mathbb{R}_+^{K \times B} \mid \mathbf{Q}\mathbf{1}_B = \frac{1}{K}\mathbf{1}_K, \mathbf{Q}^\top \mathbf{1}_K = \frac{1}{B}\mathbf{1}_B \right\}$$

SwAV: scheme

$$\mathbf{C} = [\mathbf{c}_1, \dots, \mathbf{c}_K]$$

Cluster prototypes (“centroids”)

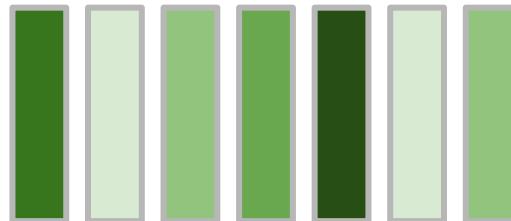
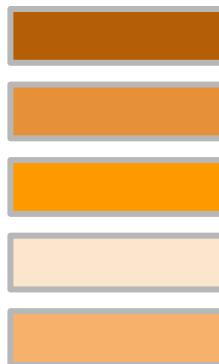
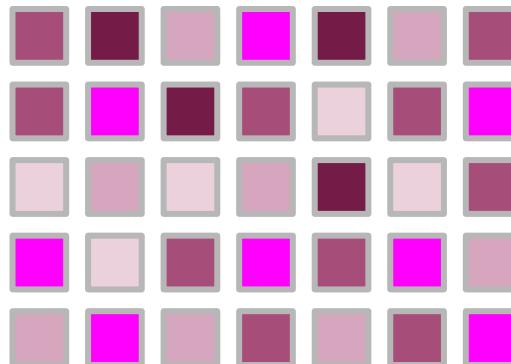


Image representations

$$\mathbf{Z} = [\mathbf{z}_1, \dots, \mathbf{z}_B]$$



$$\mathbf{Q} \in \mathbb{R}_+^{K \times B}$$

Cluster
assignments

$$\max_{\mathbf{Q} \in \mathcal{Q}} \text{Tr} (\mathbf{Q}^\top \mathbf{C}^\top \mathbf{Z}) + \varepsilon H(\mathbf{Q})$$

$$H(\mathbf{Q}) = - \sum_{ij} \mathbf{Q}_{ij} \log \mathbf{Q}_{ij}$$

$$\mathcal{Q} = \left\{ \mathbf{Q} \in \mathbb{R}_+^{K \times B} \mid \mathbf{Q}\mathbf{1}_B = \frac{1}{K}\mathbf{1}_K, \mathbf{Q}^\top \mathbf{1}_K = \frac{1}{B}\mathbf{1}_B \right\}$$

$$\mathbf{Q}^* = \text{Diag}(\mathbf{u}) \exp \left(\frac{\mathbf{C}^\top \mathbf{Z}}{\varepsilon} \right) \text{Diag}(\mathbf{v})$$

Sinkhorn–Knopp
algorithm

[Caron et al., 2020](#)

SwAV: scheme

$$\mathbf{C} = [\mathbf{c}_1, \dots, \mathbf{c}_K]$$

Cluster prototypes (“centroids”)

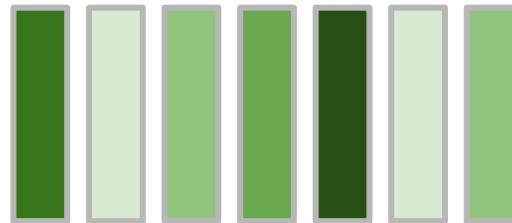
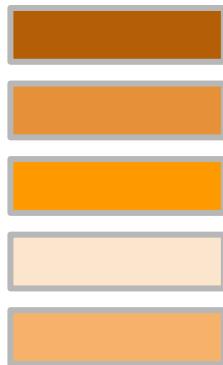
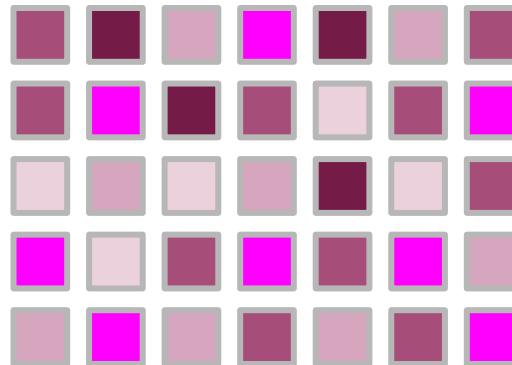


Image representations

$$\mathbf{Z} = [\mathbf{z}_1, \dots, \mathbf{z}_B]$$

$$\mathbf{Q} \in \mathbb{R}_+^{K \times B}$$

Cluster
assignments



$$\mathbf{Q}^* = \text{Diag}(\mathbf{u}) \exp\left(\frac{\mathbf{C}^\top \mathbf{Z}}{\varepsilon}\right) \text{Diag}(\mathbf{v})$$

$$\mathbf{p}_t^{(k)} = \frac{\exp\left(\frac{1}{\tau} \mathbf{z}_t^\top \mathbf{c}_k\right)}{\sum_{k'} \exp\left(\frac{1}{\tau} \mathbf{z}_t^\top \mathbf{c}_{k'}\right)}$$

$$\ell(\mathbf{z}_t, \mathbf{q}_s) = - \sum_k \mathbf{q}_s^{(k)} \log \mathbf{p}_t^{(k)}$$

SwAV: scheme

$$\mathbf{C} = [\mathbf{c}_1, \dots, \mathbf{c}_K]$$

Cluster prototypes (“centroids”)

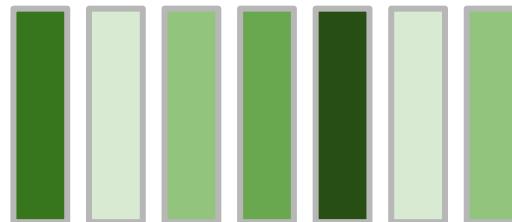
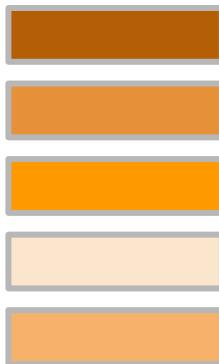
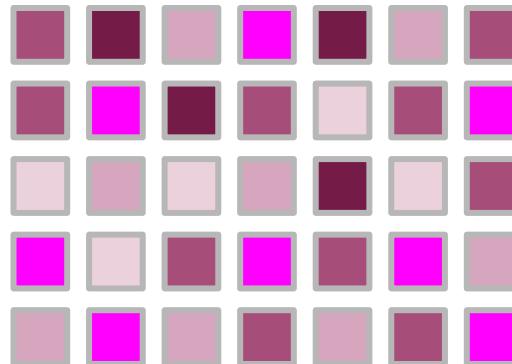


Image representations

$$\mathbf{Z} = [\mathbf{z}_1, \dots, \mathbf{z}_B]$$

$$\mathbf{Q} \in \mathbb{R}_+^{K \times B}$$

Cluster assignments



$$\mathbf{Q}^* = \text{Diag}(\mathbf{u}) \exp\left(\frac{\mathbf{C}^\top \mathbf{Z}}{\varepsilon}\right) \text{Diag}(\mathbf{v})$$

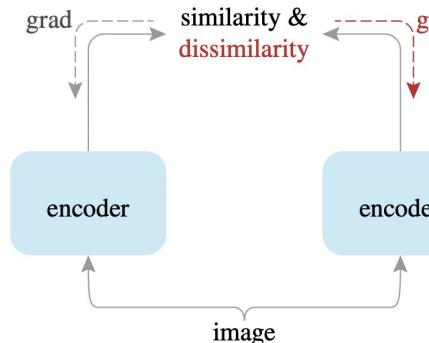
$$\mathbf{p}_t^{(k)} = \frac{\exp\left(\frac{1}{\tau} \mathbf{z}_t^\top \mathbf{c}_k\right)}{\sum_{k'} \exp\left(\frac{1}{\tau} \mathbf{z}_t^\top \mathbf{c}_{k'}\right)}$$

$$\ell(\mathbf{z}_t, \mathbf{q}_s) = - \sum_k \mathbf{q}_s^{(k)} \log \mathbf{p}_t^{(k)}$$

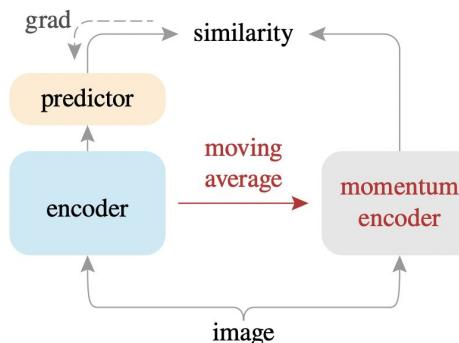
$$L(\mathbf{z}_t, \mathbf{z}_s) = \ell(\mathbf{z}_t, \mathbf{q}_s) + \ell(\mathbf{z}_s, \mathbf{q}_t)$$

[Caron et al., 2020](#)

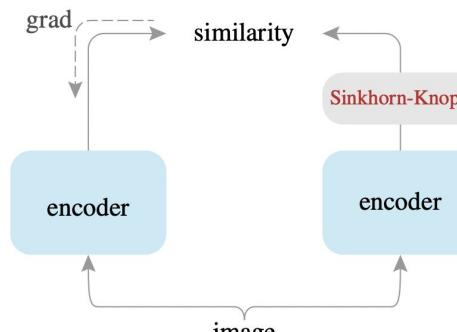
Comparison



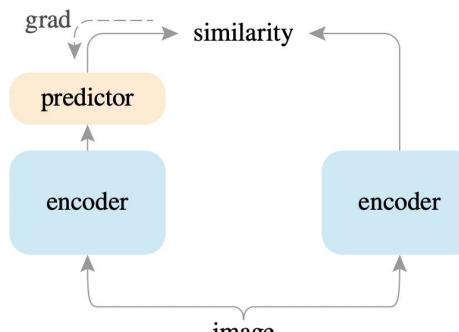
SimCLR



BYOL



SwAV



SimSiam

[Chen and He, 2020](#)

Results: ImageNet LP, VOC & COCO

method	batch size	negative pairs	momentum encoder	100 ep	200 ep	400 ep	800 ep
SimCLR (repro.+)	4096	✓		66.5	68.3	69.8	70.4
MoCo v2 (repro.+)	256	✓	✓	67.4	69.9	71.0	72.2
BYOL (repro.)	4096		✓	66.5	70.6	73.2	74.3
SwAV (repro.+)	4096			66.5	69.1	70.7	71.8
SimSiam	256			68.1	70.0	70.8	71.3

pre-train	VOC 07 detection			VOC 07+12 detection			COCO detection			COCO instance seg.		
	AP ₅₀	AP	AP ₇₅	AP ₅₀	AP	AP ₇₅	AP ₅₀	AP	AP ₇₅	AP ₅₀ ^{mask}	AP ₇₅ ^{mask}	
scratch	35.9	16.8	13.0	60.2	33.8	33.1	44.0	26.4	27.8	46.9	29.3	30.8
ImageNet supervised	74.4	42.4	42.7	81.3	53.5	58.8	58.2	38.2	41.2	54.7	33.3	35.2
SimCLR (repro.+)	75.9	46.8	50.1	81.8	55.5	61.4	57.7	37.9	40.9	54.6	33.3	35.3
MoCo v2 (repro.+)	77.1	48.5	52.5	82.3	57.0	63.3	58.8	39.2	42.5	55.5	34.3	36.6
BYOL (repro.)	77.1	47.0	49.9	81.4	55.3	61.1	57.8	37.9	40.9	54.3	33.2	35.0
SwAV (repro.+)	75.5	46.5	49.6	81.5	55.4	61.4	57.6	37.6	40.3	54.2	33.1	35.1
SimSiam, base	75.5	47.0	50.2	82.0	56.4	62.8	57.5	37.9	40.9	54.2	33.2	35.2
SimSiam, optimal	77.3	48.5	52.5	82.4	57.0	63.7	59.3	39.2	42.1	56.0	34.4	36.7

Results: downstream classification

Method	Food101	CIFAR10	CIFAR100	Birdsnap	SUN397	Cars	Aircraft	VOC2007	DTD	Pets	Caltech-101	Flowers
<i>Linear evaluation:</i>												
BYOL (ours)	75.3	91.3	78.4	57.2	62.2	67.8	60.6	82.5	75.5	90.4	94.2	96.1
SimCLR (repro)	72.8	90.5	74.4	42.4	60.6	49.3	49.8	81.4	75.7	84.6	89.3	92.6
SimCLR [8]	68.4	90.6	71.6	37.4	58.8	50.3	50.3	80.5	74.5	83.6	90.3	91.2
Supervised-IN [8]	72.3	93.6	78.3	53.7	61.9	66.7	61.0	82.8	74.9	91.5	94.5	94.7
<i>Fine-tuned:</i>												
BYOL (ours)	88.5	97.8	86.1	76.3	63.7	91.6	88.1	85.4	76.2	91.7	93.8	97.0
SimCLR (repro)	87.5	97.4	85.3	75.0	63.9	91.4	87.6	84.5	75.4	89.4	91.7	96.6
SimCLR [8]	88.2	97.7	85.9	75.9	63.5	91.3	88.1	84.1	73.2	89.2	92.1	97.0
Supervised-IN [8]	88.3	97.5	86.4	75.8	64.3	92.1	86.0	85.0	74.6	92.1	93.3	97.6
Random init [8]	86.9	95.9	80.2	76.1	53.6	91.4	85.9	67.3	64.8	81.5	72.6	92.0

Results: semi-supervised

Method	Top-1		Top-5		Method	Architecture	Param.	Top-1		Top-5	
	1%	10%	1%	10%				1%	10%	1%	10%
Supervised [77]	25.4	56.4	48.4	80.4	CPC v2 [32]	ResNet-161	305M	-	-	77.9	91.2
InstDisc	-	-	39.2	77.4	SimCLR [8]	ResNet-50 (2×)	94M	58.5	71.7	83.0	91.2
PIRL [35]	-	-	57.2	83.8	BYOL (ours)	ResNet-50 (2×)	94M	62.2	73.5	84.1	91.7
SimCLR [8]	48.3	65.6	75.5	87.8	SimCLR [8]	ResNet-50 (4×)	375M	63.0	74.4	85.8	92.6
BYOL (ours)	53.2	68.8	78.4	89.0	BYOL (ours)	ResNet-50 (4×)	375M	69.1	75.7	87.9	92.5
					BYOL (ours)	ResNet-200 (2×)	250M	71.2	77.7	89.5	93.7

(a) ResNet-50 encoder.

(b) Other ResNet encoder architectures.

Table 2: Semi-supervised training with a fraction of ImageNet labels.