Self-Supervised Learning

2021 연구실 하계 세미나

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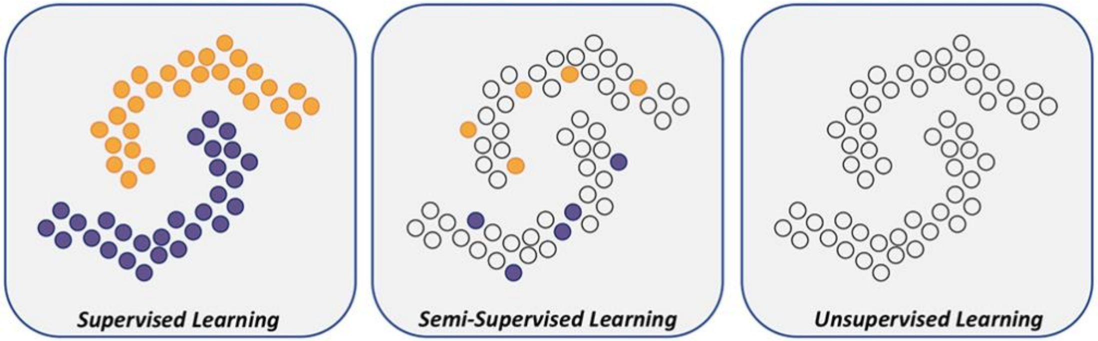
Outline

- What is Self-Supervised Learning?
- Why we need Self-Supervised Learning?
- Trend of the self-supervised learning
- Bootstrap your own latent
- Exploring Simple Siamese Representation Learning
- References

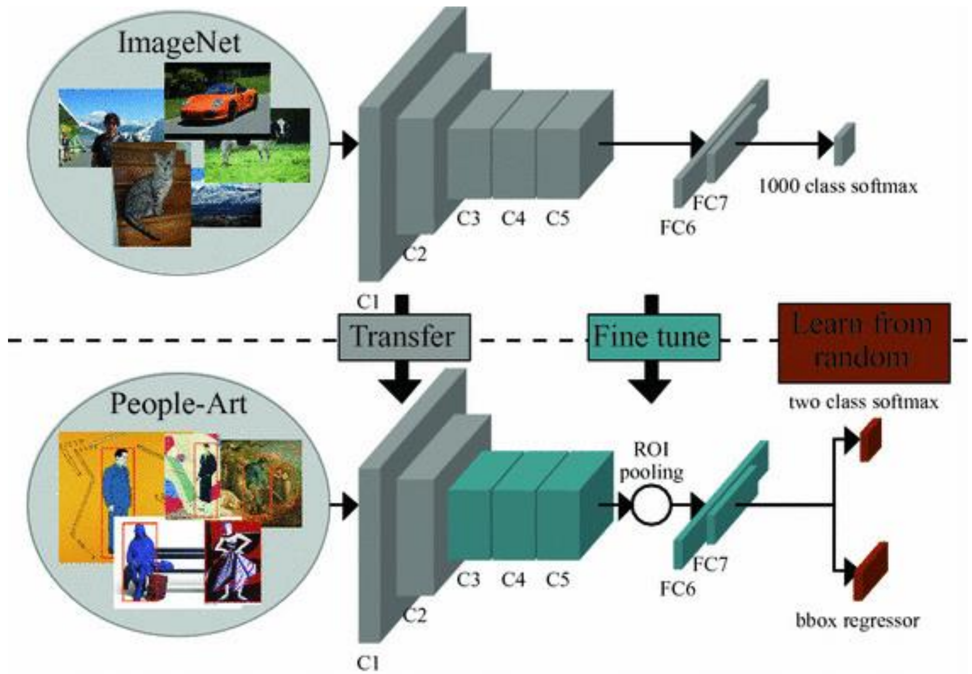
Self-Supervised Learning

- What is Self-Supervised Learning?
  - Supervised Learning
    - 모든 학습 데이터에 label이 존재
  - Semi-Supervised Learning
    - 일부 학습 데이터에 label이 존재
  - Unsupervised Learning
    - 학습 데이터에 label이 존재하지 않음
    - Self-supervised learning은 unsupervised learning의 일부
      - 스스로 Supervision을 주어서 학습을 진행



Self-Supervised Learning

- Why we need Self-Supervised Learning?
  - Visual Representation
    - 일반적으로 deep learning model 학습 시 pretrained weight 를 사용
      - Computer vision task의 경우 일반적으로 ImageNet pretrained weight를 사용
      - Pretrained weight를 사용했을 때와 사용하지 않았을 때의 성능 차이가 큼

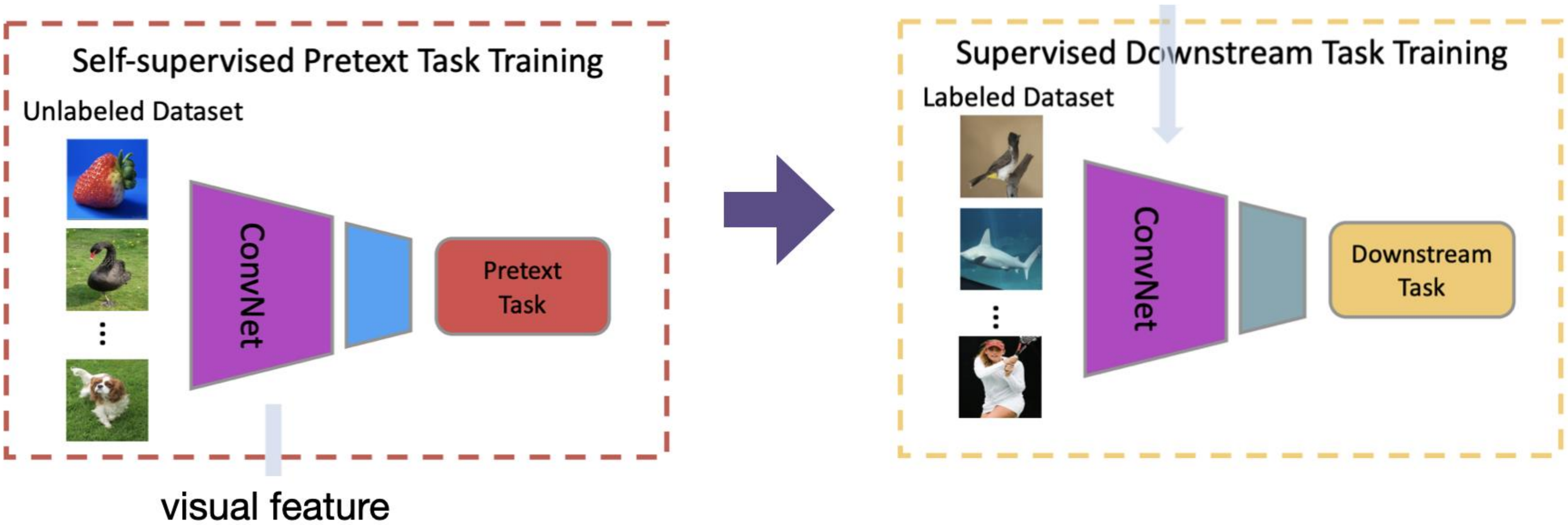


Self-Supervised Learning

- Why we need Self-Supervised Learning?
  - Visual Representation
    - 일반적인 RGB 영상이 아닌 특수한 영상을 사용하는 deep learning model의 경우 ImageNet pretrain이 아닌 해당 data 에 대한 pretrain 후, 학습된 weight 를 사용하는 것이 성능 향상에 유리
      - Pretrained model이 해당 data에 대한 feature extraction을 잘하기 때문
      - Ex) 의료 영상, ToF 영상 등
    - 특수한 data의 경우 양은 많이 존재하나, labeling 되어 있지 않은 경우가 많음
      - Labeling에는 많은 cost가 필요

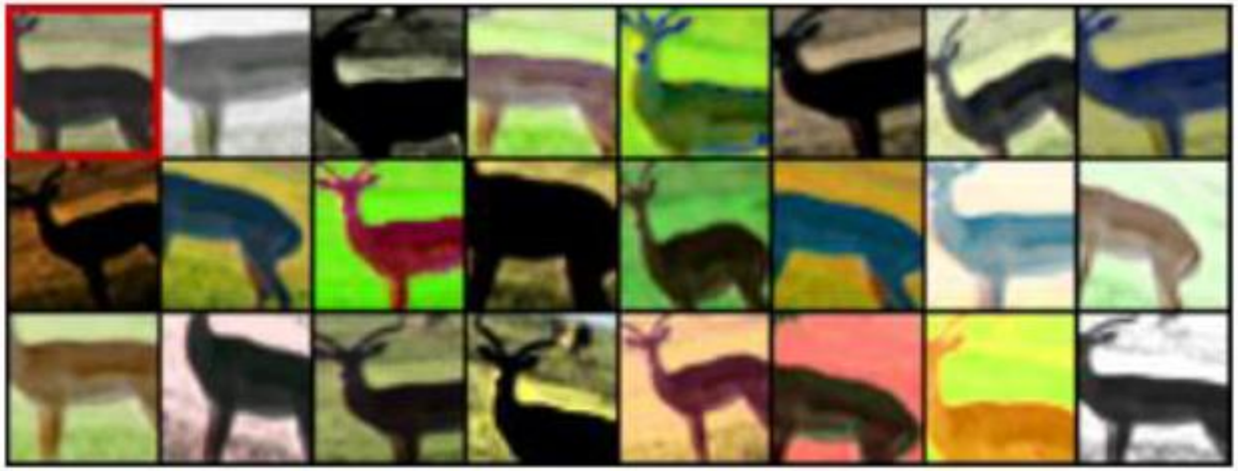
Self-Supervised Learning

- Trend of the self-supervised learning
  - Pretext Tasks (~ 2018)
    - 사용자가 정의한 간단한 문제인 Pretext Tasks 를 통해 visual representation 을 학습한 후, 해당 network 를 실제 사용할 Downstream Task 에 적용하는 방법
    - Supervised learning 으로 학습할 때보다 낮은 성능을 보임
    - Pretext task 를 잘 풀도록 학습되었을 뿐 이미지의 일반적인 시각적 특징을 잡아내지는 못함



Self-Supervised Learning

- Trend of the self-supervised learning
  - Pretext Tasks (~ 2018)
    - Exemplar [1] (NIPS 2014)
      - Image 내에 object 가 존재하는 영역 하나를 patch 로 crop 하여 augmentation
      - Augmented patches 는 전부 같은 class 로 판단하도록 학습
        - ✓ Image 수가 class 수가 되기 때문에 과도한 class 수가 존재
        - ✓ 학습 시 많은 memory 필요



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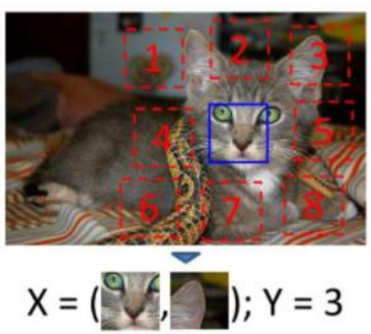
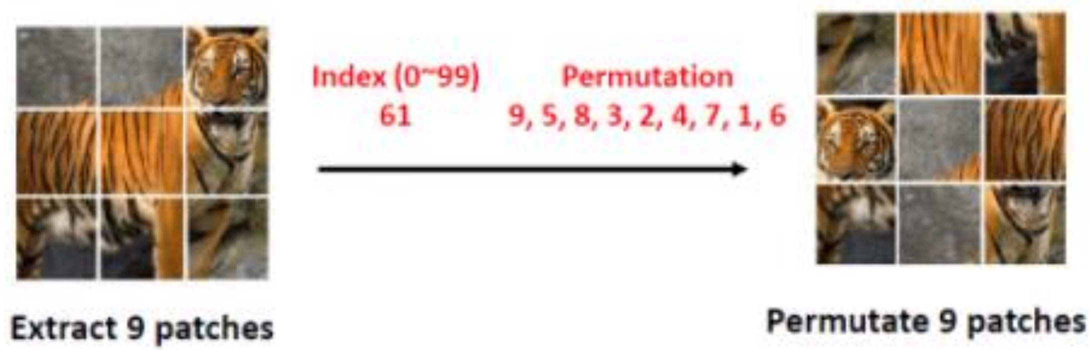
Self-Supervised Learning

- Trend of the self-supervised learning
  - Pretext Tasks (~ 2018)
    - Context Prediction [2] (ICCV 2015)
      - 9개의 patch 를 가운데 patch 를 기준으로 나머지 patch 의 상대적 위치를 classification 하도록 학습
    - Jigsaw Puzzle [3] (ECCV 2016)
      - 9개의 patch 의 순서를 섞은 후, 원래의 순서를 찾아가도록 학습



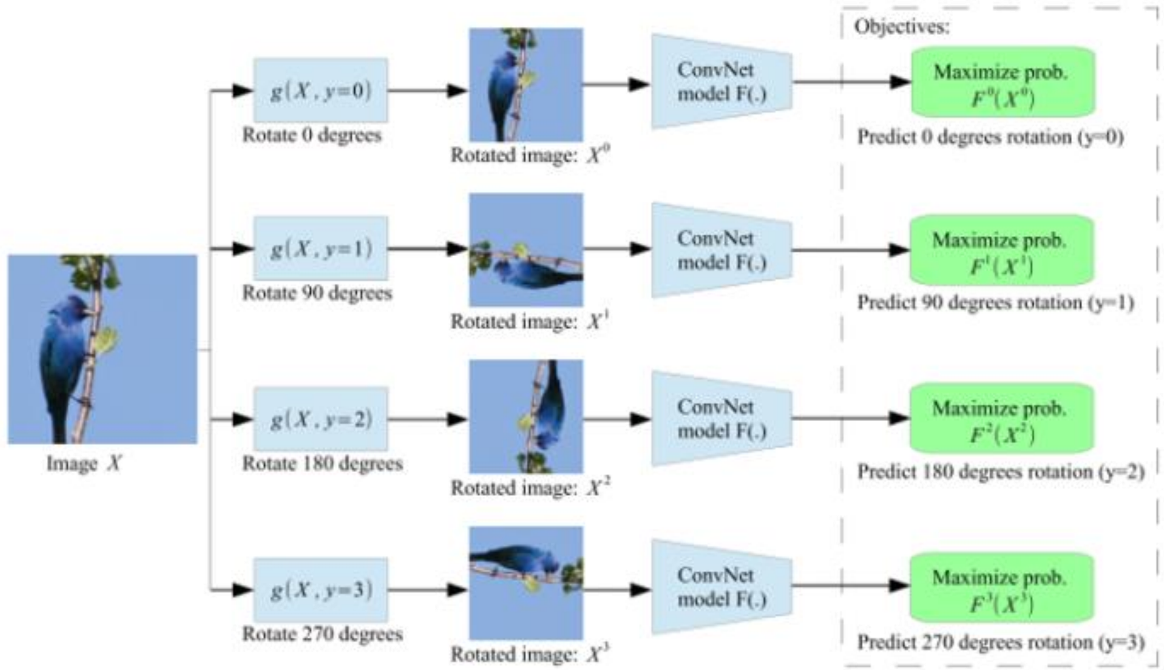
< Context Prediction >



< Jigsaw Puzzle >

Self-Supervised Learning

- Trend of the self-supervised learning
  - Pretext Tasks (~ 2018)
    - Rotation [4] (ICLR 2018)
      - Rotation 된 image가 원래 image에서 얼마나 rotation 되었는지를 classification 하도록 함.

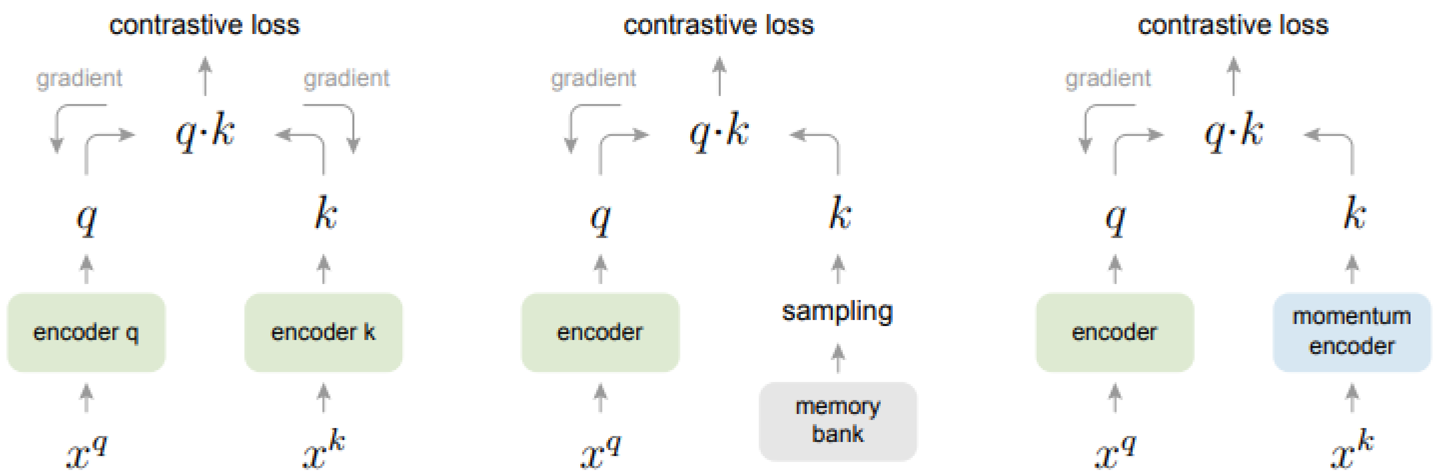


Self-Supervised Learning

- Trend of the self-supervised learning
  - Contrastive Learning (2019 ~ 2020)
    - Pretext task 를 정의하지 않고, 같은 image 에 서로 다른 augmentation 을 적용한 positive pair feature representation 는 서로 가깝게, 다른 image 에 다른 augmentation 을 적용한 negative pair 의 feature representation 은 서로 멀어지게 학습하는 것
    - Supervised ImageNet pretrained model 을 사용할 때와 비슷하거나 오히려 높은 성능 달성
    - 여러 가지 문제점 존재
      - Collapsing
        - ✓ 입력을 모두 같은 값으로 수렴시키는 문제 발생
        - ✓ 이를 해결하기 위해 학습 시 large batch size (256 ~ 8192) 사용
      - Negative pair를 정의하는 augmentation 을 어떤 것을 사용하는지에 따라 성능 차이가 심함
        - ✓ 적절한 augmentation 선정 필요

Self-Supervised Learning

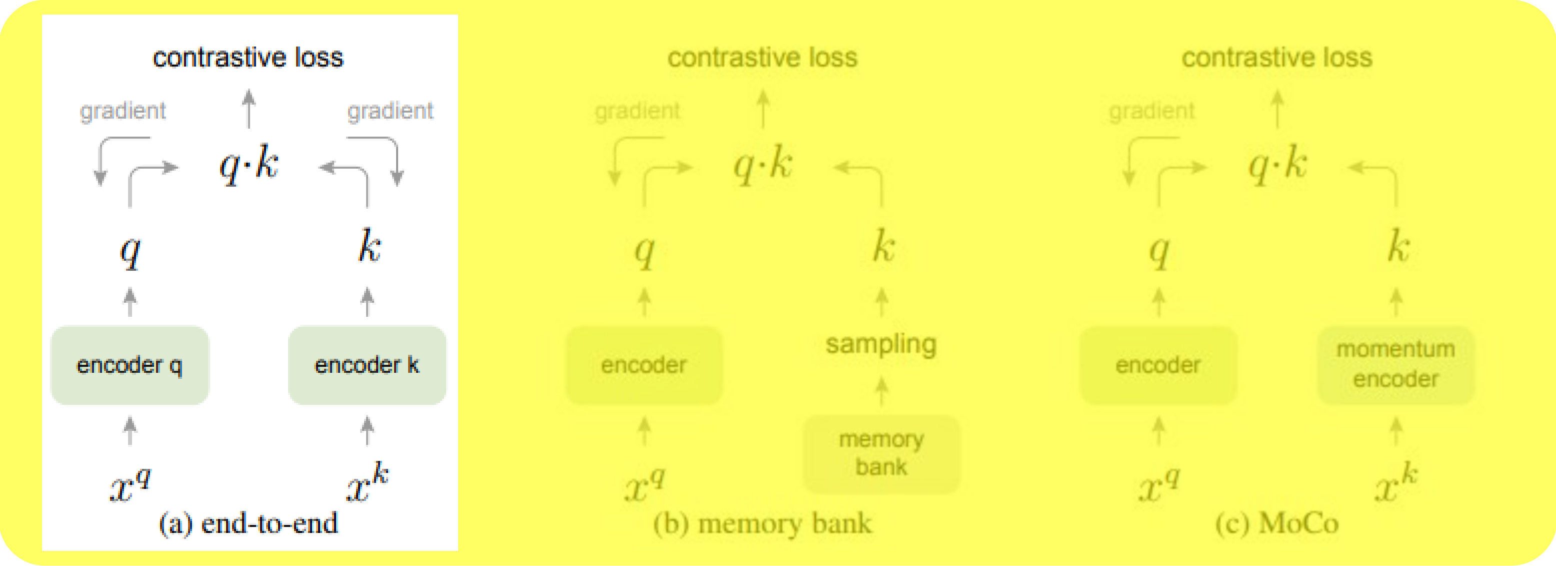
- Trend of the self-supervised learning
  - Contrastive Learning (2019 ~ 2020)
    - MoCo [5] (CVPR 2020)
      - 기존 방식 중 end-to-end 방식은 large batch size 필요
      - Memory bank 는 inconsistency 발생
      - Momentum encoder 를 사용하여 mini-batch 로 inconsistency 가 발생하지 않는 contrastive learning 방식 제안



(a) end-to-end (b) memory bank (c) MoCo

Self-Supervised Learning

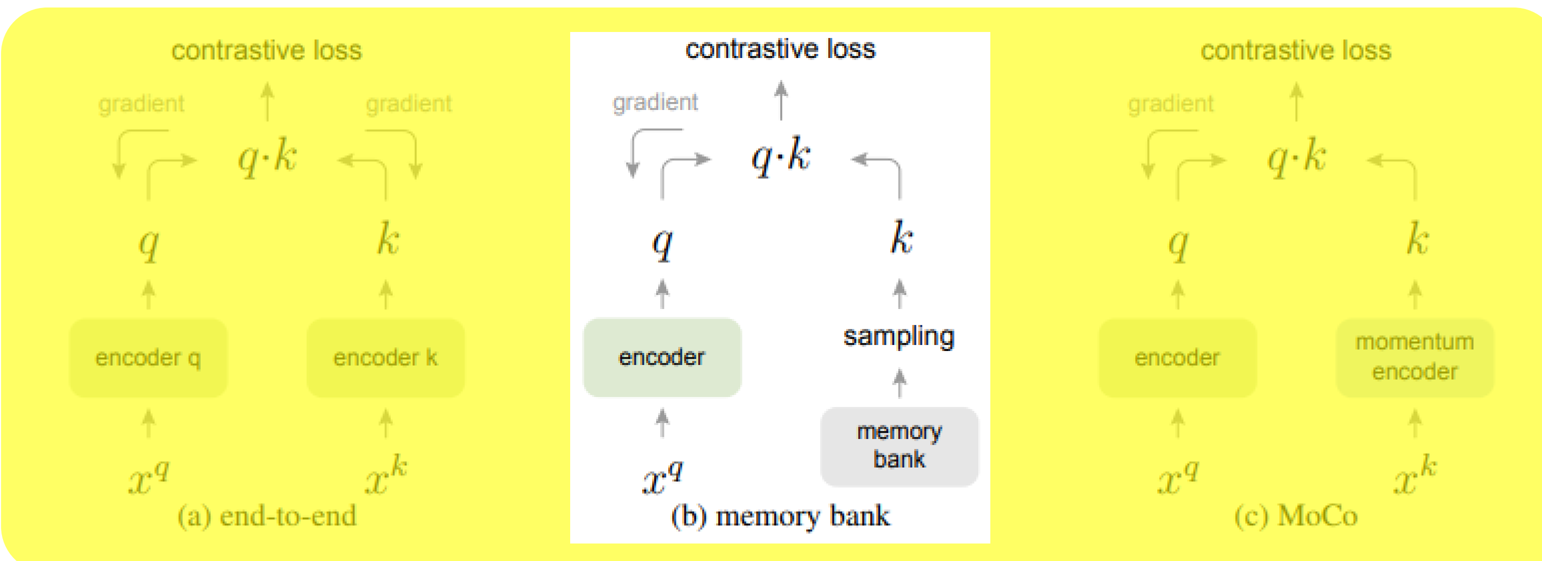
- Trend of the self-supervised learning
  - Contrastive Learning (2019 ~ 2020)
    - MoCo [5] (CVPR 2020)
      - End-to-end 방식
        - ✓ Batch size 를 크게 가져가 많은 negative sample 을 만들고, 각각의 encoder 를 모두 backpropagation 하는 방식을 채택
          - Batch size 를 크게 가져가야 함 (Memory limit)



(a) end-to-end (b) memory bank (c) MoCo

Self-Supervised Learning

- Trend of the self-supervised learning
  - Contrastive Learning (2019 ~ 2020)
    - MoCo [5] (CVPR 2020)
      - Memory bank 방식
        - ✓ 모든 image 에 대해 encoder 를 통과시킨 feature representation 을 추출하고, 해당 vector 를 key 로 하여 memory bank 에 저장 후 sampling 하여 사용
          - Batch size 를 작게 가져갈 수 있으나, inconsistency 발생

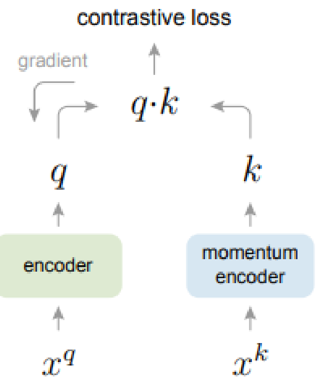


(a) end-to-end (b) memory bank (c) MoCo

Self-Supervised Learning

- Trend of the self-supervised learning
  - Contrastive Learning (2019 ~ 2020)
    - MoCo [5] (CVPR 2020)
      - Dynamic dictionary
        - ✓ Mini-batch 보다 큰 size 의 dictionary size 를 지정하고, momentum encoder 를 통과하여 추출된 feature 를 FIFO 방식으로 queuing 하여 사용
      - Momentum encoder
        - ✓ Momentum encoder 는 backpropagation 하지 않음
          - Backpropagation 시 성능이 떨어지는 것을 실험적으로 확인
        - ✓ Encoder 에서 학습된 weight 에 momentum 을 주어 update

$$\theta_{\mathrm{k}} \leftarrow m\theta_{\mathrm{k}} + (1-m)\theta_{\mathrm{q}}.$$



(c) MoCo

Self-Supervised Learning

- Trend of the self-supervised learning
  - Contrastive Learning (2019 ~ 2020)
    - MoCo [5] (CVPR 2020)
      - Downstream task 에서 supervised pretrained model 과 비슷하거나 더 높은 결과를 보임

pre-train	COCO keypoint detection AP^{kp}	AP^{kp}_{50}	AP^{kp}_{75}
random init.	65.9	86.5	71.7
super. IN-1M	65.8	86.9	71.9
MoCo IN-1M	66.8 (+1.0)	87.4 (+0.5)	72.5 (+0.6)
MoCo IG-1B	66.9 (+1.1)	87.8 (+0.9)	73.0 (+1.1)

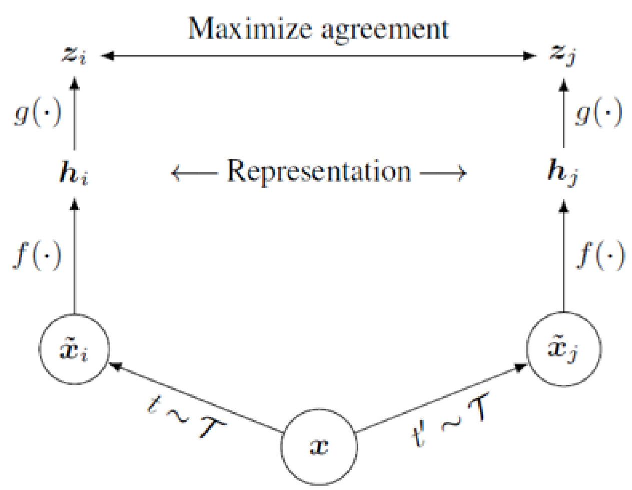
pre-train	LVIS v0.5 instance segmentation AP^{mk}	AP^{mk}_{50}	AP^{mk}_{75}
random init.	22.5	34.8	23.8
super. IN-1M†	24.4	37.8	25.8
MoCo IN-1M	24.1 (−0.3)	37.4 (−0.4)	25.5 (−0.3)
MoCo IG-1B	24.9 (+0.5)	38.2 (+0.4)	26.4 (+0.6)

pre-train	COCO dense pose estimation AP^{dp}	AP^{dp}_{50}	AP^{dp}_{75}
random init.	39.4	78.5	35.1
super. IN-1M	48.3	85.6	50.6
MoCo IN-1M	50.1 (+1.8)	86.8 (+1.2)	53.9 (+3.3)
MoCo IG-1B	50.6 (+2.3)	87.0 (+1.4)	54.3 (+3.7)

	Cityscapes instance seg.		Semantic seg. (mIoU)	
pre-train	AP^{mk}	AP^{mk}_{50}	Cityscapes	VOC
random init.	25.4	51.1	65.3	39.5
super. IN-1M	32.9	59.6	74.6	74.4
MoCo IN-1M	32.3 (−0.6)	59.3 (−0.3)	75.3 (+0.7)	72.5 (−1.9)
MoCo IG-1B	32.9 (0.0)	60.3 (+0.7)	75.5 (+0.9)	73.6 (−0.8)

Self-Supervised Learning

- Trend of the self-supervised learning
  - Contrastive Learning (2019 ~ 2020)
    - SimCLR [6] (ICML 2020)
      - Large batch size 를 사용하는 end-to-end 방식 (batch size 4096 ~ 8192)
      - MoCo 보다 높은 성능 달성
      - Encoder 이후 MLP 로 이루어진 projection head 를 추가
      - Augmentation 이 contrastive learning에 미치는 영향 분석

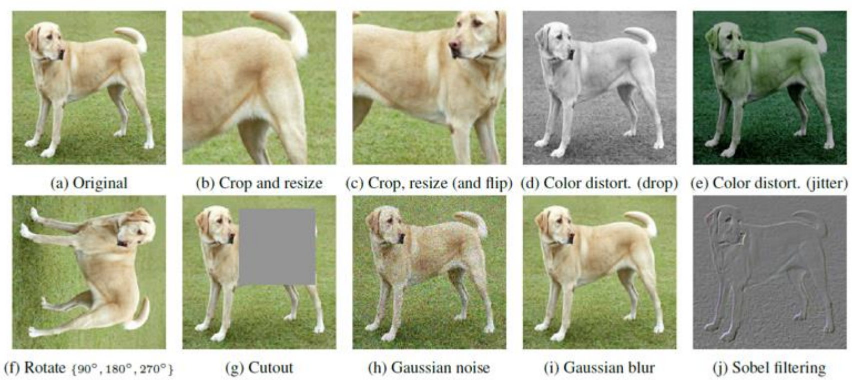


Self-Supervised Learning

- Trend of the self-supervised learning
  - Contrastive Learning (2019 ~ 2020)
    - SimCLR [6] (ICML 2020)
      - Large batch size
        - ✓ 4096 를 기본으로 8192 까지 적용
        - ✓ 각 image 마다 2개의 서로 다른 augmentation 을 적용하여 batch size 가 N일 때, 2N 개의 sample 생성
        - ✓ 입력 x 에 대한 positive sample 은 1개, negative sample 은 2N-2개 만큼 생성됨
        - ✓ Batch size 가 클수록 negative sample 개수가 많아져 성능 증가
        - ✓ Large batch 에서 안정적으로 학습이 가능하도록 LARS optimization 적용
        - ✓ Multi- GPU를 이용한 학습 시 각 device 별로 batch normalization 을 진행하지 않고, 모든 device 의 평균, 표준편차를 통합하여 사용
          - Positive sample 이 1개이기 때문에 positive sample 이 존재하는 device 가 1개이기 때문

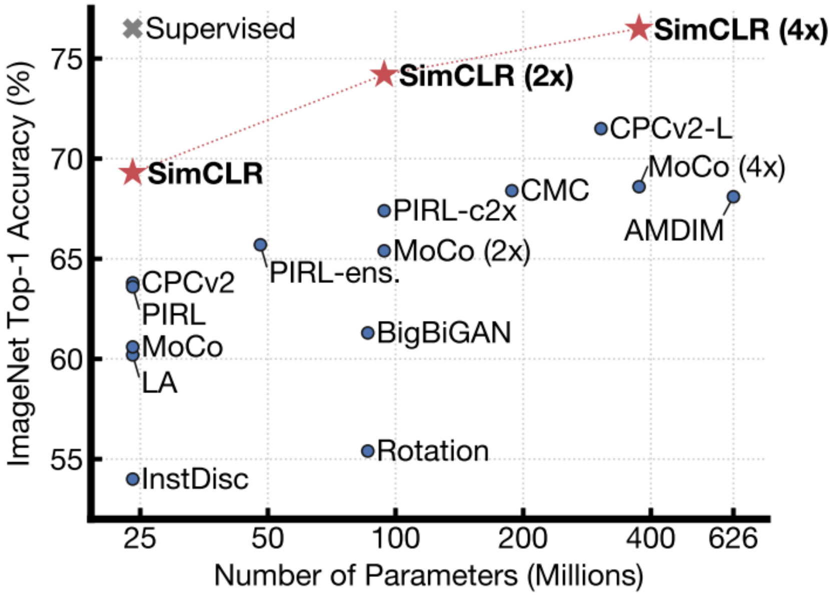
Self-Supervised Learning

- Trend of the self-supervised learning
  - Contrastive Learning (2019 ~ 2020)
    - SimCLR [6] (ICML 2020)
      - Augmentation
        - ✓ 2개의 augmentation 을 선택할 때, 어떠한 augmentation 을 사용하는지에 따라 성능 차이가 심함
        - ✓ Crop 과 color distortion 을 선택하였을 때 가장 성능이 높음
          - Color distortion 을 사용하지 않을 경우, augmentation 을 하더라도 augmentation된 영상들 간의 색 배합은 같기 때문에 visual representation 을 찾아내는 것이 아닌 색 배합만을 찾아냄.



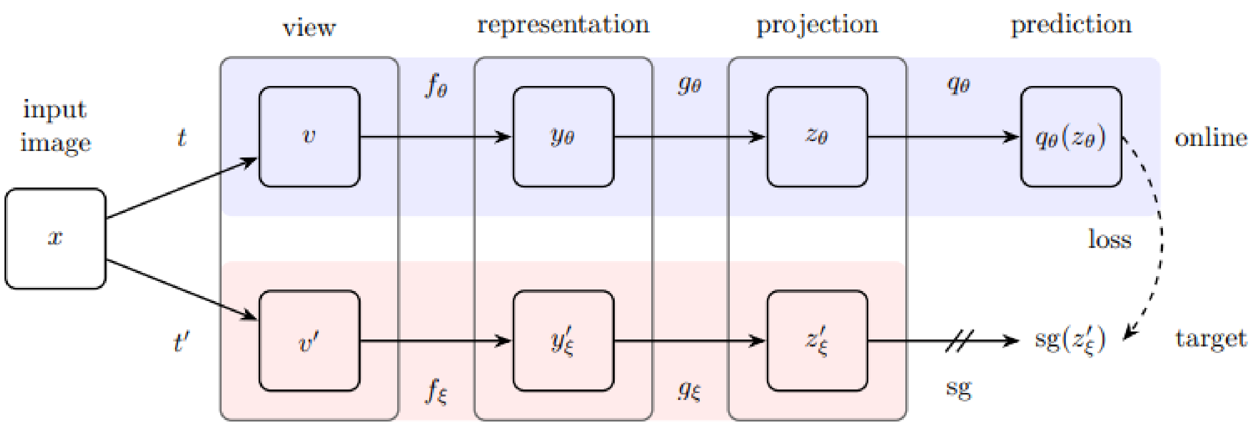
Self-Supervised Learning

- Trend of the self-supervised learning
  - Contrastive Learning (2019 ~ 2020)
    - SimCLR [6] (ICML 2020)
      - MoCo 보다 높은 성능을 보이며, supervised와 근접한 성능을 보임
      - Large batch size 로 인한 memory limit 은 여전히 문제



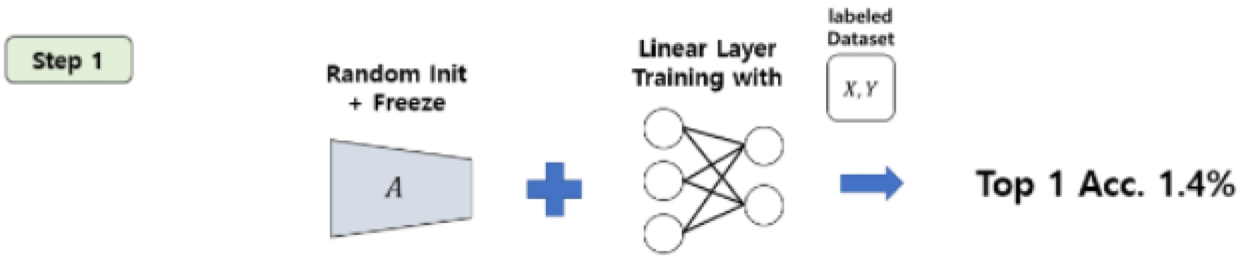
Self-Supervised Learning

- Trend of the self-supervised learning
  - Other (2020 ~)
    - Bootstrap your own latent: A new approach to self-supervised Learning [7] (NIPS 2020)
      - Negative sample 을 사용하지 않는 self-supervised learning 기법 제안
        - ✓ Batch size 를 줄일 수 있음
        - ✓ Negative sample 을 위한 augmentation 종류에 robust 해짐
      - 기존 contrastive learning 과 비슷한 Siamese network 를 이용
      - SOTA 성능 달성



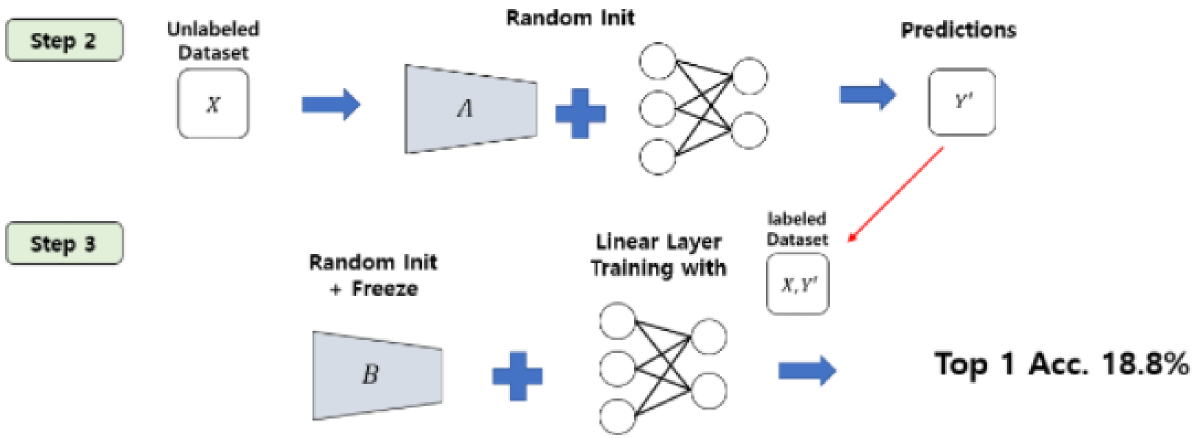
Self-Supervised Learning

- Bootstrap your own latent: A new approach to self-supervised Learning (NIPS 2020)
  - Motivation
    - Negative sample 을 사용하지 않고 image 로부터 visual representation 을 학습하는 것을 목표로 실험을 제안
      - Step 1
        - ✓ Random initialize 된 model 을 학습하지 않고, freeze 한 뒤 linear layer 를 붙여 학습
          - 학습되지 않는 backbone (feature extractor) 를 사용하여 classification 정확도 확인
          - 1.4%의 top-1 accuracy 달성



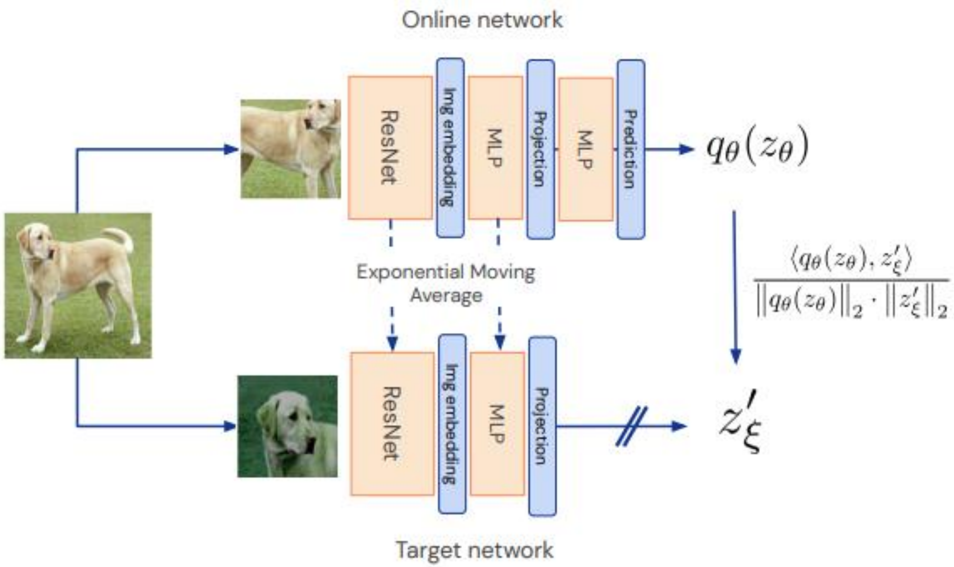
Self-Supervised Learning

- Bootstrap your own latent: A new approach to self-supervised Learning (NIPS 2020)
  - Motivation
    - Step 2
      - ✓ Random initialized backbone + MLP(predictor) 에 unlabeled dataset이 통과한 prediction 확보
    - Step 3
      - ✓ 새로운 random initialized model B를 step 2 에서 확보한 prediction 을 target 으로 학습
        - 18.8% 의 top-1 accuracy 달성
        - 부정확한 target 을 배우도록 학습하더라도 큰 폭으로 성능이 향상



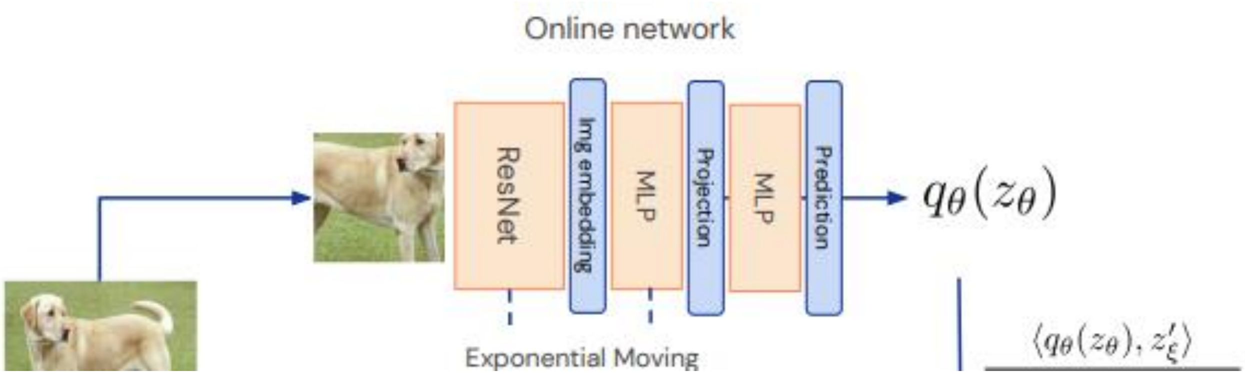
Self-Supervised Learning

- Bootstrap your own latent: A new approach to self-supervised Learning (NIPS 2020)
  - Model Architecture
    - Online network
      - Encoder (feature extractor) + projector + predictor
    - Target network
      - Encoder (feature extractor) + projector



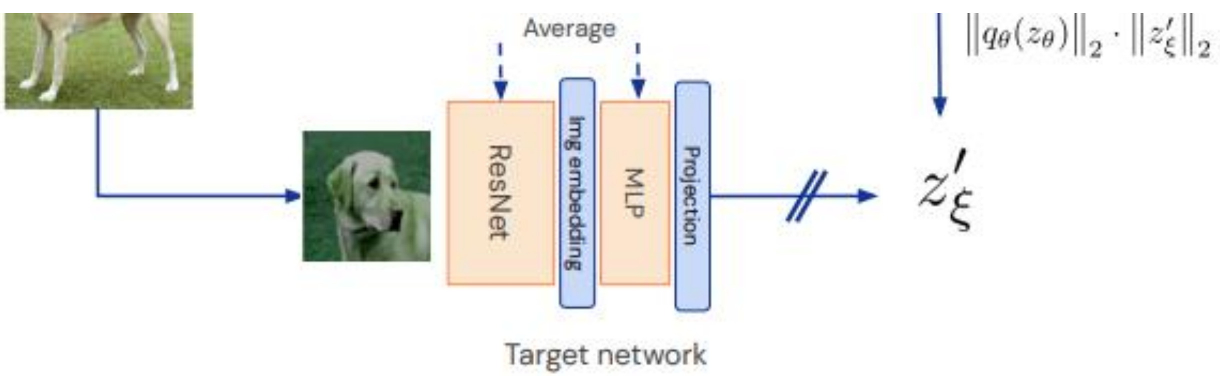
Self-Supervised Learning

- Bootstrap your own latent: A new approach to self-supervised Learning (NIPS 2020)
  - Model Architecture
    - Online network
      - Target network 가 제공한 target 을 prediction 하며 학습하는 network
      - Backpropagation 을 진행
      - Projector 와 predictor 는 모두 MLP 사용



Self-Supervised Learning

- Bootstrap your own latent: A new approach to self-supervised Learning (NIPS 2020)
  - Model Architecture
    - Target network
      - Encoder (feature extractor) + projector
      - Online network 가 학습할 target 제공
      - Stop-gradient
        - ✓ Backpropagation 하지 않음
        - ✓ Online network 의 weight 에 exponential moving average 를 적용하여 weight update
          - Stable 한 학습 가능 (stable 한 target 제공 가능)
          - Stop gradient 미적용시 collapsing 발생



Self-Supervised Learning

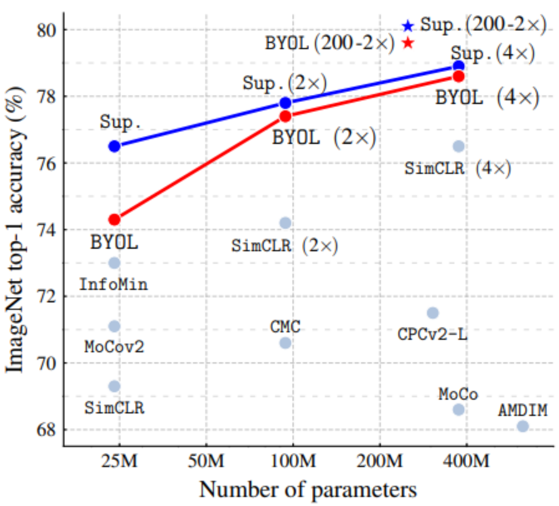
- Bootstrap your own latent: A new approach to self-supervised Learning (NIPS 2020)
  - Model Architecture
    - Symmetric Loss
      - Augmented image 를 online network 와 target network 에 바꿔 입력하여 loss 계산
      - Cosine similarity 사용

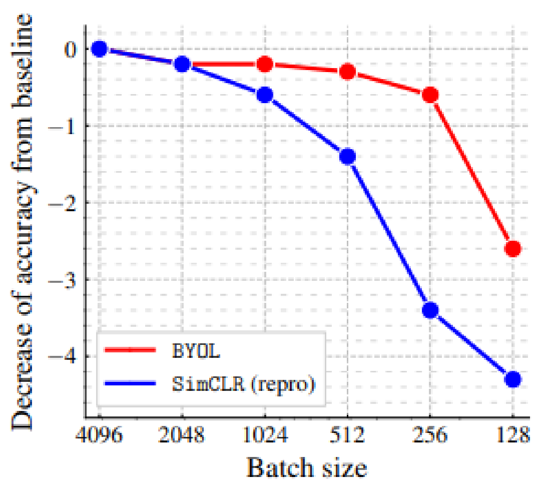
$$\mathcal{L}_{\theta,\xi} \triangleq \left\|\overline{q_\theta}(z_\theta) - \bar{z}'_\xi\right\|_2^2 = 2 - 2 \cdot \frac{\langle q_\theta(z_\theta), z'_\xi\rangle}{\left\|q_\theta(z_\theta)\right\|_2 \cdot \left\|z'_\xi\right\|_2}.$$

$$\mathcal{L}^{\texttt{BYOL}}_{\theta,\xi} = \mathcal{L}_{\theta,\xi} + \widetilde{\mathcal{L}}_{\theta,\xi}$$

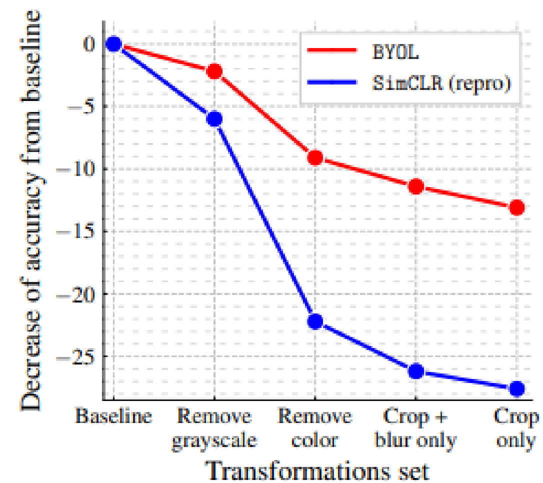
Self-Supervised Learning

- Bootstrap your own latent: A new approach to self-supervised Learning (NIPS 2020)
  - Experimental results
    - MoCo, SimCLR 을 넘어서는 성능을 보임
    - Batch size 가 256까지 감소하여도 성능 유지
    - 기존 contrastive learning 보다 augmentation 의 변화에 robust 함





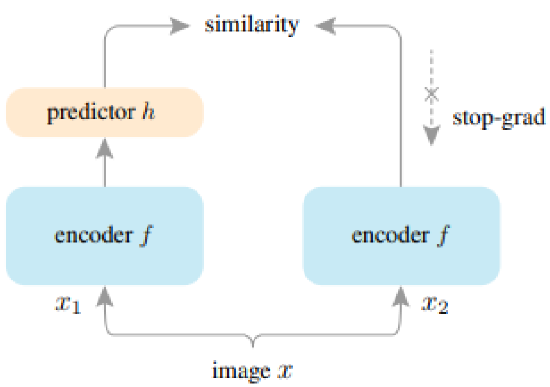
(a) Impact of batch size



(b) Impact of progressively removing transformations

Self-Supervised Learning

- Exploring Simple Siamese Representation Learning [8] (CVPR 2021)
  - Motivation
    - Unsupervised learning 에서 많이 사용되는 Siamese network 를 collapsing 이 발생하지 않게 사용할 수 있는 가장 simple 한 형태 제시
      - Negative sample pairs 를 사용하지 않음
      - large batch 를 사용하지 않음
      - Momentum encoders 를 사용하지 않음
    - Siamese network 에서 collapsing 이 일어나는 원인 실험적 분석
      - Stop-gradient 가 essential 한 role 을 가지고 있음.

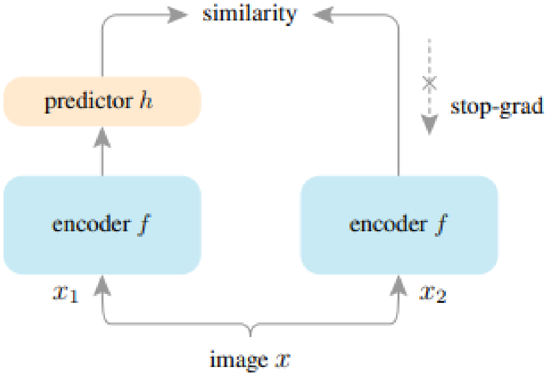


Self-Supervised Learning

- Exploring Simple Siamese Representation Learning (CVPR 2021)
  - Method
    - Siamese network 구조로 되어 있으나, 하나의 network 에만 predictor h 가 존재
    - Predictor 가 존재하지 않는 network 는 stop gradient 적용
    - Encoder 는 feature extractor + projector (MLP) 로 이루어져 있으며, 두 encoder 는 weight share
  - Loss function
    - Cosine similarity 사용
    - Symmetric 하게 cosine similarity 적용

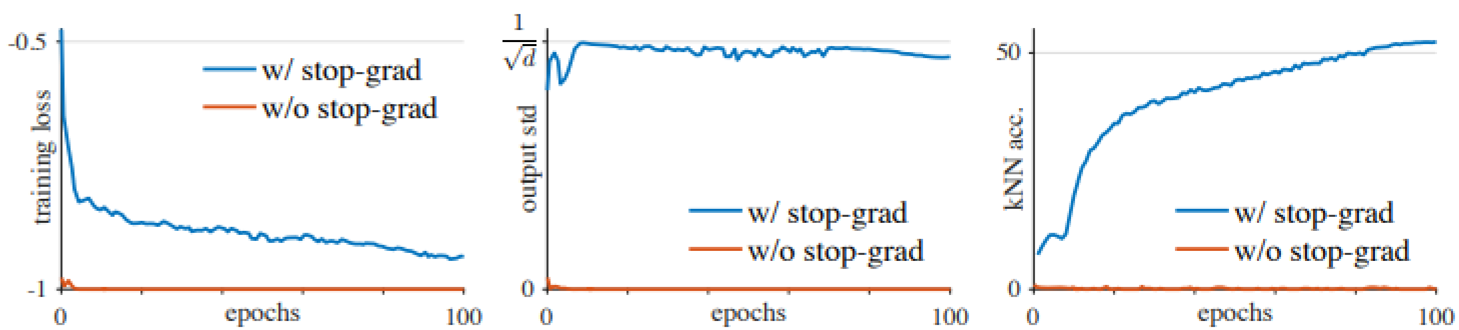
$$\mathcal{D}(p_1, z_2) = -\frac{p_1}{\|p_1\|_2} \cdot \frac{z_2}{\|z_2\|_2}$$

$$\mathcal{L} = \frac{1}{2}\mathcal{D}(p_1, \texttt{stopgrad}(z_2)) + \frac{1}{2}\mathcal{D}(p_2, \texttt{stopgrad}(z_1))$$



Self-Supervised Learning

- Exploring Simple Siamese Representation Learning (CVPR 2021)
  - Empirical Study
    - Stop Gradient
      - Stop gradient 제거 시 encoder 의 output 이 loss를 낮추기 위해 constant value 만을 출력하는 collapsing 발생
        - ✓ Loss 는 최솟값인 -1로 수렴
        - ✓ Standard deviation 이 0으로 수렴 (collapsing)
      - 모델 구조 등을 변경(MLP layer 수, batch norm 적용 여부) 하여도 stop gradient 가 적용되지 않았을 때에는 항상 collapsing 발생
        - ✓ 원인은 알 수 없으나, stop gradient 가 collapsing 해결에 essential 한 role 을 담당함



	acc. (%)
w/ stop-grad	67.7±0.1
w/o stop-grad	0.1

Self-Supervised Learning

- Exploring Simple Siamese Representation Learning (CVPR 2021)
  - Empirical Study
    - Predictor
      - Predictor 제거 시 collapsing 발생
        - ✓ Loss = $\frac{1}{2}\mathcal{D}(z_1, \texttt{stopgrad}(z_2)) + \frac{1}{2}\mathcal{D}(z_2, \texttt{stopgrad}(z_1))$
          - $\mathcal{D}(z_1, z_2)$ 와 동일한 gradient direction 및 ½ downscale
        - ✓ Stop gradient 를 제거한 것과 동일한 효과
    - Batch size
      - Batch size 는 성능에 영향을 미치나, collapsing 의 원인은 아님
      - SimSiam 에서는 작은 batch size 에서도 좋은 성능을 보임

	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).

batch size	64	128	256	512	1024	2048	4096
acc. (%)	66.1	67.3	68.1	68.1	68.0	67.9	64.0

Table 2. **Effect of batch sizes** (ImageNet linear evaluation accuracy with 100-epoch pre-training).

Self-Supervised Learning

- Exploring Simple Siamese Representation Learning (CVPR 2021)
  - Empirical Study
    - Batch Normalization
      - 성능에 영향을 미치지만, collapsing 의 원인은 아님
        - ✓ Projector 는 모든 MLP 에 batch norm 을 적용
        - ✓ Predictor 는 batch norm 을 적용하지 않음
          - 적용시 unstable 한 학습 결과를 보임
    - Similarity Function
      - Loss function 을 cosine similarity 대신 cross-entropy 를 적용하여도 어느 정도 성능을 보임
    - Symmetrization
      - asymmetric 으로 loss 를 적용하여도 어느 정도 성능을 보임

	case	proj. MLP's BN hidden	proj. MLP's BN output	pred. MLP's BN hidden	pred. MLP's BN output	acc. (%)
(a)	none	-	-	-	-	34.6
(b)	hidden-only	✓	-	✓	-	67.4
(c)	default	✓	✓	✓	-	68.1
(d)	all	✓	✓	✓	✓	unstable

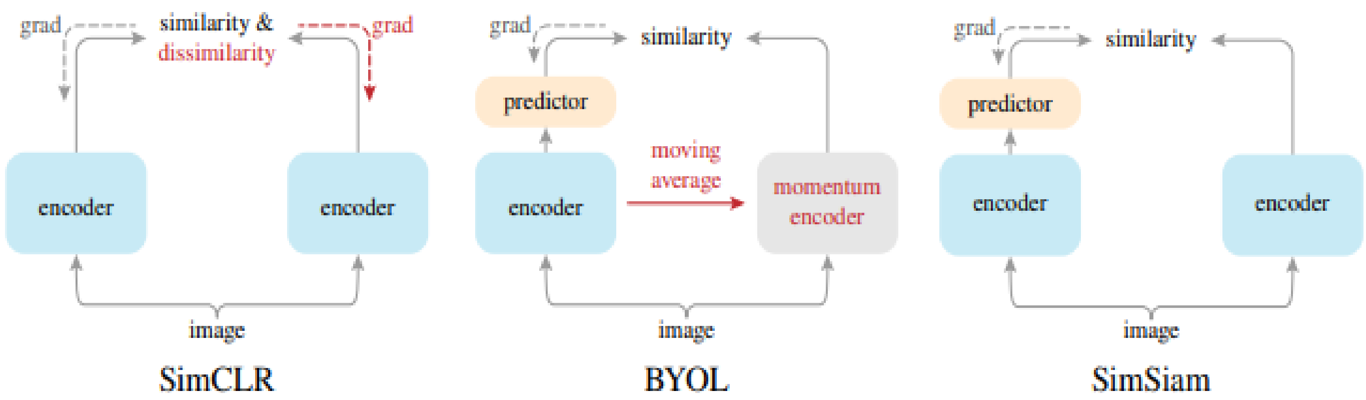
Table 3. **Effect of batch normalization on MLP heads** (ImageNet linear evaluation accuracy with 100-epoch pre-training).

	cosine	cross-entropy
acc. (%)	68.1	63.2

	sym.	asym.	asym. 2×
acc. (%)	68.1	64.8	67.3

Self-Supervised Learning

- Exploring Simple Siamese Representation Learning (CVPR 2021)
  - Methodology Comparisons
    - SimCLR
      - Negative pair 사용, large batch size
      - Stop gradient 미적용
      - Predictor 미적용
    - BYOL
      - Momentum encoder 사용



Self-Supervised Learning

- Exploring Simple Siamese Representation Learning (CVPR 2021)
  - Experimental results
    - 기존 contrastive learning 및 supervised learning 보다 높은 성능 달성

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

Table 4. **Comparisons on ImageNet linear classification**. All are based on **ResNet-50** pre-trained with **two 224×224 views**. Evaluation is on a single crop. All competitors are from our reproduction, and "+" denotes *improved* reproduction *vs*. original papers (see supplement).

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^{mask}_{50}	AP^{mask}	AP^{mask}_{75}
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**

Table 5. **Transfer Learning**. All unsupervised methods are based on 200-epoch pre-training in ImageNet. *VOC 07 detection*: Faster

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Thank you