

# An Introduction to Self-Supervised Learning

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# Supervised Learning

- Data: (x, y) x is input, y is output/response (label)
- Goal: Learn a function to map x -> y
- Examples:
  - Classification,
  - regression,
  - object detection,
  - semantic segmentation,
  - image captioning, etc.



# **Unsupervised** Learning

#### **Data**: ×

Just input data, no output labels!

• **Goal**: Learn some underlying hidden structure of the data

#### • Examples:

- Clustering,
- dimensionality reduction (manifold learning),
- Density (probability) estimation,
- Generative models:
  - Autoencoder
  - GANs, etc.

#### **Generative Models**

Given training data, generate new samples from same distribution





Training data ~  $p_{data}(x)$ 

Generated samples  $\sim p_{model}(x)$ 

Want to learn  $p_{model}(x)$  similar to  $p_{data}(x)$ 

# Today: Self-Supervised Learning

#### Data: x

- Just input data, no output labels!
- Data labeling is expensive and thus high-quality labeled dataset is limited.
- Both Self-Supervised Learning (SSL) and Generative model learn good data representation from unlabelled dataset.
- Generative learning aims to model data distribution p<sub>data</sub>(x), or generating data.
- Self-supervised learning methods solve "pretext" tasks that produce good features for downstream tasks:
  - Pretext task: (x<sub>-1</sub>, x<sub>i</sub>) or (x, T(x))
  - Learning good representation makes it easier to transfer useful information to a variety of downstream tasks.
    - e.g. A downstream task has only a few examples.
    - e.g. Zero-shot transfer to new tasks.

# Self-supervised pretext tasks

Example: learn to predict image transformations / complete corrupted images



- Solving the pretext tasks allow the model to learn good features.
- We can automatically generate labels for the pretext tasks.

# Evaluation of self-supervised learning



1. Learn good feature extractors from selfsupervised pretext tasks, e.g., predicting image rotations 2. Attach a shallow network on the feature extractor; train the shallow network on the target task with small amount of labeled data

#### **Methods of Self-Supervised Learning**

- Self-prediction
- Contrastive learning

## Self-Prediction

- Self-prediction: Given an individual data sample, the task is to predict one part of the sample given the other part.
- The part to be predicted pretends to be missing.



"Intra-sample" prediction: reconstruction

# **Contrastive Learning**

- Contrastive learning: Given multiple data samples, the task is to predict the relationship among them.
- The multiple samples can be selected from the dataset based on some known logics (e.g. the order of words / sentences), or fabricated by altering the original version.



"Inter-sample" prediction: similar or not?

# **Self-prediction**

#### Self-Prediction

Self-prediction construct prediction tasks within every individual data sample: to predict a part of the data from the rest while pretending we don't know that part.



# Self-Prediction: Autoregressive Generation

- The autoregressive model predicts future behavior based on past behavior. Any data that comes with an innate sequential order can be modeled with regression.
- Examples:
  - Audio (WaveNet, WaveRNN)
  - Autoregressive language modeling (GPT, XLNet)
  - Images in raster scan (PixelCNN, PixelRNN, iGPT)





## Self-Prediction: Masked Generation

- We mask a random portion of information and pretend it is missing, irrespective of the natural sequence. The model learns to predict the missing portion given other unmasked information.
- Examples:
  - Masked language modeling (BERT)
  - Images with masked patch (denoising autoencoder, context autoencoder, colorization)







## Example: Masked AutoEncoder (MAE)



Figure 1. **Our MAE architecture**. During pre-training, a large random subset of image patches (*e.g.*, 75%) is masked out. The encoder is applied to the small subset of *visible patches*. Mask tokens are introduced *after* the encoder, and the full set of encoded patches and mask tokens is processed by a small decoder that reconstructs the original image in pixels. After pre-training, the decoder is discarded and the encoder is applied to uncorrupted images (full sets of patches) for recognition tasks.

- A large random subset of image patches (75%) is masked out.
- Masked token is introduced after Encoder.



#### Example: Masked AutoEncoder (MAE)

[Source: He et al. 2021. arXiv:2111.06377. Masked Autoencoders Are Scalable Vision Learners]



Figure 5. **Masking ratio**. A high masking ratio (75%) works well for both fine-tuning (top) and linear probing (bottom). The y-axes are ImageNet-1K validation accuracy (%) in all plots in this paper.

 High masking ratio (75%) works well.



# Self-Prediction: Innate Relationship Prediction

- Some transformation (e.g. rotation, inpainting, jigsaw puzzle, coloring) of one data sample should maintain the original information or follow the desired innate logic.
- Examples:
  - Order of image patches (e.g., relative position, jigsaw puzzle)
  - Image rotation
  - Counting features across patches





## Pretext task: predict rotations

Hypothesis: a model could recognize the correct rotation of an object only if it has the "visual commonsense" of what the object should look like unperturbed.



 $90^{\circ}$  rotation

 $270^{\circ}$  rotation

 $180^{\circ}$  rotation

 $0^{\circ}$  rotation

 $270^{\circ}$  rotation

# **Rotation** prediction

- Self-supervised learning by rotating the entire input images.
- The model learns to predict which rotation is applied (4-way classification)



## Evaluation on semi-supervised learning



- Self-supervised learning on CIFAR10 (entire training set).
- Freeze conv1 + conv2 Learn conv3 + linear layers with subset of labeled CIFAR10 data (classification).

 <u>Gidaris</u>, et al. ICLR 2018, arXiv:1803.07728

# **Evaluation of transfer learning**

		Classif (%n	fication nAP)	Detection (%mAP)	Segmentation (%mIoU)	
	Trained layers	fc6-8	all	all	all	Pretrained with full
1	ImageNet labels	78.9	79.9	56.8	48.0	ImageNet supervision
	Random Random rescaled Krähenbühl et al. (2015)	39.2	53.3 56.6	43.4 45.6	19.8 32.6	<ul> <li>No pretraining</li> </ul>
	Egomotion (Agrawal et al., 2015) Context Encoders (Pathak et al., 2016b) Tracking (Wang & Gupta, 2015) Context (Doersch et al., 2015) Colorization (Zhang et al., 2016a) BIGAN (Donahue et al., 2016) Jigsaw Puzzles (Noroozi & Favaro, 2016) NAT (Bojanowski & Joulin, 2017)	31.0 34.6 55.6 55.1 61.5 52.3 - 56.7	54.2 56.5 63.1 65.3 65.6 60.1 67.6 65.3	43.9 44.5 47.4 51.1 46.9 46.9 53.2 49.4	29.7 35.6 34.9 37.6	Self-supervised learning on <b>ImageNet</b> (entire training set) with AlexNet.
	Split-Brain (Zhang et al., 2016b) ColorProxy (Larsson et al., 2017) Counting (Noroozi et al., 2017)	63.0	67.1 65.9 67.7	46.7 51.4	36.0 38.4 36.6	Finetune on labeled data from <b>Pascal VOC 2007</b> .
	(Ours) Kotinet	/0.8/	12.91	54.4	39.1	

Self-supervised learning with rotation prediction

source: Gidaris et al. 2018

## Visualize learned features



## Pretext task: predict relative patch locations



(Image source: Doersch et al., ICCV 2015)

### Pretext task: solving "jigsaw puzzles"



(Image source: Noroozi & Favaro, 2016)

# Pretext task: predict missing pixels (inpainting)



Context Encoders: Feature Learning by Inpainting (Pathak et al., 2016)

# Learning to inpaint by reconstruction

Learning to reconstruct the missing pixels



Image Source: Pathak et al., 2016

## Learning to inpaint by reconstruction

Loss = reconstruction + adversarial learning

Adversarial loss between "real" images and inpainted images

$$egin{aligned} L(x) &= L_{recon}(x) + L_{adv}(x) \ L_{recon}(x) &= ||M*(x-F_{ heta}((1-M)*x))||_2^2 \ L_{adv} &= \max_D \mathbb{E}[\log(D(x))] + \log(1-D(F(((1-M)*x)))] \end{aligned}$$





#### reconstruction

adversarial

recon + adv

## Transfer features to classification

 Self-supervised learning on ImageNet training set, transfer to classification (Pascal VOC 2007), detection (Pascal VOC 2007), and semantic segmentation (Pascal VOC 2012)

Pretraining Method	Supervision	Pretraining time	Classification	Detection	Segmentation
ImageNet [26]	1000 class labels	3 days	78.2%	56.8%	48.0%
Random Gaussian	initialization	< 1 minute	53.3%	43.4%	19.8%
Autoencoder	-	14 hours	53.8%	41.9%	25.2%
Agrawal et al. [1]	egomotion	10 hours	52.9%	41.8%	-
Wang <i>et al</i> . [39]	motion	1 week	58.7%	47.4%	-
Doersch <i>et al</i> . [7]	relative context	4 weeks	55.3%	46.6%	-
Ours	context	14 hours	56.5%	44.5%	30.0%

## Pretext task: image coloring



Source: Richard Zhang / Phillip Isola

#### Learning features from colorization: Split-brain Autoencoder

Cross-channel prediction



Source: Richard Zhang / Phillip Isola

#### Learning features from colorization: Split-brain Autoencoder

Example:



Source: Richard Zhang / Phillip Isola

## Pretext task: video coloring

- Idea: model the temporal coherence of colors in videos
- Hypothesis: learning to color video frames should allow model to learn to track regions or objects without labels!

#### reference frame

## how should I color these frames? Should be the same color!











t = 3

Vondrick et al., 2018

# Pretext task: video coloring

Idea: model the temporal coherence of colors in videos



Vondrick et al., 2018

# Summary

- Pretext tasks focus on "visual common sense", e.g., predict rotations, inpainting, rearrangement, and colorization.
- The models are forced learn good features about natural images, e.g., semantic representation of an object category, in order to solve the pretext tasks.
- We don't care about the performance of these pretext tasks, but rather how useful the learned features are for downstream tasks (classification, detection, segmentation).
- Problems:
  - 1) coming up with individual pretext tasks is tedious, and
  - 2) the learned representations may not be general.

## Pretext tasks from image transformations



- Learned representations may be tied to a specific pretext task!
- Can we come up with a more general pretext task?

# A more general pretext task?







# **Contrastive learning**

# **Contrastive Learning**

The goal of contrastive representation learning is to learn such an embedding space in which similar sample pairs stay close to each other while dissimilar ones are far apart.



# Early work on metric and contrastive learning

Metric learning (Xing et al. 2002)

$$d_A(x,y) = ||x - y||_A = \sqrt{(x - y)^T A(x - y)}$$

Contrastive Loss (Chopra & Hadsell et al. 2005)

- i. If  $Y_{ij} = 0$ , then update W to decrease  $D_W = \|G_W(\vec{X_i}) - G_W(\vec{X_j})\|_2$
- ii. If  $Y_{ij} = 1$ , then update W to increase  $D_W = \|G_W(\vec{X}_i) - G_W(\vec{X}_j)\|_2$

#### Triplet loss (Schroff et al. 2015)







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## **Contrastive Learning of Images**



## A Modern Formulation

For x: reference sample; x+ positive sample; x- negative sample

$$\operatorname{score}(f(x), f(x^+)) >> \operatorname{score}(f(x), f(x^-))$$

Given a chosen score function, we aim to learn an encoder function f that yields high score for positive pairs (x, x+) and low scores for negative pairs (x, x-).

# Contrastive loss function

Given 1 positive sample and N-1 negative samples, cross-entropy loss:

$$L = -\mathbb{E}_{X} \left[ \log \frac{\overline{\exp(s(f(x), f(x^{+}))}}{\exp(s(f(x), f(x^{+})) + \sum_{j=1}^{N-1} \exp(s(f(x), f(x_{j}^{-})))} \right]$$

$$score for the score for the N-1 negative pairs
$$\exp(s(f(x), f(x^{+})) + \sum_{j=1}^{\cdots} \exp(s(f(x), f(x_{j}^{-})))\right]$$

$$ightarrow x_{1}^{-}$$

$$x \quad x_{2}^{-}$$

$$ightarrow x_{3}^{-}$$

$$\vdots$$$$

## InfoNCE loss

Loss function given 1 positive sample and N - 1 negative samples:  $L = -\mathbb{E}_X \left[ \log \frac{\exp(s(f(x), f(x^+)))}{\exp(s(f(x), f(x^+)) + \sum_{j=1}^{N-1} \exp(s(f(x), f(x_j^-)))} \right]$ 

Commonly known as the InfoNCE loss (van den Oord et al., 2018) A *lower bound* on the mutual information between f(x) and  $f(x^+)$  $MI[f(x), f(x^+)] - \log(N) \ge -L$ 

The larger the negative sample size (N), the tighter the bound

Detailed derivation: Poole et al., 2019

Detailed derivation: Poole et al., 2019

# SimCLR: A Simple Framework for Contrastive Learning

osine similarity as the score nction:  $s_{i,j} = rac{z_i^T z_j}{||z_i||\,||z_j||}$ 

loss

(X)

encoder

affinity

encoder

enerate positive samples through  $\mathbf{z} \in \mathbb{R}^{2N}$  augmentation:

- random cropping, random color distortion, and random blur,2N

use encoder  ${\it f}$  and projection ead  ${\it g}$  (discarded after training) re trained with contrastive loss 2N



Figure 2. A simple framework for contrastive learning of visual representations. Two separate data augmentation operators are sampled from the same family of augmentations ( $t \sim T$  and  $t' \sim T$ ) and applied to each data example to obtain two correlated views. A base encoder network  $f(\cdot)$  and a projection head  $g(\cdot)$  are trained to maximize agreement using a contrastive loss. After training is completed, we throw away the projection head  $g(\cdot)$  and use encoder  $f(\cdot)$  and representation h for downstream tasks.

Source: Chen et al., ICML 2020

# Training linear classifier on SimCLR features



- Train feature encoder on ImageNet (entire training set) using SimCLR.
- Freeze feature encoder, train a linear classifier on top with labeled data.

Chen et al. ICML 2020

# Semi-supervised learning on SimCLR features

		Label fraction		
Method	Architecture	1%	10%	
		Top 5		
Supervised baseline	ResNet-50	48.4	80.4	
Methods using other labe	l-propagation:			
Pseudo-label	ResNet-50	51.6	82.4	
VAT+Entropy Min.	ResNet-50	47.0	83.4	
UDA (w. RandAug)	ResNet-50	-	88.5	
FixMatch (w. RandAug)	ResNet-50	-	89.1	
S4L (Rot+VAT+En. M.)	ResNet-50 (4 $\times$ )	-	91.2	
Methods using representa	representation learning only:			
InstDisc	ResNet-50	39.2	77.4	
BigBiGAN	RevNet-50 $(4 \times)$	55.2	78.8	
PIRL	ResNet-50	57.2	83.8	
CPC v2	ResNet-161(*)	77.9	91.2	
SimCLR (ours)	ResNet-50	75.5	87.8	
SimCLR (ours)	ResNet-50 (2 $\times$ )	83.0	91.2	
SimCLR (ours)	ResNet-50 ( $4\times$ )	85.8	92.6	

 Train feature encoder on ImageNet (entire training set) using SimCLR.

Finetune the encoder with 1% / 10% of labeled data on ImageNet.

Chen et al. ICML 2020

Table 7. ImageNet accuracy of models trained with few labels.

# SimCLR: projection head





- Linear / non-linear projection heads improve representation learning.
- A possible explanation:
  - contrastive learning objective may discard useful information for downstream tasks
  - representation space z is trained to be invariant to data transformation.
  - by leveraging the projection head g(·), more information can be preserved in the h representation space

#### Chen et al. ICML 2020

## SimCLR needs large batch size!



*Figure 9.* Linear evaluation models (ResNet-50) trained with different batch size and epochs. Each bar is a single run from scratch.<sup>10</sup>

- Large training batch size is crucial for SimCLR!
- Large batch size causes large memory footprint during backpropagation: requires distributed training on TPUs (ImageNet experiments)



# Momentum Contrastive Learning (MoCo)



#### Key differences to SimCLR:

- Keep a running queue of keys (negative samples).
- Compute gradients and update the encoder only through the queries.
- Decouple min-batch size with the number of keys: can support a large number of negative samples.
- The key encoder is slowly progressing through the momentum update rules:

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

#### He et al. CVPR 2020

# MoCo v2

- A hybrid of ideas from SimCLR and MoCo:
  - From SimCLR: non-linear projection head and strong data augmentation.
  - From MoCo: momentum-updated queues that allow training on a large number of negative samples (no TPU required!).

#### **Improved Baselines with Momentum Contrastive Learning**

Xinlei ChenHaoqi FanRoss GirshickKaiming HeFacebook AI Research (FAIR)



## MoCo v2 vs. SimCLR

		ImageNet					
case	MLP	aug+	cos	epochs	batch	acc.	
MoCo v1 [6]				200	256	60.6	
SimCLR [2]	$\checkmark$	$\checkmark$	$\checkmark$	200	256	61.9	
SimCLR [2]	$\checkmark$	$\checkmark$	$\checkmark$	200	8192	66.6	
MoCo v2	$\checkmark$	$\checkmark$	$\checkmark$	200	256	67.5	
results of longer unsupervised training follow:							
SimCLR [2]	$\checkmark$	$\checkmark$	$\checkmark$	1000	4096	69.3	
MoCo v2	$\checkmark$	$\checkmark$	$\checkmark$	800	256	71.1	

Table 2. MoCo vs. SimCLR: ImageNet linear classifier accuracy (**ResNet-50, 1-crop 224** $\times$ **224**), trained on features from unsupervised pre-training. "aug+" in SimCLR includes blur and stronger color distortion. SimCLR ablations are from Fig. 9 in [2] (we thank the authors for providing the numerical results).

mechanism	batch	memory / GPU	time / 200-ep.
MoCo	256	5.0G	53 hrs
end-to-end	256	7.4G	65 hrs
end-to-end	4096	93.0G <sup>†</sup>	n/a

Table 3. **Memory and time cost** in 8 V100 16G GPUs, implemented in PyTorch. <sup>†</sup>: based on our estimation.

- Non-linear projection head and strong data augmentation are crucial for contrastive learning.
- Decoupling mini-batch size with negative sample size allows MoCo-V2 to outperform SimCLR with smaller batch size (256 vs. 8192).
- ... all with much smaller memory footprint! ("end-to-end" means SimCLR here)

Chen et al. 2020

#### MoCo v3: the State of the Art

#### An Empirical Study of Training Self-Supervised Vision Transformers

Xinlei Chen\* Saining Xie\* Kaiming He Facebook AI Research (FAIR)

Code: https://github.com/facebookresearch/moco-v3

#### Abstract

This paper does not describe a novel method. Instead, it studies a straightforward, incremental, yet must-know baseline given the recent progress in computer vision: selfsupervised learning for Vision Transformers (ViT). While the training recipes for standard convolutional networks have been highly mature and robust, the recipes for ViT are yet to be built, especially in the self-supervised scenarios where training becomes more challenging. In this work, we go back to basics and investigate the effects of several fundamental components for training self-supervised ViT. We observe that instability is a major issue that degrades accuracy, and it can be hidden by apparently good results. We reveal that these results are indeed partial failure, and they can be improved when training is made more stable. We benchmark ViT results in MoCo v3 and several other selfsupervised frameworks, with ablations in various aspects. We discuss the currently positive evidence as well as challenges and open questions. We hope that this work will provide useful data points and experience for future research.

framework	model	params	acc. (%)
linear probing:			
iGPT [9]	iGPT-L	1362M	69.0
iGPT [9]	iGPT-XL	6801M	72.0
MoCo v3	ViT-B	86M	76.7
MoCo v3	ViT-L	304M	77.6
MoCo v3	ViT-H	632M	78.1
MoCo v3	ViT-BN-H	632M	79.1
MoCo v3	ViT-BN-L/7	304M	81.0
end-to-end fine-tuning:			
masked patch pred. [16]	ViT-B	86M	79.9 <sup>†</sup>
MoCo v3	ViT-B	86M	83.2
Μοζο ν3	ViT-L	304M	84.1

Table 1. State-of-the-art Self-supervised Transformers in ImageNet classification, evaluated by linear probing (top panel) or end-to-end fine-tuning (bottom panel). Both iGPT [9] and masked patch prediction [16] belong to the masked auto-encoding paradigm. MoCo v3 is a contrastive learning method that compares two ( $224 \times 224$ ) crops. ViT-B, -L, -H are the Vision Transformers proposed in [16]. ViT-BN is modified with BatchNorm, and "/7" denotes a patch size of  $7 \times 7$ . <sup>†</sup>: pre-trained in JFT-300M.

#### Chen et al. ICCV 2021

#### From Instance to Sequence ...





#### Instance-level contrastive learning:

contrastive learning based on positive & negative instances. Examples: SimCLR, MoCo

#### Sequence-level contrastive learning:

contrastive learning based on sequential / temporal orders. Example: Contrastive Predictive Coding (CPC)

# Contrastive Predictive Coding (CPC)



- Contrastive: contrast between "right" and "wrong" sequences using contrastive learning.
- Predictive: the model has to predict future patterns given the current context.
- Coding: the model learns useful feature vectors, or "code", for downstream tasks, similar to other self-supervised methods.
- Can be applied to a variety of learning problems, but not as effective in learning image representations compared to instance-level methods.
- Source: van den Oord et al. 2018 arXiv:1807.03748

## Contrastive Language–Image Pre-training (CLIP)



Contrastive learning between image and natural language sentences, enables zeroshot learning.

Radford et al., 2021

# A Short History of Contrastive Representation Learning

- Common loss functions:
  - Contrastive loss (Chopra et al. 2005)
  - Triplet loss (Schroff et al. 2015; FaceNet)
  - Lifted structured loss (Song et al. 2015)
  - Multi-class n-pair loss (Sohn 2016)
  - Noise contrastive estimation ("NCE"; Gutmann & Hyvarinen 2010)
  - InfoNCE (van den Oord, et al. 2018)
  - Soft-nearest neighbors loss (Salakhutdinov & Hinton 2007, Frosst et al. 2019)

# Summary: SimCLR

- SimCLR: a simple framework for contrastive representation learning
- Key ideas: non-linear projection head to allow flexible representation learning
- Simple to implement, effective in learning visual representation
- Requires large training batch size to be effective; large memory footprint



Source: Chen et al., 2020

## Summary: MoCo

- MoCo (v1, v2): contrastive learning using momentum sample encoder
- Decouples negative sample size from minibatch size; allows large batch training without TPU
- MoCo-v2 combines the key ideas from SimCLR, i.e., nonlinear projection head, strong data augmentation, with momentum contrastive learning



Figure 1. A **batching** perspective of two optimization mechanisms for contrastive learning. Images are encoded into a representation space, in which pairwise affinities are computed.

He et al., 2020; Chen et al., 2020

# Thank you!

