

# Lecture 14: Self-Supervised Learning

# Administrative

- Assignment 4 due in Feb 22th

# Recall: Supervised

**Data:**  $(x, y)$

$x$  is the input data,  $y$  is the output label.

**Goal:** Learn a function  $f: x \rightarrow y$

**Example:** in image classification,  $x$  is the image and  $y$  is the object category

# Problem: Supervised Learning is Expensive!

Assume that we want to label re-label ImageNet's 1.4 Million images.

How much will it cost?

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How much will it cost?

(1,400,000 images)  
× (10 seconds/image)  
× (1/3600 hours/second)  
× (\$15 / hour)

(Small to medium sized dataset)  
(Fast annotation)  
(Low wage paid to annotator)

# Problem: Supervised Learning is Expensive!

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$$\begin{array}{ll} (1,400,000 \text{ images}) & (\text{Small to medium sized dataset}) \\ \times (10 \text{ seconds/image}) & (\text{Fast annotation}) \\ \times (1/3600 \text{ hours/second}) & \\ \times (\$15 / \text{hour}) & (\text{Low wage paid to annotator}) \\ \hline = \$58,333 & \end{array}$$

Assumptions:

- one annotator per image,
- no benefits / payroll tax / crowdsourcing fee for annotators;
- not accounting for front end developer time to set up tasks for annotators.
- Real costs could easily be 3x this or more: **>\\$175,000**

# Problem: Supervised Learning is Expensive!

Assume that we want to label CLIP's **1B** images. (GPT also needs billions of documents)

How much will it cost?

(1,000,000,000 images)

(Small to medium sized dataset)

× (10 seconds/image)

(Fast annotation)

× (1/3600 hours/second)

(Low wage paid to annotator)

× (\$15 / hour)

= **\$41,666,667**

**41 Million dollars (again, not including all other costs)**

# Supervised Learning is Not How We Learn

Babies don't get supervision  
for everything they see!



[Baby image](#) is CCO public domain

# Solution: self-supervised learning

Lets build methods that learn from “raw” data – no annotations required

**Unsupervised Learning:** Model isn’t told what to predict. Older terminology, not used as much today.

**Self-Supervised Learning:** Model is trained to predict some naturally occurring signal in the raw data rather than human annotations.

# Solution: self-supervised learning

Lets build methods that learn from "raw" data – no annotations required

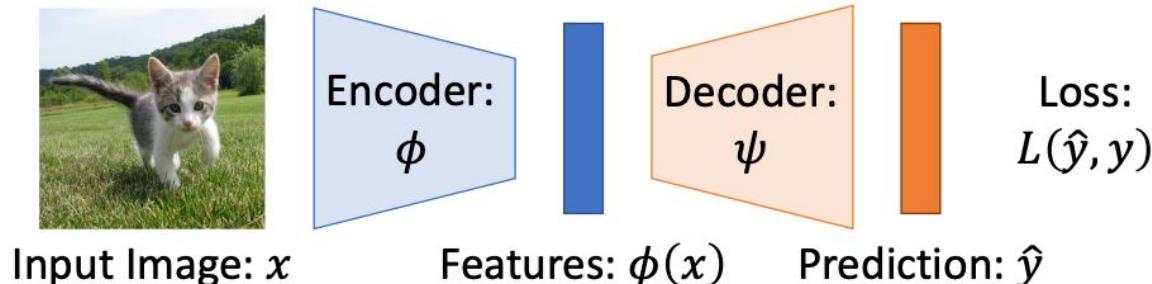
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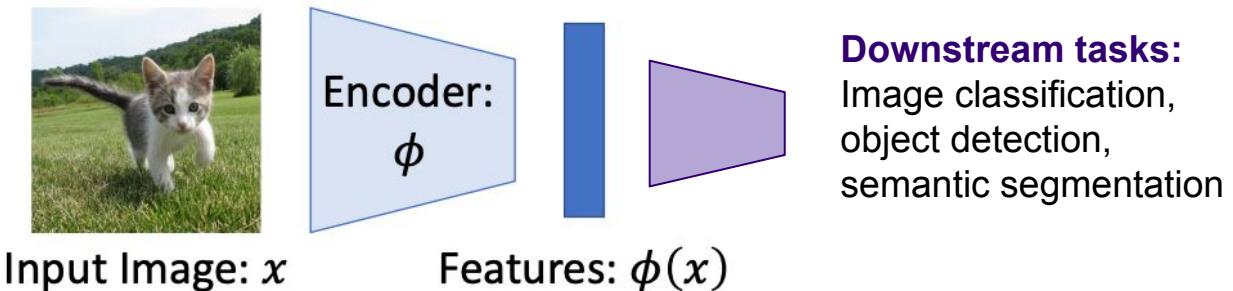
**Semi-Supervised Learning:** Train jointly with some labeled data and (a lot) of unlabeled data.

# Self-Supervised Learning: Pretext then Transfer

**Step 1:** Pretrain a network on a pretext task that doesn't require supervision

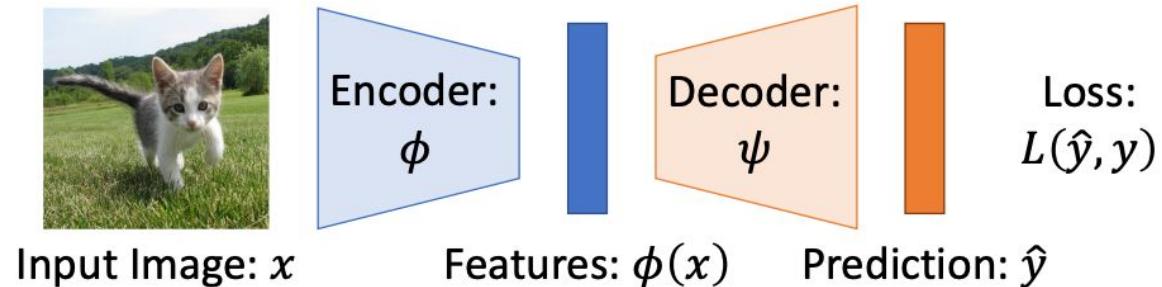


**Step 2:** Transfer encoder to downstream tasks via linear classifiers, KNN, finetuning

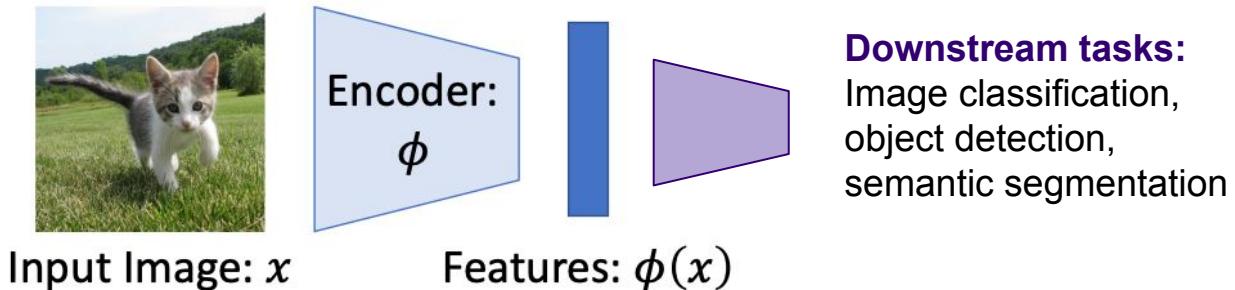


# Goal of Self-Supervised Learning: Define pre-text tasks that do better than supervised learning

**Step 1:** Pretrain a network on a pretext task that doesn't require supervision



**Step 2:** Transfer encoder to downstream tasks via linear classifiers, KNN, finetuning



# Self-Supervised Learning: Pretext Tasks

**Generative:** Predict part of the input signal

- Autoencoders (sparse, denoising, masked)
- Autoregressive
- GANs
- Colorization
- Inpainting

**Discriminative:** Predict something about the input signal

- Context prediction
- Rotation
- Clustering
- Contrastive

**Multimodal:** Use some additional signal in addition to RGB images

- Video
- 3D
- Sound
- Language

# Self-Supervised Learning: Pretext Tasks

## Today

**Generative:** Predict part of the input signal

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# Self-supervised pretext tasks

Example: learn to predict image transformations / complete corrupted images

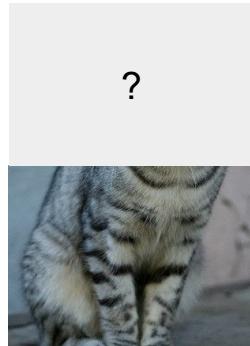
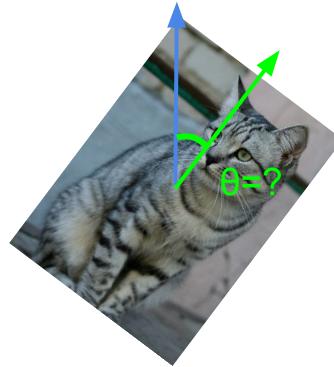


image completion



rotation prediction



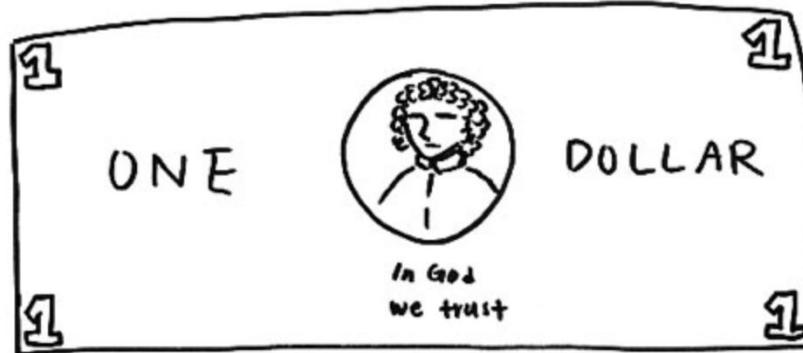
"jigsaw puzzle"



colorization

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

# Generative Self-supervised Learning



Left: Drawing of a dollar bill from memory. Right: Drawing subsequently made with a dollar bill present. Image source: [Epstein, 2016](#)

Learning to generate pixel-level details is often unnecessary; learn high-level semantic features with pretext tasks instead

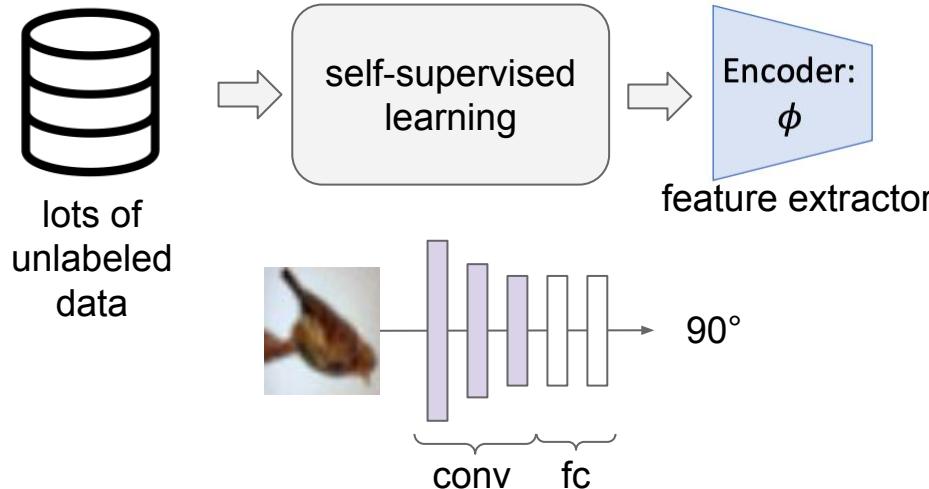
Source: [Anand, 2020](#)

# How to evaluate a self-supervised learning method?

We usually don't care about the performance of the self-supervised learning task, e.g., we don't care if the model learns to predict image rotation perfectly.

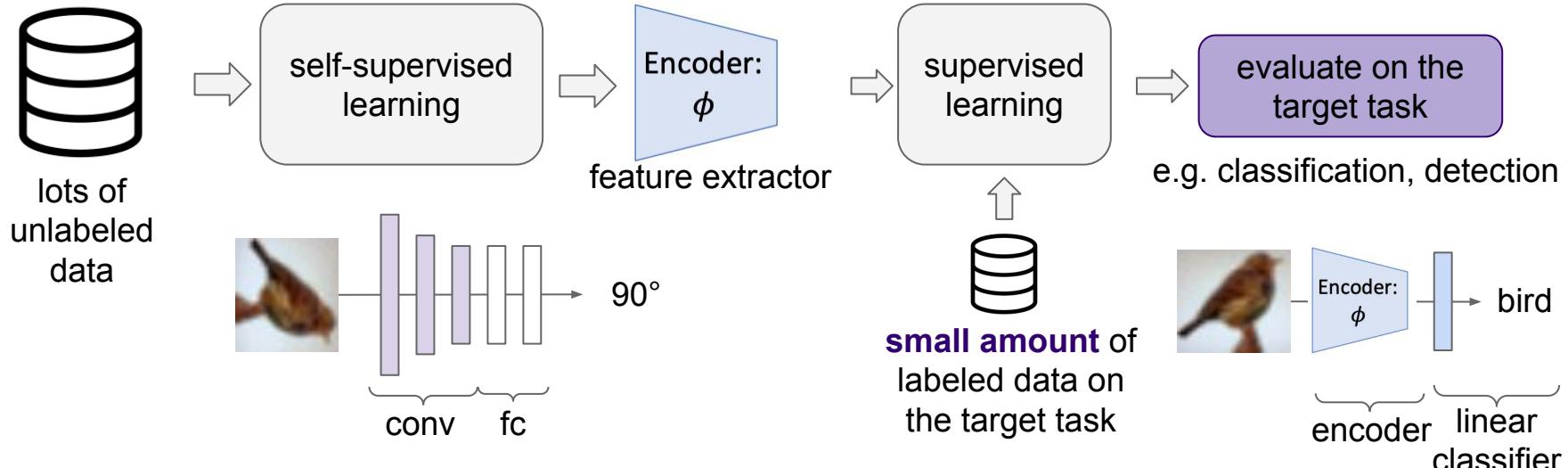
Evaluate the learned feature encoders on downstream *target tasks*

# How to evaluate a self-supervised learning method?



**Step 1:** Pretrain a network on a pretext task that doesn't require supervision

# How to evaluate a self-supervised learning method?

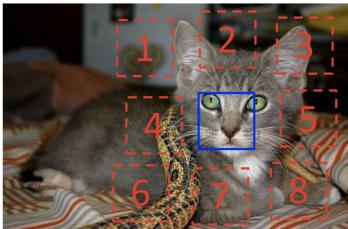


**Step 1:** Pretrain a network on a pretext task that doesn't require supervision

**Step 2:** Transfer encoder to downstream tasks via linear classifiers, KNN, finetuning

# Broader picture

## computer vision



Doersch et al., 2015

## robot / reinforcement learning



Dense Object Net (Florence and Manuelli et al., 2018)

## language modeling

### Language Models are Few-Shot Learners

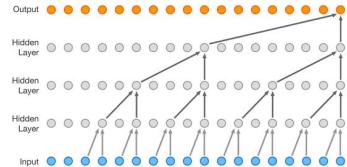
Tom B. Brown\* Benjamin Mann\* Nick Ryder\* Melanie Subbiah\*  
Jared Kaplan† Prafulla Dhariwal Arvind Neelakantan Pranav Shyam Girish Sastry  
Amanda Askell Sandhini Agarwal Ariel Herbert-Voss Gretchen Krueger Tom Henighan  
Rewon Child Aditya Ramesh Daniel M. Ziegler Jeffrey Wu Clemens Winter  
Christopher Hesse Mark Chen Eric Sigler Mateusz Litwin Scott Gray  
Benjamin Chess Jack Clark Christopher Berner  
Sam McCandlish Alec Radford Ilya Sutskever Dario Amodei  
OpenAI

#### Abstract

Recent work has demonstrated substantial gains on many NLP tasks and benchmarks by pre-training on a large corpus of text followed by fine-tuning on a specific task. While typically task-agnostic in architecture, this method still requires task-specific fine-tuning datasets of thousands or tens of thousands of examples. By contrast, humans can generally perform a new language task from only a few examples – scaling up a system which can learn “syntax” to “semantics” is currently thought to be difficult to do. Here we show that scaling up a language model greatly improves task-agnostic few-shot performance, sometimes even reaching competitiveness with prior state-of-the-art fine-tuning approaches. Specifically, we train GPT-3, an autoregressive language model with 175 billion parameters, 10x larger than any previous non-sparse language model, and test its performance in the few-shot setting. For all tasks, GPT-3 is trained without gradient descent or fine-tuning, with tasks and few-shot demonstrations specified purely via text interaction with the model. GPT-3 achieves strong performance on many NLP datasets, including translation, question-answering, and close tasks, as well as several tasks that require on-the-fly reasoning or domain adaptation, such as understanding words, using a novel word in a sentence, or performing 3-digit arithmetic. At the same time, we also identify datasets where GPT-3 faces challenges in learning simple analogies, as well as some datasets where GPT-3 faces methodological issues related to training on large web corpora. Finally, we find that GPT-3 can generate samples of news articles which human evaluators have difficulty distinguishing from articles written by humans. We discuss broader societal impacts of this finding and of GPT-3 in general.

GPT3 (Brown, Mann, Ryder, Subbiah et al., 2020)

## speech synthesis



Wavenet (van den Oord et al., 2016)

# Today's Agenda

## **Pretext tasks from image transformations**

- Rotation, inpainting, rearrangement, coloring

## **Contrastive representation learning**

- Intuition and formulation
- Instance contrastive learning: SimCLR and MOCO

# Today's Agenda

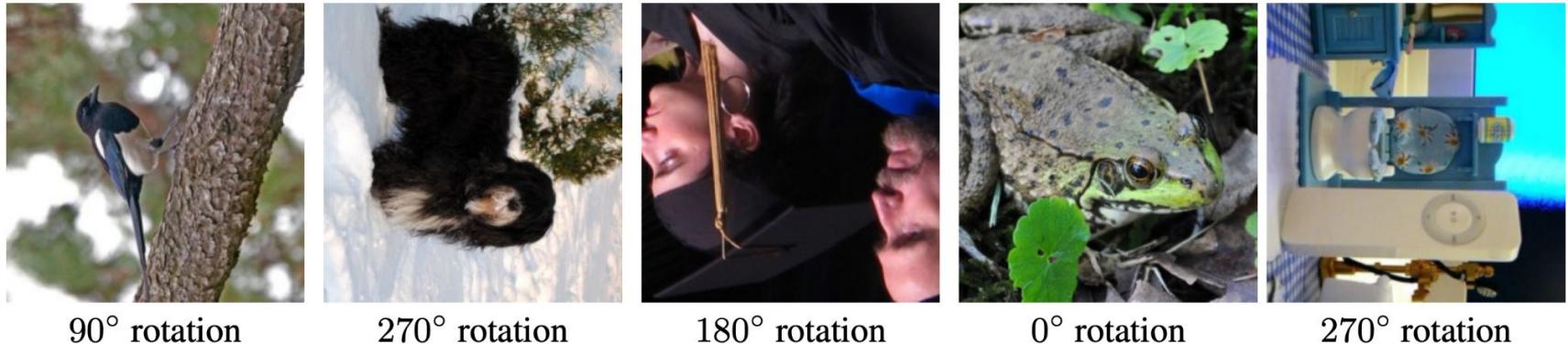
## **Pretext tasks from image transformations**

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## **Contrastive representation learning**

- Intuition and formulation
- Instance contrastive learning: SimCLR and MOCO

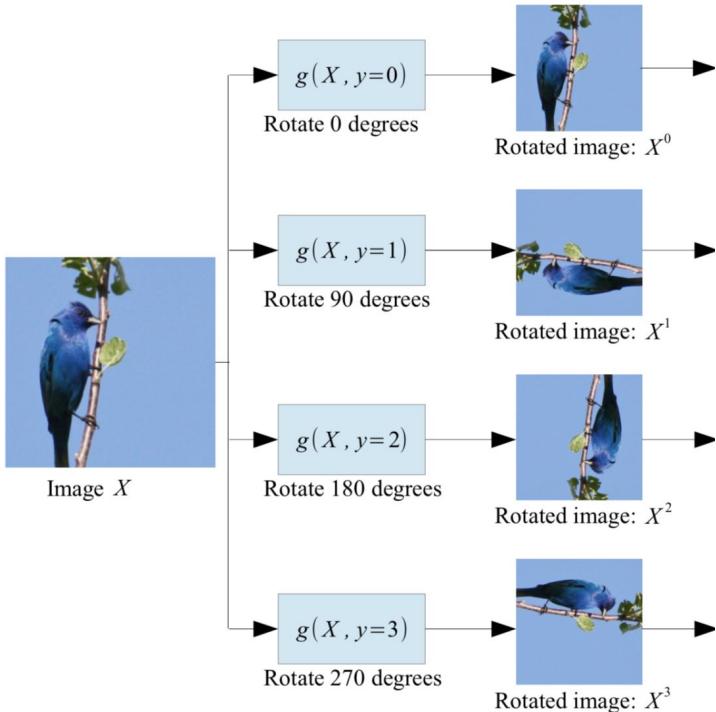
# Pretext task: predict rotations



**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.

(Image source: [Gidaris et al. 2018](#))

# Pretext task: predict rotations

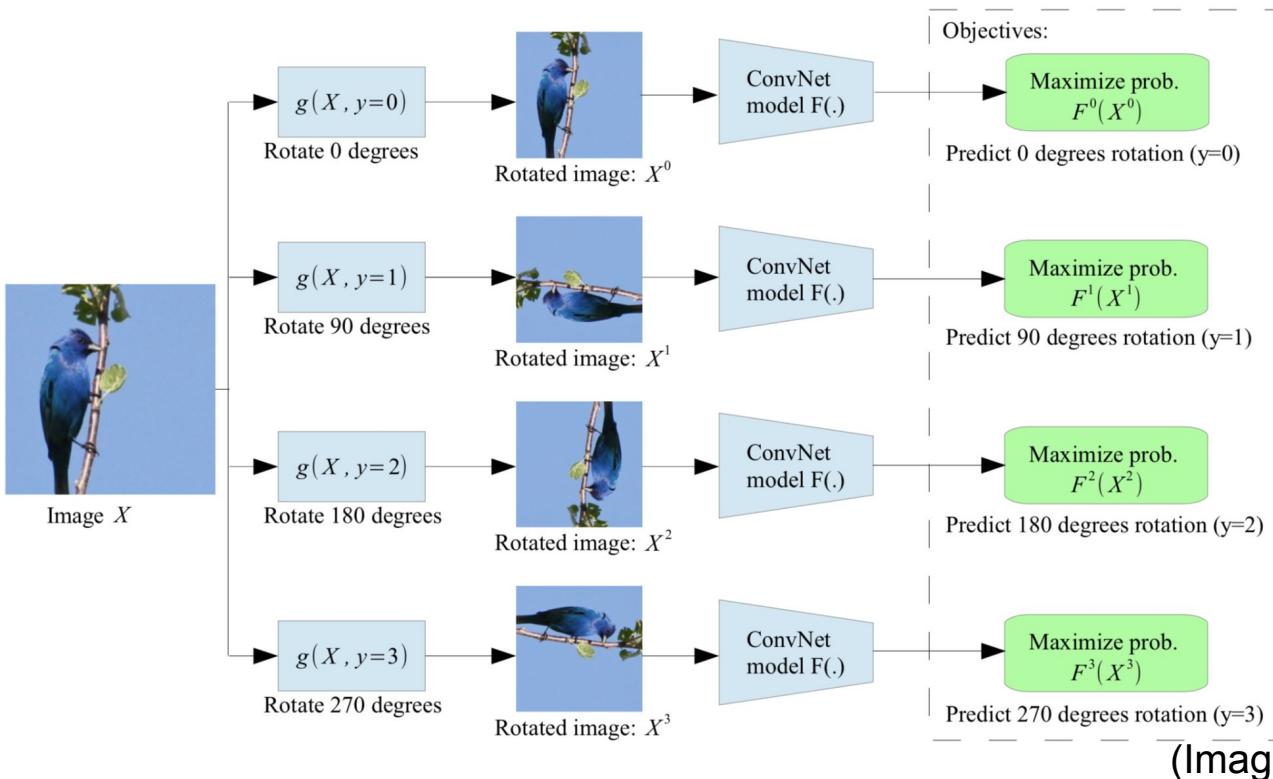


Self-supervised learning by rotating the entire input images.

The model learns to predict which rotation is applied (4-way classification)

(Image source: [Gidaris et al. 2018](#))

# Pretext task: predict rotations

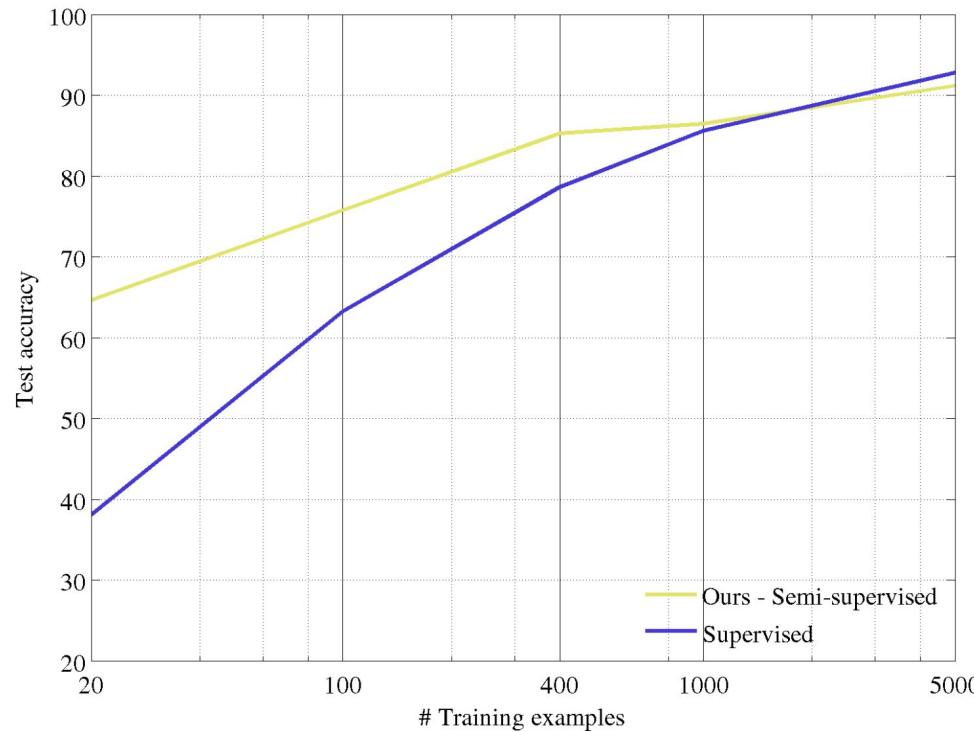


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The model learns to predict which rotation is applied (4-way classification)

(Image source: [Gidaris et al. 2018](#))

# 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).

(Image source: [Gidaris et al. 2018](#))

# Transfer learned features to supervised learning

	Classification (%mAP)	Detection (%mAP)	Segmentation (%mIoU)
Trained layers	fc6-8	all	all
ImageNet labels	78.9	79.9	56.8
Random		53.3	43.4
Random rescaled Krähenbühl et al. (2015)	39.2	56.6	45.6
Egomotion (Agrawal et al., 2015)	31.0	54.2	43.9
Context Encoders (Pathak et al., 2016b)	34.6	56.5	44.5
Tracking (Wang & Gupta, 2015)	55.6	63.1	47.4
Context (Doersch et al., 2015)	55.1	65.3	51.1
Colorization (Zhang et al., 2016a)	61.5	65.6	46.9
BIGAN (Donahue et al., 2016)	52.3	60.1	46.9
Jigsaw Puzzles (Noroozi & Favaro, 2016)	-	67.6	53.2
NAT (Bojanowski & Joulin, 2017)	56.7	65.3	49.4
Split-Brain (Zhang et al., 2016b)	63.0	67.1	46.7
ColorProxy (Larsson et al., 2017)		65.9	
Counting (Noroozi et al., 2017)	-	67.7	51.4
(Ours) RotNet	<b>70.87</b>	<b>72.97</b>	<b>54.4</b>
			<b>39.1</b>

Self-supervised learning with rotation prediction

Pretrained with full  
ImageNet supervision

No pretraining

Self-supervised learning on  
**ImageNet** (entire training  
set) with AlexNet.

Finetune on labeled data  
from **Pascal VOC 2007**.

source: [Gidaris et al. 2018](#)

# Visualize learned visual attentions



Conv1  $27 \times 27$    Conv3  $13 \times 13$    Conv5  $6 \times 6$

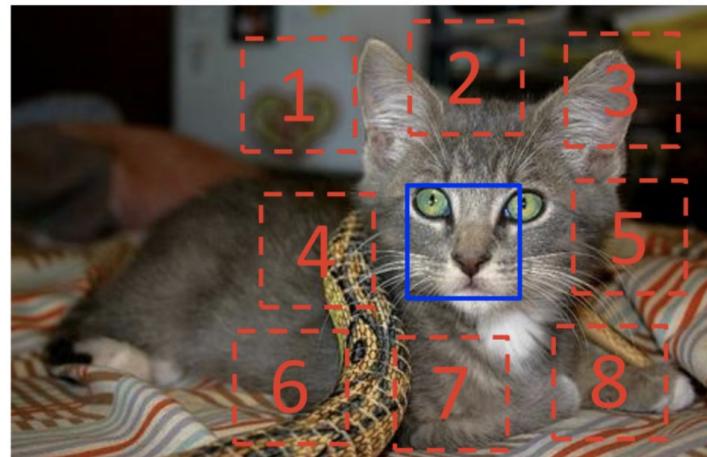
Conv1  $27 \times 27$    Conv3  $13 \times 13$    Conv5  $6 \times 6$

(a) Attention maps of supervised model

(b) Attention maps of our self-supervised model

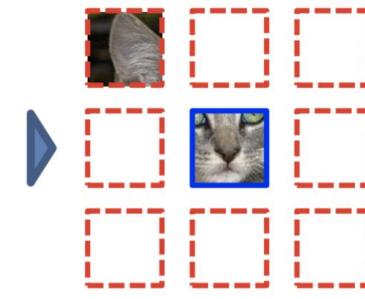
(Image source: [Gidaris et al. 2018](#))

# Pretext task: predict relative patch locations



$$X = (\text{[cat eye]}, \text{[cat ear]}); Y = 3$$

Example:



Question 1:

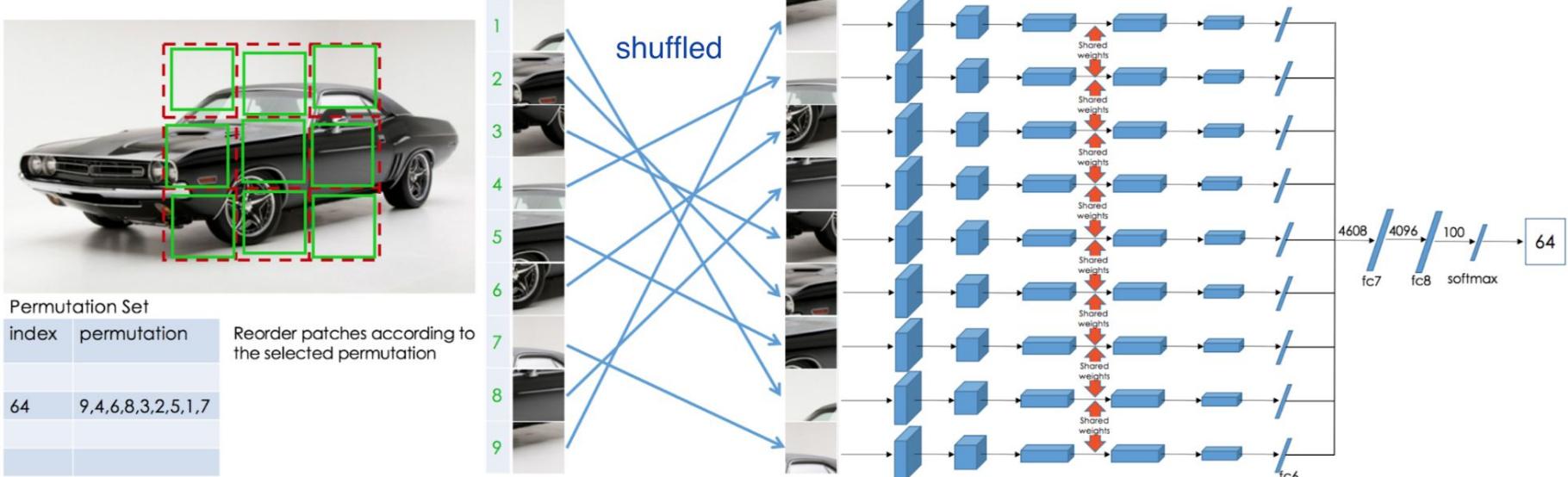


Question 2:



(Image source: [Doersch et al., 2015](#))

# Pretext task: solving “jigsaw puzzles”



(Image source: [Noroozi & Favaro, 2016](#))

# Transfer learned features to supervised learning

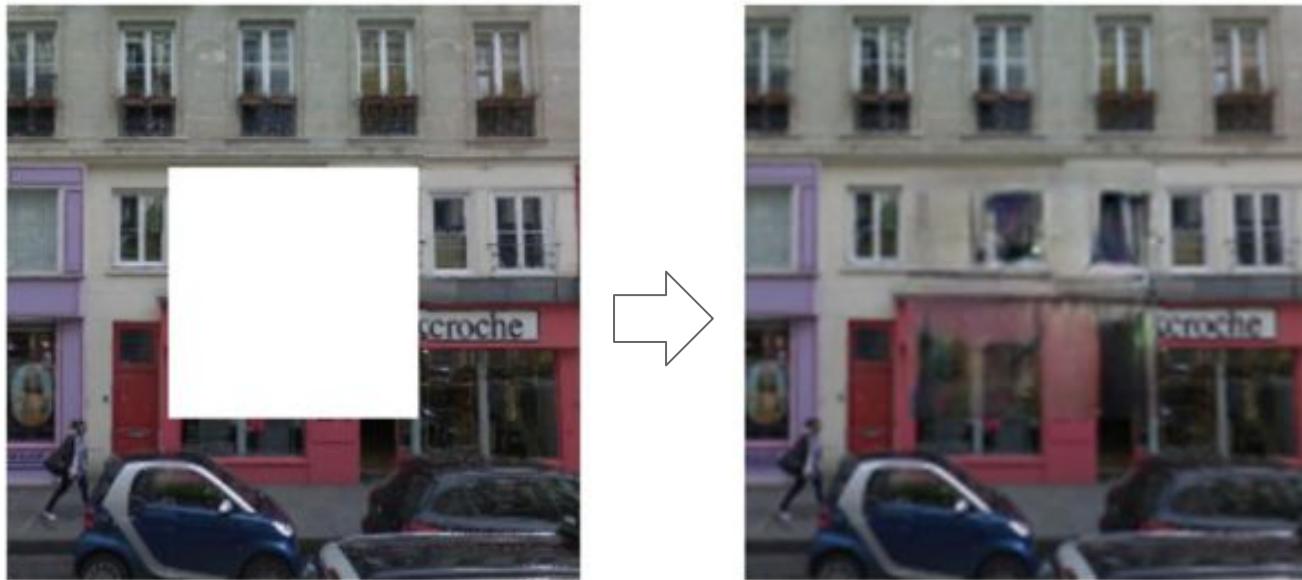
Table 1: Results on PASCAL VOC 2007 Detection and Classification. The results of the other methods are taken from Pathak *et al.* [30].

Method	Pretraining time	Supervision	Classification	Detection	Segmentation
Krizhevsky <i>et al.</i> [25]	3 days	1000 class labels	<b>78.2%</b>	<b>56.8%</b>	<b>48.0%</b>
Wang and Gupta[39]	1 week	motion	58.4%	44.0%	-
Doersch <i>et al.</i> [10]	4 weeks	context	55.3%	46.6%	-
Pathak <i>et al.</i> [30]	14 hours	context	56.5%	44.5%	29.7%
Ours	2.5 days	context	<b>67.6%</b>	<b>53.2%</b>	<b>37.6%</b>

“Ours” is feature learned from solving image Jigsaw puzzles (Noroozi & Favaro, 2016). Doersch et al. is the method with relative patch location

(source: [Noroozi & Favaro, 2016](#))

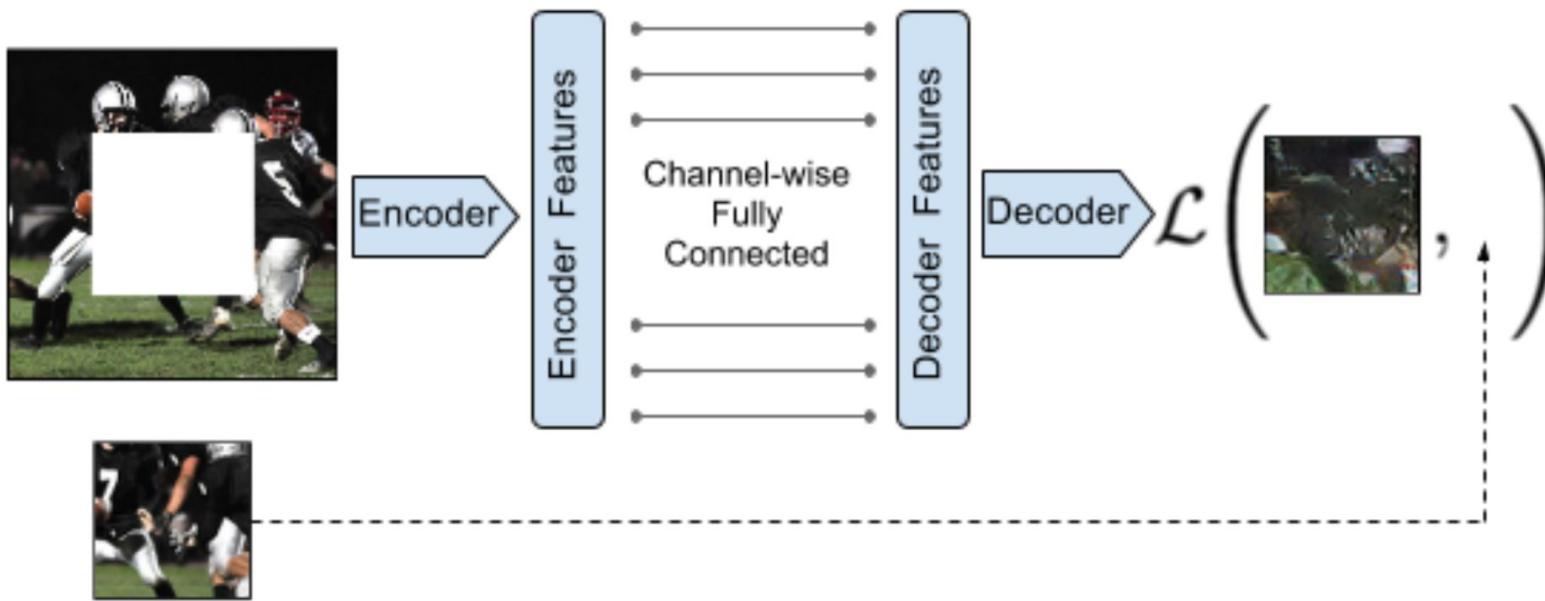
# Pretext task: predict missing pixels (inpainting)



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

Source: [Pathak et al., 2016](#)

# Learning to inpaint by reconstruction



Learning to reconstruct the missing pixels

Source: [Pathak et al., 2016](#)

# Inpainting evaluation



Input (context)



reconstruction

Source: [Pathak et al., 2016](#)

# Learning to inpaint by reconstruction

Loss = reconstruction + adversarial learning

$$L(x) = L_{recon}(x) + L_{adv}(x)$$

$$L_{recon}(x) = \left\| M * (x - F_\theta((1 - M) * x)) \right\|_2^2$$

$$L_{adv} = \max_D \mathbb{E}[\log(D(x))] + \log(1 - D(F((1 - M) * x)))]$$

Adversarial loss between “real” images and *inpainted images*

Source: [Pathak et al., 2016](#)

# Inpainting evaluation



Input (context)

reconstruction

adversarial

recon + adv

Source: [Pathak et al., 2016](#)

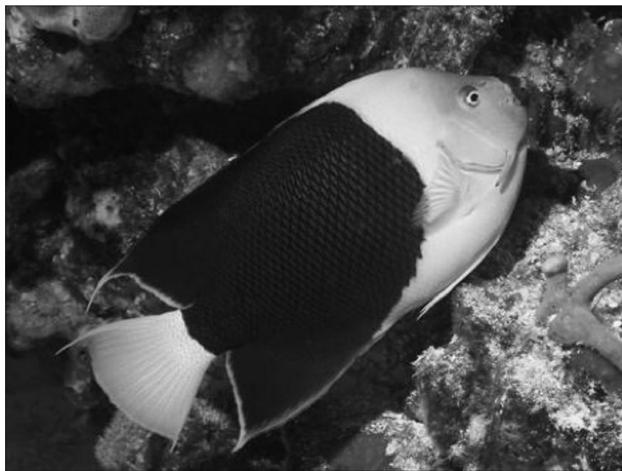
# Transfer learned features to supervised learning

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 <i>et al.</i> [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%

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

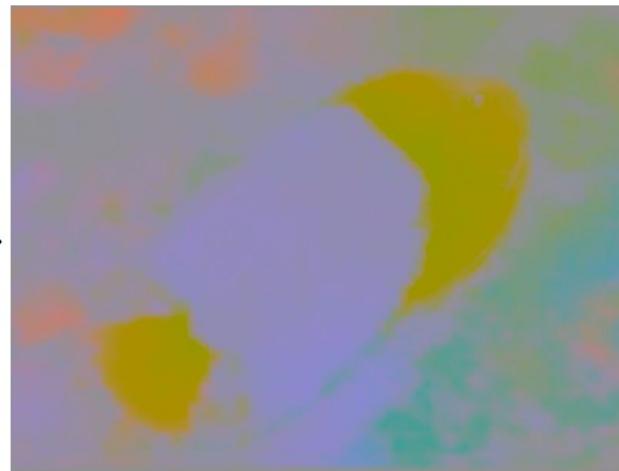
Source: [Pathak et al., 2016](#)

# Pretext task: image coloring



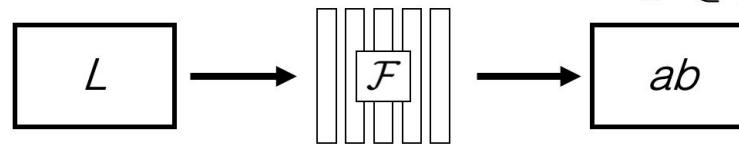
Grayscale image:  $L$  channel

$$\mathbf{X} \in \mathbb{R}^{H \times W \times 1}$$



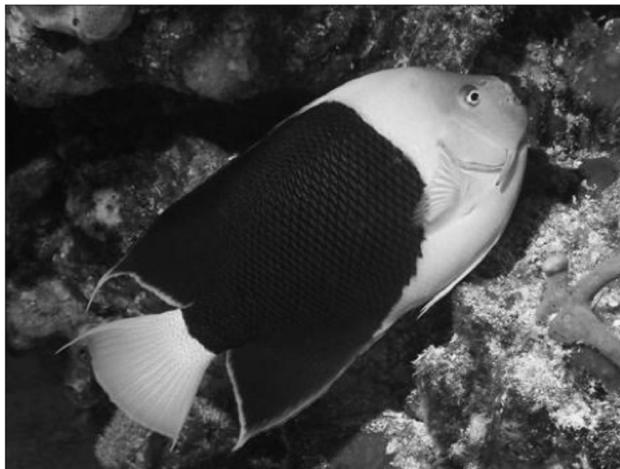
Color information:  $ab$  channels

$$\hat{\mathbf{Y}} \in \mathbb{R}^{H \times W \times 2}$$



Source: Richard Zhang / Phillip Isola <sup>5</sup>

# Pretext task: image coloring



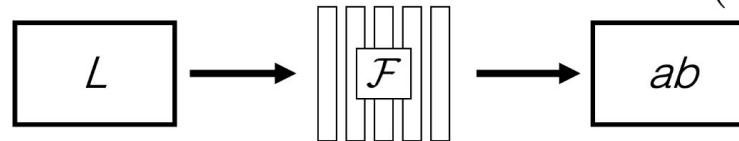
Grayscale image:  $L$  channel

$$\mathbf{X} \in \mathbb{R}^{H \times W \times 1}$$



Concatenate  $(L, ab)$  channels

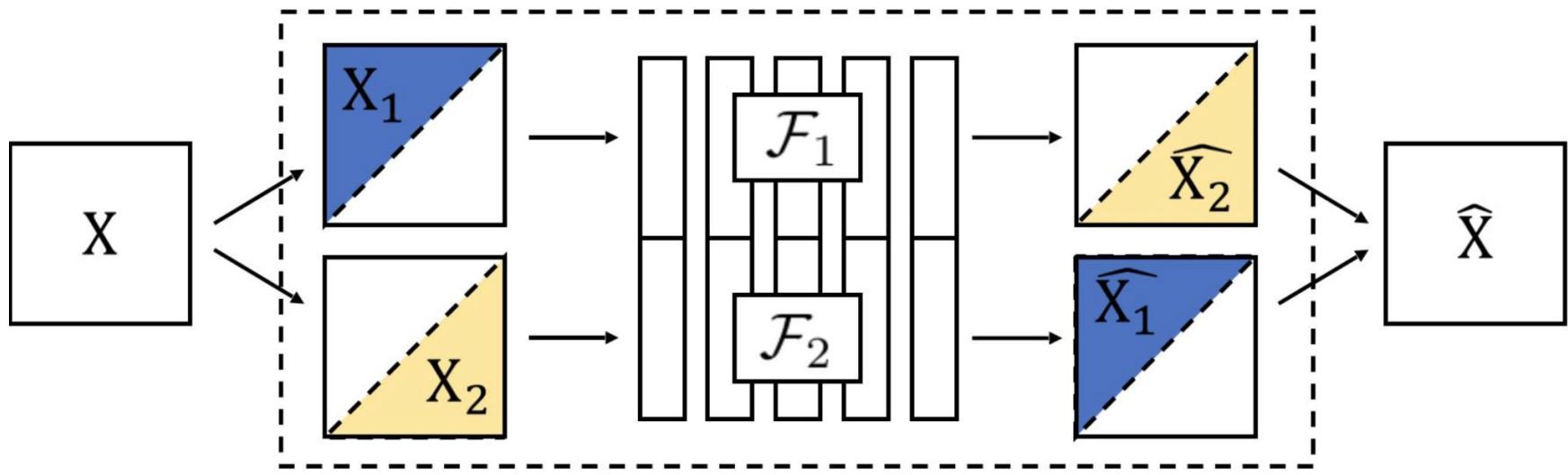
$$(\mathbf{X}, \hat{\mathbf{Y}})$$



Source: Richard Zhang / Phillip Isola

# Learning features from colorization: Split-brain Autoencoder

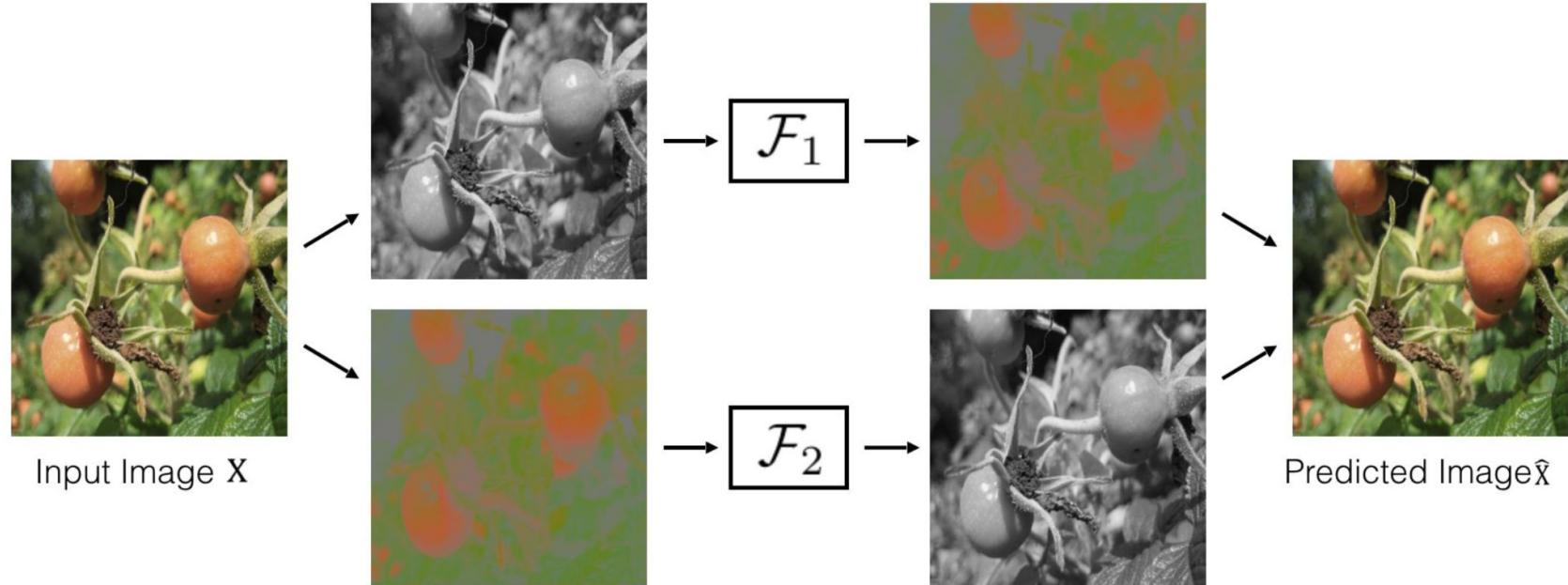
**Idea:** cross-channel predictions



Split-Brain Autoencoder

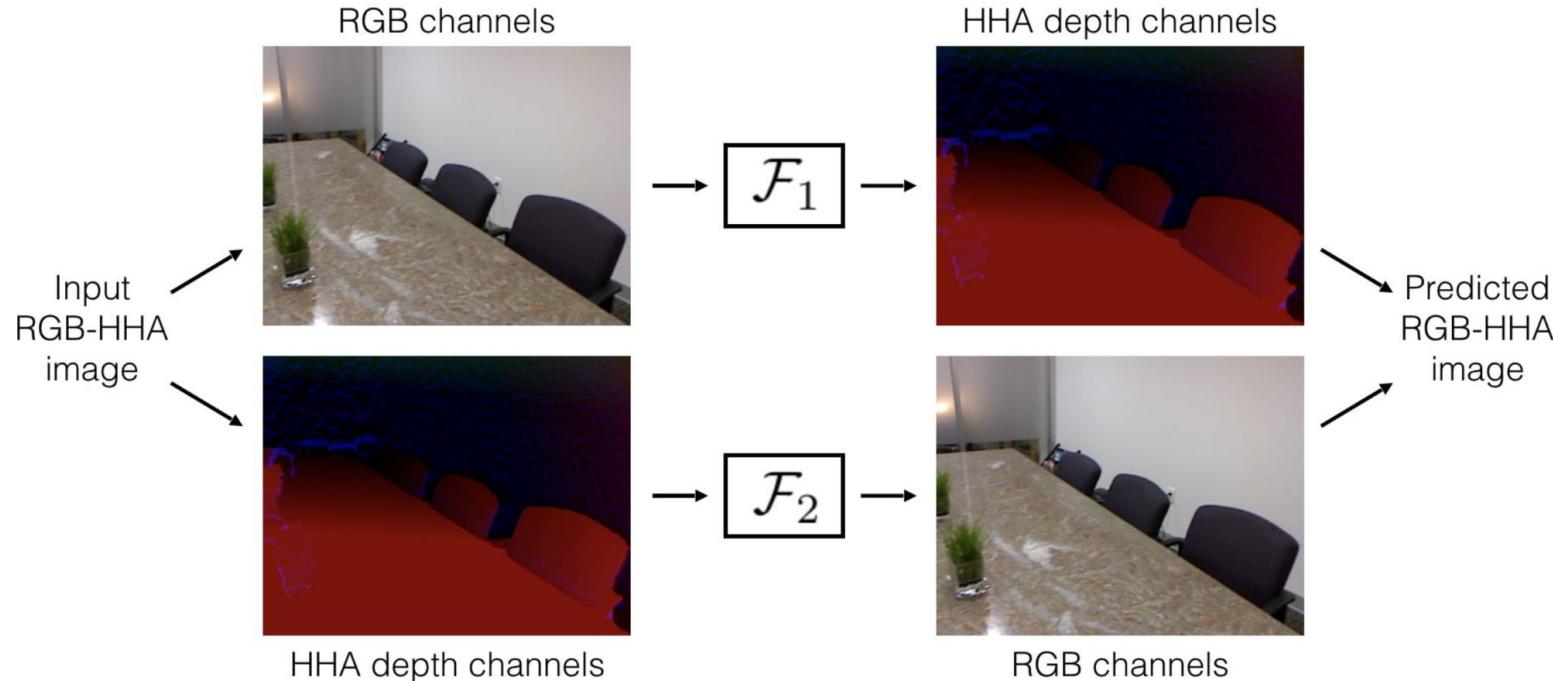
Source: Richard Zhang / Phillip Isola

# Learning features from colorization: Split-brain Autoencoder



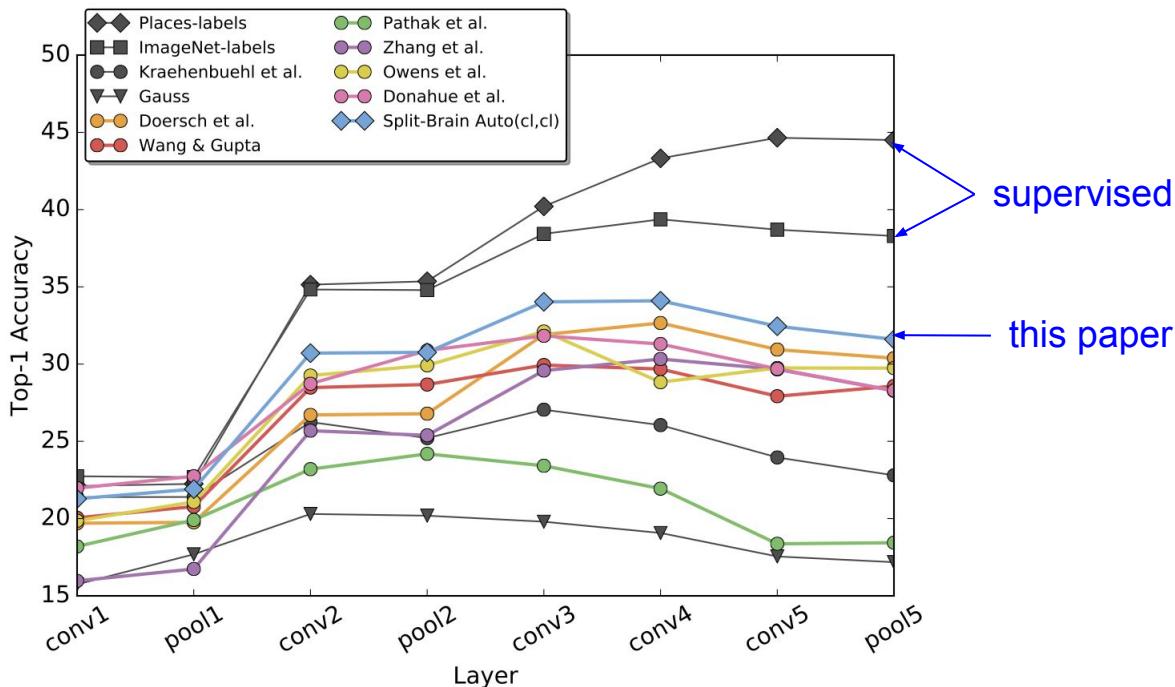
Source: Richard Zhang / Phillip Isola

# Learning features from colorization: Split-brain Autoencoder



Source: Richard Zhang / Phillip Isola

# Transfer learned features to supervised learning



Self-supervised learning on **ImageNet** (entire training set).

Use concatenated features from  $F_1$  and  $F_2$

Labeled data is from the **Places** (Zhou 2016).

Source: [Zhang et al., 2017](#)

# Real world application: image coloring



Source: Richard Zhang / Phillip Isola

# Pretext task: image coloring



Source: Richard Zhang / Phillip Isola

# Pretext task: video coloring

**Idea:** model the *temporal coherence* of colors in videos

reference frame



$t = 0$

how should I color these frames?



$t = 1$



$t = 2$



$t = 3$

...

Source: [Vondrick et al., 2018](#)

# Pretext task: video coloring

**Idea:** model the *temporal coherence* of colors in videos

reference frame



$t = 0$

how should I color these frames?

**Should be the same color!**



$t = 1$



$t = 2$



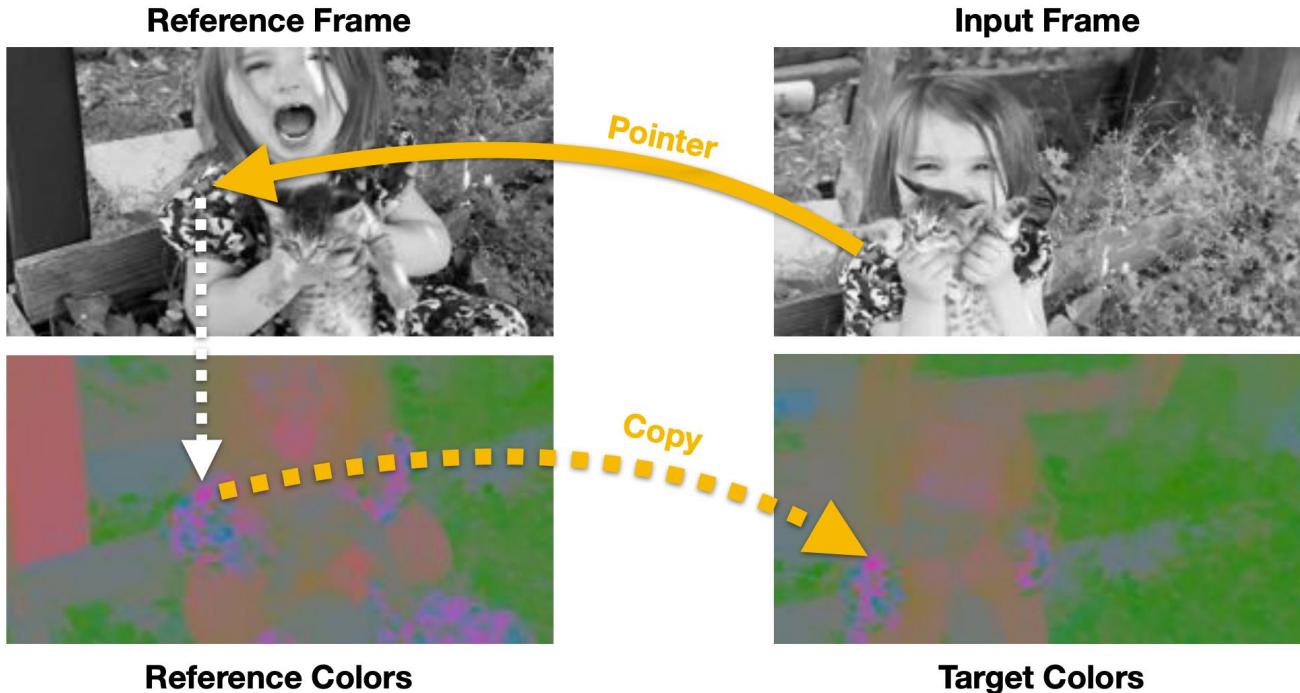
$t = 3$

...

**Hypothesis:** learning to color video frames should allow model to learn to track regions or objects without labels!

Source: [Vondrick et al., 2018](#)

# Learning to color videos



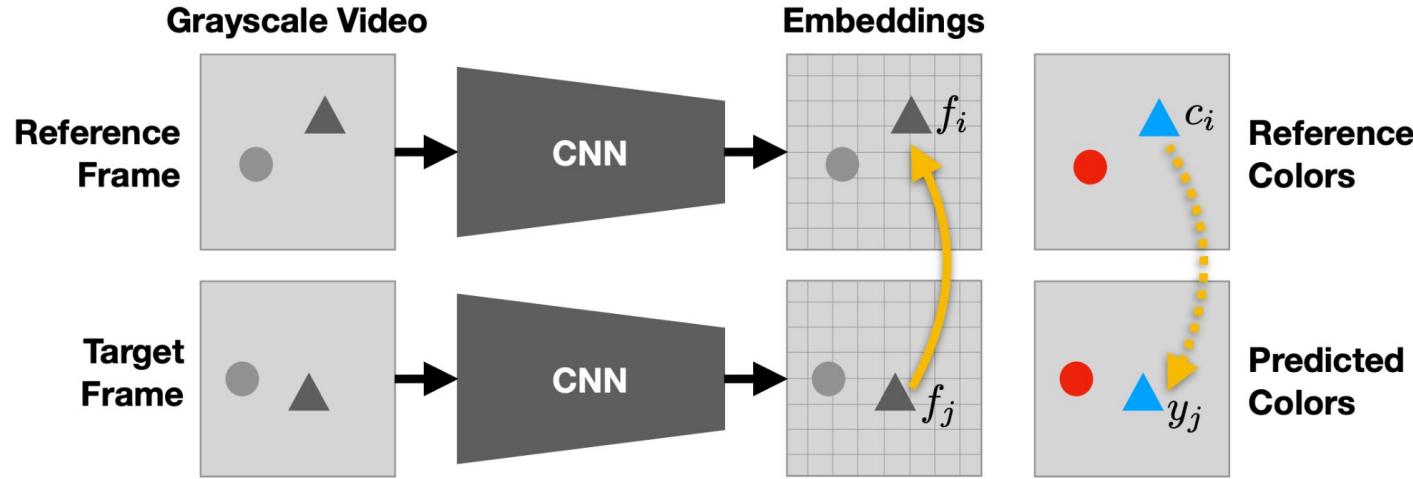
## Learning objective:

Establish mappings between reference and target frames in a learned feature space.

Use the mapping as “pointers” to copy the correct color (LAB).

Source: [Vondrick et al., 2018](#)

# Learning to color videos

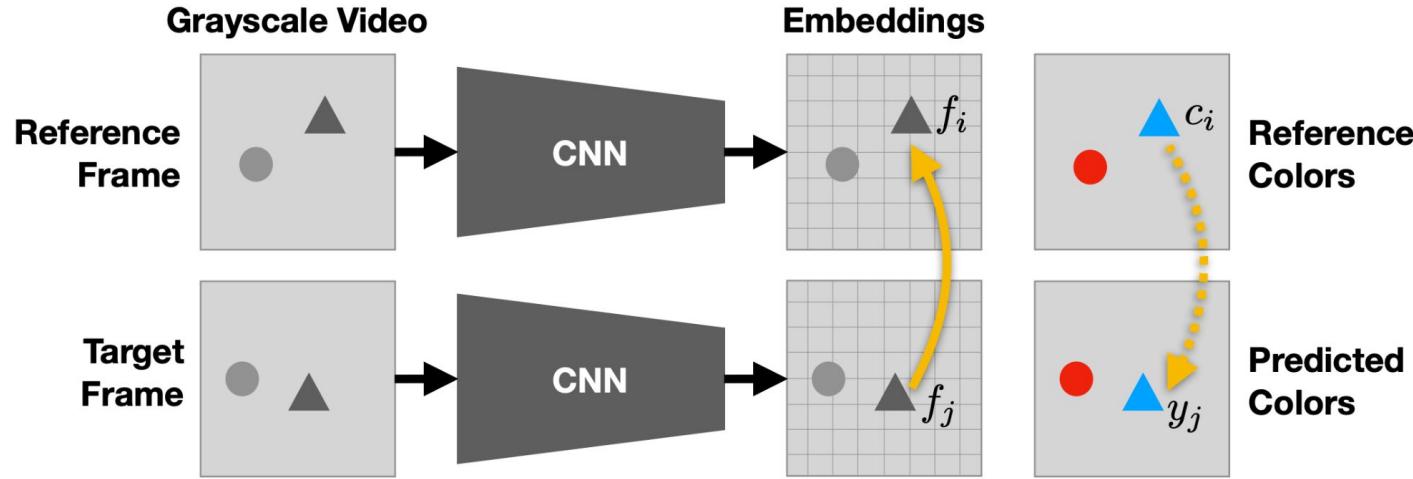


attention map on the  
reference frame

$$A_{ij} = \frac{\exp(f_i^T f_j)}{\sum_k \exp(f_k^T f_j)}$$

Source: [Vondrick et al., 2018](#)

# Learning to color videos



attention map on the  
reference frame

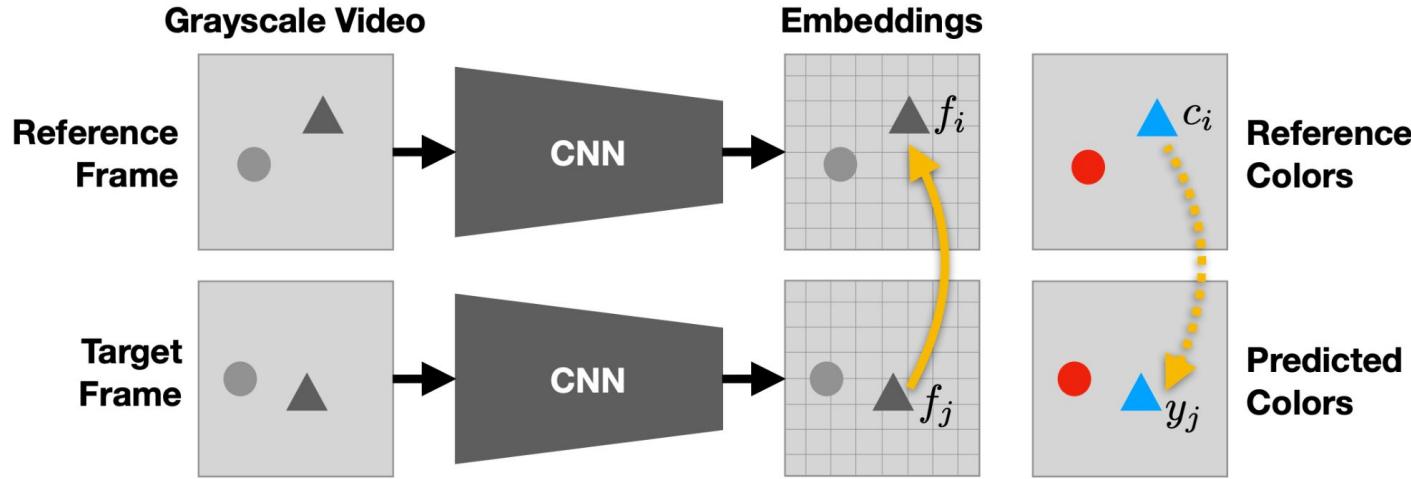
predicted color = weighted  
sum of the reference color

$$A_{ij} = \frac{\exp(f_i^T f_j)}{\sum_k \exp(f_k^T f_j)}$$

$$y_j = \sum_i A_{ij} c_i$$

Source: [Vondrick et al., 2018](#)

# Learning to color videos



attention map on the  
reference frame

predicted color = weighted  
sum of the reference color

loss between predicted color  
and ground truth color

$$A_{ij} = \frac{\exp(f_i^T f_j)}{\sum_k \exp(f_k^T f_j)}$$

$$y_j = \sum_i A_{ij} c_i$$

$$\min_{\theta} \sum_j \mathcal{L}(y_j, c_j)$$

Source: [Vondrick et al., 2018](#)

# Colorizing videos (qualitative)

reference frame



target frames (gray)



predicted color



Source: [Google AI blog post](#)

# Colorizing videos (qualitative)

reference frame



target frames (gray)



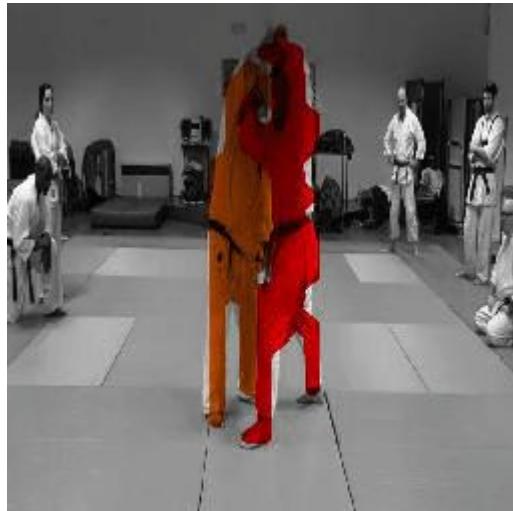
predicted color



Source: [Google AI blog post](#)

# Tracking emerges from colorization

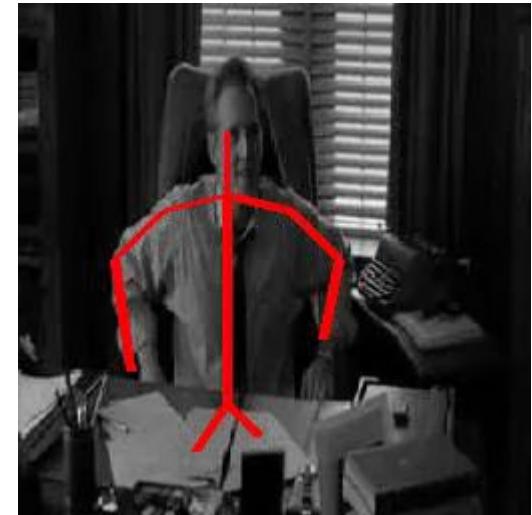
Propagate segmentation masks using learned attention



Source: [Google AI blog post](#)

# Tracking emerges from colorization

Propagate pose keypoints using learned attention



Source: [Google AI blog post](#)

# Summary: pretext tasks from image transformations

- 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).

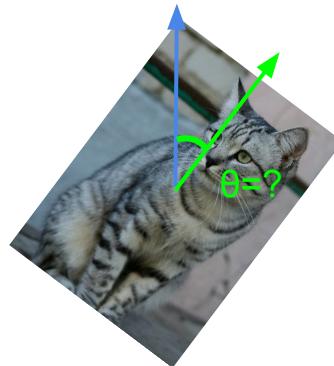
# Summary: pretext tasks from image transformations

- 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 generally useful for all downstream tasks.

# Pretext tasks from image transformations



image completion



rotation prediction



“jigsaw puzzle”

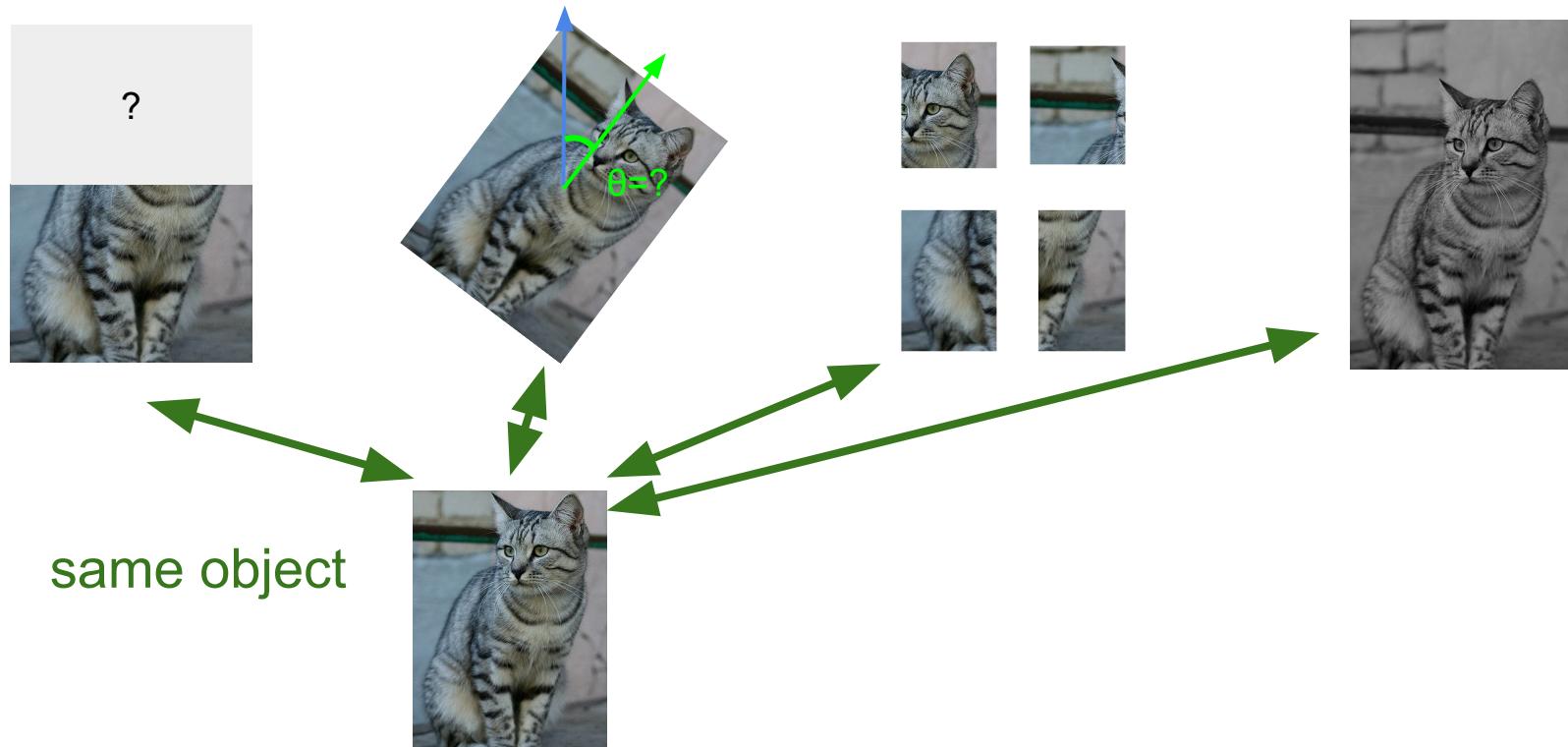


colorization

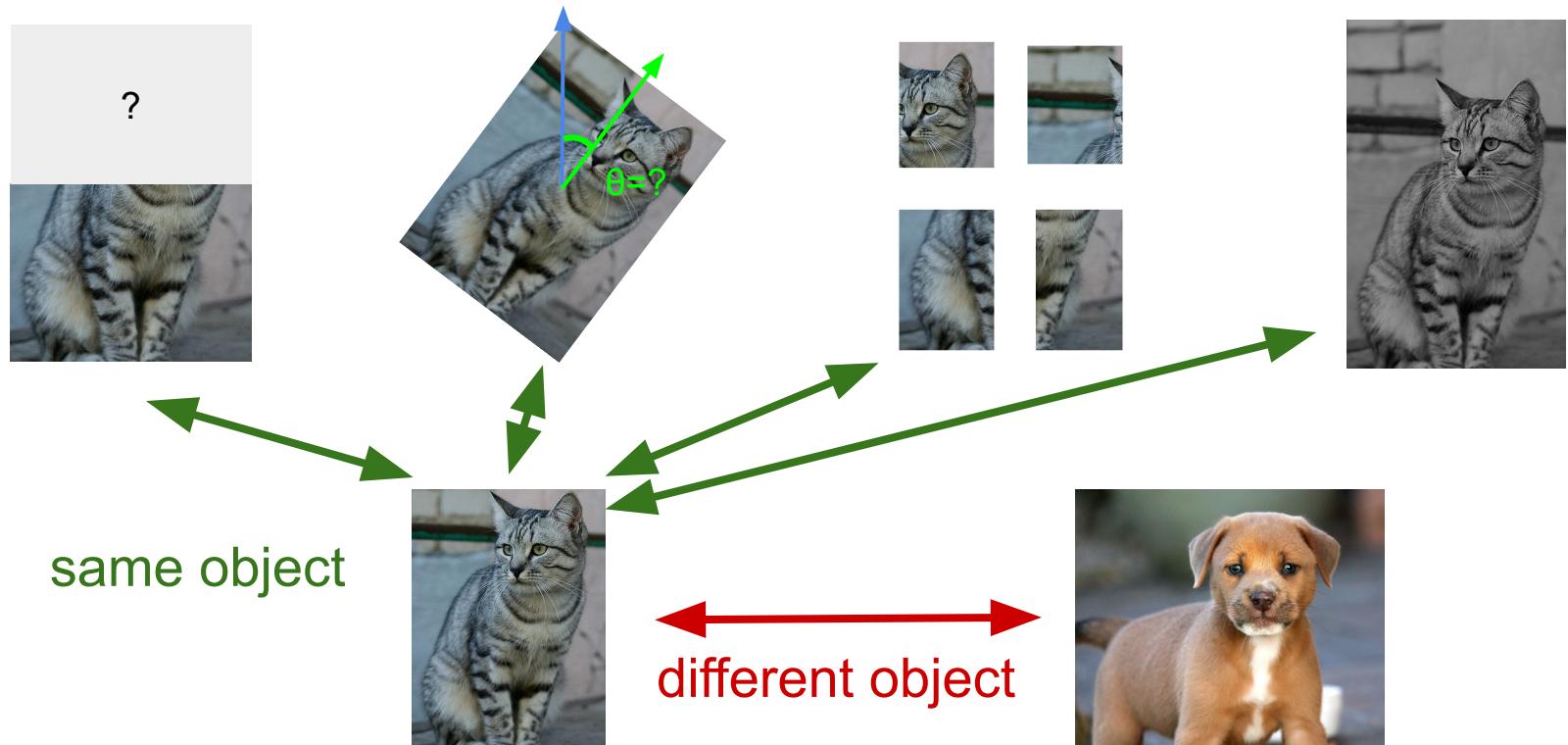
Learned representations may be tied to a specific pretext task!

Can we come up with a more general pretext task?

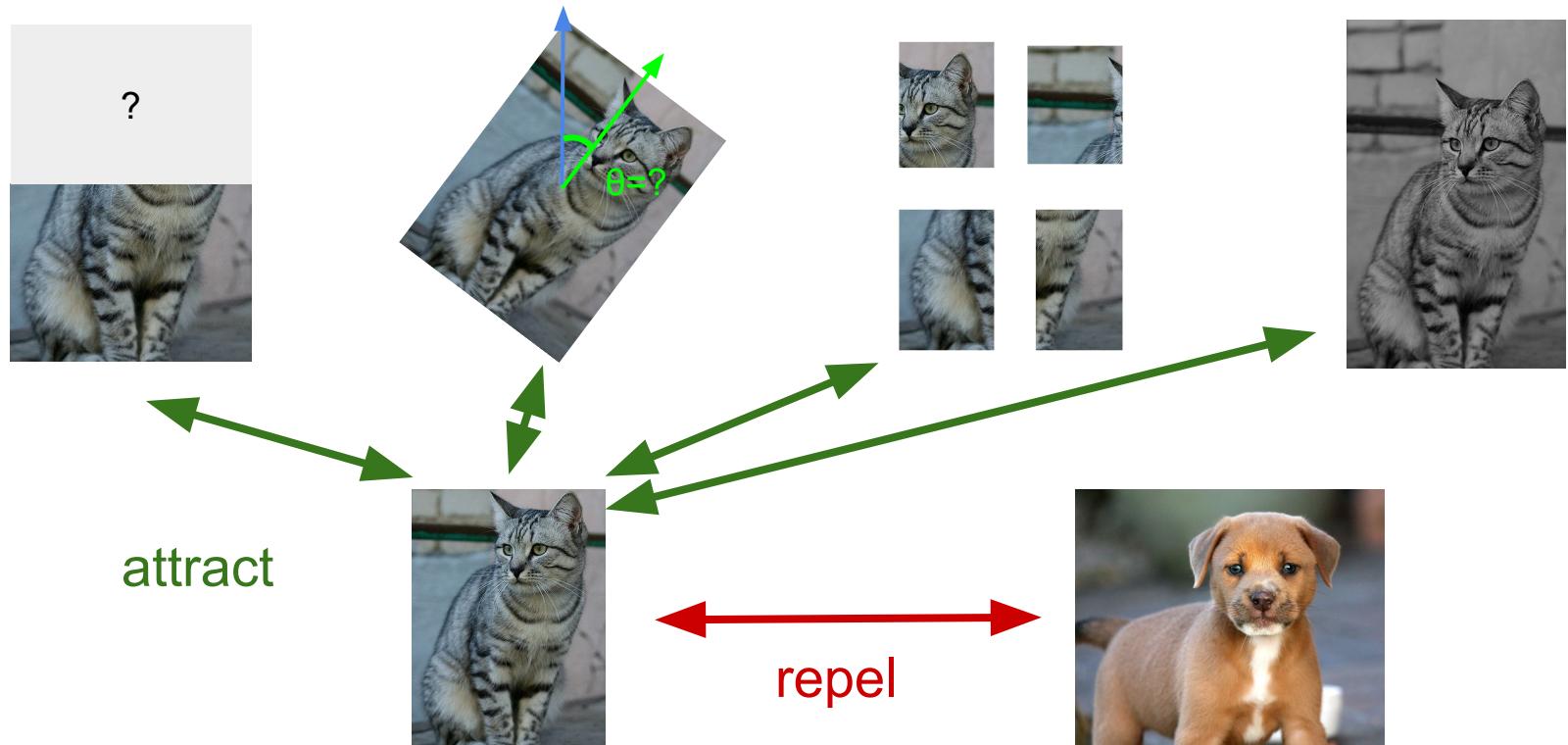
# A more general pretext task?



# A more general pretext task?



# Contrastive Representation Learning



# Today's Agenda

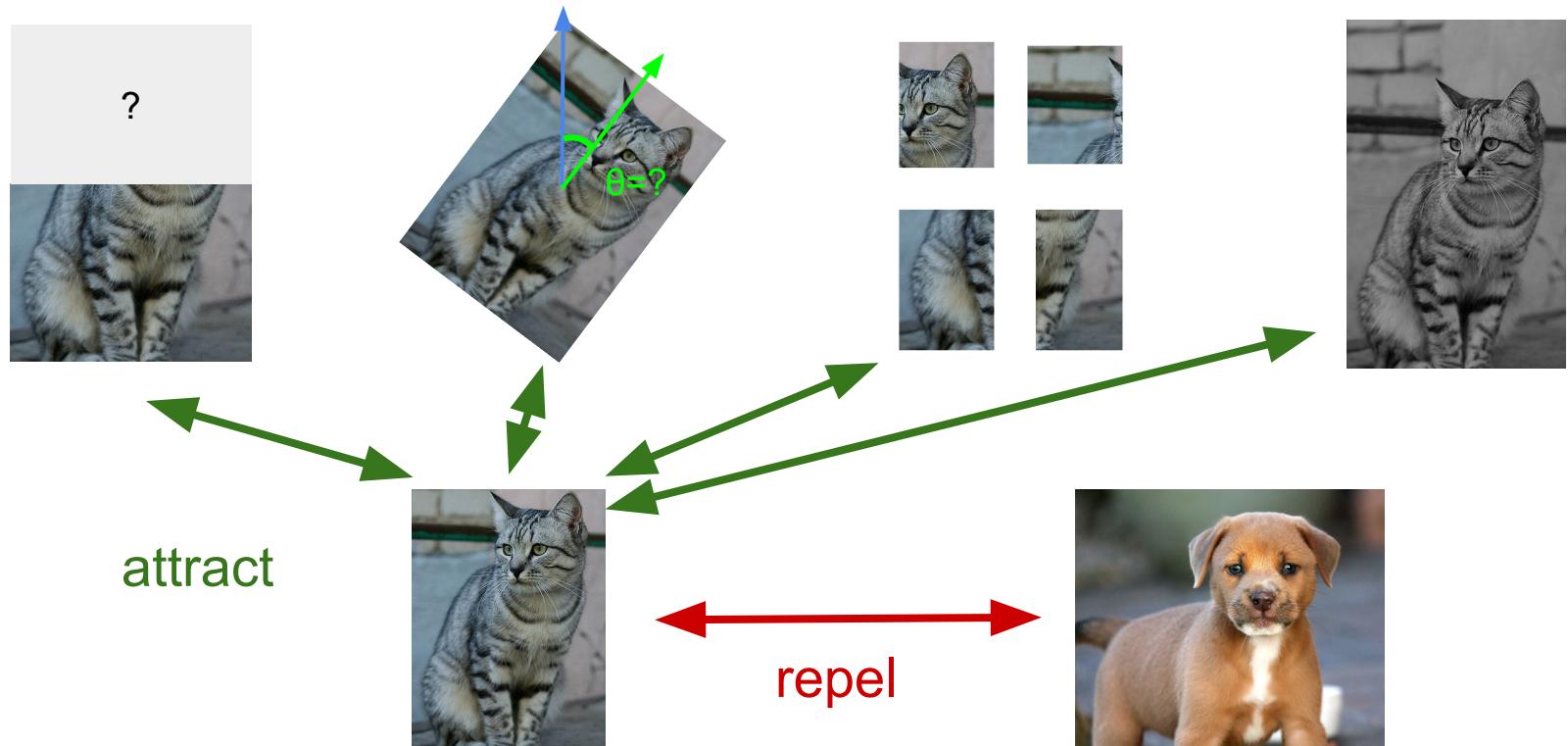
## Pretext tasks from image transformations

- Rotation, inpainting, rearrangement, coloring

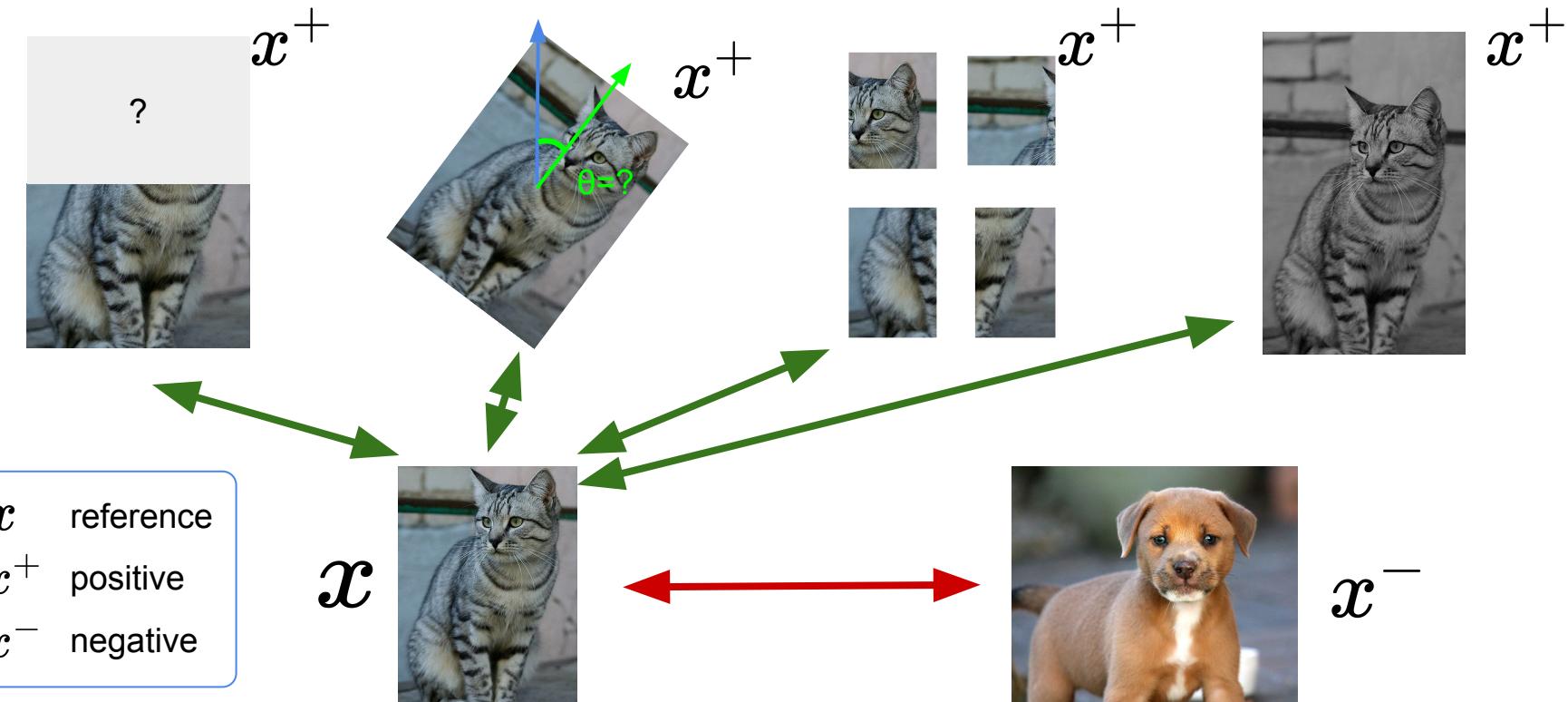
## Contrastive representation learning

- Intuition and formulation
- Instance contrastive learning: SimCLR and MOCO
- Sequence contrastive learning: CPC

# Contrastive Representation Learning



# Contrastive Representation Learning



# A formulation of contrastive learning

What we want:

$$\text{score}(f(x), f(x^+)) \gg \text{score}(f(x), f(x^-))$$

$x$ : reference sample;  $x^+$  positive sample;  $x^-$  negative sample

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  $(x, x^-)$ .

# A formulation of contrastive learning

Loss function given 1 positive sample and  $N - 1$  negative samples:

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

Q. What does this loss function remind you of?

# A formulation of contrastive learning

Loss function given 1 positive sample and  $N - 1$  negative samples:

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

 $x$  $x^+$  $x$  $x_1^-$  $x_2^-$  $x_3^-$  $\dots$

# A formulation of contrastive learning

Loss function given 1 positive sample and  $N - 1$  negative samples:

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

score for the positive pair      score for the N-1 negative pairs

## This seems familiar ...

# A formulation of contrastive learning

Loss function given 1 positive sample and  $N - 1$  negative samples:

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

score for the positive pair
score for the N-1 negative pairs

This seems familiar ...

# Cross entropy loss for a N-way softmax classifier!

I.e., learn to find the positive sample from the N samples

# A formulation of contrastive learning

Loss function given 1 positive sample and  $N - 1$  negative samples:

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

Very similar to the softmax classifier we talked about a few lectures ago.

- We want to compare the reference image against all other positive and negative images.
- We can exponentiate and normalize these scores like we did with the softmax classifier.
- And we get the above similar equation.

# A formulation of contrastive learning

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  $f(x^+)$

$$MI[f(x), f(x^+)] - \log(N) \geq -L$$

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

Detailed derivation: [Poole et al., 2019](#)

# SimCLR: A Simple Framework for Contrastive Learning

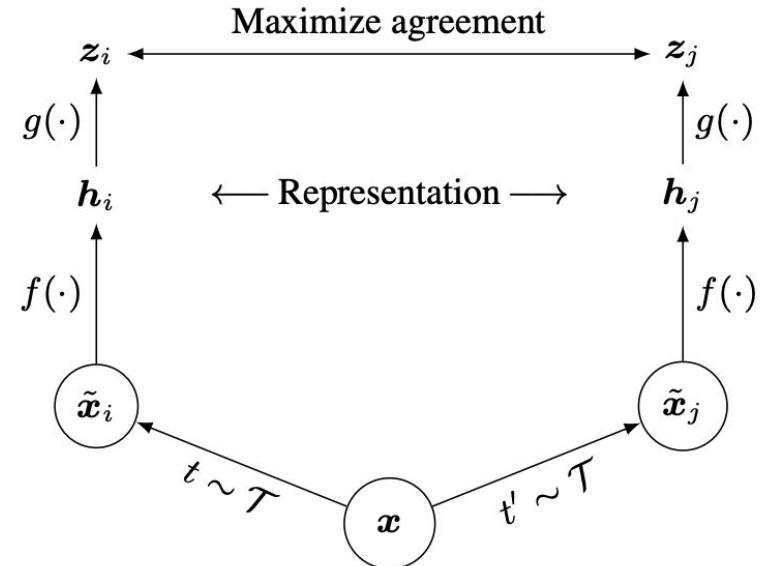
Cosine similarity as the score function:

$$s(u, v) = \frac{u^T v}{\|u\| \|v\|}$$

Use a projection network  $h(\cdot)$  to project features to a space where contrastive learning is applied

Generate positive samples through data augmentation:

- random cropping, random color distortion, and random blur.



Source: [Chen et al., 2020](#)

# SimCLR: generating positive samples from data augmentation



(a) Original



(b) Crop and resize



(c) Crop, resize (and flip)



(d) Color distort. (drop)



(e) Color distort. (jitter)



(f) Rotate  $\{90^\circ, 180^\circ, 270^\circ\}$



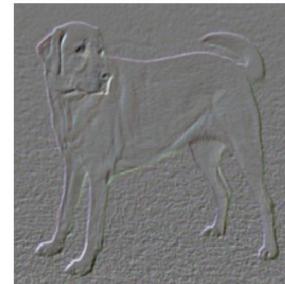
(g) Cutout



(h) Gaussian noise



(i) Gaussian blur



(j) Sobel filtering

Source: [Chen et al., 2020](#)

# SimCLR

Generate a positive pair  
by sampling data  
augmentation functions

---

**Algorithm 1** SimCLR's main learning algorithm.

---

```
input: batch size  $N$ , constant  $\tau$ , structure of  $f, g, \mathcal{T}$ .
for sampled minibatch  $\{\mathbf{x}_k\}_{k=1}^N$  do
    for all  $k \in \{1, \dots, N\}$  do
        draw two augmentation functions  $t \sim \mathcal{T}, t' \sim \mathcal{T}$ 
        # the first augmentation
         $\tilde{\mathbf{x}}_{2k-1} = t(\mathbf{x}_k)$ 
         $\mathbf{h}_{2k-1} = f(\tilde{\mathbf{x}}_{2k-1})$  # representation
         $\mathbf{z}_{2k-1} = g(\mathbf{h}_{2k-1})$  # projection
        # the second augmentation
         $\tilde{\mathbf{x}}_{2k} = t'(\mathbf{x}_k)$ 
         $\mathbf{h}_{2k} = f(\tilde{\mathbf{x}}_{2k})$  # representation
         $\mathbf{z}_{2k} = g(\mathbf{h}_{2k})$  # projection
    end for
    for all  $i \in \{1, \dots, 2N\}$  and  $j \in \{1, \dots, 2N\}$  do
         $s_{i,j} = \mathbf{z}_i^\top \mathbf{z}_j / (\|\mathbf{z}_i\| \|\mathbf{z}_j\|)$  # pairwise similarity
    end for
    define  $\ell(i, j)$  as  $\ell(i, j) = -\log \frac{\exp(s_{i,j}/\tau)}{\sum_{k=1}^{2N} \mathbb{1}_{[k \neq i]} \exp(s_{i,k}/\tau)}$ 
     $\mathcal{L} = \frac{1}{2N} \sum_{k=1}^N [\ell(2k-1, 2k) + \ell(2k, 2k-1)]$ 
    update networks  $f$  and  $g$  to minimize  $\mathcal{L}$ 
end for
return encoder network  $f(\cdot)$ , and throw away  $g(\cdot)$ 
```

---

\*We use a slightly different formulation in the assignment.  
You should follow the assignment instructions.

Source: [Chen et al., 2020](#)

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Generate a positive pair  
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InfoNCE loss:  
Use all non-positive samples in the batch as  $x^-$

Source: [Chen et al., 2020](#)

# SimCLR

Generate a positive pair  
by sampling data  
augmentation functions

Iterate through and  
use each of the  $2N$   
sample as reference,  
compute average loss

---

**Algorithm 1** SimCLR's main learning algorithm.

---

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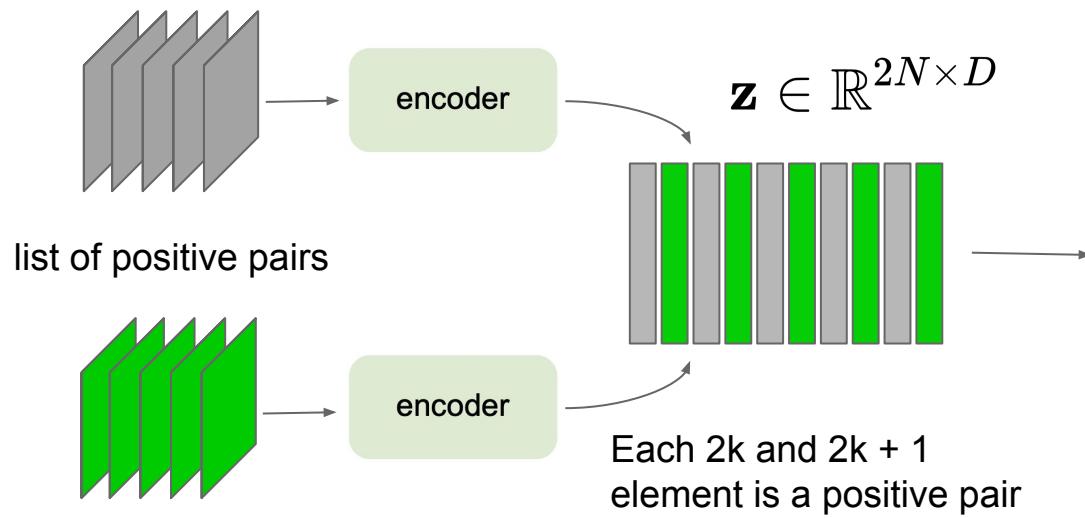
InfoNCE loss:  
Use all non-positive samples in the batch as  $x^-$

Source: [Chen et al., 2020](#)

# SimCLR: mini-batch training

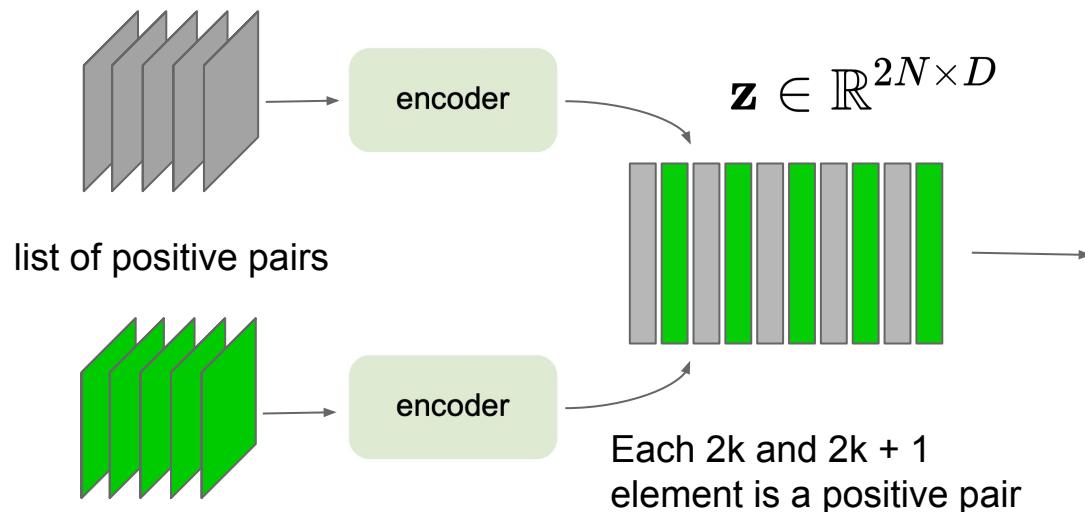
$$s_{i,j} = \frac{z_i^T z_j}{\|z_i\| \|z_j\|}$$

“Affinity matrix”



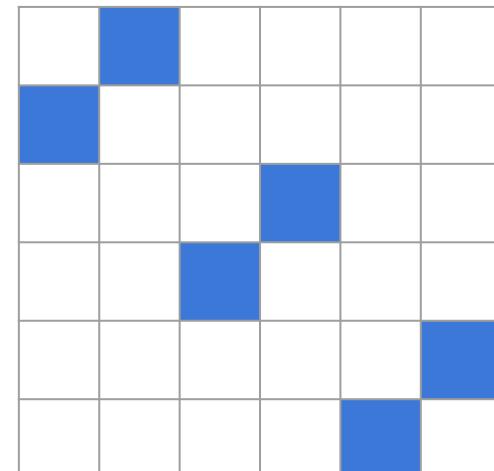
\*We use a slightly different formulation in the assignment.  
You should follow the assignment instructions.

# SimCLR: mini-batch training

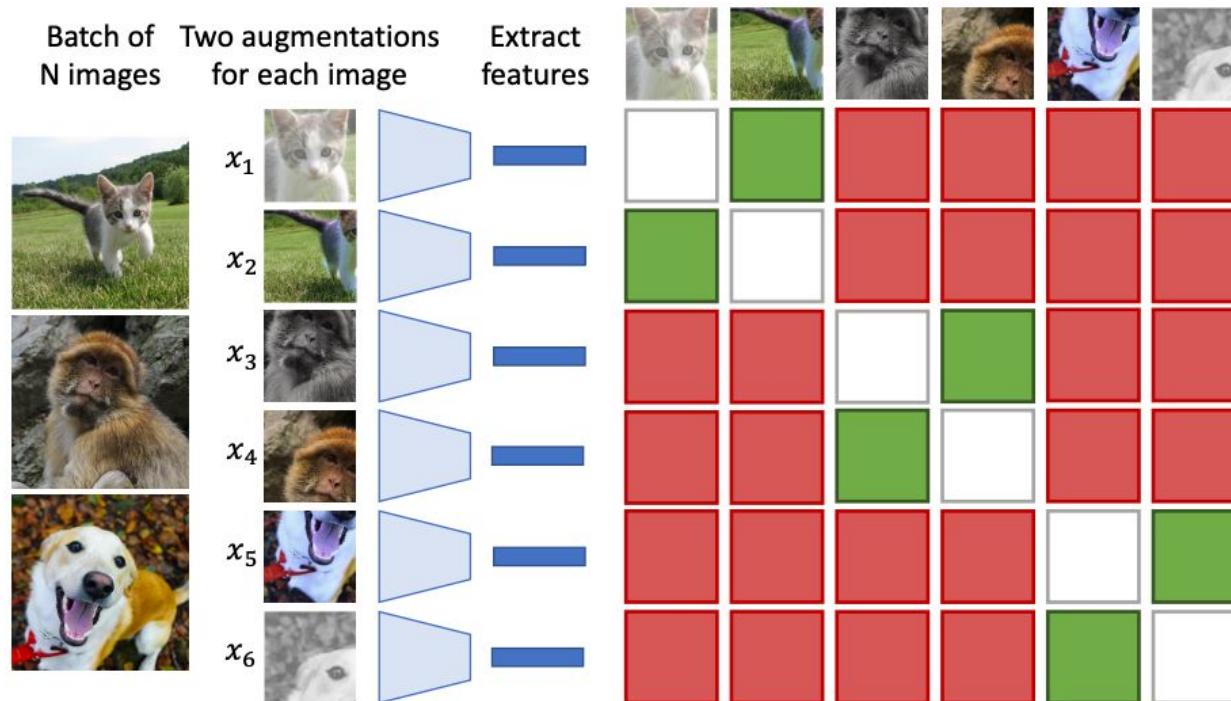


$$s_{i,j} = \frac{\mathbf{z}_i^T \mathbf{z}_j}{\|\mathbf{z}_i\| \|\mathbf{z}_j\|}$$

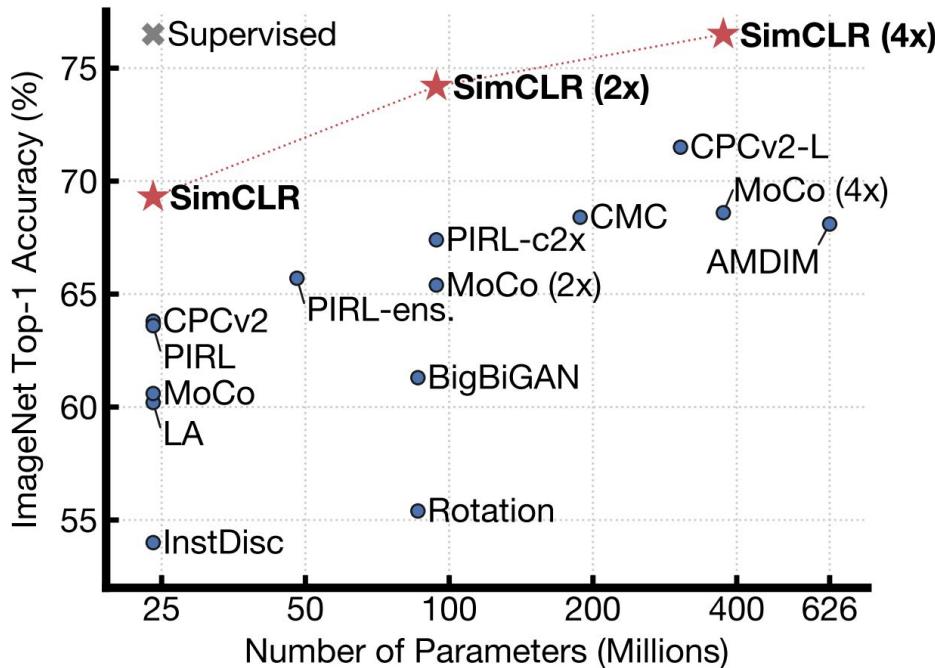
“Affinity matrix”



# SimCLR: what a batch looks like



# 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.

Source: [Chen et al., 2020](#)

# Semi-supervised learning on SimCLR features

Method	Architecture	Label fraction		
		1%	10%	Top 5
Supervised baseline	ResNet-50	48.4	80.4	
<i>Methods using other label-propagation:</i>				
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×)	-	91.2	
<i>Methods using representation learning only:</i>				
InstDisc	ResNet-50	39.2	77.4	
BigBiGAN	RevNet-50 (4×)	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×)	83.0	91.2	
SimCLR (ours)	ResNet-50 (4×)	<b>85.8</b>	<b>92.6</b>	

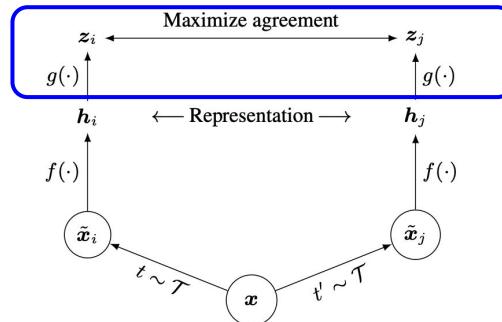
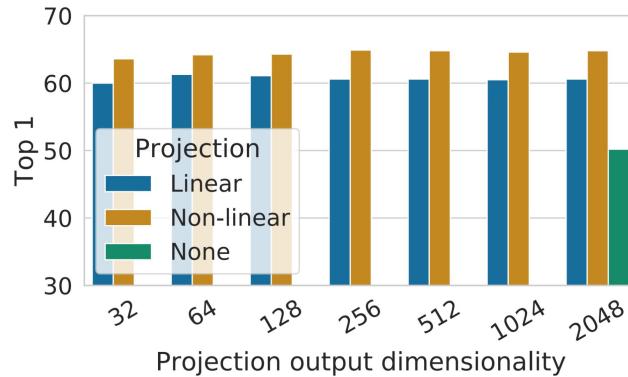
Table 7. ImageNet accuracy of models trained with few labels.

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

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

Source: [Chen et al., 2020](#)

# SimCLR design choices: projection head



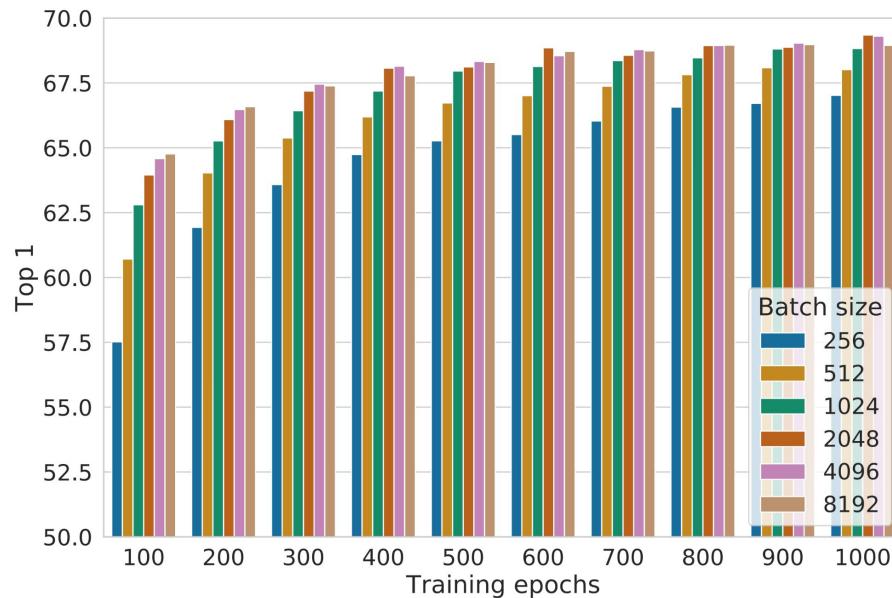
Linear / non-linear projection heads improve representation learning.

A possible explanation:

- contrastive learning objective may discard useful information for downstream tasks
- representation space  $\mathbf{z}$  is trained to be invariant to data transformation.
- by leveraging the projection head  $\mathbf{g}(\cdot)$ , more information can be preserved in the  $\mathbf{h}$  representation space

Source: [Chen et al., 2020](#)

# SimCLR design choices: large batch size



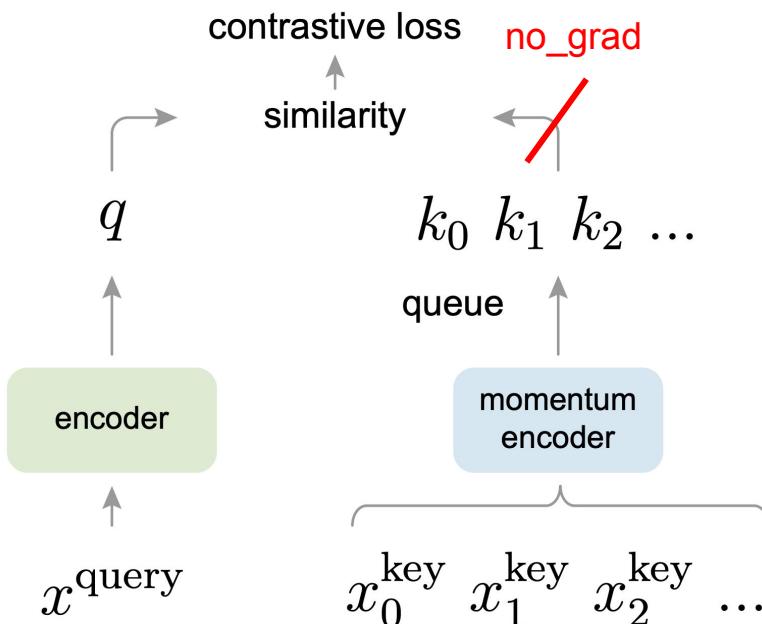
Large training batch size is crucial for SimCLR!

Large batch size causes large memory footprint during backpropagation:  
**requires distributed training on TPUs (ImageNet experiments)**

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>

Source: [Chen et al., 2020](#)

# Momentum Contrastive Learning (MoCo)

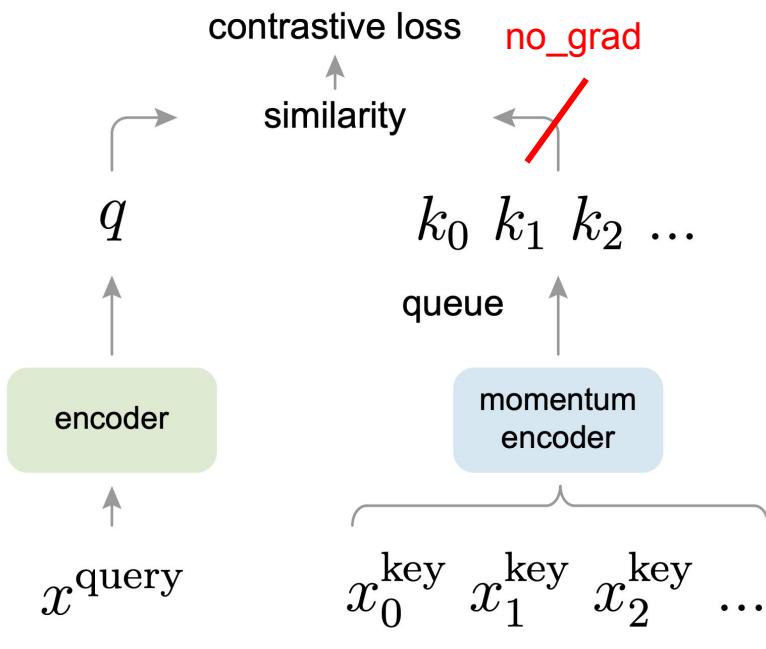


## Key differences to SimCLR:

- 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**.

Source: [He et al., 2020](#)

# 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:

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

Source: [He et al., 2020](#)

# MoCo

Generate a positive pair  
by sampling data  
augmentation functions

No gradient through  
the negative samples

Update the FIFO  
negative sample queue

---

## Algorithm 1 Pseudocode of MoCo in a PyTorch-like style.

---

```
# f_q, f_k: encoder networks for query and key
# queue: dictionary as a queue of K keys (CxK)
# m: momentum
# t: temperature

f_k.params = f_q.params # initialize
for x in loader: # load a minibatch x with N samples
    x_q = aug(x) # a randomly augmented version
    x_k = aug(x) # another randomly augmented version

    q = f_q.forward(x_q) # queries: NxC
    k = f_k.forward(x_k) # keys: NxC
    k = k.detach() # no gradient to keys

    # positive logits: Nx1
    l_pos = bmm(q.view(N, 1, C), k.view(N, C, 1))

    # negative logits: NxK
    l_neg = mm(q.view(N, C), queue.view(C, K))

    # logits: Nx(1+K)
    logits = cat([l_pos, l_neg], dim=1)

    # contrastive loss, Eqn.(1)
    labels = zeros(N) # positives are the 0-th
    loss = CrossEntropyLoss(logits/t, labels)

    # SGD update: query network
    loss.backward()
    update(f_q.params)

    # momentum update: key network
    f_k.params = m*f_k.params+(1-m)*f_q.params

    # update dictionary
    enqueue(queue, k) # enqueue the current minibatch
    dequeue(queue) # dequeue the earliest minibatch
```

bmm: batch matrix multiplication; mm: matrix multiplication; cat: concatenation.

Use the running  
queue of keys as the  
negative samples

InfoNCE loss

Update f\_k through  
momentum

Source: [He et al., 2020](#)

# “MoCo V2”

## Improved Baselines with Momentum Contrastive Learning

Xinlei Chen Haoqi Fan Ross Girshick Kaiming He  
Facebook AI Research (FAIR)

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!).

Source: [Chen et al., 2020](#)

# MoCo vs. SimCLR vs. MoCo V2

## Key takeaways:

- Non-linear projection head and strong data augmentation are crucial for contrastive learning.

case	MLP	unsup. pre-train aug+	cos	epochs	ImageNet acc.	VOC detection		
						AP <sub>50</sub>	AP	AP <sub>75</sub>
supervised					76.5	81.3	53.5	58.8
MoCo v1				200	60.6	81.5	55.9	62.6
(a)	✓			200	66.2	82.0	56.4	62.6
(b)		✓		200	63.4	82.2	56.8	63.2
(c)	✓	✓		200	67.3	<b>82.5</b>	57.2	63.9
(d)	✓	✓	✓	200	67.5	82.4	57.0	63.6
(e)	✓	✓	✓	<b>800</b>	<b>71.1</b>	<b>82.5</b>	<b>57.4</b>	<b>64.0</b>

Table 1. **Ablation of MoCo baselines**, evaluated by ResNet-50 for (i) ImageNet linear classification, and (ii) fine-tuning VOC object detection (mean of 5 trials). “MLP”: with an MLP head; “aug+”: with extra blur augmentation; “cos”: cosine learning rate schedule.

Source: [Chen et al., 2020](#)

# MoCo vs. SimCLR vs. MoCo V2

case	MLP	aug+	cos	unsup. pre-train epochs	batch	ImageNet acc.
MoCo v1 [6]				200	256	60.6
SimCLR [2]	✓	✓	✓	200	256	61.9
SimCLR [2]	✓	✓	✓	200	8192	66.6
<b>MoCo v2</b>	✓	✓	✓	200	256	<b>67.5</b>
<i>results of longer unsupervised training follow:</i>						
SimCLR [2]	✓	✓	✓	1000	4096	69.3
<b>MoCo v2</b>	✓	✓	✓	800	256	<b>71.1</b>

Table 2. **MoCo vs. SimCLR**: ImageNet linear classifier accuracy (**ResNet-50, 1-crop 224×224**), 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).

## Key takeaways:

- 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).

Source: [Chen et al., 2020](#)

# MoCo vs. SimCLR vs. MoCo V2

## Key takeaways:

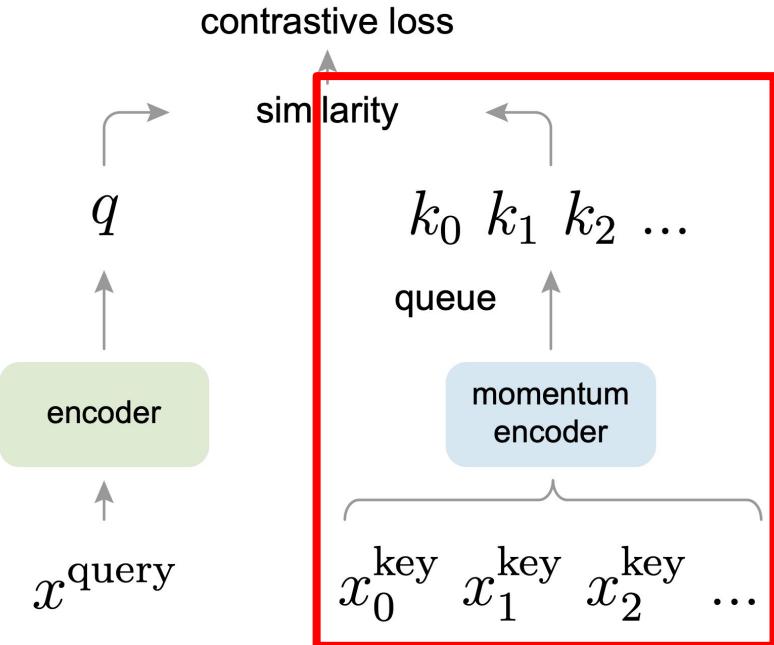
- Non-linear projection head and strong data augmentation are crucial for contrastive learning.
- Decoupling mini-batch size with negative sample size allows MoCo-V2 to outperform SimCLR with smaller batch size (256 vs. 8192).
- ... all with much smaller memory footprint! (“end-to-end” means SimCLR here)

mechanism	batch	memory / GPU	time / 200-ep.
MoCo	256	<b>5.0G</b>	<b>53 hrs</b>
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.

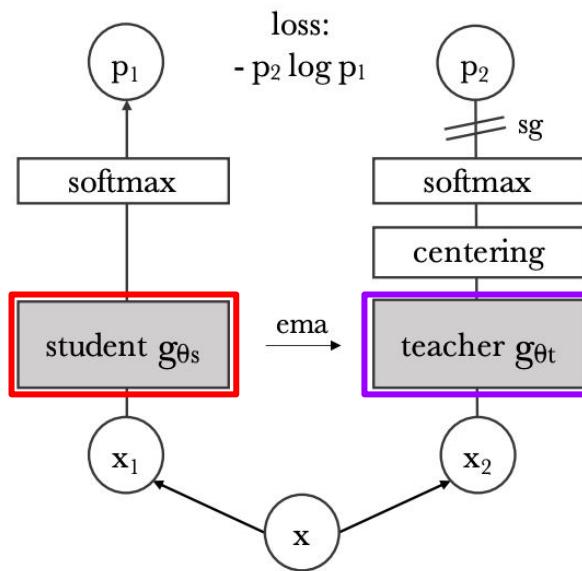
Source: [Chen et al., 2020](#)

# Problem with MoCoV2: Need to keep around a set of negatives



Do we need these  
negatives?

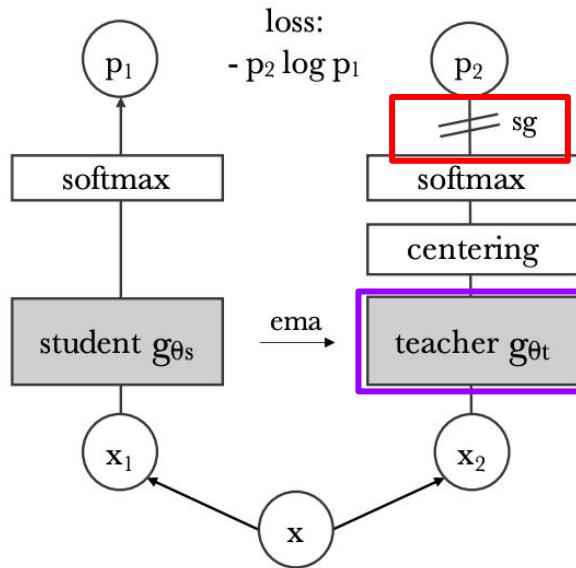
# Solution: DINO: self-distillation with no labels



- Similar to SimCLR and MOCO but with one big difference: no negatives
- Reformulates contrastive learning as knowledge distillation between a **student** and a **teacher** model.

Source: Caron et al. Emerging Properties in Self-Supervised Vision Transformers. 2021

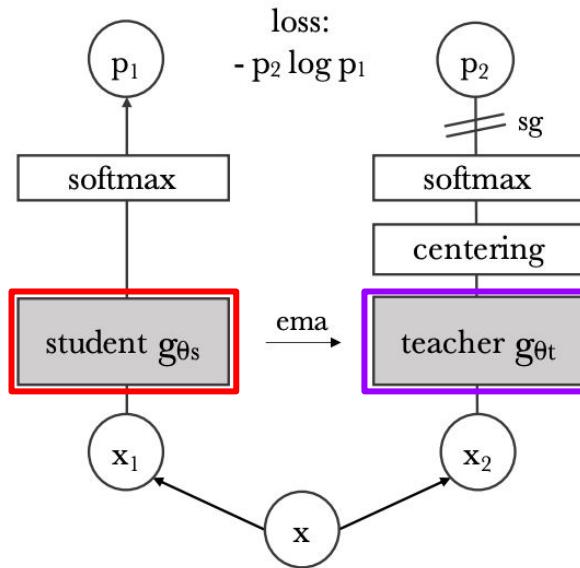
# Solution: DINO: self-distillation with no labels



- The **teacher** model is not trained: **sg** stands for stop-gradient: meaning that gradients are prevented from flowing back.

Source: Caron et al. Emerging Properties in Self-Supervised Vision Transformers. 2021

# Problem: But how do we choose the teacher model?



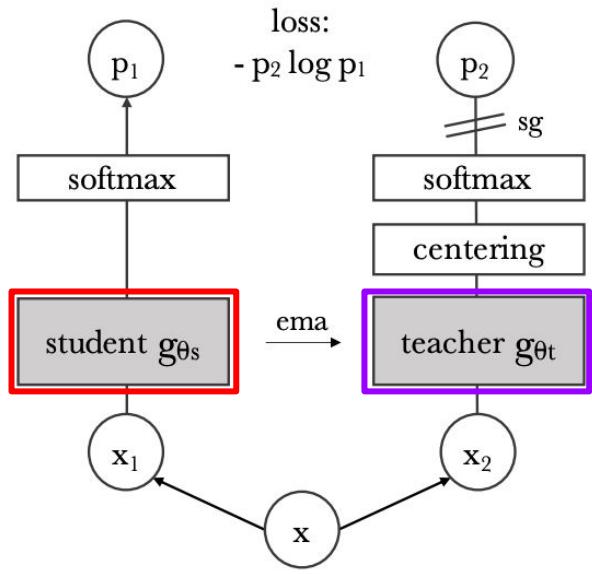
- The **teacher** model is like the momentum encoder. It is a running average of the student model

$$\theta_t \leftarrow \lambda \theta_t + (1 - \lambda) \theta_s$$

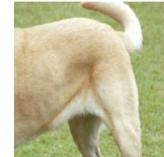
- The teacher sees a **global view** augmentation of the image
- Student only sees augmented **local crops** of the image

Source: Caron et al. Emerging Properties in Self-Supervised Vision Transformers. 2021

# Problem: But how do we choose the teacher model?



Local augmented crops

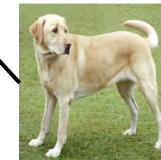


$x_1$

Global augmented views



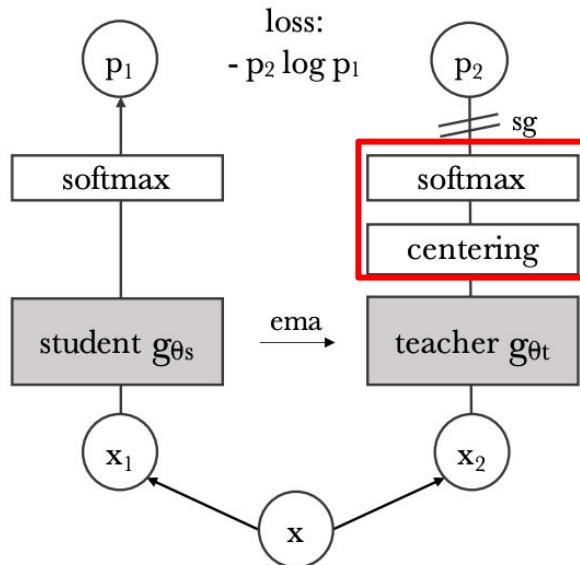
$x_2$



$x$

Source: Caron et al. Emerging Properties in Self-Supervised Vision Transformers. 2021

# Problem: But how do we choose the teacher model?



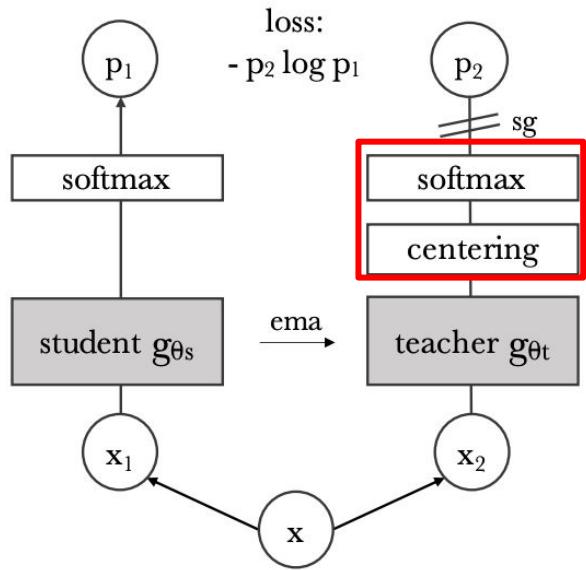
Training tricks:

- **Centering:** prevents one dimension from dominating.
  - A constant value  $c$  is added to all dimensions of the teacher's output.
  - $c$  is a running average of outputs

$$g_t(x) \leftarrow g_t(x) + c, c \leftarrow mc + (1 - m) \frac{1}{B} \sum_{i=1}^B g_{\theta_t}(x_i)$$

Source: Caron et al. Emerging Properties in Self-Supervised Vision Transformers. 2021

# Problem: But how do we choose the teacher model?



Training tricks:

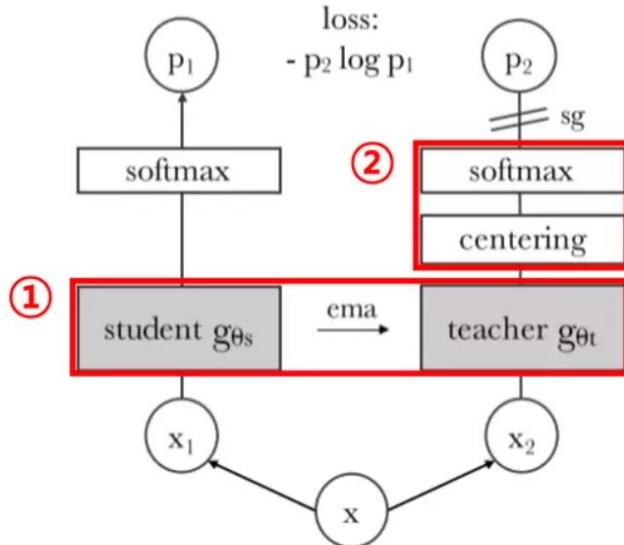
- **Sharpening:**

- A temperature ( $\text{Tau}$ ) hyperparameter is used to sharpen the distributions towards one dimension.

$$\frac{\exp(g_{\theta_s}(x)^{(i)} / \tau_s)}{\sum_{k=1}^K \exp(g_{\theta_s}(x)^{(k)} / \tau_s)}$$

Source: Caron et al. Emerging Properties in Self-Supervised Vision Transformers. 2021

# DINO code



**Algorithm 1** DINO PyTorch pseudocode w/o multi-crop.

```
# gs, gt: student and teacher networks
# C: center (K)
# tps, tpt: student and teacher temperatures
# l, m: network and center momentum rates
gt.params = gs.params
for x in loader: # load a minibatch x with n samples
    x1, x2 = augment(x), augment(x) # random views

    s1, s2 = gs(x1), gs(x2) # student output n-by-K
    t1, t2 = gt(x1), gt(x2) # teacher output n-by-K

    loss = H(t1, s2)/2 + H(t2, s1)/2
    loss.backward() # back-propagate

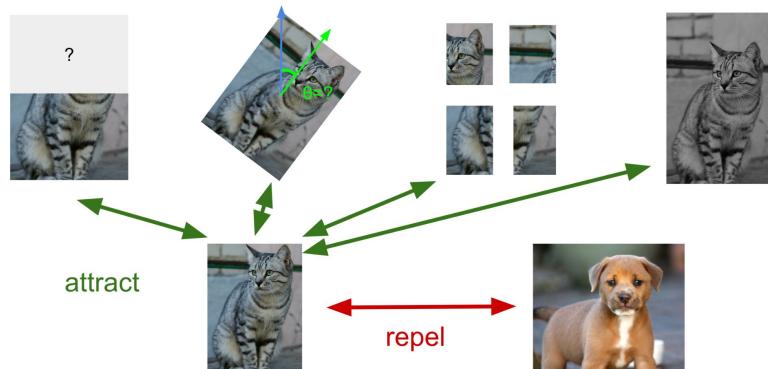
    # student, teacher and center updates
    update(gs) # SGD
    gt.params = l*gt.params + (1-l)*gs.params
    C = m*C + (1-m)*cat([t1, t2]).mean(dim=0)

def H(t, s):
    t = t.detach() # stop gradient
    s = softmax(s / tps, dim=1)
    t = softmax((t - C) / tpt, dim=1) # center + sharpen
    return - (t * log(s)).sum(dim=1).mean()
```

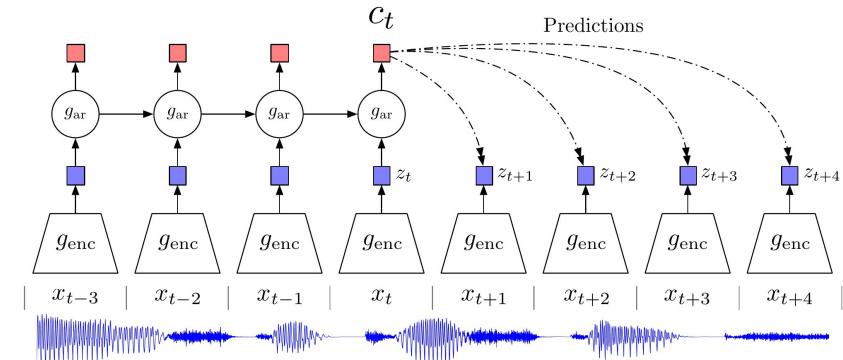
# Results: DINO

Method	Arch.	Param.	im/s	Linear	$k$ -NN
Supervised	RN50	23	1237	79.3	79.3
SCLR [12]	RN50	23	1237	69.1	60.7
MoCov2 [15]	RN50	23	1237	71.1	61.9
InfoMin [67]	RN50	23	1237	73.0	65.3
BarlowT [81]	RN50	23	1237	73.2	66.0
OBoW [27]	RN50	23	1237	73.8	61.9
BYOL [30]	RN50	23	1237	74.4	64.8
DCv2 [10]	RN50	23	1237	75.2	67.1
SwAV [10]	RN50	23	1237	75.3	65.7
<b>DINO</b>	RN50	23	1237	<b>75.3</b>	<b>67.5</b>

# Instance vs. Sequence Contrastive Learning



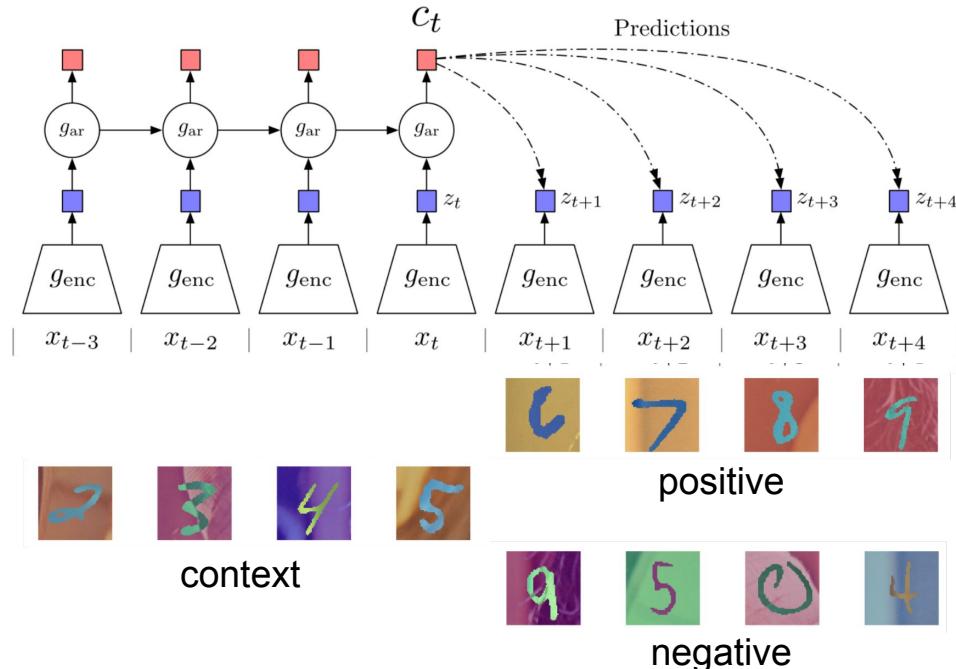
**Instance-level contrastive learning:**  
contrastive learning based on  
**positive & negative instances.**  
Examples: SimCLR, MoCo



Source: [van den Oord et al., 2018](#)

**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.

Figure [source](#)

Source: [van den Oord et al., 2018](#),

# Contrastive Predictive Coding (CPC)

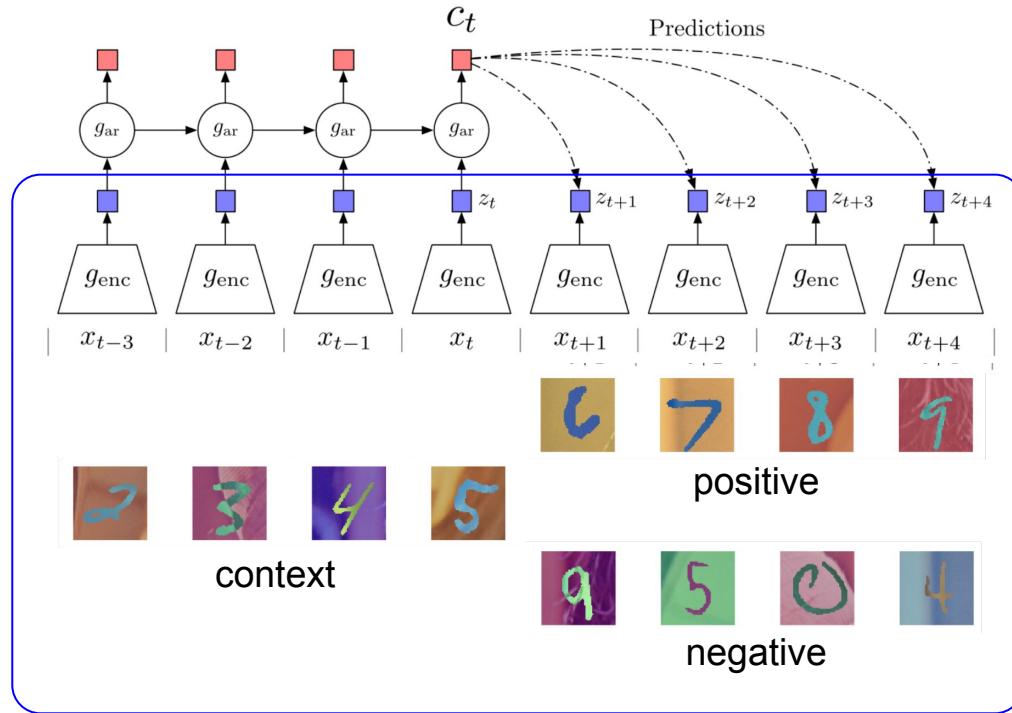
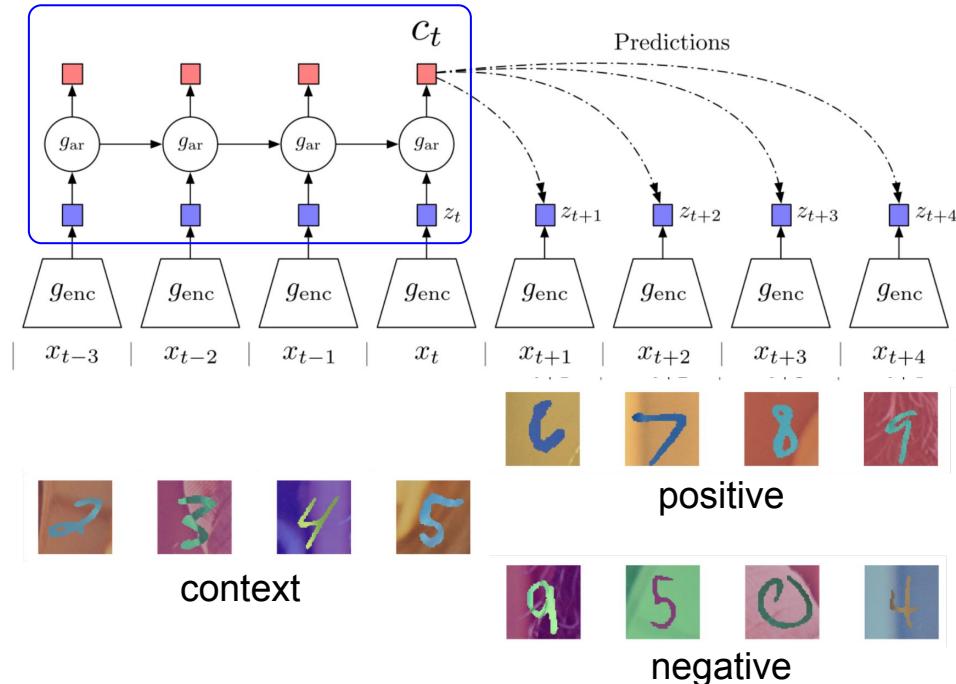


Figure [source](#)

1. Encode all samples in a sequence into vectors  $\mathbf{z}_t = \mathbf{g}_{enc}(\mathbf{x}_t)$

Source: [van den Oord et al., 2018](#),

# Contrastive Predictive Coding (CPC)

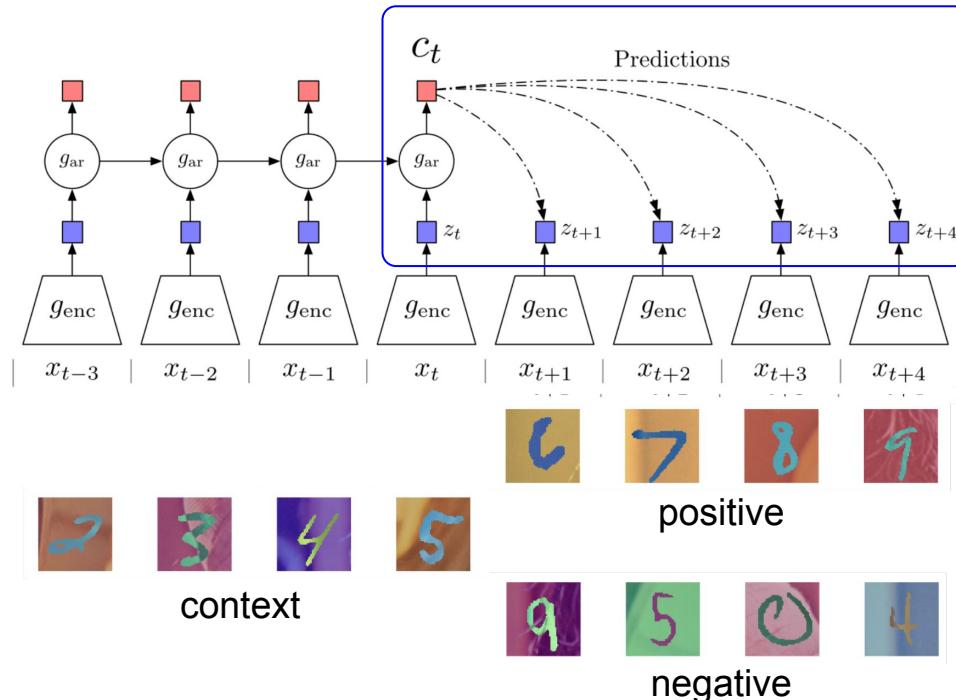


1. Encode all samples in a sequence into vectors  $\mathbf{z}_t = \mathbf{g}_{enc}(\mathbf{x}_t)$
2. Summarize context (e.g., half of a sequence) into a context code  $\mathbf{c}_t$  using an auto-regressive model ( $\mathbf{g}_{ar}$ ). The original paper uses GRU-RNN here.

Figure [source](#)

Source: [van den Oord et al., 2018](#),

# Contrastive Predictive Coding (CPC)



1. Encode all samples in a sequence into vectors  $\mathbf{z}_t = \mathbf{g}_{enc}(\mathbf{x}_t)$
2. Summarize context (e.g., half of a sequence) into a context code  $\mathbf{c}_t$  using an auto-regressive model ( $\mathbf{g}_{ar}$ )
3. Compute InfoNCE loss between the context  $\mathbf{c}_t$  and future code  $\mathbf{z}_{t+k}$  using the following **time-dependent score function**:

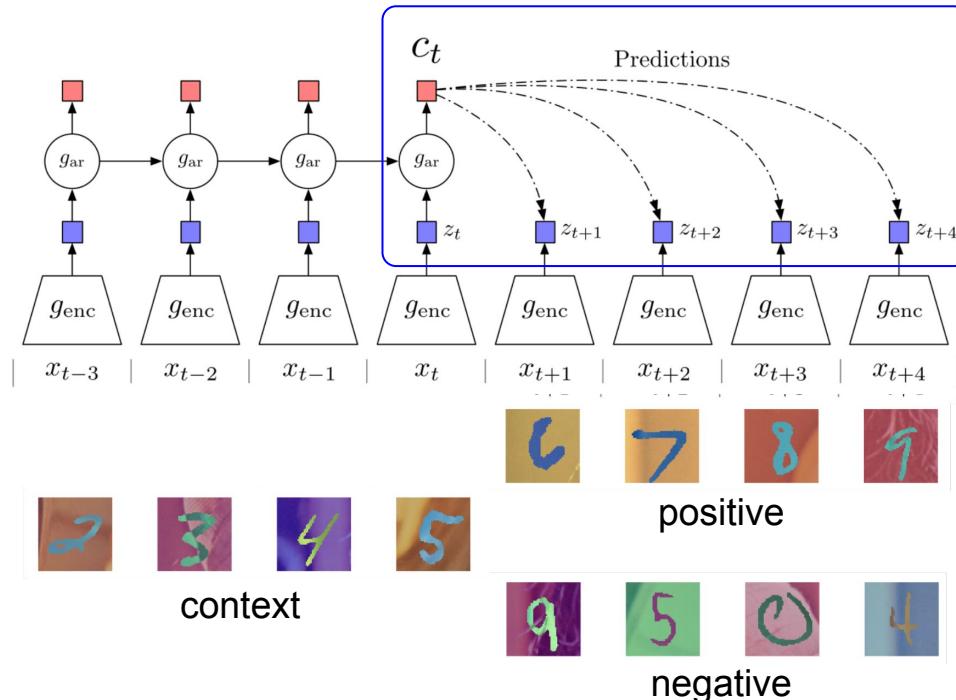
$$s_k(z_{t+k}, c_t) = z_{t+k}^T W_k c_t$$

, where  $W_k$  is a trainable matrix.

Figure [source](#)

Source: [van den Oord et al., 2018](#),

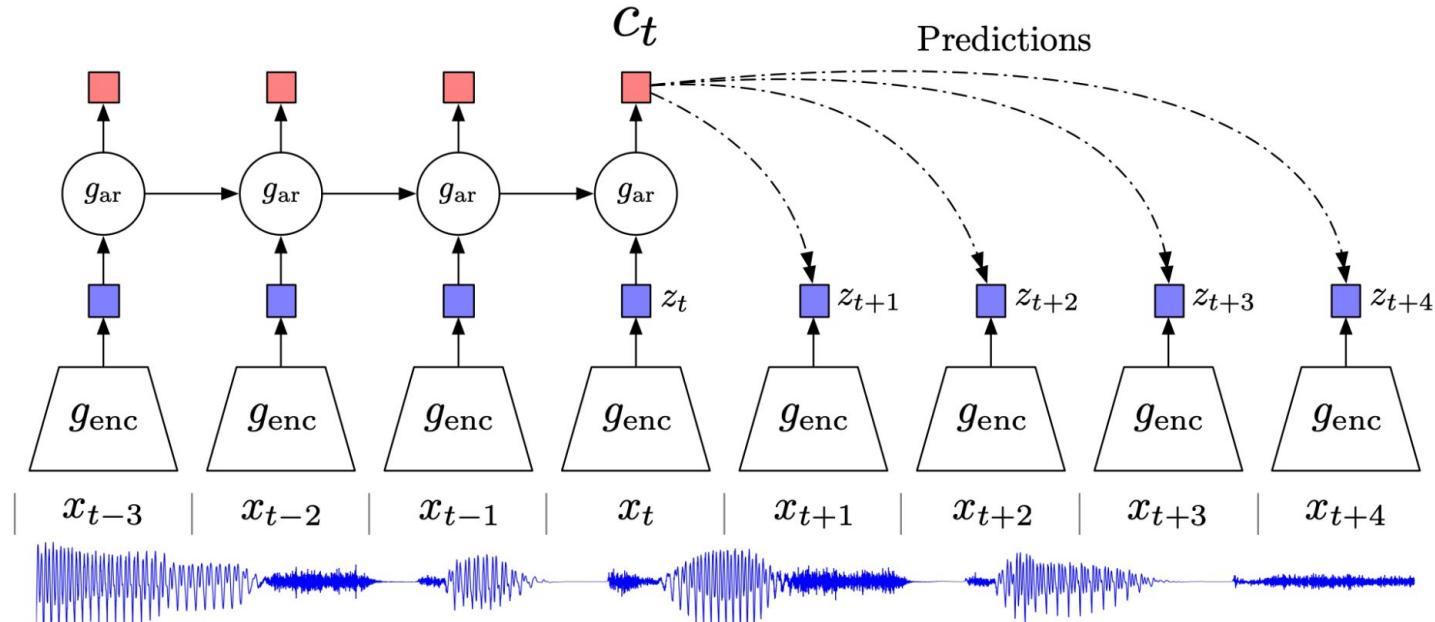
# Contrastive Predictive Coding (CPC)



1. Encode all samples in a sequence into vectors  $\mathbf{z}_t = \mathbf{g}_{enc}(\mathbf{x}_t)$
2. Summarize context (e.g., half of a sequence) into a context code  $\mathbf{c}_t$  using an auto-regressive model ( $\mathbf{g}_{ar}$ )
3. Predict  $\mathbf{z}_{t+k}$  using  $\mathbf{c}$  and trainable weights. Loss is similarity to true  $\mathbf{z}_{t+k}$  value over similarity to contrasting option

Figure [source](#)

# CPC example: modeling audio sequences



Source: [van den Oord et al., 2018](#),

# CPC example: modeling audio sequences

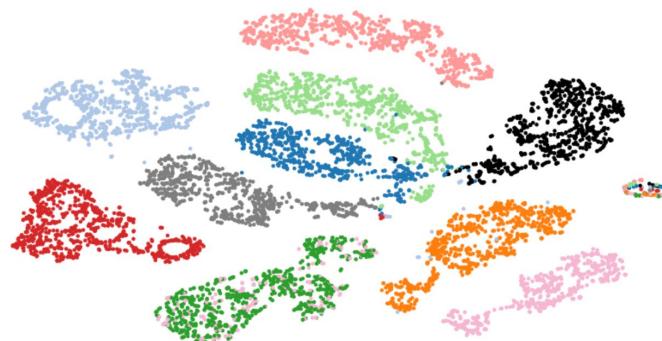


Figure 2: t-SNE visualization of audio (speech) representations for a subset of 10 speakers (out of 251). Every color represents a different speaker.

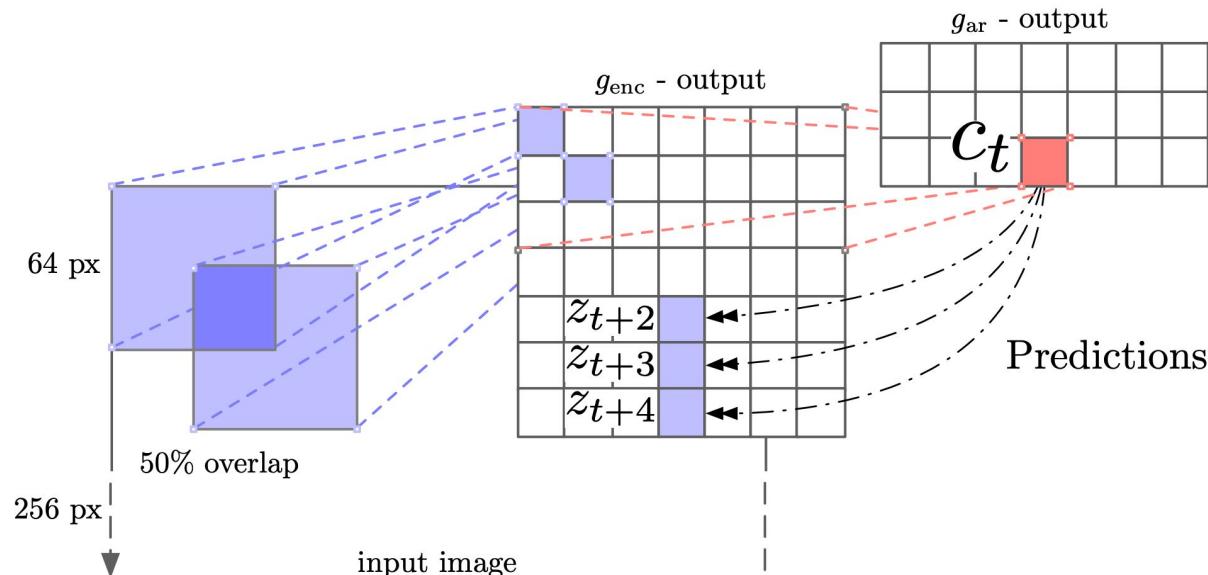
Method	ACC
<b>Phone classification</b>	
Random initialization	27.6
MFCC features	39.7
CPC	64.6
Supervised	74.6
<b>Speaker classification</b>	
Random initialization	1.87
MFCC features	17.6
CPC	97.4
Supervised	98.5

Linear classification on trained representations (LibriSpeech dataset)

Source: [van den Oord et al., 2018](#),

# CPC example: modeling visual context

Idea: split image into patches, model rows of patches from top to bottom as a sequence. I.e., use top rows as context to predict bottom rows.



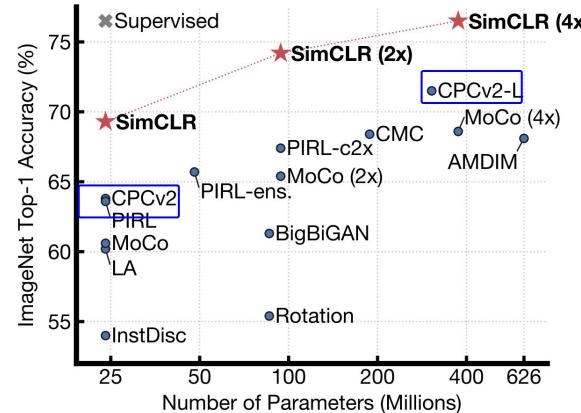
Source: [van den Oord et al., 2018](#),

# CPC example: modeling visual context

Method	Top-1 ACC
<b>Using AlexNet conv5</b>	
Video [28]	29.8
Relative Position [11]	30.4
BiGan [35]	34.8
Colorization [10]	35.2
Jigsaw [29] *	38.1
<b>Using ResNet-V2</b>	
Motion Segmentation [36]	27.6
Exemplar [36]	31.5
Relative Position [36]	36.2
Colorization [36]	39.6
<b>CPC</b>	<b>48.7</b>

Table 3: ImageNet top-1 unsupervised classification results. \*Jigsaw is not directly comparable to the other AlexNet results because of architectural differences.

- Compares favorably with other pretext task-based self-supervised learning method.
- Doesn't do as well compared to newer instance-based contrastive learning methods on image feature learning.



Source: [van den Oord et al., 2018](#),

# Summary: Contrastive Representation Learning

A general formulation for contrastive learning:

$$\text{score}(f(x), f(x^+)) \gg \text{score}(f(x), f(x^-))$$

InfoNCE loss: N-way classification among positive and 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](#))

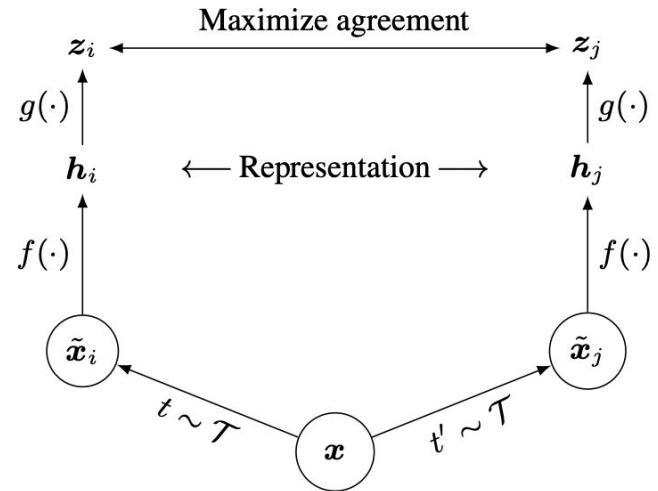
A *lower bound* on the mutual information between  $f(x)$  and  $f(x^+)$

$$MI[f(x), f(x^+)] - \log(N) \geq -L$$

# Summary: Contrastive Representation Learning

**SimCLR**: a simple framework for contrastive representation learning

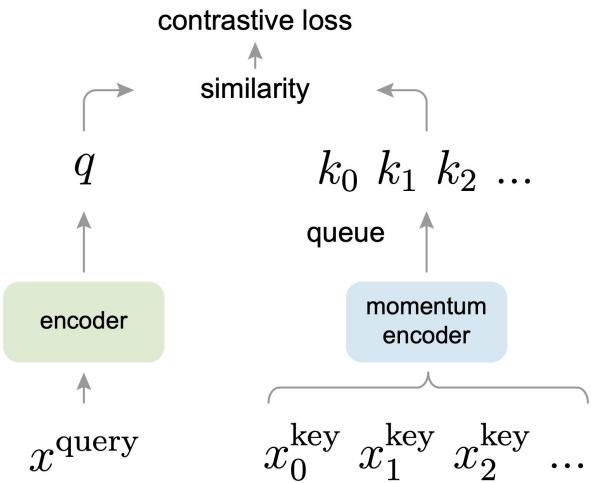
- **Key ideas**: non-linear projection head to allow flexible representation learning
- Simple to implement, effective in learning visual representation
- Requires large training batch size to be effective; large memory footprint



# Summary: Contrastive Representation Learning

**MoCo** (v1, v2): contrastive learning using momentum sample encoder

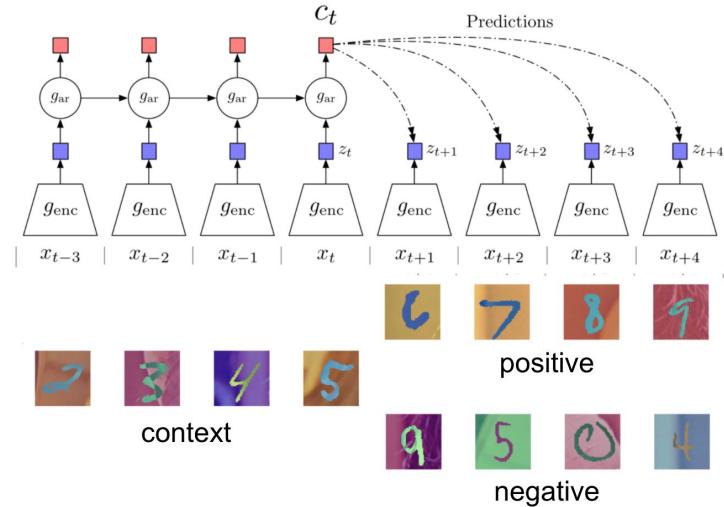
- Decouples negative sample size from minibatch size; allows large batch training without TPU
- MoCo-v2 combines the key ideas from SimCLR, i.e., nonlinear projection head, strong data augmentation, with momentum contrastive learning



# Summary: Contrastive Representation Learning

CPC: sequence-level contrastive learning

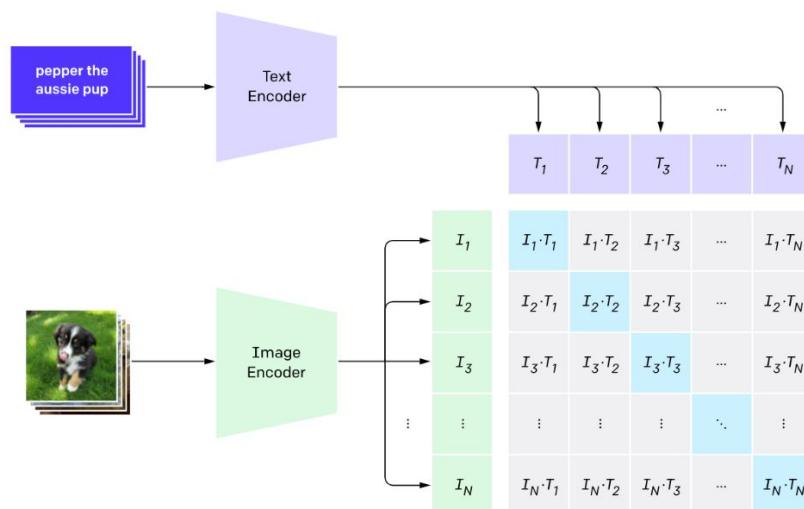
- Contrast “right” sequence with “wrong” sequence.
- InfoNCE loss with a time-dependent score function.
- Can be applied to a variety of learning problems, but not as effective in learning image representations compared to instance-level methods.



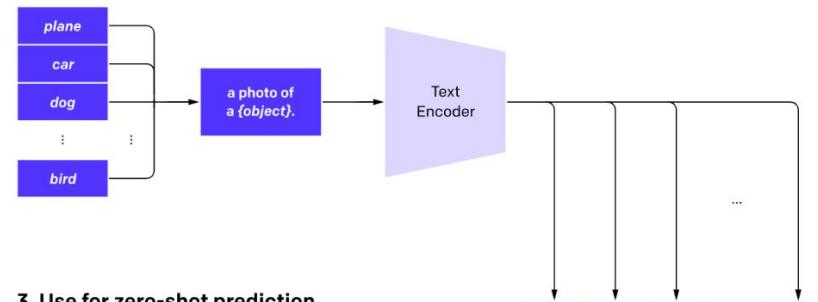
# Other examples: will be covered in next lecture

Contrastive learning between image and natural language sentences

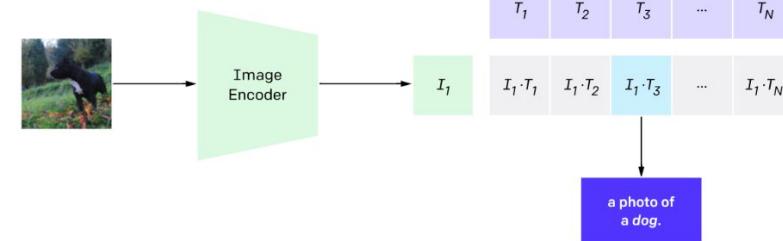
## 1. Contrastive pre-training



## 2. Create dataset classifier from label text



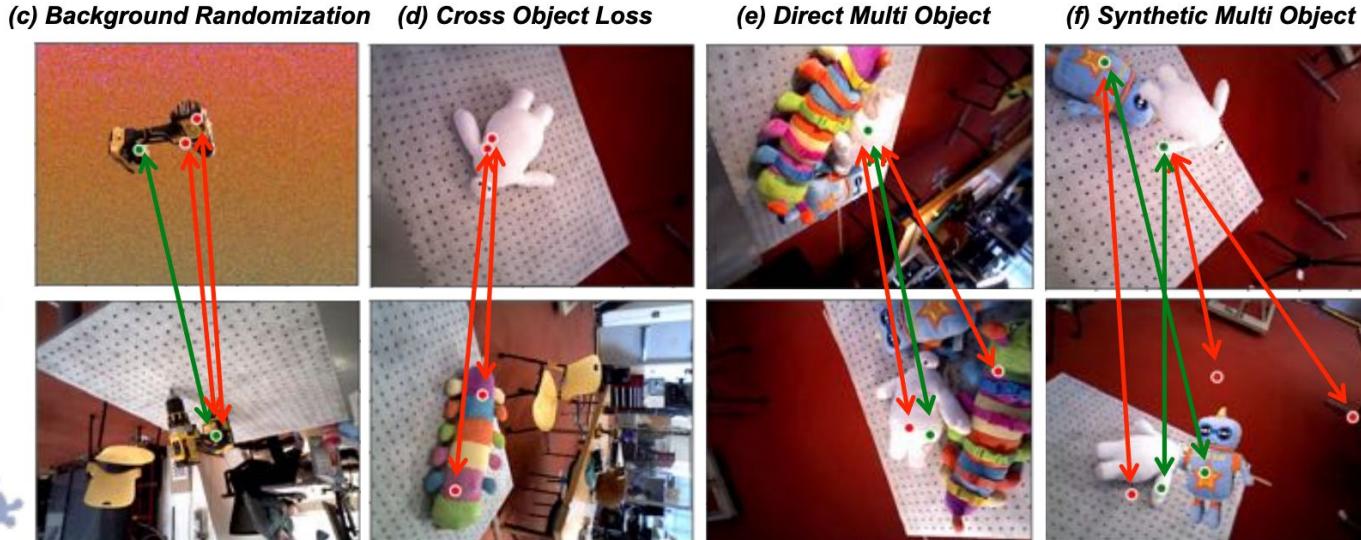
## 3. Use for zero-shot prediction



CLIP (*Contrastive Language–Image Pre-training*) Radford *et al.*, 2021

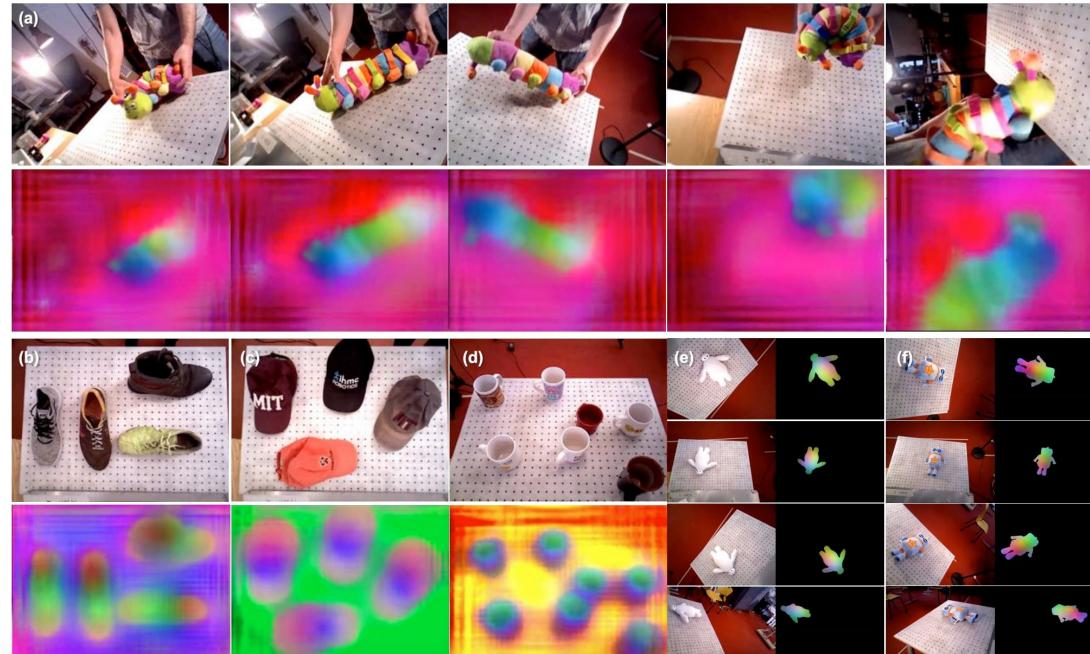
# Other examples

Contrastive learning on pixel-wise feature descriptors



Dense Object Net, Florence et al., 2018

# Other examples



Dense Object Net, Florence et al., 2018

# Other examples



**Next time: LLMs**

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

# Self-Supervised Learning

General idea: pretend there is a part of the data you don't know and train the neural network to predict that.

Y. LeCun

## Self-Supervised Learning

- ▶ Predict any part of the input from any other part.
- ▶ Predict the **future** from the **past**.
- ▶ Predict the **future** from the **recent past**.
- ▶ Predict the **past** from the **present**.
- ▶ Predict the **top** from the **bottom**.
- ▶ Predict the **occluded** from the **visible**
- ▶ **Pretend there is a part of the input you don't know and predict that.**

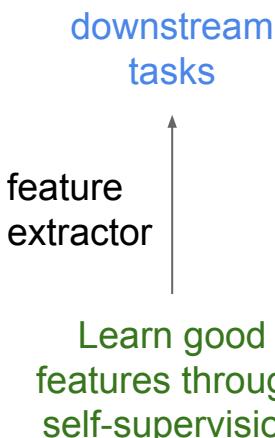
Time →

← Past      Present      Future →

# “The Cake of Learning”

## How Much Information is the Machine Given during Learning?

Y. LeCun



- ▶ “Pure” Reinforcement Learning (**cherry**)
  - ▶ The machine predicts a scalar reward given once in a while.
  - ▶ **A few bits for some samples**
  
- ▶ Supervised Learning (**icing**)
  - ▶ The machine predicts a category or a few numbers for each input
  - ▶ Predicting human-supplied data
  - ▶ **10→10,000 bits per sample**



- ▶ Self-Supervised Learning (**cake génoise**)
  - ▶ The machine predicts any part of its input for any observed part.
  - ▶ Predicts future frames in videos
  - ▶ **Millions of bits per sample**

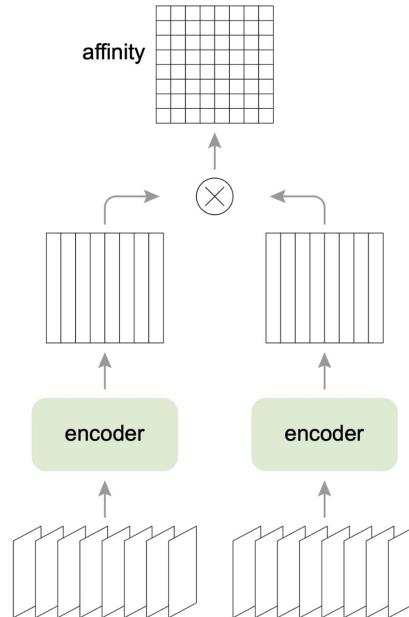
© 2019 IEEE International Solid-State Circuits Conference

1.1: Deep Learning Hardware: Past, Present, & Future

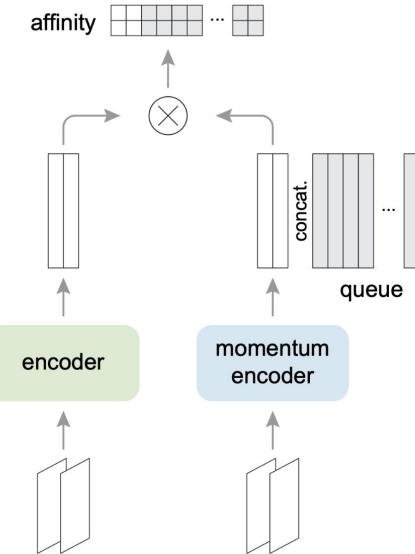
59

Source: Lecun 2019 Keynote at ISSCC

# Can we do better?



SimCLR



**Momentum Contrast  
(MoCo)**

Source: [Chen et al., 2020b](#)