CS 4803-DL / 7643-A: LECTURE 22
DANFEI XU

Topics:

- Self-supervised Learning
    - **Pretext task from image transformation**
    - **Contrastive learning**

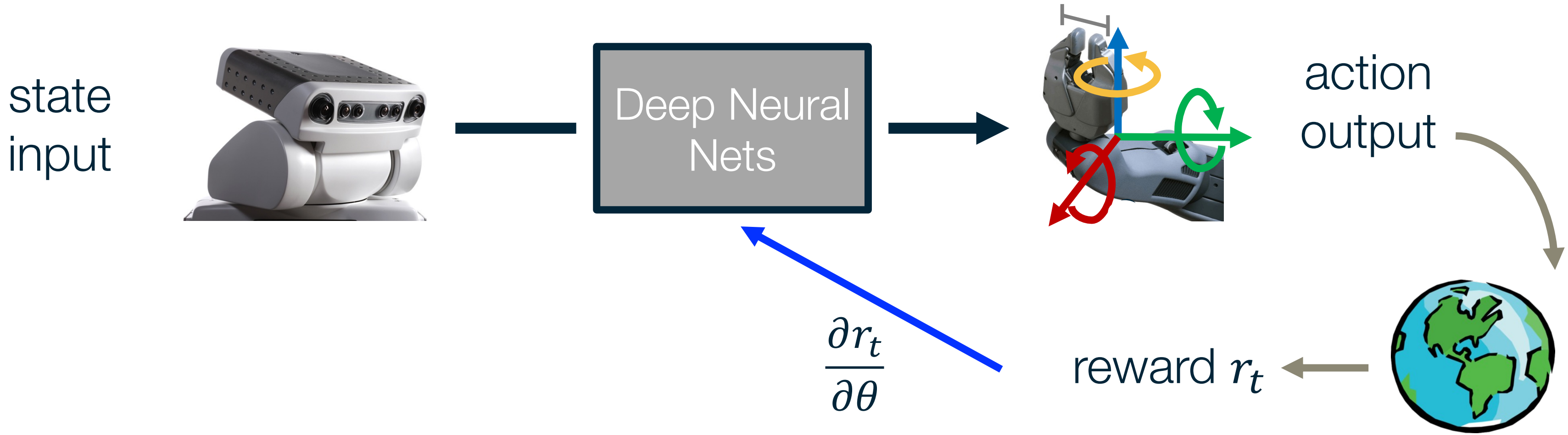
Administrative

Final project report due EOD Dec 4th, grace period EOD Dec 6th

Poster session Dec 6th 12:30-2pm

- Two sessions, 35min each. You’ll get assigned at the event.
- Check out other posters if you are presenting at a different session.
- We will have hors d'oeuvre and dessert available.
- We will announce a **best project award** at the end of the poster session (1:45-2pm).
- The event is open to the GT community. Expect many attendees, so bring your best work. And tell your friends to come too!

Deep Learning for Decision Making



state input

Deep Neural Nets

action output

reward r_t

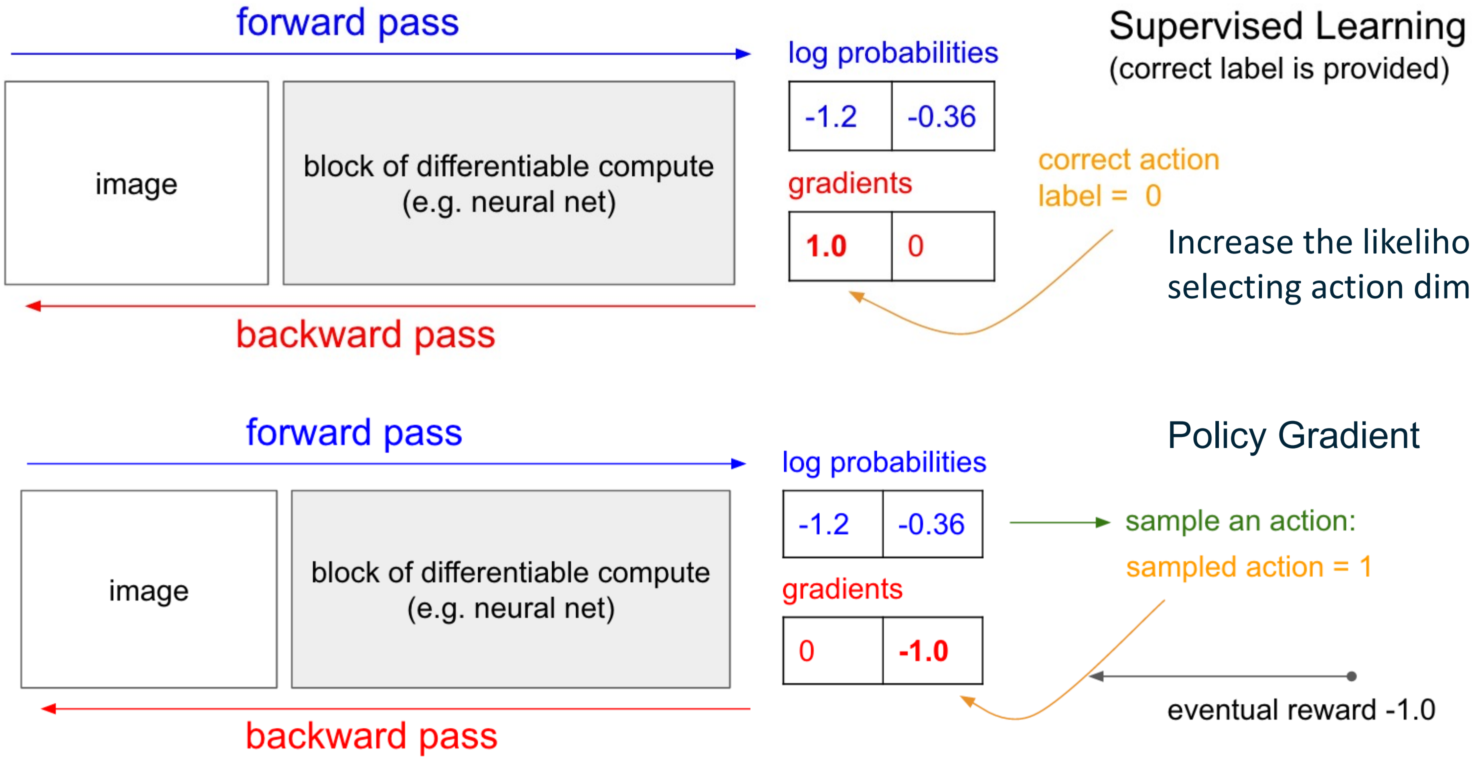
$\frac{\partial r_t}{\partial \theta}$

Problem: we don’t know the correct action label to supervise the output!

All we know is the step-wise task reward

Can we directly backprop reward???

Policy Gradient: Just backprop from reward (sort of)!



Supervised Learning

(correct label is provided)

forward pass

image

block of differentiable compute
(e.g. neural net)

log probabilities

-1.2	-0.36

gradients

1.0	0

correct action
label = 0

backward pass

Increase the likelihood of selecting action dim = 0!

Policy Gradient

forward pass

image

block of differentiable compute
(e.g. neural net)

log probabilities

-1.2	-0.36

sample an action:

sampled action = 1

gradients

0	**-1.0**

eventual reward -1.0

backward pass

Image Source: http://karpathy.github.io/2016/05/31/rl/

Decrease the likelihood of selecting action dim = 1!

Brief derivation of policy gradient (REINFORCE)

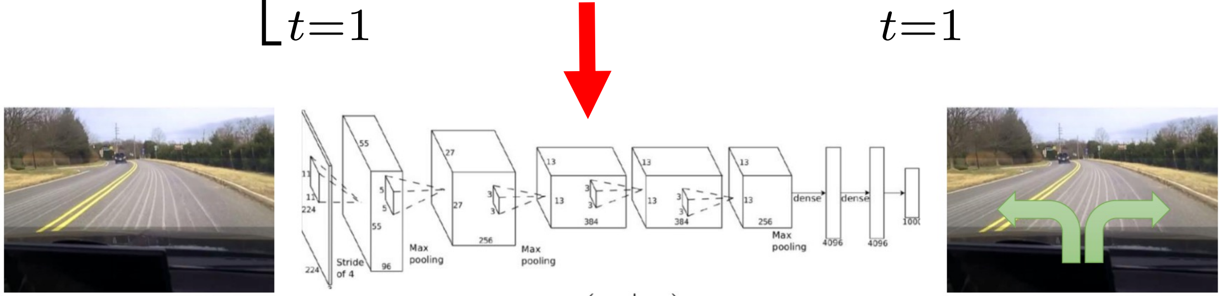
$$\pi_\theta(\tau) = p(s_0)\prod_{t=0}^{T} p_\theta\left(a_t \mid s_t\right)\cdot p\left(s_{t+1} \mid s_t, a_t\right)$$

$$\nabla_\theta J(\theta) = \mathbb{E}_{\tau\sim p_\theta(\tau)}[\underbrace{\nabla_\theta \log \pi_\theta(\tau)}\mathcal{R}(\tau)]$$

$$\nabla_\theta\left[\cancel{\log p(s_0}) + \sum_{t=1}^{T} \log \pi_\theta(a_t|s_t) + \sum_{t=1}^{T} \cancel{\log p(s_{t+1} \mid s_t, a_t})\right]$$

Doesn't depend on Transition probabilities!

$$= \mathbb{E}_{\tau\sim p_\theta(\tau)}\left[\sum_{t=1}^{T} \nabla_\theta \log \pi_\theta(a_t|s_t) \cdot \sum_{t=1}^{T} \mathcal{R}(s_t, a_t)\right]$$



$\mathbf{s}_t$ $\pi_\theta(\mathbf{a}_t|\mathbf{s}_t)$ $\mathbf{a}_t$

Can use continuous action space!

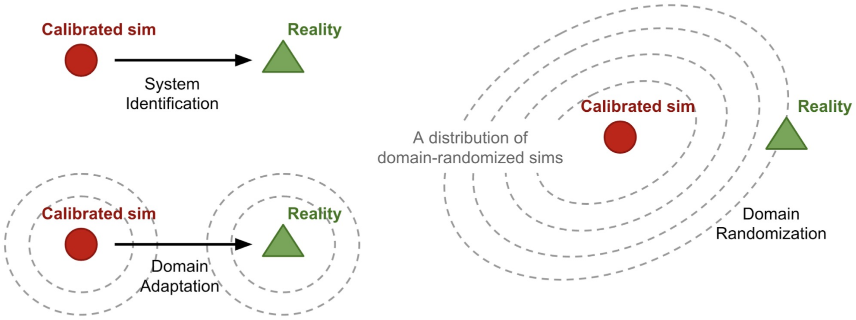
Policy Gradient Methods

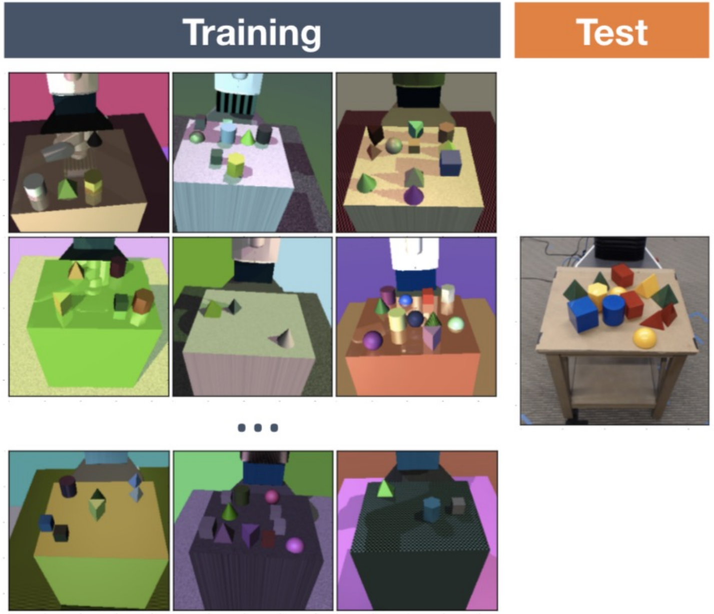
- REINFORCE: $\nabla_\theta J(\pi_\theta) = \mathrm{E}_{a\sim\pi_\theta}[\nabla_\theta \log \pi_\theta(a|s) R(s,a)]$
- Actor-critic (AC): $\nabla_\theta J(\pi_\theta) = \mathrm{E}_{a\sim\pi_\theta}[\nabla_\theta \log \pi_\theta(a|s) Q(s,a)]$
- Advantage Actor-critic (A2C): $\nabla_\theta J(\pi_\theta) = \mathrm{E}_{a\sim\pi_\theta}[\nabla_\theta \log \pi_\theta(a|s) A(s,a)]$

Simulation to Real World Transfer (Sim2Real)

Issue: simulators is a *very crude* approximation of the real world!

Idea: domain randomization





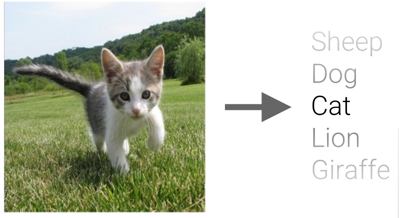
https://lilianweng.github.io/posts/2019-05-05-domain-randomization/

Recap: Reinforcement Learning

- It turns out we *can* directly backprop from reward (sort of)!
- Naïve policy gradient (REINFORCE) has high variance due to the use of episodic reward. Credit assignment is hard.
- Use Action Value Function (Q) instead!
  - Actor-Critic: learn Q value function jointly with policy
  - Advantage Actor-Critic: estimate advantage A using V value function
- Advanced policy gradient methods: TRPO, PPO
- Still pretty expensive to train! Mostly used in simulation.

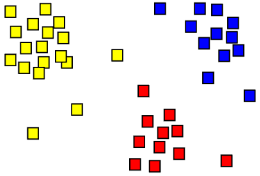
Supervised Learning

- Train Input: $\{X, Y\}$
- Learning output: $f: X \rightarrow Y$, $P(y|x)$
- e.g. classification



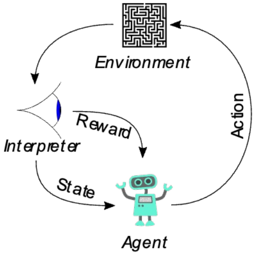
Unsupervised Learning

- Input: $\{X\}$
- Learning output: $P(x)$
- Example: Clustering, density estimation, generative modeling



Reinforcement Learning

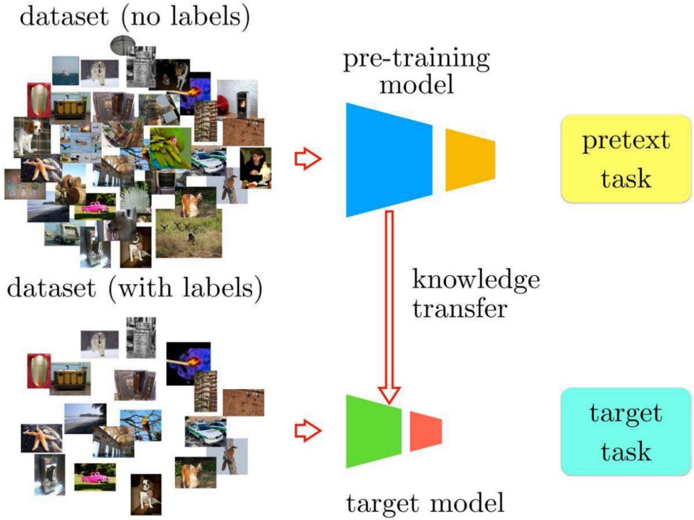
- Evaluative feedback in the form of **reward**
- No supervision on the right action



Self-supervised Learning

In short: still supervised learning, with two important distinctions:

1. Learn from labels generated *autonomously* instead of human annotations.
2. The goal is to learn *good representations* for *other target tasks.*



Source: Noroozi *et al.*, 2018

Self-supervised pretext tasks

Example: learn to predict image transformations / complete corrupted images

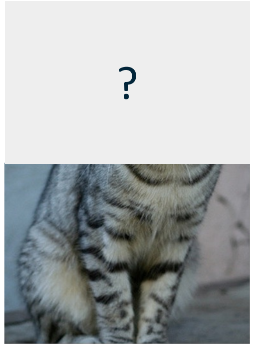
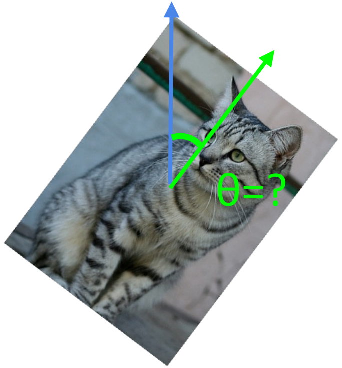
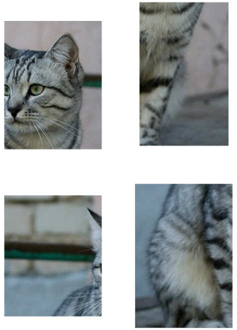


image completion



rotation prediction

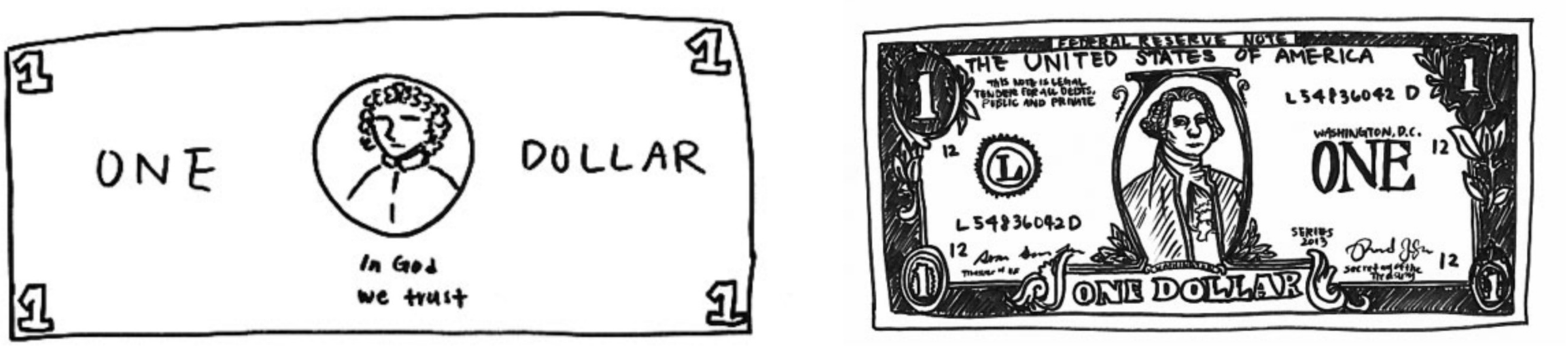


“jigsaw puzzle”

colorization

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

Generative vs. 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

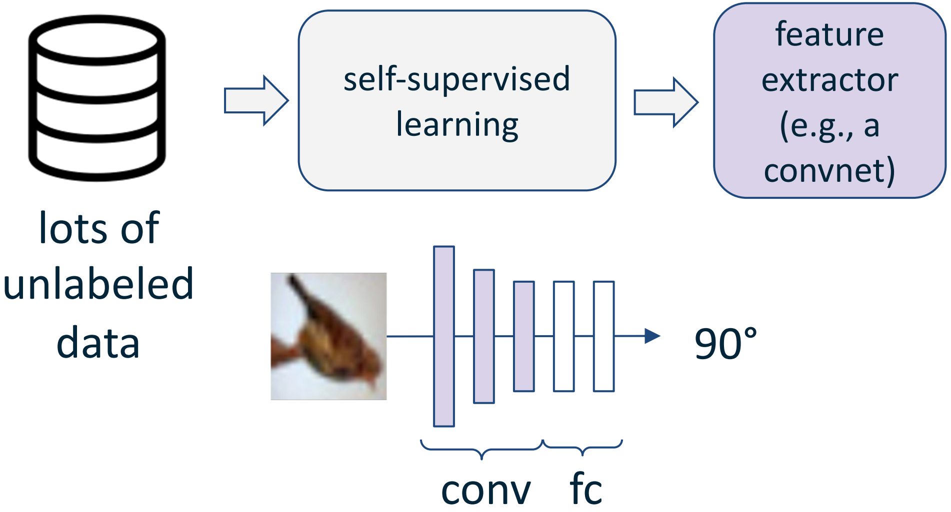
Source: Anand, 2020

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?



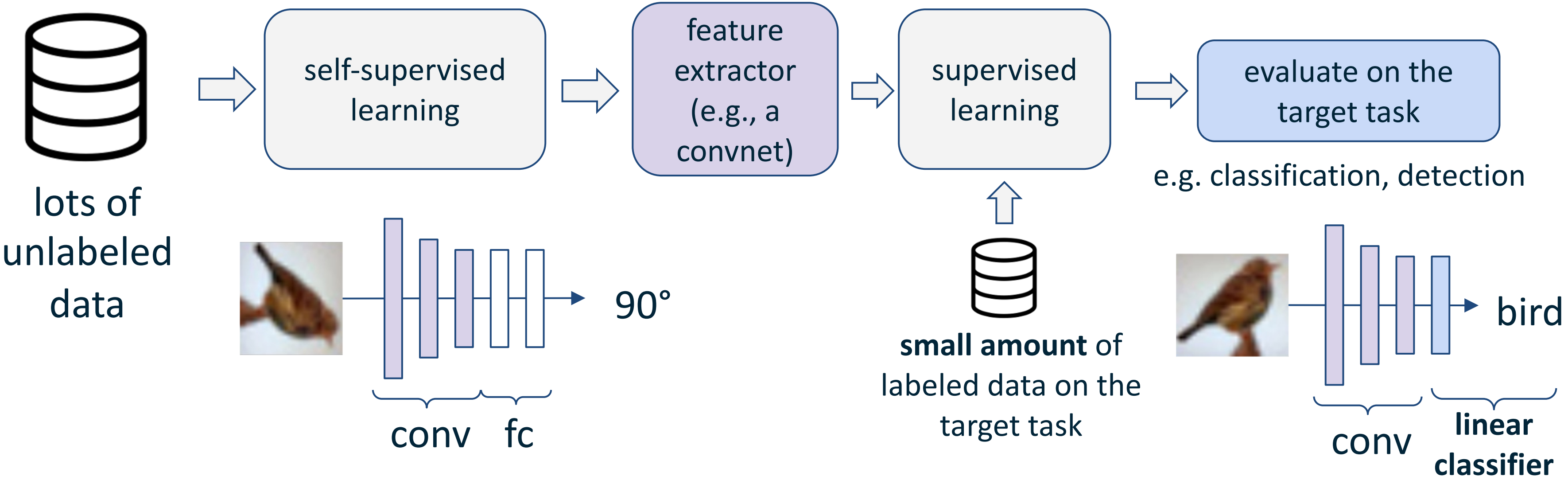
lots of unlabeled data

self-supervised learning

feature extractor (e.g., a convnet)

1. Learn good feature extractors from self-supervised pretext tasks, e.g., predicting image rotations

How to evaluate a self-supervised learning method?



lots of unlabeled data

self-supervised learning

feature extractor (e.g., a convnet)

supervised learning

evaluate on the target task

e.g. classification, detection

small amount of labeled data on the target task

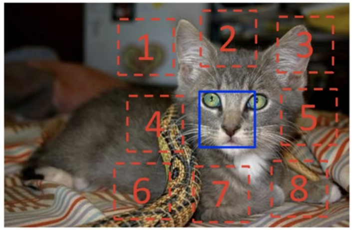
1. Learn good feature extractors from self-supervised pretext tasks, e.g., predicting image rotations

2. Attach a shallow network on the feature extractor; train the shallow network on the target task with small amount of labeled data

Broader picture

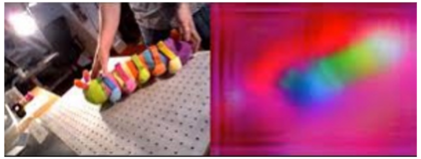
Today's lecture

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**

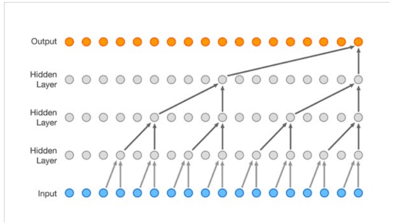
OpenAI

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 or from simple instructions – something which current NLP systems still largely struggle to do. Here we show that scaling up language models 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 more than any previous non-sparse language model, and test its performance in the few-shot setting. For all tasks, GPT-3 is applied without any gradient updates 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 cloze tasks, as well as several tasks that require on-the-fly reasoning or domain adaptation, such as unscrambling words, using a novel word in a sentence, or performing 3-digit arithmetic. At the same time, we also identify some datasets where GPT-3's few-shot learning still struggles, 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
- Sequence contrastive learning: CPC

Today’s Agenda

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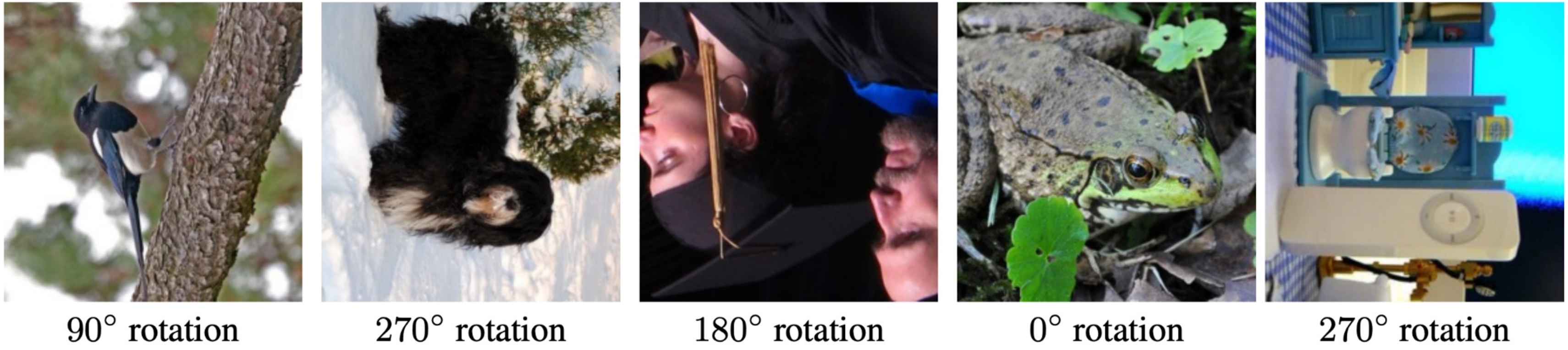
- Intuition and formulation
- Instance contrastive learning: SimCLR and MOCO
- Sequence contrastive learning: CPC

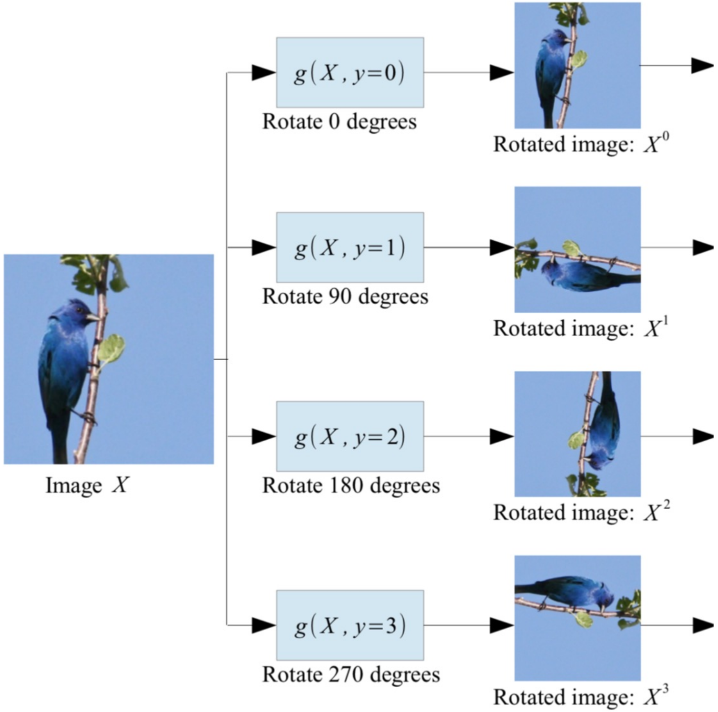
Pretext task: predict rotations



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

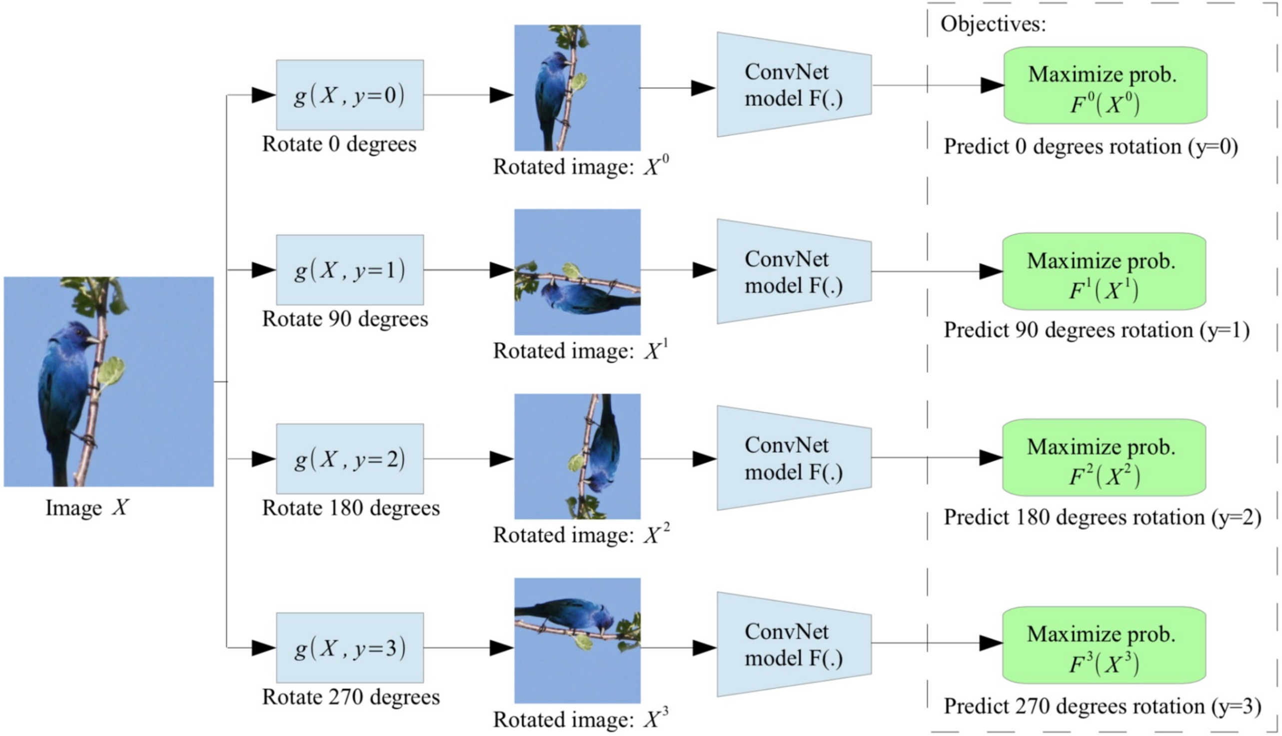


Self-supervised learning by rotating the entire input images.

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

(Image source: Gidaris et al. 2018)

Pretext task: predict rotations

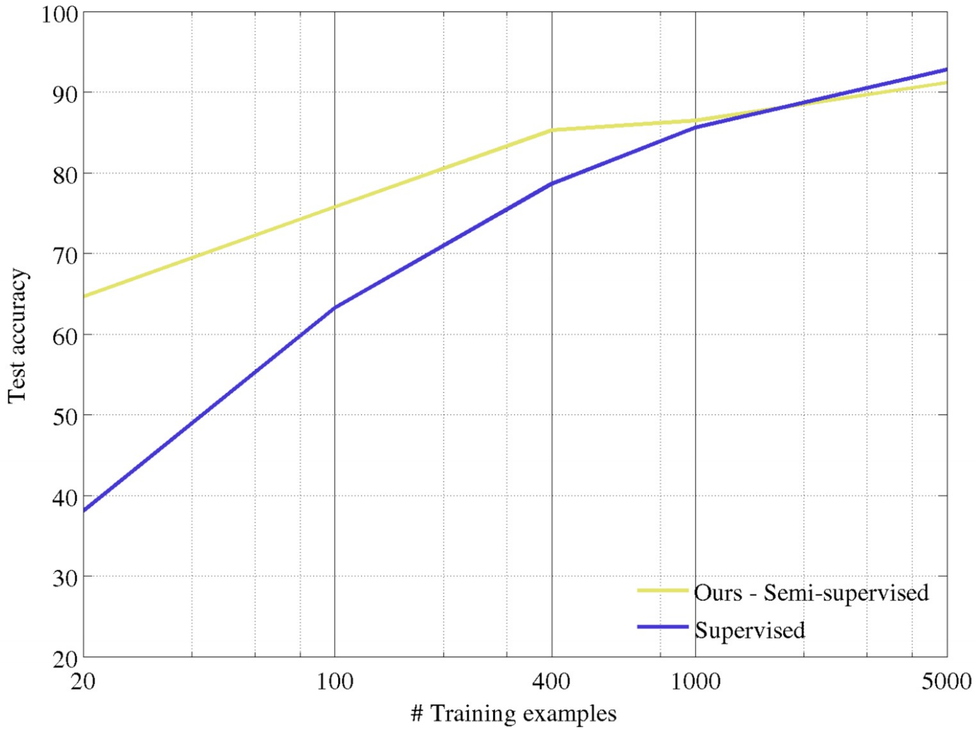


Self-supervised learning by rotating the entire input images.

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

(Image source: Gidaris et al. 2018)

Evaluation on semi-supervised learning

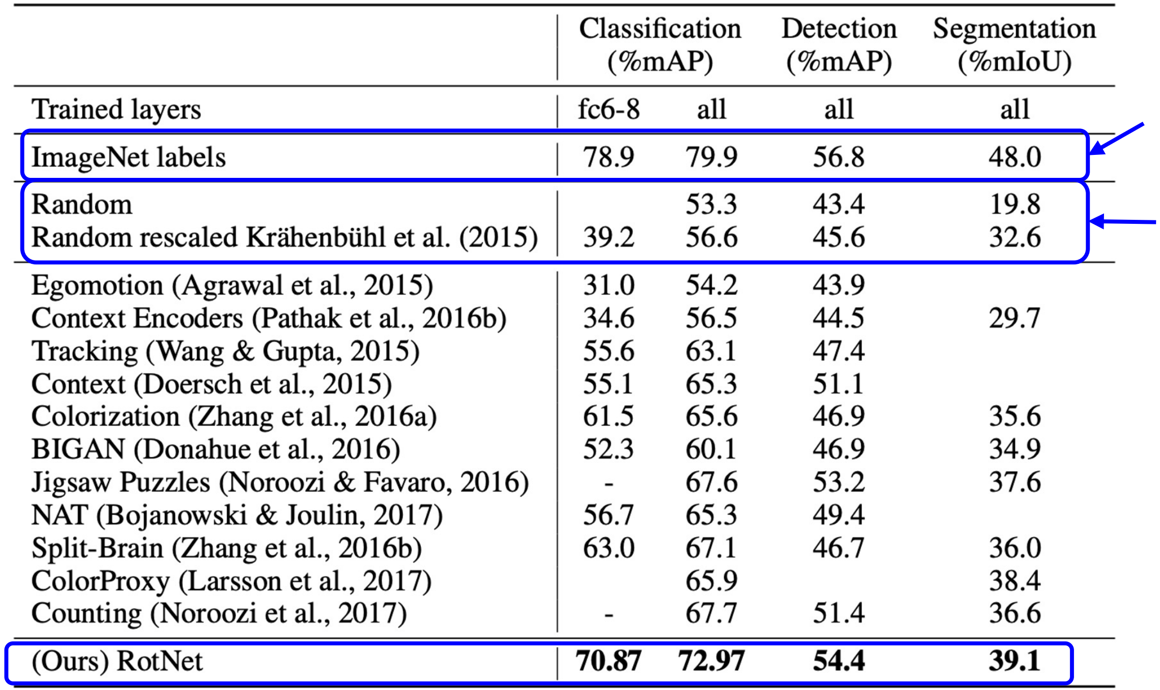


Self-supervised learning on **CIFAR10** (entire training set).

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	all
ImageNet labels	78.9	79.9	56.8	48.0
Random		53.3	43.4	19.8
Random rescaled Krähenbühl et al. (2015)	39.2	56.6	45.6	32.6
Egomotion (Agrawal et al., 2015)	31.0	54.2	43.9	
Context Encoders (Pathak et al., 2016b)	34.6	56.5	44.5	29.7
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	35.6
BIGAN (Donahue et al., 2016)	52.3	60.1	46.9	34.9
Jigsaw Puzzles (Noroozi & Favaro, 2016)	-	67.6	53.2	37.6
NAT (Bojanowski & Joulin, 2017)	56.7	65.3	49.4	
Split-Brain (Zhang et al., 2016b)	63.0	67.1	46.7	36.0
ColorProxy (Larsson et al., 2017)		65.9		38.4
Counting (Noroozi et al., 2017)	-	67.7	51.4	36.6
(Ours) RotNet	**70.87**	**72.97**	**54.4**	**39.1**

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**.

Self-supervised learning with rotation prediction

source: Gidaris et al. 2018

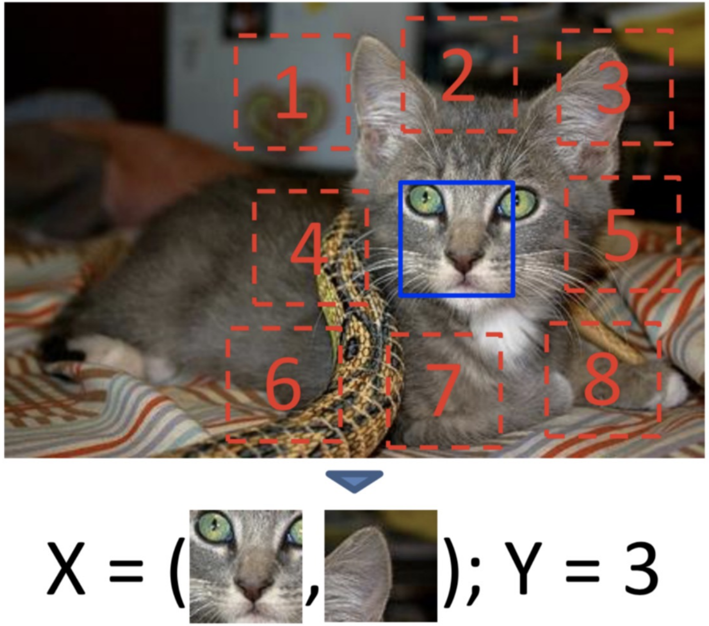
Visualize learned visual attentions

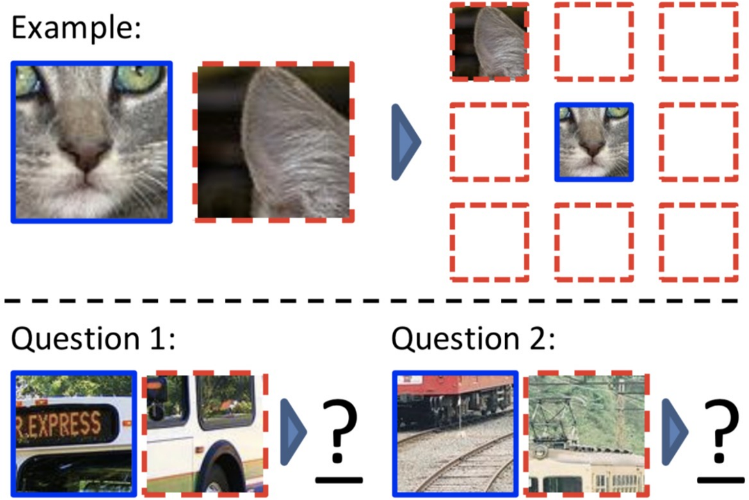
(a) **Attention maps of supervised model**

(b) **Attention maps of our self-supervised model**

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

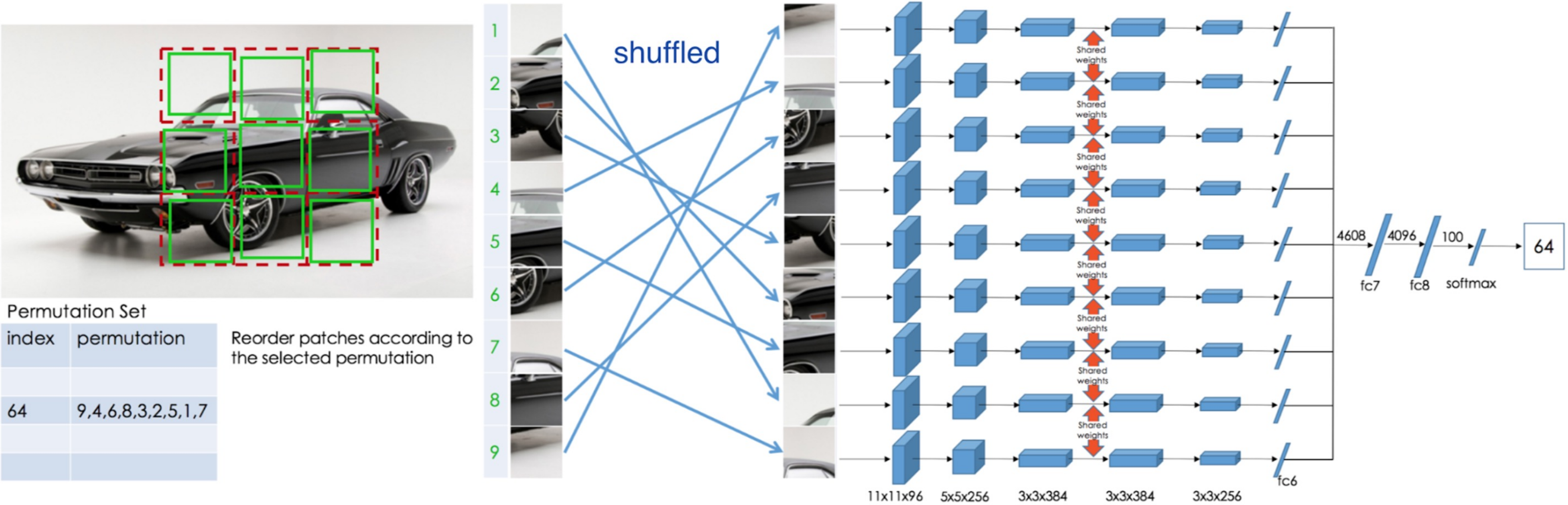
Pretext task: predict relative patch locations





(Image source: Doersch et al., 2015)

Pretext task: solving “jigsaw puzzles”



Permutation Set

index	permutation
64	9,4,6,8,3,2,5,1,7

Reorder patches according to the selected permutation

(Image source: Noroozi & Favaro, 2016)

Transfer learned features to supervised learning

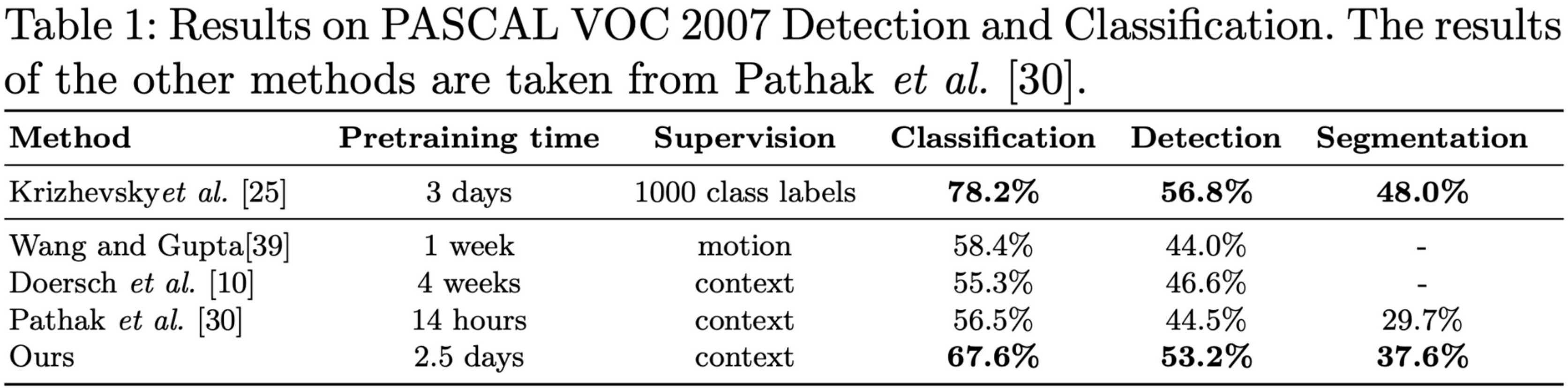


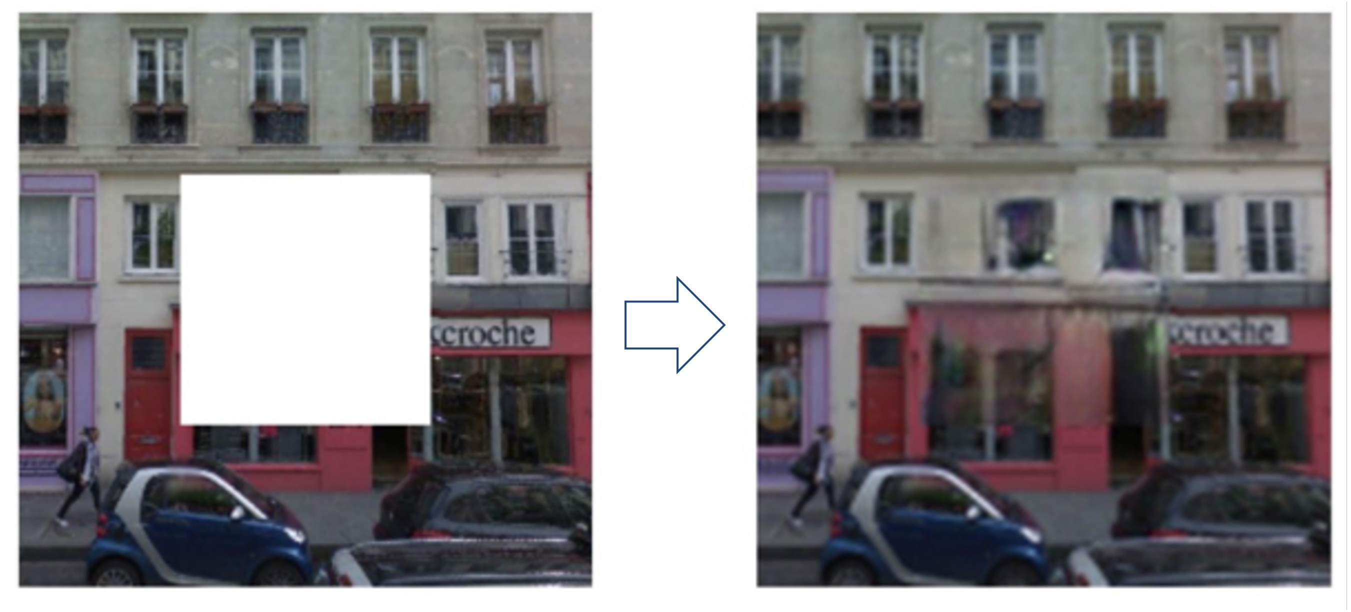
Table 1: Results on PASCAL VOC 2007 Detection and Classification. The results of the other methods are taken from Pathak *et al.* [30].

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

“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)

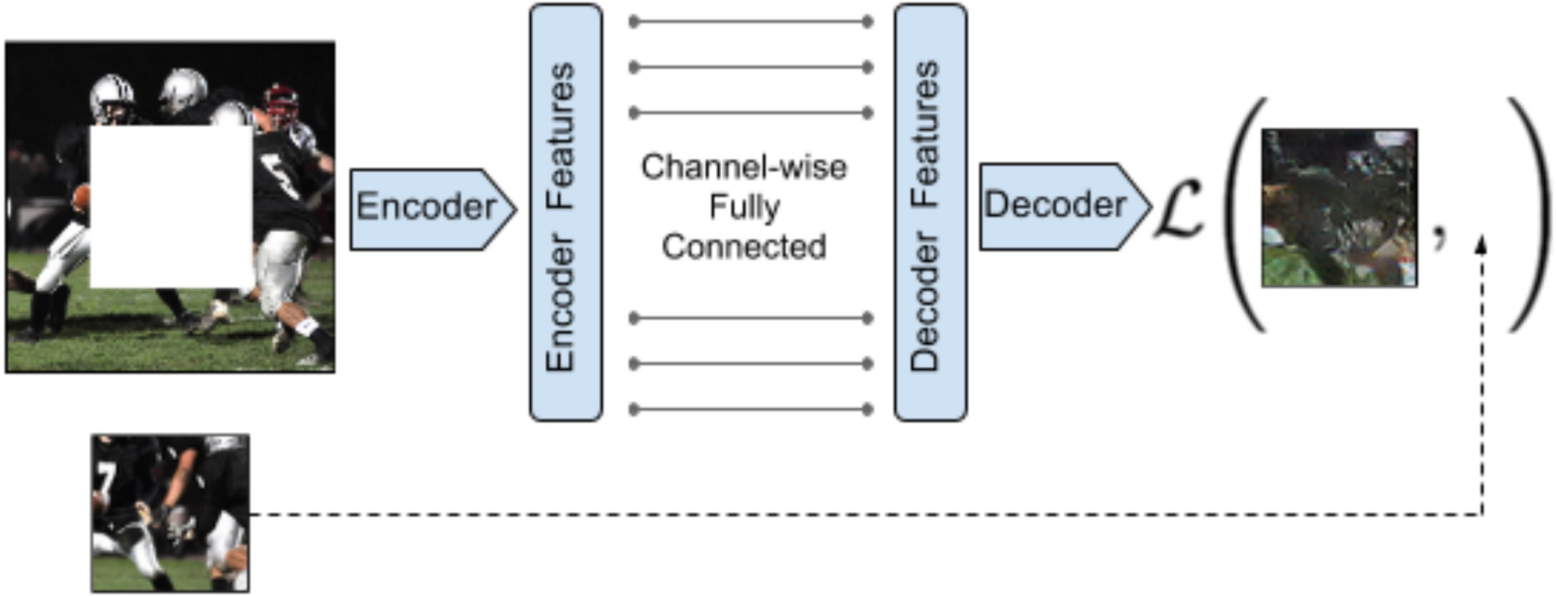
Pretext task: predict missing pixels (inpainting)



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

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

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

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

Adversarial loss between "real" images and *inpainted images*

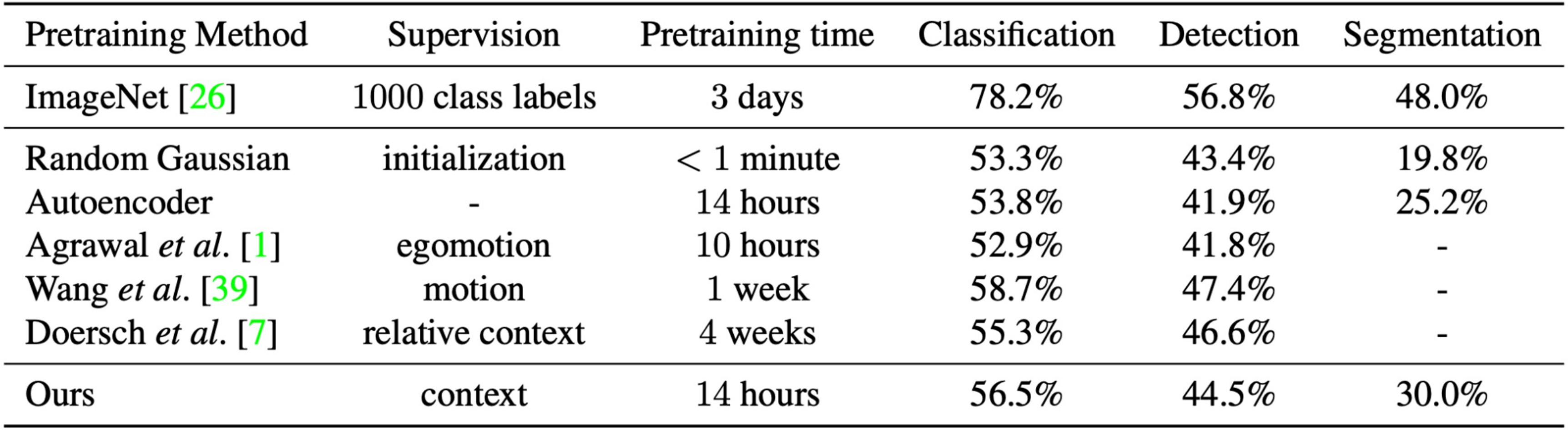
Source: Pathak et al., 2016

Inpainting evaluation

Input (context) reconstruction adversarial recon + adv

Source: Pathak et al., 2016

Transfer learned features to supervised learning

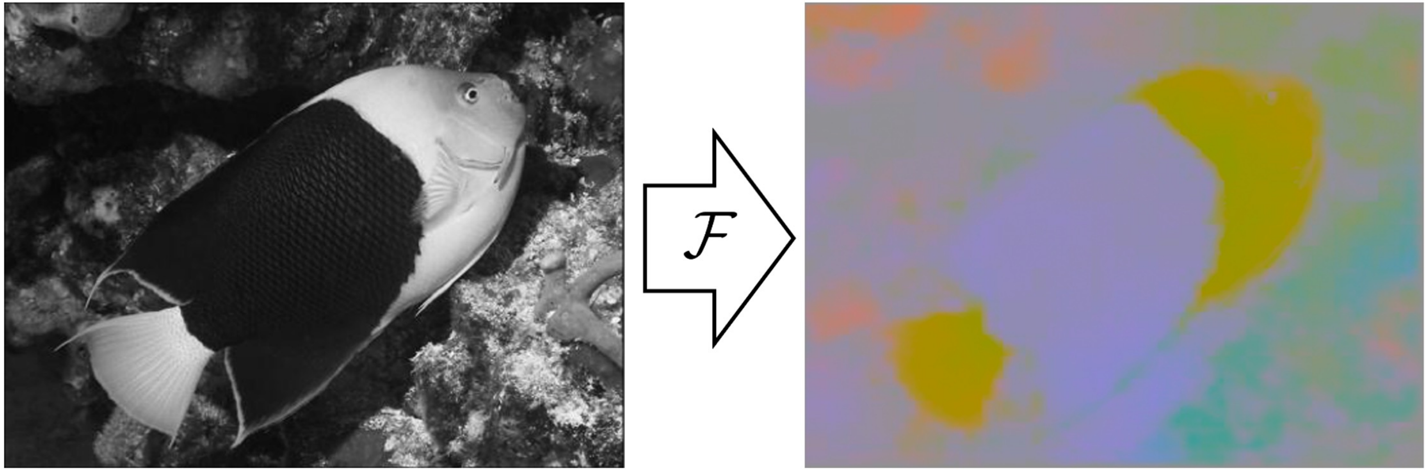


Pretraining Method	Supervision	Pretraining time	Classification	Detection	Segmentation
ImageNet [26]	1000 class labels	3 days	78.2%	56.8%	48.0%
Random Gaussian	initialization	< 1 minute	53.3%	43.4%	19.8%
Autoencoder	-	14 hours	53.8%	41.9%	25.2%
Agrawal *et al.* [1]	egomotion	10 hours	52.9%	41.8%	-
Wang *et al.* [39]	motion	1 week	58.7%	47.4%	-
Doersch *et al.* [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

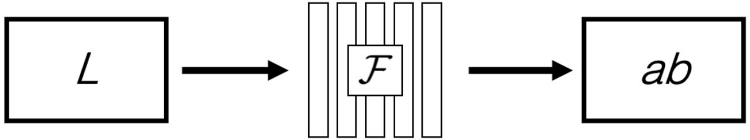


Grayscale image: *L* channel

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

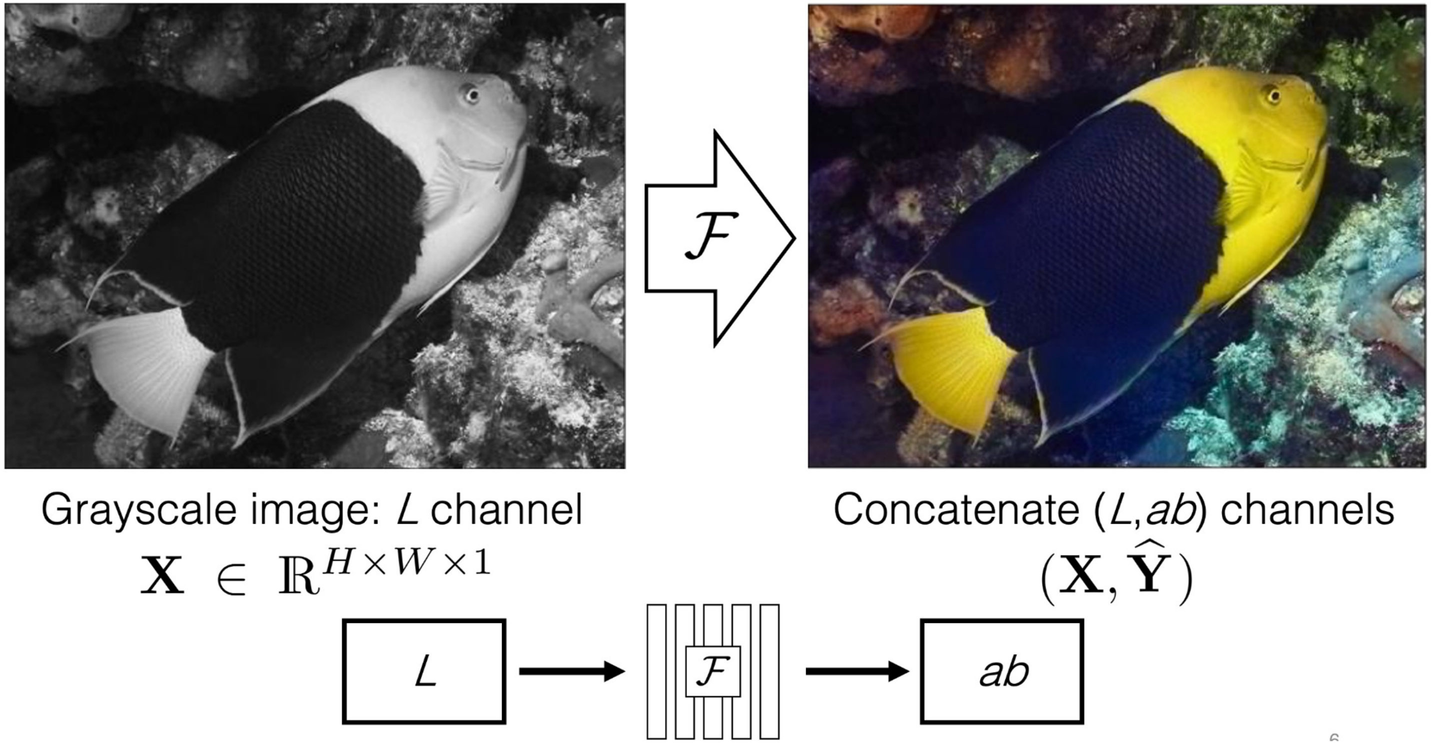
Color information: *ab* channels

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



Source: Richard Zhang / Phillip Isola

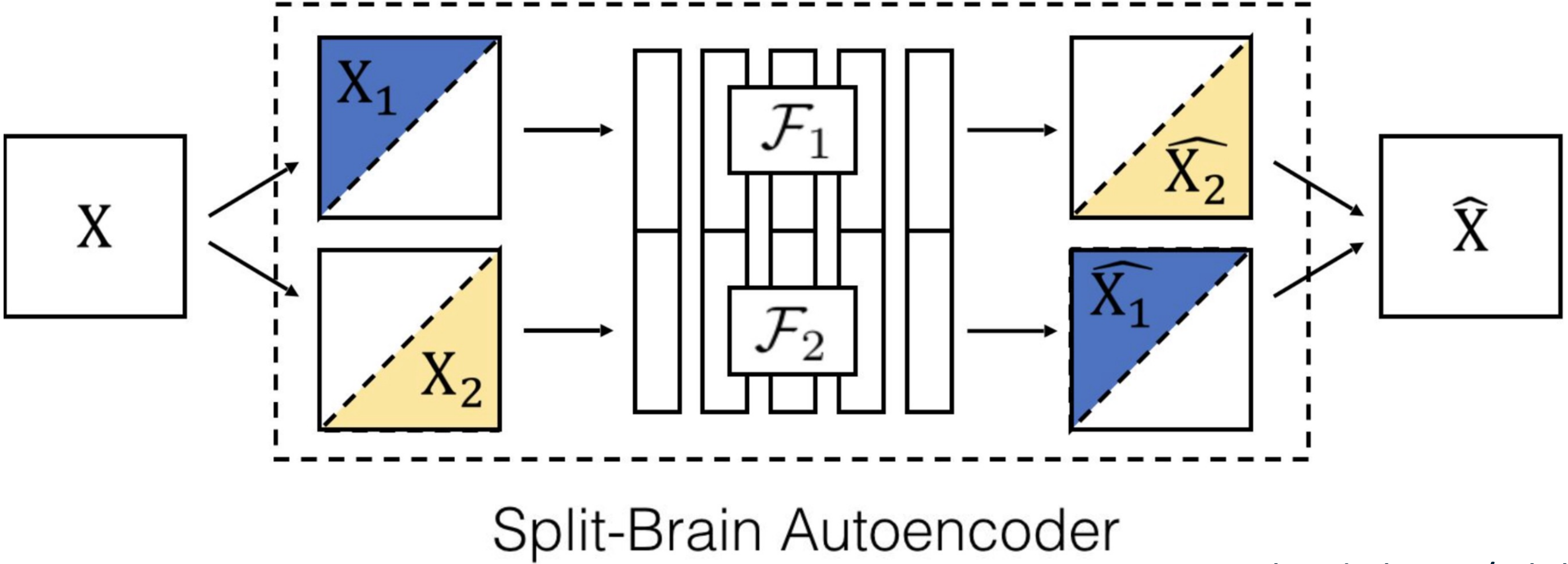
Pretext task: image coloring



Source: Richard Zhang / Phillip Isola

Learning features from colorization: Split-brain Autoencoder

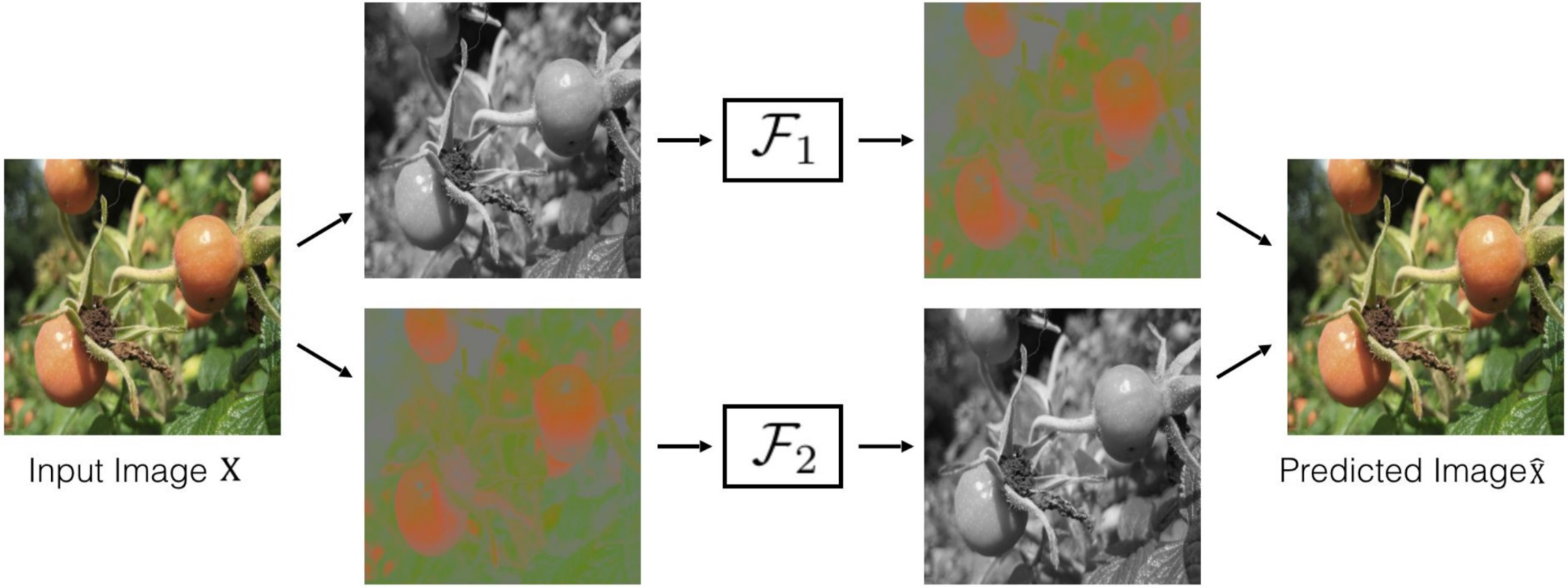
Idea: cross-channel predictions



Split-Brain Autoencoder

Source: Richard Zhang / Phillip Isola

Learning features from colorization: Split-brain Autoencoder



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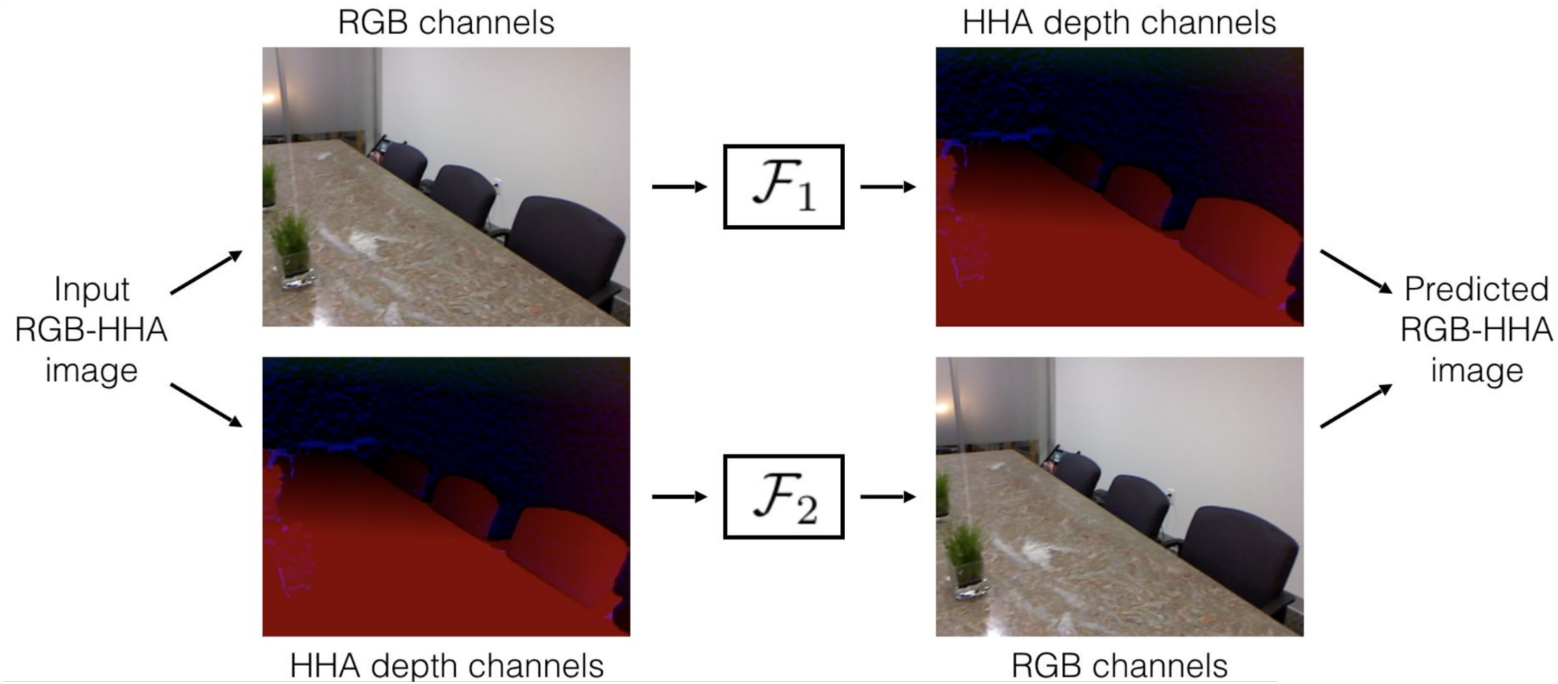
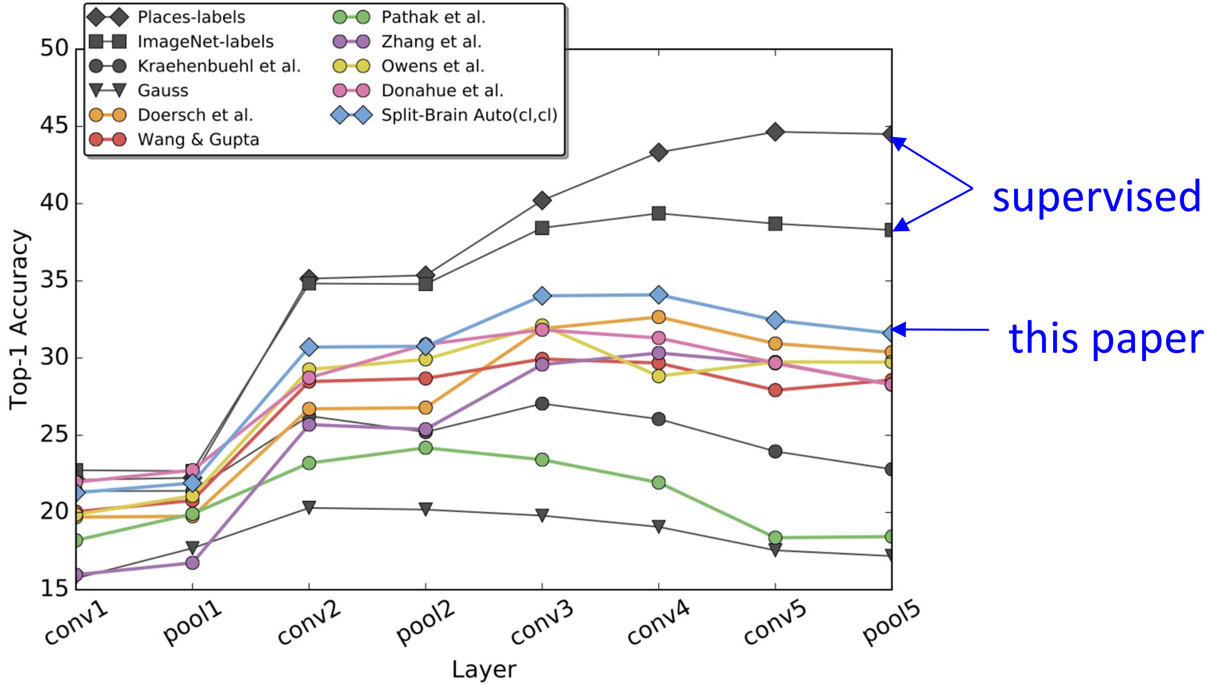


Source: Richard Zhang / Phillip Isola

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

Pretext task: 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

how should I color these frames?

$t = 0$

$t = 1$

$t = 2$

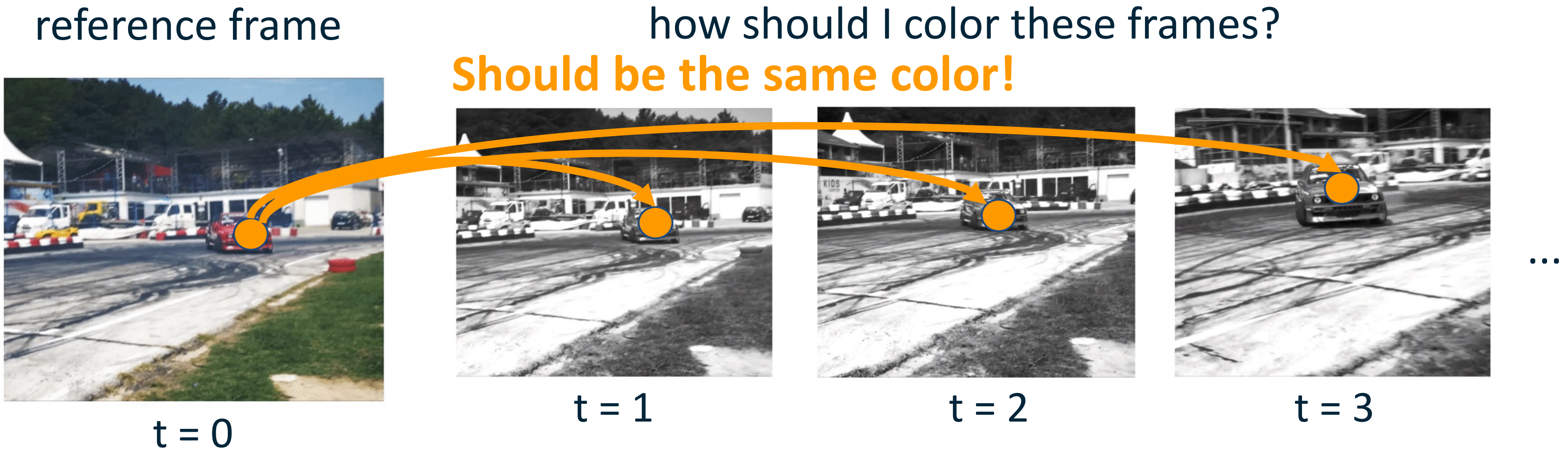
$t = 3$

…

Source: [Vondrick et al., 2018]

Pretext task: video coloring

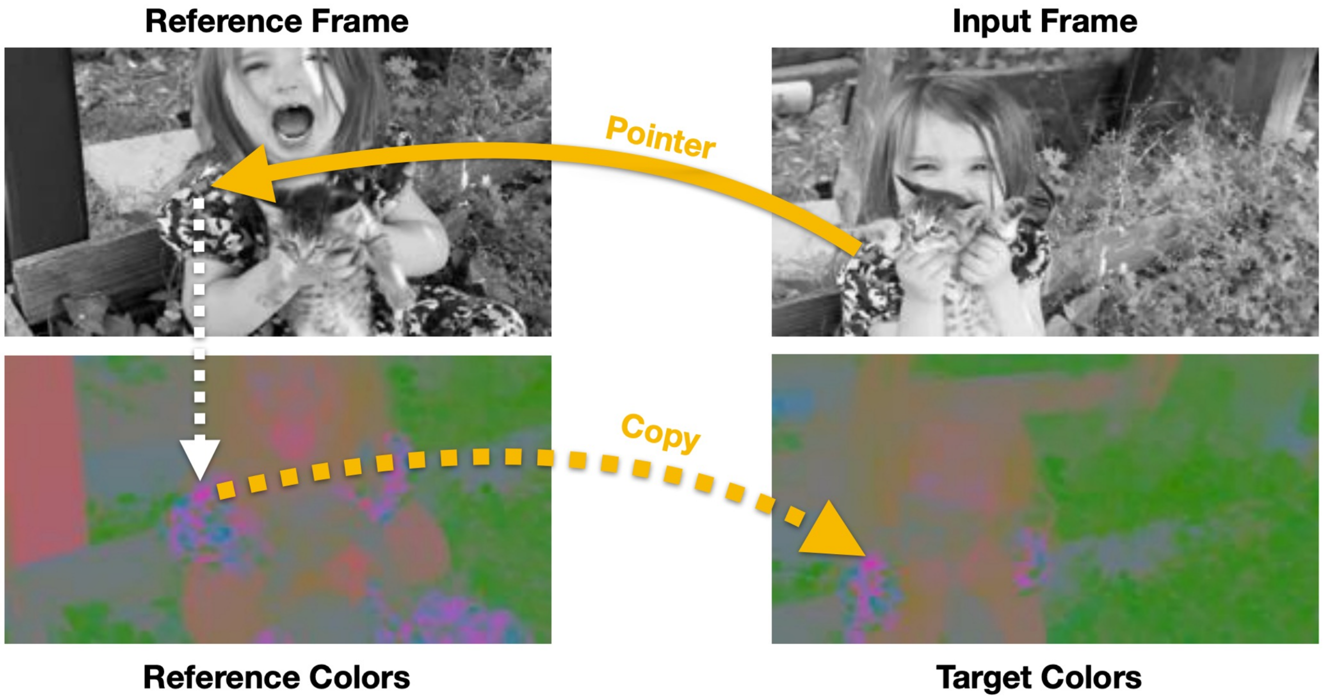
Idea: model the *temporal coherence* of colors in videos



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

Source: Vondrick et al., 2018

Learning to color videos



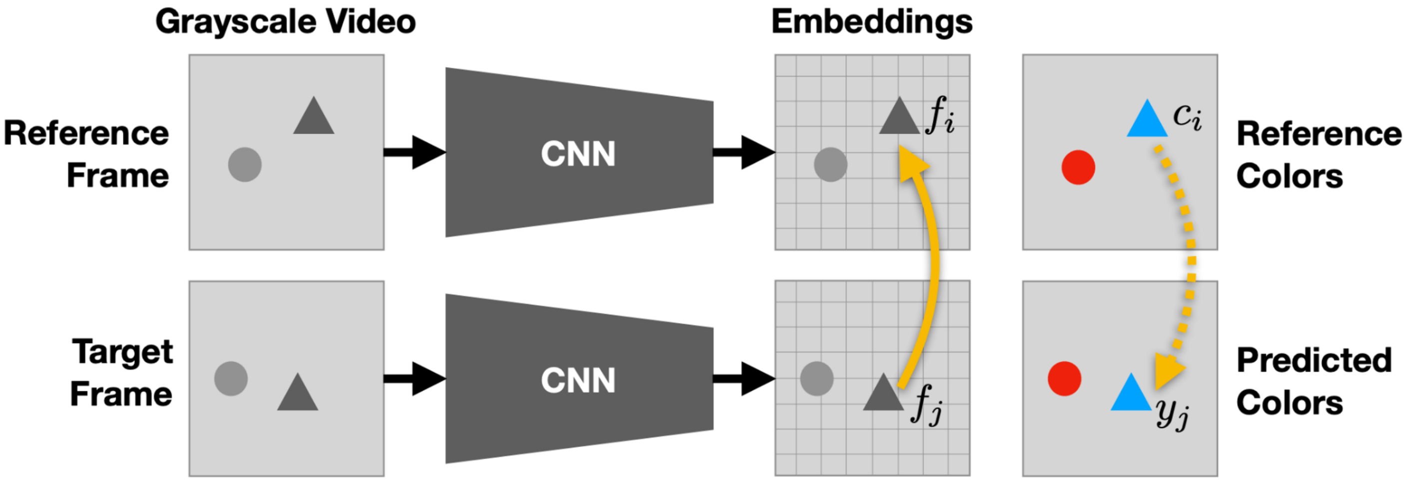
Learning objective:

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

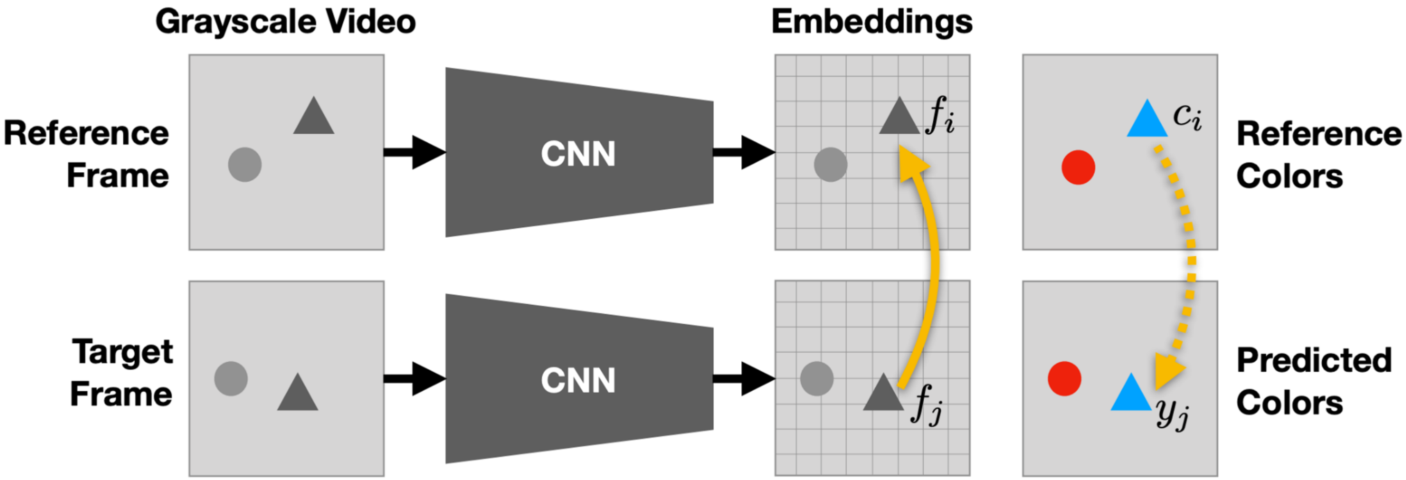


attention map on the reference frame

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

Source: Vondrick et al., 2018

Learning to color videos



attention map on the reference frame

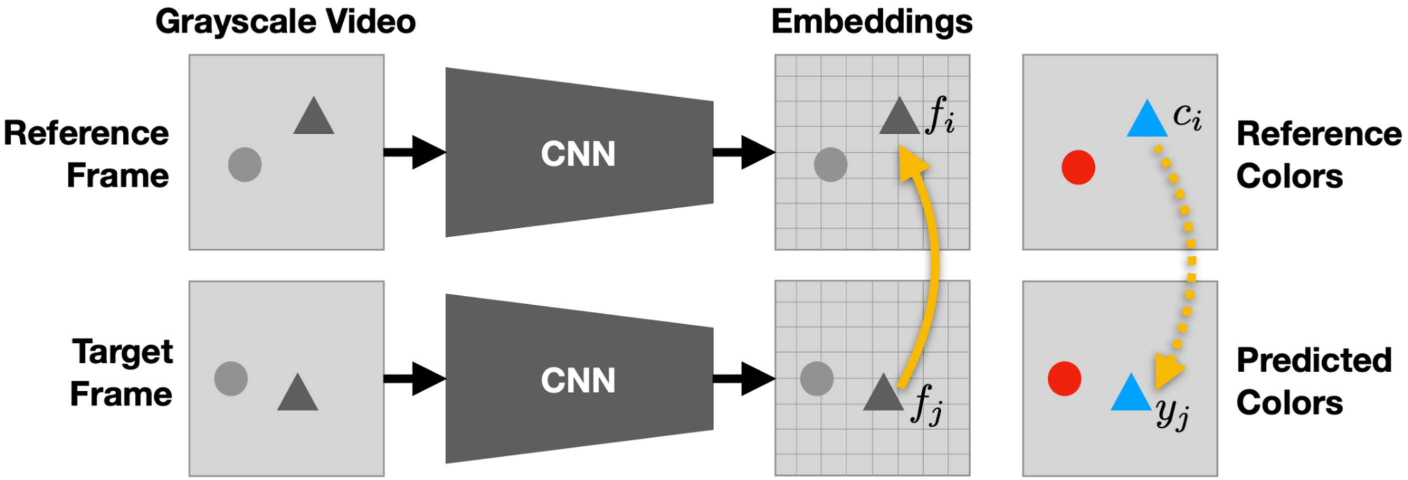
$$A_{ij} = \frac{\exp\left(f_i^T f_j\right)}{\sum_k \exp\left(f_k^T f_j\right)}$$

predicted color = weighted sum of the reference color

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

Source: Vondrick et al., 2018

Learning to color videos



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predicted color = weighted sum of the reference color

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

loss between predicted color and ground truth color

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

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

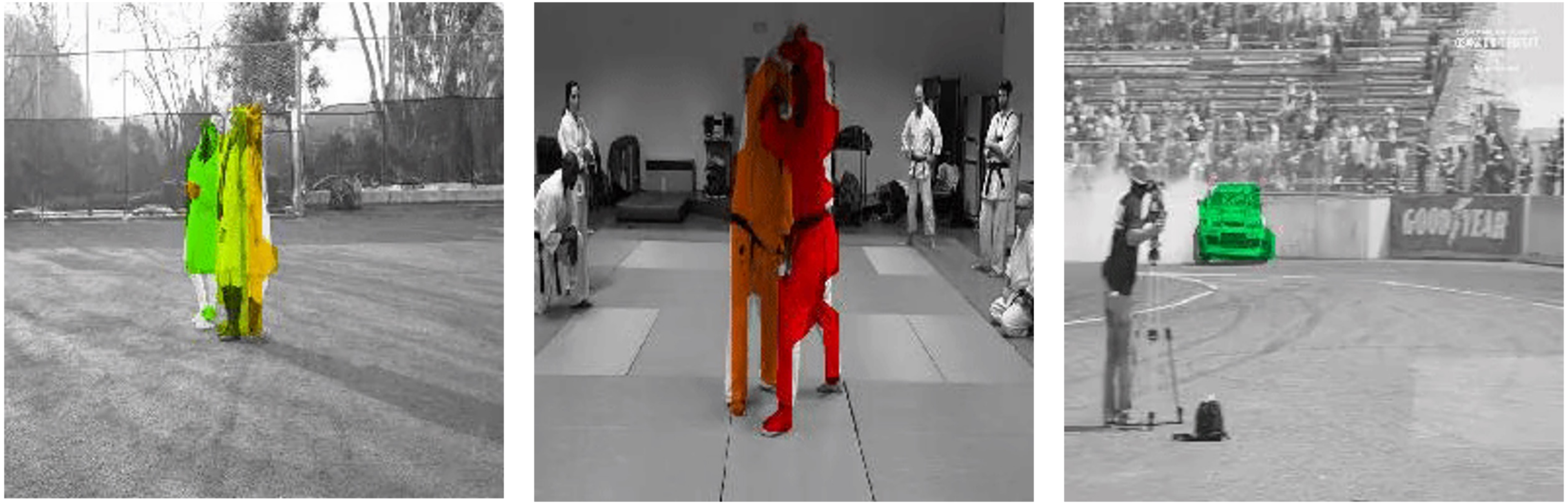
target frames (gray)

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 general.

Pretext tasks from image transformations

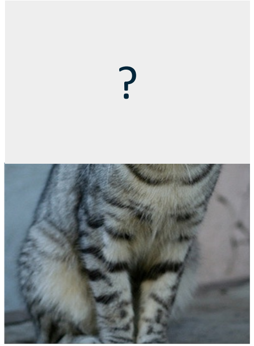
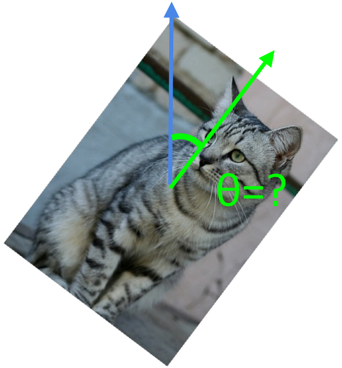


image
completion



rotation
prediction

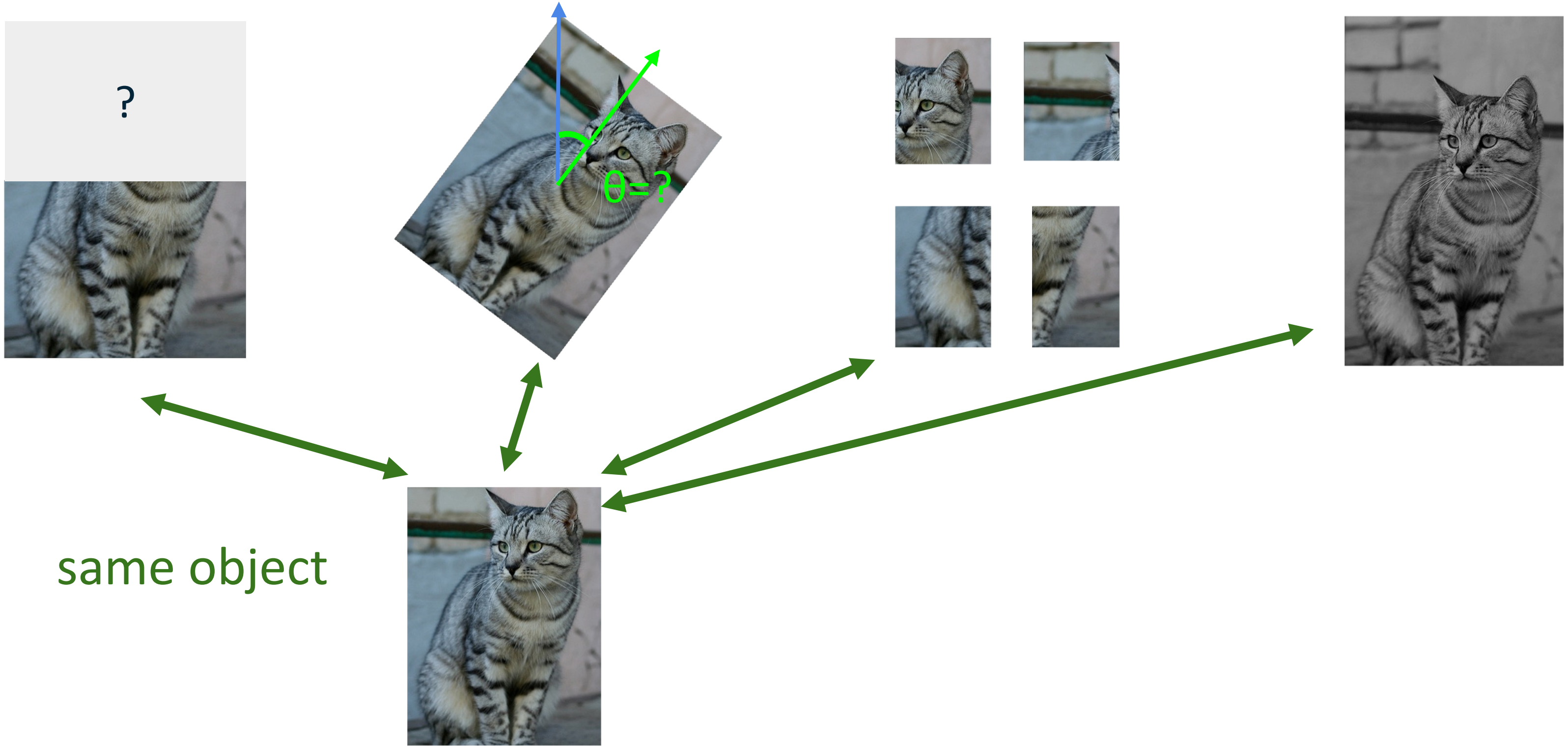
“jigsaw puzzle”

colorization

Learned representations may be tied to a specific pretext task!

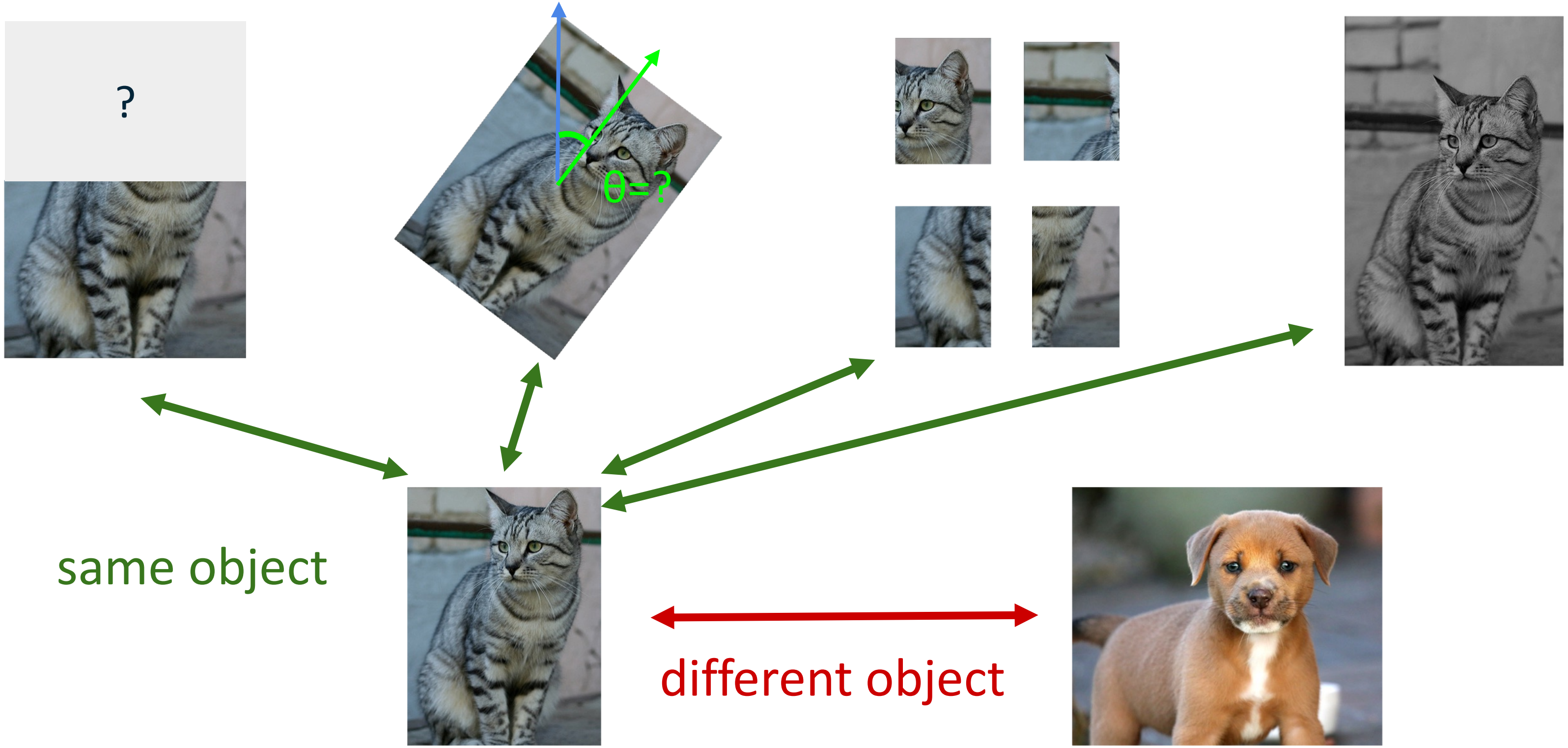
Can we come up with a more general pretext task?

A more general pretext task?



same object

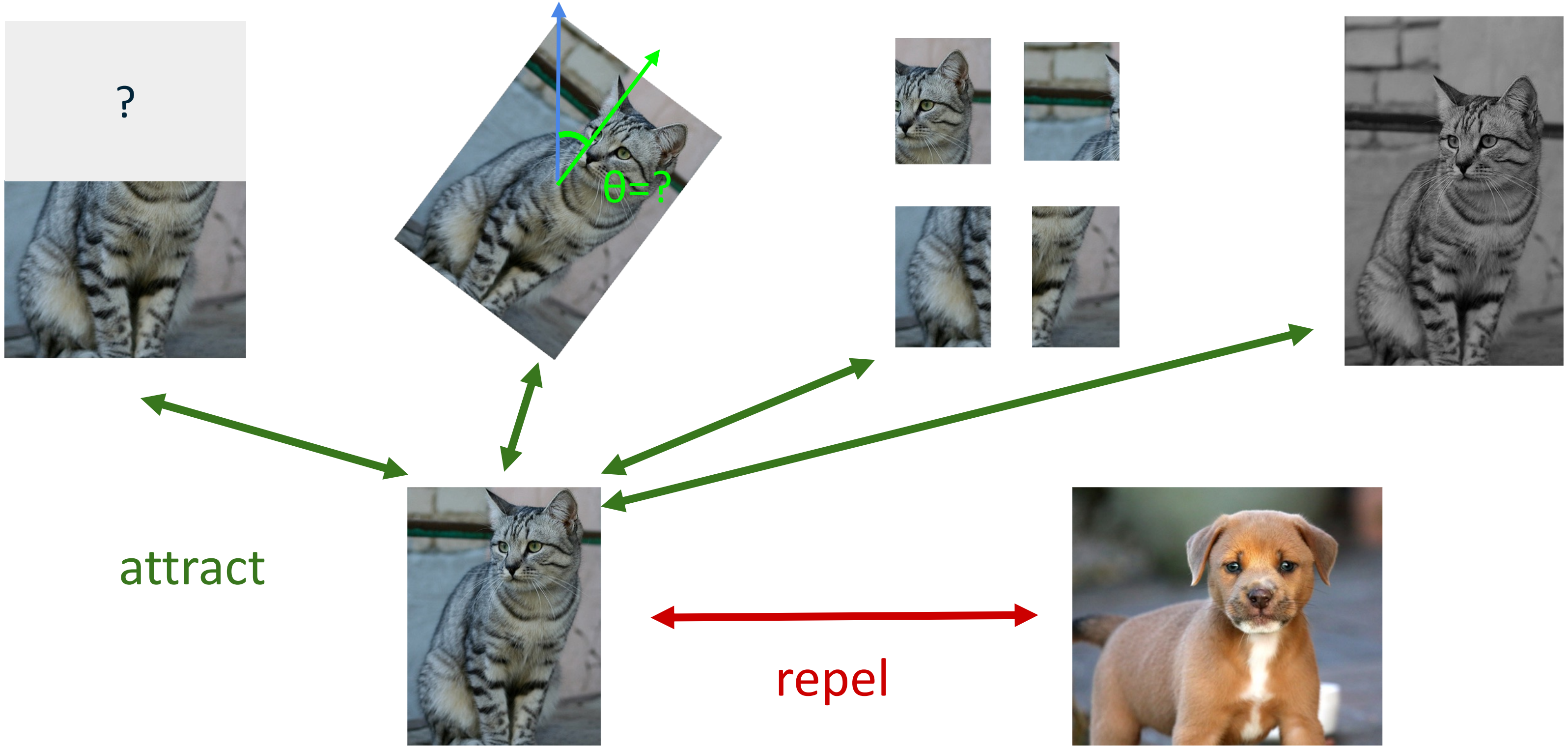
A more general pretext task?



same object

different object

Contrastive Representation Learning



attract

repel

Today's Agenda

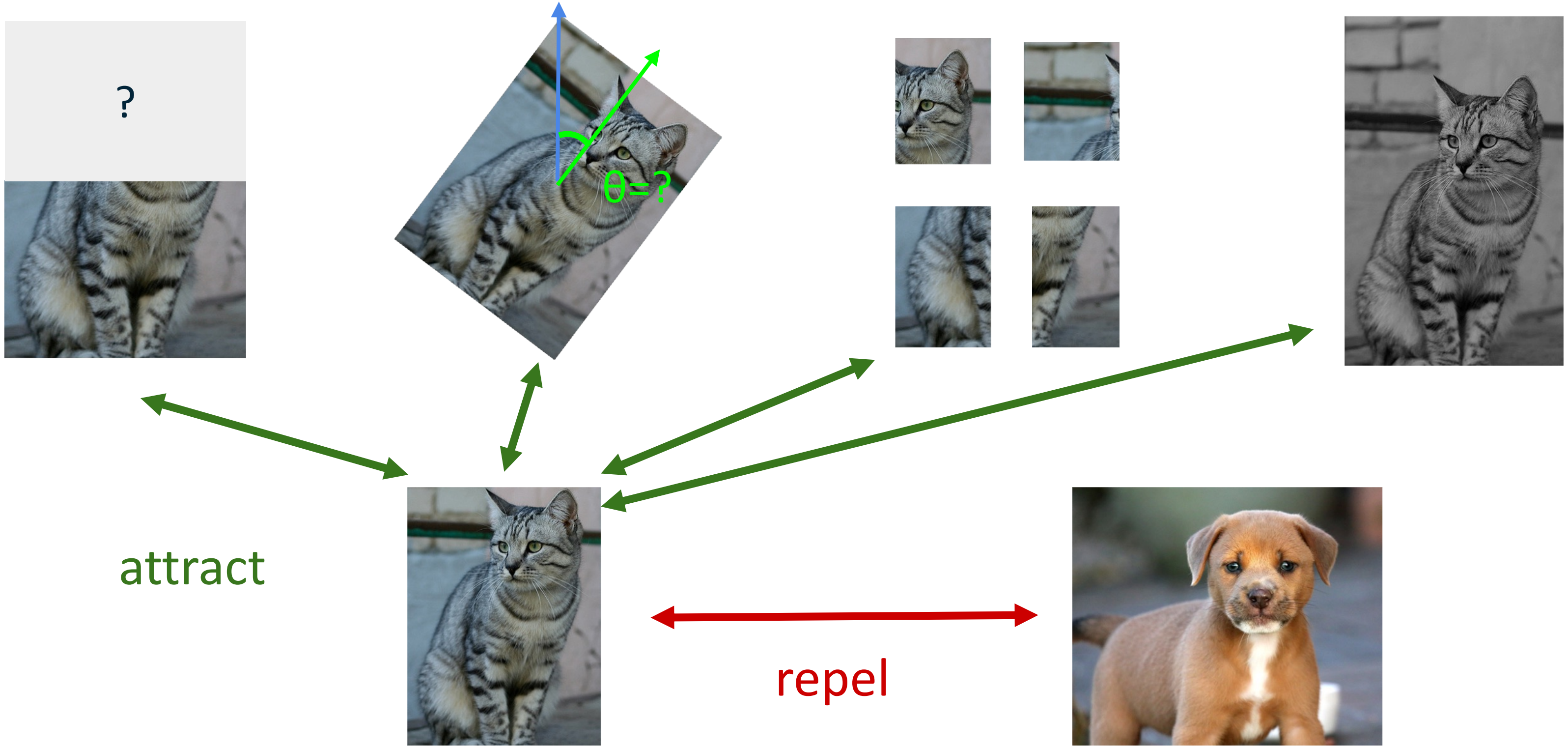
Pretext tasks from image transformations

- Rotation, inpainting, rearrangement, coloring

Contrastive representation learning

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

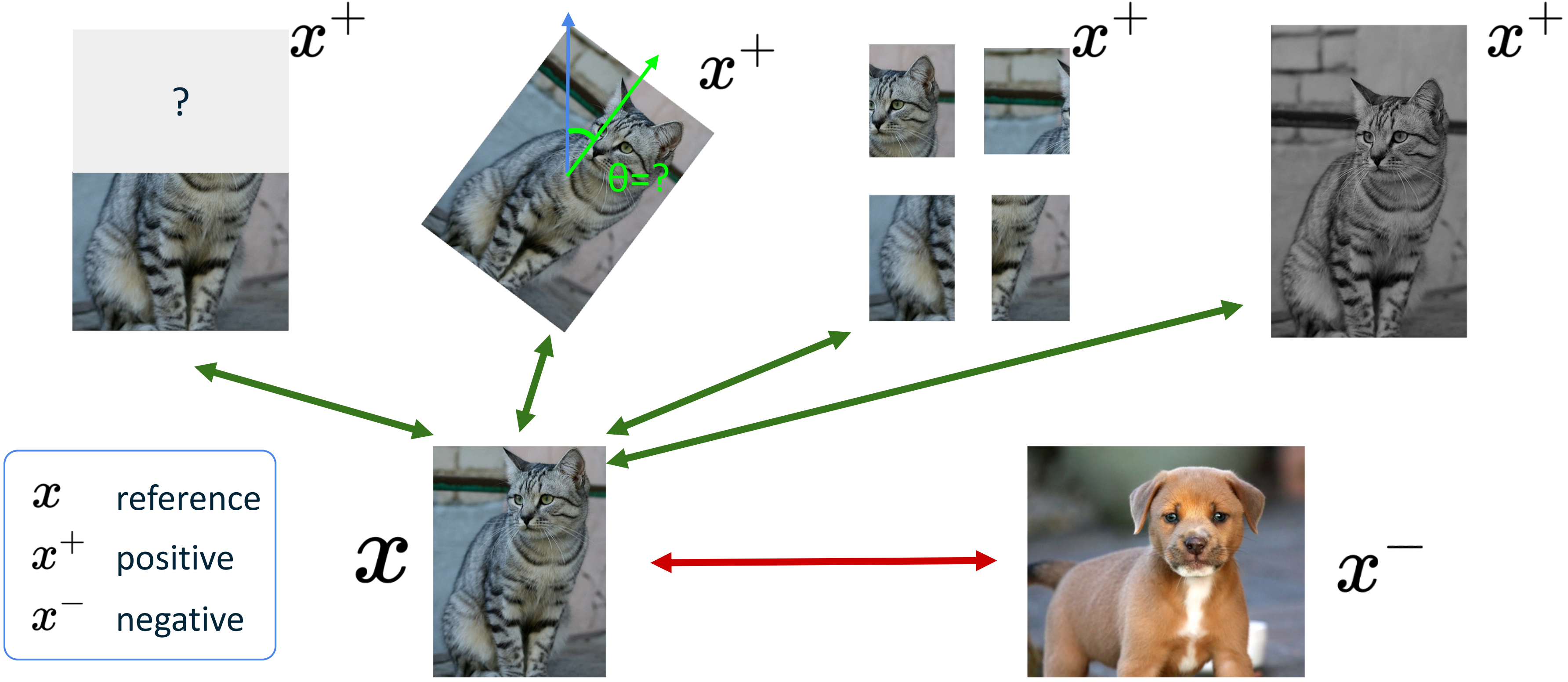
Contrastive Representation Learning



attract

repel

Contrastive Representation Learning



x	reference
x^+	positive
x^-	negative

A formulation of contrastive learning

What we want:

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

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:

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

A formulation of contrastive learning

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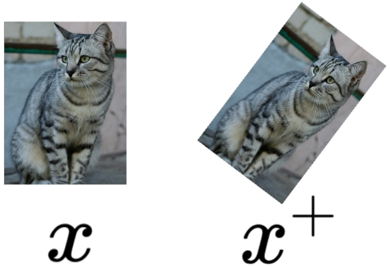

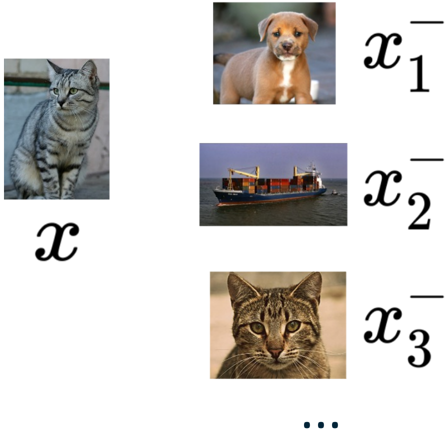

A formulation of contrastive learning

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

$$L = -\mathbb{E}_X \left[\log \frac{\overline{\exp(s(f(x), f(x^+)))}}{\underbrace{\exp(s(f(x), f(x^+)))}_{\text{score for the positive pair}} + \underbrace{\sum_{j=1}^{N-1} \exp(s(f(x), f(x_j^-)))}_{\text{score for the N-1 negative pairs}}} \right]$$

This seems familiar …

A formulation of contrastive learning

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

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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:

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

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

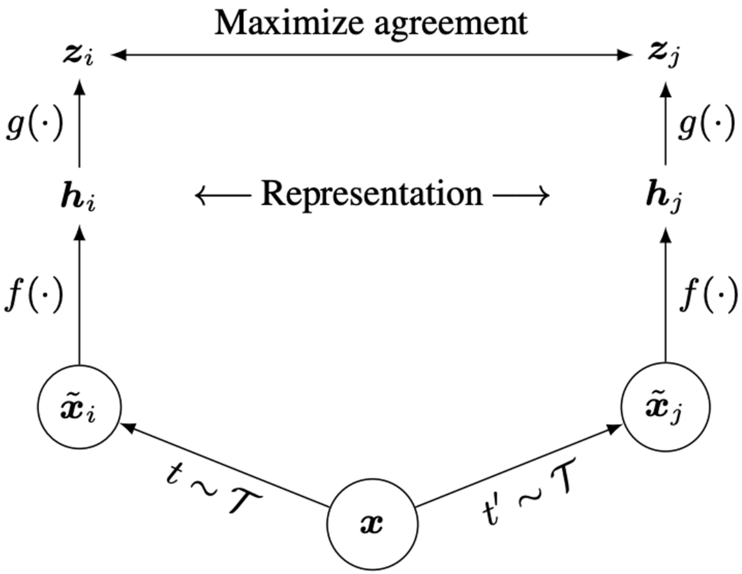
Cosine similarity as the score function:

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

Use a projection network ***h(·)*** 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

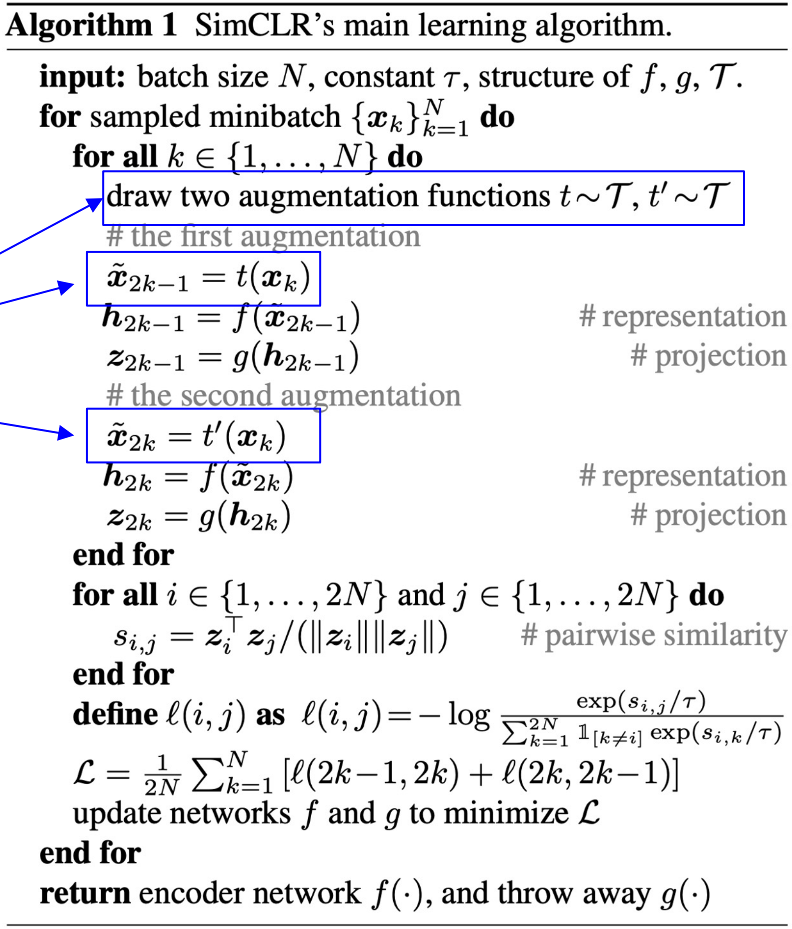
SimCLR: generating positive samples from data augmentation

(a) Original (b) Crop and resize (c) Crop, resize (and flip) (d) Color distort. (drop) (e) Color distort. (jitter)

(f) Rotate {90°, 180°, 270°} (g) Cutout (h) Gaussian noise (i) Gaussian blur (j) Sobel filtering

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

SimCLR



Algorithm 1 SimCLR's main learning algorithm.

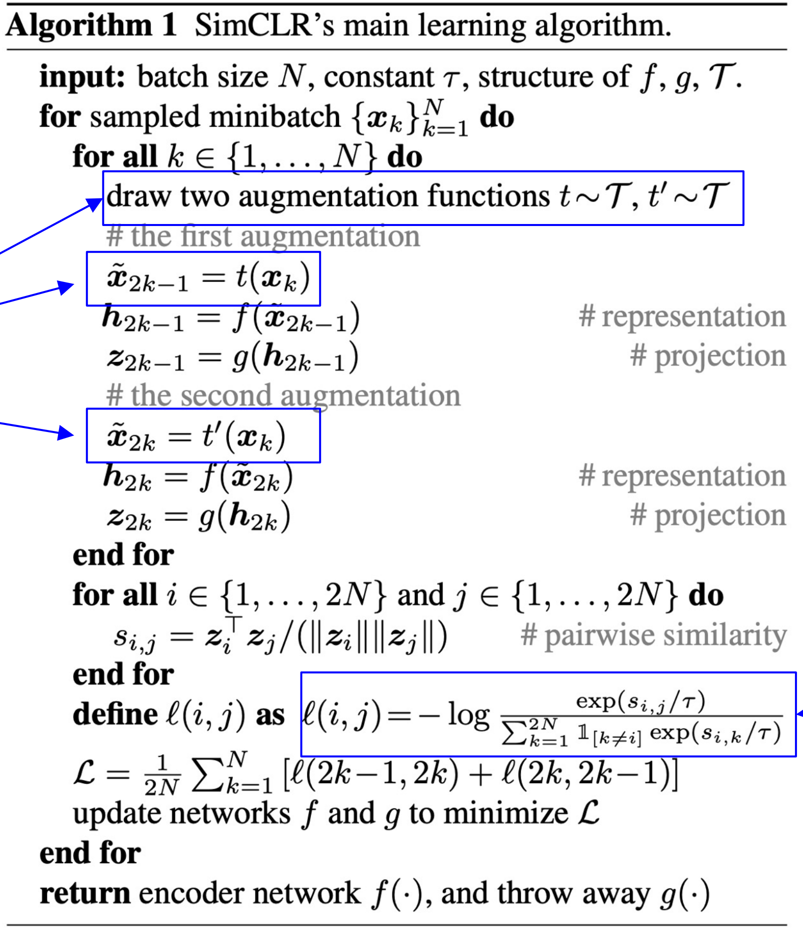
```
input: batch size $N$, constant $\tau$, structure of $f$, $g$, $\mathcal{T}$.
for sampled minibatch $\{\boldsymbol{x}_k\}_{k=1}^{N}$ do
    for all $k \in \{1, \ldots, N\}$ do
        draw two augmentation functions $t \sim \mathcal{T}$, $t' \sim \mathcal{T}$
        # the first augmentation
        $\tilde{\boldsymbol{x}}_{2k-1} = t(\boldsymbol{x}_k)$
        $\boldsymbol{h}_{2k-1} = f(\tilde{\boldsymbol{x}}_{2k-1})$                # representation
        $\boldsymbol{z}_{2k-1} = g(\boldsymbol{h}_{2k-1})$                # projection
        # the second augmentation
        $\tilde{\boldsymbol{x}}_{2k} = t'(\boldsymbol{x}_k)$
        $\boldsymbol{h}_{2k} = f(\tilde{\boldsymbol{x}}_{2k})$                # representation
        $\boldsymbol{z}_{2k} = g(\boldsymbol{h}_{2k})$                # projection
    end for
    for all $i \in \{1, \ldots, 2N\}$ and $j \in \{1, \ldots, 2N\}$ do
        $s_{i,j} = \boldsymbol{z}_i^\top \boldsymbol{z}_j / (\|\boldsymbol{z}_i\| \|\boldsymbol{z}_j\|)$        # 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 $g(\cdot)$
```

Generate a positive pair by sampling data augmentation functions

Source: Chen et al., 2020

SimCLR

Generate a positive pair by sampling data augmentation functions



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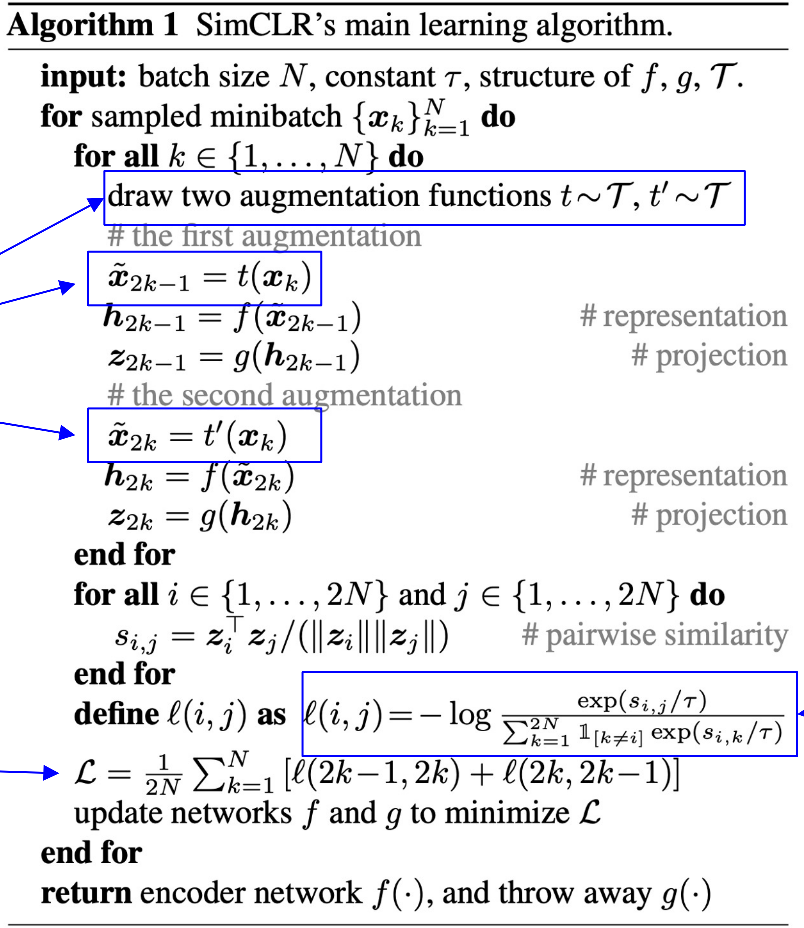
InfoNCE loss:
Use all non-positive samples in the batch as x^-

Source: Chen et al., 2020

SimCLR



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    update networks $f$ and $g$ to minimize $\mathcal{L}$
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return encoder network $f(\cdot)$, and throw away $g(\cdot)$
```

Generate a positive pair by sampling data augmentation functions

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

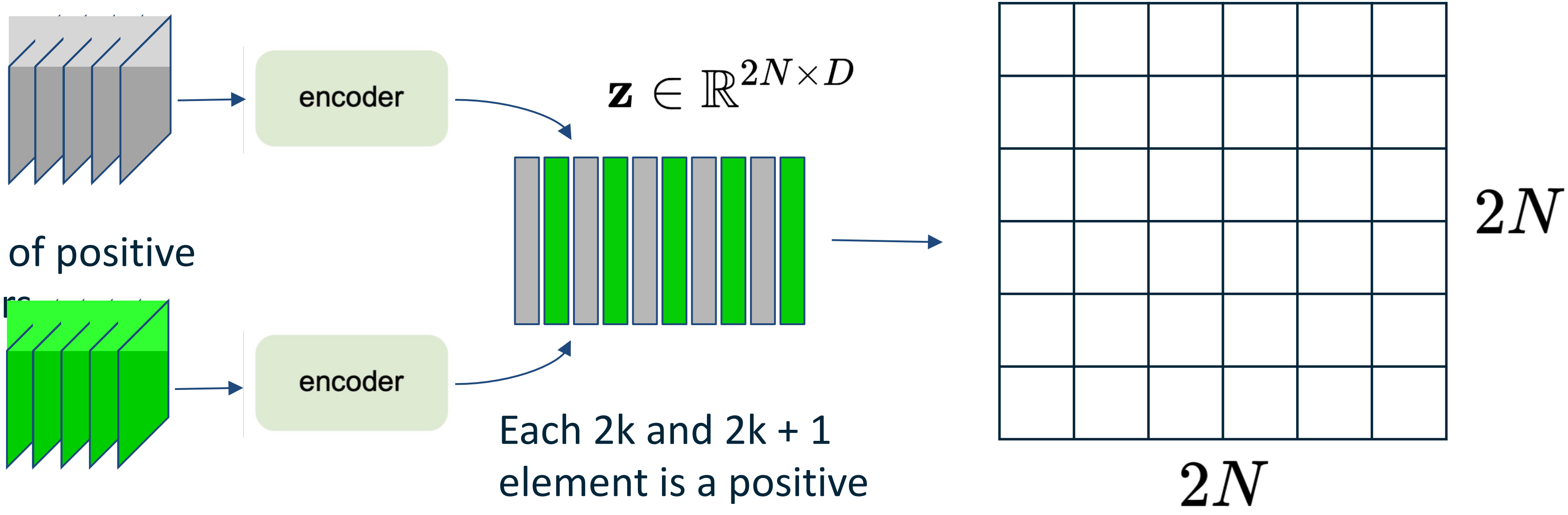
InfoNCE loss:
Use all non-positive samples in the batch as x^-

Source: Chen et al., 2020

SimCLR: mini-batch training

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

“Affinity matrix”



list of positive pairs

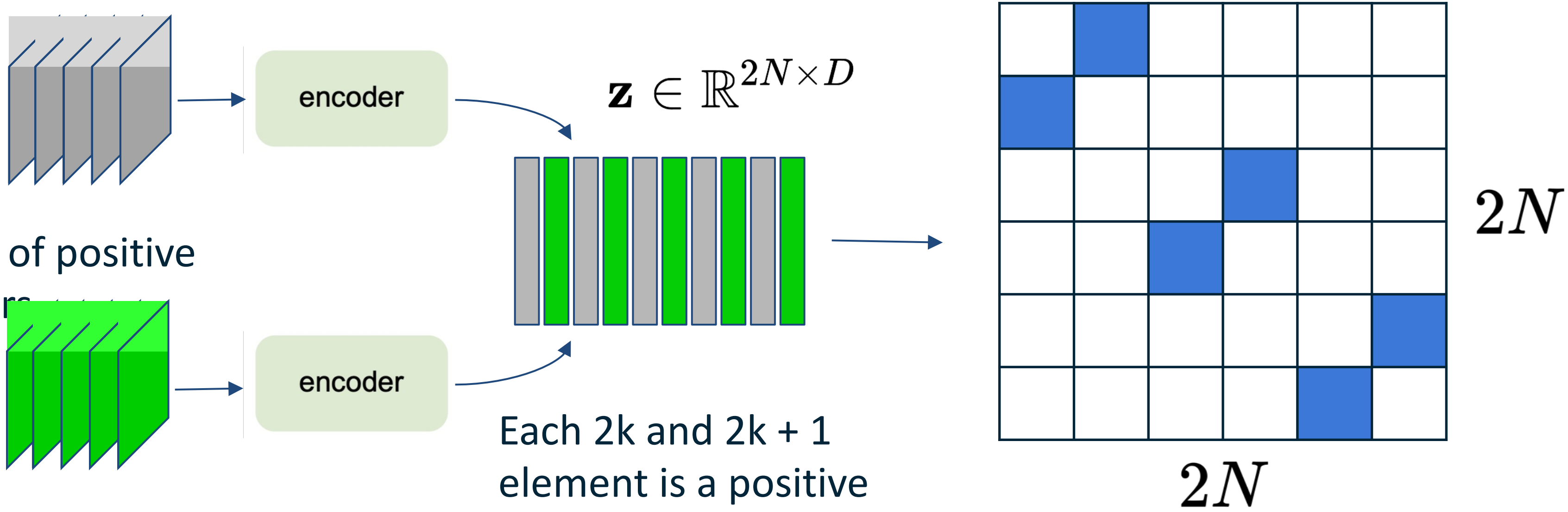
$\mathbf{z} \in \mathbb{R}^{2N \times D}$

Each 2k and 2k + 1 element is a positive pair

SimCLR: mini-batch training

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

“Affinity matrix”



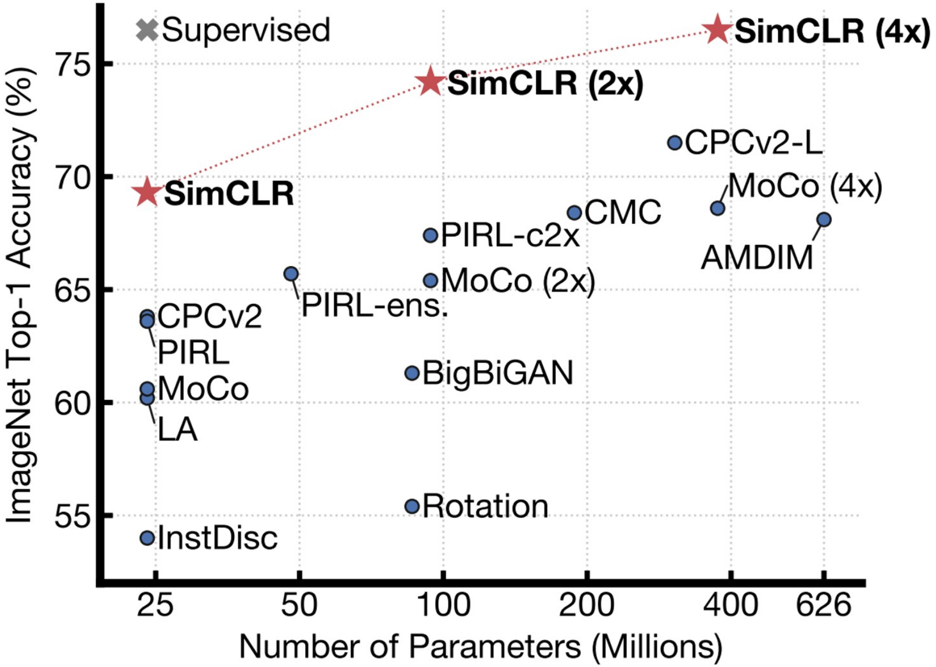
list of positive pairs

$\mathbf{z} \in \mathbb{R}^{2N\times D}$

Each 2k and 2k + 1 element is a positive pair

🟦 = classification label for each row

Training linear classifier on SimCLR features

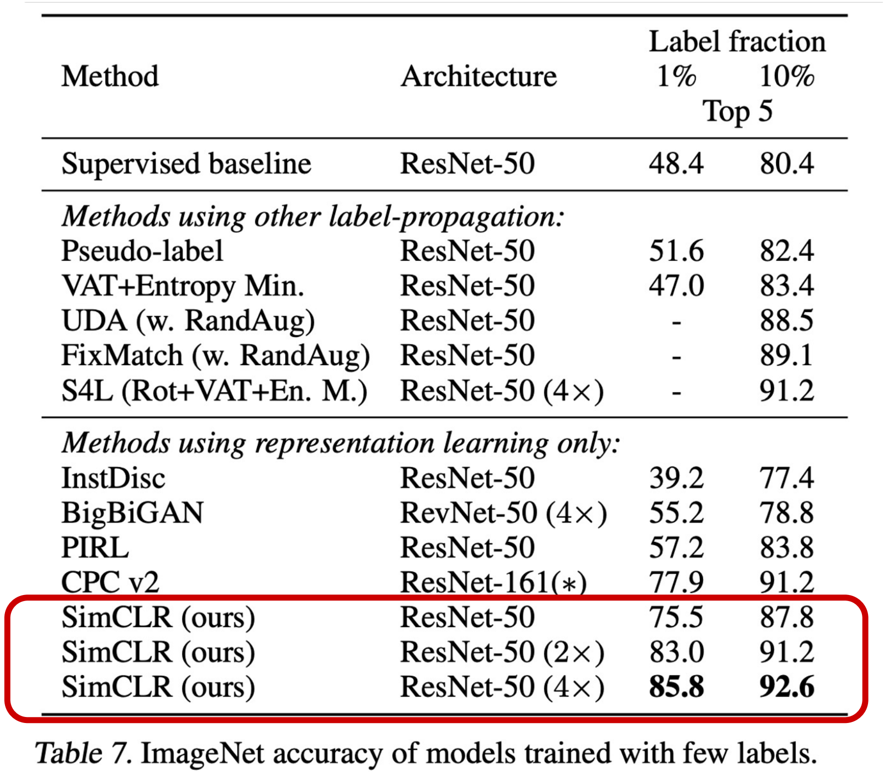


Train feature encoder on **ImageNet** (entire training set) using SimCLR.

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%	Label fraction 10%
		Top 5	
Supervised baseline	ResNet-50	48.4	80.4
Methods using other label-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×)	-	91.2
Methods using representation learning only:			
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×)	**85.8**	**92.6**

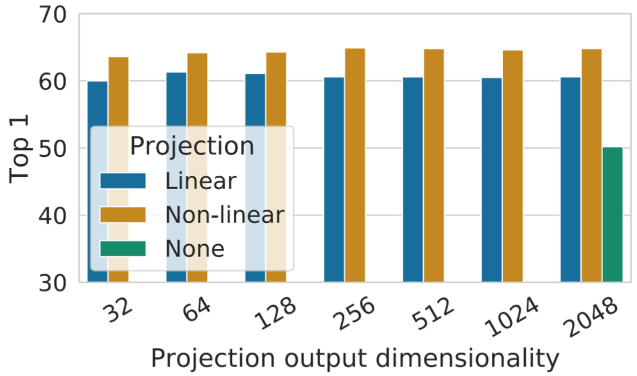
Table 7. ImageNet accuracy of models trained with few labels.

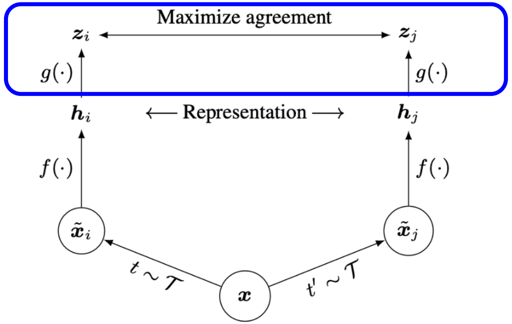
Train feature encoder on **ImageNet** (entire training set) using SimCLR.

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 ***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

Source: Chen et al., 2020

SimCLR design choices: large batch size

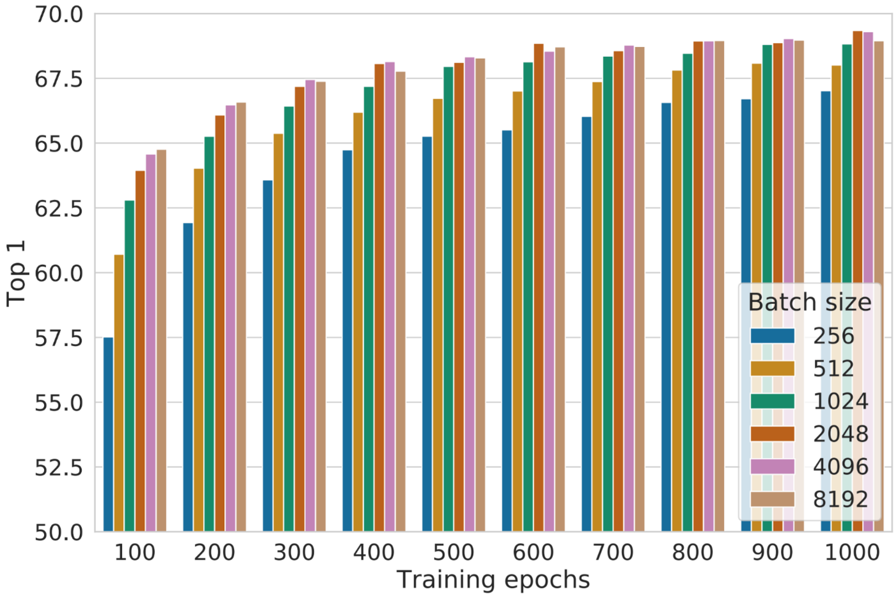


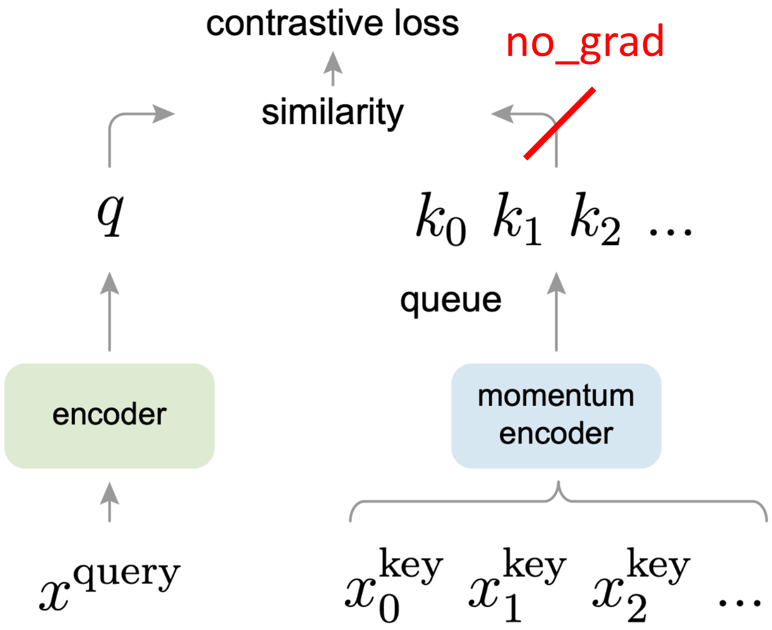
Figure 9. Linear evaluation models (ResNet-50) trained with different batch size and epochs. Each bar is a single run from scratch.[10]

Large training batch size is crucial for SimCLR!

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

Source: [Chen et al., 2020]

Momentum Contrastive Learning (MoCo)

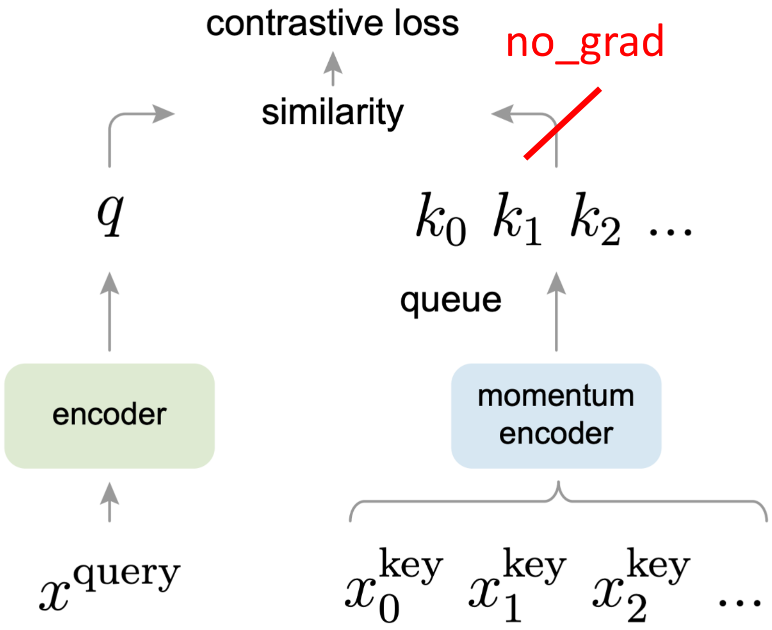


Key differences to SimCLR:

- Keep a running queue of keys (negative samples).
- Compute gradients and update the encoder only through the queries.
- Decouple mini-batch size with the number of keys: can support a large number of negative samples.

Source: He et al., 2020

Momentum Contrastive Learning (MoCo)



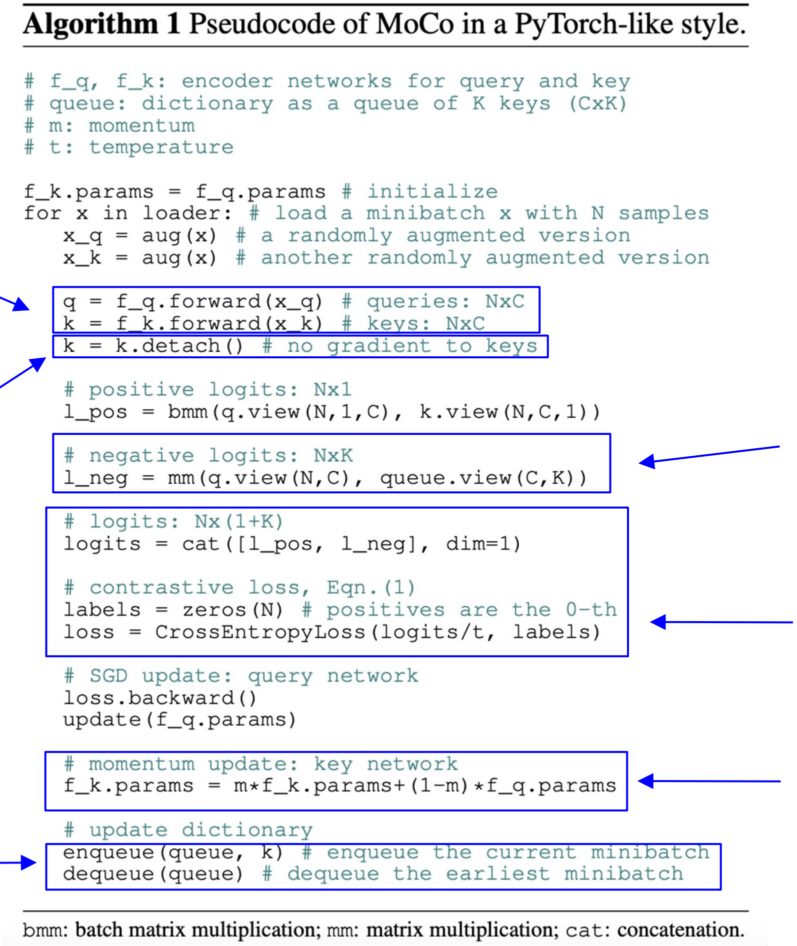
Key differences to SimCLR:

- 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:

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

Source: He et al., 2020

MoCo



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.

Generate a positive pair by sampling data augmentation functions

No gradient through the positive sample

Use the running queue of keys as the negative samples

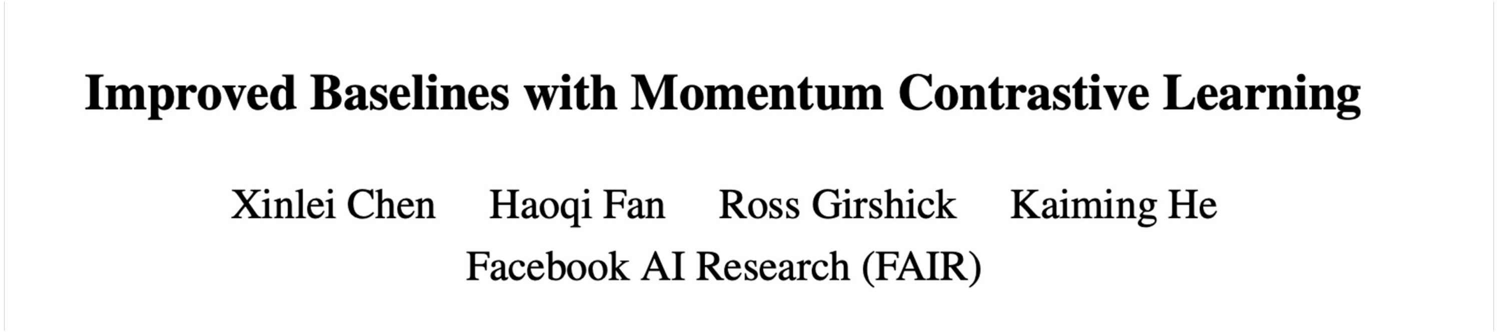
InfoNCE loss

Update f_k through momentum

Update the FIFO negative sample queue

Source: He et al., 2020

“MoCo V2”



Improved Baselines with Momentum Contrastive Learning

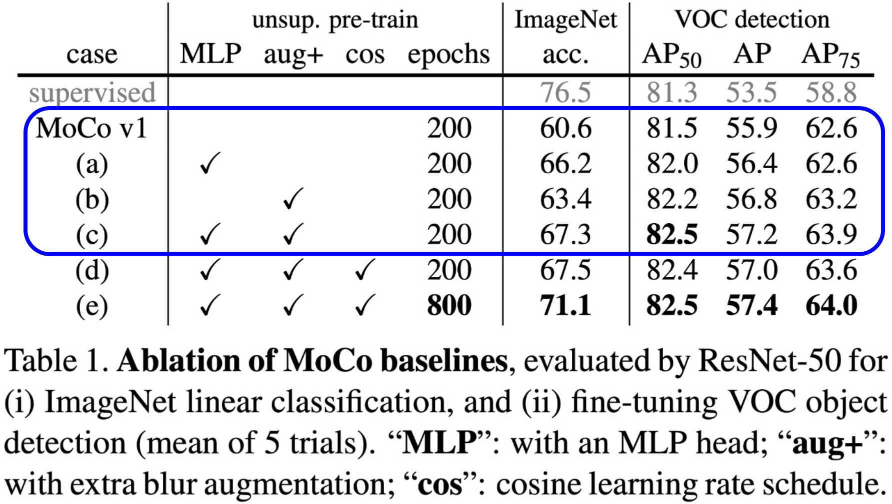
Xinlei Chen Haoqi Fan Ross Girshick Kaiming He
Facebook AI Research (FAIR)

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



case	unsup. pre-train				ImageNet	VOC detection		
	MLP	aug+	cos	epochs	acc.	AP_{50}	AP	AP_{75}
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	**82.5**	57.2	63.9
(d)	✓	✓	✓	200	67.5	82.4	57.0	63.6
(e)	✓	✓	✓	**800**	**71.1**	**82.5**	**57.4**	**64.0**

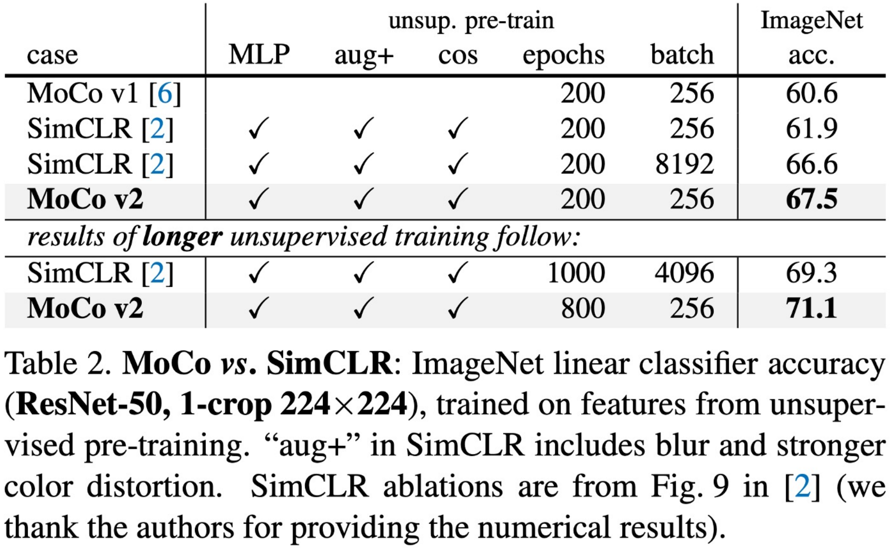
Table 1. **Ablation of MoCo baselines**, evaluated by ResNet-50 for (i) ImageNet linear classification, and (ii) fine-tuning VOC object detection (mean of 5 trials). "**MLP**": with an MLP head; "**aug+**": with extra blur augmentation; "**cos**": cosine learning rate schedule.

Key takeaways:

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

Source: Chen et al., 2020

MoCo vs. SimCLR vs. MoCo V2



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

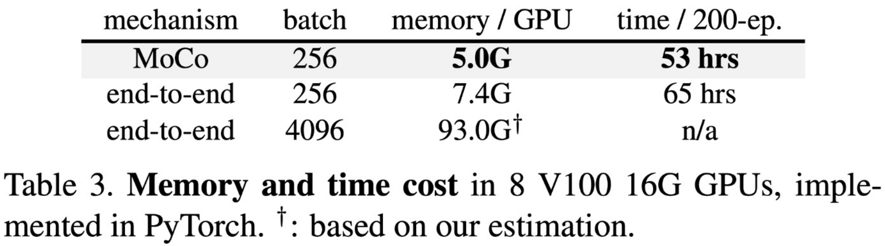
Table 2. **MoCo *vs.* SimCLR**: ImageNet linear classifier accuracy (**ResNet-50, 1-crop 224×224**), trained on features from unsupervised pre-training. "aug+" in SimCLR includes blur and stronger color distortion. SimCLR ablations are from Fig. 9 in [2] (we thank the authors for providing the numerical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



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[†]	n/a

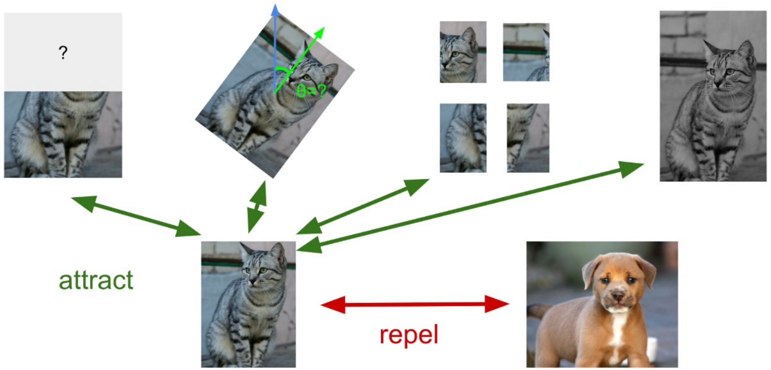
Table 3. **Memory and time cost** in 8 V100 16G GPUs, implemented in PyTorch. [†]: based on our estimation.

Key takeaways:

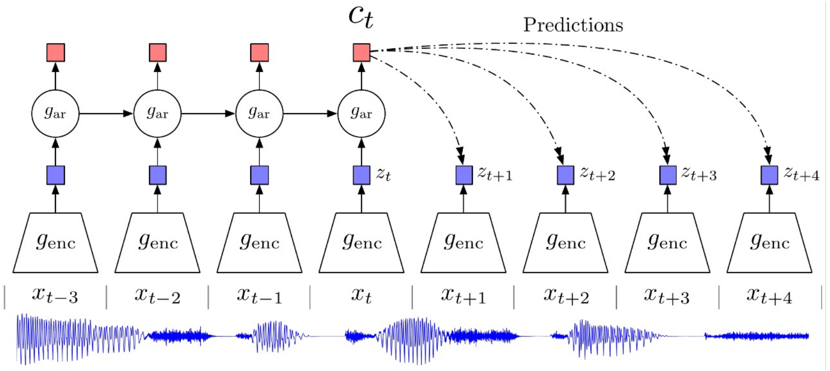
- Non-linear projection head and strong data augmentation are crucial for contrastive learning.
- Decoupling mini-batch size with negative sample size allows MoCo-V2 to outperform SimCLR with smaller batch size (256 vs. 8192).
- … all with much smaller memory footprint! (“end-to-end” means SimCLR here)

Source: Chen et al., 2020

Instance vs. Sequence Contrastive Learning



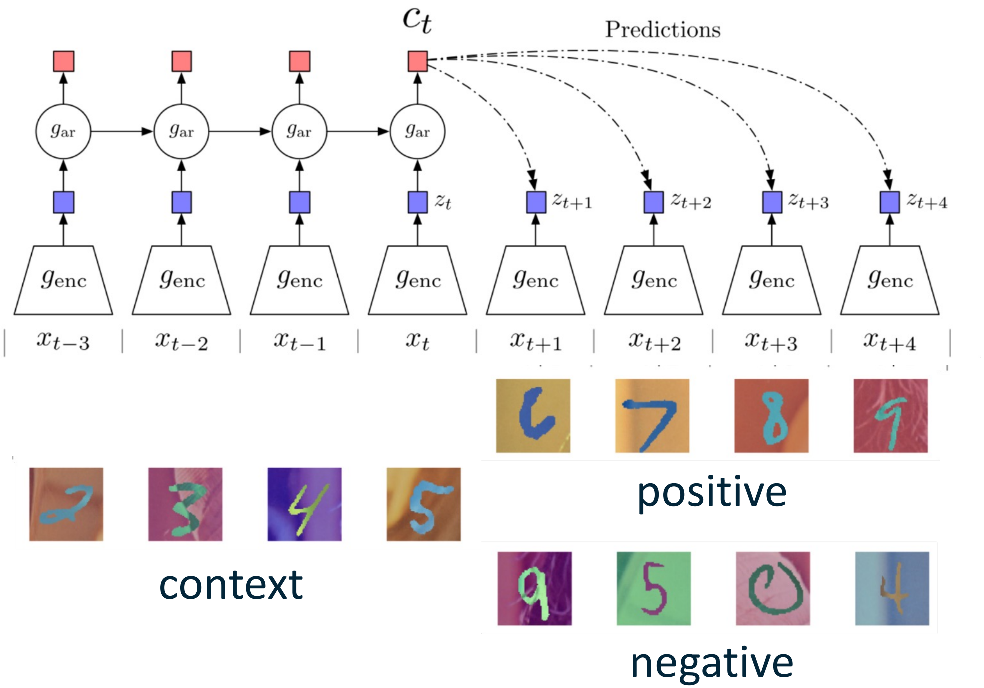
Instance-level contrastive learning:
contrastive learning based on
positive & negative instances.
Examples: SimCLR, MoCo



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)

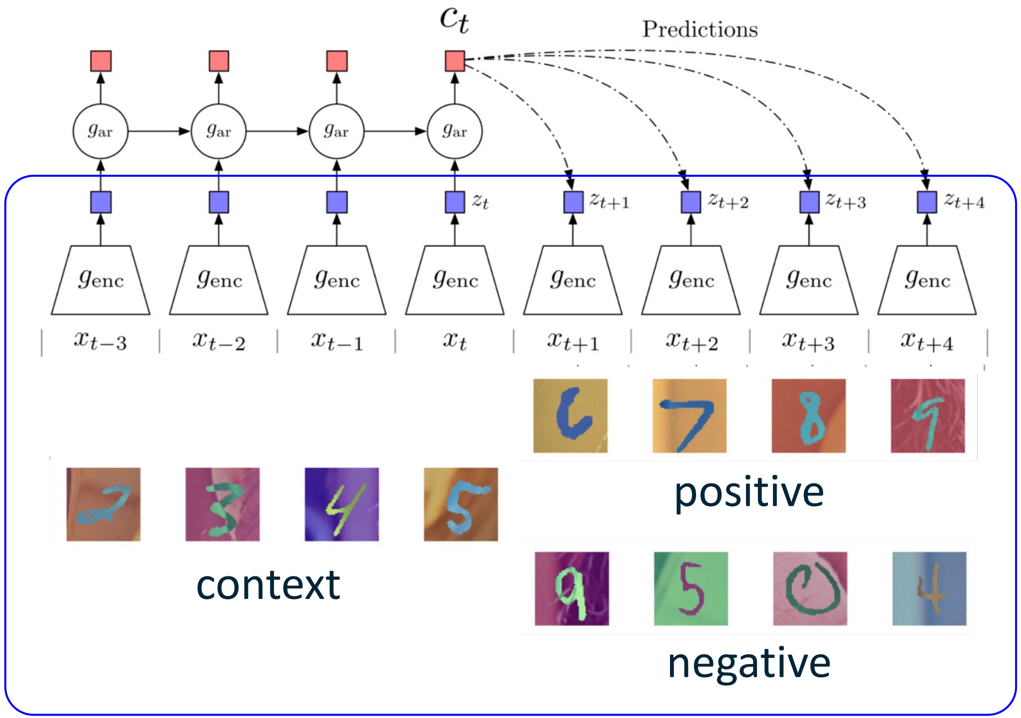
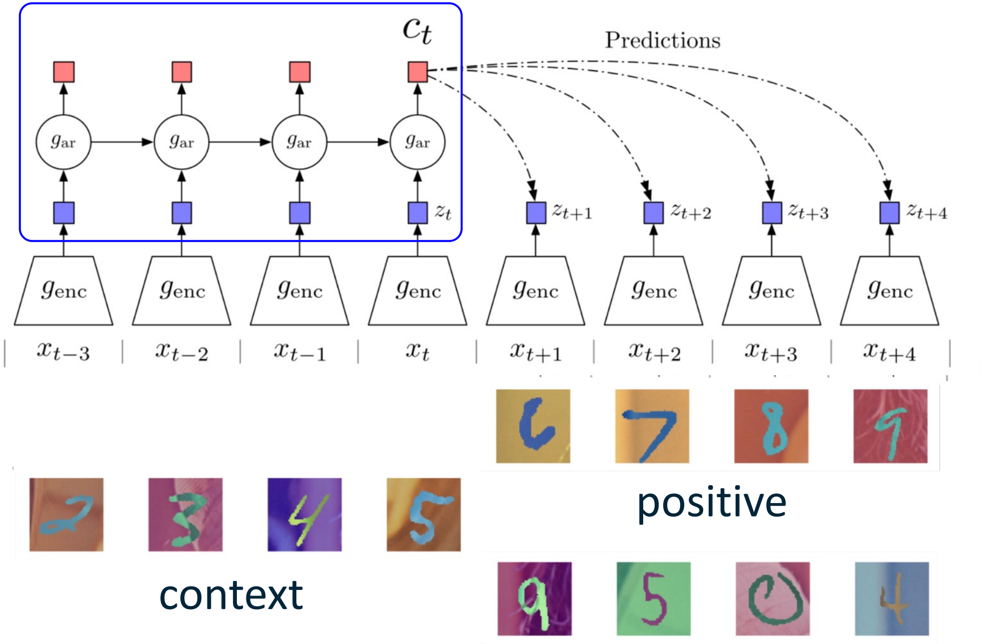


Figure source

1. Encode all samples in a sequence into vectors $z_t = g_{enc}(x_t)$

Source: van den Oord et al., 2018,

Contrastive Predictive Coding (CPC)



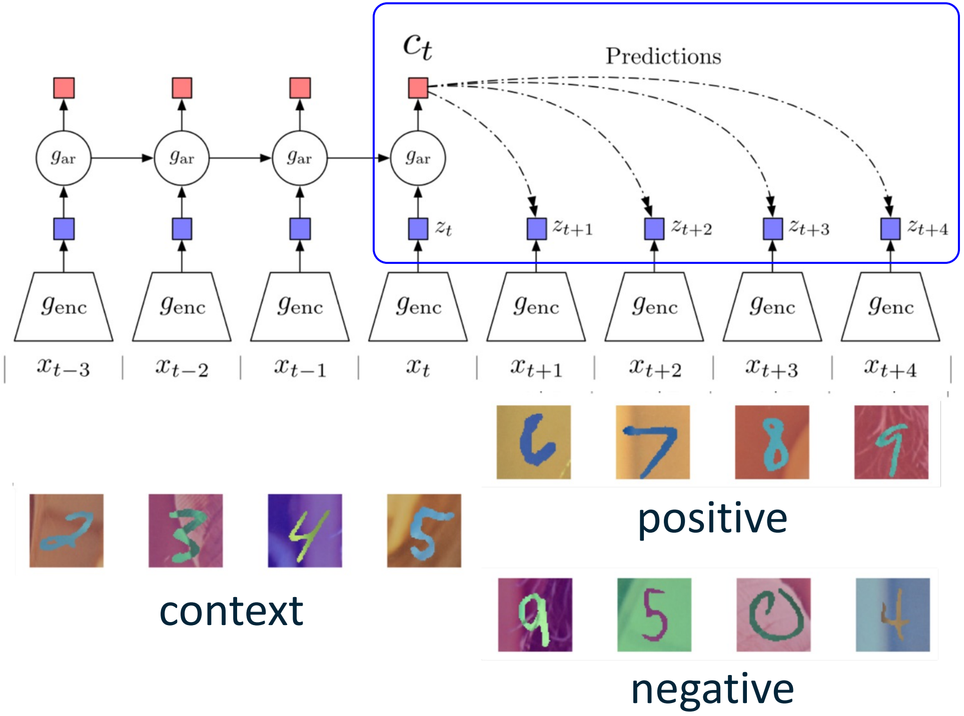
1. Encode all samples in a sequence into vectors $\boldsymbol{z_t = g_{enc}(x_t)}$

2. Summarize context (e.g., half of a sequence) into a context code $\boldsymbol{c_t}$ using an auto-regressive model ($\boldsymbol{g_{ar}}$).

Figure source

Source: van den Oord et al., 2018,

Contrastive Predictive Coding (CPC)



1. Encode all samples in a sequence into vectors $\boldsymbol{z_t = g_{enc}(x_t)}$

2. Summarize context (e.g., half of a sequence) into a context code $\boldsymbol{c_t}$ using an auto-regressive model ($\boldsymbol{g_{ar}}$).

3. Compute InfoNCE loss between the context $\boldsymbol{c_t}$ and future code $\boldsymbol{z_{t+k}}$ using the following time-dependent score function:

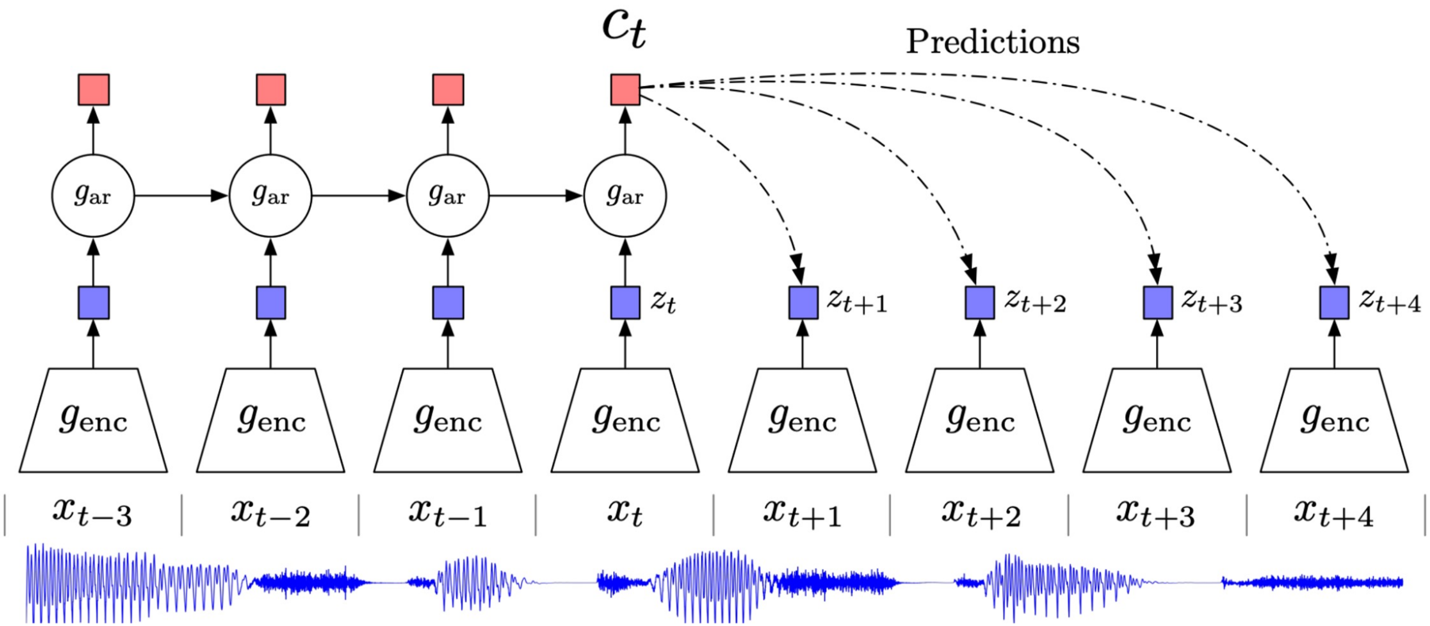
$$s_k(z_{t+k}, c_t) = z_{t+k}^T W_k c_t$$

, where W_k is a trainable matrix.

Figure source

Source: van den Oord et al., 2018,

CPC example: modeling audio sequences



Source: van den Oord et al., 2018,

CPC example: modeling audio sequences

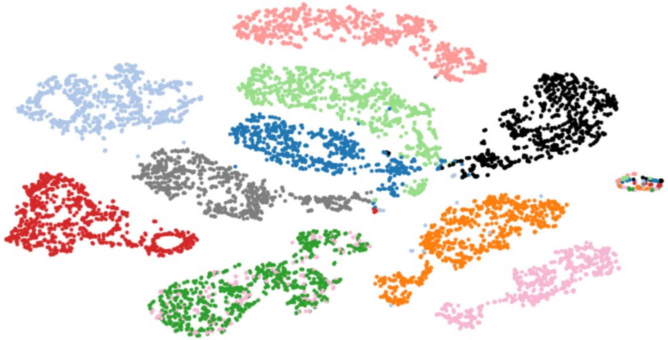
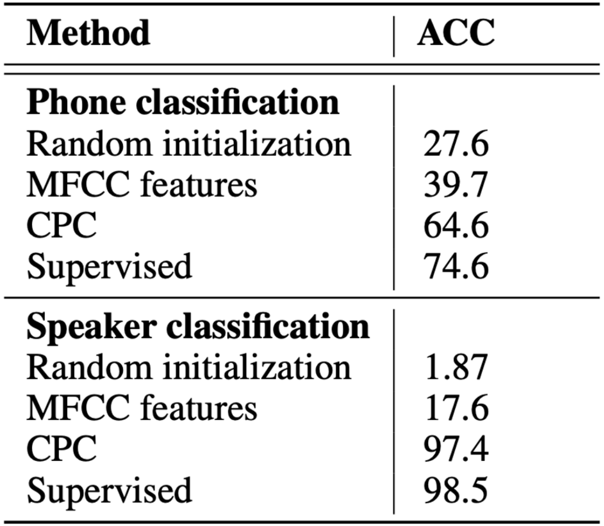


Figure 2: t-SNE visualization of audio (speech) representations for a subset of 10 speakers (out of 251). Every color represents a different speaker.



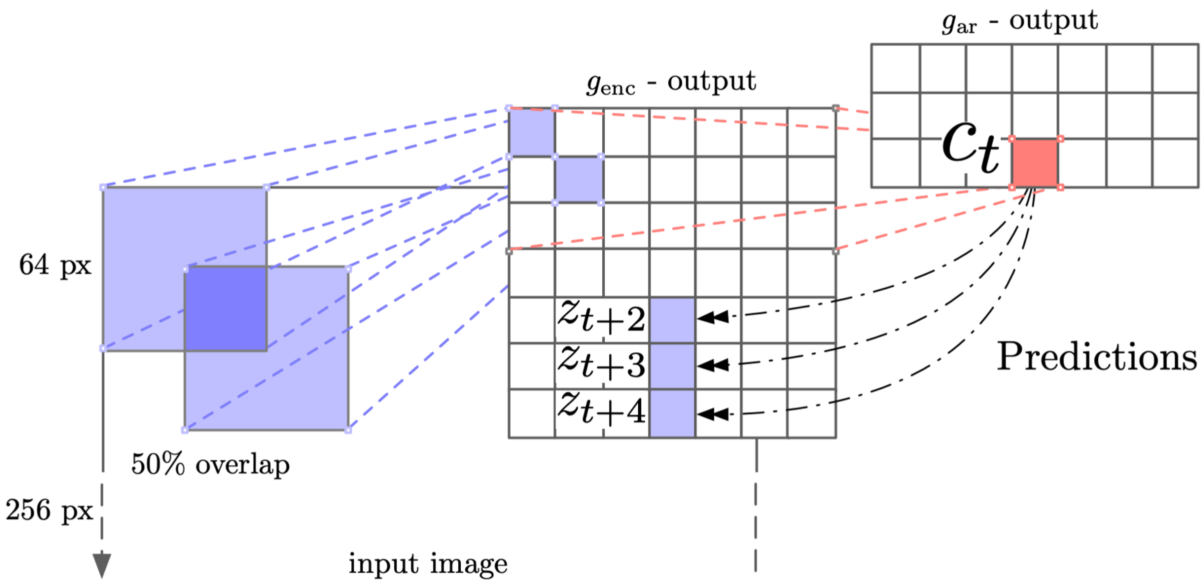
Method	**ACC**
Phone classification	
Random initialization	27.6
MFCC features	39.7
CPC	64.6
Supervised	74.6
Speaker classification	
Random initialization	1.87
MFCC features	17.6
CPC	97.4
Supervised	98.5

Linear classification on trained representations (LibriSpeech dataset)

Source: van den Oord et al., 2018,

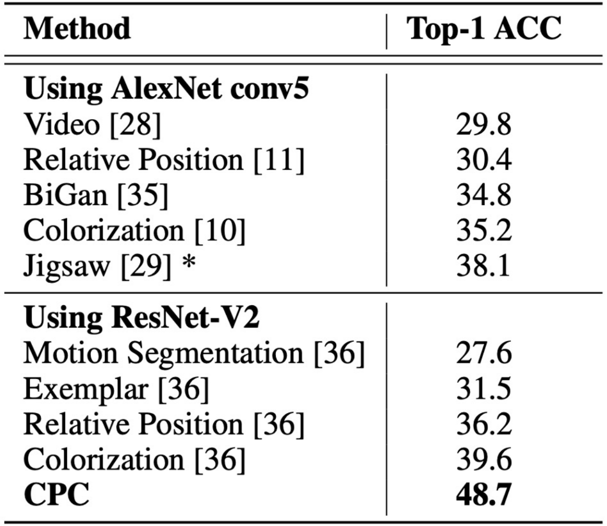
CPC example: modeling visual context

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,

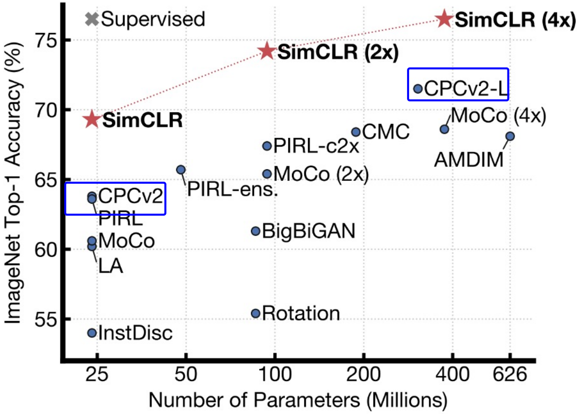
CPC example: modeling visual context



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

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:

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

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)

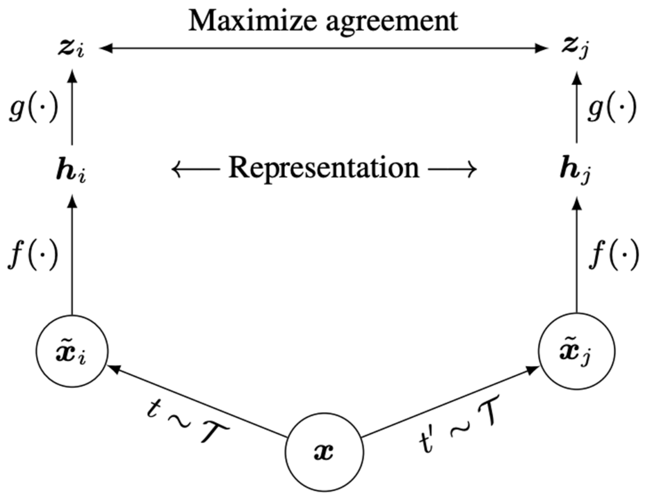
A *lower bound* on the mutual information between *f(x)* and *f(x⁺)*

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

Summary: Contrastive Representation Learning

SimCLR: a simple framework for contrastive representation learning

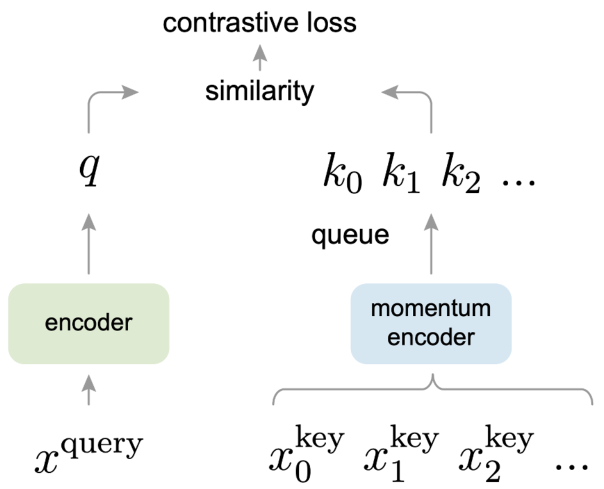
- **Key ideas**: non-linear projection head to allow flexible representation learning
- Simple to implement, effective in learning visual representation
- Requires large training batch size to be effective; large memory footprint



Summary: Contrastive Representation Learning

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

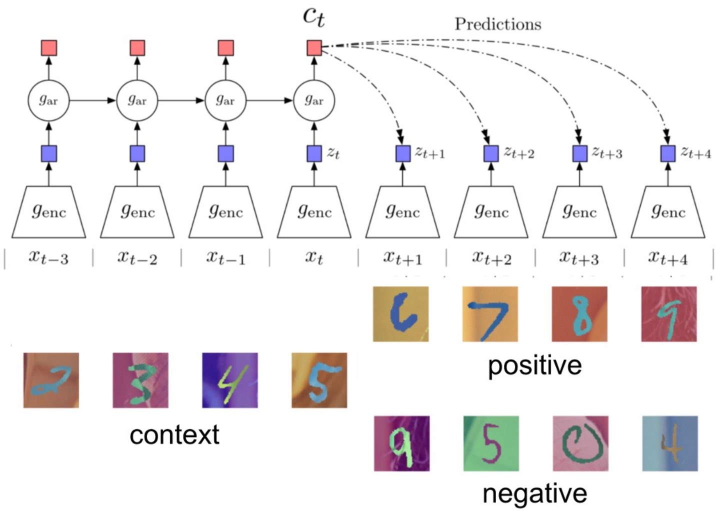
- Decouples negative sample size from minibatch size; allows large batch training without TPU
- MoCo-v2 combines the key ideas from SimCLR, i.e., nonlinear projection head, strong data augmentation, with momentum contrastive learning



Summary: Contrastive Representation Learning

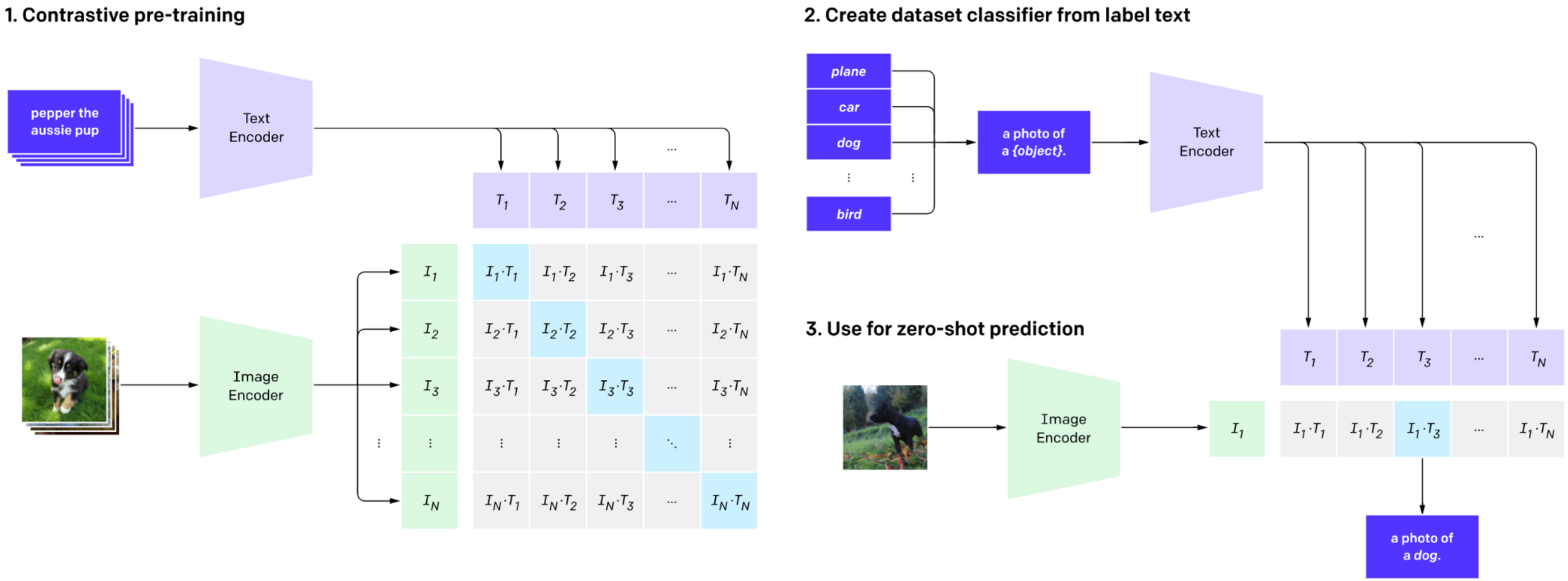
CPC: sequence-level contrastive learning

- 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

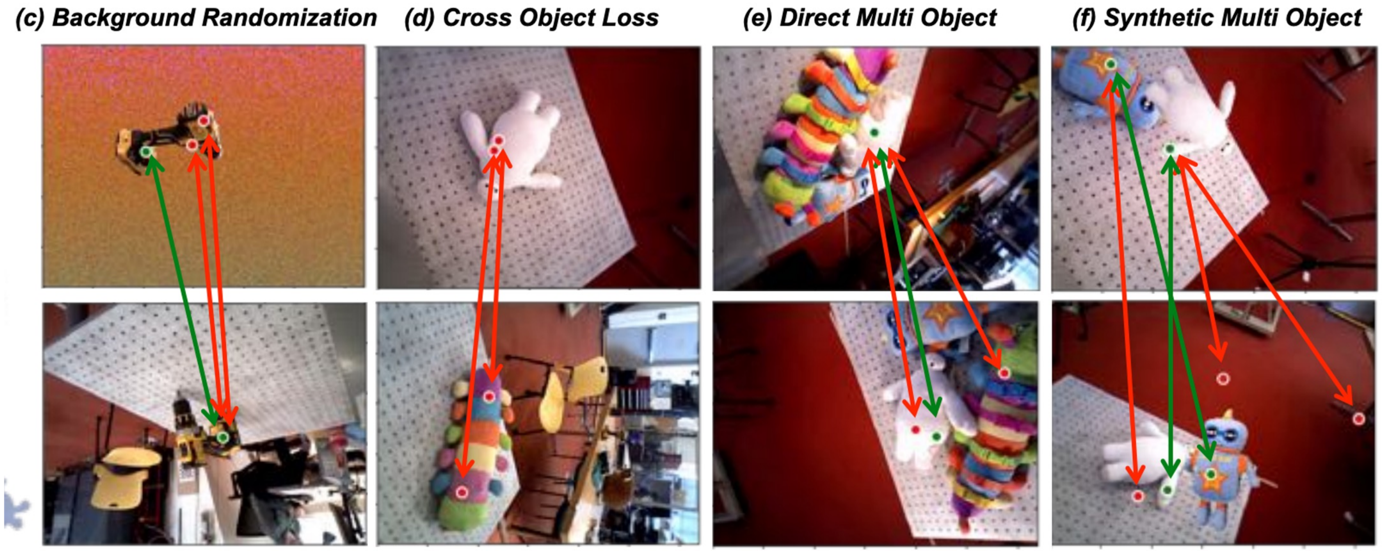
Contrastive learning between image and natural language sentences



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

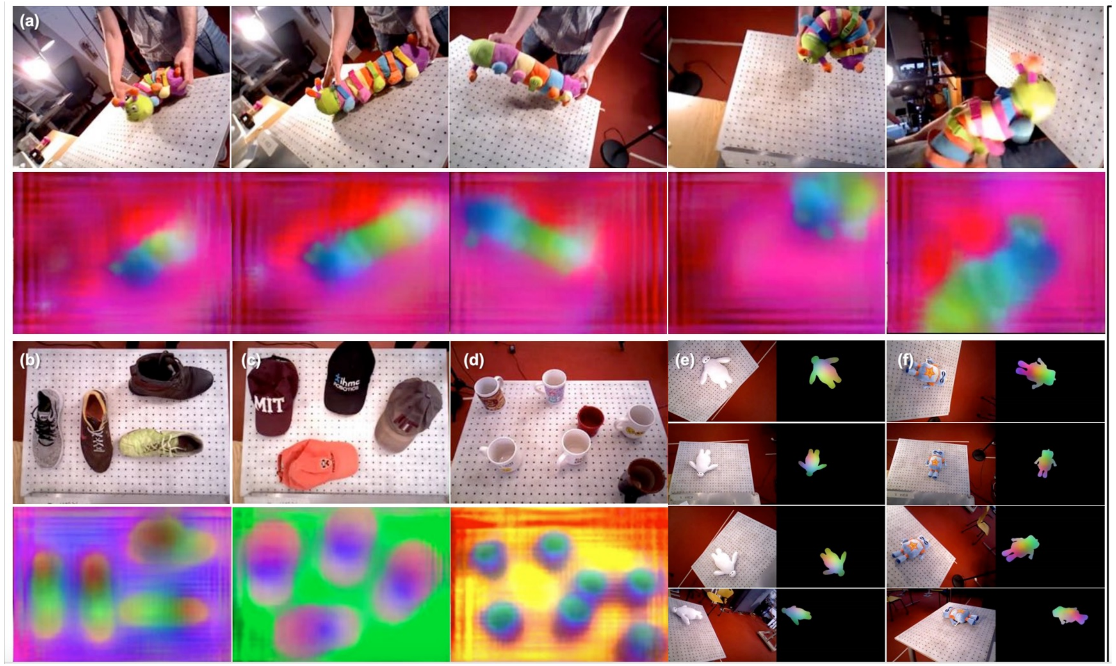
Other examples

Contrastive learning on pixel-wise feature descriptors



Dense Object Net, Florence et al., 2018

Other examples



Dense Object Net, Florence et al., 2018

Final Lecture: Robot Learning Overview and Deep Learning Frontiers