CS 4644/7643: Lecture 19
Danfei Xu

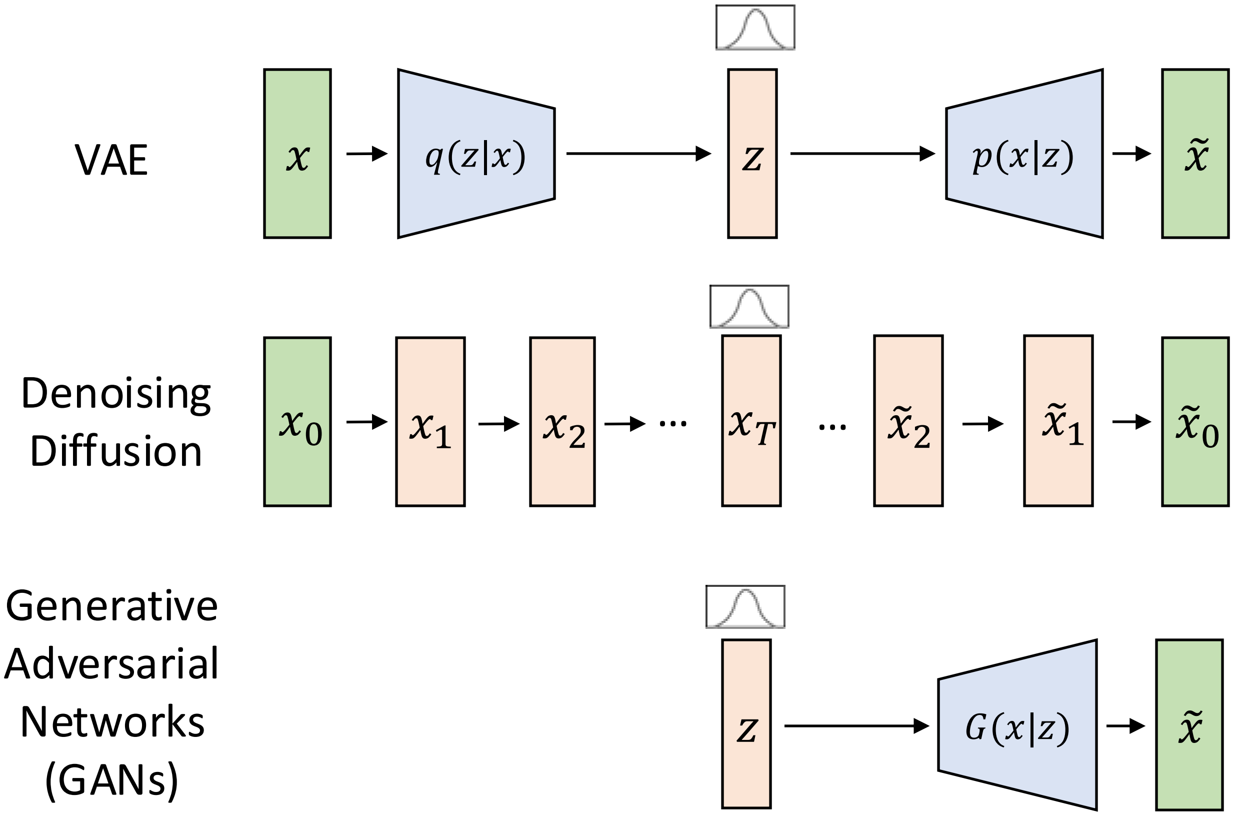
Topics:

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

Administrative

- HW4 / PS4 out. Due Nov 12th**.** Grace Period ends 14th**.**
- **Start the coding part NOW** --- it takes some time to run GAN / diffusion model training on Colab GPUs.
- Milestone Report due Nov 4th. **NO GRACE PERIOD**

Denoising Diffusion: Image to Noise and Back



The Denoising Diffusion Process

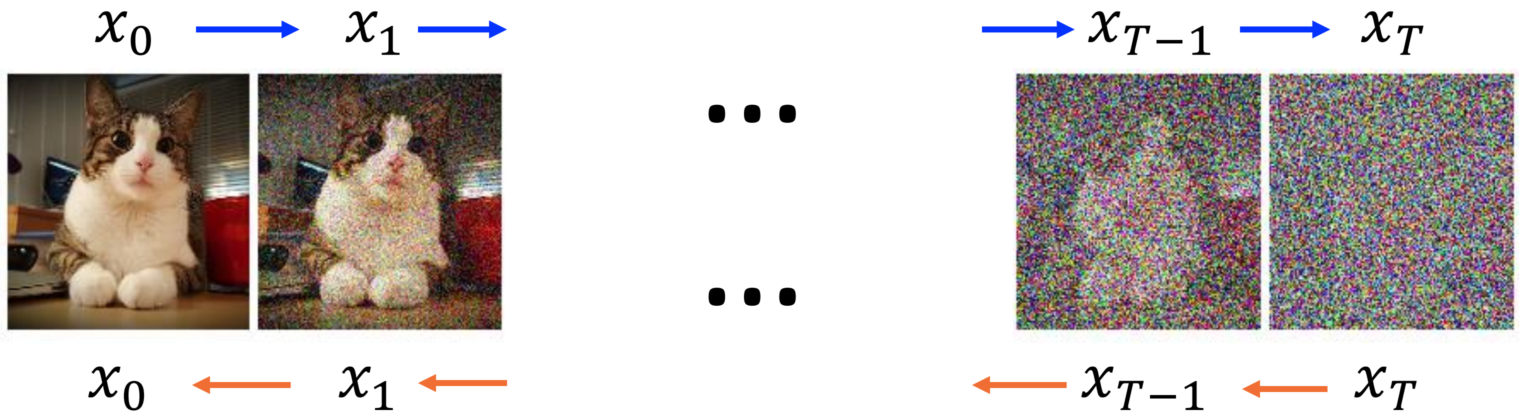


image from
dataset

The “forward diffusion” process:
add Gaussian noise each step

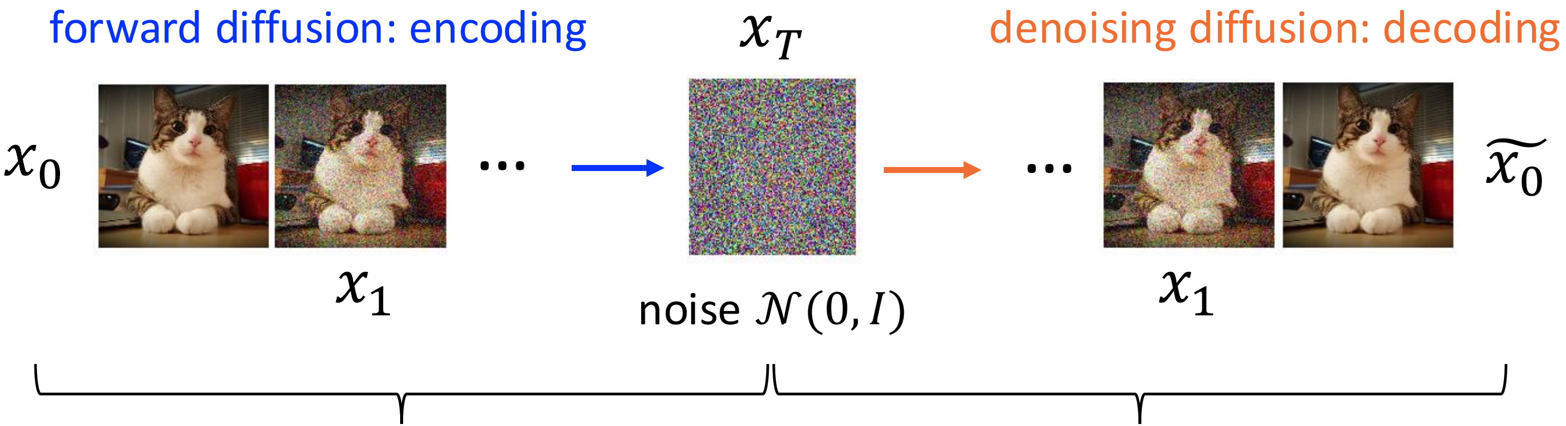
noise $\mathcal{N}(0, I)$

$x_0 \longrightarrow x_1 \longrightarrow \cdots \longrightarrow x_{T-1} \longrightarrow x_T$

$x_0 \longleftarrow x_1 \longleftarrow \cdots \longleftarrow x_{T-1} \longleftarrow x_T$

The “denoising diffusion” process:
generate an image from noise by
denoising the gaussian noises

Connection to VAEs



forward diffusion: encoding

x_T

denoising diffusion: decoding

x_0

x_1

noise $\mathcal{N}(0, I)$

x_1

$\widetilde{x_0}$

Known / predefined:

$q(x_{1:T}|x_0)$

Unknown / learned:

$$p_\theta(x_{0:T}) = p(x_T)\prod_{t=1}^{T} p_\theta(x_{t-1}|x_t)$$

Similar to VAEs, use the denoising decoding process to generate new images.

The Diffusion (Encoding) Process

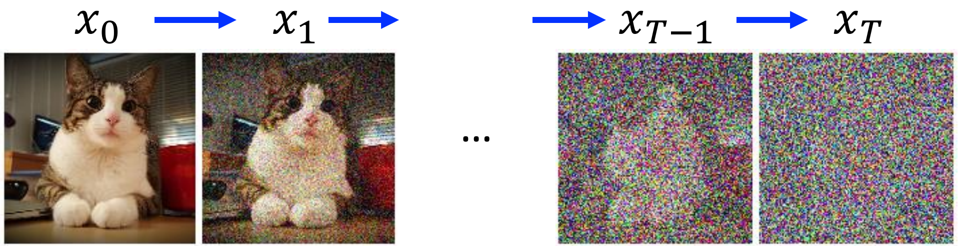
The **known** forward process $x_0 \longrightarrow x_1 \longrightarrow \cdots \longrightarrow x_T$

$$q(x_{1:T}|x_0) = \prod_{t=1}^{T} q(x_t|x_{t-1})$$ Probability Chain Rule (Markov Chain)

$$q(x_t|x_{t-1}) = \mathcal{N}(x_t; (1-\beta_t)x_{t-1}, \beta_t I)$$ Conditional Gaussian

β_t is the *variance schedule* at the diffusion step t

$0 < \beta_1 < \beta_2 < \cdots < \beta_T < 1$, typical value range $[0.0001, 0.02]$, with $T = 1000$



The Denoising (Decoding) Process

The **learned** denoising process $x_0 \leftarrow x_1 \leftarrow \cdots \leftarrow x_T$

$$p_\theta(x_{0:T}) = p(x_T)\prod_{t=1}^{T} p_\theta(x_{t-1}|x_t)$$

Probability Chain Rule (Markov Chain)

$$p_\theta(x_{t-1}|x_t) = \mathcal{N}(x_{t-1}; \mu_\theta(x_t, t), \Sigma_q(t))$$

Conditional Gaussian

Want to learn time-dependent mean

Assume fixed / known variance (simplification)

How do we form a learning objective?

The Denoising (Decoding) Process

The **learned** denoising process $x_0 \leftarrow x_1 \leftarrow \cdots \leftarrow x_T$

$$p_\theta(x_{t-1}|x_t) = \mathcal{N}(x_{t-1}; \mu_\theta(x_t, t), \Sigma_q(t))$$

High-level intuition: derive a *ground truth denoising distribution* $q(x_{t-1}|x_t, x_0)$ and train a neural net $p_\theta(x_{t-1}|x_t)$ to match the distribution.

The learning objective: $\mathrm{argmin}_\theta D_{KL}(q(x_{t-1}|x_t, x_0)||p_\theta(x_{t-1}|x_t))$

What does it look like? $q(x_{t-1}|x_t, x_0) = \mathcal{N}\left(x_{t-1}; \mu_q(t), \Sigma_q(t)\right)$

$$\mu_q(t) = \frac{1}{\sqrt{\alpha_t}}\left(x_t - \frac{\beta_t}{\sqrt{(1-\bar{\alpha}_t)}}\epsilon\right), \qquad \epsilon \sim \mathcal{N}(0, I) \leftarrow$$

Recall: Gaussian reparameterization trick

The "ground truth" noise that brought x_{t-1} to x_t

The Denoising (Decoding) Process

The **learned** denoising process $x_0 \leftarrow x_1 \leftarrow \cdots \leftarrow x_T$

$$p_\theta(x_{t-1}|x_t) = \mathcal{N}(x_{t-1}; \mu_\theta(x_t, t), \Sigma_q(t))$$

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What does it look like? $q(x_{t-1}|x_t, x_0) = \mathcal{N}\left(x_{t-1}; \mu_q(t), \Sigma_q(t)\right)$

Assuming identical variance $\Sigma_q(t)$, we have:

$$\mathrm{argmin}_\theta D_{KL}(q(x_{t-1}|x_t, x_0)||p_\theta(x_{t-1}|x_t)) = \mathrm{argmin}_\theta w||\mu_q(t) - \mu_\theta(x_t, t)||$$

Should be variance-dependent, but constant works better in practice

$p(x) = \int p(x|z)p(z)dz$ Intractable to estimate!

$$\log p(x) = \mathrm{E}_q\left[\log \frac{p(x|z)p(z)}{q(z|x)}\right] + D_{KL}(q(z|x)||p(z|x))$$

$$\geq \mathrm{E}_q\left[\log \frac{p(x|z)p(z)}{q(z|x)}\right]$$ Evidence Lower Bound (ELBO)

$$\log p(x_0) \geq \mathrm{E}_q\left[\log \frac{p(x_0|x_{1:T})p(x_{1:T})}{q(x_{1:T}|x_0)}\right]$$ $x = x_0,\ z = x_{1:T}$

$$= \mathrm{E}_q\left[\log \frac{p(x_T)\prod_{t=1}^{T} p_\theta(x_{t-1}|x_t)}{\prod_{t=1}^{T} q(x_t|x_{t-1})}\right]$$

… (derivation omitted, see Sohl-Dickstein *et al.,* 2015 Appendix B)

$$= -\mathrm{E}_q[D_{KL}(q(x_T|x_0)||p(x_T))] \boxed{-\sum_{t=2}^{T} D_{KL}(q(x_{t-1}|x_t, x_0)||p_\theta(x_{t-1}|x_t))} + \log p_\theta(x_0|x_1)$$

Maximize the agreement between the predicted reverse diffusion distribution p_θ and the "ground truth" reverse diffusion distribution q

Deep Unsupervised Learning using Nonequilibrium Thermodynamics, Sohl-Dickstein *et al.*, 2015

Learning the Denoising Process

The **learned** denoising process $x_0 \leftarrow x_1 \leftarrow \cdots \leftarrow x_T$

$$p_\theta(x_{0:T}) = p(x_T)\prod_{t=1}^{T} p_\theta(x_{t-1}|x_t)$$

$$p_\theta(x_{t-1}|x_t) = \mathcal{N}(x_{t-1}; \mu_\theta(x_t, t), \Sigma(t))$$

Conditional Gaussian

Learning objective: $\text{argmin}_\theta ||\mu_q(t) - \mu_\theta(x_t, t)||$

$$\mu_q(t) = \frac{1}{\sqrt{\alpha_t}}\left(x_t - \frac{\beta_t}{\sqrt{(1-\bar{\alpha}_t)}}\epsilon\right), \qquad \epsilon \sim \mathcal{N}(0, I)$$

known during inference

Unknown during inference

Recall: this is the “ground truth” noise that brought x_0 to x_t

Idea: just learn ϵ with $\epsilon_\theta(x_t, t)$!

Learning the Denoising Process

The **learned** denoising process $x_0 \leftarrow x_1 \leftarrow \cdots \leftarrow x_T$

$$p_\theta(x_{0:T}) = p(x_T) \prod_{t=1}^{T} p_\theta(x_{t-1} | x_t)$$

$$p_\theta(x_{t-1} | x_t) = \mathcal{N}(x_{t-1}; \mu_\theta(x_t, t), \Sigma(t))$$

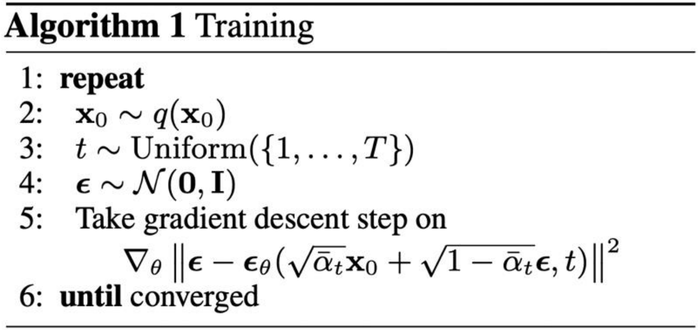
Conditional Gaussian

Simplified learning objective: $\mathrm{argmin}_\theta || \epsilon - \epsilon_\theta\left(\sqrt{\bar{\alpha}_t} x_0 + \sqrt{1 - \bar{\alpha}_t}\epsilon, t\right) ||$

Inference time: $\mu_\theta(x_t, t) = \frac{1}{\sqrt{\alpha_t}}\left(x_t - \frac{\beta_t}{\sqrt{(1 - \bar{\alpha}_t)}} \epsilon_\theta(x_t, t)\right)$

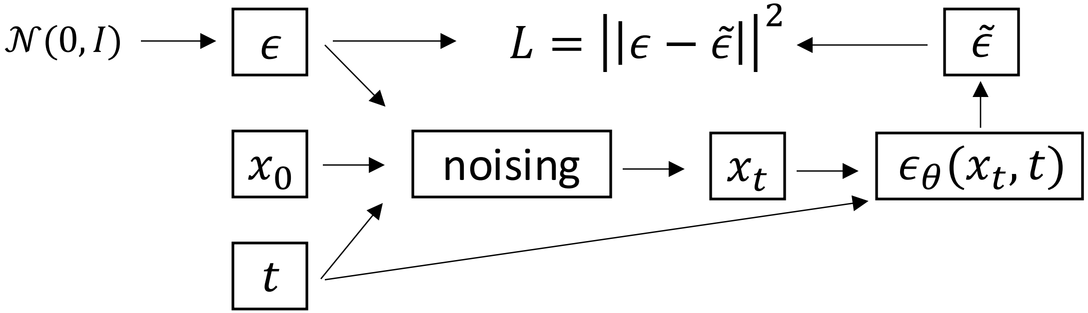
Predicted “denoising noise”

The Denoising Diffusion Algorithm



Algorithm 1 Training

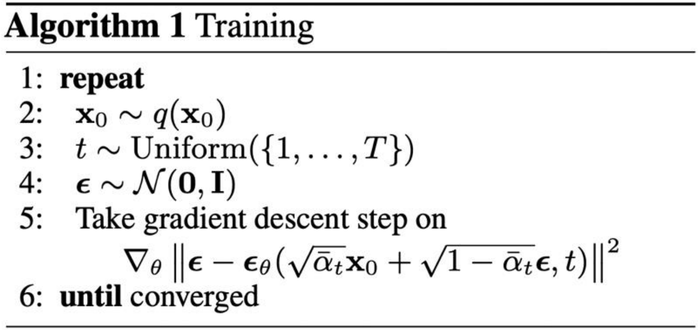
```
repeat
  $\mathbf{x}_0 \sim q(\mathbf{x}_0)$
  $t \sim \mathrm{Uniform}(\{1, \ldots, T\})$
  $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
  Take gradient descent step on
      $\nabla_\theta \left\| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}, t) \right\|^2$
until converged
```



Compute regression loss

The Denoising Diffusion Probabilistic Models, Ho *et al.*, 2020

The Denoising Diffusion Algorithm



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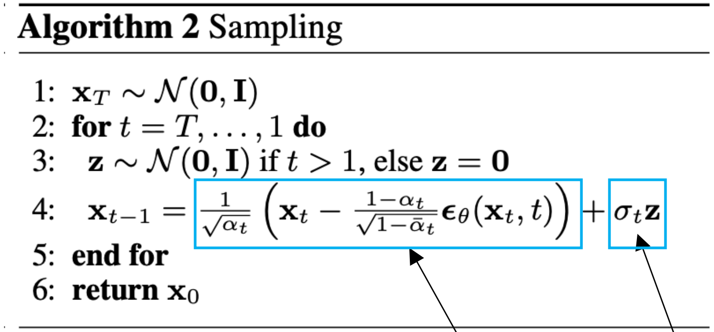
```

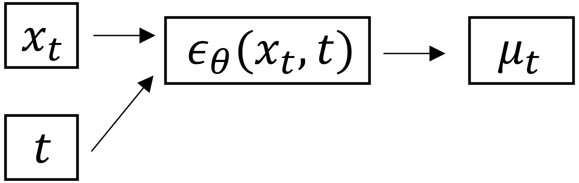


Algorithm 2 Sampling

```
$\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
for $t = T, \ldots, 1$ do
  $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ if $t > 1$, else $\mathbf{z} = \mathbf{0}$
  $\mathbf{x}_{t-1} = \boxed{\frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)\right)} + \boxed{\sigma_t \mathbf{z}}$
end for
return $\mathbf{x}_0$
```

$$\sigma_t = \sqrt{\beta}_t$$

$$p_\theta(x_{t-1}|x_t) = \mathcal{N}(x_{t-1}; \mu(t), \Sigma(t))$$



x_t

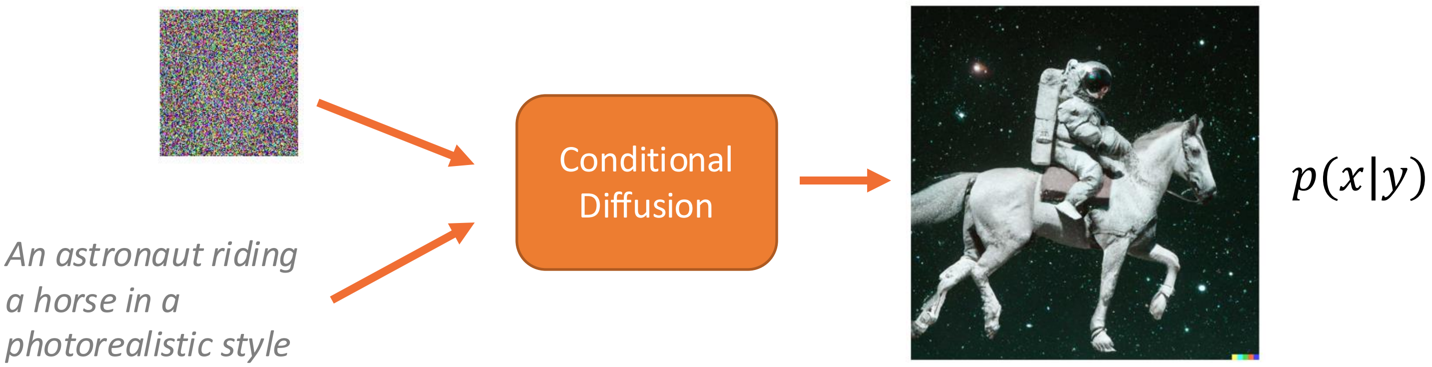
t

$\epsilon_\theta(x_t, t)$

μ_t

The Denoising Diffusion Probabilistic Models, Ho *et al.*, 2020

Conditional Diffusion Models



An astronaut riding a horse in a photorealistic style

Conditional Diffusion

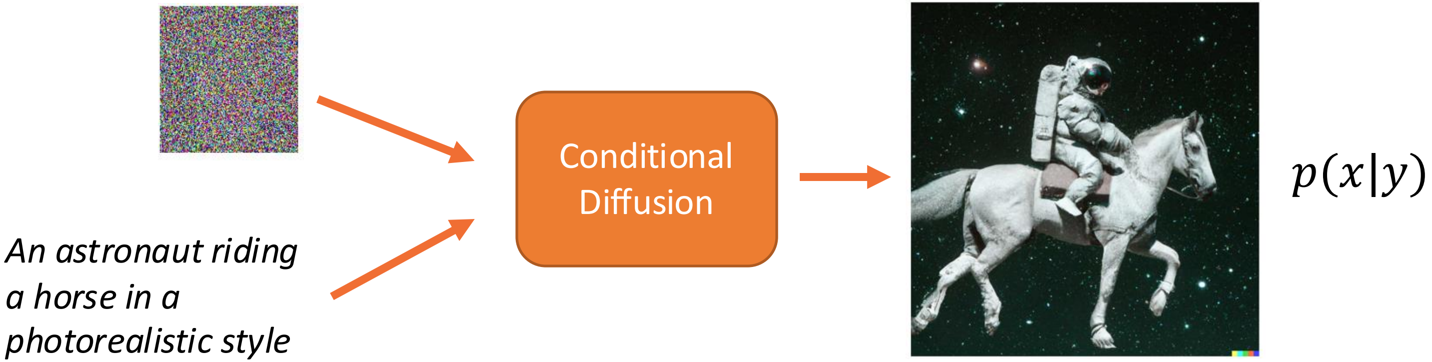
$p(x|y)$

Simple idea: just condition the model on some text labels y!

$$\epsilon_\theta(x_t, y, t)$$

Problem: Very blurry generation

Classifier-free Guided Diffusion



An astronaut riding a horse in a photorealistic style

Conditional Diffusion

$p(x|y)$

Classifier-free Guided Diffusion: estimate the gradient of the classifier model with conditional diffusion models!

$$\nabla_{x_t} \log f_\varphi(y|x_t) = -\frac{1}{\sqrt{1-\bar{\alpha}_t}}\left(\epsilon_\theta(x_t, t, y) - \epsilon_\theta(x_t, t)\right)$$

$$\bar{\epsilon}_\theta(x_t, t, y) = (w+1)\epsilon_\theta(x_t, t, y) - w\epsilon_\theta(x_t, t)$$

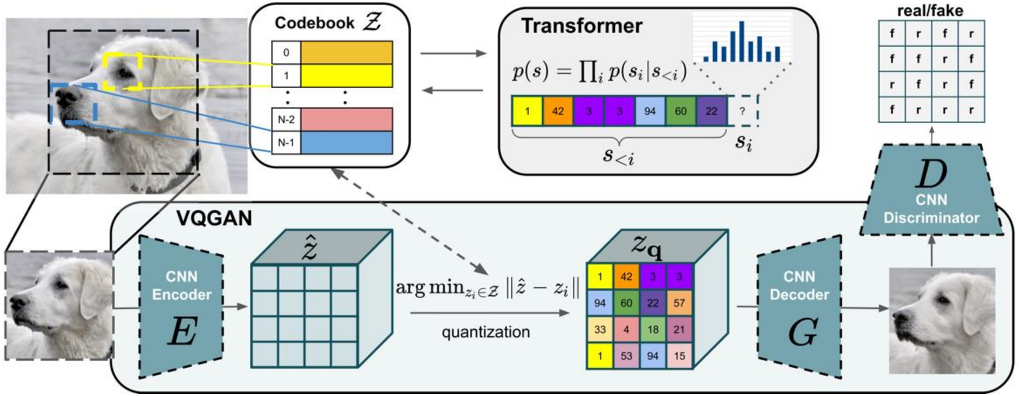
Linearly combine denoisers from an unconditional distribution and a conditional distribution

Ho and Salimans, 2022

Latent-space Diffusion

Problem: Hard to learn diffusion process on high-resolution images

Solution: learn a low-dimensional latent space using a ViT-based autoencoder and *do diffusion on the latent space*!



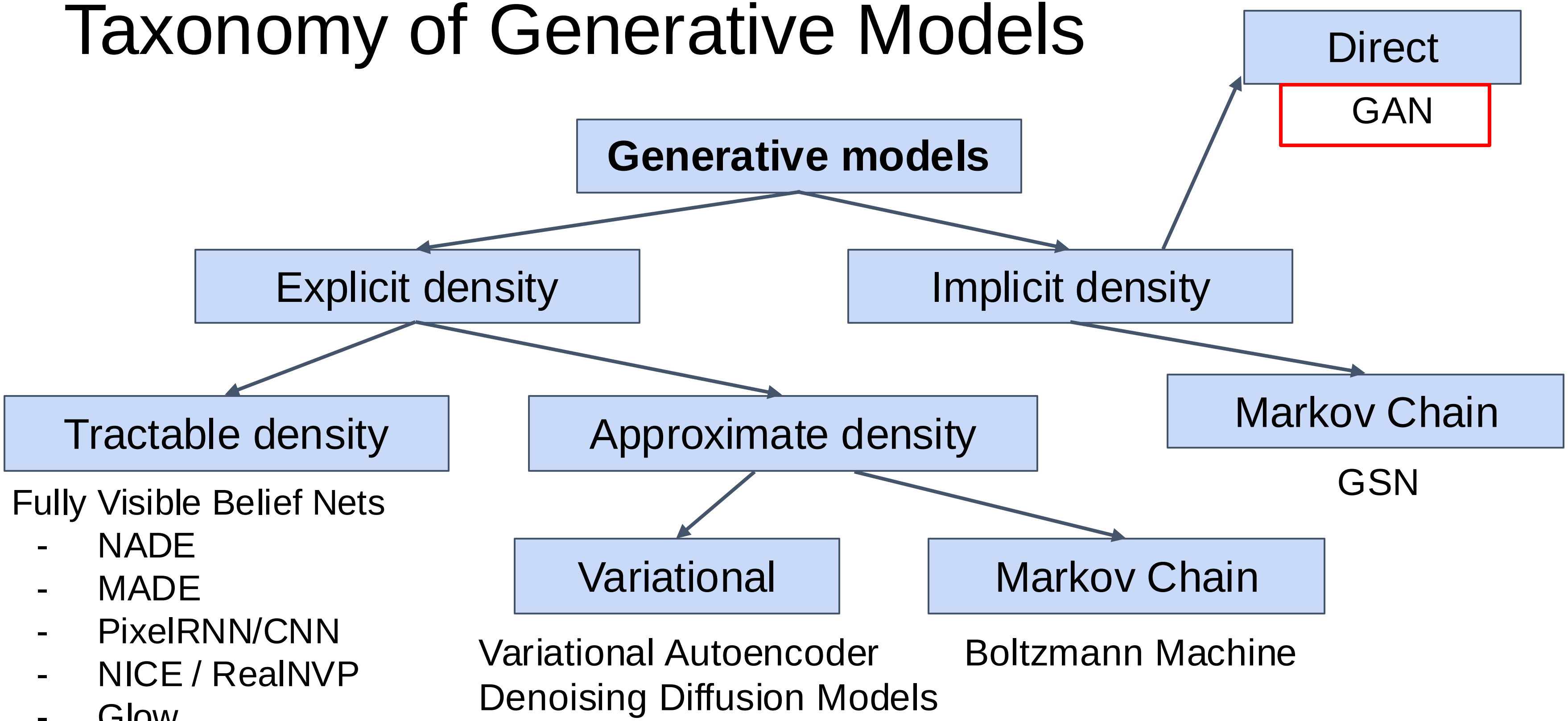
The latent space autoencoder

Esser and Rombach *et al.*, 2021

Summary

- Denoising Diffusion model is a type of generative model that learns the process of “denoising” a known noise source (Gaussian).
- We can construct a learning problem by deriving the evidence lower bound (ELBO) of the denoising process.
- The learning objective is to minimize the KL divergence between the “ground truth” and the learned denoising distribution.
- A simplified learning objective is to estimate the noise of the forward diffusion process.
- The diffusion process can be guided to generate targeted samples.
- Can be applied to many different domains. Same underlying principle.
- Very hot topic!

Taxonomy of Generative Models



Generative models

Explicit density

Implicit density

Direct

GAN

Tractable density

Approximate density

Markov Chain

GSN

Fully Visible Belief Nets
- NADE
- MADE
- PixelRNN/CNN
- NICE / RealNVP
- Glow
- Ffjord

Variational

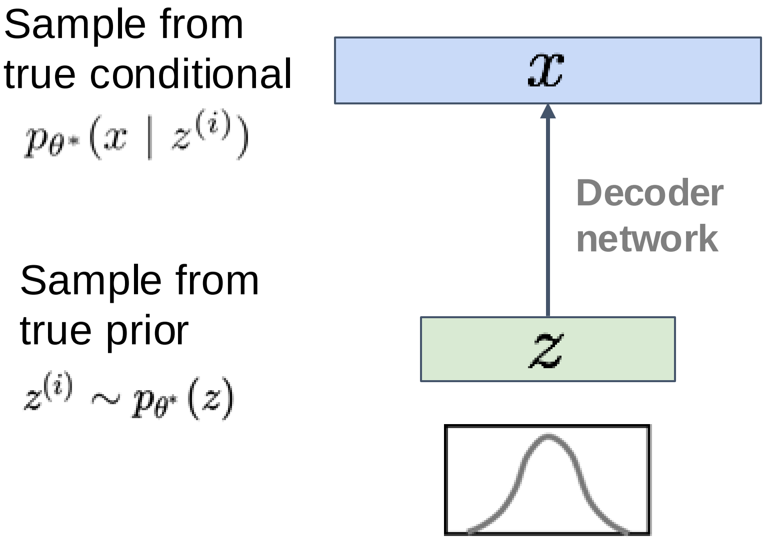
Variational Autoencoder
Denoising Diffusion Models

Markov Chain

Boltzmann Machine

Figure copyright and adapted from Ian Goodfellow, Tutorial on Generative Adversarial Networks, 2017.

Recall: Variational Autoencoders



Sample from true conditional

$p_{\theta^*}(x \mid z^{(i)})$

Sample from true prior

$z^{(i)} \sim p_{\theta^*}(z)$

We want to estimate the true parameters θ^* of this generative model given training data x.

How should we represent this model?

Assume p(z) is *known* and ***simple***, e.g. isotropic Gaussian. Reasonable for latent attributes, e.g. pose, how much smile.

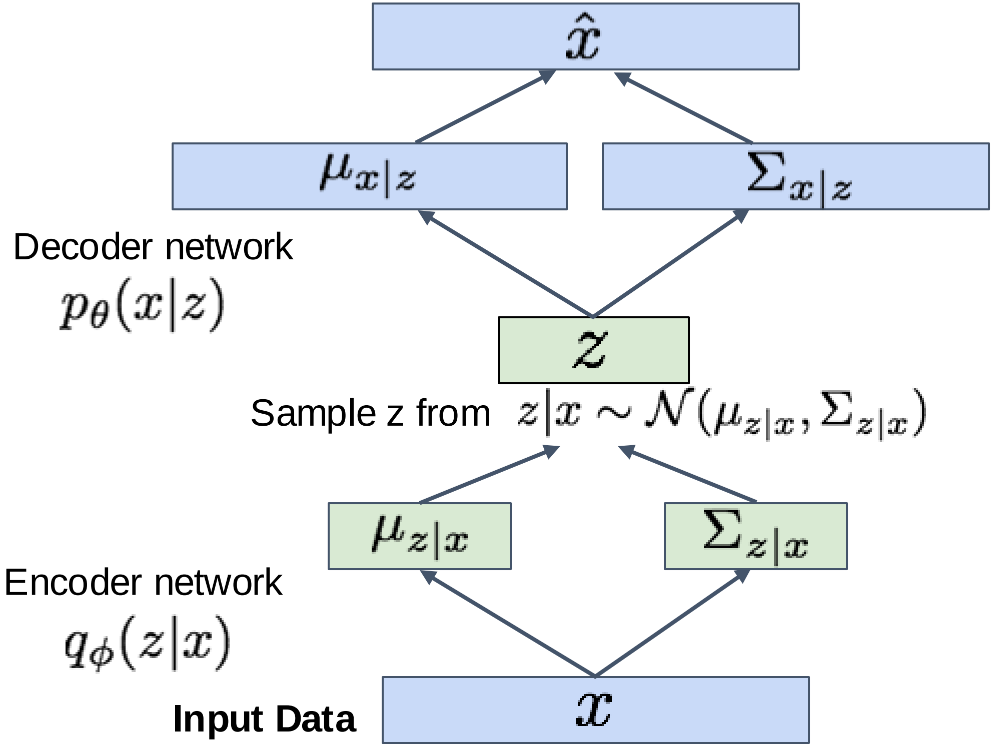
Conditional p(x|z) is ***complex*** (generates image) => represent with neural network

Kingma and Welling, “Auto-Encoding Variational Bayes”, ICLR 2014

Recall: Variational Autoencoders

Overall, we are trying to match a distribution p(z) to a new distribution p(x|z).

We need an approximate posterior q(z|x) to tell us which z corresponds to which x.

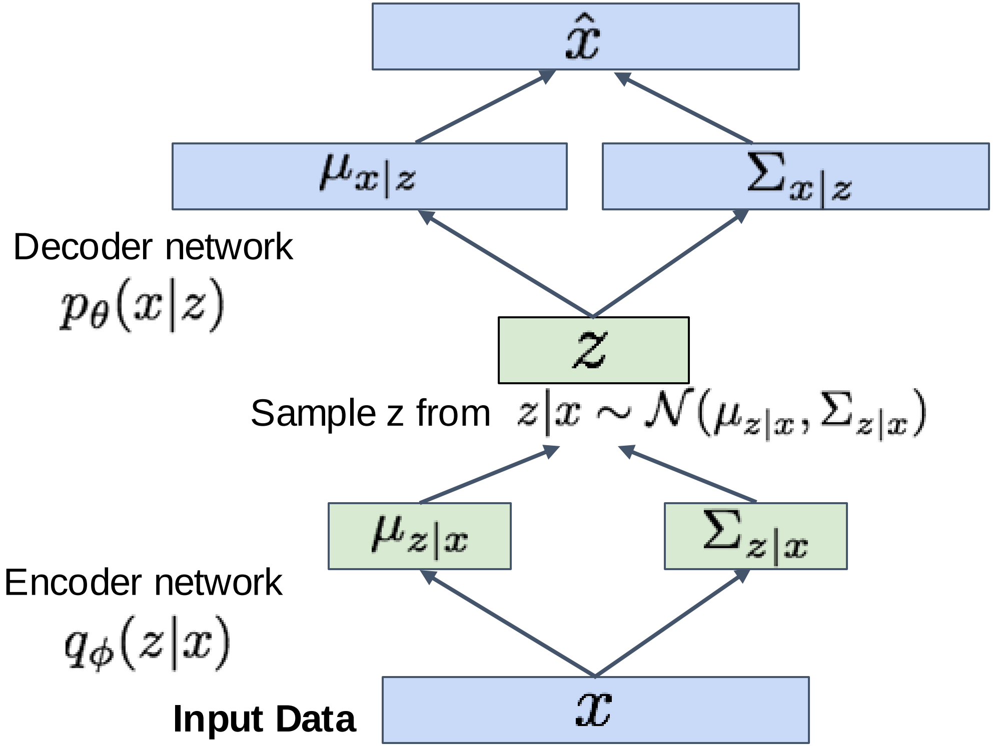


Recall: Variational Autoencoders

Overall, we are trying to match a distribution p(z) to a new distribution p(x|z).

We need an approximate posterior q(z|x) to tell us which z in the prior corresponds to which x.

What if we can learn this mapping (prior z to samples x) directly?



$\hat{x}$

$\mu_{x|z}$

$\Sigma_{x|z}$

Decoder network

$p_\theta(x|z)$

z

Sample z from $z|x \sim \mathcal{N}(\mu_{z|x}, \Sigma_{z|x})$

$\mu_{z|x}$

$\Sigma_{z|x}$

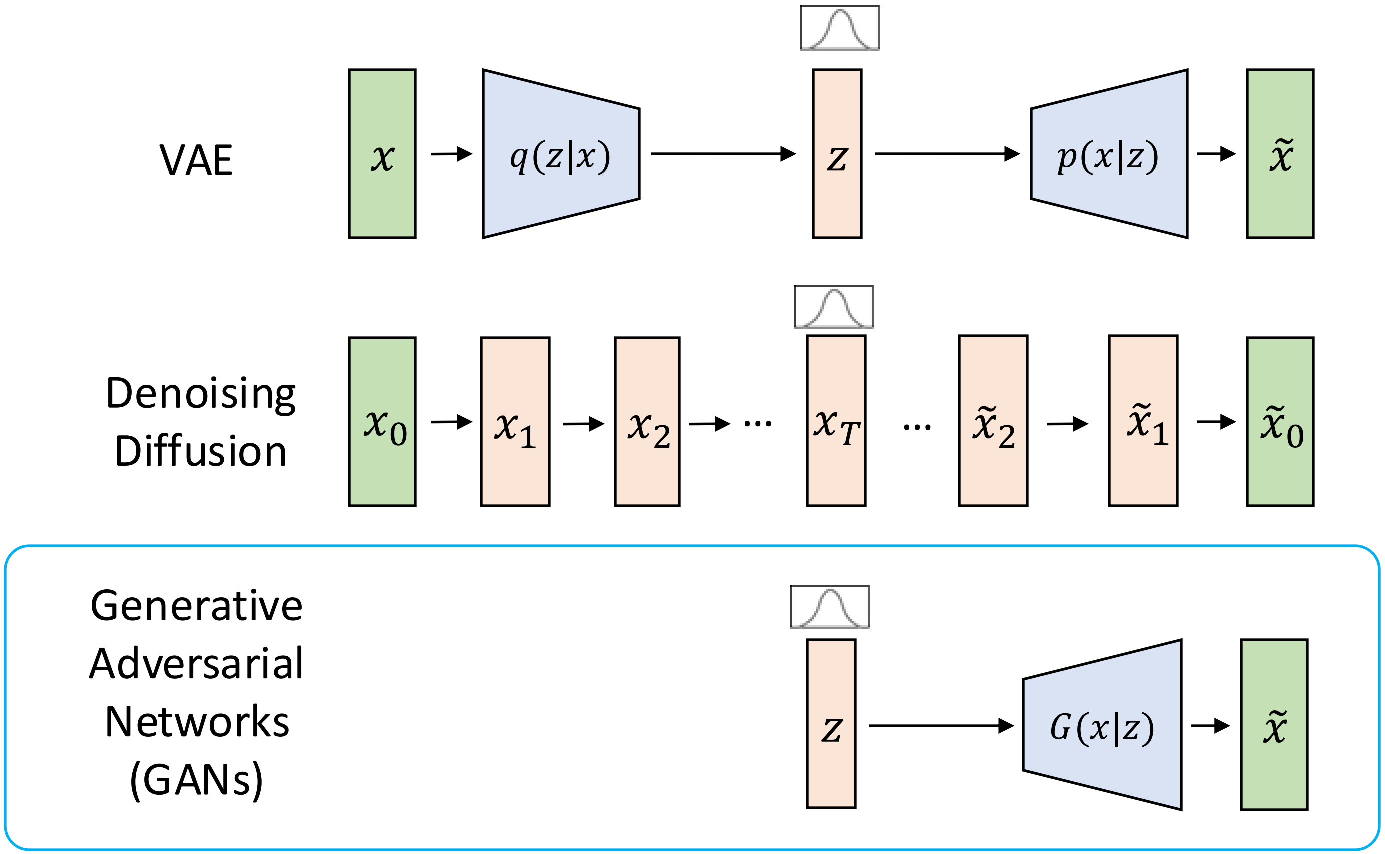
Encoder network

$q_\phi(z|x)$

Input Data

x

GANs: Learning generate samples directly



VAE

$x \rightarrow q(z|x) \rightarrow z \rightarrow p(x|z) \rightarrow \tilde{x}$

Denoising Diffusion

$x_0 \rightarrow x_1 \rightarrow x_2 \rightarrow \cdots x_T \cdots \tilde{x}_2 \rightarrow \tilde{x}_1 \rightarrow \tilde{x}_0$

Generative Adversarial Networks (GANs)

$z \rightarrow G(x|z) \rightarrow \tilde{x}$

Generative Adversarial Networks

Ian Goodfellow et al., “Generative Adversarial Nets”, NIPS 2014

Problem: Want to sample from complex, high-dimensional training distribution. No direct way to do this!

Solution: Sample from a simple distribution we can easily sample from, e.g. random noise. Learn transformation to training distribution.

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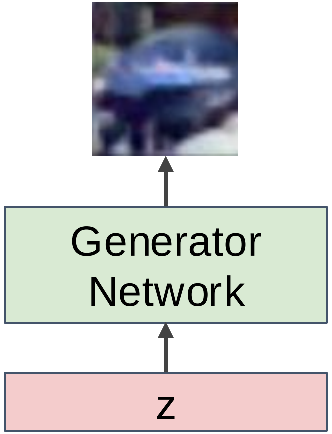

Output: Sample from training distribution

Generator Network

Input: Random noise

z

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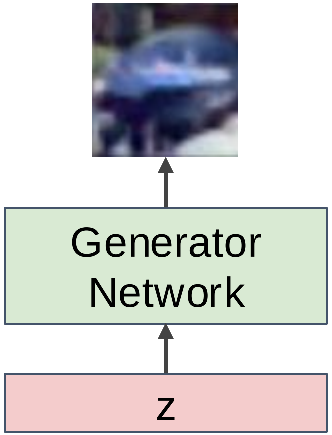
But we don’t know which sample z maps to which training image -> can’t learn by reconstructing training images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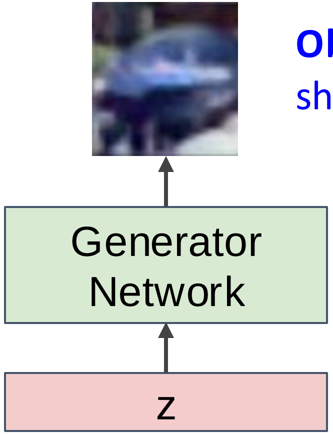


Input: Random noise

Objective: generated images should look “real”

Generative Adversarial Networks

Ian Goodfellow et al., “Generative Adversarial Nets”, NIPS 2014

Problem: Want to sample from complex, high-dimensional training distribution. No direct way to do this!

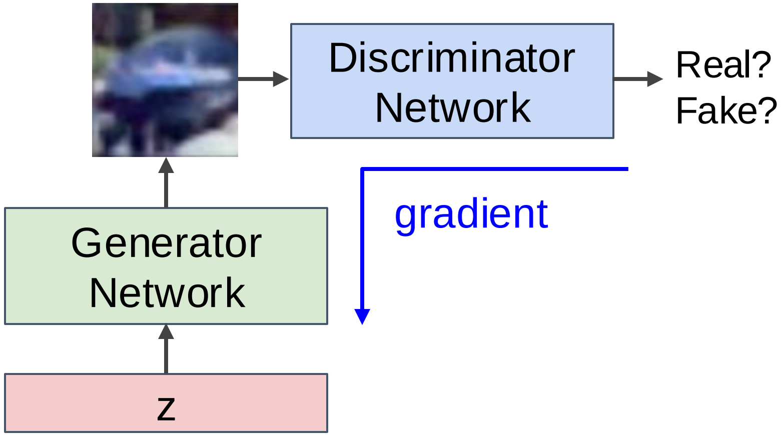
Solution: Sample from a simple distribution we can easily sample from, e.g. random noise. Learn transformation to training distribution.

But we don’t know which sample z maps to which training image -> can’t learn by reconstructing training images

Solution: Use a discriminator network to tell whether the generate image is within data distribution (“real”) or not

Output: Sample from training distribution

Input: Random noise



Discriminator Network

Real?
Fake?

gradient

Generator Network

z

Training GANs: Two-player game

Ian Goodfellow et al., “Generative Adversarial Nets”, NIPS 2014

Discriminator network: try to distinguish between real and fake images
Generator network: try to fool the discriminator by generating real-looking images

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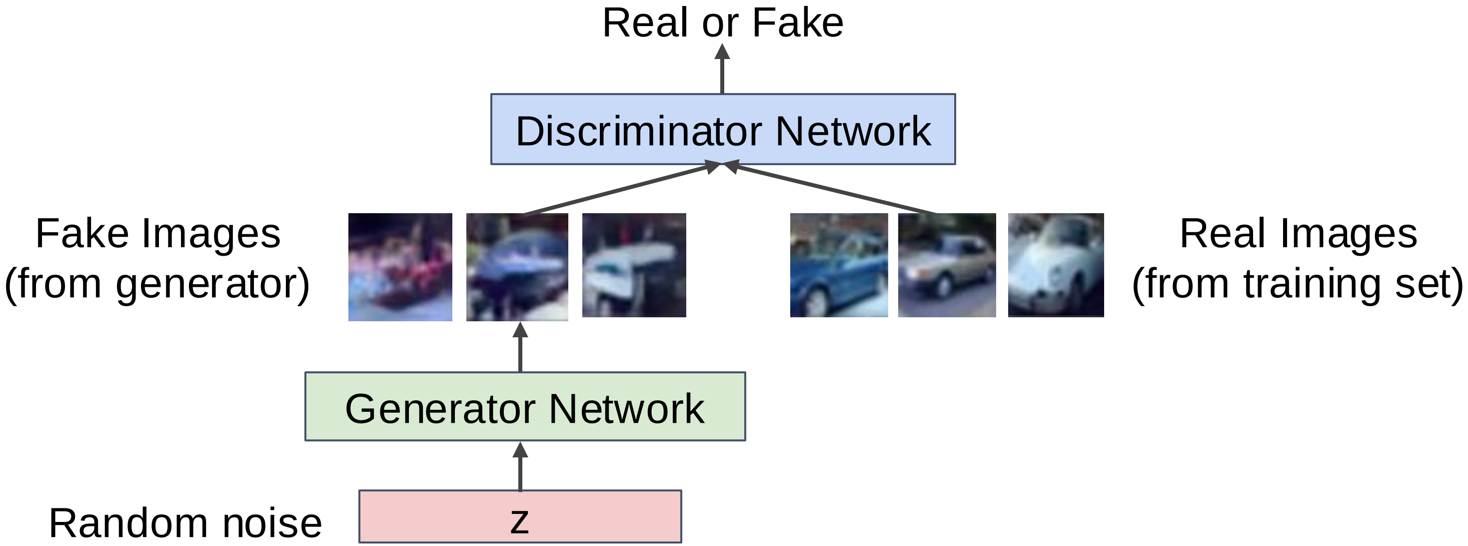

Fake and real images copyright Emily Denton et al. 2015. Reproduced with permission.

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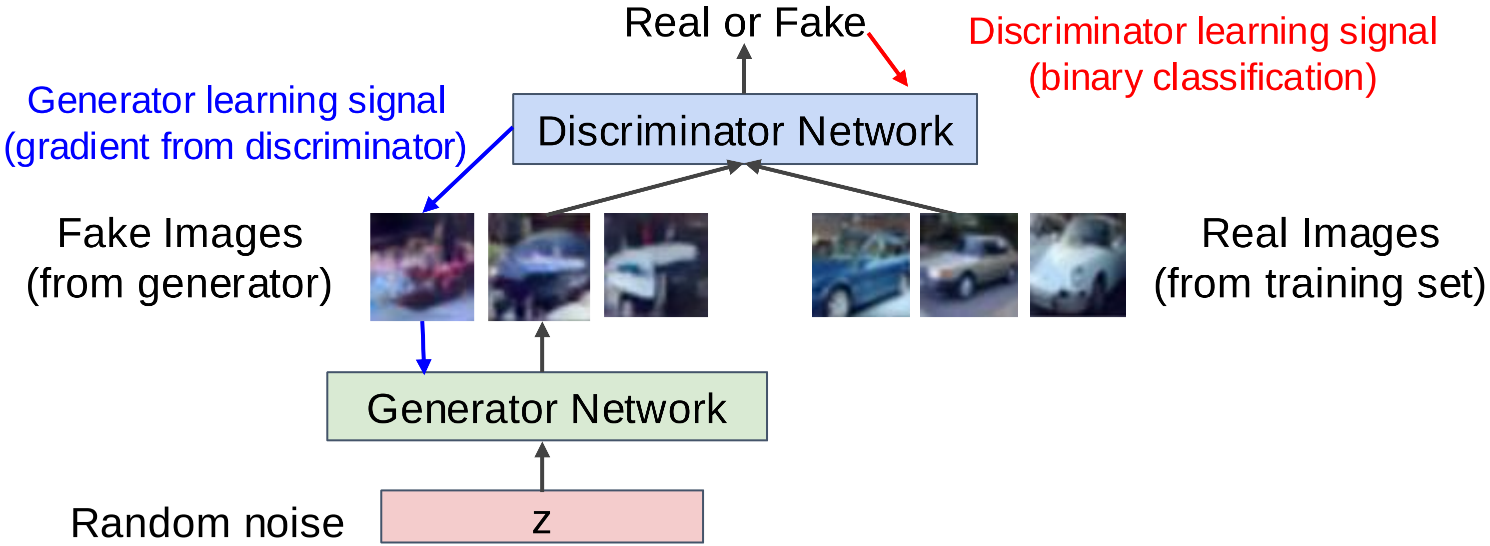

Real or Fake

Discriminator learning signal
(binary classification)

Generator learning signal
(gradient from discriminator)

Discriminator Network

Fake Images
(from generator)

Real Images
(from training set)

Generator Network

Random noise

z

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Generator network: try to fool the discriminator by generating real-looking images

Train jointly in **minimax game**

Minimax objective function:

$$\min_{\theta_g} \max_{\theta_d} \left[\mathbb{E}_{x \sim p_{data}} \log D_{\theta_d}(x) + \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z))) \right]$$

Generator objective

Discriminator objective

Training GANs: Two-player game

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Train jointly in **minimax game**

Discriminator outputs likelihood in (0,1) of real image

Minimax objective function:

$$\min_{\theta_g}\max_{\theta_d}\left[\mathbb{E}_{x\sim p_{data}}\log \underbrace{D_{\theta_d}(x)}_{\text{Discriminator output for real data x}} + \mathbb{E}_{z\sim p(z)}\log(\underbrace{1-D_{\theta_d}(G_{\theta_g}(z))}_{\text{Discriminator output for generated fake data G(z)}})\right]$$

$\uparrow$

Classify all real images as real

Classify all generated images as fake

Training GANs: Two-player game

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Discriminator outputs likelihood in (0,1) of real image

Minimax objective function:

$$\min_{\theta_g} \max_{\theta_d} \left[\mathbb{E}_{x\sim p_{data}} \log D_{\theta_d}(x) + \mathbb{E}_{z\sim p(z)} \log(1 - D_{\theta_d}(\underbrace{G_{\theta_g}(z)}))\right]$$

Generator: learn to fool discriminator. Minimize $\log(1 - p_{\theta_d}(x_{gen}))$

Training GANs: Two-player game

Ian Goodfellow et al., “Generative Adversarial Nets”, NIPS 2014

Discriminator network: try to distinguish between real and fake images
Generator network: try to fool the discriminator by generating real-looking images

Train jointly in **minimax game**

Discriminator outputs likelihood in (0,1) of real image

Minimax objective function:

$$\min_{\theta_g} \max_{\theta_d} \left[\mathbb{E}_{x \sim p_{data}} \log D_{\theta_d}(x) + \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z))) \right]$$

- Discriminator (θ_d) wants to **maximize objective** such that D(x) is close to 1 (real) and D(G(z)) is close to 0 (fake)
- Generator (θ_g) wants to **minimize objective** such that D(G(z)) is close to 1 (discriminator is fooled into thinking generated G(z) is real)

Training GANs: Two-player game

Ian Goodfellow et al., “Generative Adversarial Nets”, NIPS 2014

Minimax objective function:

$$\min_{\theta_g} \max_{\theta_d} \left[\mathbb{E}_{x \sim p_{data}} \log D_{\theta_d}(x) + \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z))) \right]$$

Alternate between:

1. **Gradient ascent** on discriminator

$$\max_{\theta_d} \left[\mathbb{E}_{x \sim p_{data}} \log D_{\theta_d}(x) + \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z))) \right]$$

2. **Gradient descent** on generator

$$\min_{\theta_g} \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z)))$$

Training GANs: Two-player game

Ian Goodfellow et al., “Generative Adversarial Nets”, NIPS 2014

Minimax objective function:

$$\min_{\theta_g} \max_{\theta_d} \left[\mathbb{E}_{x \sim p_{data}} \log D_{\theta_d}(x) + \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z))) \right]$$

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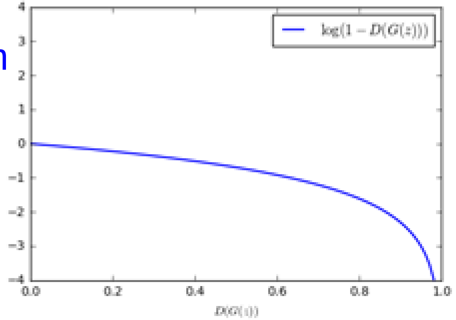
2. **Gradient descent** on generator

$$\min_{\theta_g} \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z)))$$

In practice, optimizing this generator objective does not work well!

When sample is likely fake, want to learn from it to improve generator (move to the right on X axis).



Training GANs: Two-player game

Ian Goodfellow et al., "Generative Adversarial Nets", NIPS 2014

Minimax objective function:

$$\min_{\theta_g} \max_{\theta_d} \left[\mathbb{E}_{x \sim p_{data}} \log D_{\theta_d}(x) + \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z))) \right]$$

Alternate between:

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$$\max_{\theta_d} \left[\mathbb{E}_{x \sim p_{data}} \log D_{\theta_d}(x) + \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z))) \right]$$

2. **Gradient descent** on generator

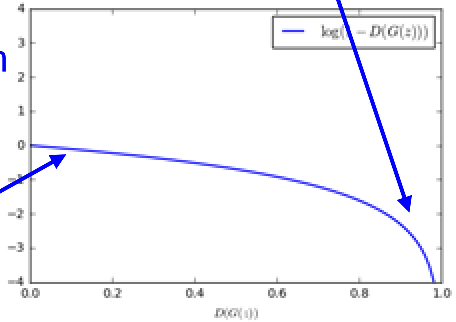
$$\min_{\theta_g} \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z)))$$

In practice, optimizing this generator objective does not work well!

When sample is likely fake, want to learn from it to improve generator (move to the right on X axis).

But gradient in this region is relatively flat!

Gradient signal dominated by region where sample is already good



Training GANs: Two-player game

Ian Goodfellow et al., “Generative Adversarial Nets”, NIPS 2014

Minimax objective function:

$$\min_{\theta_g} \max_{\theta_d} \left[\mathbb{E}_{x \sim p_{data}} \log D_{\theta_d}(x) + \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z))) \right]$$

Alternate between:

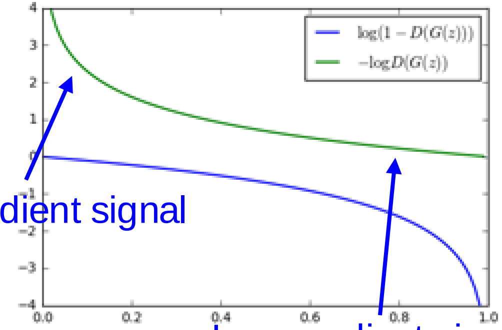
1. **Gradient ascent** on discriminator

$$\max_{\theta_d} \left[\mathbb{E}_{x \sim p_{data}} \log D_{\theta_d}(x) + \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z))) \right]$$

2. **Instead: Gradient ascent** on generator, different objective

$$\max_{\theta_g} \mathbb{E}_{z \sim p(z)} \log(D_{\theta_d}(G_{\theta_g}(z)))$$

Instead of minimizing likelihood of discriminator being correct, now maximize likelihood of discriminator being wrong.
Same objective of fooling discriminator, but now higher gradient signal for bad samples => works much better! Standard in practice.



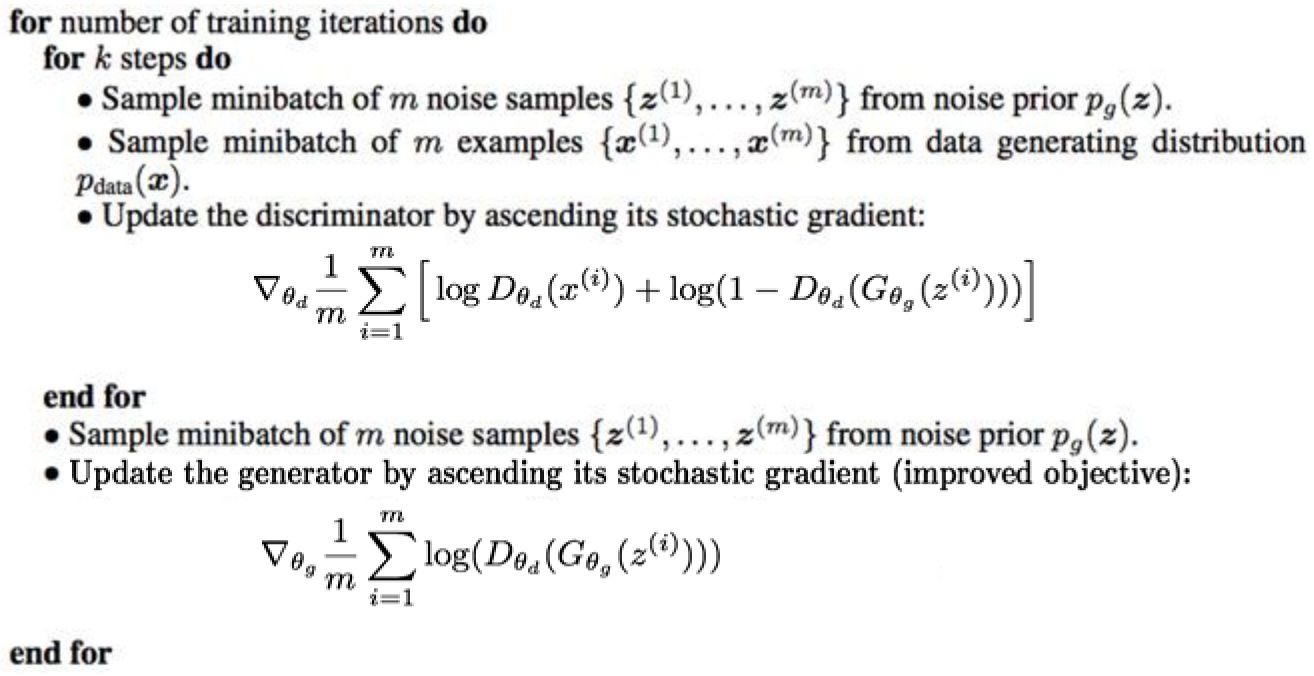
High gradient signal

Low gradient signal

Training GANs: Two-player game

Ian Goodfellow et al., “Generative Adversarial Nets”, NIPS 2014

Putting it together: GAN training algorithm



```
for number of training iterations do
    for $k$ steps do
        • Sample minibatch of $m$ noise samples $\{\boldsymbol{z}^{(1)}, \dots, \boldsymbol{z}^{(m)}\}$ from noise prior $p_g(\boldsymbol{z})$.
        • Sample minibatch of $m$ examples $\{\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(m)}\}$ from data generating distribution $p_{\text{data}}(\boldsymbol{x})$.
        • Update the discriminator by ascending its stochastic gradient:
            $\nabla_{\theta_d} \frac{1}{m} \sum_{i=1}^{m} \left[ \log D_{\theta_d}(x^{(i)}) + \log(1 - D_{\theta_d}(G_{\theta_g}(z^{(i)}))) \right]$
    end for
    • Sample minibatch of $m$ noise samples $\{\boldsymbol{z}^{(1)}, \dots, \boldsymbol{z}^{(m)}\}$ from noise prior $p_g(\boldsymbol{z})$.
    • Update the generator by ascending its stochastic gradient (improved objective):
        $\nabla_{\theta_g} \frac{1}{m} \sum_{i=1}^{m} \log(D_{\theta_d}(G_{\theta_g}(z^{(i)})))$
end for
```

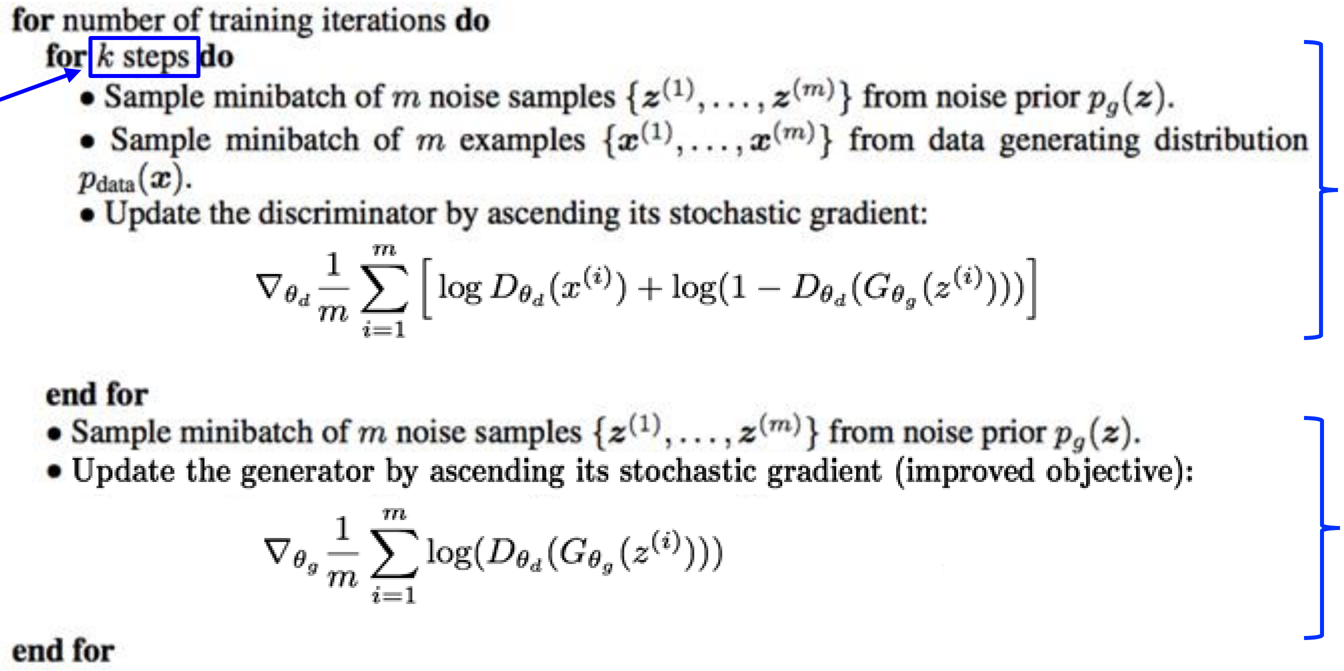
Training GANs: Two-player game

Ian Goodfellow et al., “Generative Adversarial Nets”, NIPS 2014

Putting it together: GAN training algorithm

Some find k=1 more stable, others use k > 1, no best rule.

Followup work (e.g. Wasserstein GAN, BEGAN) alleviates this problem, better stability!



```
for number of training iterations do
    for $k$ steps do
        • Sample minibatch of $m$ noise samples $\{z^{(1)}, \dots, z^{(m)}\}$ from noise prior $p_g(z)$.
        • Sample minibatch of $m$ examples $\{x^{(1)}, \dots, x^{(m)}\}$ from data generating distribution $p_{\text{data}}(x)$.
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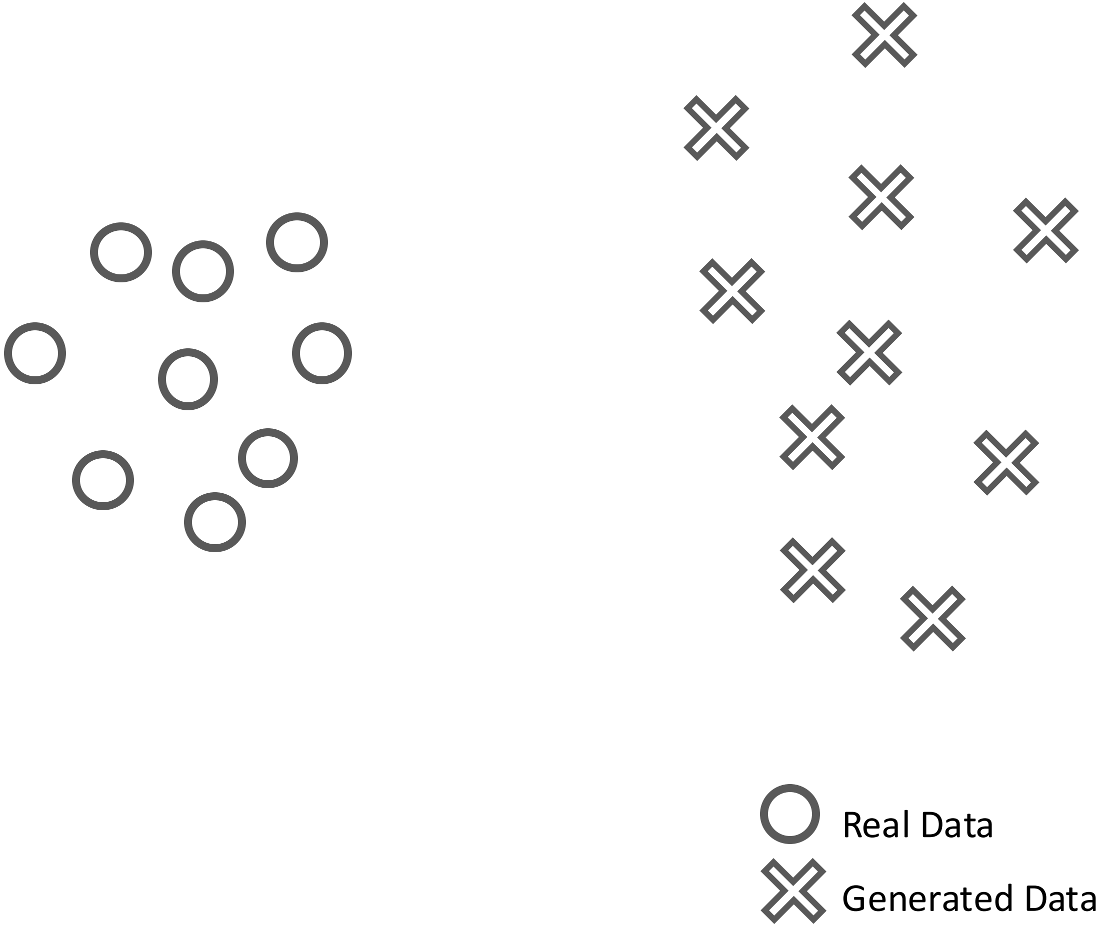
    end for
    • Sample minibatch of $m$ noise samples $\{z^{(1)}, \dots, z^{(m)}\}$ from noise prior $p_g(z)$.
    • Update the generator by ascending its stochastic gradient (improved objective):
        $\nabla_{\theta_g} \frac{1}{m} \sum_{i=1}^{m} \log(D_{\theta_d}(G_{\theta_g}(z^{(i)})))$
end for
```

Update discriminator

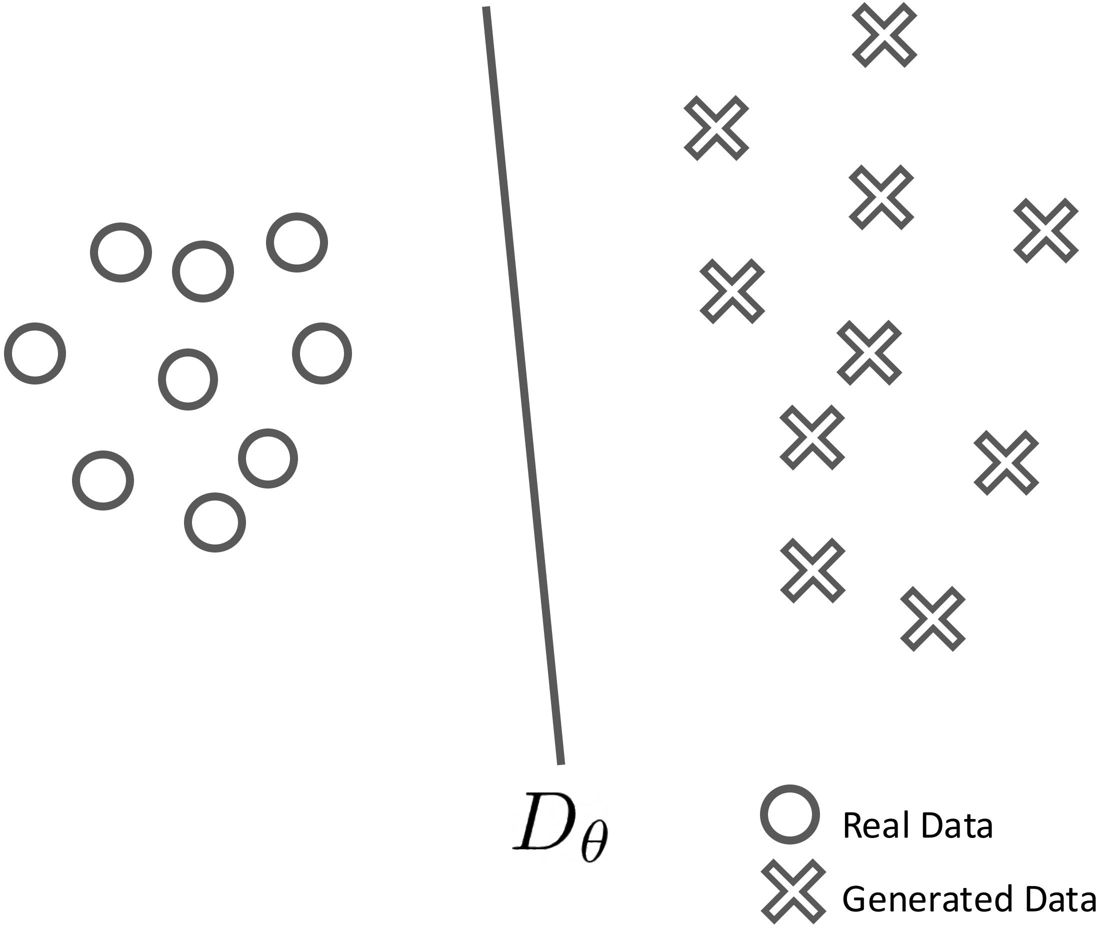
Update generator

Arjovsky et al. "Wasserstein gan." arXiv preprint arXiv:1701.07875 (2017)
Berthelot, et al. "Began: Boundary equilibrium generative adversarial networks." arXiv preprint arXiv:1703.10717 (2017)

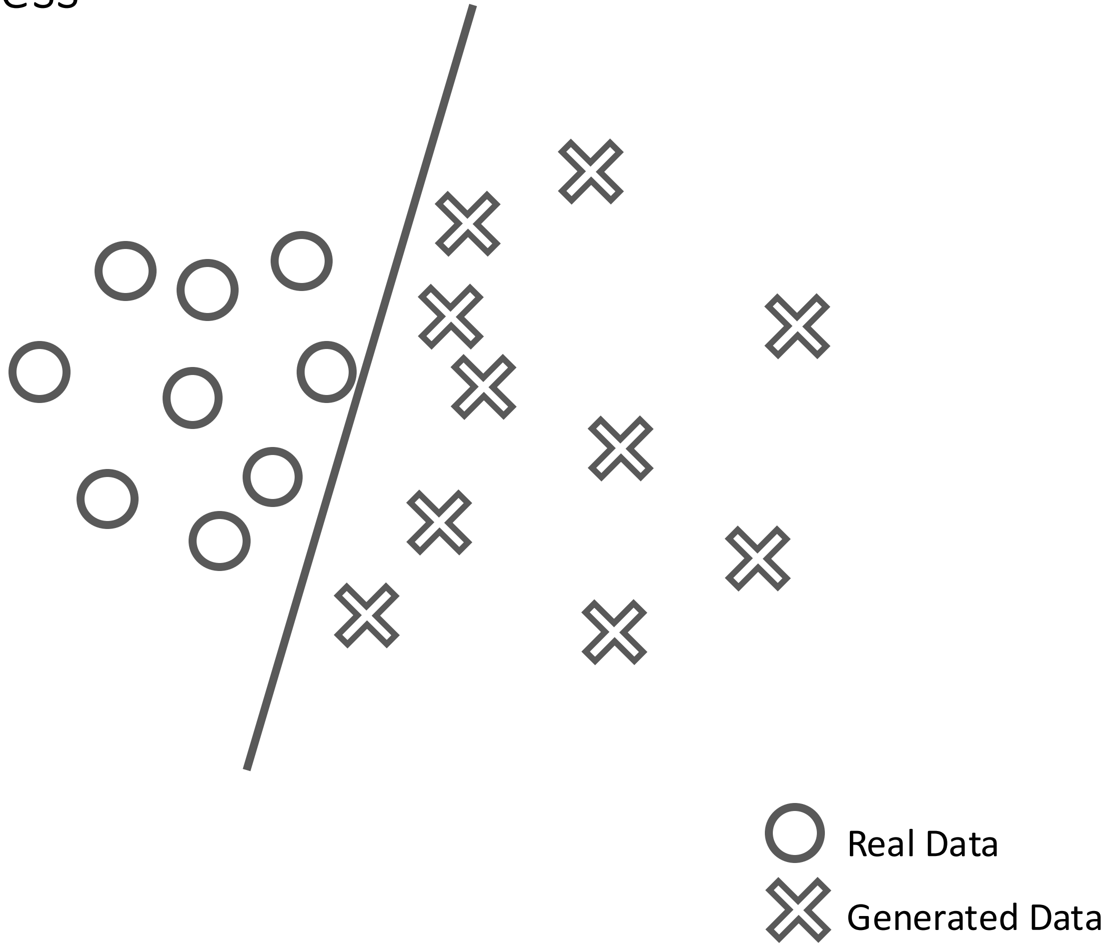
GAN Learning Process



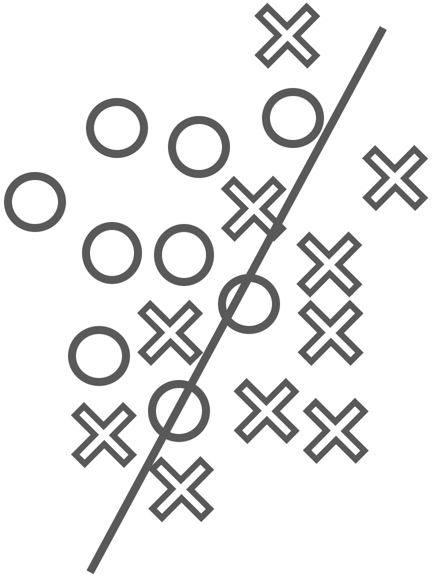
GAN Learning Process



GAN Learning Process



GAN Learning Process



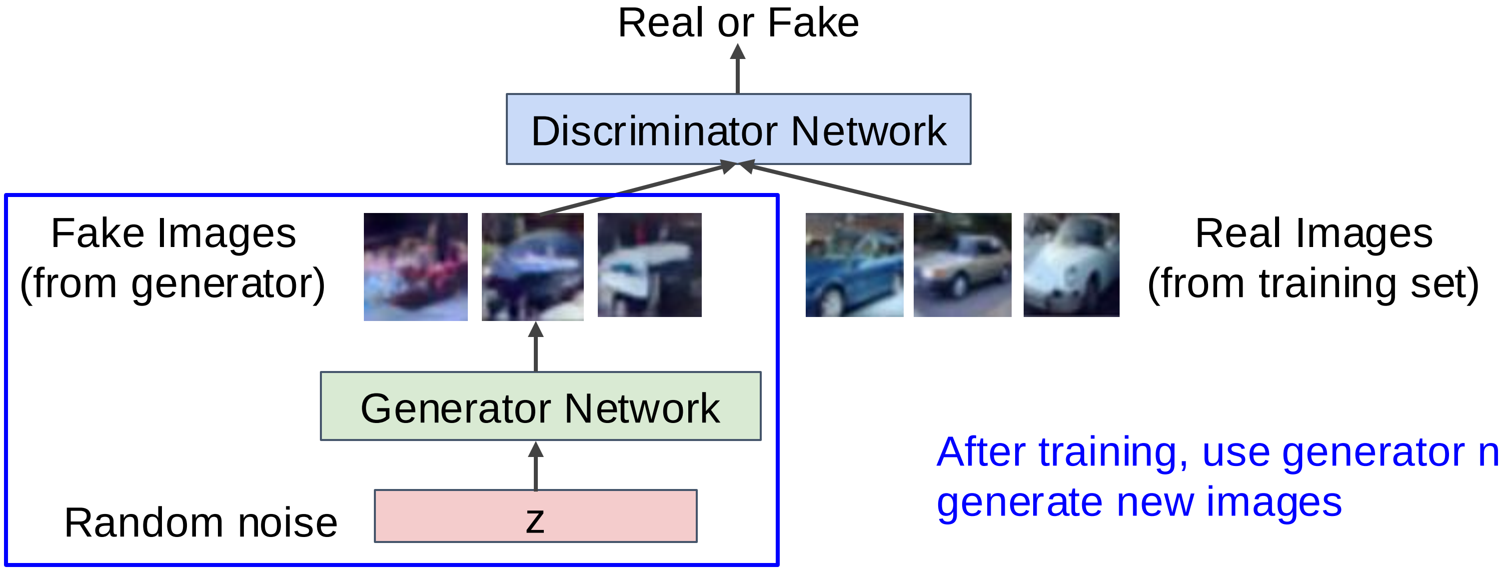
○ Real Data

✕ Generated Data

Training GANs: Two-player game

Ian Goodfellow et al., “Generative Adversarial Nets”, NIPS 2014

Generator network: try to fool the discriminator by generating real-looking images
Discriminator network: try to distinguish between real and fake images



Real or Fake

Discriminator Network

Fake Images
(from generator)

Real Images
(from training set)

Generator Network

Random noise

z

After training, use generator network to generate new images

Fake and real images copyright Emily Denton et al. 2015. Reproduced with permission.

Ian Goodfellow et al., “Generative Adversarial Nets”, NIPS 2014

Generative Adversarial Nets

Generated samples

Nearest neighbor from training set

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Ian Goodfellow et al., “Generative Adversarial Nets”, NIPS 2014

Generative Adversarial Nets

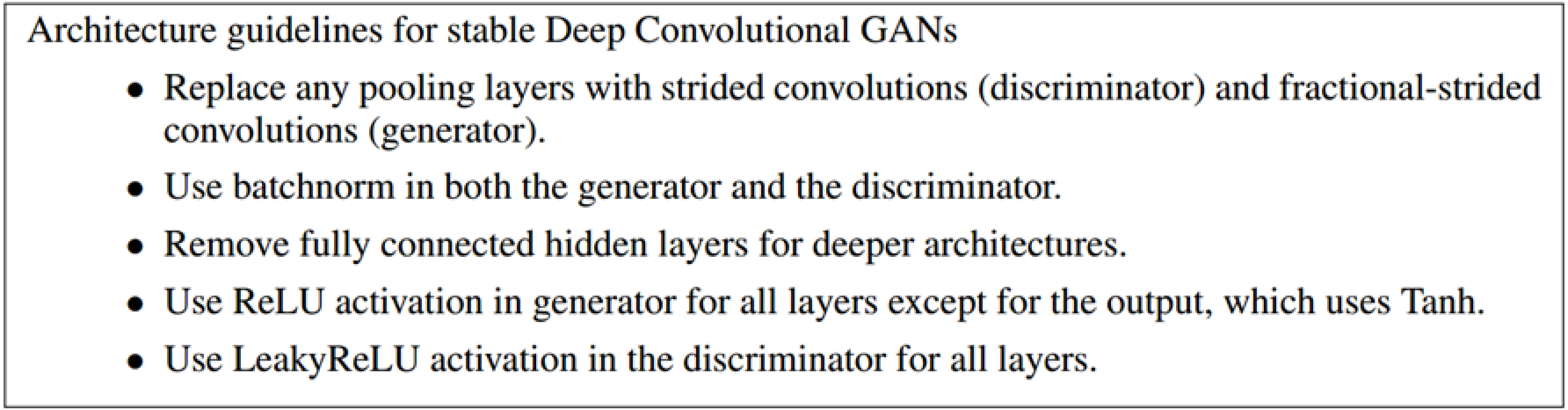
Generated samples (CIFAR-10)

Nearest neighbor from training set

Figures copyright Ian Goodfellow et al., 2014. Reproduced with permission.

Generative Adversarial Nets: Convolutional Architectures

Generator is an upsampling network with fractionally-strided convolutions
Discriminator is a convolutional network



Architecture guidelines for stable Deep Convolutional GANs

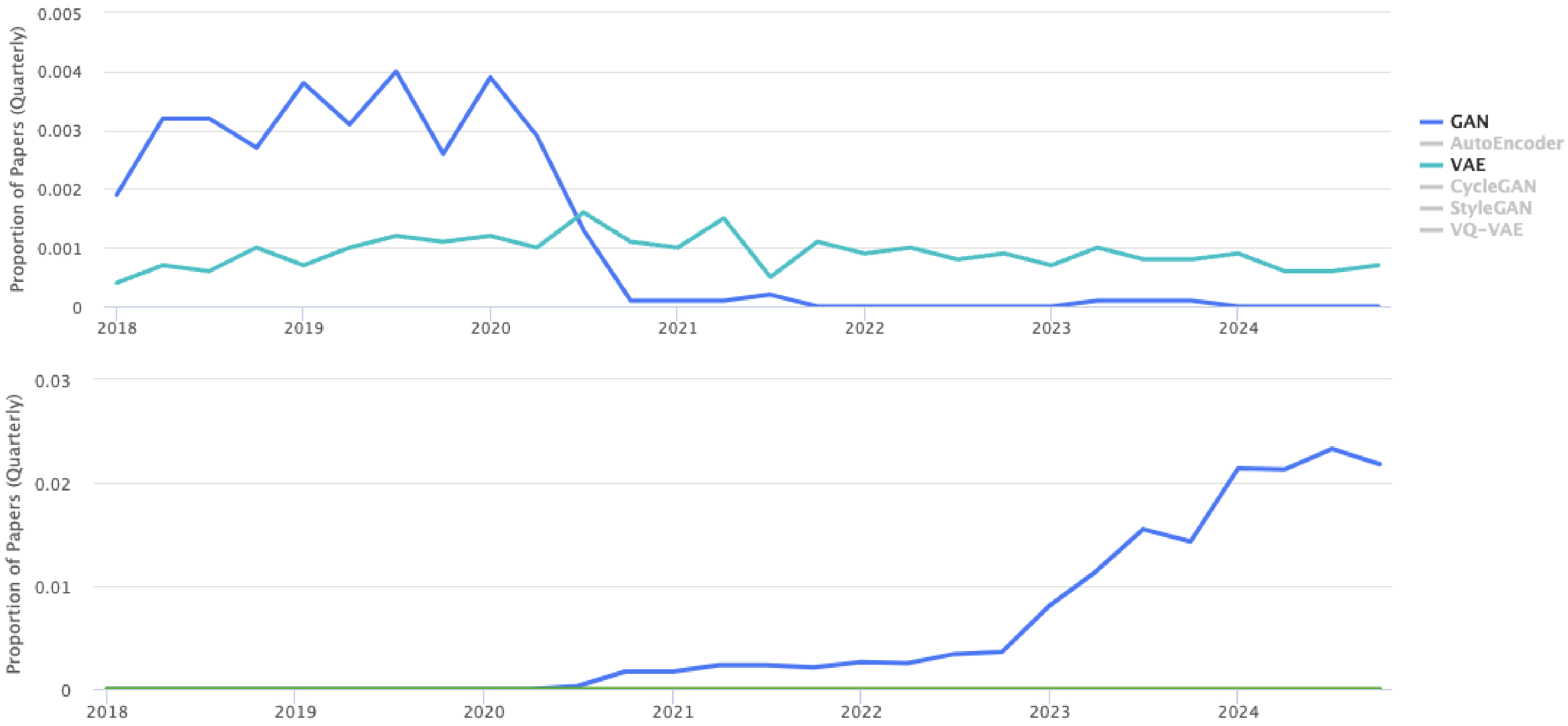
- Replace any pooling layers with strided convolutions (discriminator) and fractional-strided convolutions (generator).
- Use batchnorm in both the generator and the discriminator.
- Remove fully connected hidden layers for deeper architectures.
- Use ReLU activation in generator for all layers except for the output, which uses Tanh.
- Use LeakyReLU activation in the discriminator for all layers.

Radford et al, “Unsupervised Representation Learning with Deep Convolutional Generative Adversarial Networks”, ICLR 2016

2019: BigGAN

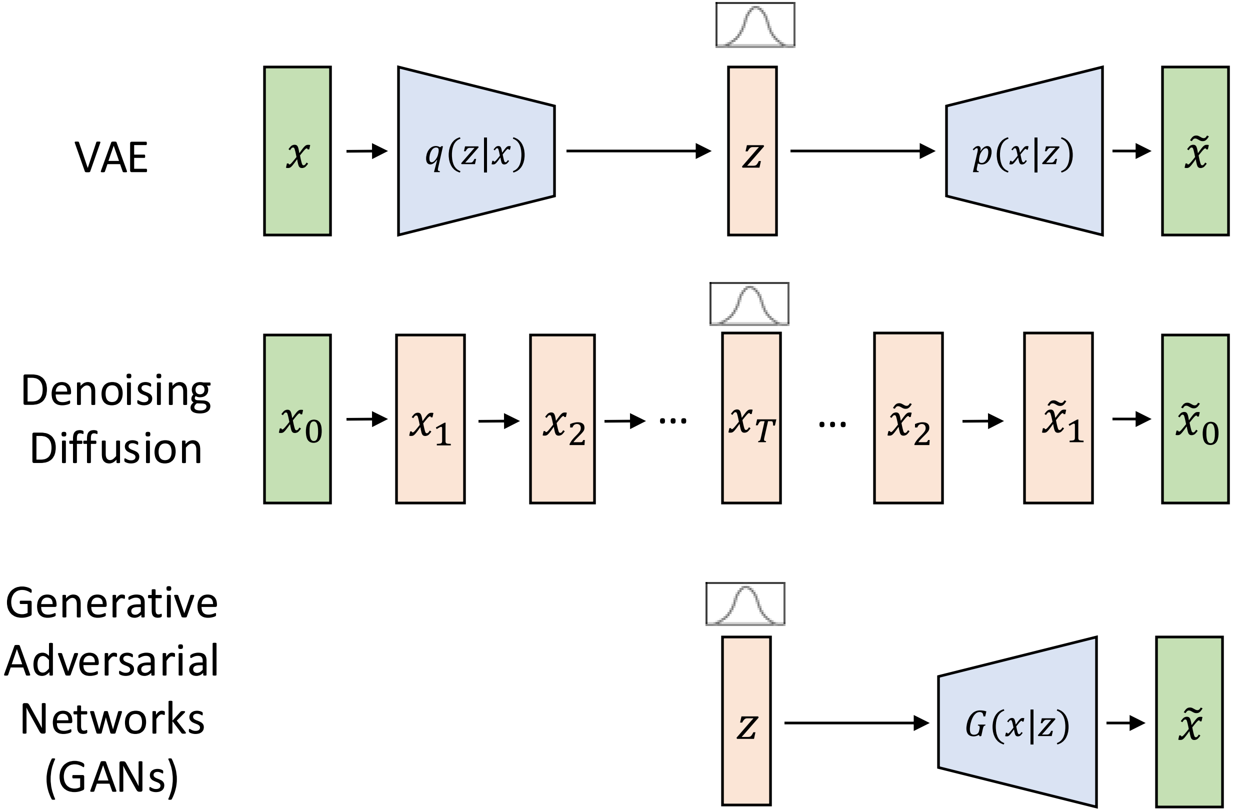
Brock et al., 2019

GANs were popular …



Source: https://paperswithcode.com

Deep Generative Models

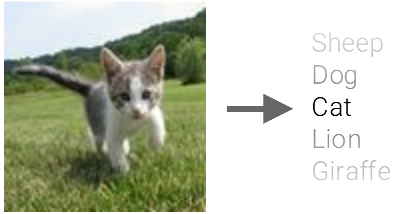


Generative Models: Closing Thoughts

- Learn without supervision = ability to leverage large, raw dataset
- Realism: Generate plausible samples given dataset
- Diversity: Generate diverse samples (avoid mode collapse)
- Controllability: Generate based on instruction / conditioning
- Healthy combination of theory and deep learning magic
- Generative Modeling is extremely hot in 2024. More will come …

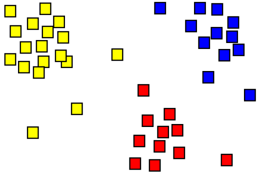
Supervised Learning

- 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

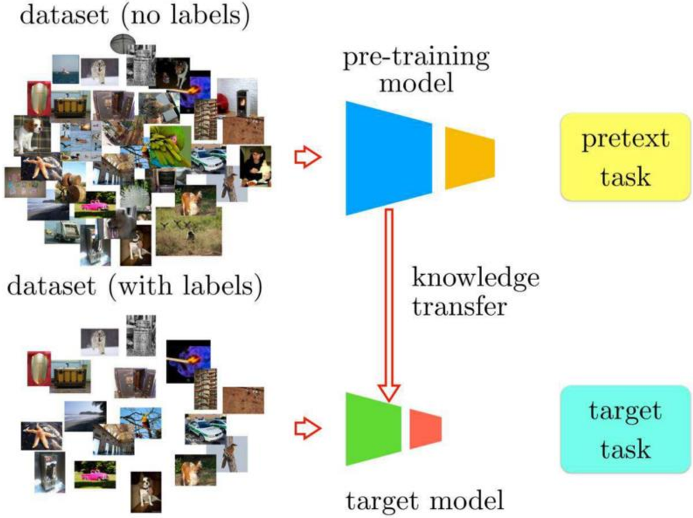
Self-Supervised Learning:

Create your own supervision

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

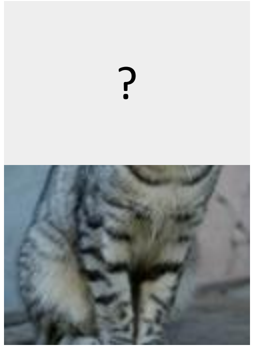
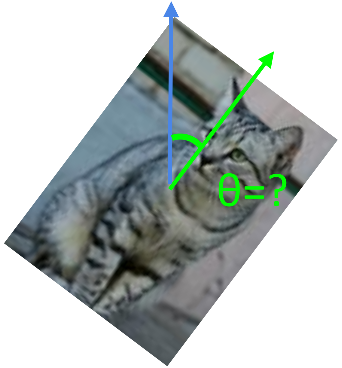


image completion



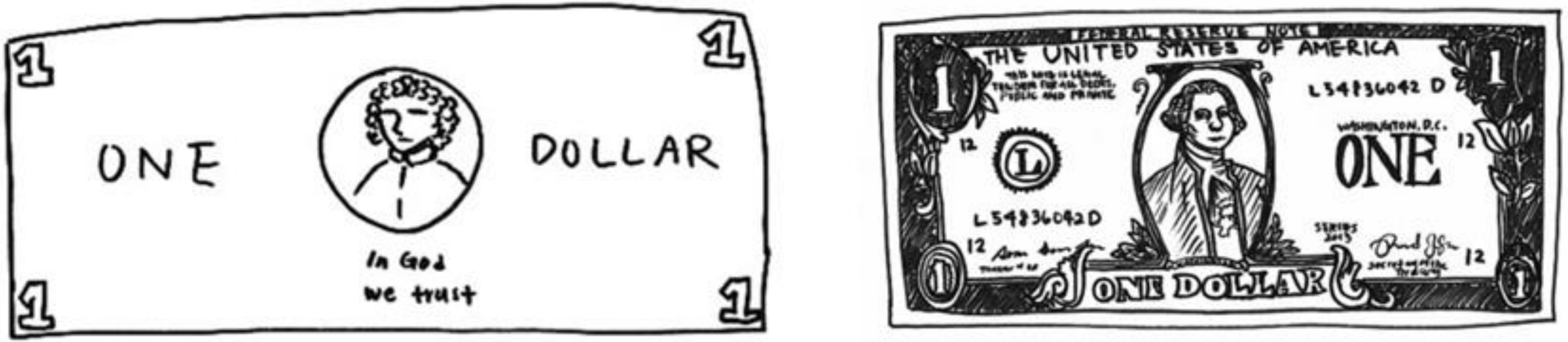
rotation prediction

“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

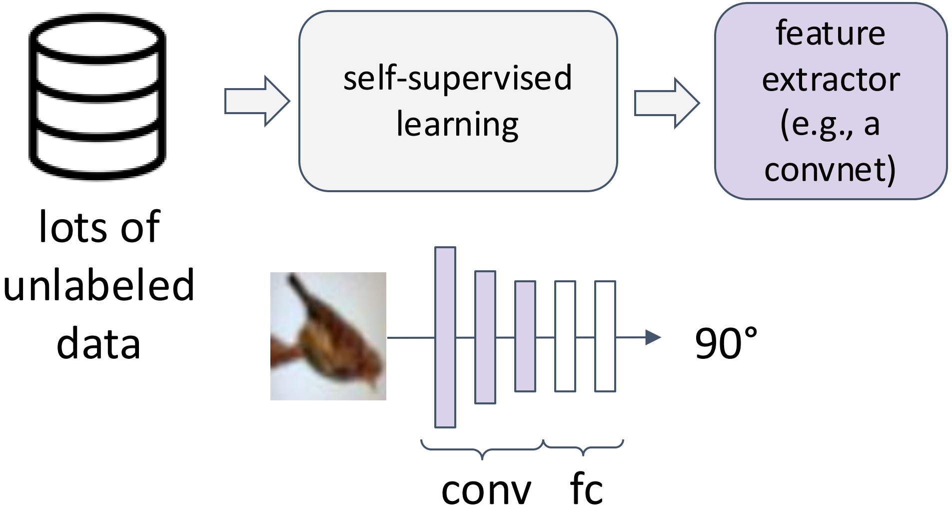
Source: [Anand, 2020]()

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?



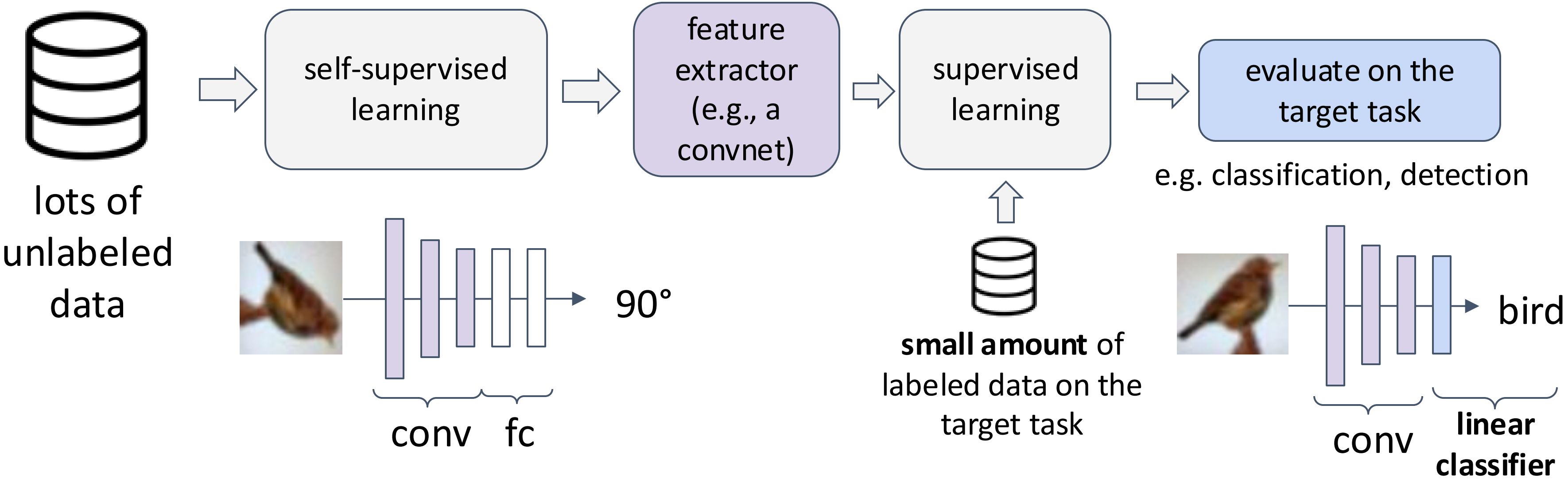
lots of unlabeled data

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

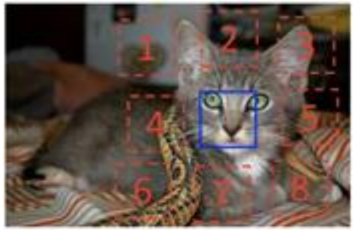
1. Learn good feature extractors from self-supervised pretext tasks, e.g., predicting image rotations

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

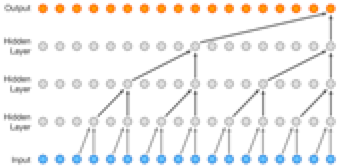
OpenAI

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

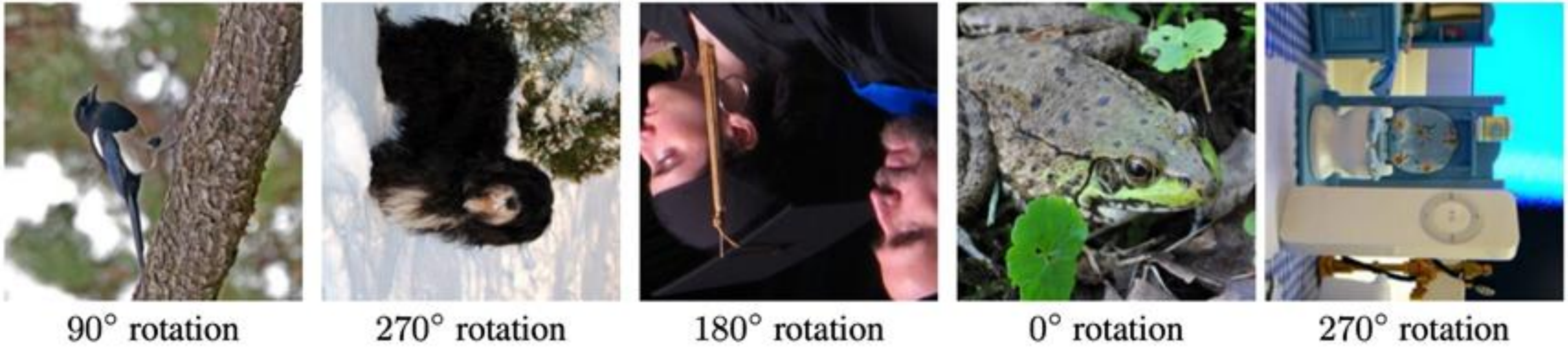
Pretext tasks from image transformations

- Rotation, inpainting, rearrangement, coloring

Contrastive representation learning

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

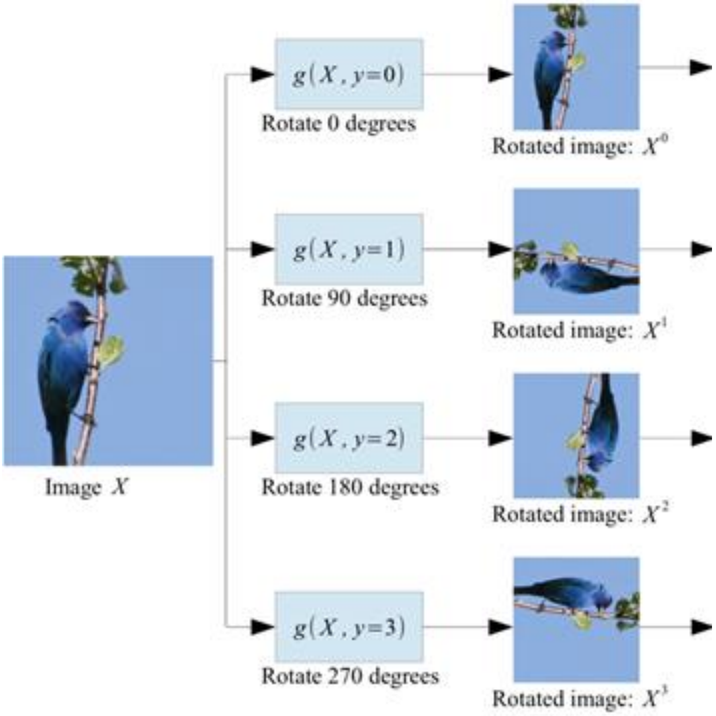
Pretext task: predict rotations



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

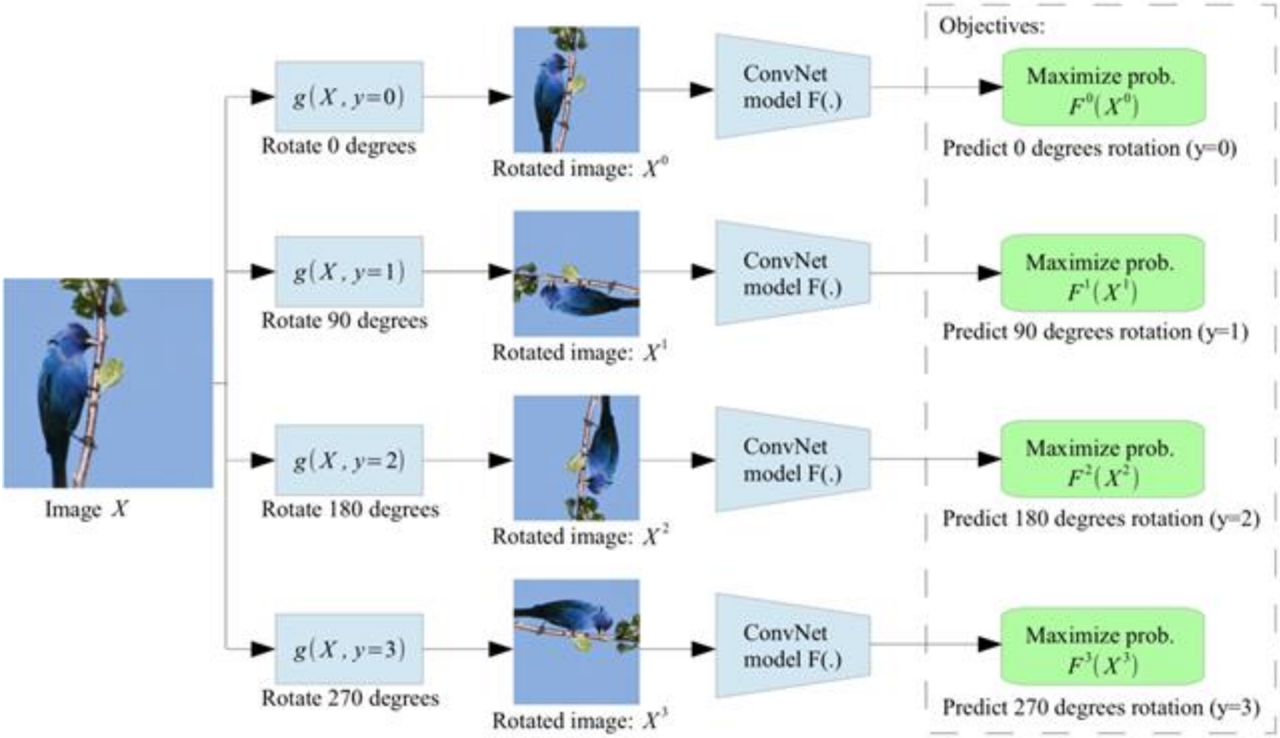


Self-supervised learning by rotating the entire input images.

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

(Image source: Gidaris et al. 2018)

Pretext task: predict rotations

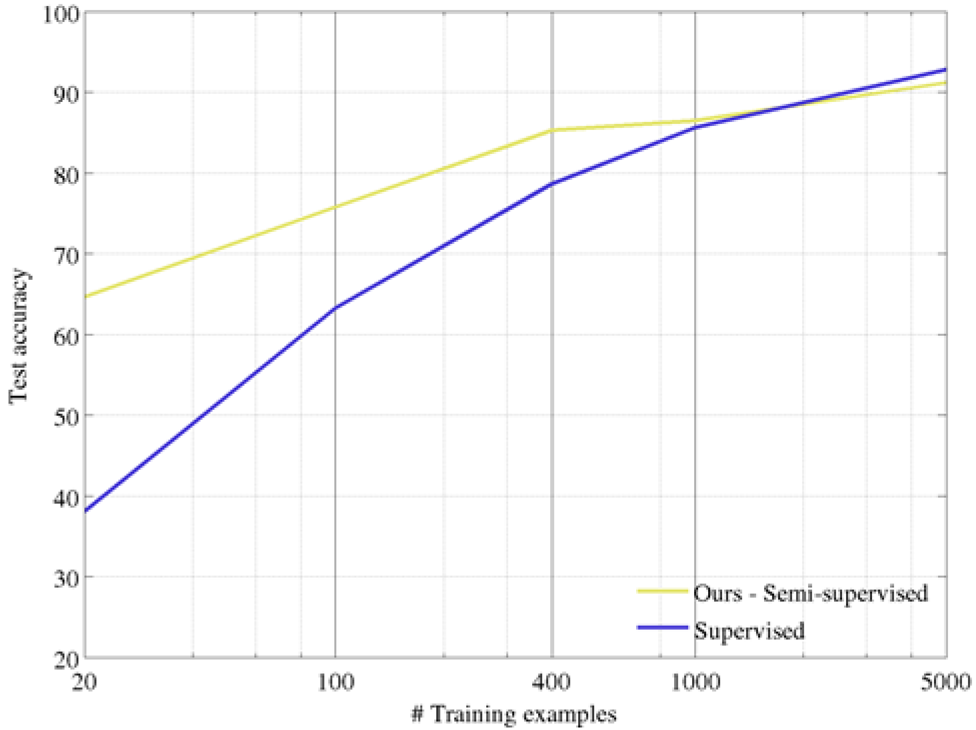


Self-supervised learning by rotating the entire input images.

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

(Image source: Gidaris et al. 2018)

Evaluation on semi-supervised learning

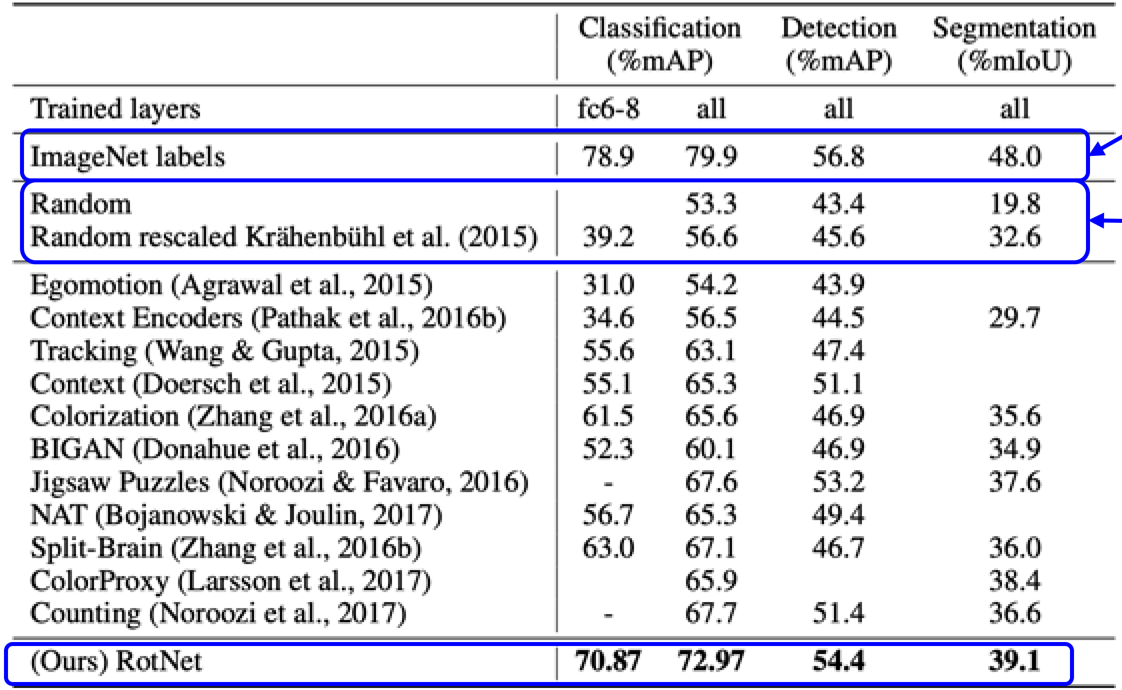


Self-supervised learning on **CIFAR10** (entire training set).

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

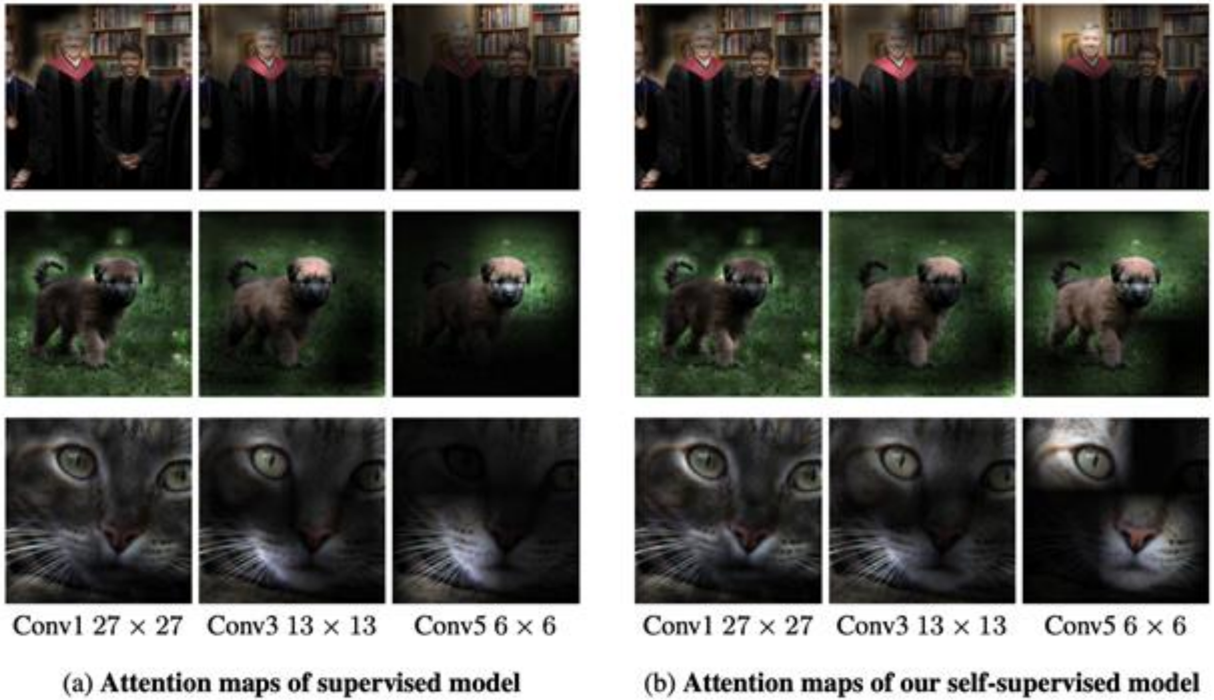
Self-supervised learning on **ImageNet** (entire training set) with AlexNet.

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

Self-supervised learning with rotation prediction

source: Gidaris et al. 2018

Visualize learned visual attentions

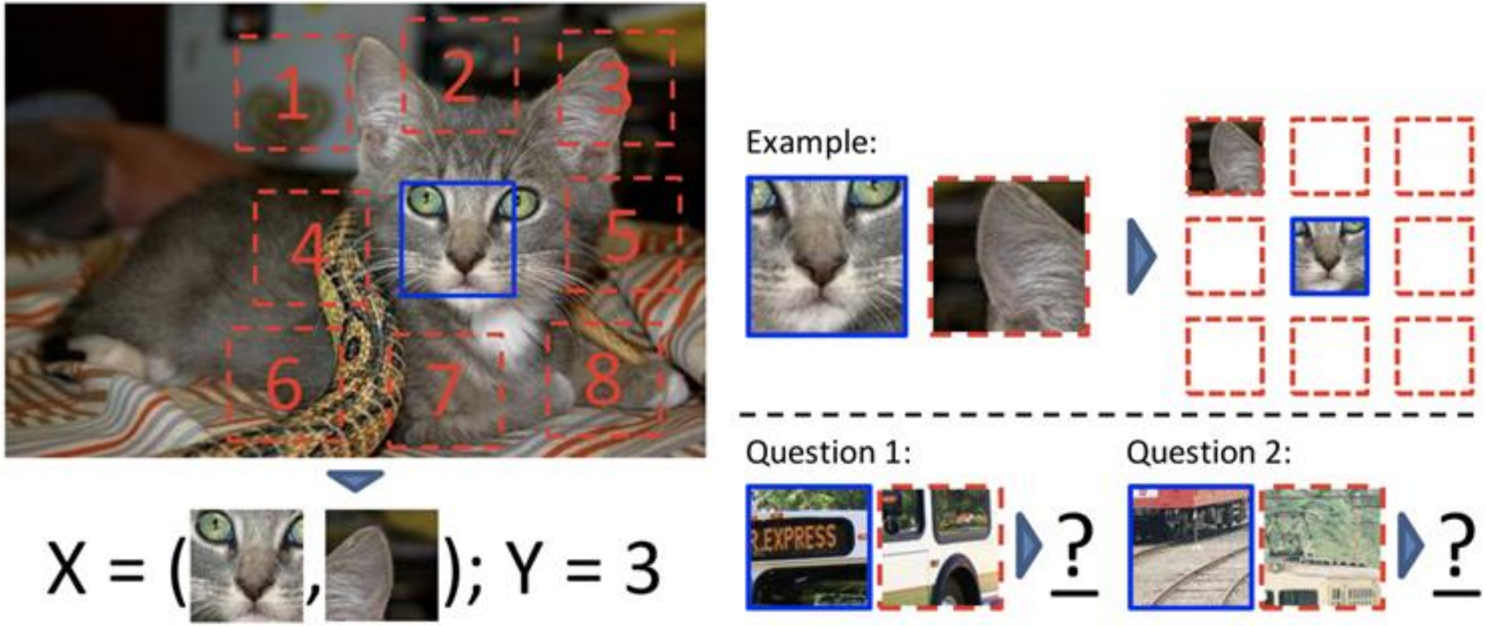


(a) **Attention maps of supervised model**

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

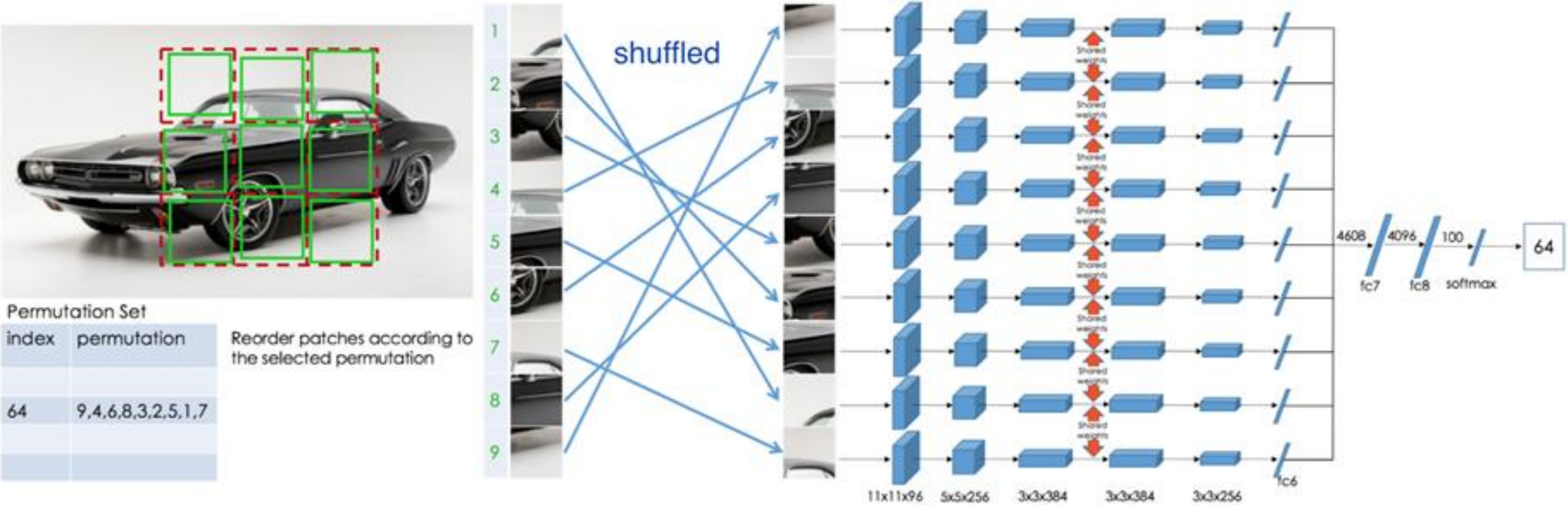
(Image source: Gidaris et al. 2018)

Pretext task: predict relative patch locations



(Image source: [Doersch et al., 2015](https://arxiv.org/abs/1505.05192))

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

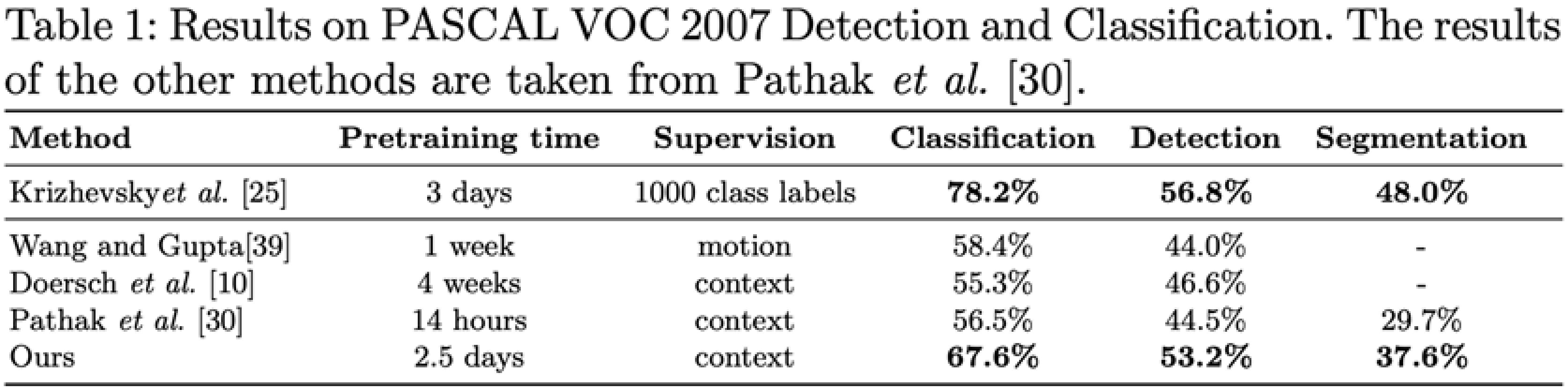


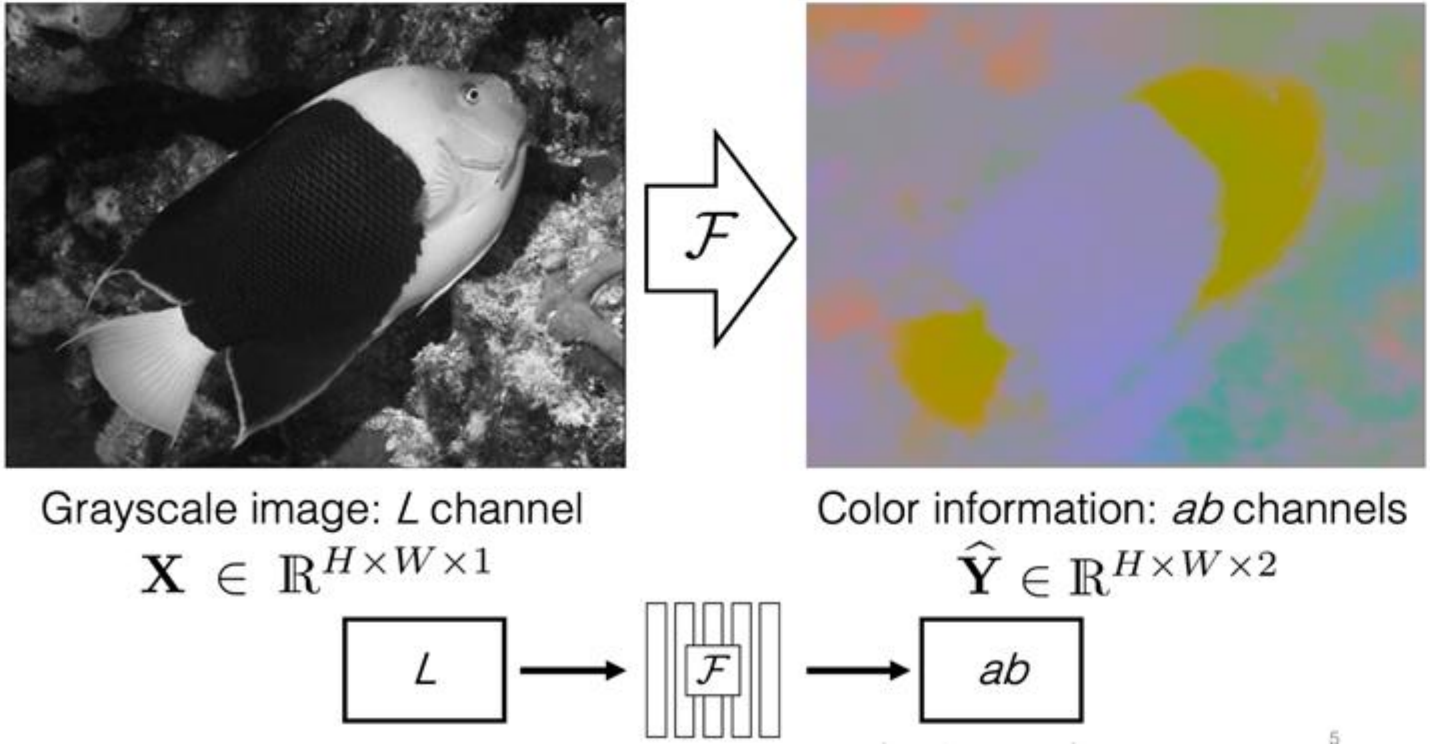
Table 1: Results on PASCAL VOC 2007 Detection and Classification. The results of the other methods are taken from Pathak *et al.* [30].

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: image coloring



Grayscale image: *L* channel

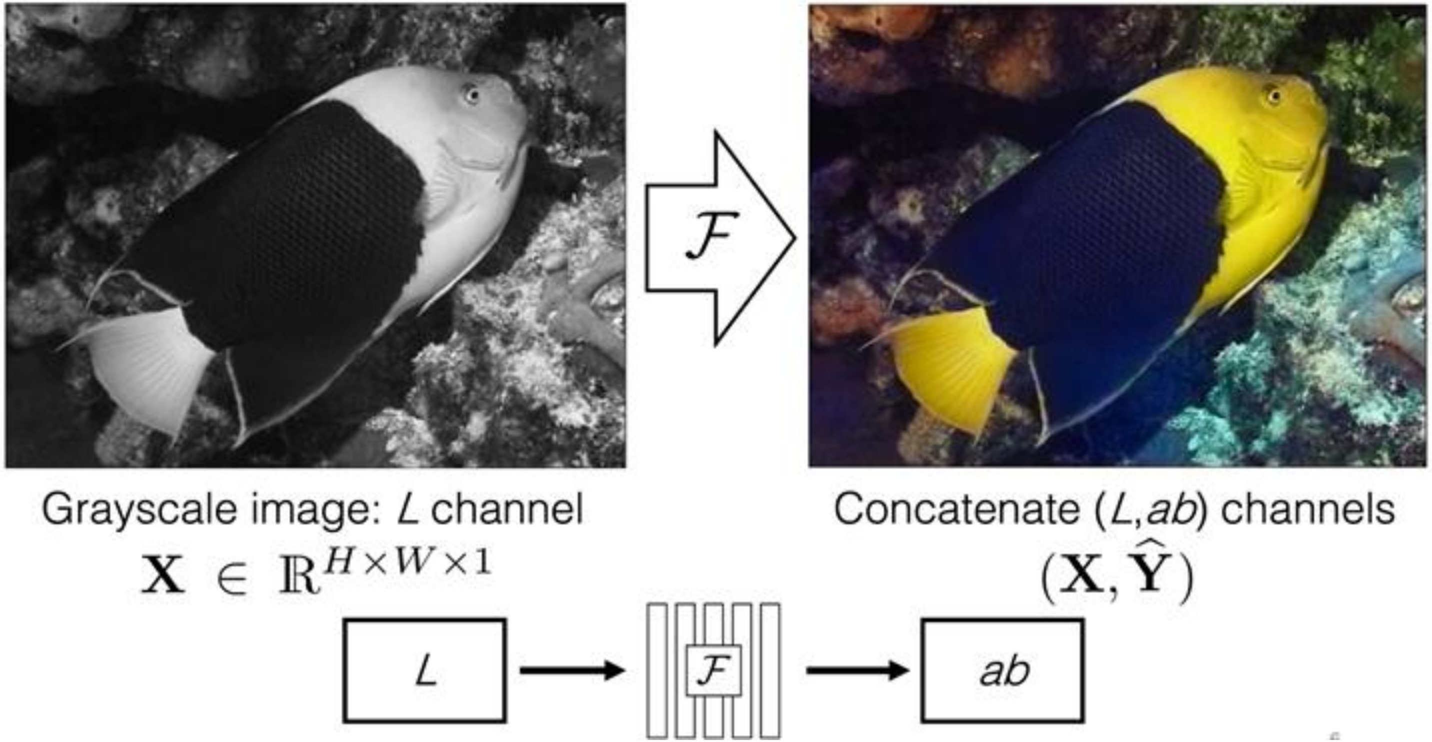
$\mathbf{X} \in \mathbb{R}^{H \times W \times 1}$

Color information: *ab* channels

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

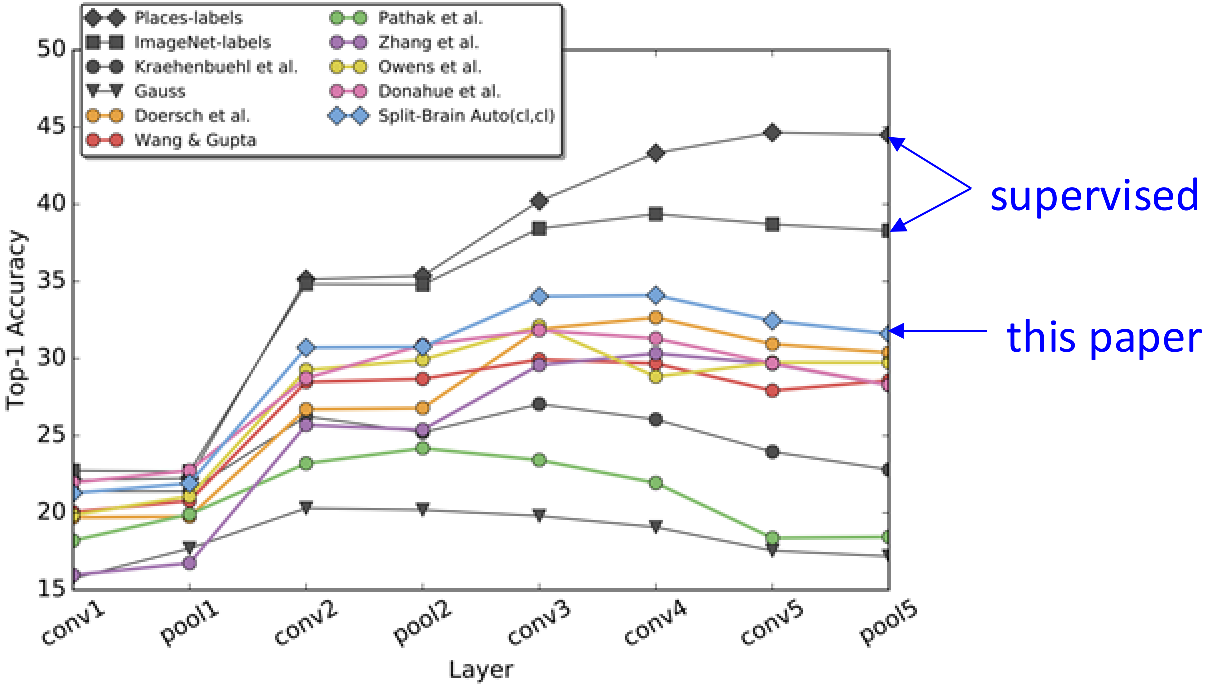
Source: Richard Zhang / Phillip Isola

Pretext task: image coloring



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

t = 0

how should I color these frames?

t = 1

t = 2

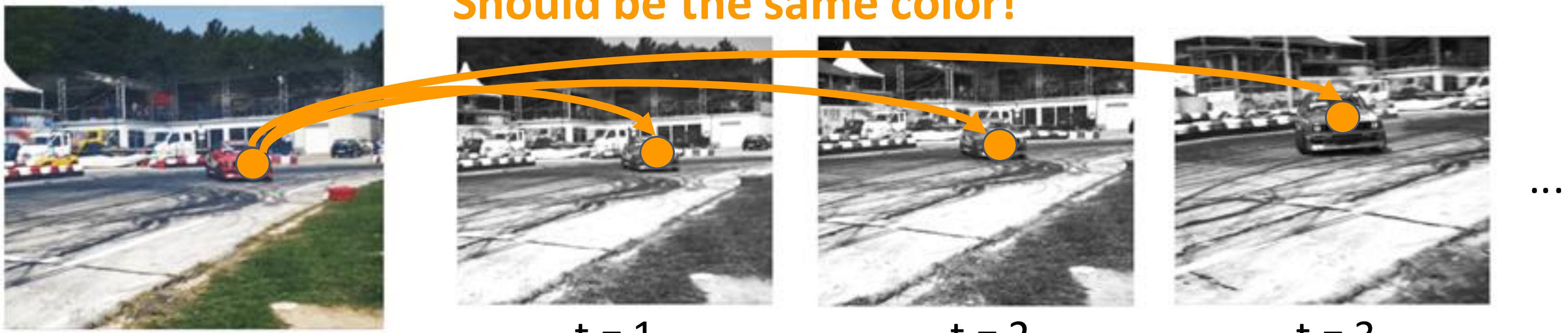
t = 3

...

Source: [Vondrick et al., 2018]

Pretext task: video coloring

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



reference frame

how should I color these frames?

Should be the same color!

t = 0

t = 1

t = 2

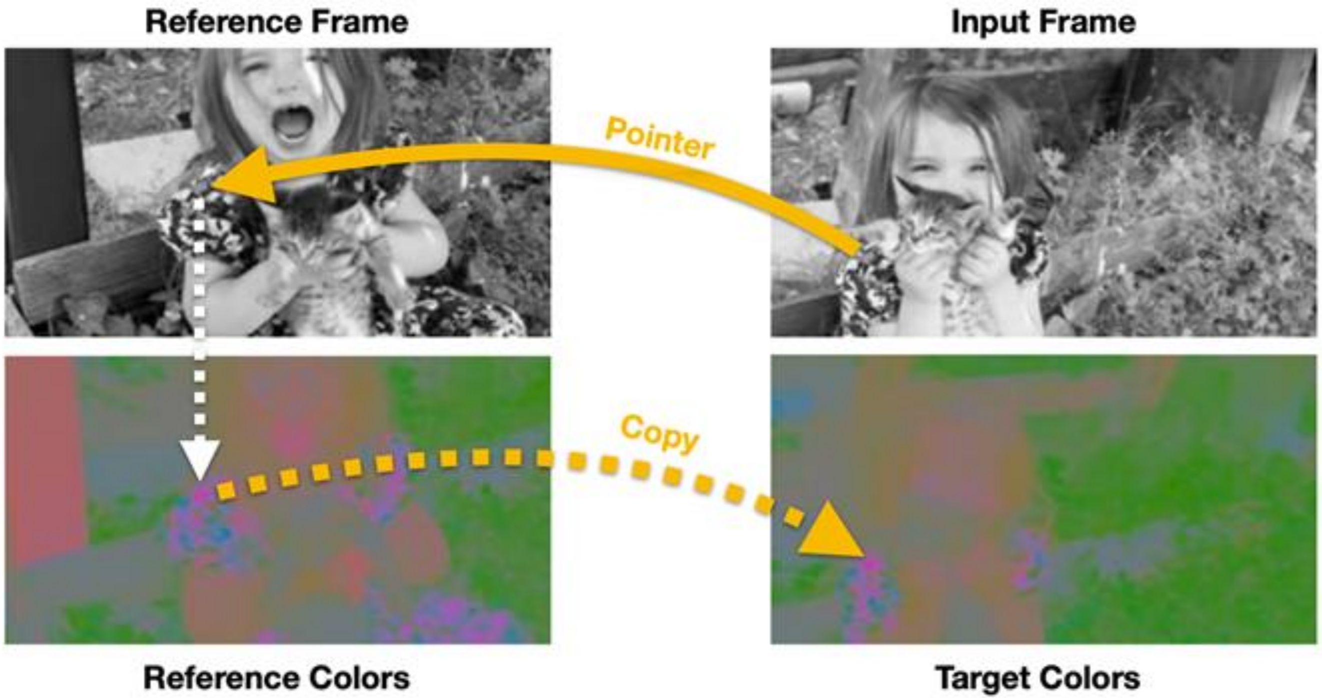
t = 3

...

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



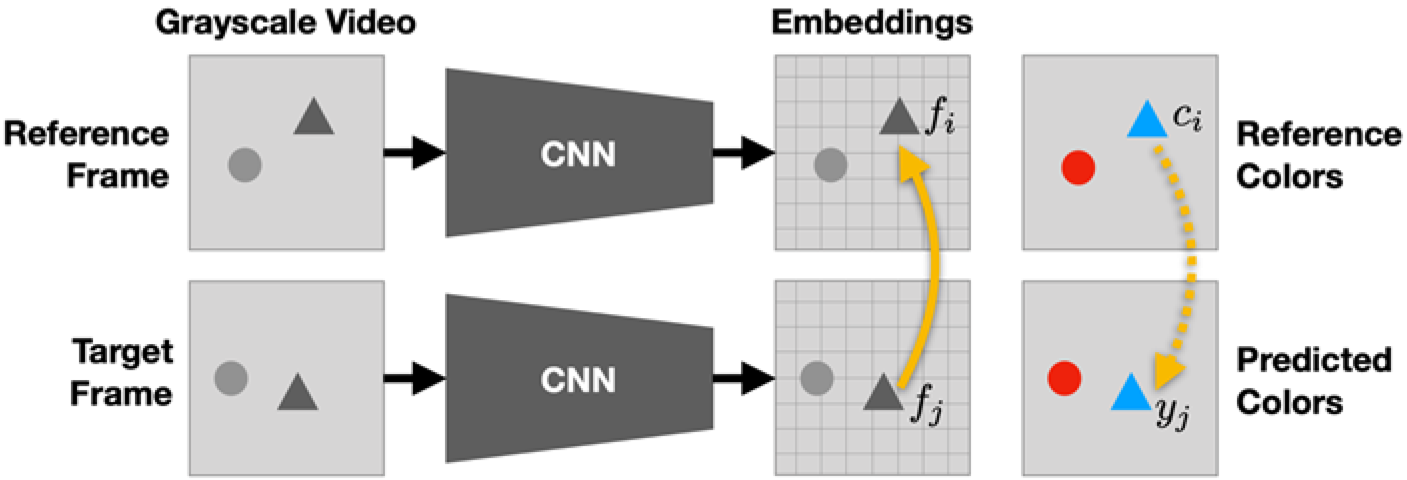
Learning objective:

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

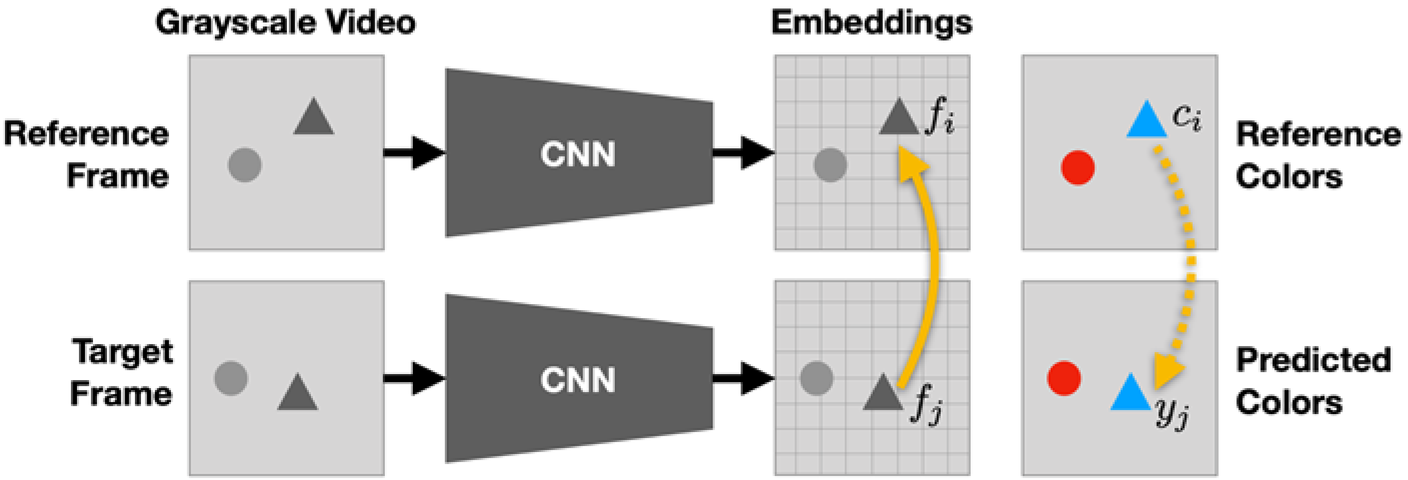


attention map on the reference frame

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

Source: Vondrick et al., 2018

Learning to color videos



attention map on the reference frame

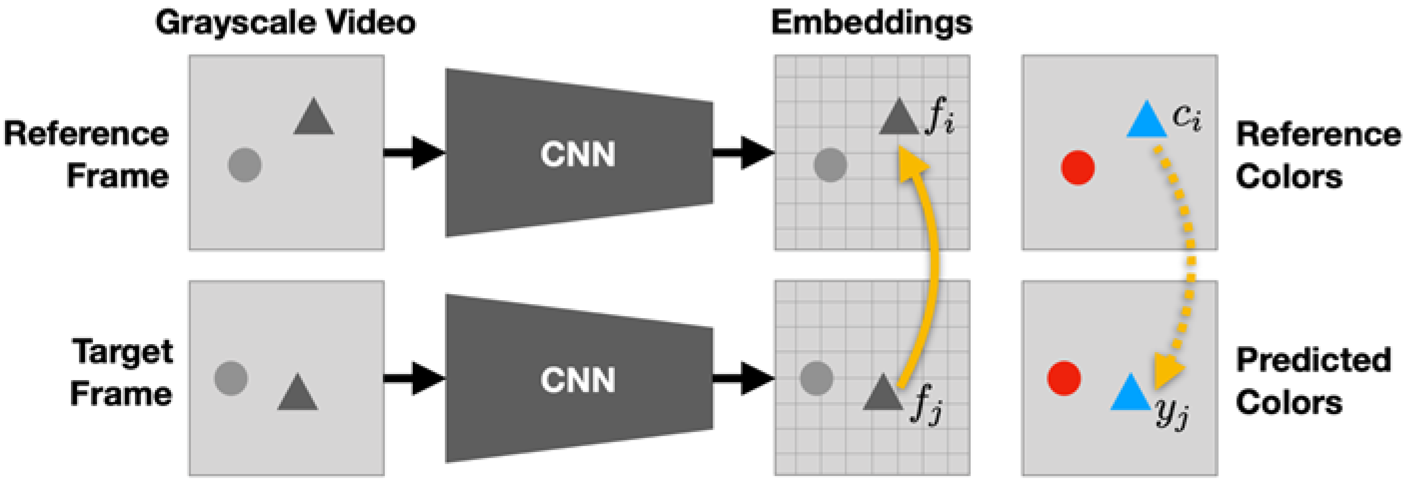
$$A_{ij} = \frac{\exp\left(f_i^T f_j\right)}{\sum_k \exp\left(f_k^T f_j\right)}$$

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

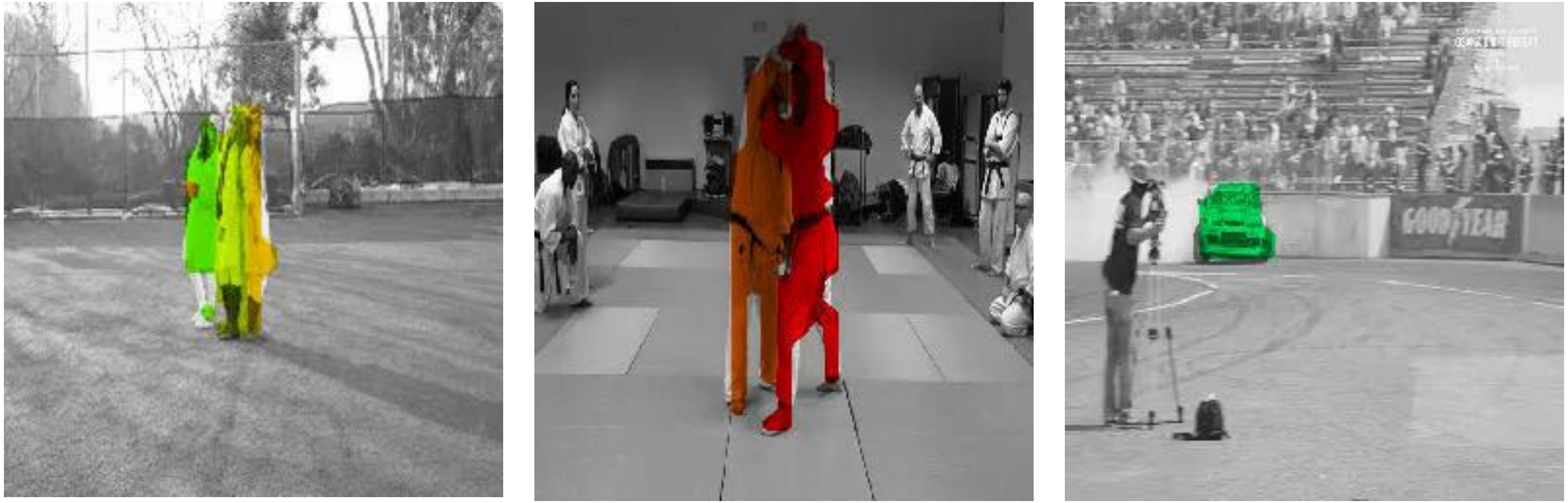
target frames (gray)

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

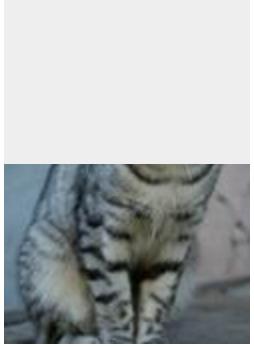


image
completion

rotation
prediction

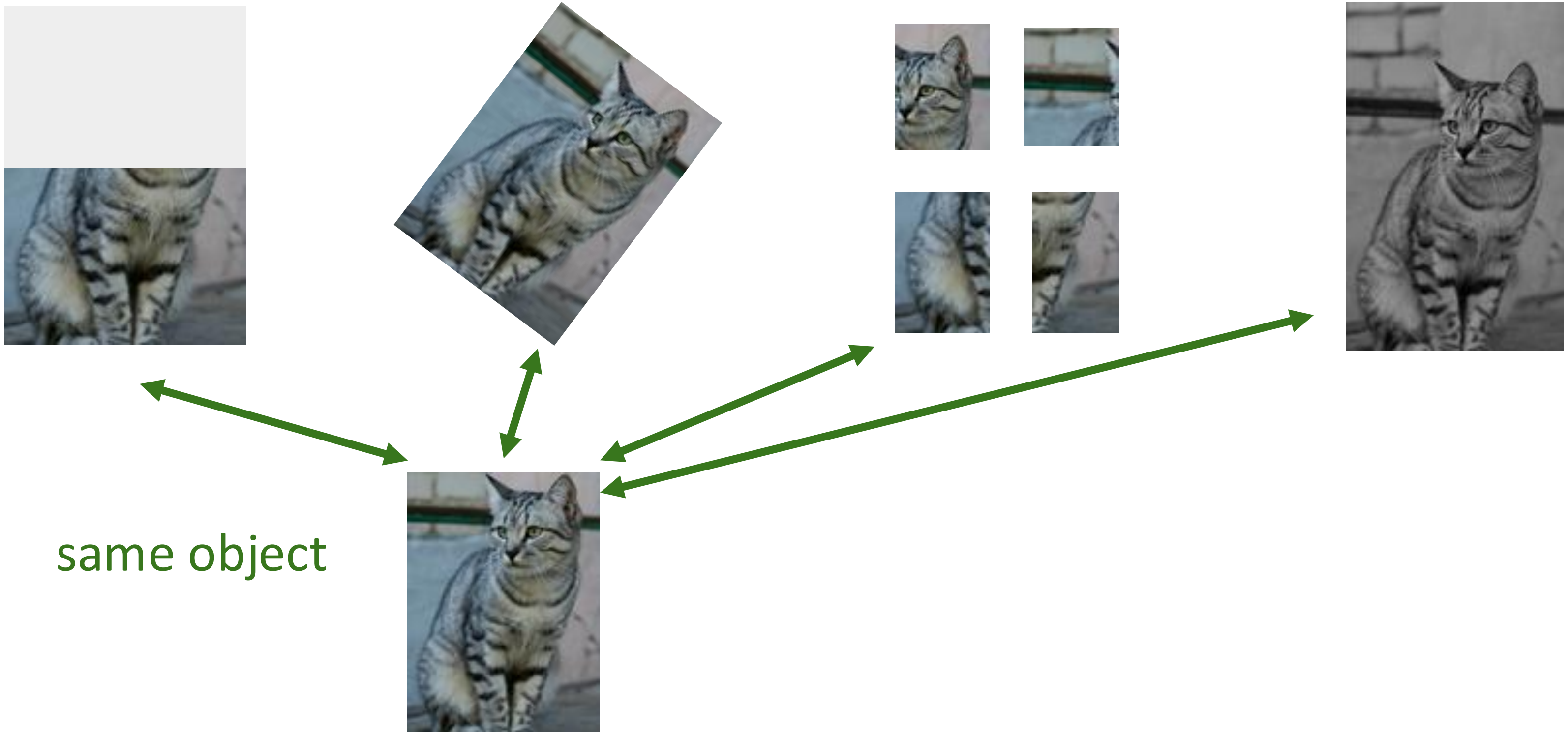
"jigsaw puzzle"

colorization

Learned representations may be tied to a specific pretext task!

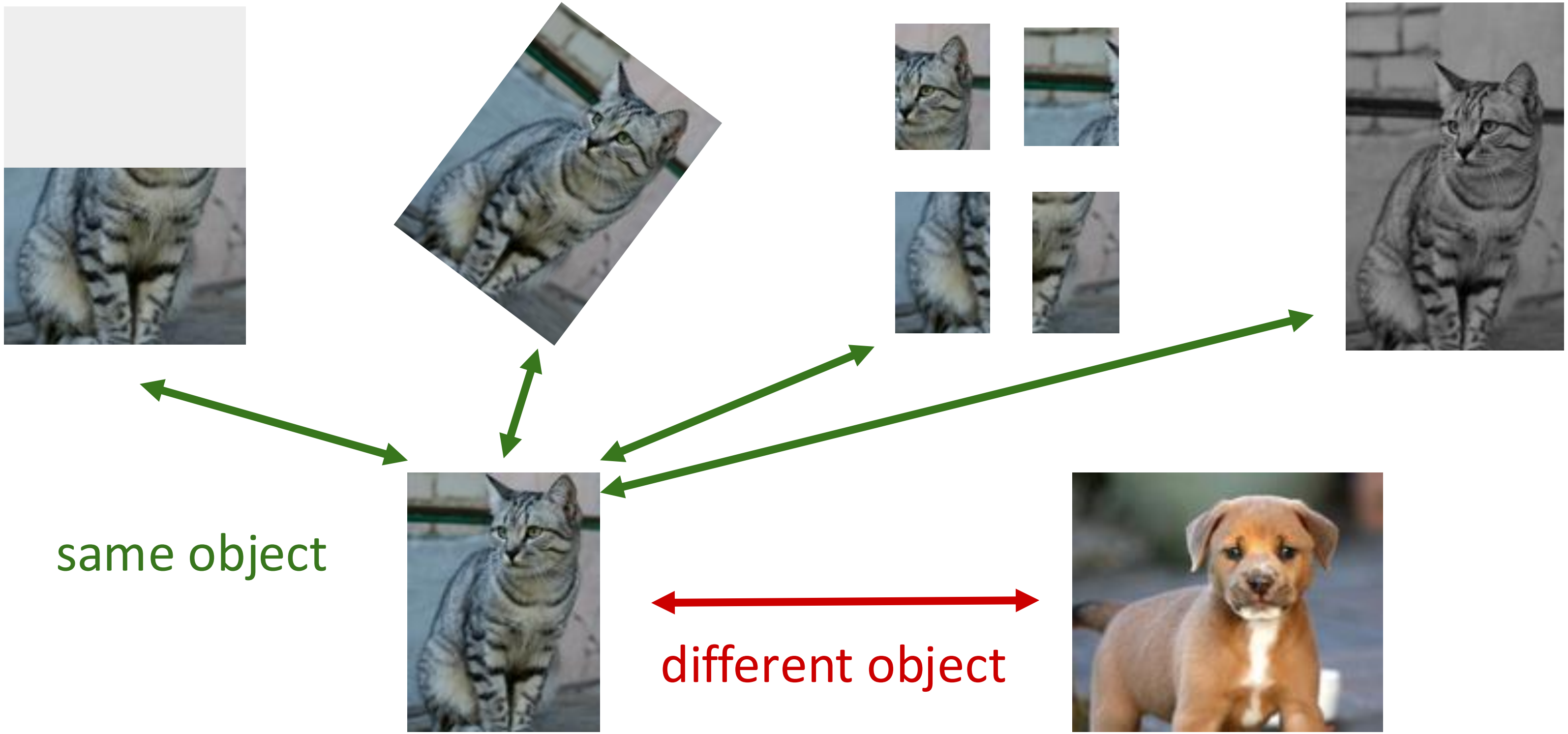
Can we come up with a more general pretext task?

A more general pretext task?



same object

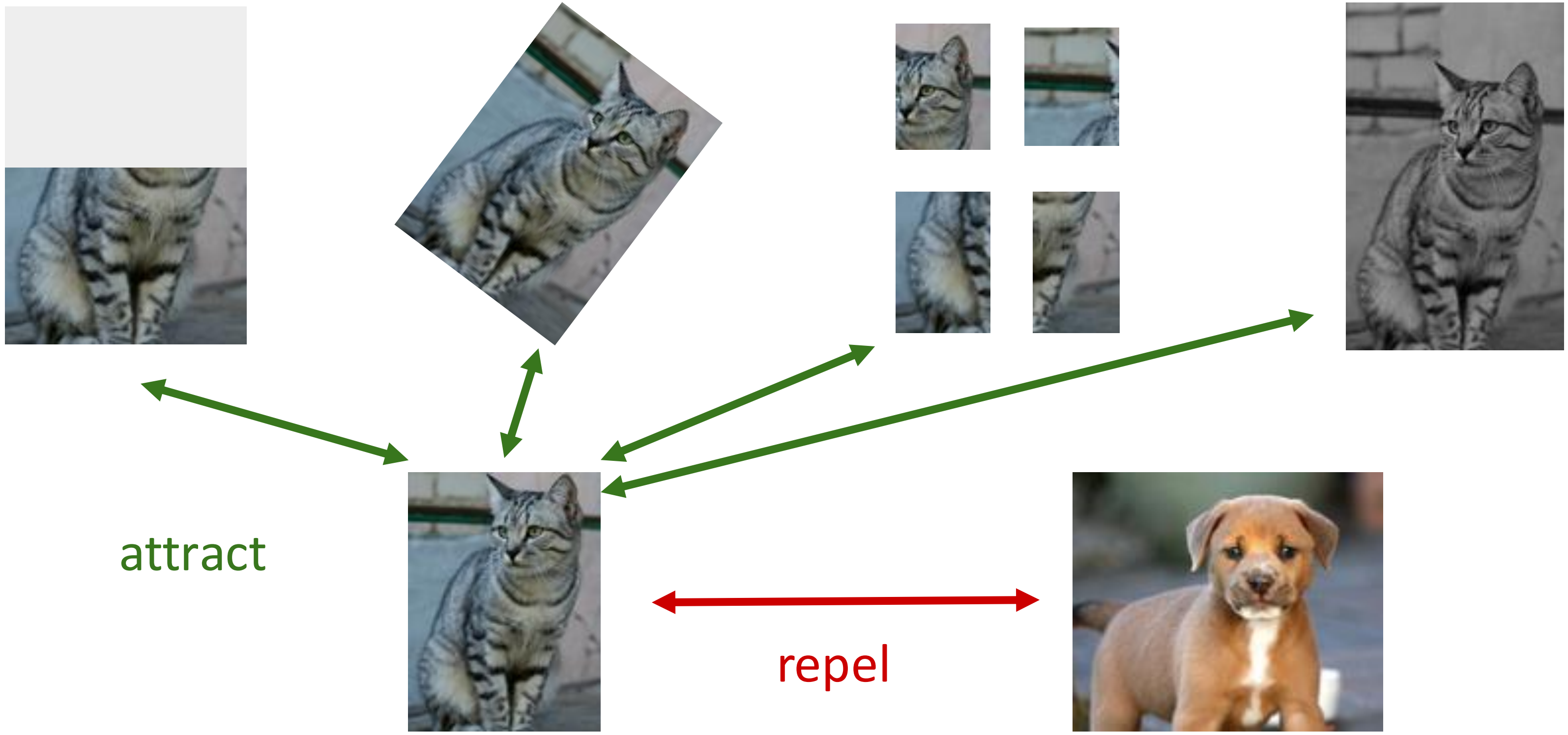
A more general pretext task?



same object

different object

Contrastive Representation Learning



Today’s Agenda

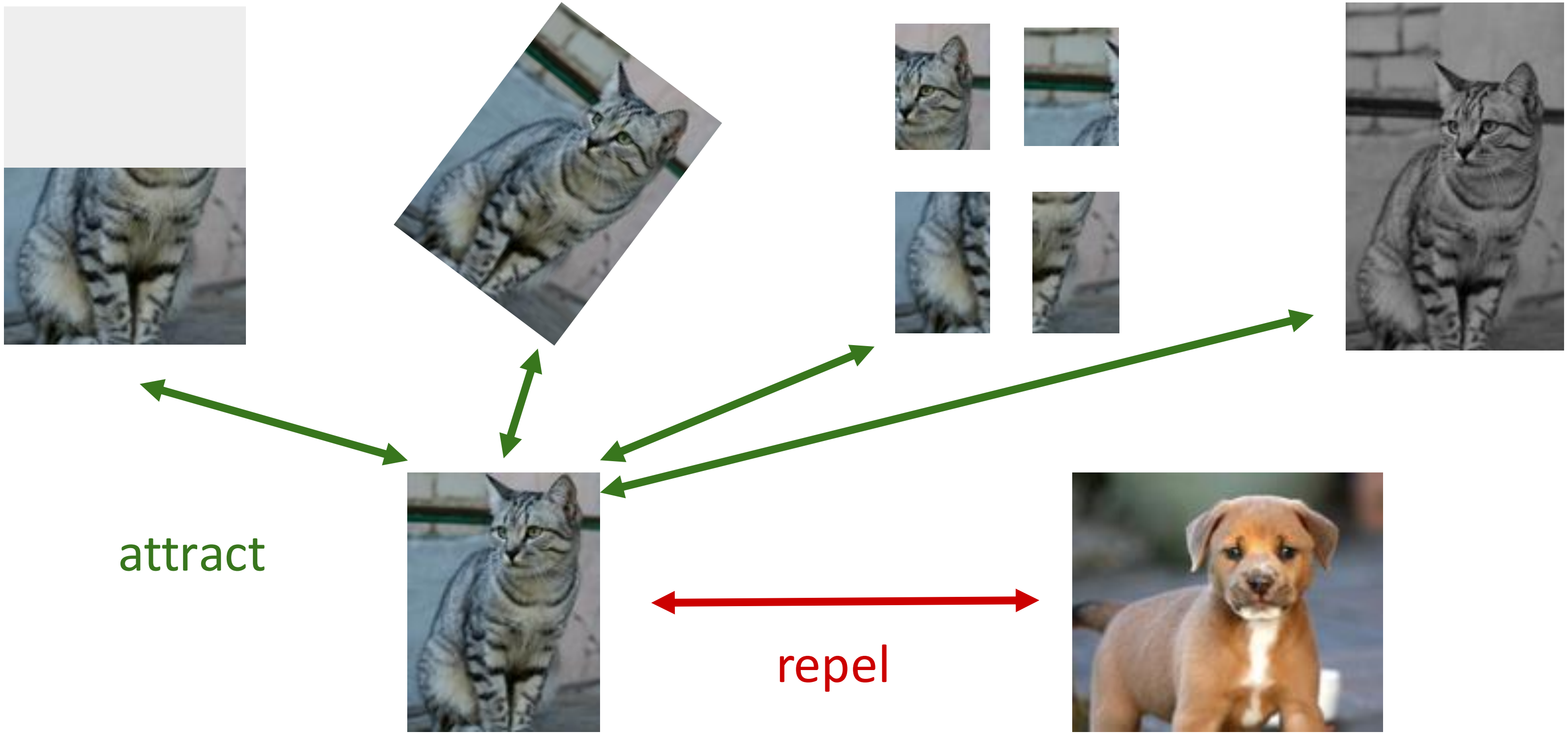
Pretext tasks from image transformations

- Rotation, inpainting, rearrangement, coloring

Contrastive representation learning

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

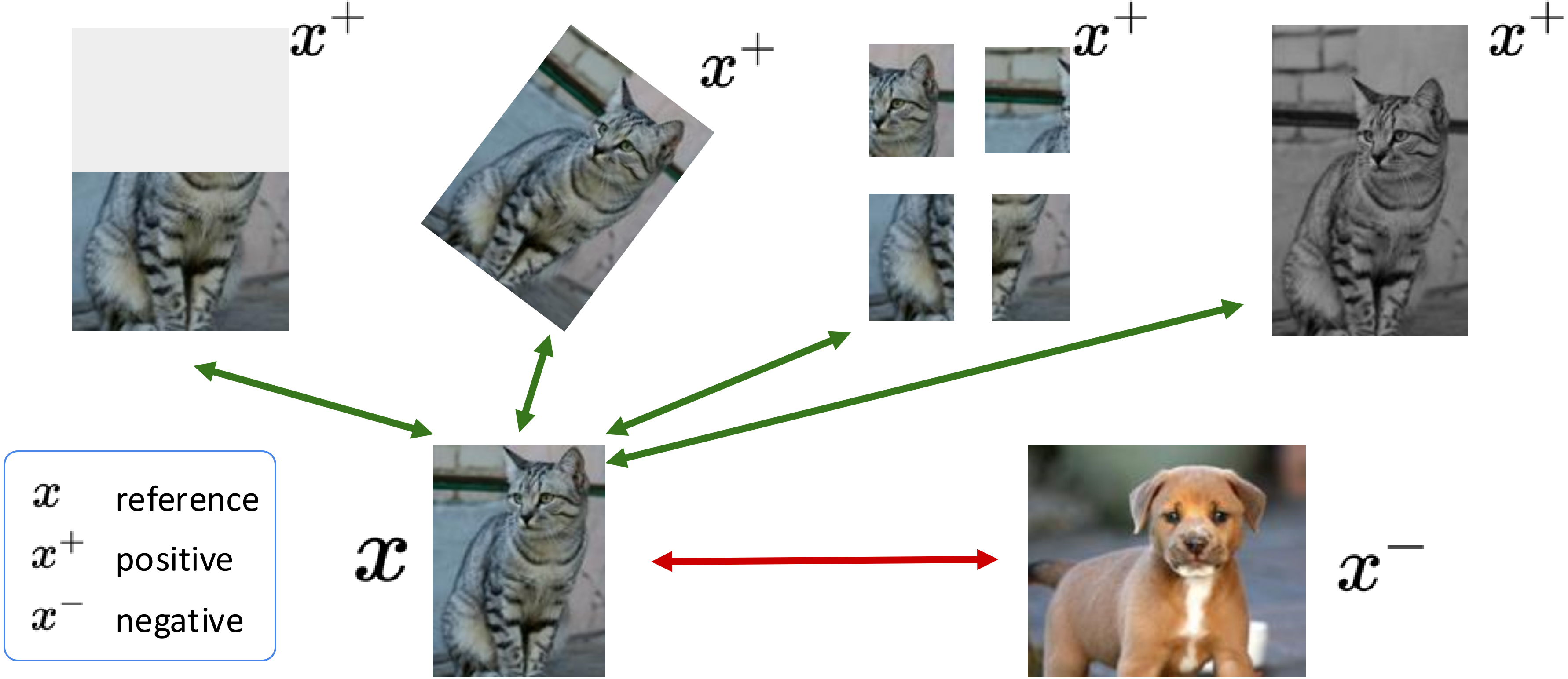
Contrastive Representation Learning



attract

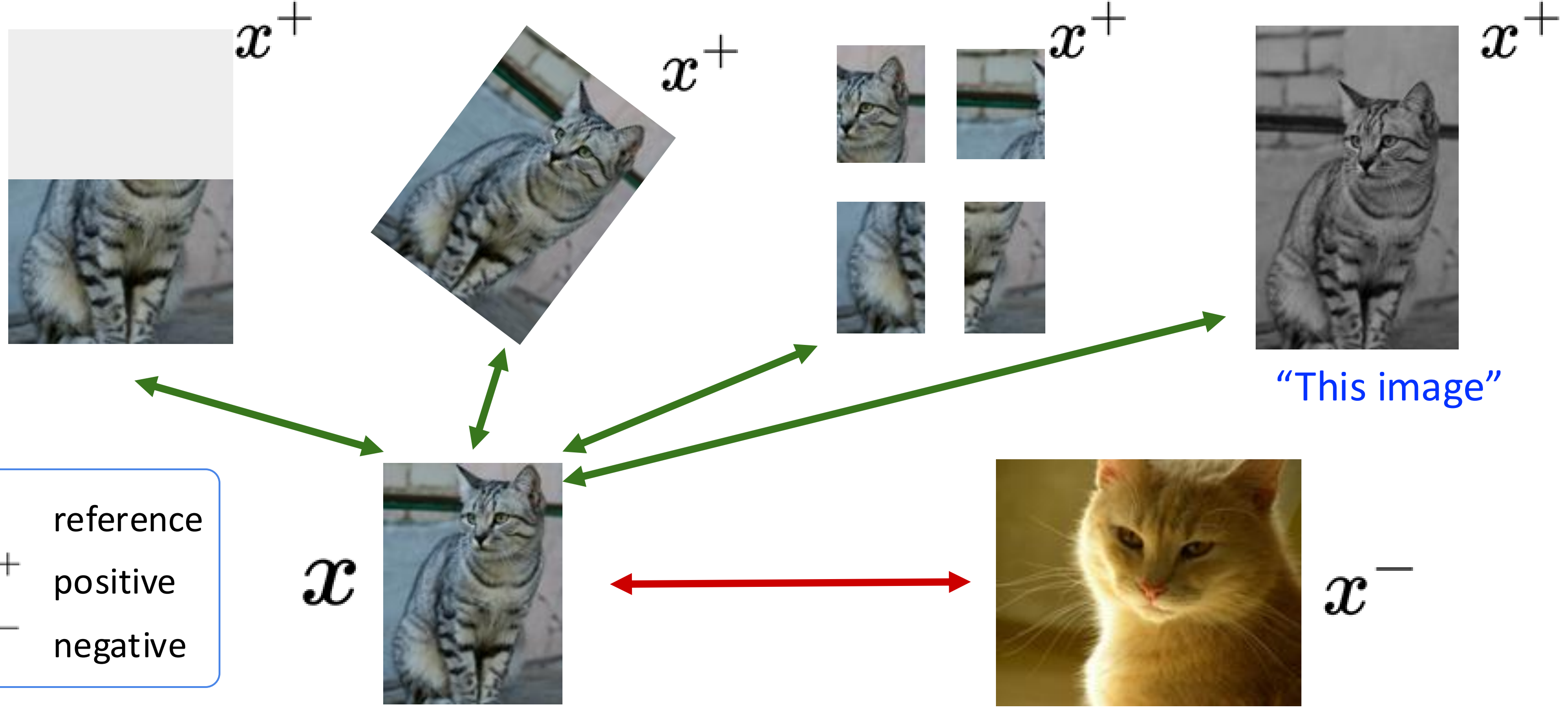
repel

Contrastive Representation Learning



x	reference
x^+	positive
x^-	negative

Contrastive Representation Learning



x reference
x^+ positive
x^- negative

A formulation of contrastive learning

What we want:

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

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:

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

A formulation of contrastive learning

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

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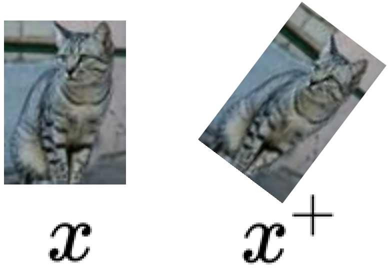
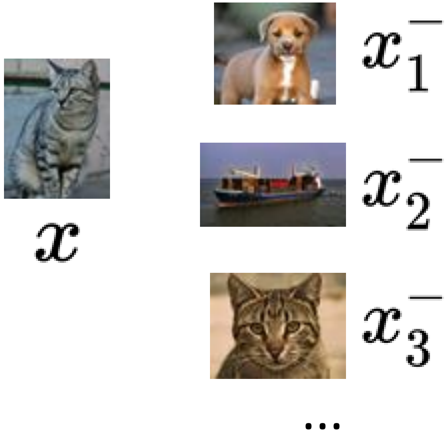




A formulation of contrastive learning

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:

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

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:

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

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

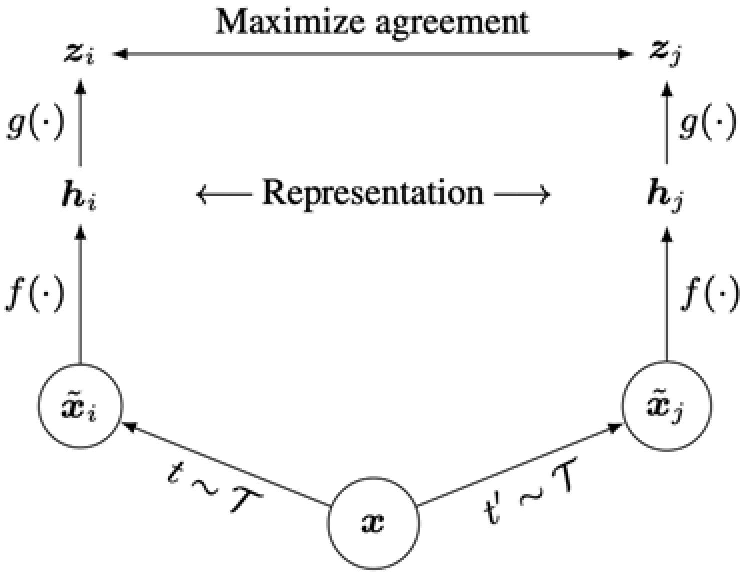
Cosine similarity as the score function:

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

Use a projection network ***h(·)*** to project features to a space where contrastive learning is applied

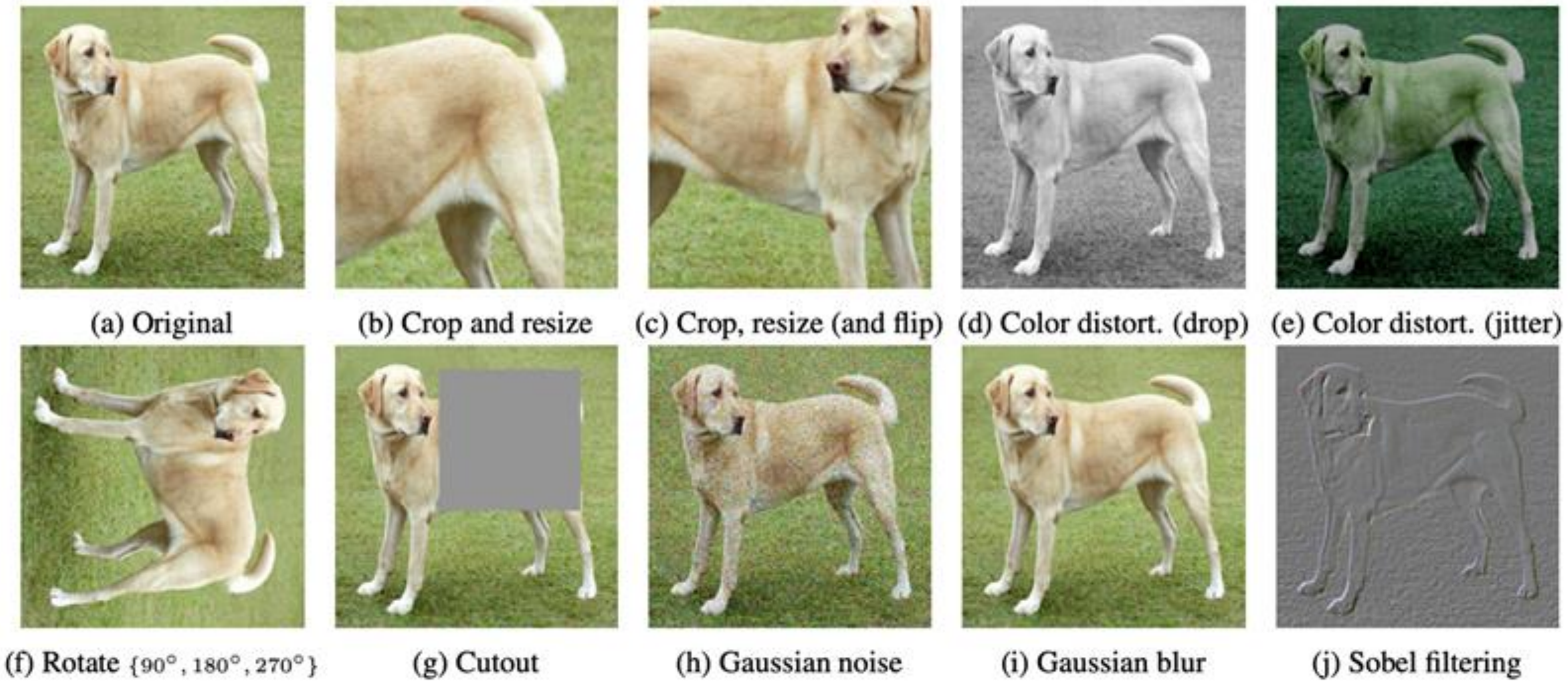
Generate positive samples through data augmentation:

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



Source: Chen et al., 2020

SimCLR: generating positive samples from data augmentation

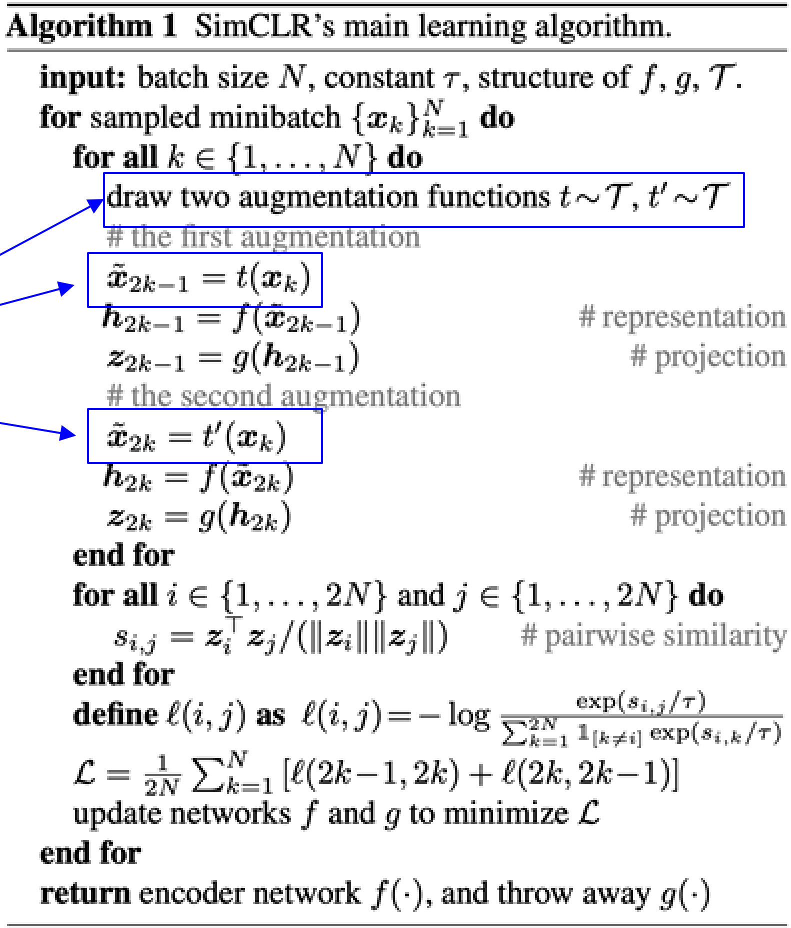


(a) Original (b) Crop and resize (c) Crop, resize (and flip) (d) Color distort. (drop) (e) Color distort. (jitter)

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

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

SimCLR



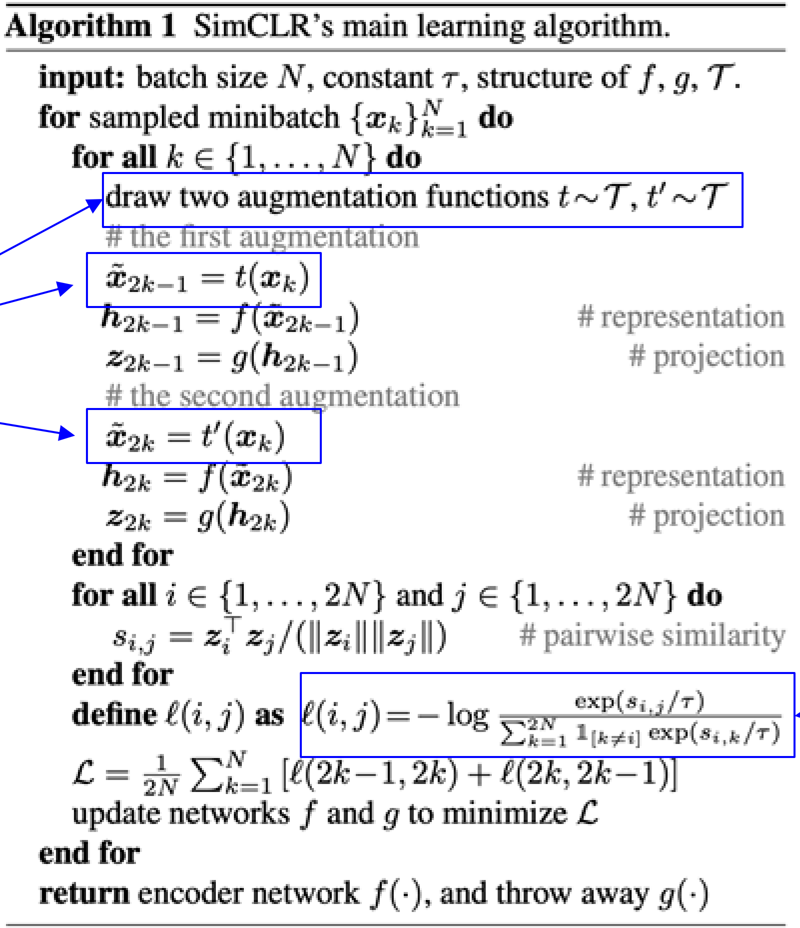
```
Algorithm 1  SimCLR's main learning algorithm.
input: batch size $N$, constant $\tau$, structure of $f$, $g$, $\mathcal{T}$.
for sampled minibatch $\{\boldsymbol{x}_k\}_{k=1}^N$ do
    for all $k \in \{1, \ldots, N\}$ do
        draw two augmentation functions $t \sim \mathcal{T}$, $t' \sim \mathcal{T}$
        # 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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```

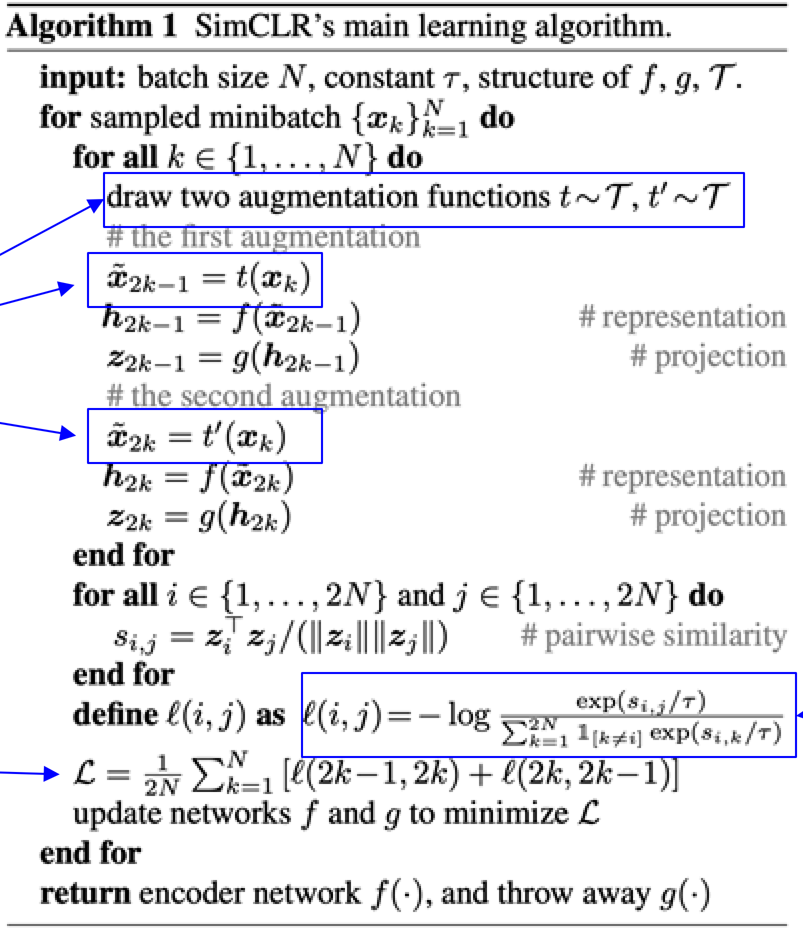
InfoNCE loss:
Use all non-positive samples in the batch as x^-

Source: Chen et al., 2020

SimCLR

Generate a positive pair by sampling data augmentation functions

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



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```
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```
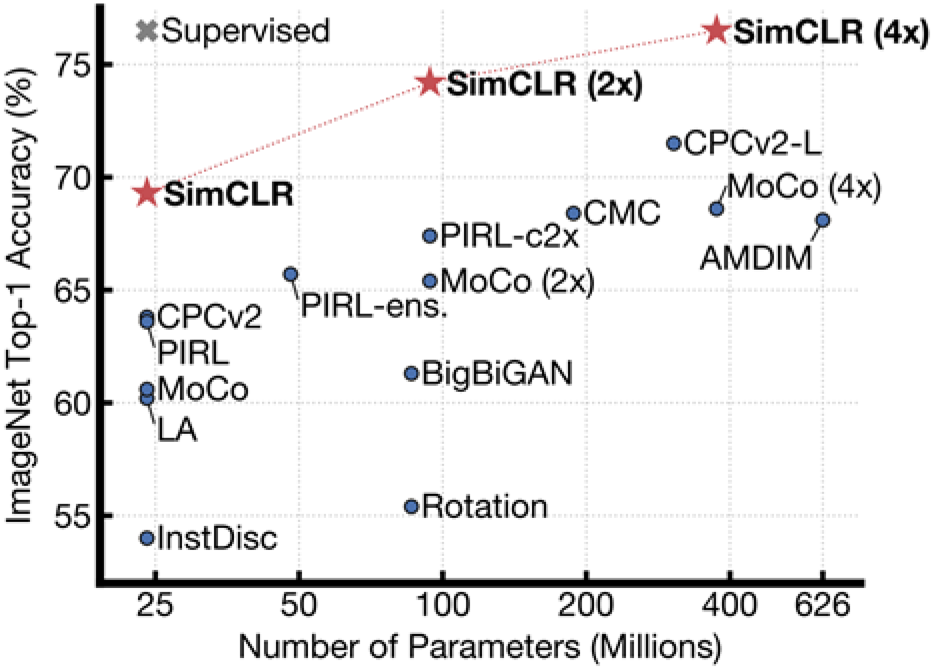

InfoNCE loss:
Use all non-positive samples in the batch as x^-

Source: Chen et al., 2020

Training linear classifier on SimCLR features

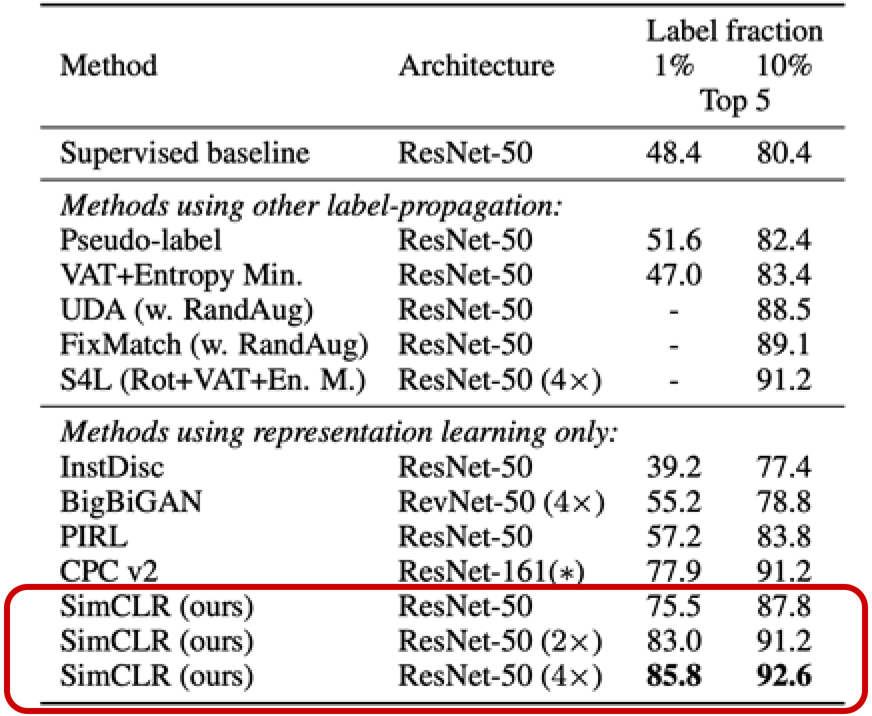


Train feature encoder on **ImageNet** (entire training set) using SimCLR.

Freeze feature encoder, train a linear classifier on top with labeled data.

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
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**

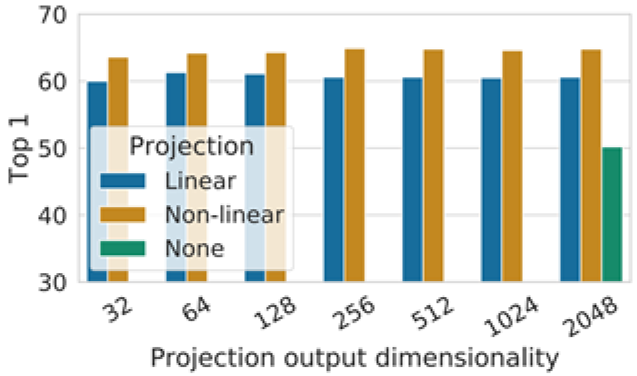
Table 7. ImageNet accuracy of models trained with few labels.

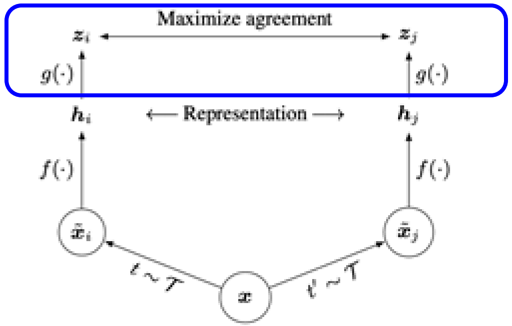
Train feature encoder on **ImageNet** (entire training set) using SimCLR.

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

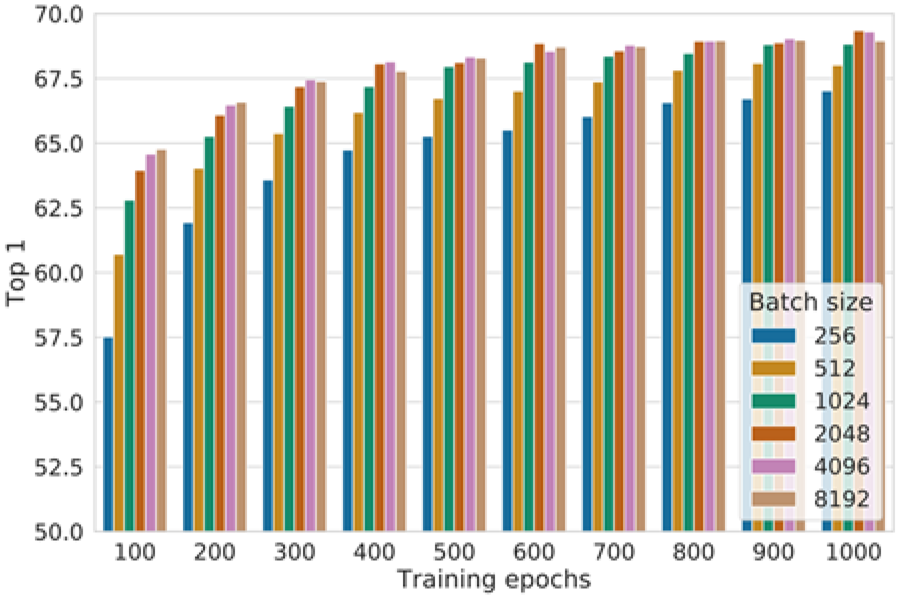


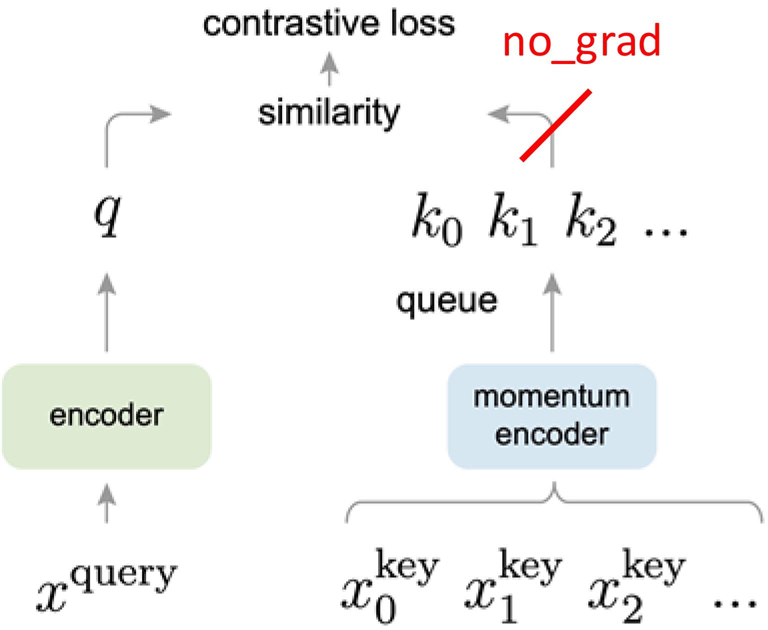
Figure 9. Linear evaluation models (ResNet-50) trained with different batch size and epochs. Each bar is a single run from scratch.[10]

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)

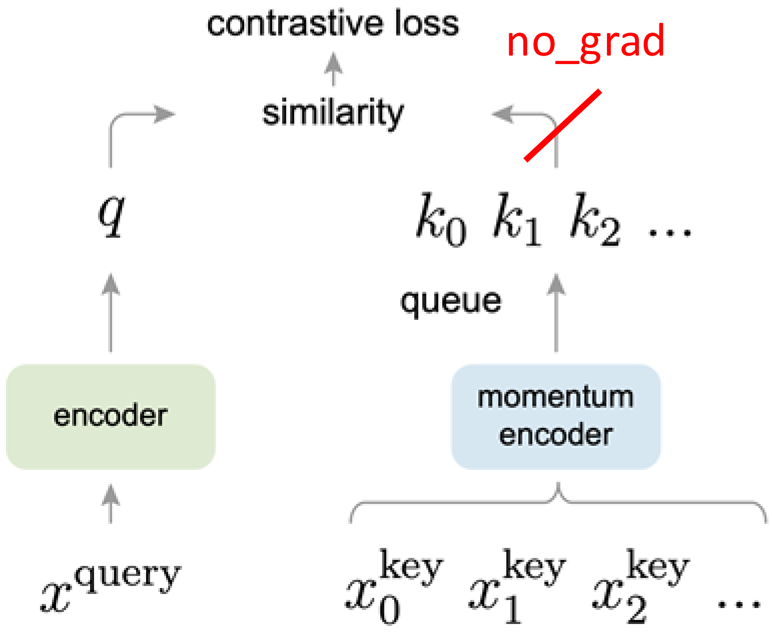


Key differences to SimCLR:

- Keep a running queue of keys (negative samples).
- Compute gradients and update the encoder only through the queries.
- Decouple 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)



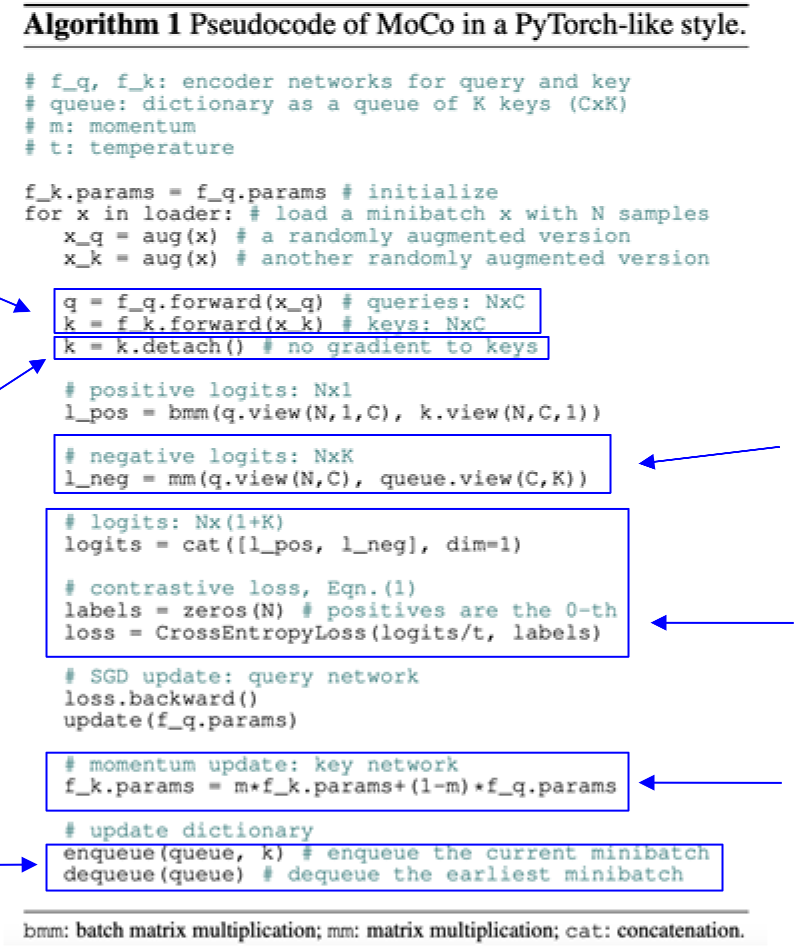
Key differences to SimCLR:

- 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:

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

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

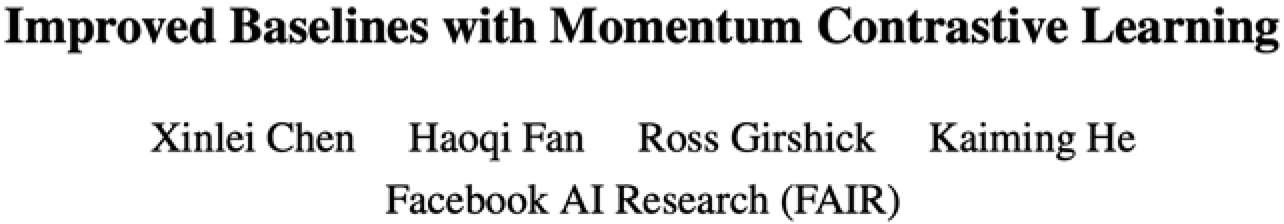
InfoNCE loss

Update f_k through momentum

Update the FIFO negative sample queue

Source: He et al., 2020

“MoCo V2”



Improved Baselines with Momentum Contrastive Learning

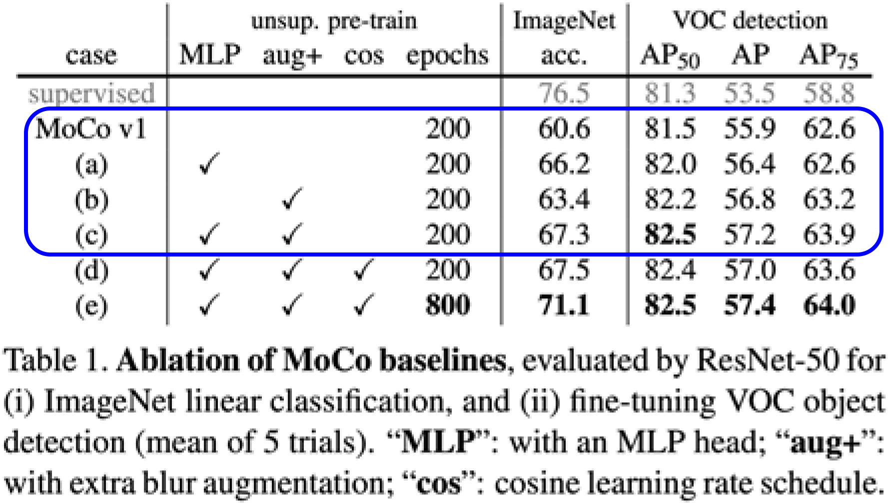
Xinlei Chen Haoqi Fan Ross Girshick Kaiming He
Facebook AI Research (FAIR)

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**

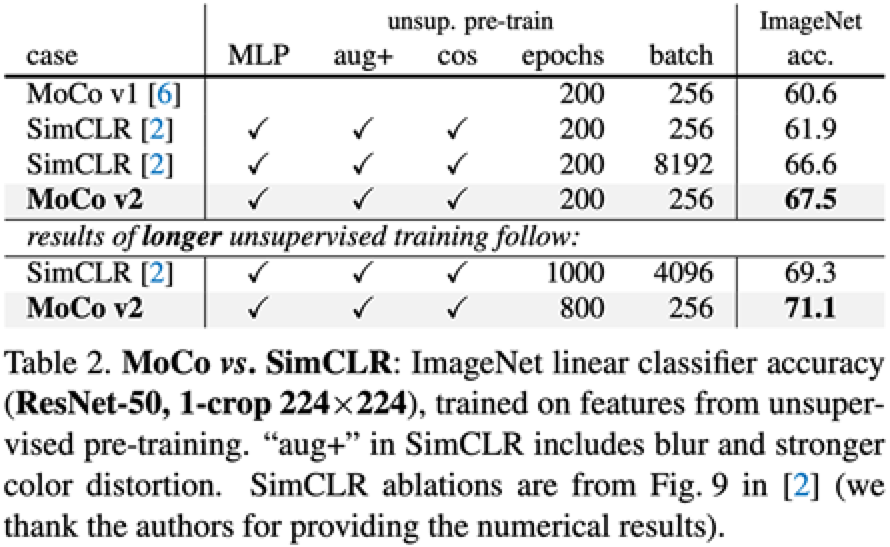
Table 1. **Ablation of MoCo baselines**, evaluated by ResNet-50 for (i) ImageNet linear classification, and (ii) fine-tuning VOC object detection (mean of 5 trials). "**MLP**": with an MLP head; "**aug+**": with extra blur augmentation; "**cos**": cosine learning rate schedule.

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**

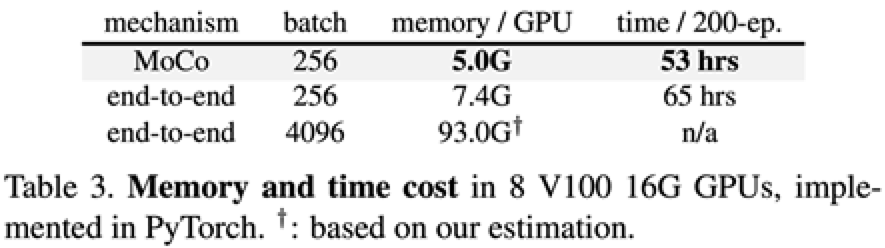
Table 2. **MoCo *vs.* SimCLR**: ImageNet linear classifier accuracy (**ResNet-50, 1-crop 224×224**), trained on features from unsupervised pre-training. "aug+" in SimCLR includes blur and stronger color distortion. SimCLR ablations are from Fig. 9 in [2] (we thank the authors for providing the numerical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

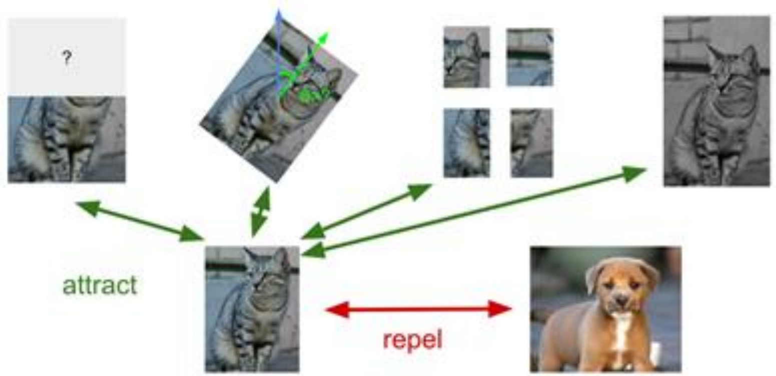
Table 3. **Memory and time cost** in 8 V100 16G GPUs, implemented in PyTorch. †: based on our estimation.

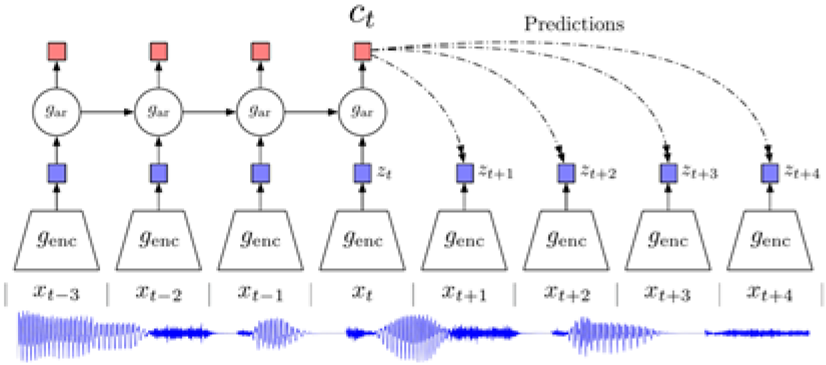
Key takeaways:

- 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



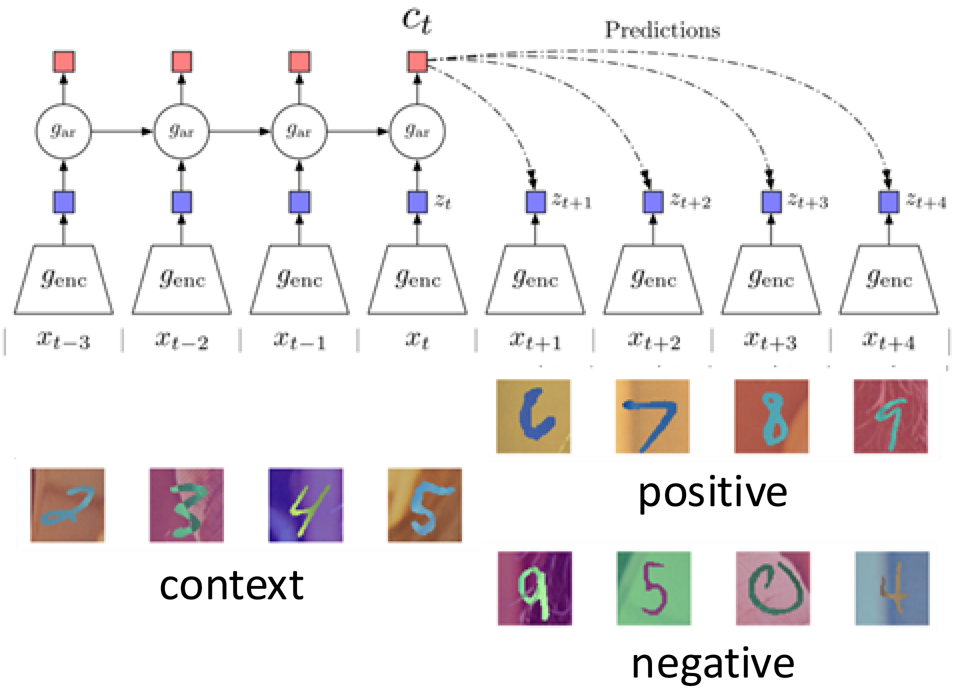


Source: van den Oord et al., 2018

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

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

Contrastive Predictive Coding (CPC)



Contrastive: contrast between “right” and “wrong” sequences using contrastive learning.

Predictive: the model has to predict future patterns given the current context.

Coding: the model learns useful feature vectors, or “code”, for downstream tasks, similar to other self-supervised methods.

Figure source

Source: van den Oord et al., 2018,

Contrastive Predictive Coding (CPC)

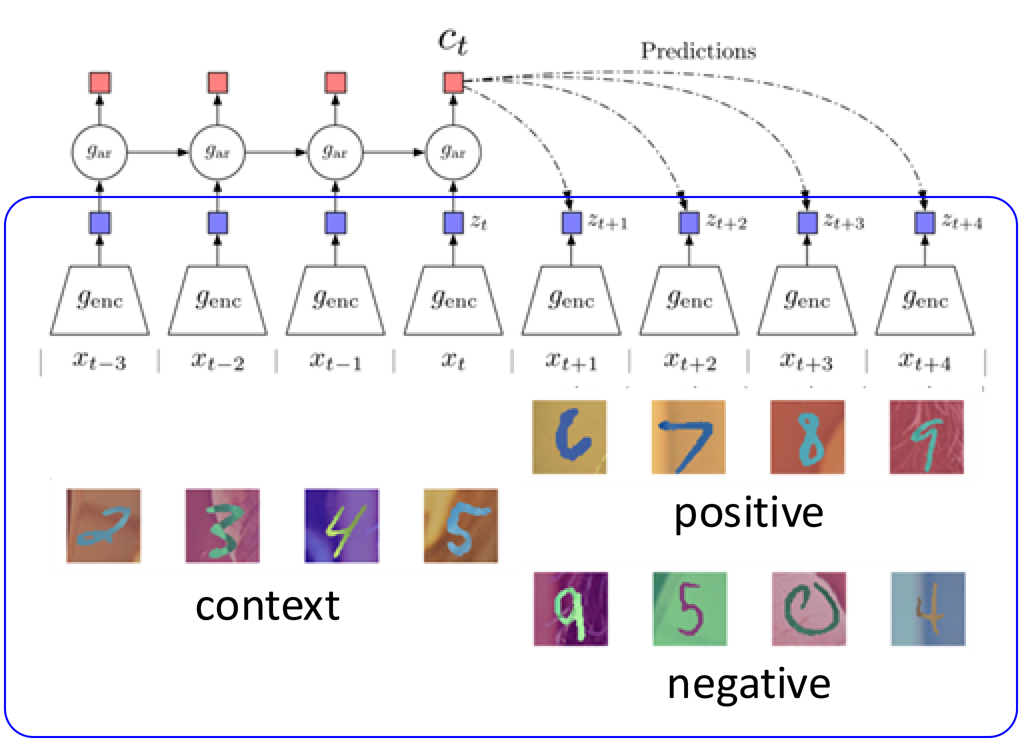
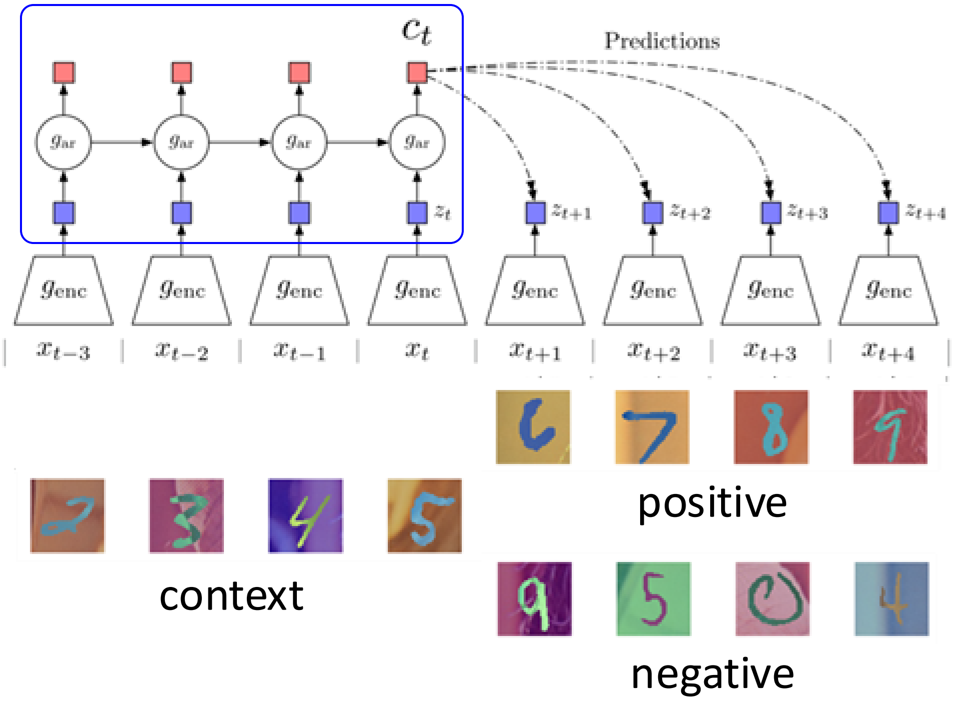


Figure source

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)



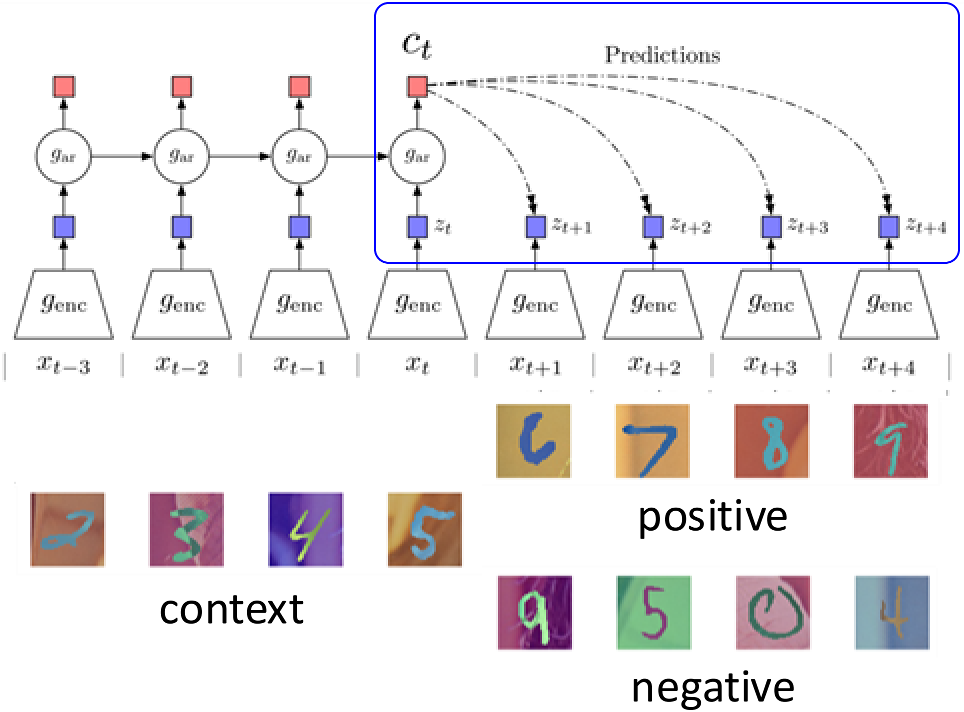
1. Encode all samples in a sequence into vectors $z_t = g_{enc}(x_t)$

2. Summarize context (e.g., half of a sequence) into a context code c_t using an auto-regressive model (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:

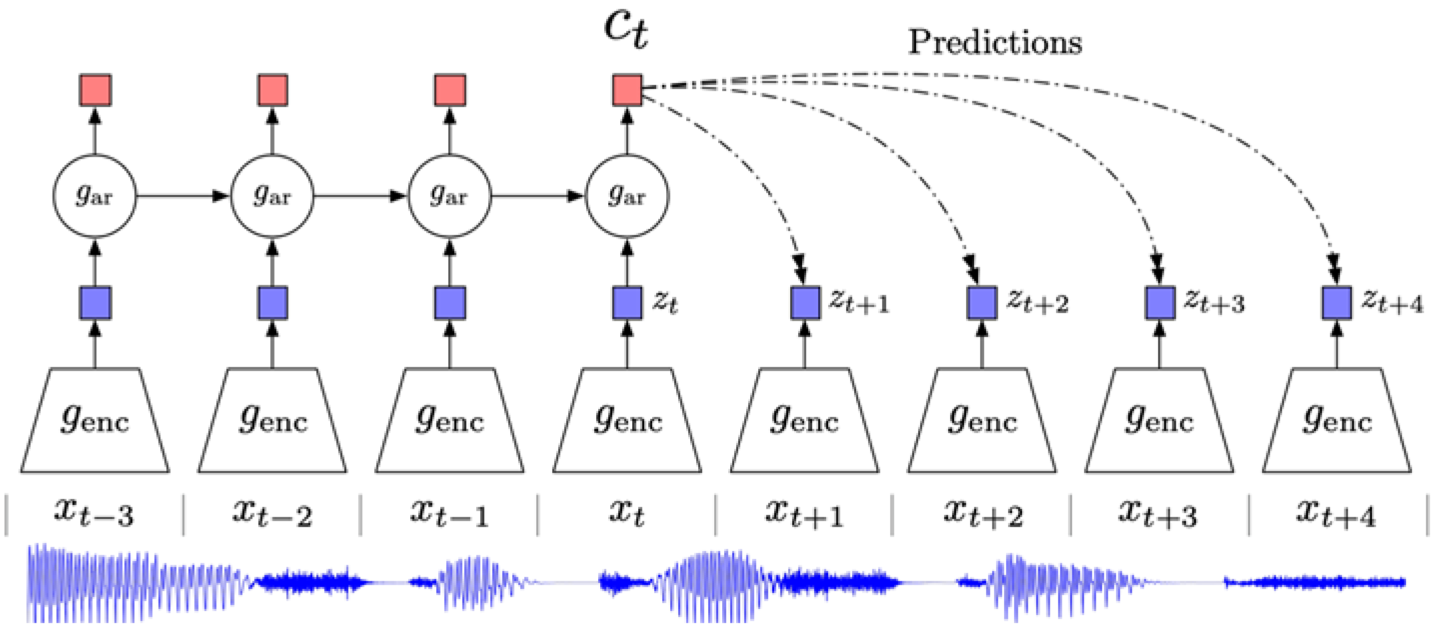
$$s_k(z_{t+k}, c_t) = z_{t+k}^T W_k c_t$$

, 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

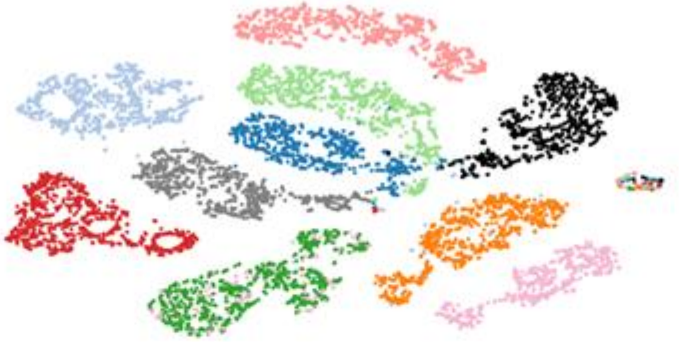
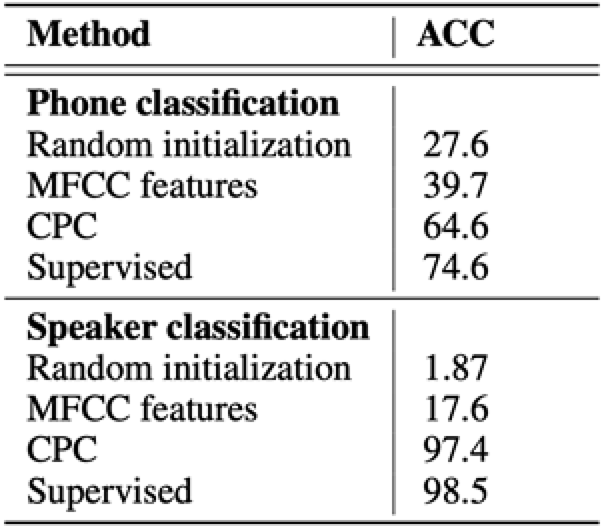


Figure 2: t-SNE visualization of audio (speech) representations for a subset of 10 speakers (out of 251). Every color represents a different speaker.



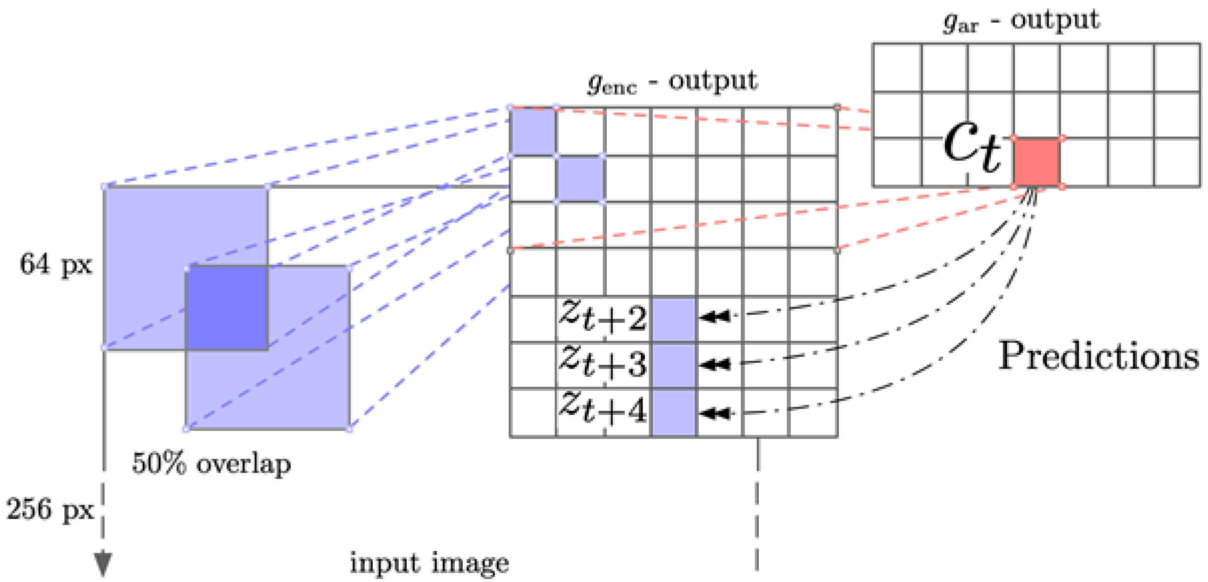
Method	ACC
Phone classification	
Random initialization	27.6
MFCC features	39.7
CPC	64.6
Supervised	74.6
Speaker classification	
Random initialization	1.87
MFCC features	17.6
CPC	97.4
Supervised	98.5

Linear classification on trained representations (LibriSpeech dataset)

Source: van den Oord et al., 2018,

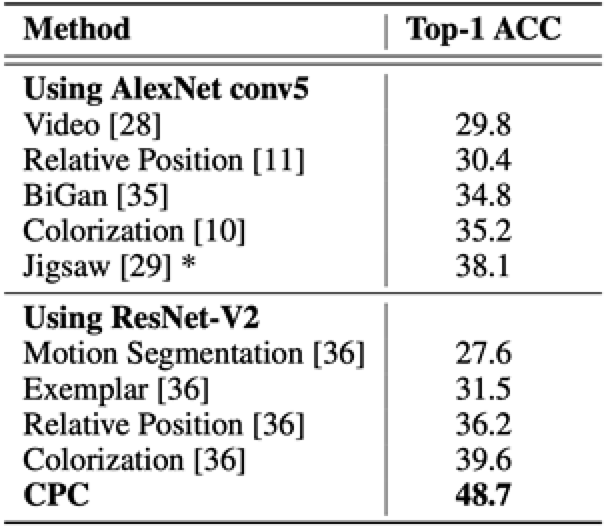
CPC example: modeling visual context

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,

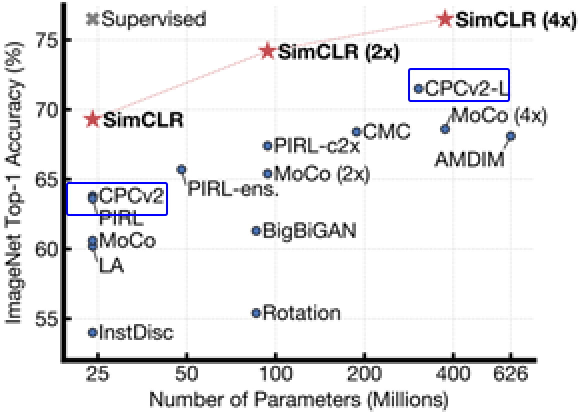
CPC example: modeling visual context



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)

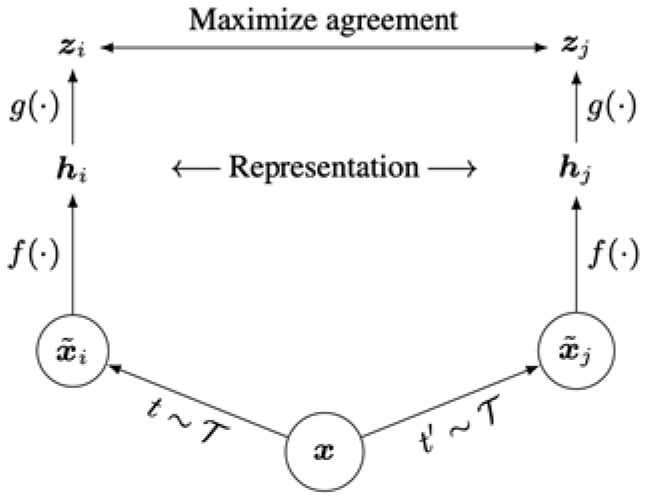
A *lower bound* on the mutual information between *f(x)* and *f(x⁺)*

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

Summary: Contrastive Representation Learning

SimCLR: a simple framework for contrastive representation learning

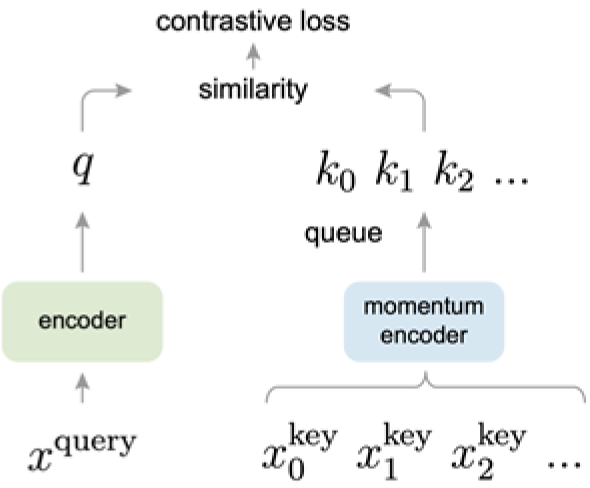
- **Key ideas**: non-linear projection head to allow flexible representation learning
- Simple to implement, effective in learning visual representation
- Requires large training batch size to be effective; large memory footprint



Summary: Contrastive Representation Learning

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

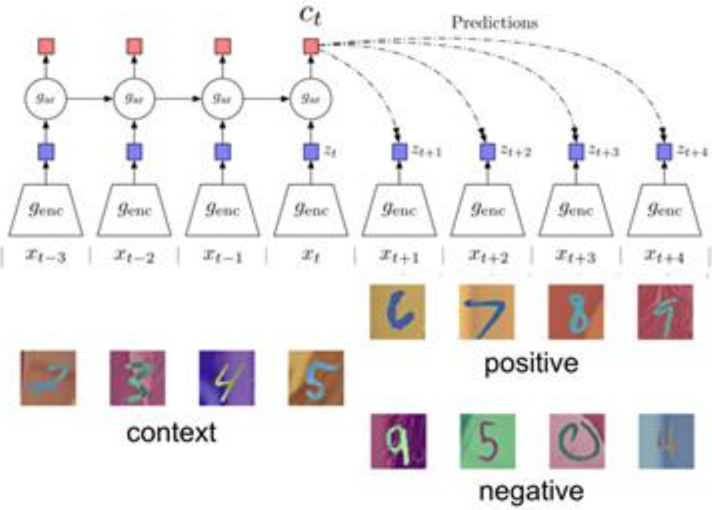
- Decouples negative sample size from minibatch size; allows large batch training without TPU
- MoCo-v2 combines the key ideas from SimCLR, i.e., nonlinear projection head, strong data augmentation, with momentum contrastive learning



Summary: Contrastive Representation Learning

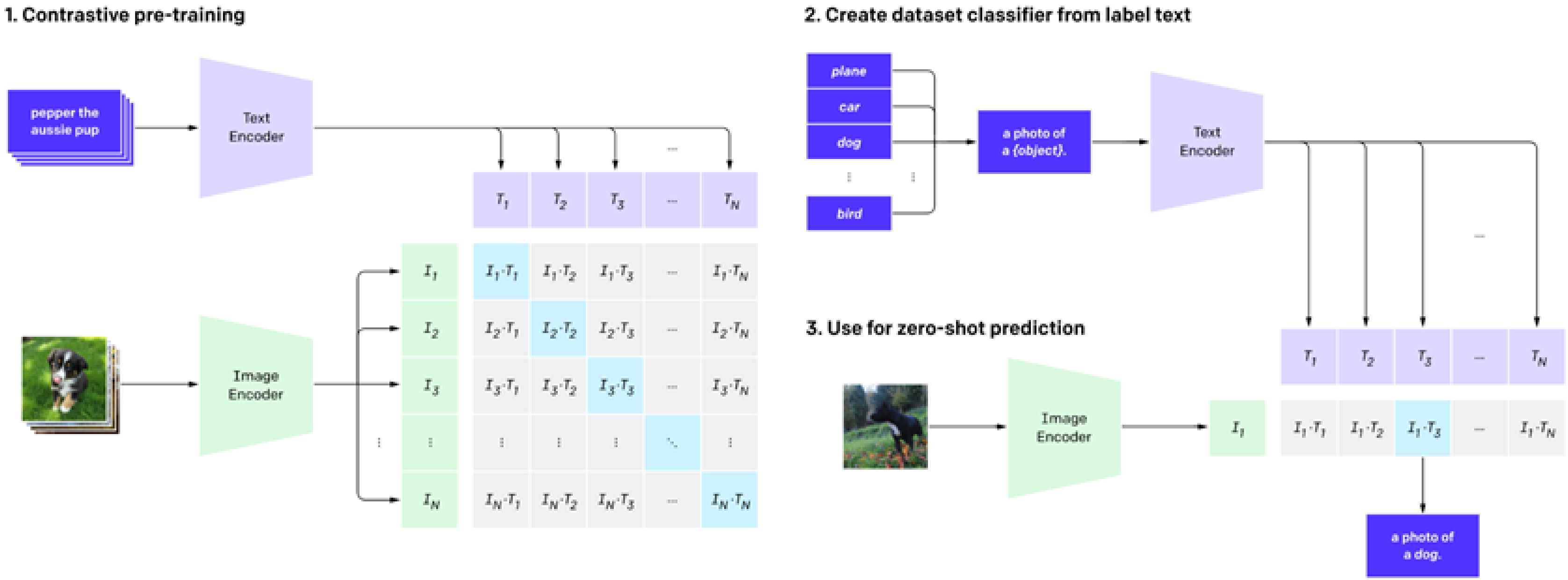
CPC: sequence-level contrastive learning

- 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

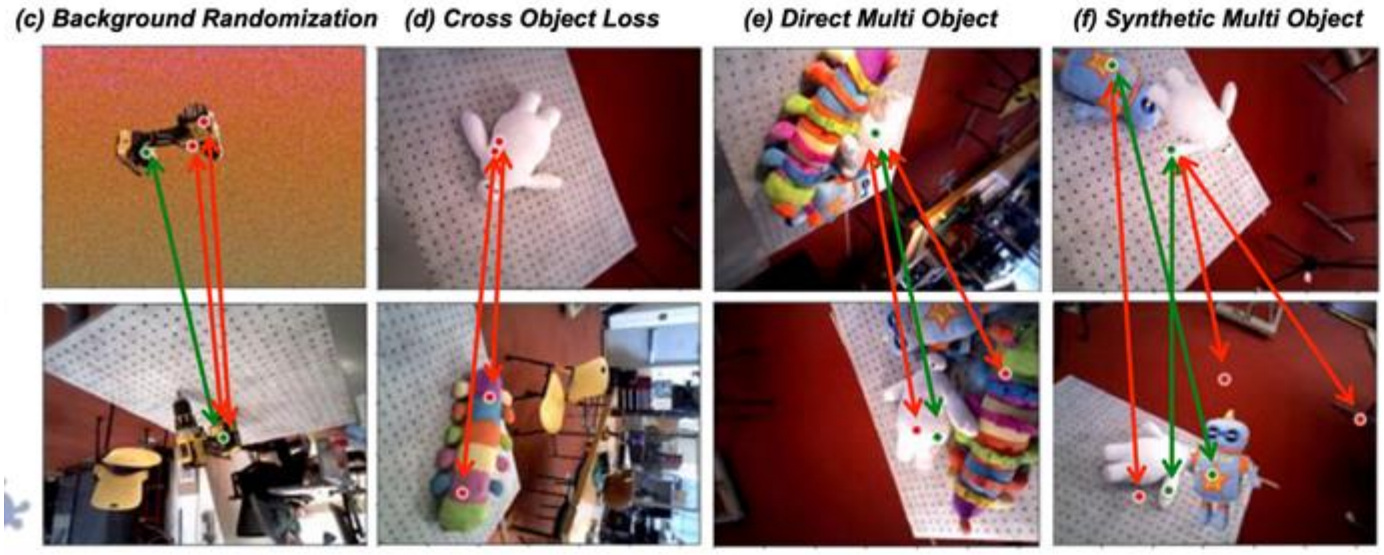
Contrastive learning between image and natural language sentences



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

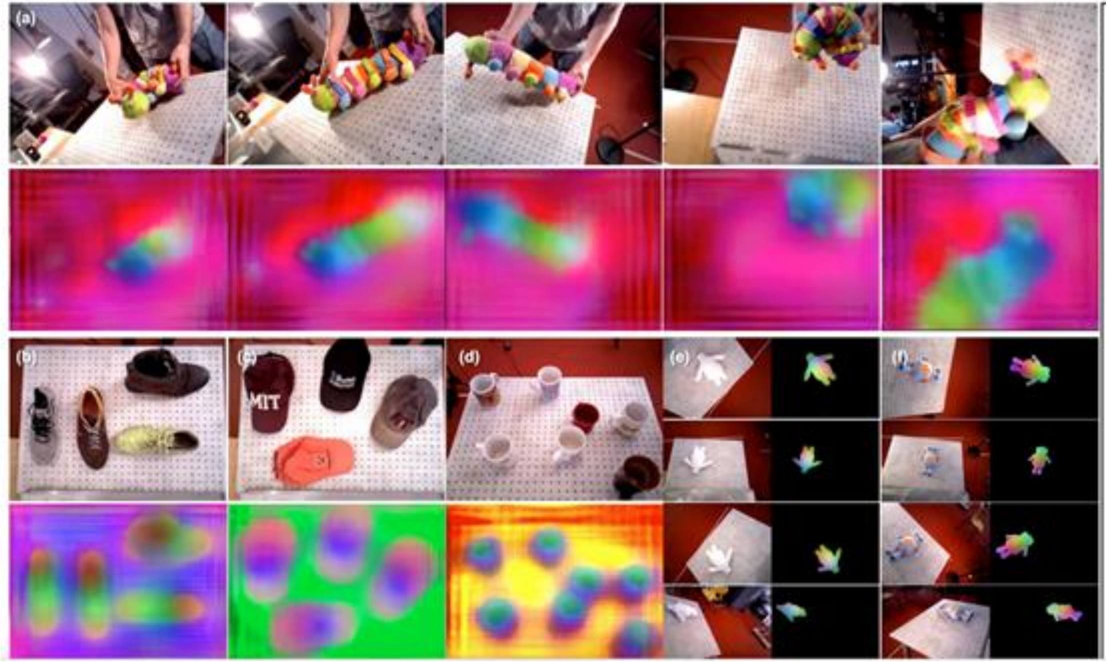
Other examples

Contrastive learning on pixel-wise feature descriptors



Dense Object Net, Florence et al., 2018

Other examples



Dense Object Net, Florence et al., 2018