Self-Supervised Representation Learning for Images

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Types of Machine learning

	+	−
• Supervised	**the most accurate** type. simple learning process.	limited number **labelled** datasets.
• Unsupervised	use large collections of **unlabeled data.**	usually works much **less efficiently.**

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• Unsupervised	use large collections of **unlabeled data.**	usually works much **less efficiently.**
• Semi-Supervised	**bigger datasets** than SL, **higher accuracy** than UsL.	still need **human-labeled** data.
• **Self-Supervised.**	?	?

What Self-Supervised Learning is?

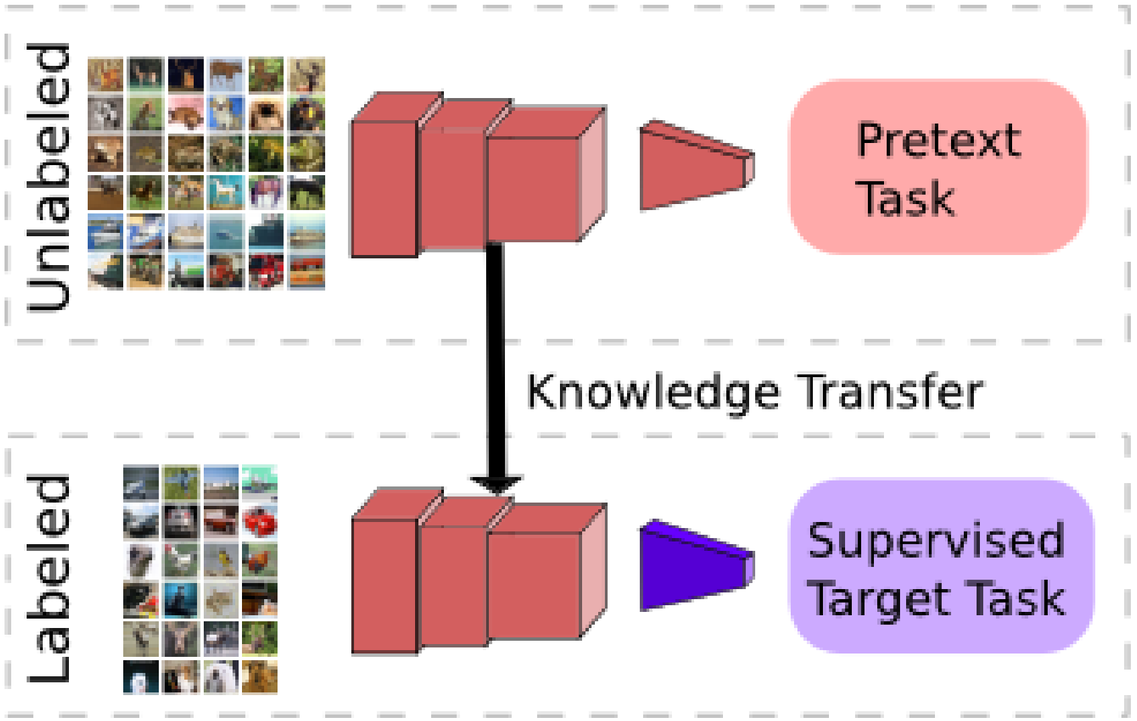
Goal: Downstream task - main supervised-learning task that utilizes a pre-trained model or component.

Motivation: Automatically label unlabeled data. Learn high-quality representation.

Idea: To solve downstream task we will solve **pretext tasks** as a supervised learning task and learn intermediate representation with the expectation that this representation can carry good semantic or structural meanings.

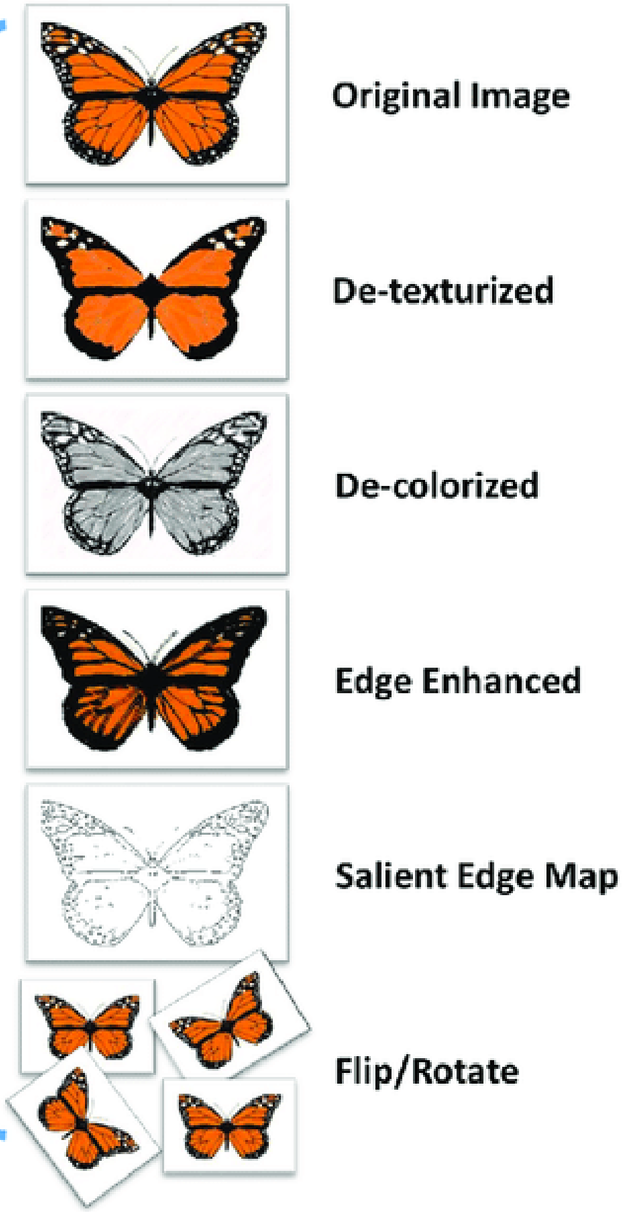
What Self-Supervised Learning is?

- **Pretext task** - a synthetic task with supervised loss function.
  Labels for pretext tasks come with the data for free!
  - Rotation
  - Exemplar-CNN
  - Relative position
  - Jigsaw puzzle
  - Contrastive Learning



Augmentations:

augmentations



- **simple** enough to keep semantic meaning unchanged.
- **complicated** enough to avoid catching trivial signals.

Rotation

The pretext task: Each input image is first rotated by a multiple of 90 at random, corresponding to [0, 90, 180, 270]. The model is trained to predict which rotation has been applied, thus a 4-class classification problem.

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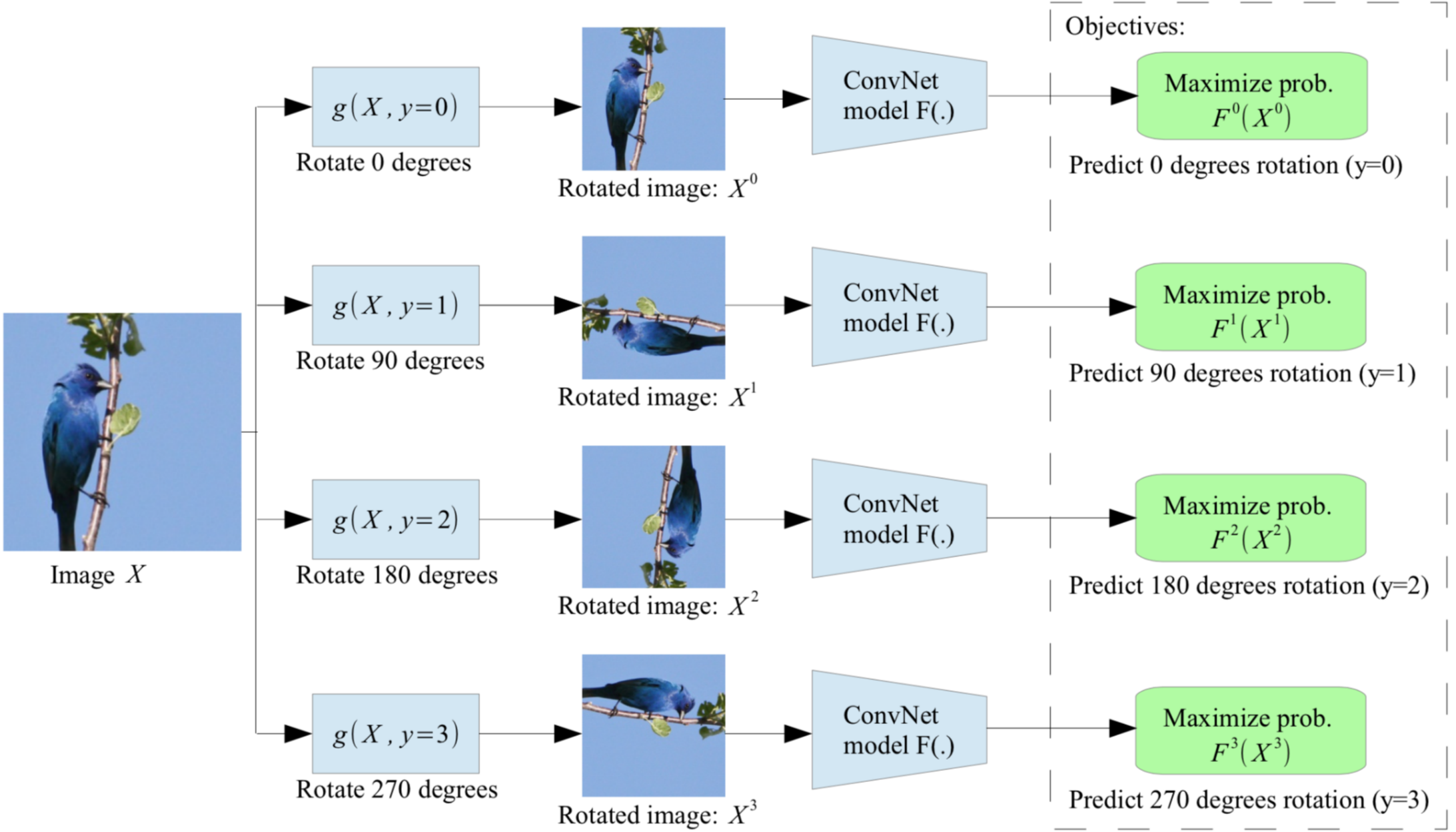
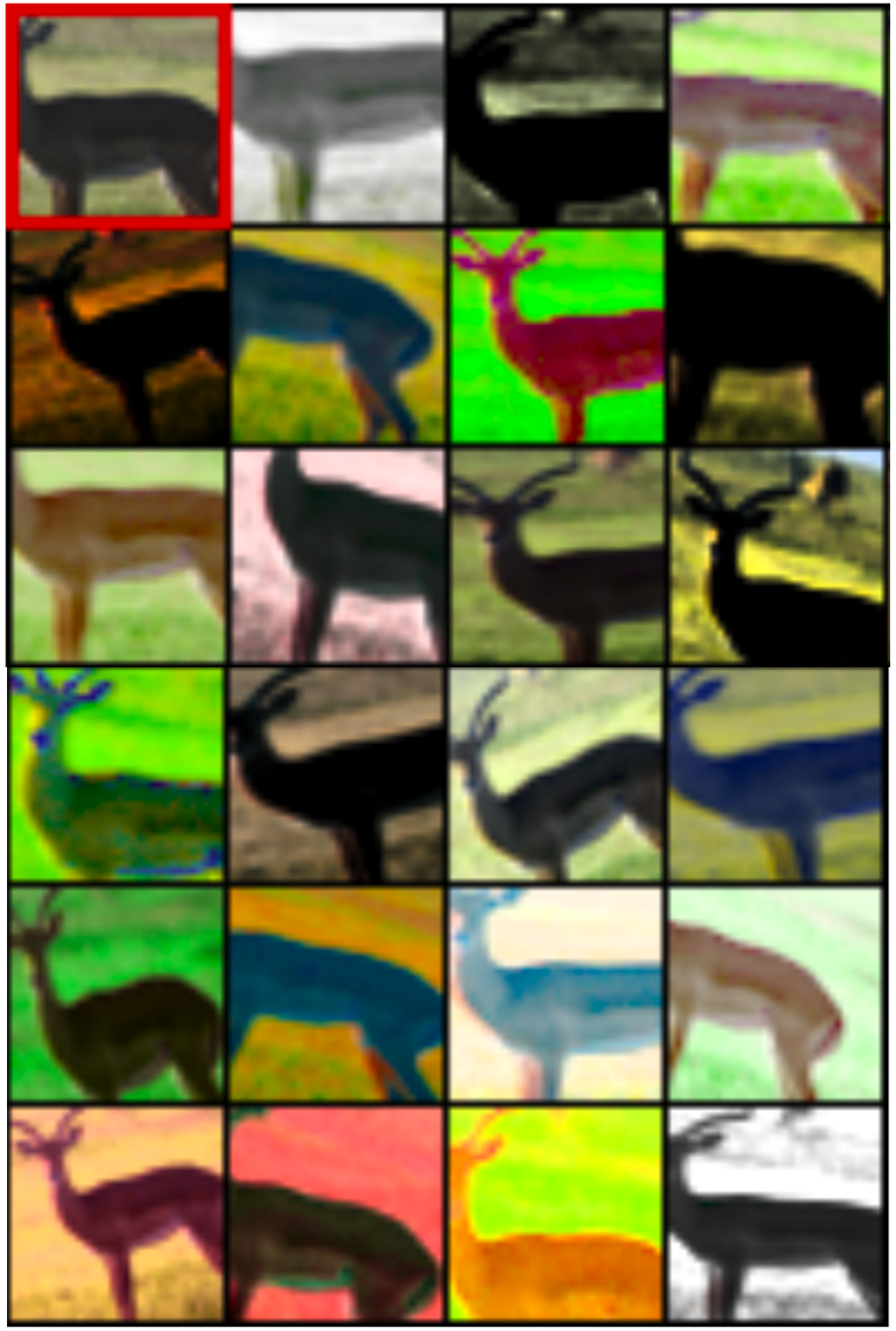
The model has to learn to recognize **high level traits**, such as heads, noses, and eyes, and the relative positions of these parts, rather than local patterns.


Objectives:
Image X
$g(X, y=0)$
Rotate 0 degrees
Rotated image: X^0
ConvNet model F(.)
Maximize prob. $F^0(X^0)$
Predict 0 degrees rotation (y=0)
$g(X, y=1)$
Rotate 90 degrees
Rotated image: X^1
ConvNet model F(.)
Maximize prob. $F^1(X^1)$
Predict 90 degrees rotation (y=1)
$g(X, y=2)$
Rotate 180 degrees
Rotated image: X^2
ConvNet model F(.)
Maximize prob. $F^2(X^2)$
Predict 180 degrees rotation (y=2)
$g(X, y=3)$
Rotate 270 degrees
Rotated image: X^3
ConvNet model F(.)
Maximize prob. $F^3(X^3)$
Predict 270 degrees rotation (y=3)

Exemplar-CNN

augmentations



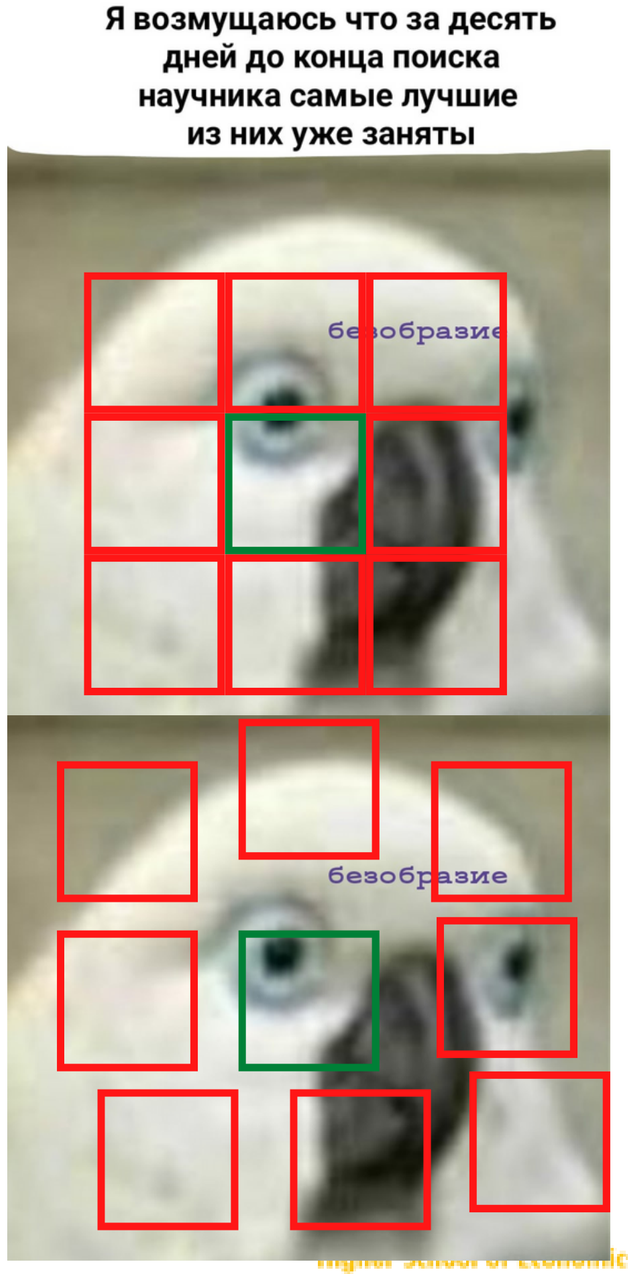
The pretext task is to discriminate between a set of surrogate classes.

Relative position

Preparation:

1. Randomly sample the first patch.
2. Considering that the first patch is placed in the middle of a 3x3 grid, and the second patch is sampled from its 8 neighboring locations around it.
3. Avoid the model only catching low-level trivial signals.

The pretext task is to predict which one of 8 neighboring locations the second patch is selected from, a classification problem over 8 classes.



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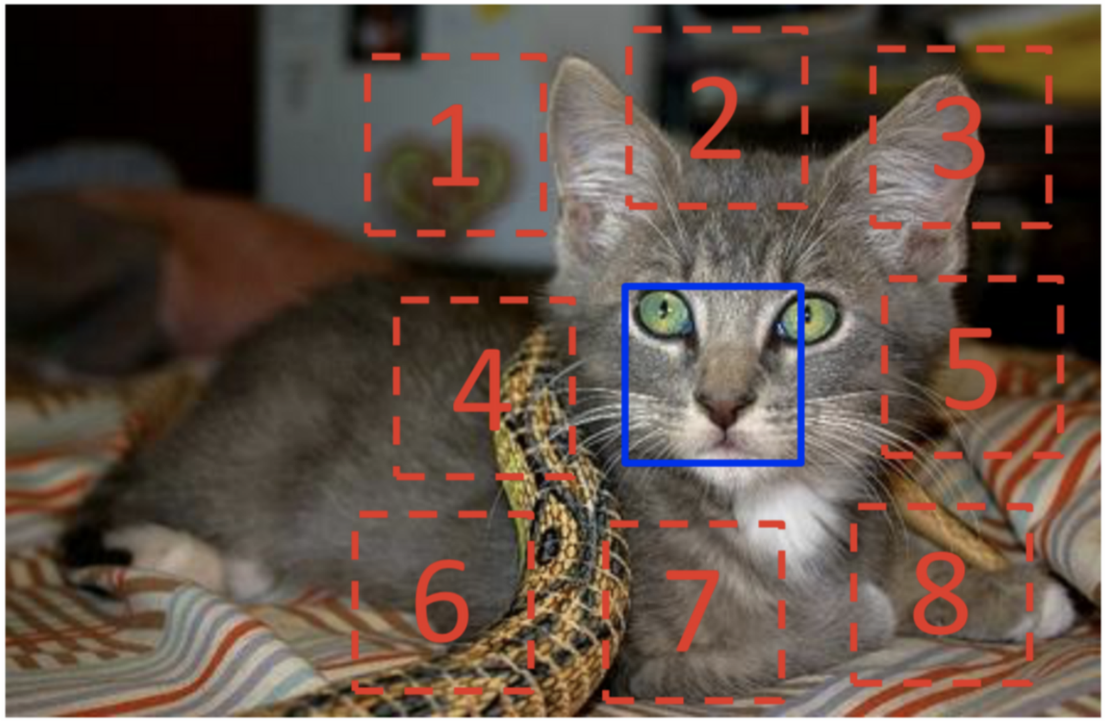
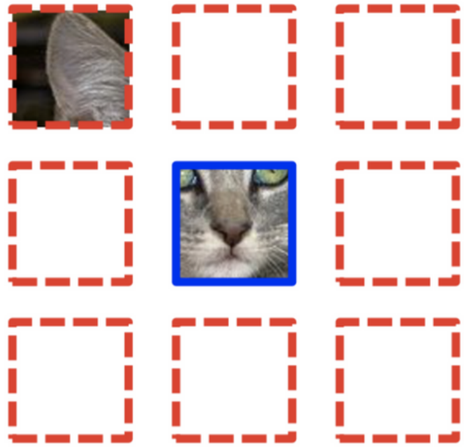


X = ( , ); Y = 3

Example:





Question 1:

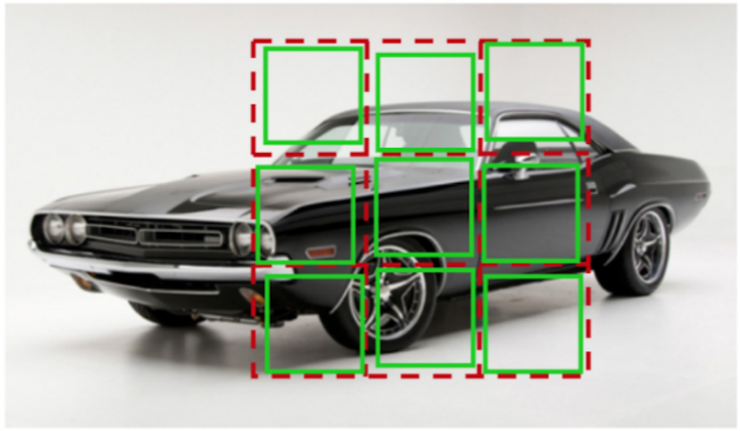
?

Question 2:

?

Jigsaw puzzle

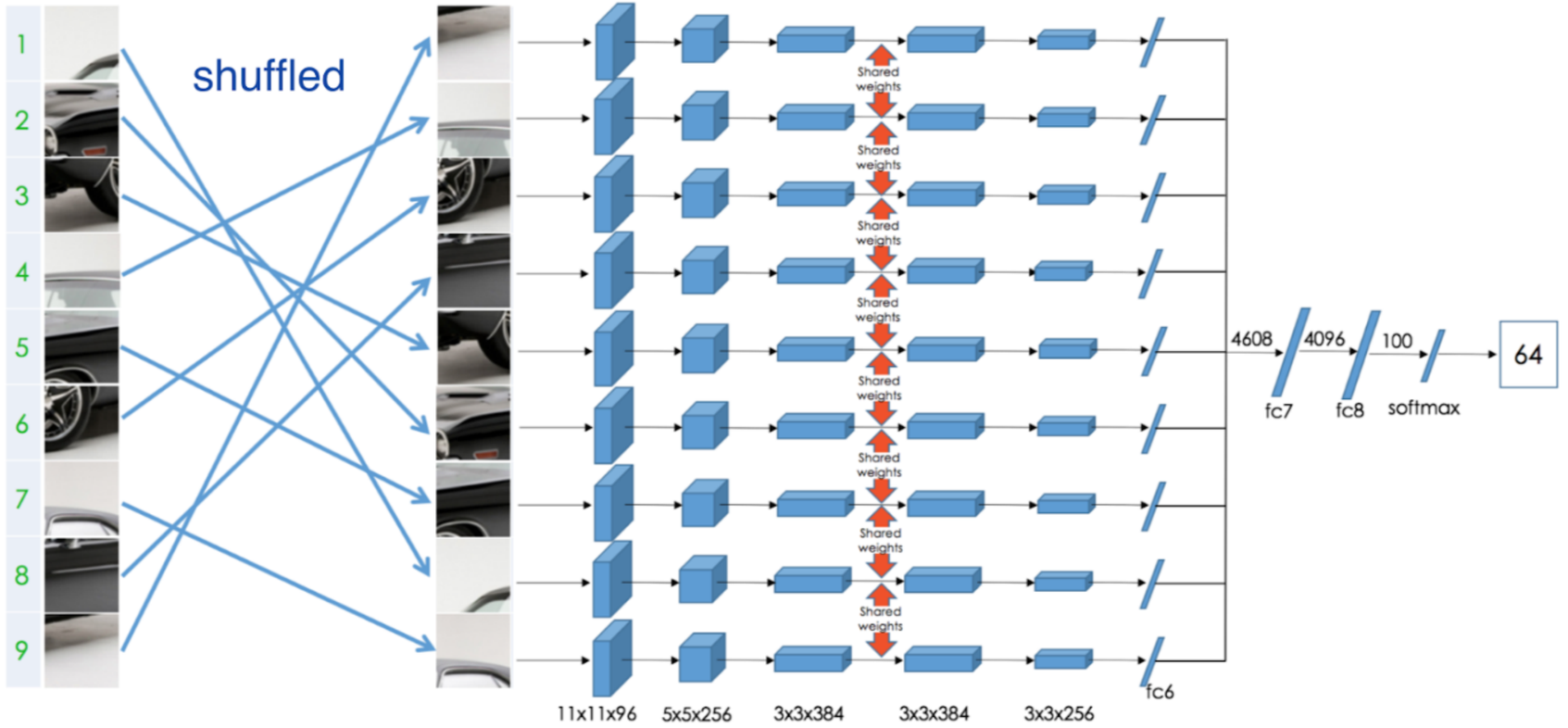
The pretext task: The model is trained to place 9 shuffled patches back to the original locations.



Permutation Set

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

Reorder patches according to the selected permutation



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Contrastive Representation Learning

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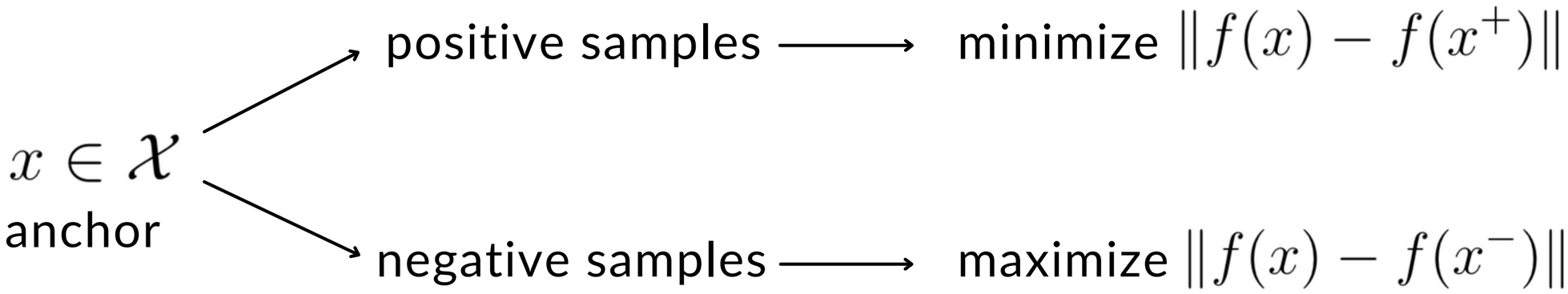
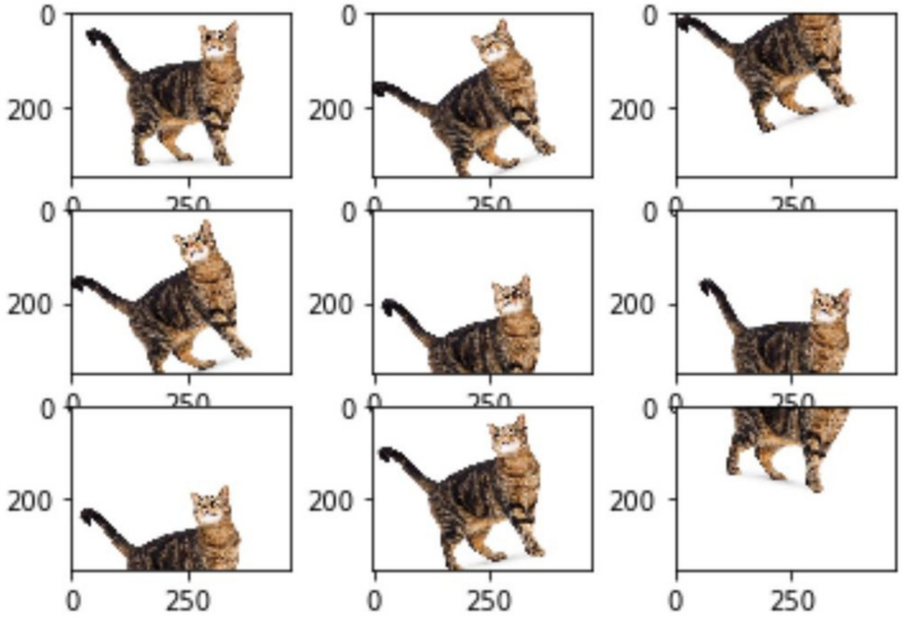
Idea: $\mathcal{X}$ - unlabeled data



Positive samples

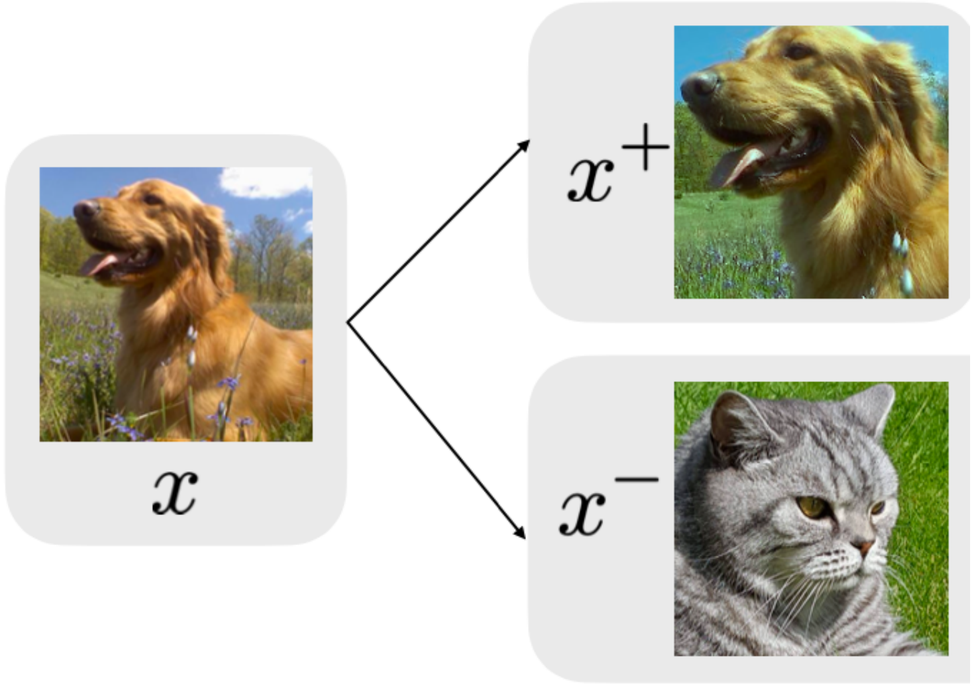
Augmentations:

- **simple** & **complicated**



Negative samples

Hard negatives: defferent labels, but similar embeddings



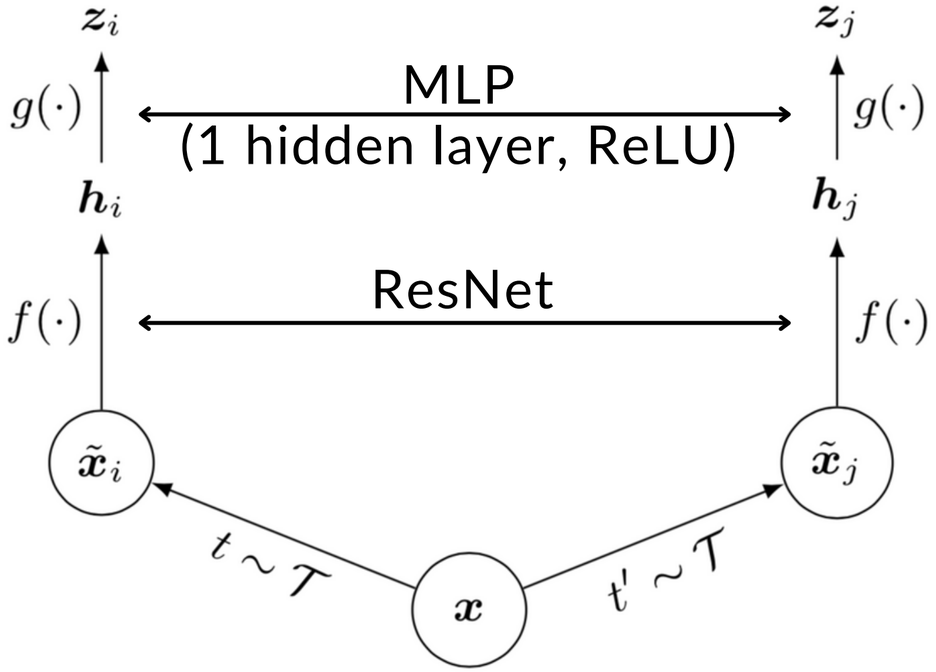
Hard negatives mining is hard when data is unlabeled.

But we can try to implicitly introduce them, for example via **large batch size.**

SimCLR

Idea:

1. Batch of size N -> batch of size 2N
2. Representations of augmented images
3. Projections of representations
4. Cosine similarity: $\text{sim}(u, v) = \frac{u^T v}{\|u\| \cdot \|v\|}$



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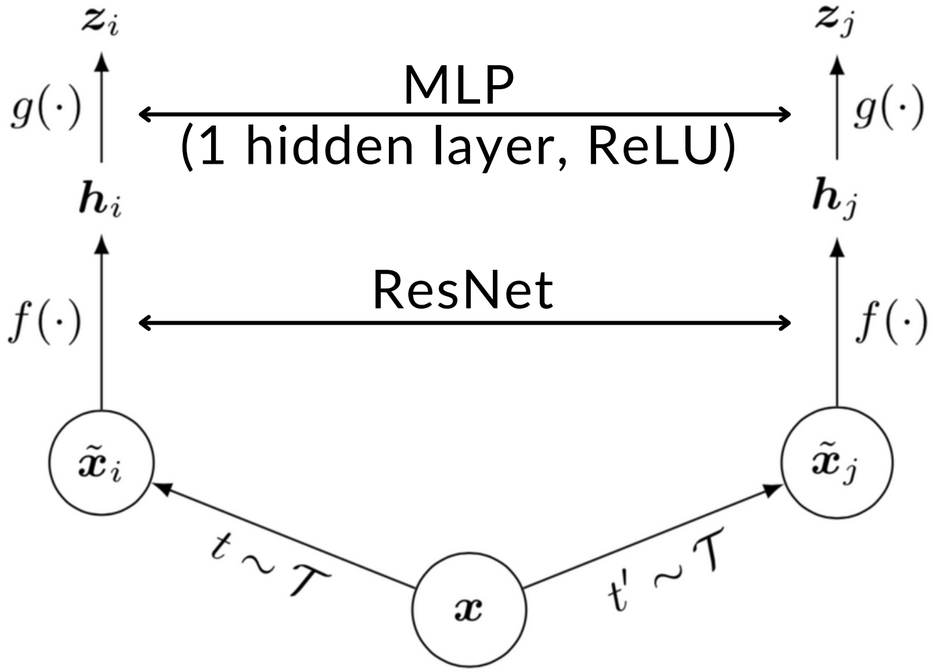

Loss: $$\mathcal{L}_{\text{SimCLR}}^{(i,j)} = -\log \frac{\exp(\text{sim}(\mathbf{z}_i, \mathbf{z}_j)/\tau)}{\sum_{k=1}^{2N} \mathbb{1}_{[k \neq i]} \exp(\text{sim}(\mathbf{z}_i, \mathbf{z}_k)/\tau)}$$

SimCLR

Computing embedding for a large amount of negative samples in every batch is **expensive**.

⇓

Memory bank - store the representation in memory to trade off data staleness for cheaper compute

MoCo (Momentum Contrast)

$\{k_0, \ldots, k_K\}$ - dictionary of encoded keys (for previous batches)

f_q - honest representation, θ_q - parameters

f_k - key encoder, θ_k - parameters

slowly progressing! $\Rightarrow$ maintain key's consistency

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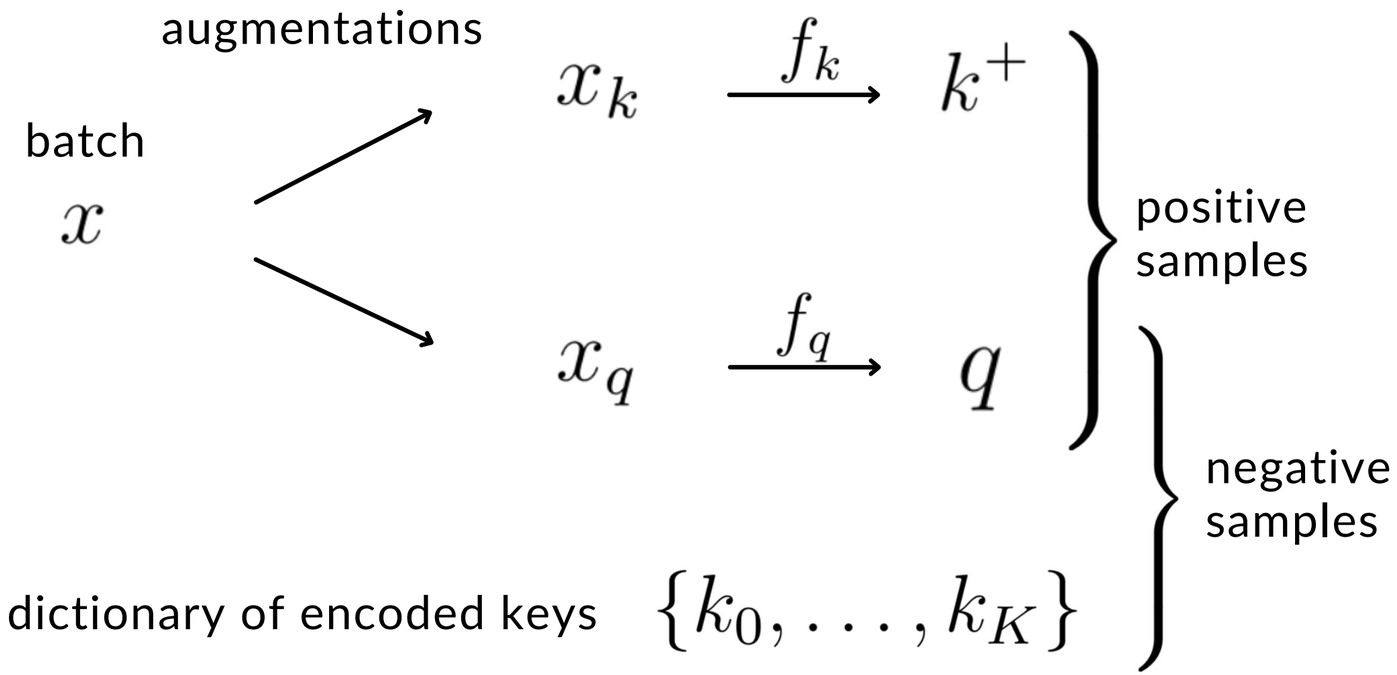
Updating encoders:

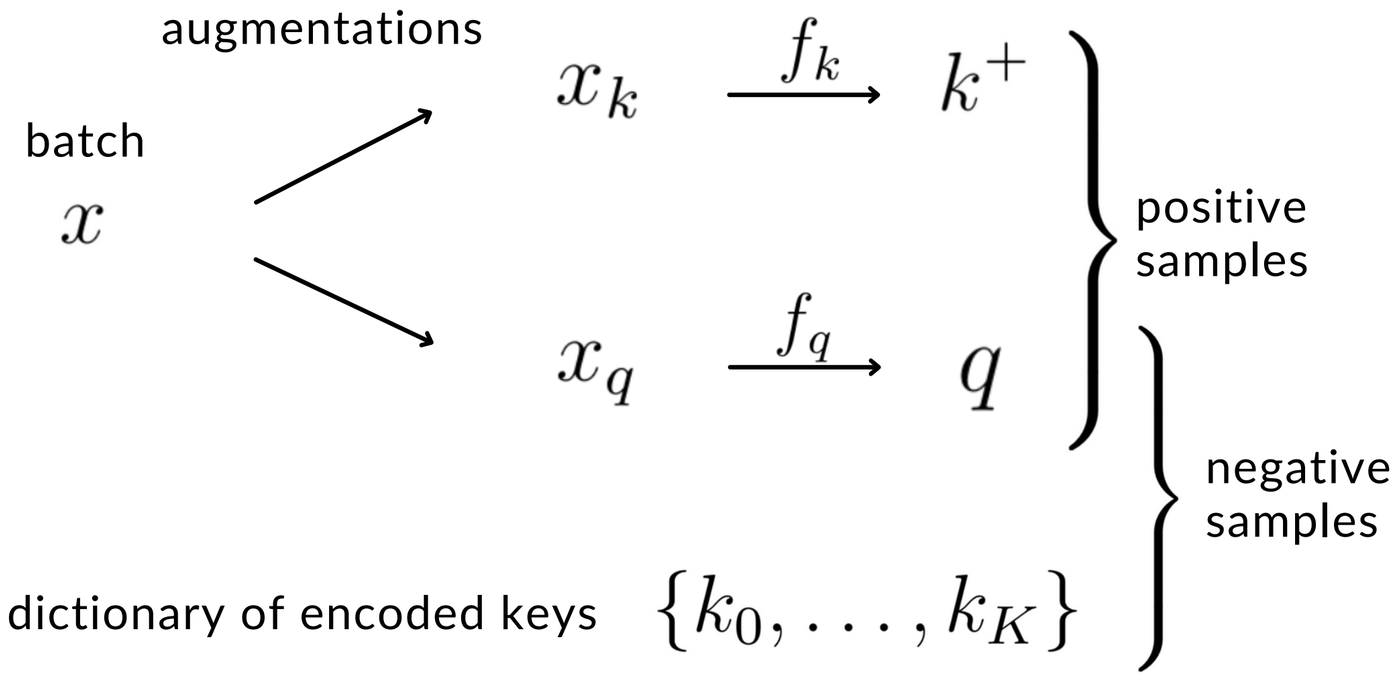
f_q - gradient

f_k - momentum: $\theta_k \leftarrow \underbrace{m\theta_k}_{m \approx 0.999} + (1-m)\theta_q$

MoCo


augmentations
batch
x
x_k
f_k
k^+
x_q
f_q
q
positive samples
negative samples
dictionary of encoded keys
$\{k_0, \ldots, k_K\}$

MoCo



Loss:

$$\mathcal{L}_q = -\log \frac{\exp(q \cdot k_+ / \tau)}{\sum_{i=0}^{K} \exp(q \cdot k_i / \tau)}$$

Updating dictionary:

dequeue the earliset batch k_0 $\longleftarrow$ $\{k_0, \ldots, k_K\}$ $\longleftarrow$ k^+ enqueue current batch

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MoCo v2

MoCo doesn't require a large batch size in order to have enough negative samples!
Can it become even better?

Key ideas of SimCLR:

1. Heavy data augmentation (+ Gaussian blur)
2. Projection layer

Apply them to MoCo $\Rightarrow$ **MoCo v2**

SimCLR vs MoCo

case	pre-train epochs	pre-train batch	ImageNet acc.
MoCo v1	200	256	60.6
SimCLR	200	256	61.9
SimCLR	200	8192	66.6
MoCo v2	200	256	**67.5**

- Large batches are not necessary
- Even better performance

What makes CRL special?

Self-supervised learning:
Learns representation by learning features, invariant to augmentations

Contrastive learning:
Learns representation by grouping similar objects together and detecting common features

Overview

- Self-Supervised Learning doesn't need human-labeled dataset.
- Don’t care about the final performance of pretext task.
- Care about the learned representation with high level traits.
- **Pretext tasks**: Rotation, Exemplar-CNN, Relative position, Jigsaw puzzle, Contrastive Learning and others!

- CLR aims at learning an embedding space
- Key factors: data augmentation and negative samples
- Large batch size (SimCLR), memory bank (MoCo)
- MoCo + key ideas of SimCLR = MoCo v2 -> better performance!

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Appendix

SimCLR

Algorithm 1 SimCLR's main learning algorithm.

input: batch size N, constant τ, 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 $g(\cdot)$

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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.

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