



Deep Learning Self-Supervised & Contrastive Learning

or how to overcome the need for huge amounts of labels

Contrastive & Self-Supervised Learning

or how to overcome the need for huge amounts of labels

A large class of contemporary ML methods rely on **human provided-labels** or rewards as the only form of **learning signal** used during the training process.

Contrastive & Self-Supervised Learning

or how to overcome the need for huge amounts of labels

This over-reliance on direct-**semantic** supervision has several perils:

- The underlying **data has a much richer structure than what sparse labels could provide.**
- Thus, purely supervised learning algorithms often require large numbers of samples to learn from, and converge to **brittle** solutions.



(a) Texture image
81.4% **Indian elephant**
10.3% indri
8.2% black swan



(b) Content image
71.1% **tabby cat**
17.3% grey fox
3.3% Siamese cat



(c) Texture-shape cue conflict
63.9% **Indian elephant**
26.4% indri
9.6% black swan

The supervision signal (simple labels) is too weak to deal with these subtleties (shape and texture).

Contrastive & Self-Supervised Learning

or how to overcome the need for huge amounts of labels

This over-reliance on direct-**semantic** supervision has several perils:

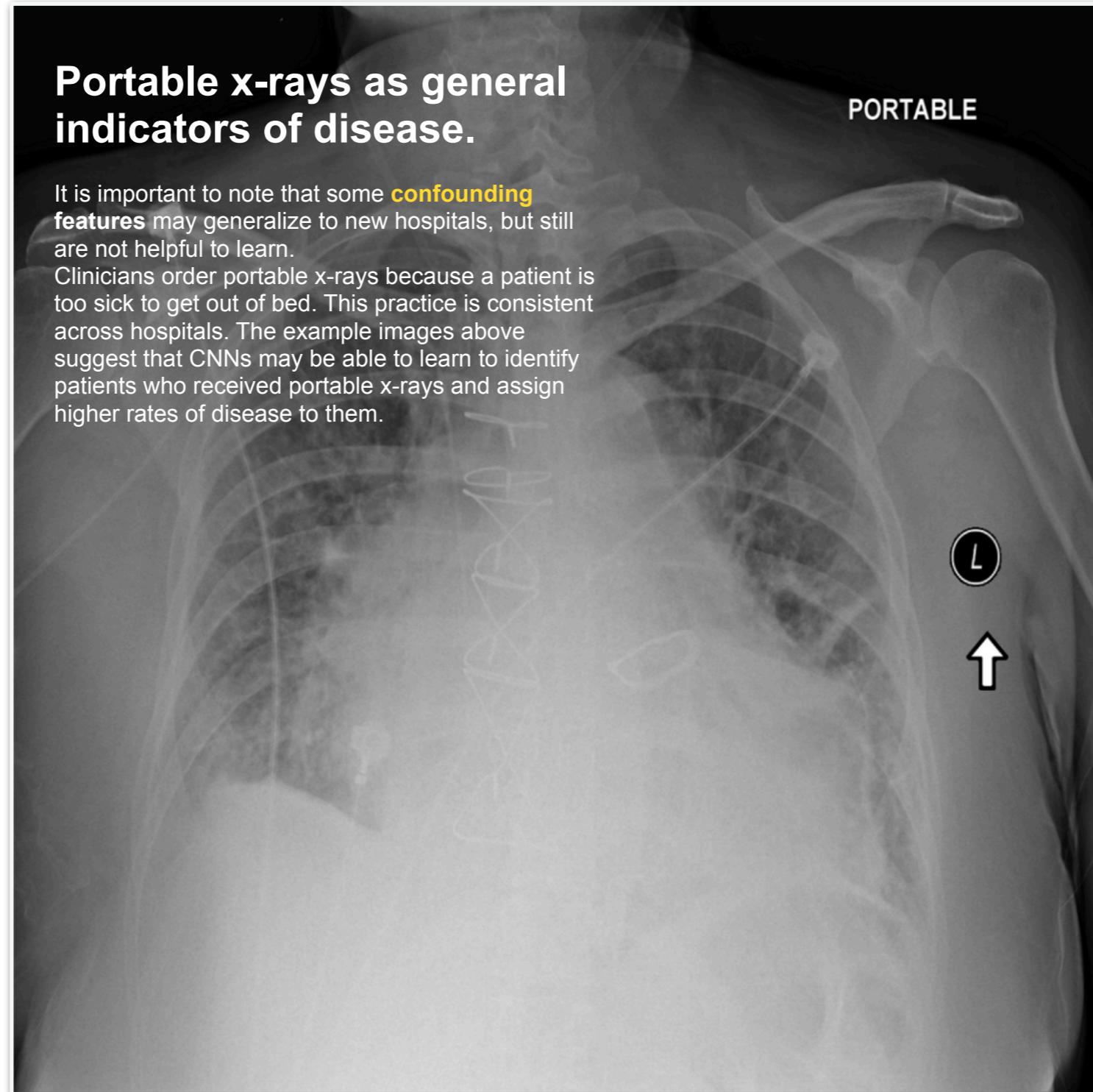
- The underlying **data has a much richer structure than what sparse labels could provide.**
 - Thus, purely supervised learning algorithms often require large numbers of samples to learn from, and converge to brittle solutions.
- It leads to **task-specific solutions**, rather than knowledge that can be repurposed.

Even with large amounts of data, supervised learning still has several blind-spots in terms of learning **useful** and **rich** representations.

Useful = robust
Rich = general

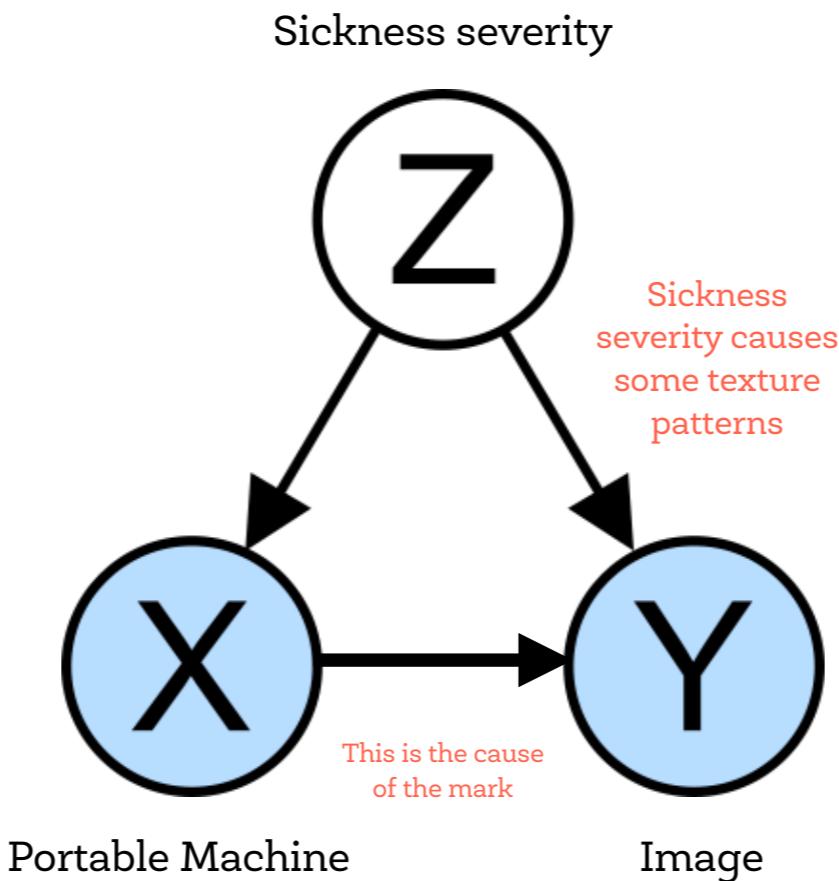
Contrastive & Self-Supervised Learning

or how to overcome the need for huge amounts of labels



Contrastive & Self-Supervised Learning

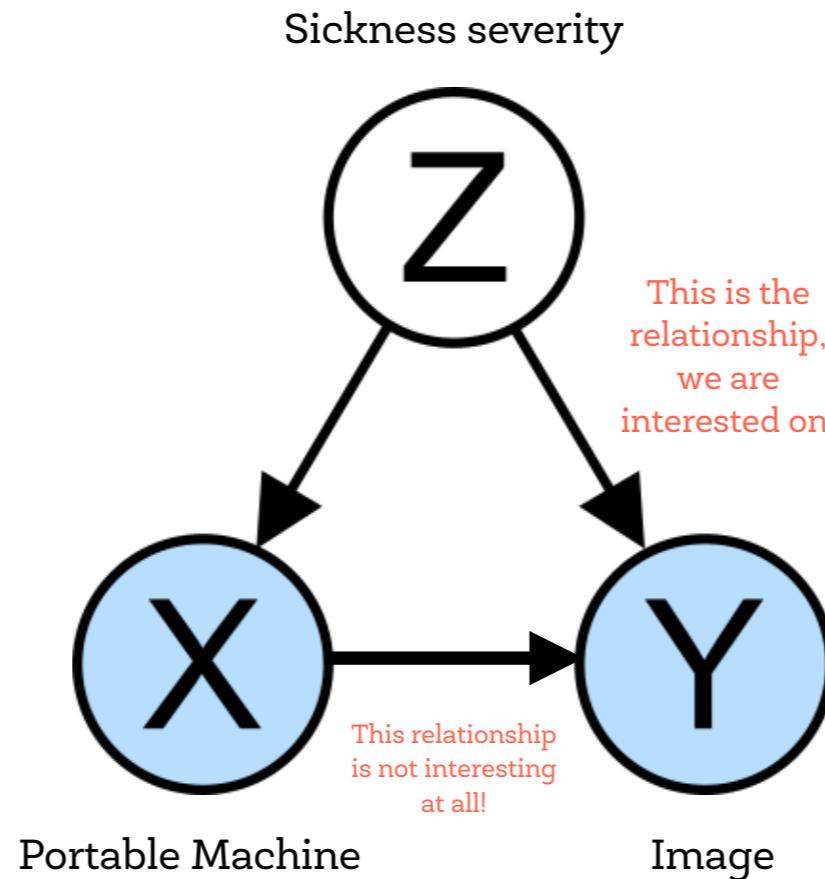
or how to overcome the need for huge amounts of labels



Spurious associations are useful for prediction, **if** we can assure that they are present in all prediction scenarios (hospitals). Otherwise, they are extremely dangerous!

Contrastive & Self-Supervised Learning

or how to overcome the need for huge amounts of labels

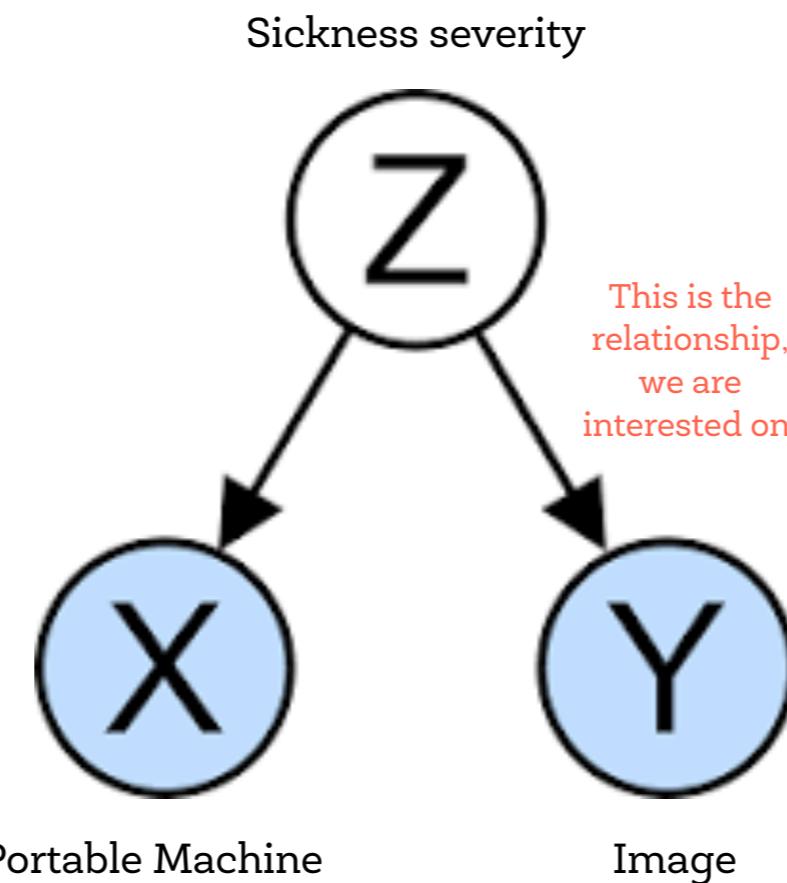


Spurious associations are useful for prediction, **if** we can assure that they are present in all prediction scenarios (hospitals). Otherwise, they are extremely dangerous!

How can we get ride of this spurious correlations?
(Open question)

Contrastive & Self-Supervised Learning

or how to overcome the need for huge amounts of labels



We can hide ALL images with a black square in the place of the mark. This results in a “mutilated” graph were image features are only caused by sickness severity.

Self-Supervised Learning

Self-Supervised Learning

Self-Supervised Learning provides a promising alternative **to learn powerful representations**, where the data itself provides the supervision for a learning algorithm.

Consider this experiment conducted where subjects were asked to draw a picture of the dollar bill as detailed as possible. Here is a drawing ‘from memory’:



A rich representation, that is useful for a variety of tasks, is not a “copy” of the original features!

And here is the drawing subsequently made with a dollar bill present:



Self-Supervised Learning

Despite having seen a dollar bill countless number of times, we don't retain a full representation of it.

In fact, we really only retain enough features of the bill **to distinguish it from other objects**.

This can be extended to **objects that have no name** or to individuals.



Caricatures of people you know are recognized more quickly and accurately than life-like drawings or photographs.

Self-Supervised Learning

Can we build **representation learning** algorithms (**not relying in semantic labels**) that don't concentrate on pixel-level details, and only encode high-level features sufficient enough to "think about" (recognize, compare, describe, etc.) different objects?



Considering the amount of **unlabelled data** (e.g. free text, all the images on the Internet) is substantially more than a limited number of human curated labelled datasets, it is kinda wasteful not to use them.

However, **unsupervised learning** is not easy and usually works much less **efficiently** than supervised learning.

Self-Supervised Learning

What if we can get **labels for free** for unlabelled data and **train unsupervised dataset in a supervised manner?**

We can achieve this by framing an **auxiliary supervised learning task** in a special form to predict only **a subset of information of the target using the rest.**

This is known as **self-supervised learning.**

Self-Supervised Learning

EXAMPLE

The default task for a language model (LM) is to **predict the next word given the past sequence**, $p(X_n | X_1, \dots X_{n-1})$.

Modern LMs adds two auxiliary tasks and both rely on self-generated labels:

Task 1: Mask language model (MLM)

From [Wikipedia](#): “A cloze test (also cloze deletion test) is an exercise, test, or assessment consisting of a portion of language with certain items, words, or signs removed (cloze text), where the participant is asked to replace the missing language item. ... The exercise was first described by W.L. Taylor in 1953.”

It is unsurprising to believe that a representation that learns the context around a word rather than just after the word is able to better capture its meaning, both syntactically and semantically. BERT encourages the model to do so by training on the “*mask language model*” task:

1. Randomly mask 15% of tokens in each sequence. Because if we only replace masked tokens with a special placeholder `[MASK]`, the special token would never be encountered during fine-tuning. Hence, BERT employed several heuristic tricks:
 - (a) with 80% probability, replace the chosen words with `[MASK]`;
 - (b) with 10% probability, replace with a random word;
 - (c) with 10% probability, keep it the same.
2. The model only predicts the missing words, but it has no information on which words have been replaced or which words should be predicted. The output size is only 15% of the input size.

Self-Supervised Learning

EXAMPLE

Task 2: Next sentence prediction

Motivated by the fact that many downstream tasks involve the understanding of relationships between sentences (i.e., [QA](#), [NLI](#)), BERT added another auxiliary task on training a *binary classifier* for telling whether one sentence is the next sentence of the other:

1. Sample sentence pairs (A, B) so that:
 - o (a) 50% of the time, B follows A;
 - o (b) 50% of the time, B does not follow A.
2. The model processes both sentences and output a binary label indicating whether B is the next sentence of A.

The training data for both auxiliary tasks above can be trivially generated from any monolingual corpus.

Hence the scale of training is unbounded.

Image-based Self-Supervised Learning

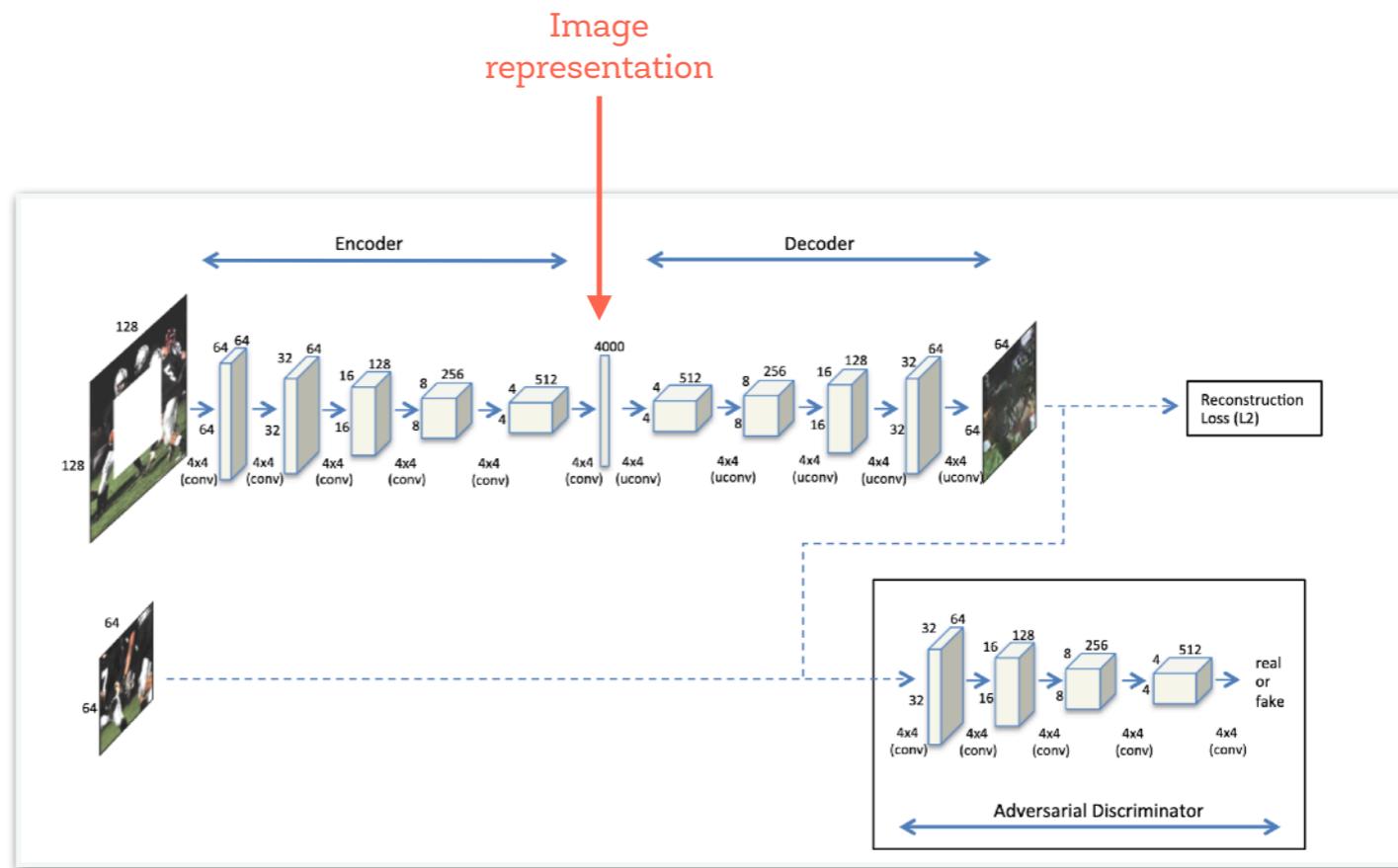
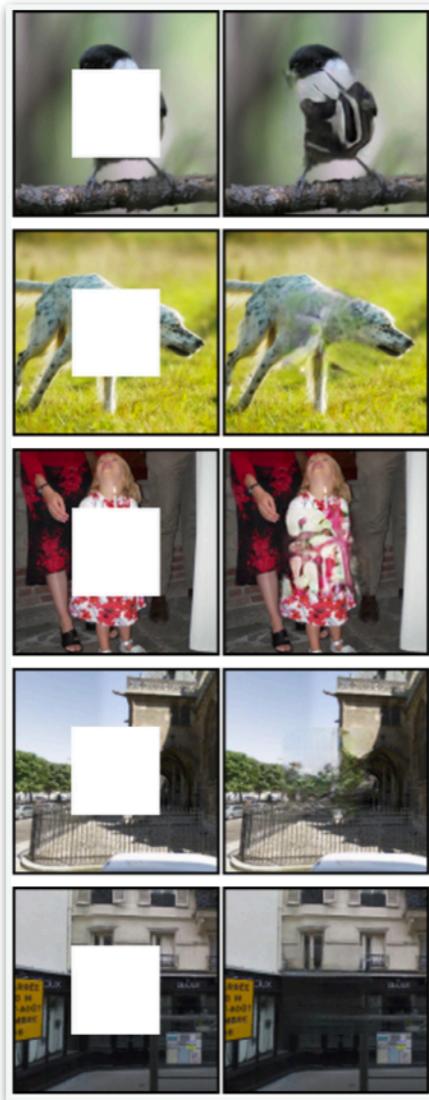
Many ideas have been proposed for self-supervised representation learning on **images**.

A common workflow is to train a model on one or multiple auxiliary tasks with unlabelled images and then **use one intermediate feature layer of this model** (usually, the output of the last convolutional layer) **to feed** a multinomial logistic regression classifier on image classification.

The final classification accuracy quantifies how good the learned representation is.

Image-based Self-Supervised Learning

Patch Inpainting



<https://arxiv.org/pdf/1604.07379.pdf>

Image-based Self-Supervised Learning

Distortion (or how to enrich a label with a surrogate task)

1. Sample N patches of size 32×32 pixels from different images at varying positions and scales, only from regions containing considerable gradients as those areas cover edges and tend to contain objects or parts of objects. They are “**exemplary**” patches.
2. Each patch is distorted by applying a variety of random transformations (i.e., translation, rotation, scaling, etc.). All the resulting distorted patches are considered to belong to the same surrogate class.
3. The pretext task is to discriminate between a set of surrogate classes. We can arbitrarily create as many surrogate classes as we want.

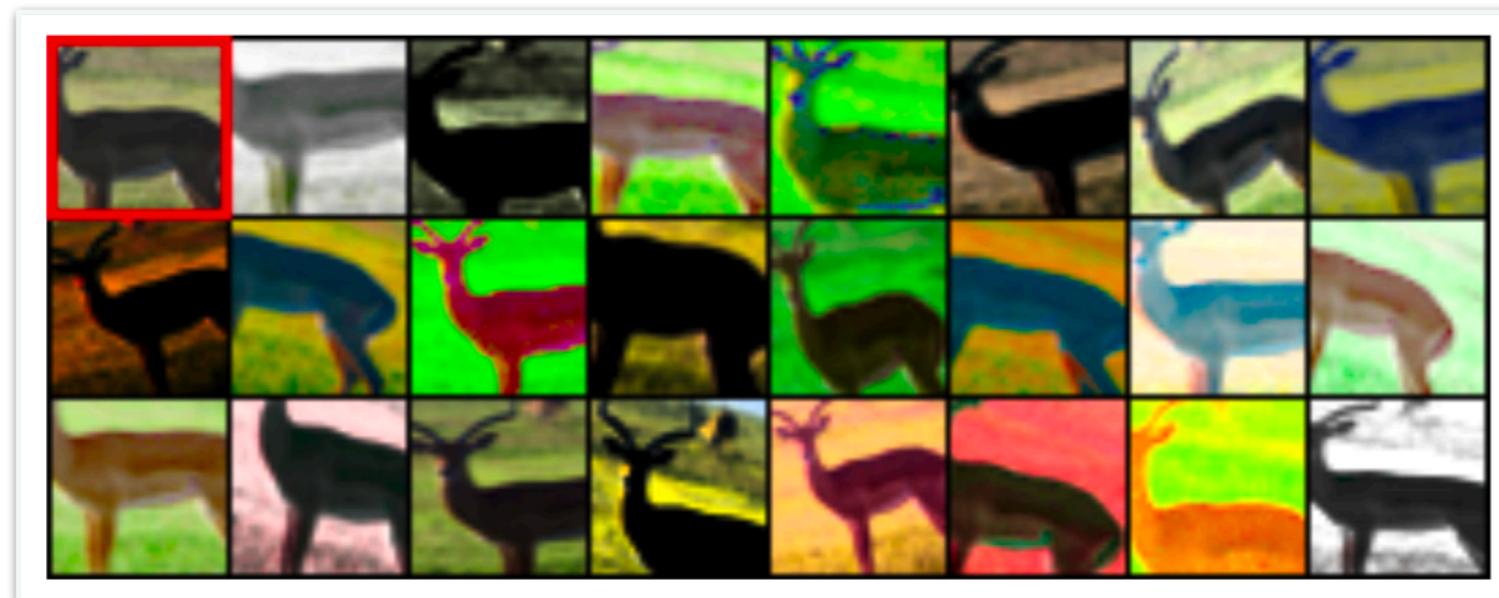
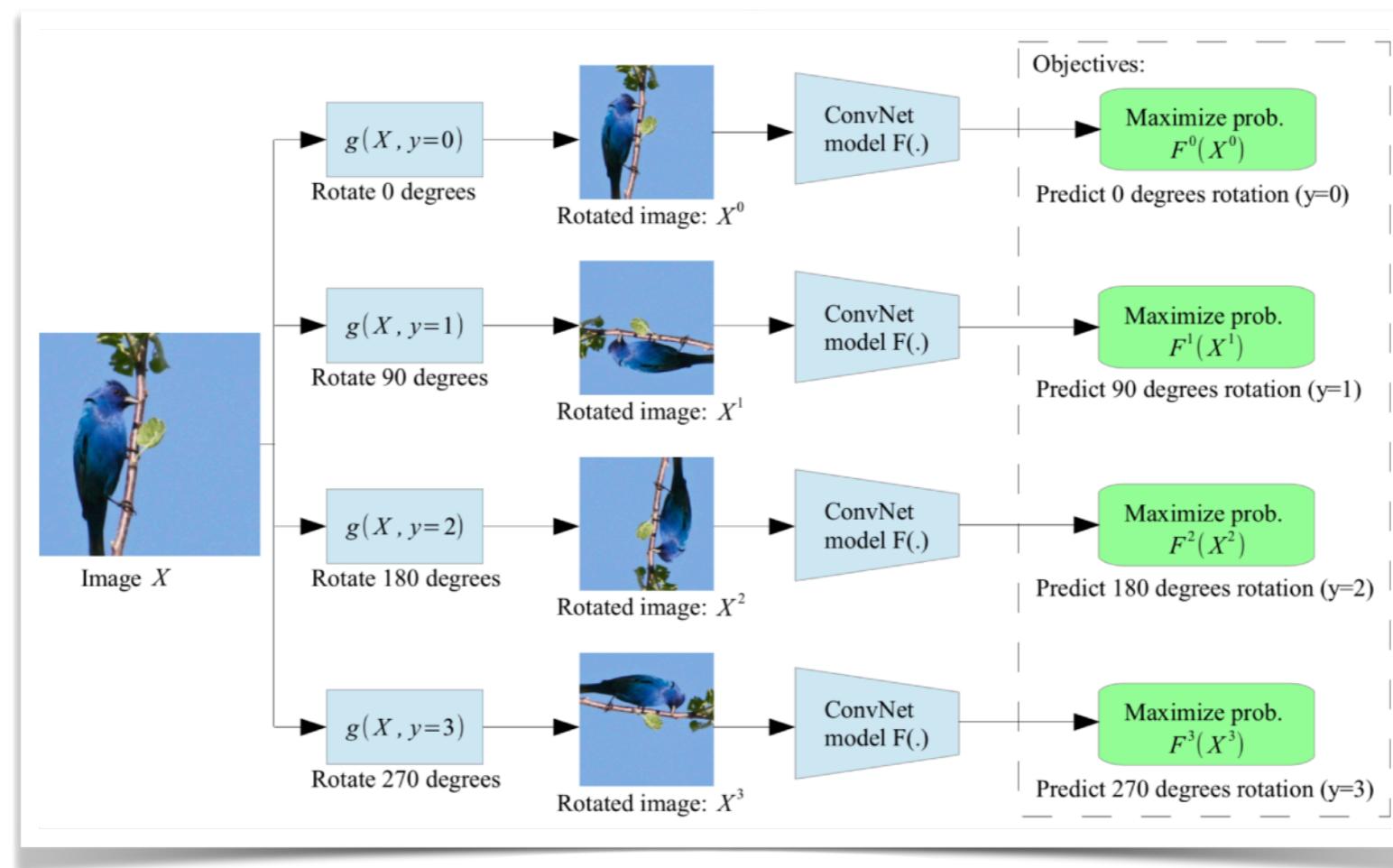


Image-based Self-Supervised Learning

Rotation

Each input image is first rotated by a multiple of 90 degrees 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**.



In order to identify the same image with different rotations, **the model has to learn to recognize high level object parts**, such as heads, noses, and eyes, and the relative positions of these parts, rather than local patterns.

Image-based Self-Supervised Learning

Patch positions

Predicting the **relative position** between two random patches from one image. A model needs to understand the spatial context of objects in order to tell the relative position between parts.

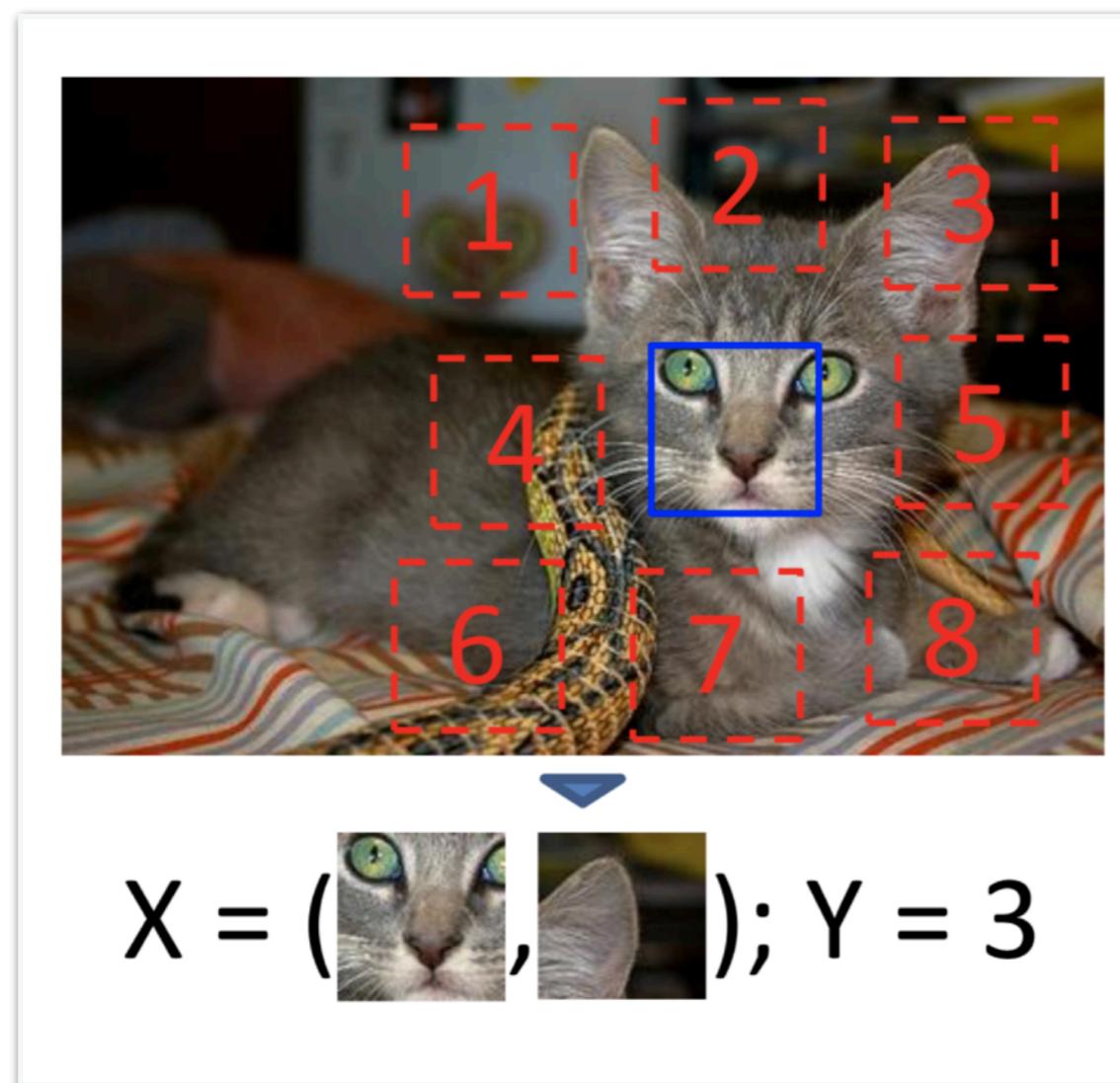


Image-based Self-Supervised Learning

Patch positions

The training patches are sampled in the following way:

1. Randomly sample the first patch without any reference to image content.
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. To avoid the model only catching **low-level trivial signals**, such as connecting a straight line across boundary or matching local patterns, additional noise is introduced by:
 - Add gaps between patches
 - Small jitters
 - Randomly downsample some patches to as little as 100 total pixels, and then upsampling it, to build robustness to pixelation.
 - **Shift green and magenta toward gray or randomly drop 2 of 3 color channels.**

Chromatic Aberration

Confounder

Image-based Self-Supervised Learning

Chromatic Aberration

Other than trivial signals like boundary patterns or textures continuing, another interesting and a bit surprising, **unexpected**, trivial solution was found, called “**chromatic aberration**”.

It is triggered by different focal lengths of lights at different wavelengths passing through the lens. In the process, there might exist **small offsets between color channels that depend on the shape of the lens**.

Hence, the model can learn to tell the relative position by simply comparing how green and magenta are separated differently in two patches. This is a trivial solution and has nothing to do with the image content.

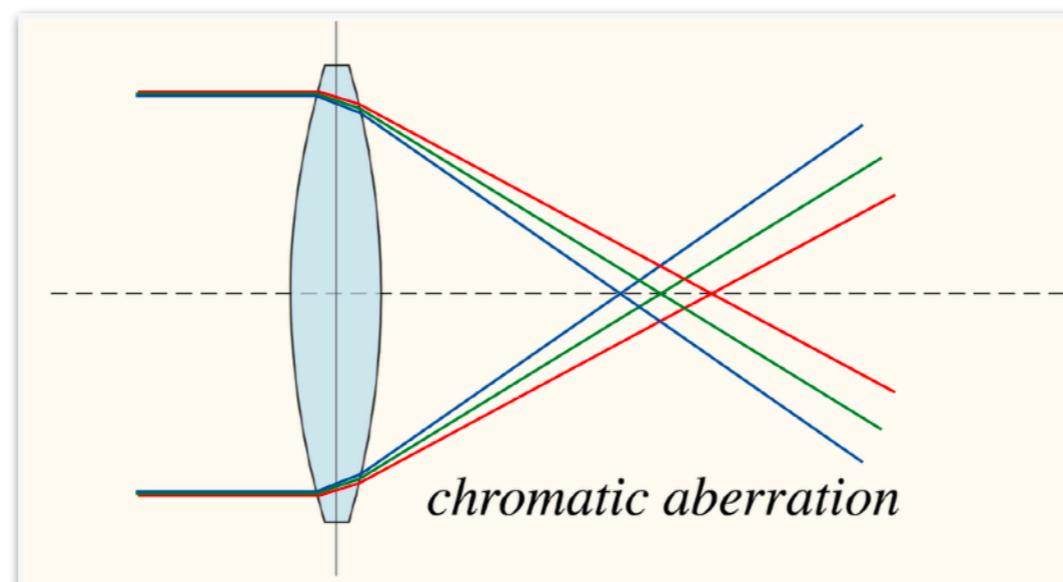


Image-based Self-Supervised Learning

Jigsaw puzzle

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

A convolutional network processes each patch independently with **shared weights** and outputs a probability vector per patch index out of a predefined set of permutations.

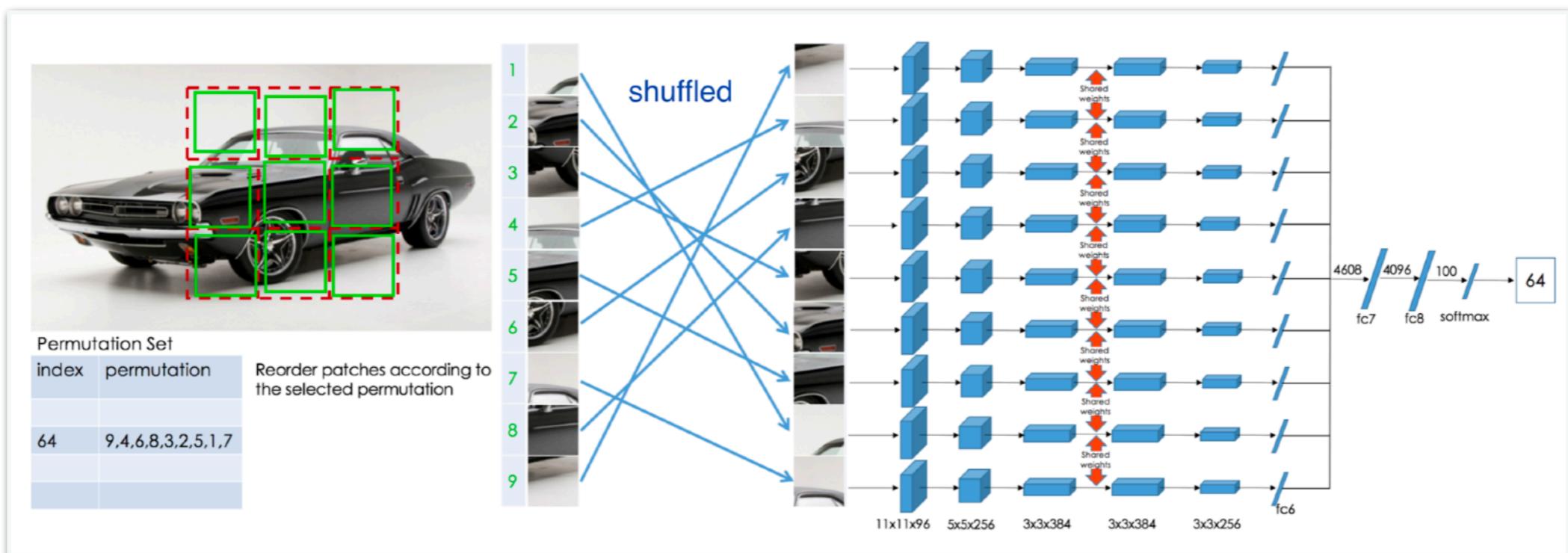


Image-based Self-Supervised Learning

Colorization

Colorization can be used as a powerful self-supervised task: a model is trained to color a grayscale input image; precisely the task is to map this image to a distribution over quantized color value outputs

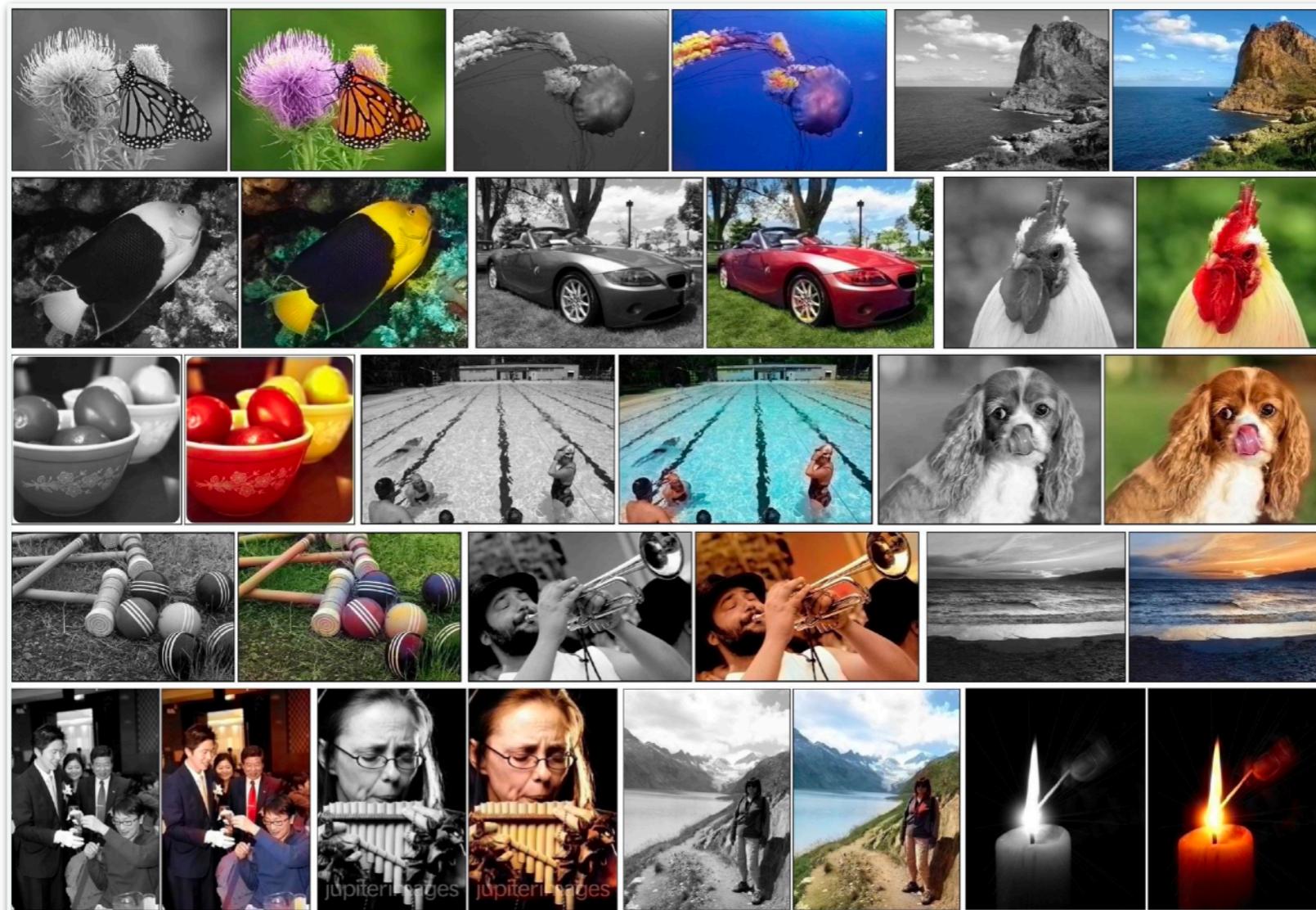


Image-based Self-Supervised Learning

Colorization

```
model = Sequential()
model.add(InputLayer(input_shape=(None, None, 1)))
model.add(Conv2D(8, (3, 3), activation='relu', padding='same', strides=2))
model.add(Conv2D(16, (3, 3), activation='relu', padding='same'))
model.add(Conv2D(16, (3, 3), activation='relu', padding='same', strides=2))
model.add(Conv2D(32, (3, 3), activation='relu', padding='same'))
model.add(Conv2D(32, (3, 3), activation='relu', padding='same', strides=2))
model.add(UpSampling2D((2, 2)))
model.add(Conv2D(32, (3, 3), activation='relu', padding='same'))
model.add(UpSampling2D((2, 2)))
model.add(Conv2D(16, (3, 3), activation='relu', padding='same'))
model.add(UpSampling2D((2, 2)))
model.add(Conv2D(2, (3,3), activation='tanh', padding='same'))
```

Main limitation: it's deterministic.
We would like a probabilistic output!

Contrastive Methods

Contrastive Methods

Contrastive methods, as the name implies, learn **representations** by contrasting **positive** and **negative** examples.

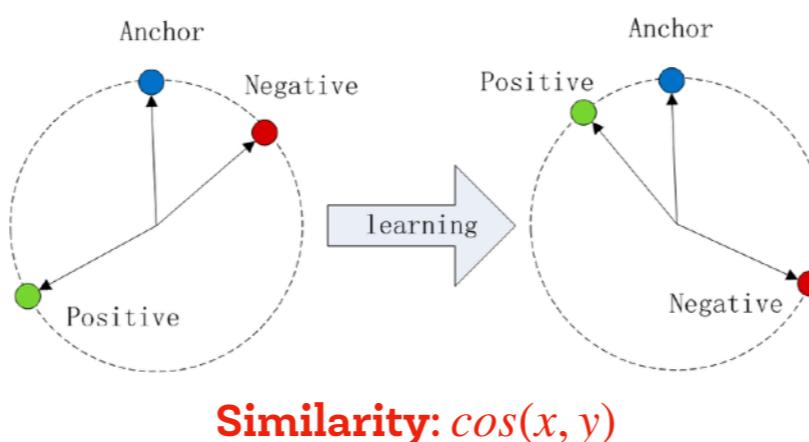
- Contrastive methods trained on unlabelled image data and evaluated with a linear classifier now surpass the accuracy of supervised AlexNet.
- **Contrastive pre-training on images successfully transfers to other downstream tasks and outperforms the supervised pre-training counterparts.**

Contrastive Methods

More formally, for any data point x , contrastive methods aim to learn an **encoder** f such that: $\text{sim}(f(x), f(x^+)) >> \text{sim}(f(x), f(x^-))$

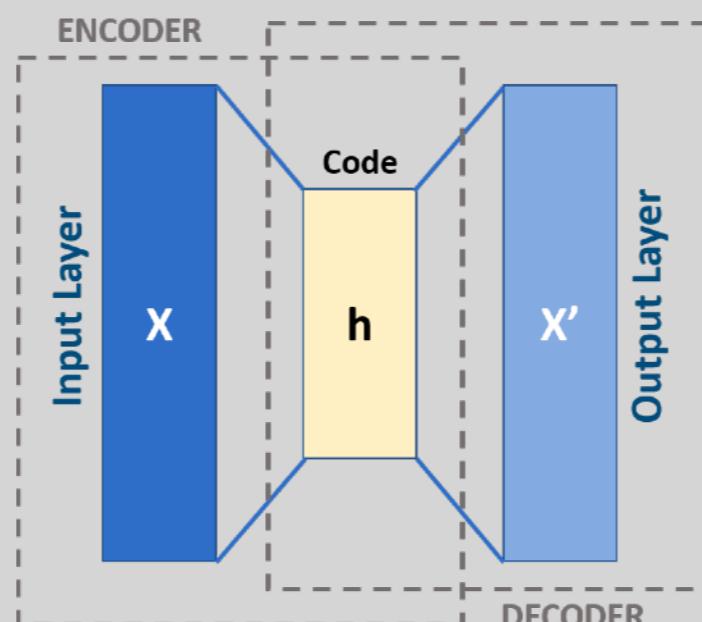
- here x^+ is data point **similar** or **congruent** to x , referred to as a **positive** sample.
- x^- is a data point **dissimilar** to x , referred to as a **negative** sample.
- the sim function is a metric that measures the similarity between two features.

x is commonly referred to as an “**anchor**” data point.



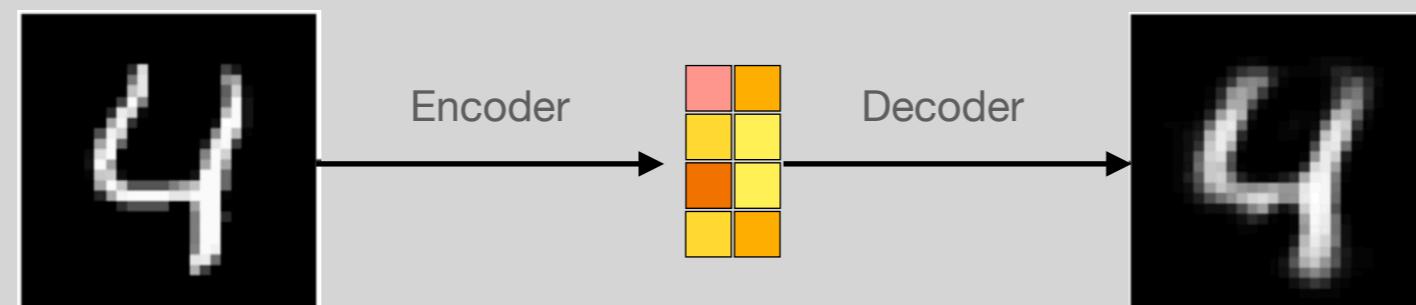
What is an encoder?

An **autoencoder** is a neural network that learns to copy its input to its output. It has an internal (hidden) layer that describes a (low dimensional) **code** used to represent the input, and it is constituted by two main parts: an **encoder** that maps the input into the code, and a **decoder** that maps the code to a reconstruction of the original input.

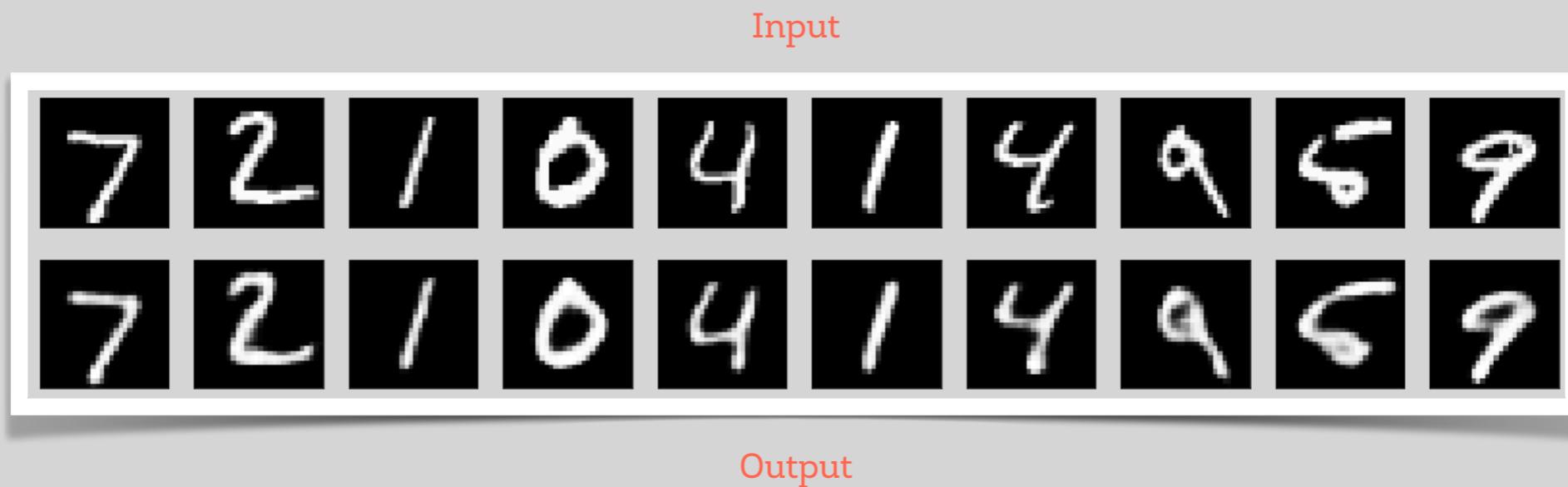


To build an autoencoder we need 3 things: an encoding method, decoding method, and a loss function to compare the output with the target.

<https://en.wikipedia.org/wiki/Autoencoder>



What is an encoder?



What is an encoder?

784 dimensions

```
1 input_img = tf.keras.layers.Input(shape=(28, 28, 1))
2
3 x = tf.keras.layers.Conv2D(16, (3, 3), activation='relu', padding='same')(input_img)
4 x = tf.keras.layers.MaxPooling2D((2, 2), padding='same')(x)
5 x = tf.keras.layers.Conv2D(8, (3, 3), activation='relu', padding='same')(x)
6 x = tf.keras.layers.MaxPooling2D((2, 2), padding='same')(x)
7 x = tf.keras.layers.Conv2D(8, (3, 3), activation='relu', padding='same')(x)
8 encoded = tf.keras.layers.MaxPooling2D((2, 2), padding='same')(x)
9
10 # at this point the representation is (4, 4, 8) i.e. 128-dimensional    128 dimensions
11
12 x = tf.keras.layers.Conv2D(8, (3, 3), activation='relu', padding='same')(encoded)
13 x = tf.keras.layers.UpSampling2D((2, 2))(x)    No parameters
14 x = tf.keras.layers.Conv2D(8, (3, 3), activation='relu', padding='same')(x)
15 x = tf.keras.layers.UpSampling2D((2, 2))(x)
16 x = tf.keras.layers.Conv2D(16, (3, 3), activation='relu')(x)
17 x = tf.keras.layers.UpSampling2D((2, 2))(x)
18 decoded = tf.keras.layers.Conv2D(1, (3, 3), activation='sigmoid', padding='same')(x)
19
20 autoencoder = tf.keras.models.Model(input_img, decoded)
21 autoencoder.compile(optimizer='adam', loss='binary_crossentropy')
```

784 dimensions
Almost binary image

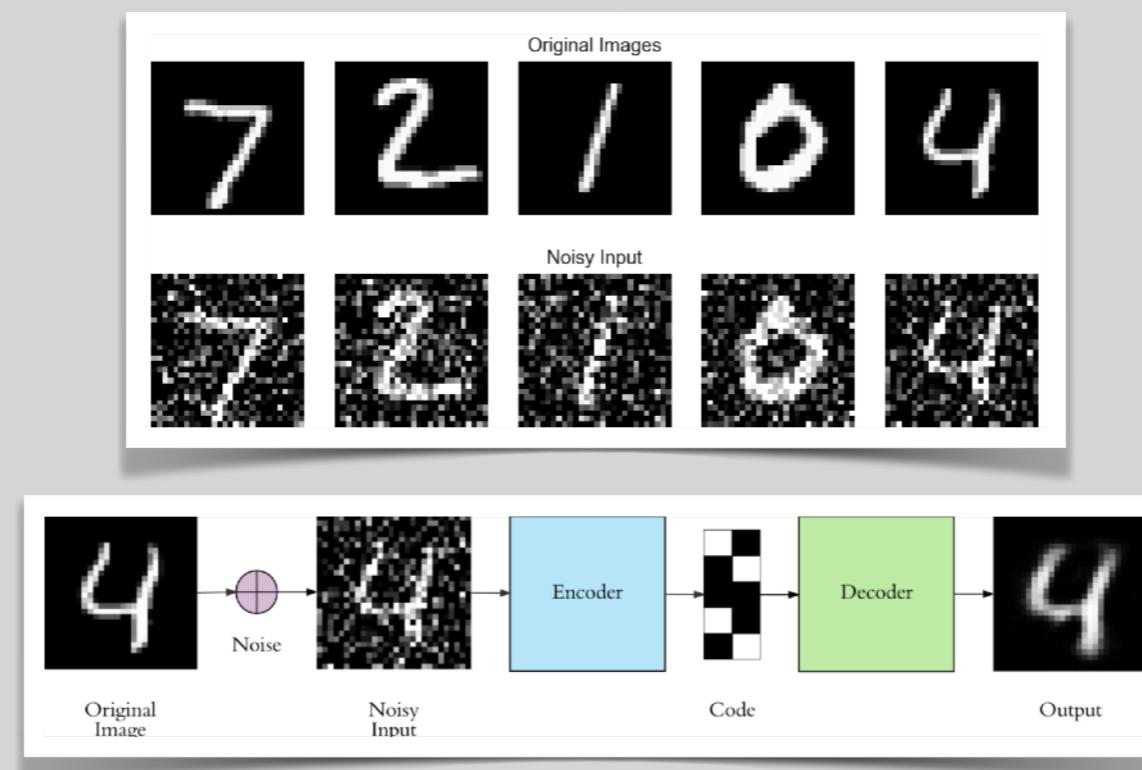


What is an encoder?

Keeping the **code layer small** forces the autoencoder to learn an intelligent representation of the data.

There is another way to force the autoencoder to learn useful features, which is adding **random noise** to its inputs and making it recover the original noise-free data.

This way the autoencoder can't simply copy the input to its output because the input also contains random noise. We are asking it to subtract the noise and produce the underlying meaningful data. This is called a **denoising autoencoder**.



Contrastive Methods

Contrastive learning is to learn a metric space between two samples in which the distance (score) between two positive samples is reduced while the distance between two negative samples is enlarged.

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

Same Class Different Class

In early versions of **loss functions** for contrastive learning, only one positive and one negative sample are involved. The trend in recent training objectives is to include multiple positive and negative pairs in one batch.

Triplet Loss

Given one anchor input \mathbf{x} , we select one positive sample \mathbf{x}^+ and one negative \mathbf{x}^- . Triplet loss learns to minimize the distance between the anchor \mathbf{x} and positive \mathbf{x}^+ and maximize the distance between the anchor \mathbf{x} and negative \mathbf{x}^- at the same time with the following equation:

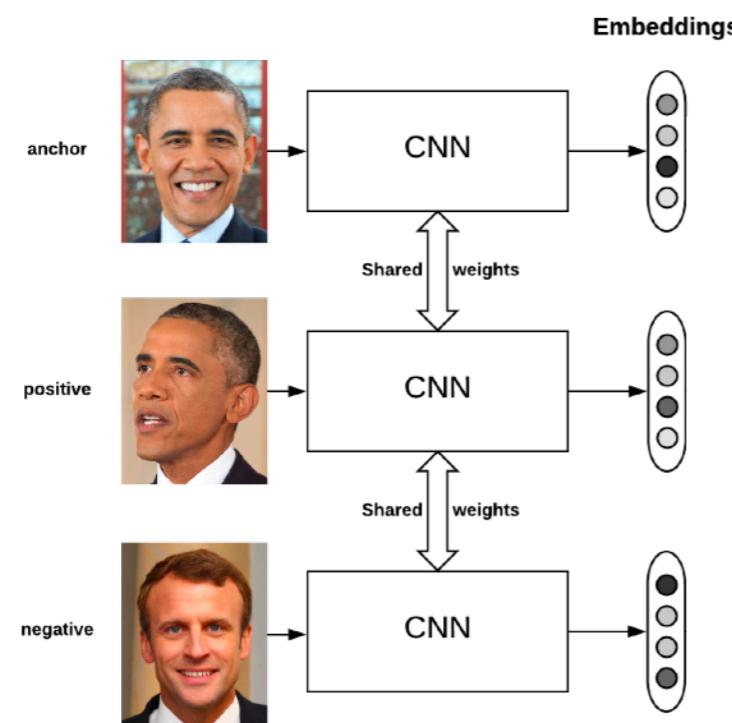
$$\mathcal{L}_{\text{triplet}}(\mathbf{x}, \mathbf{x}^+, \mathbf{x}^-) = \sum_{\mathbf{x} \in \mathcal{X}} \max \left(0, \|f(\mathbf{x}) - f(\mathbf{x}^+)\|_2^2 - \|f(\mathbf{x}) - f(\mathbf{x}^-)\|_2^2 + \epsilon \right)$$

where the margin parameter ϵ is configured as the minimum offset between distances of similar vs dissimilar pairs.

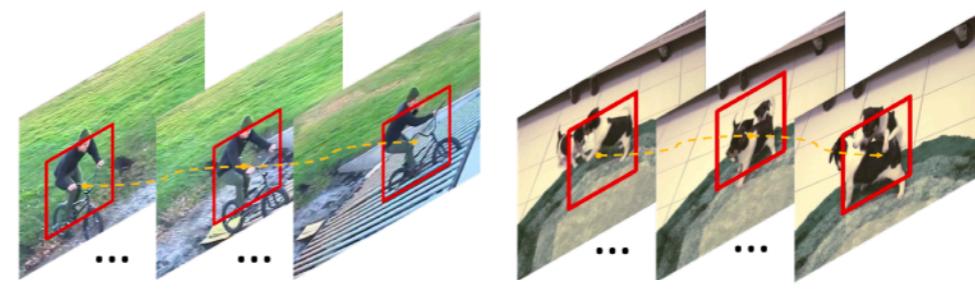
It is crucial to select challenging \mathbf{x}^- to truly improve the model.

Contrastive Methods

Positive and negative examples can be built by relying in known classes, but we can also use self-supervised signals (data augmentation, time, etc.)



Class-based contrastive method

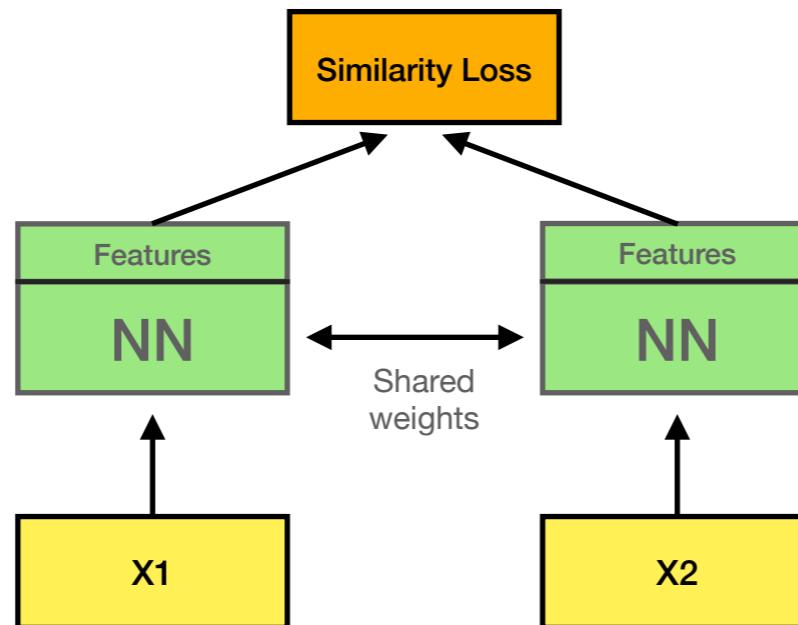


$$D \left(\begin{matrix} \text{[region from person]} \\ \text{[region from dog]} \end{matrix}, \begin{matrix} \text{[region from person]} \\ \text{[region from dog]} \end{matrix} \right) < D \left(\begin{matrix} \text{[region from person]} \\ \text{[region from dog]} \end{matrix}, \begin{matrix} \text{[region from person]} \\ \text{[region from dog]} \end{matrix} \right)$$

Self-supervised contrastive method

Contrastive Loss

One of the firsts contrastive models were **siamese networks**.

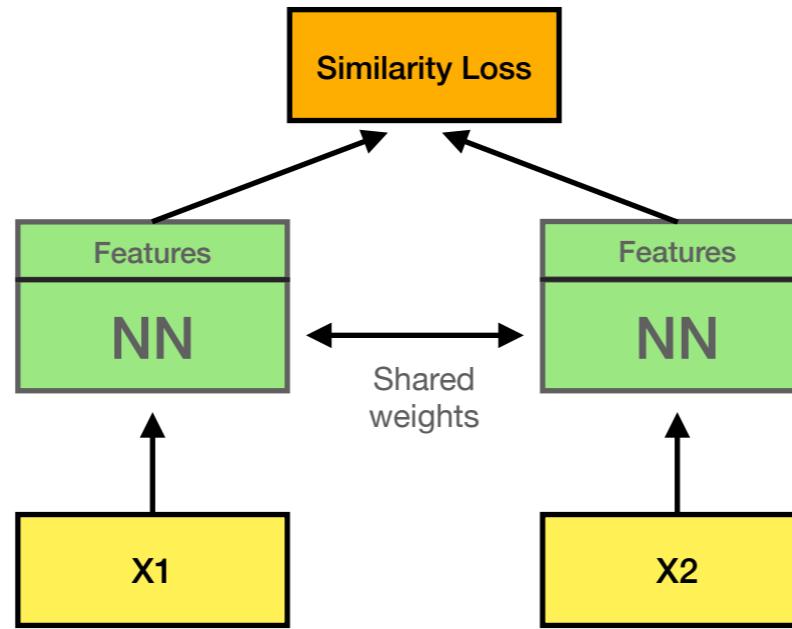


A siamese network is often shown as two different encoding networks that share weights, but in reality the same network is just used twice before doing backpropagation.



Contrastive Loss

One of the firsts contrastive models were **siamese networks**.

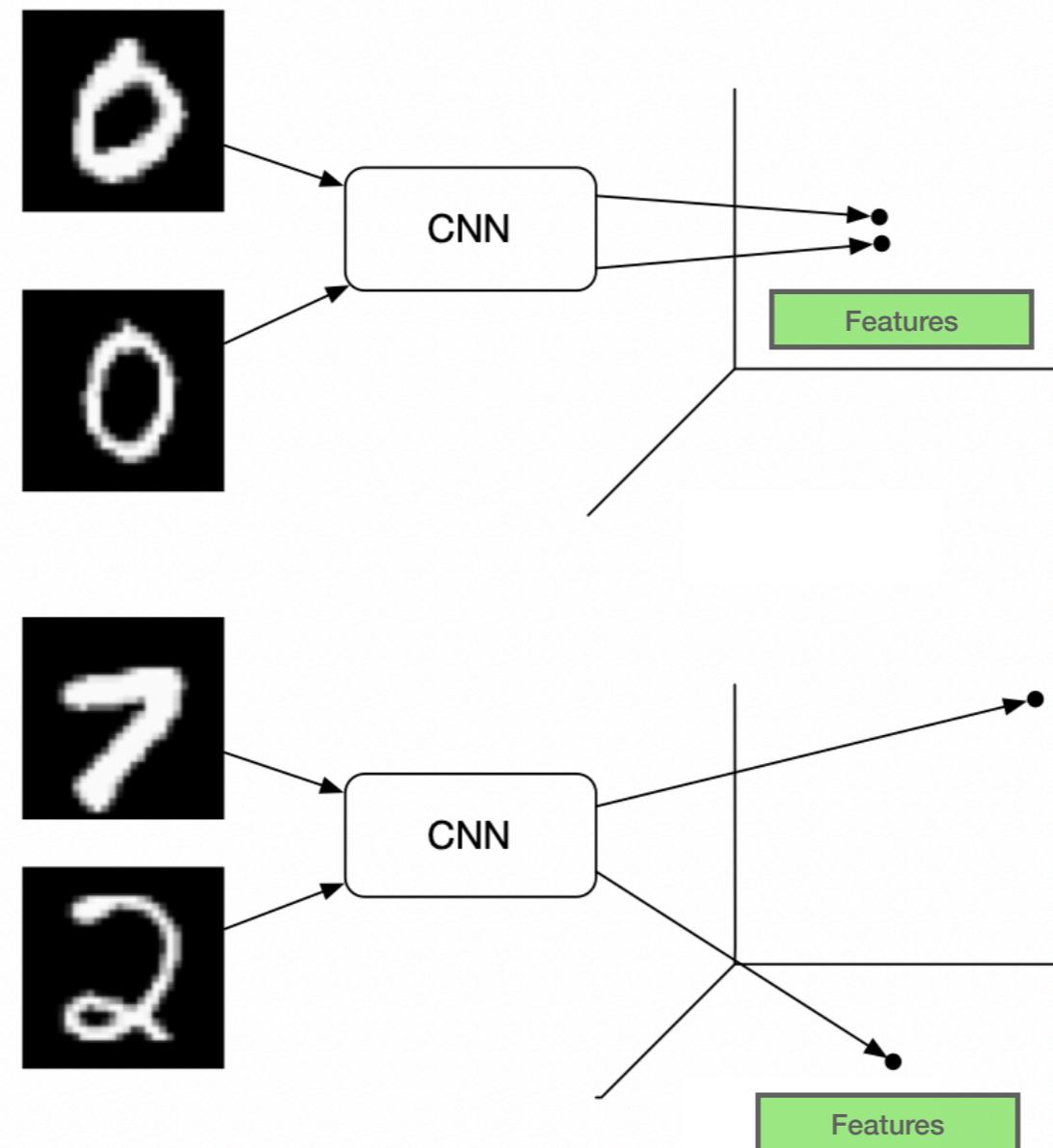


A siamese network is often shown as two different encoding networks that share weights, but in reality the same network is just used twice before doing backpropagation.

When training a siamese network, 2 or more inputs are encoded and the output features are compared. This comparison can be done in a number of ways, for example, the **pairwise ranking loss**:

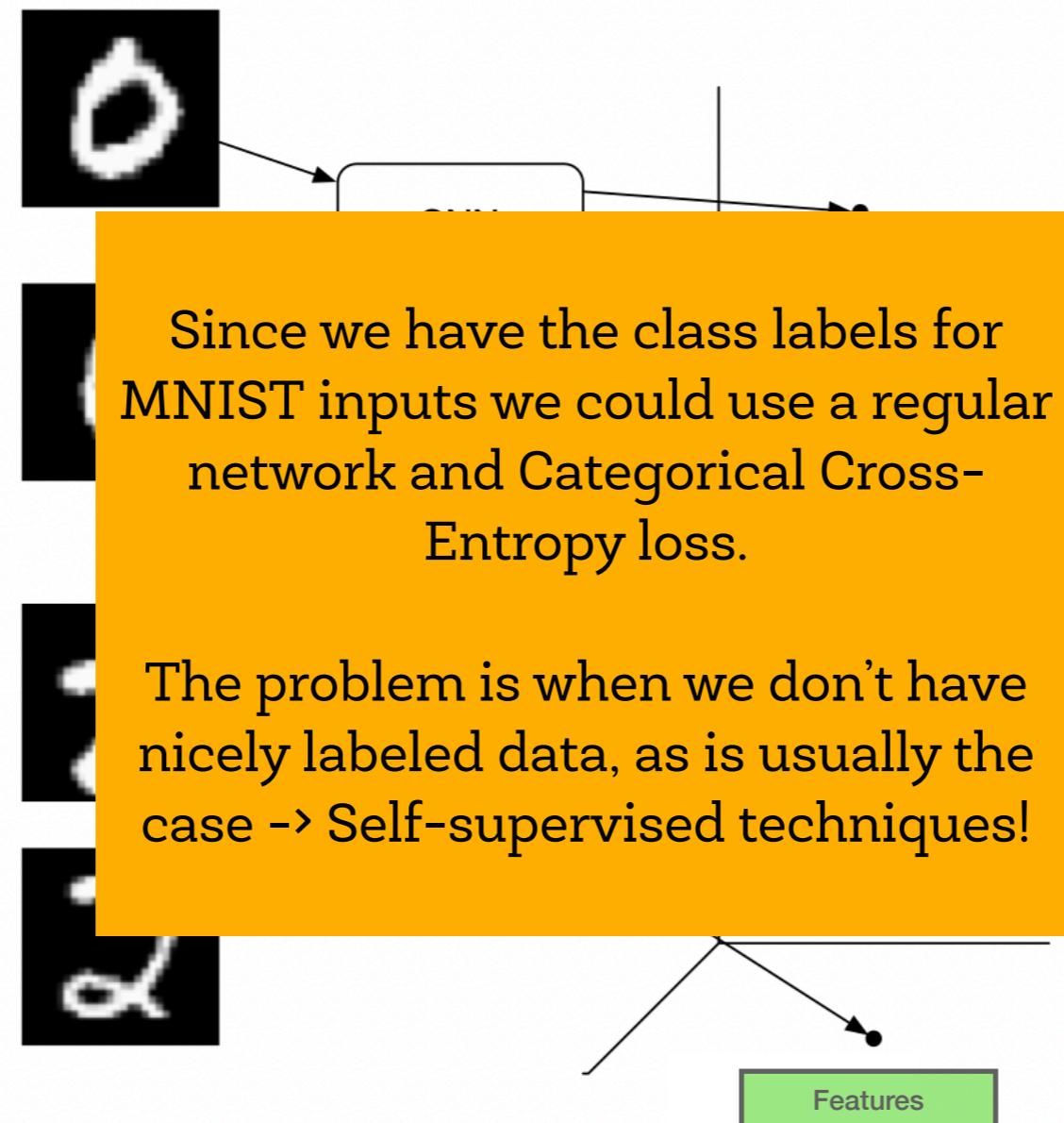
$$L(x_0, x_1, y) = y \left\| f(x_0) - f(x_1) \right\| + (1 - y) \max(0, m - \left\| f(x_0) - f(x_1) \right\|)$$

Contrastive Loss



Let's look at an example where we want to make features out of MNIST numbers. **Each image of an MNIST number should encode into a vector** that is close to vectors from images of the same class. Conversely different numbers should encode into vectors that are far from each other.

Contrastive Loss



Let's look at an example where we want to make features out of MNIST numbers. **Each image of an MNIST number should encode into a vector** that is close to vectors from images of the same class. Conversely different numbers should encode into vectors that are far from each other.

Siamese Networks

```
1
2 def loss(margin=1):
3     """Provides 'contrastive_loss' an enclosing scope with variable 'margin'.
4
5     Arguments:
6         margin: Integer, defines the baseline for distance for which pairs
7                 should be classified as dissimilar. - (default is 1).
8
9     Returns:
10        'contrastive_loss' function with data ('margin') attached.
11    """
12
13    # Contrastive loss = mean( (1-true_value) * square(prediction) +
14    #                           true_value * square( max(margin-prediction, 0) ))
15    def contrastive_loss(y_true, y_pred):
16        """Calculates the contrastive loss.
17
18        Arguments:
19            y_true: List of labels, each label is of type float32.
20            y_pred: List of predictions of same length as of y_true,
21                    each label is of type float32.
22
23        Returns:
24            A tensor containing contrastive loss as floating point value.
25        """
26
27        square_pred = tf.math.square(y_pred)
28        margin_square = tf.math.square(tf.math.maximum(margin - (y_pred), 0))
29        return tf.math.reduce_mean(
30            (1 - y_true) * square_pred + (y_true) * margin_square
31        )
32
33    return contrastive_loss
34
```

