



UNIVERSITY OF TECHNOLOGY
IN THE EUROPEAN CAPITAL OF CULTURE
CHEMNITZ

Neurocomputing

Autoencoders

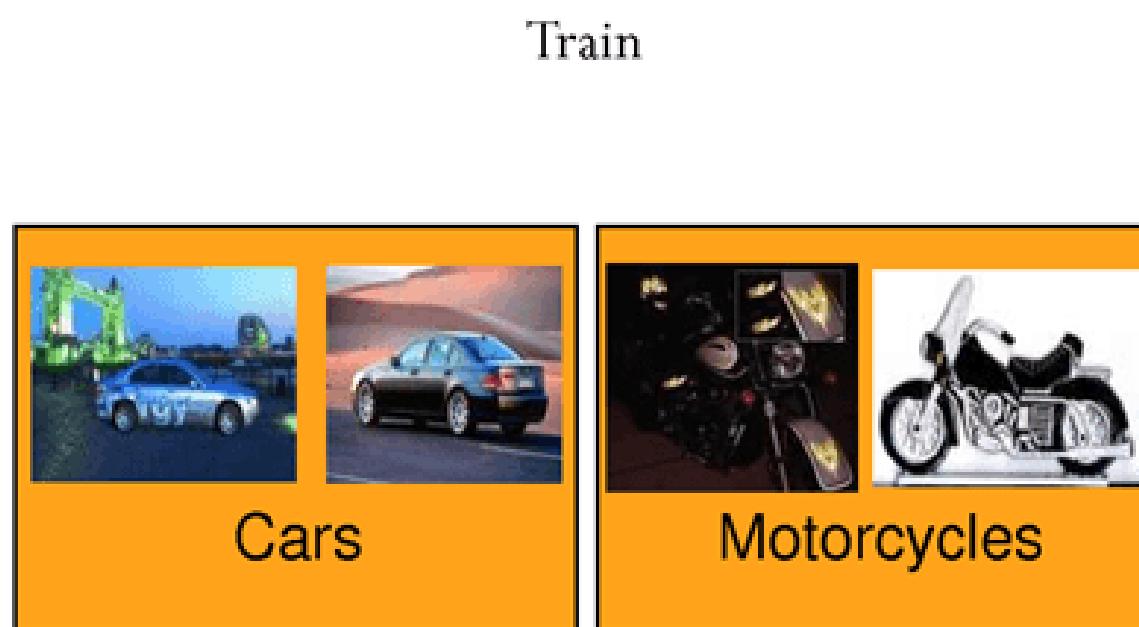
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1 - Autoencoders

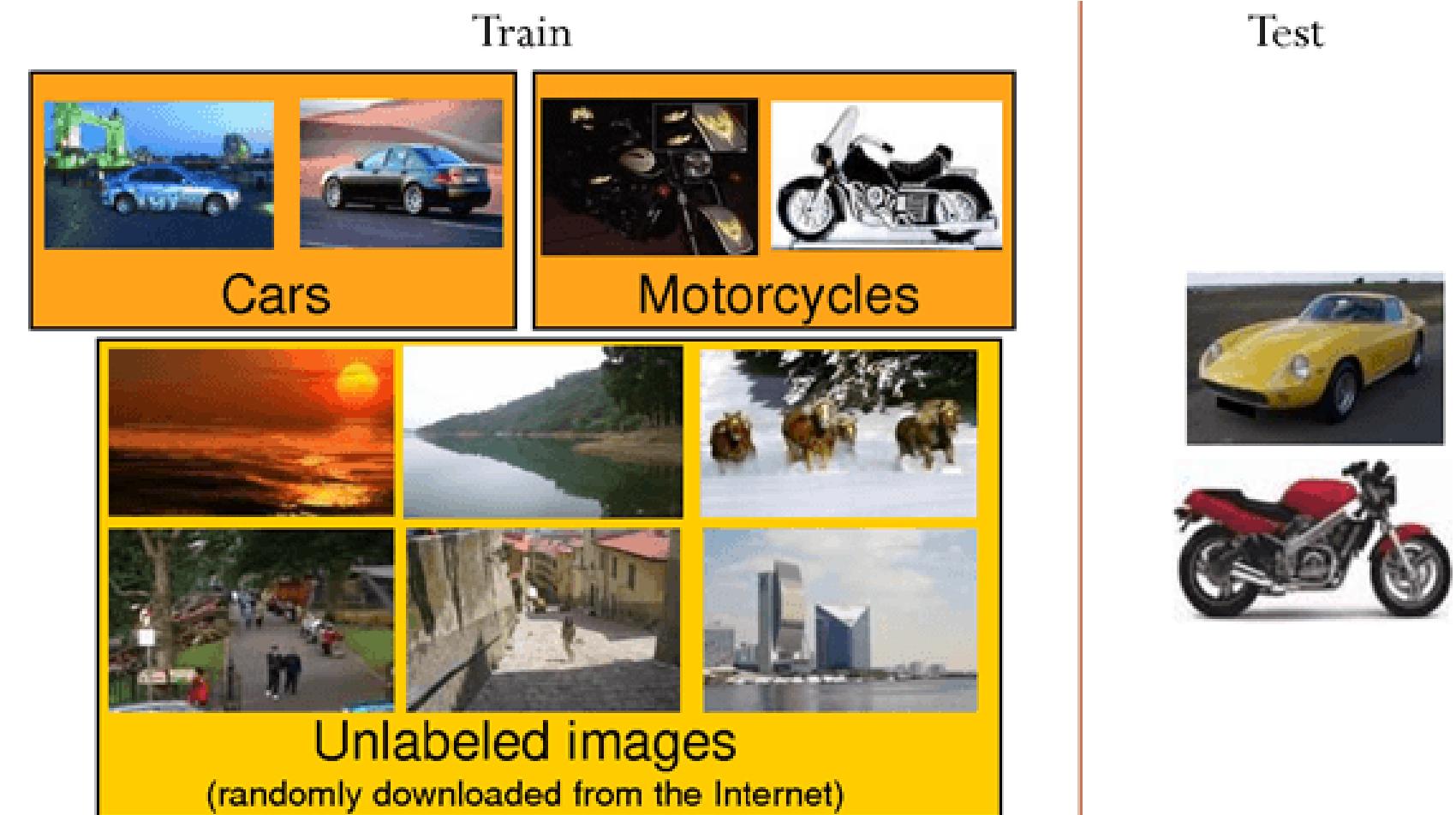
Labeled vs unlabeled data

- **Supervised learning** algorithms need a lot of labeled data (with t) in order to learn classification/regression tasks, but labeled data is very expensive to obtain (experts, crowd sourcing).
- A “bad” algorithm trained with a lot of data will perform better than a “good” algorithm trained with few data. *“It is not who has the best algorithm who wins, it is who has the most data.”*

Supervised learning



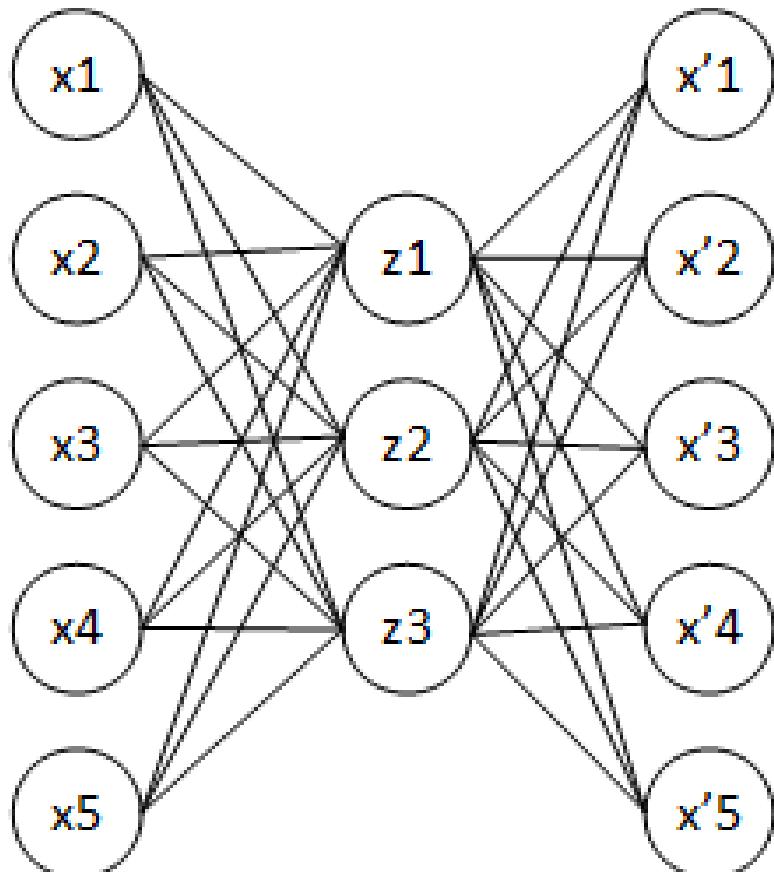
Self-taught learning



- Unlabeled data is only useful for **unsupervised learning**, but very cheap to obtain (camera, microphone, search engines). Can we combine efficiently both approaches? **Self-taught learning** or **semi-supervised learning**.

Autoencoders

- An **autoencoder** is a NN trying to learn the identity function $f(\mathbf{x}) = \mathbf{x}$ using a different number of neurons in the hidden layer than in the input layer.



- An autoencoder minimizes the **reconstruction loss** between the input \mathbf{x} and the reconstruction \mathbf{x}' , for example the mse between the two vectors:

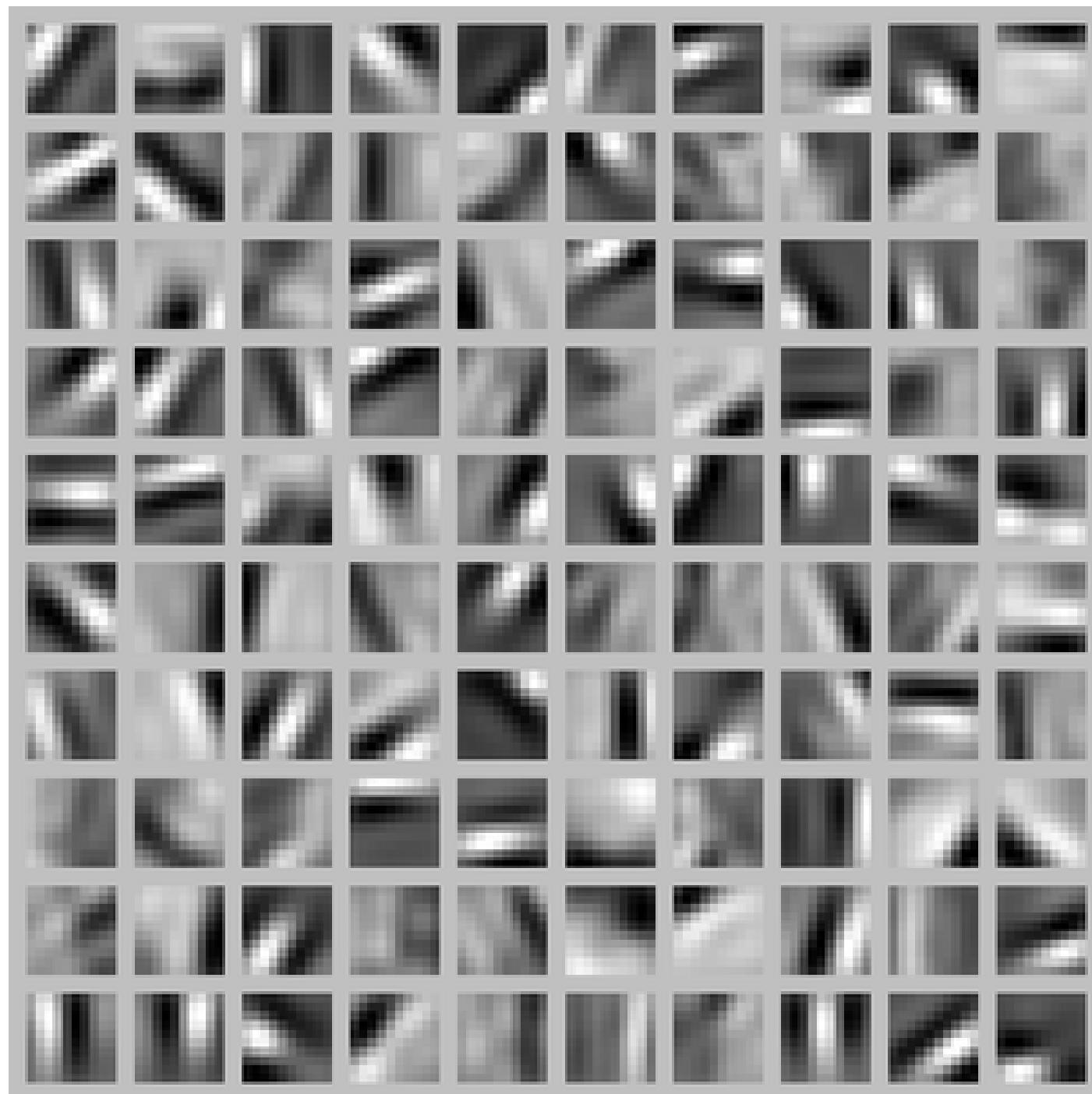
$$\mathcal{L}_{\text{reconstruction}}(\theta) = \mathbb{E}_{\mathbf{x} \in \mathcal{D}}[||\mathbf{x}' - \mathbf{x}||^2]$$

- An autoencoder uses **unsupervised learning**: the output data used for learning is the same as the input data.
 - No need for labels!

- By forcing the projection of the input data on a feature space with less dimensions (**latent space**), the network has to extract relevant **features** from the training data.
 - Dimensionality reduction, compression.

Result of training a sparse autoencoder on natural images

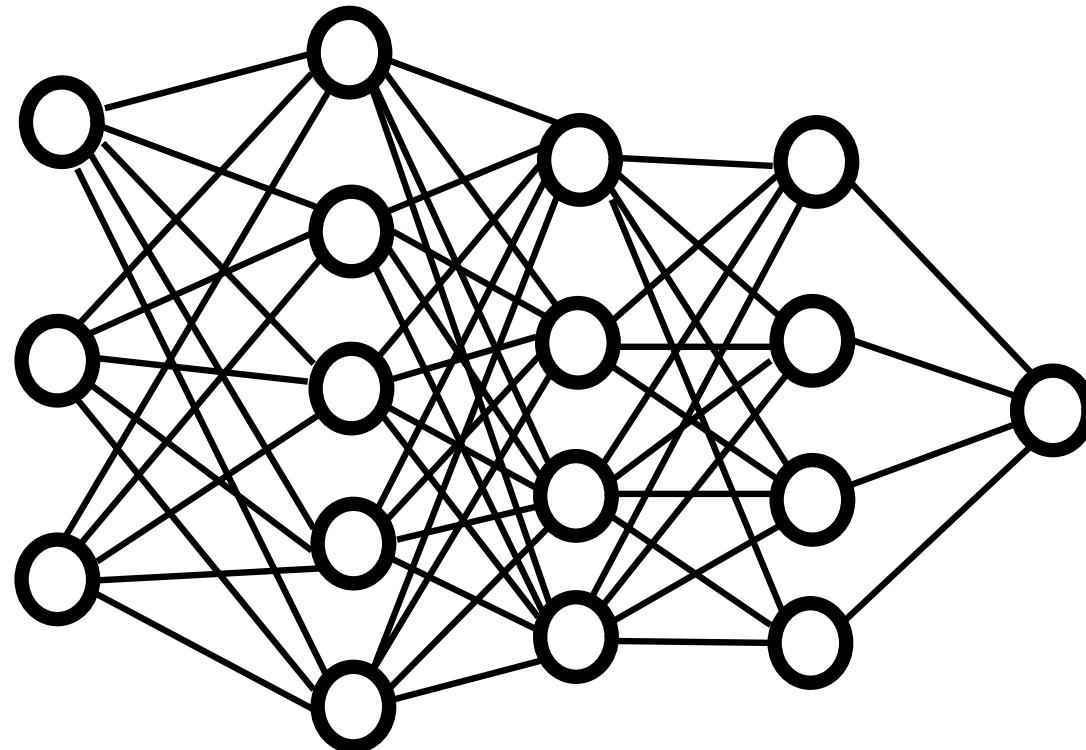
- If the latent space has more dimensions than the input space, we need to **constrain** the autoencoder so that it does not simply learn the identity mapping.
- Below is an example of a sparse autoencoder trained on natural images.



- Inputs are taken from random natural images and cut in 10×10 patches.
- 100 features are extracted in the hidden layer.
- The autoencoder is said **sparse** because it uses **L1-regularization** to make sure that only a few neurons are active in the hidden layer for a particular image.
- The learned features look like what the first layer of a CNN would learn, except that there was no labels at all!
- Can we take advantage of this to pre-train a supervised network?

2 - Stacked autoencoders

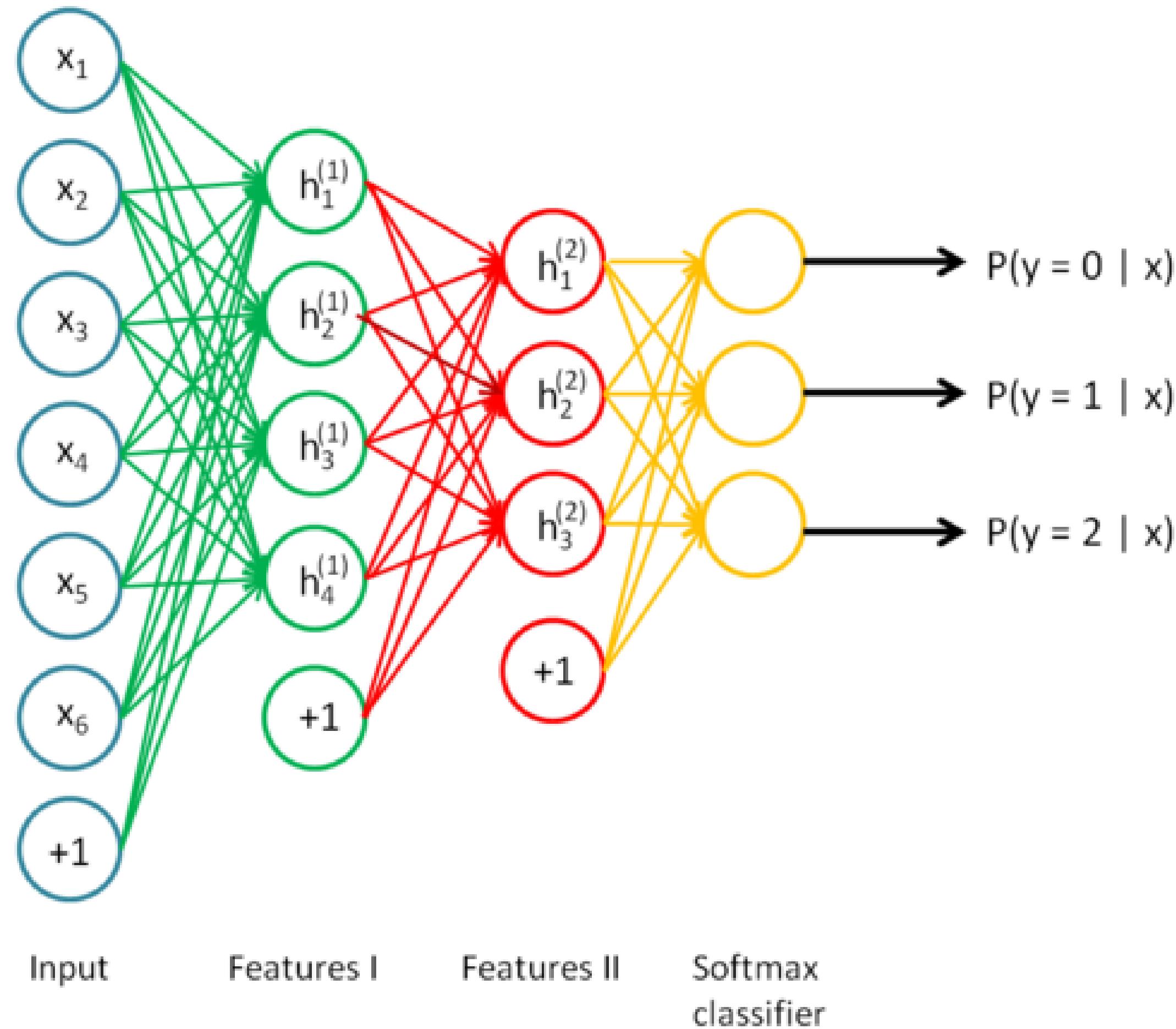
Using an autoencoder for supervised learning



- In supervised learning, deep neural networks suffer from many problems:
 - Local minima
 - Vanishing gradients
 - Long training times
- All these problems are due to the fact that the weights are randomly initialized at the beginning of training.
- **Pretraining** the weights using unsupervised learning allows to start already close to a good solution:
 - the network will need less steps to converge.
 - the gradients will vanish less.
 - less data is needed to learn a particular supervised task.

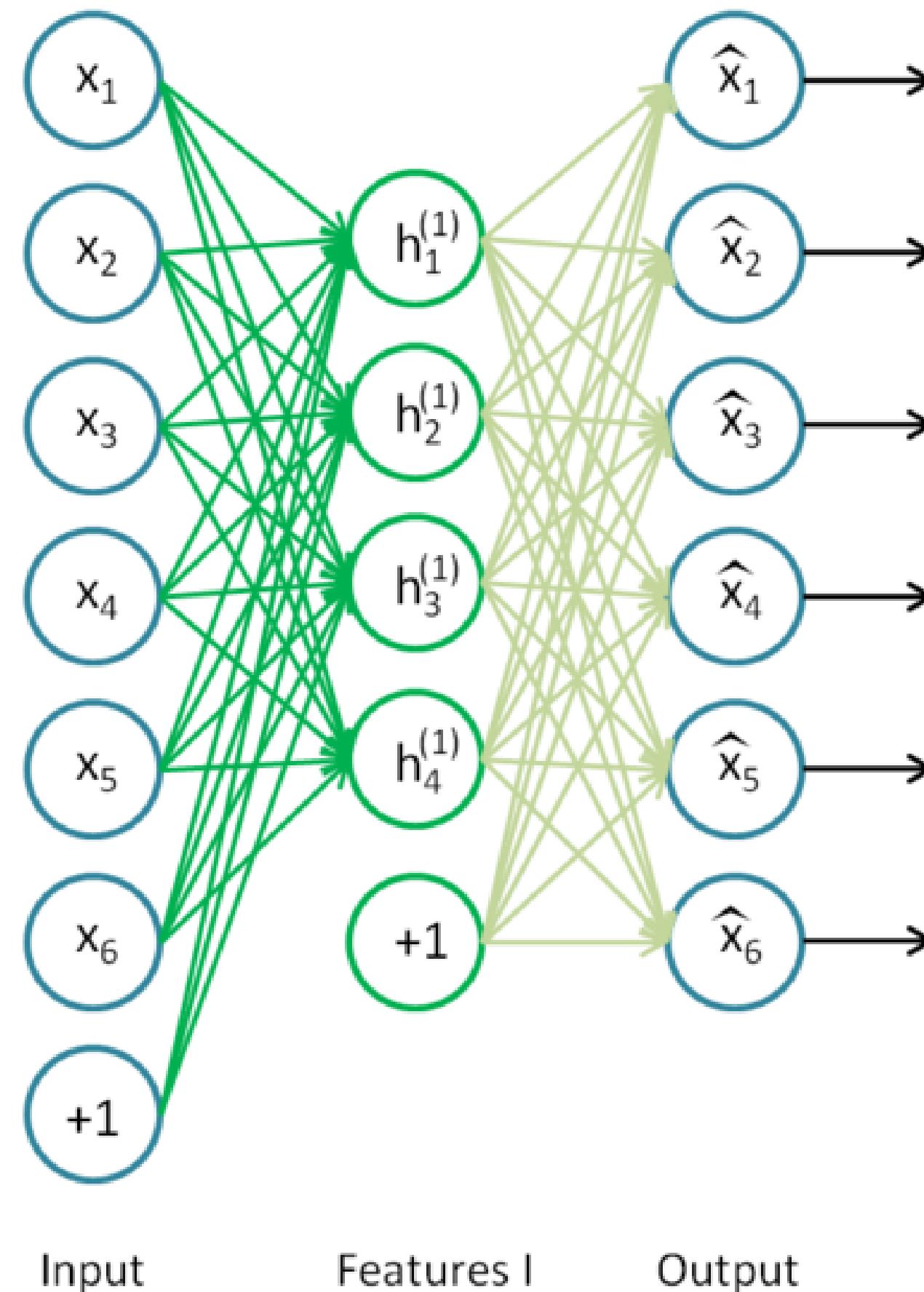
Stacked autoencoders

- Let's try to learn a **stacked autoencoder** by learning *progressively* each feature vector.



Stacked autoencoders

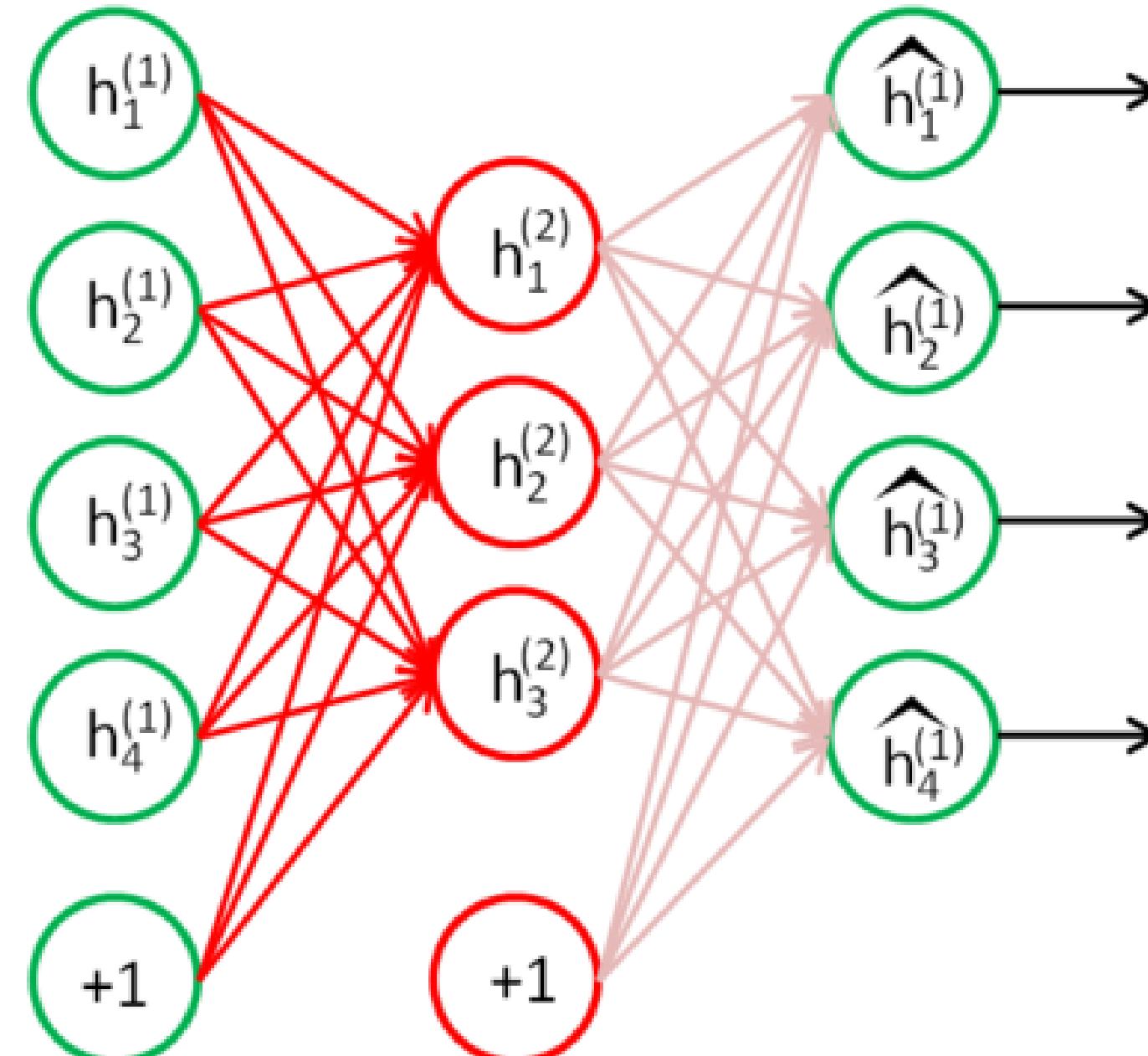
- Using unlabeled data, train an autoencoder to extract first-order features, freeze the weights and remove the decoder.



http://ufldl.stanford.edu/wiki/index.php/Stacked_Autoencoders

Stacked autoencoders

- Train another autoencoder on the same unlabeled data, but using the previous latent space as input/output.

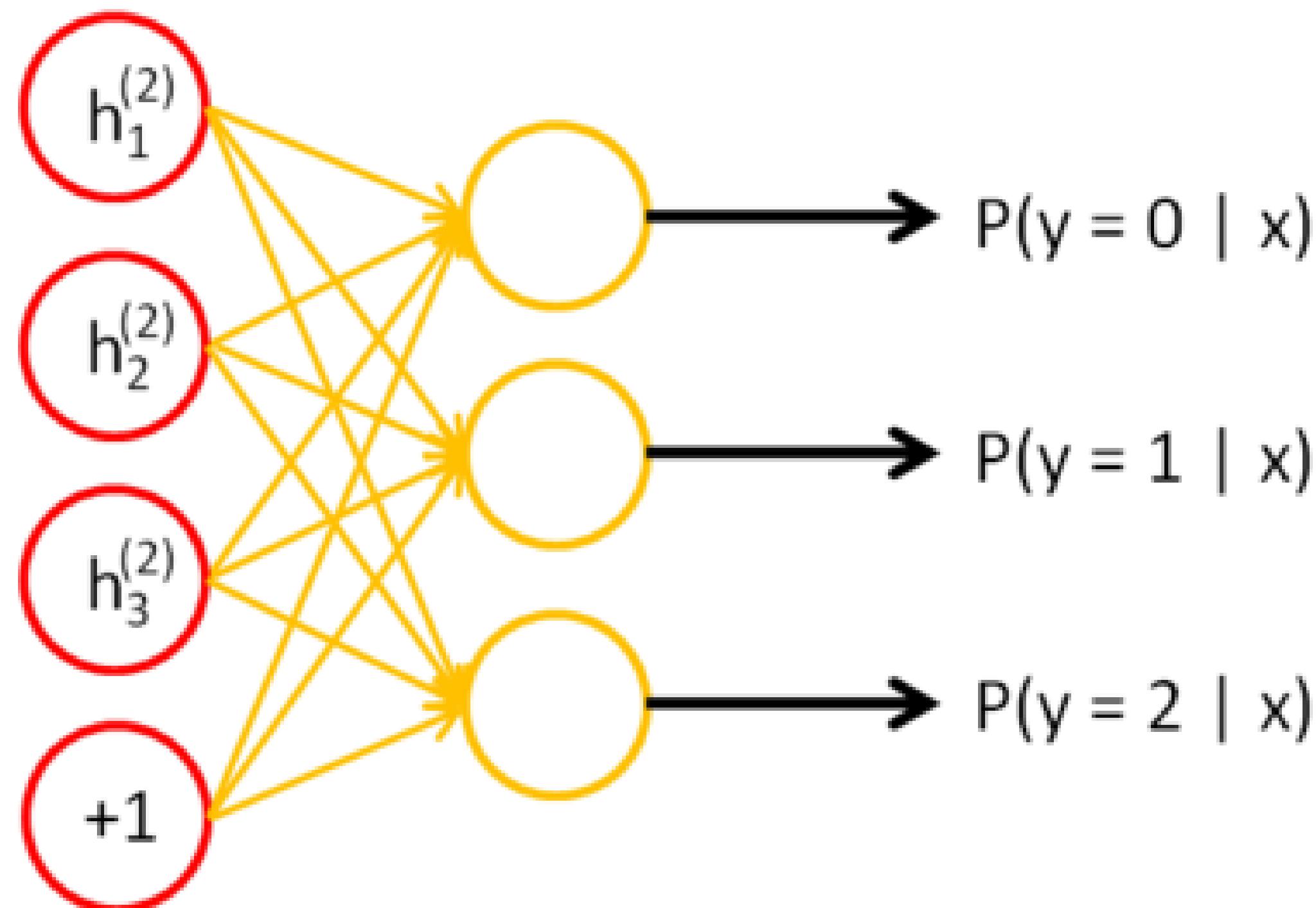


Input (Features I)	Features II	Output
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http://ufldl.stanford.edu/wiki/index.php/Stacked_Autoencoders

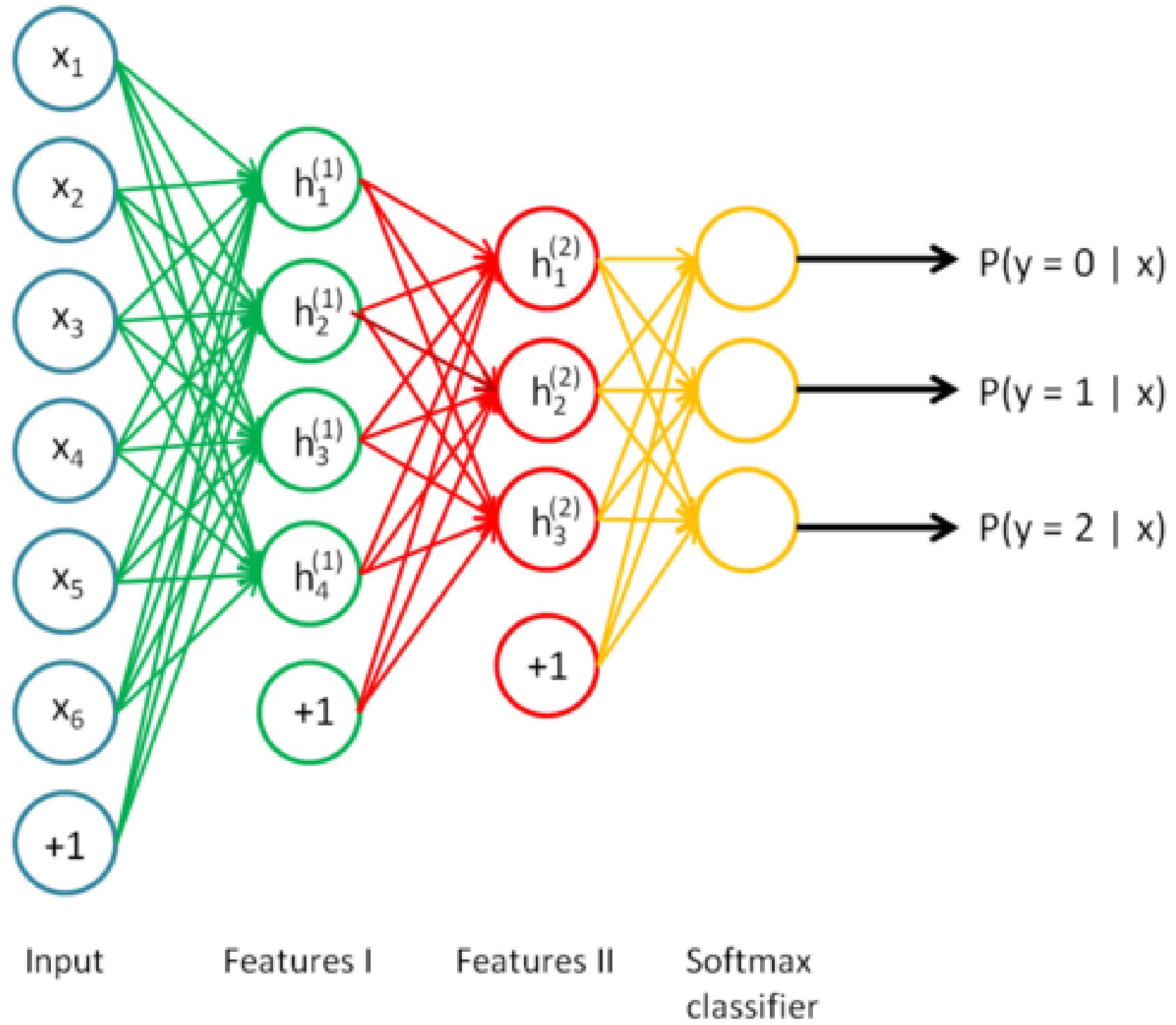
Stacked autoencoders

- Repeat the operation as often as needed, and finish with a simple classifier using the labeled data.



Input
(Features II) Softmax
classifier

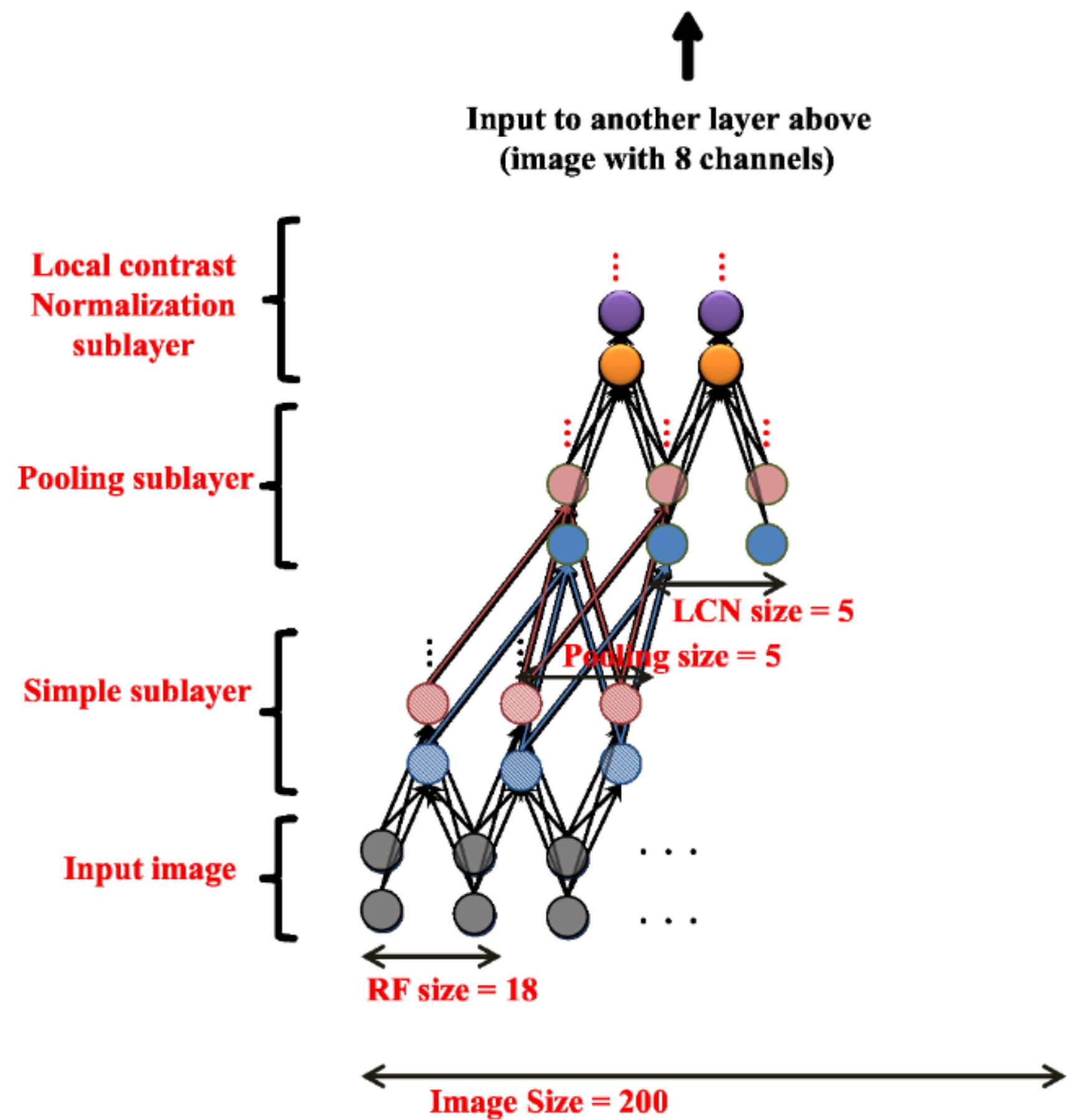
Greedy layer-wise learning



- This defines a **stacked autoencoder**, trained using **Greedy layer-wise** learning.
- Each layer progressively learns more and more complex features of the input data (edges - contour - forms - objects): **feature extraction**.
- This method allows to train a deep network on few labeled data: the network will not overfit, because the weights are already in the right region.
- It solves **gradient vanishing**, as the weights are already close to the optimal solution and will efficiently transmit the gradient backwards.
- One can keep the pre-trained weights fixed for the classification task or **fine-tune** all the weights as in a regular DNN.

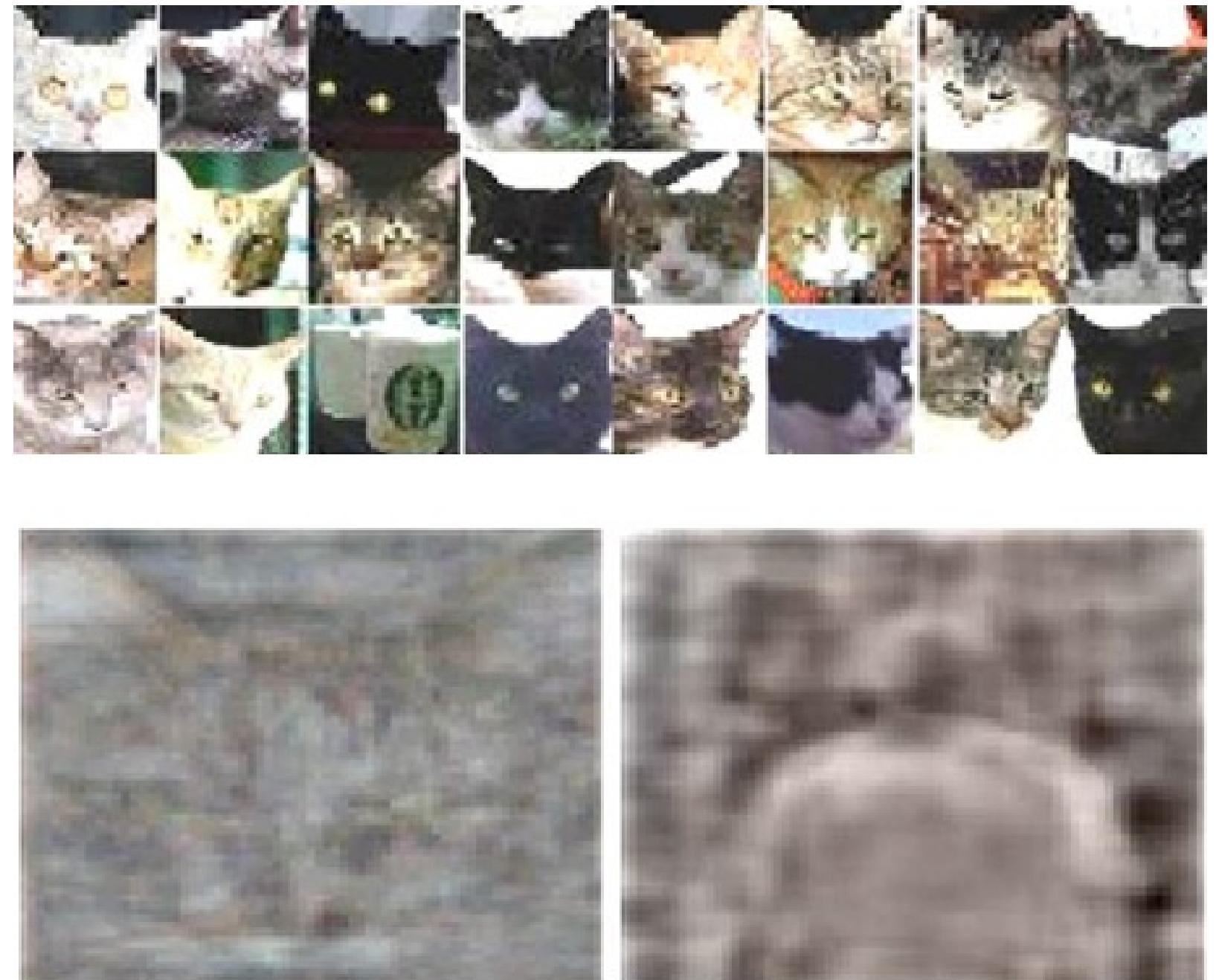
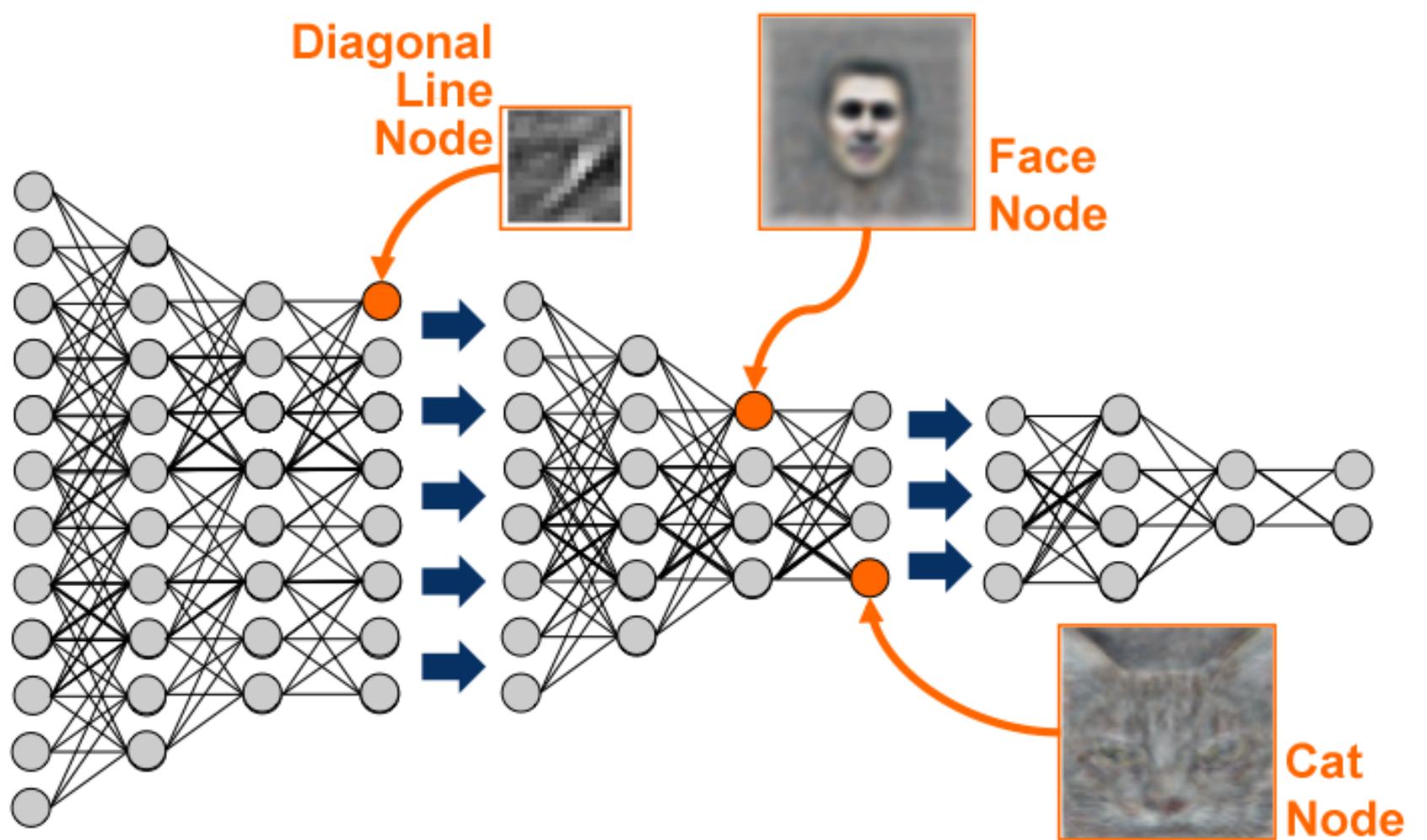
http://ufldl.stanford.edu/wiki/index.php/Stacked_Autoencoders

Application: Finding cats on the internet



- Andrew Ng and colleagues (Google, Stanford) used a similar technique to train a deep belief network on color images (200x200) taken from 10 million random unlabeled Youtube videos.
- Each layer was trained greedily. They used a particular form of autoencoder called **restricted Boltzmann machines** (RBM) and a couple of other tricks (receptive fields, contrast normalization).
- Training was distributed over 1000 machines (16.000 cores) and lasted for three days.
- There was absolutely no task: the network just had to watch youtube videos.
- After learning, they visualized what the neurons had learned.

Application: Finding cats on the internet



- After training, some neurons had learned to respond uniquely to faces, or to cats, without ever having been instructed to.
- The network can then be fine-tuned for classification tasks, improving the pre-AlexNet state-of-the-art on ImageNet by 70%.

3 - Deep autoencoders

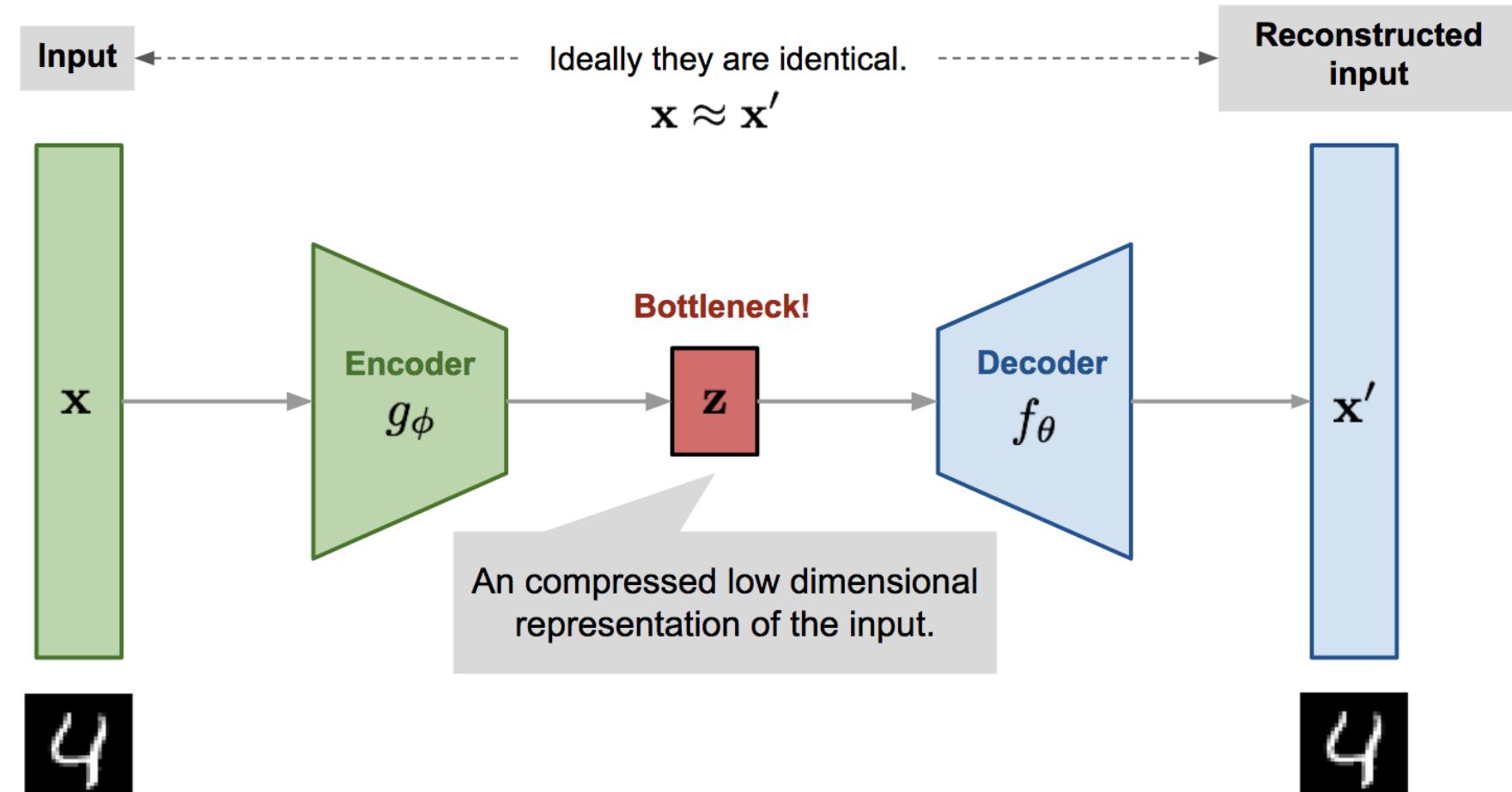
Deep autoencoders

- Autoencoders are not restricted to a single hidden layer.
- The **encoder** goes from the input space \mathbf{x} to the latent space \mathbf{z} .

$$\mathbf{z} = g_{\phi}(\mathbf{x})$$

- The **decoder** goes from the latent space \mathbf{z} to the output space \mathbf{x}' .

$$\mathbf{x}' = f_{\theta}(\mathbf{z})$$



Source: <https://lilianweng.github.io/lil-log/2018/08/12/from-autoencoder-to-beta-vae.html>

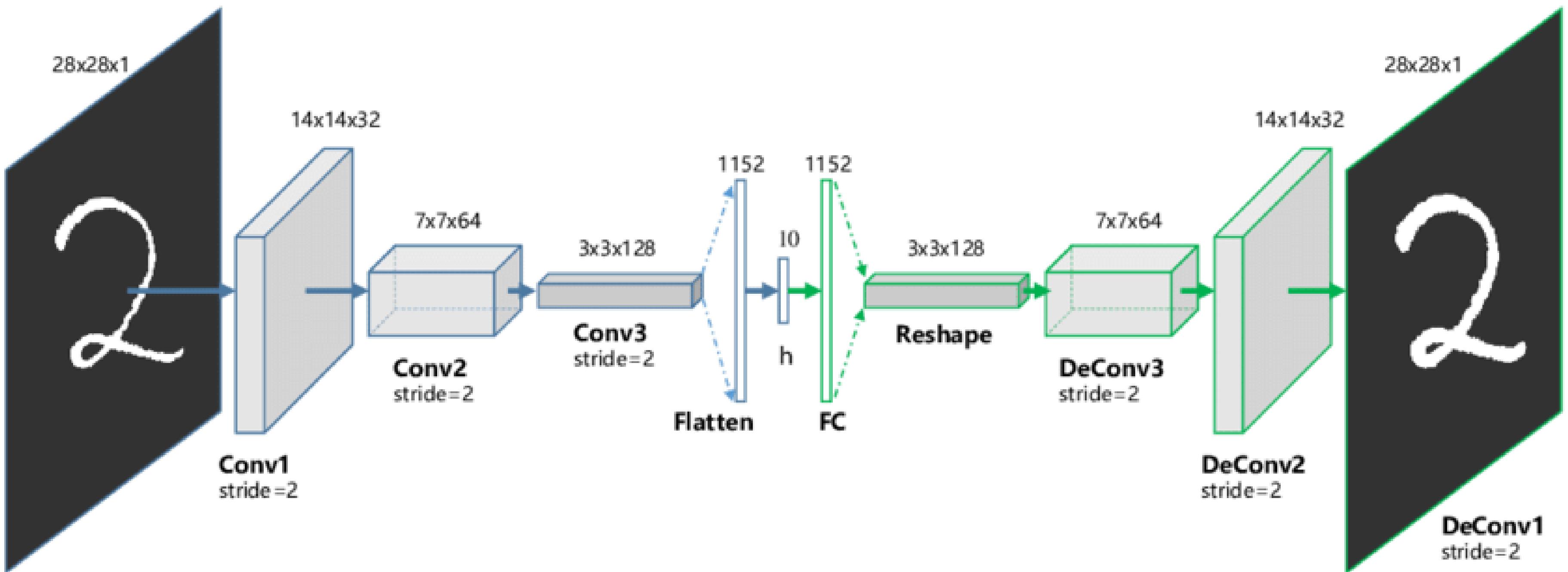
- The **latent space** is a **bottleneck** layer of lower dimensionality, learning a compressed representation of the input which has to contain enough information in order to **reconstruct** the input.
- Both the encoder with weights ϕ and the decoder with weights θ try to minimize the **reconstruction loss**:

$$\mathcal{L}_{\text{reconstruction}}(\theta, \phi) = \mathbb{E}_{\mathbf{x} \in \mathcal{D}} [||f_{\theta}(g_{\phi}(\mathbf{x})) - \mathbf{x}||^2]$$

- Learning is **unsupervised**: we only need input data.

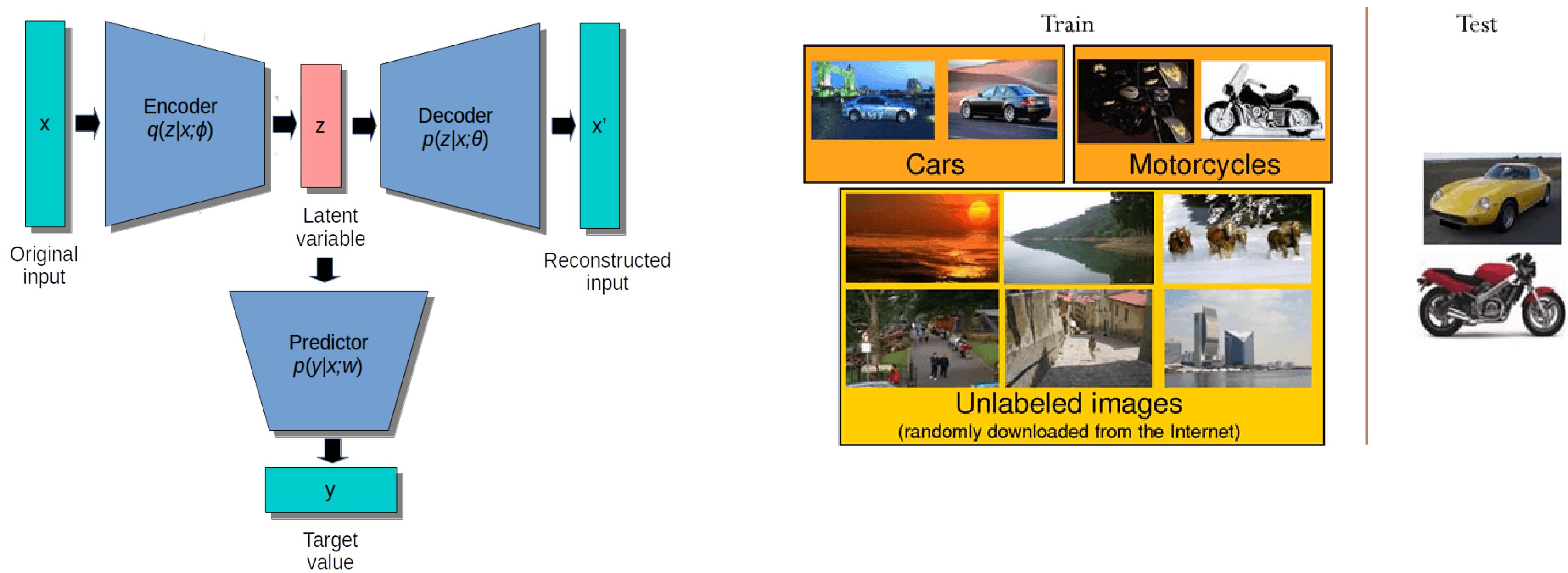
Deep autoencoders

- The encoder and decoder can be anything: fully-connected, convolutional, recurrent, etc.
- When using convolutional layers, the decoder has to **upsample** the latent space: max-unpooling or transposed convolutions can be used as in segmentation networks.



Semi-supervised learning

- In **semi-supervised** or **self-taught** learning, we can first train an autoencoder on huge amounts of unlabeled data, and then use the latent representations as an input to a shallow classifier on a small supervised dataset.

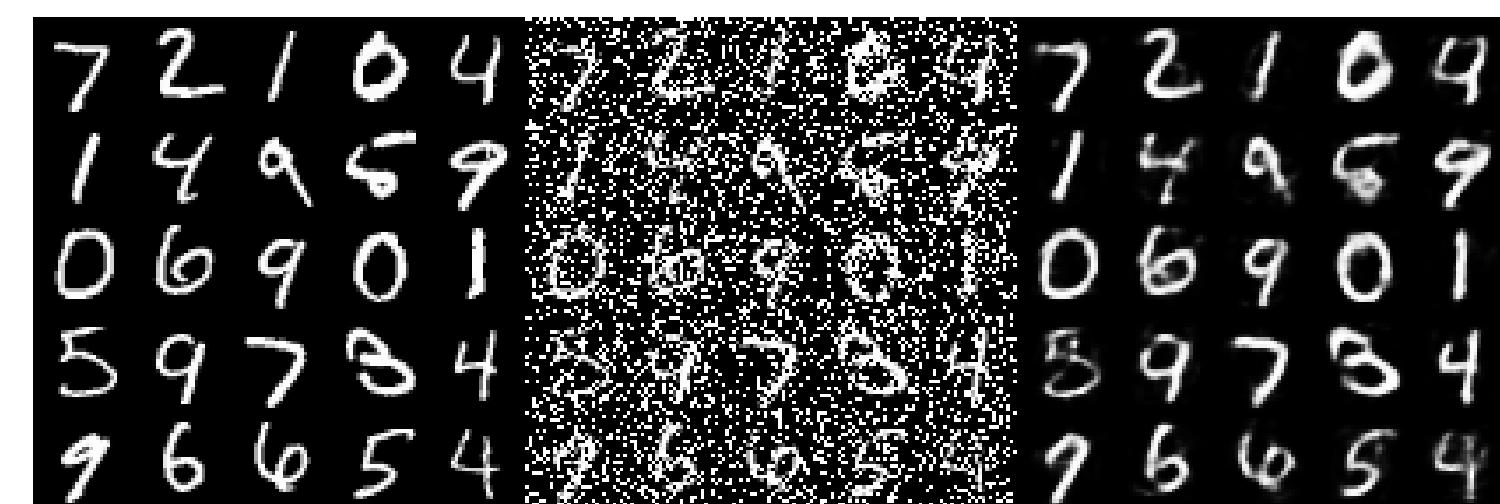
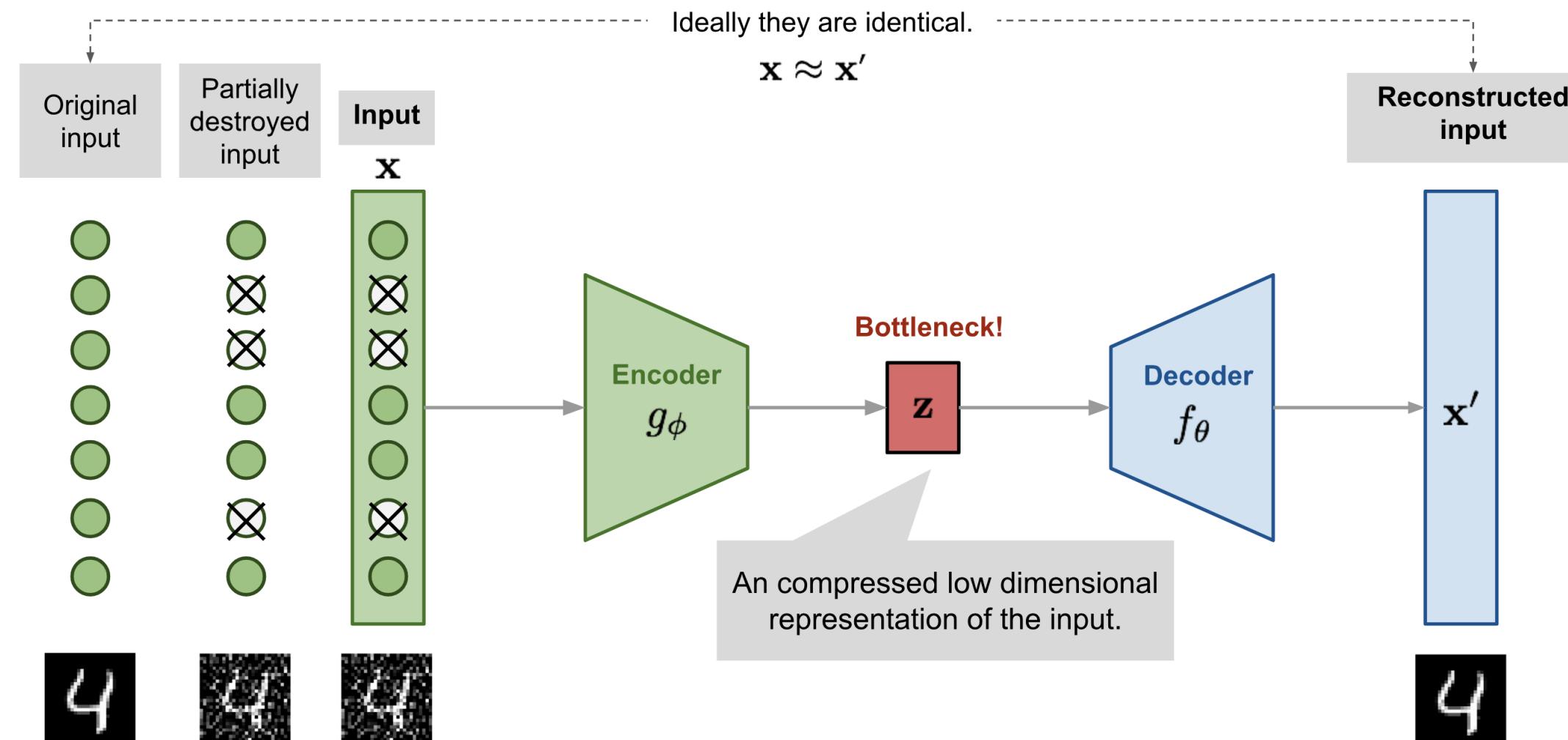


Source: <https://doi.org/10.1111/12.2303912>

- A linear classifier might even be enough if the latent space is well trained.
- The weights of the encoder can be fine-tuned with backpropagation, or remain fixed.

Denoising autoencoder

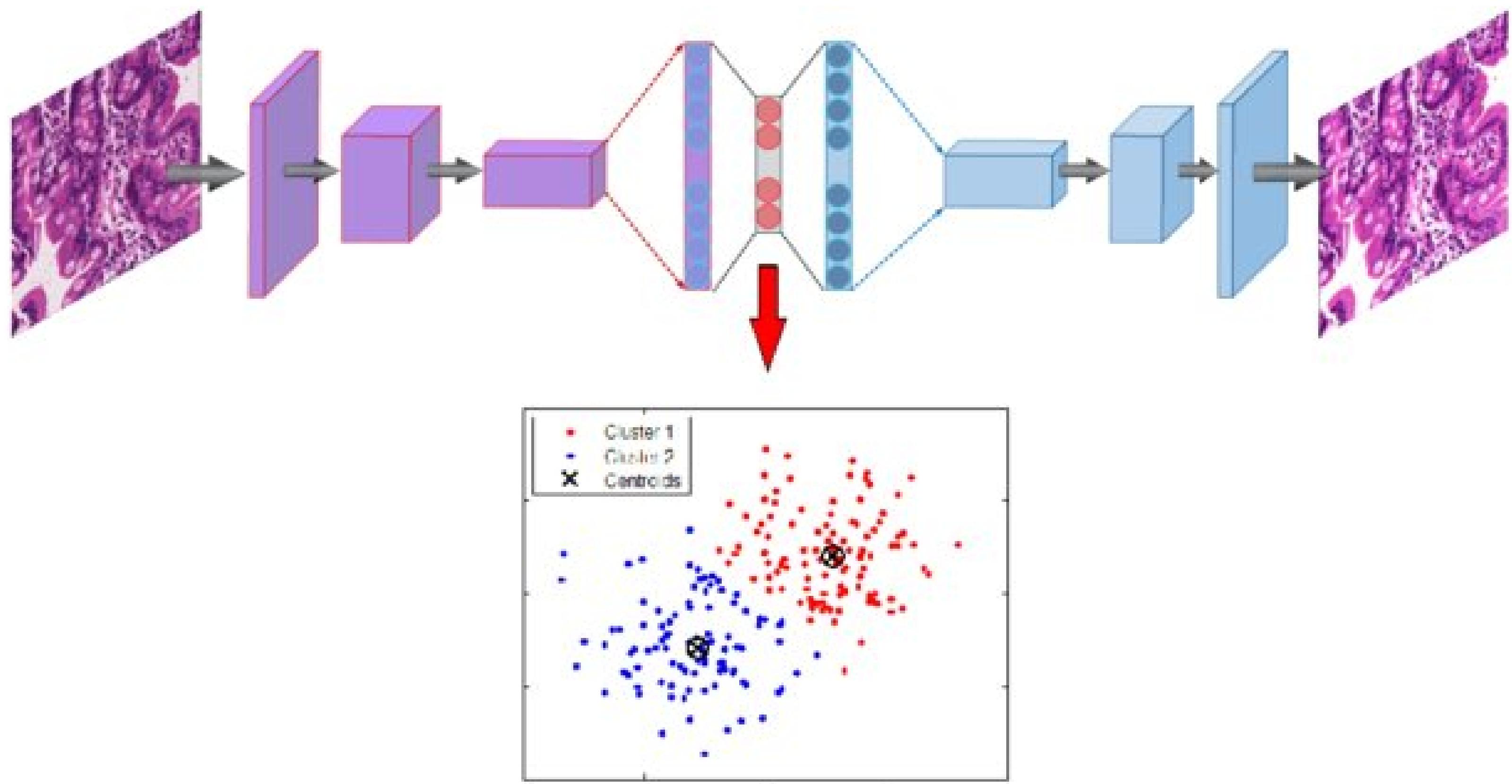
- A **denoising autoencoder** (DAE) is trained with noisy inputs (some pixels are dropped) but perfect desired outputs. It learns to suppress that noise.



Source : <https://lilianweng.github.io/lil-log/2018/08/12/from-autoencoder-to-beta-vae.html>

Deep clustering

- **Clustering** algorithms (k-means, Gaussian Mixture Models, spectral clustering, etc) can be applied in the latent space to group data points into clusters.
- If you are lucky, the clusters may even correspond to classes.

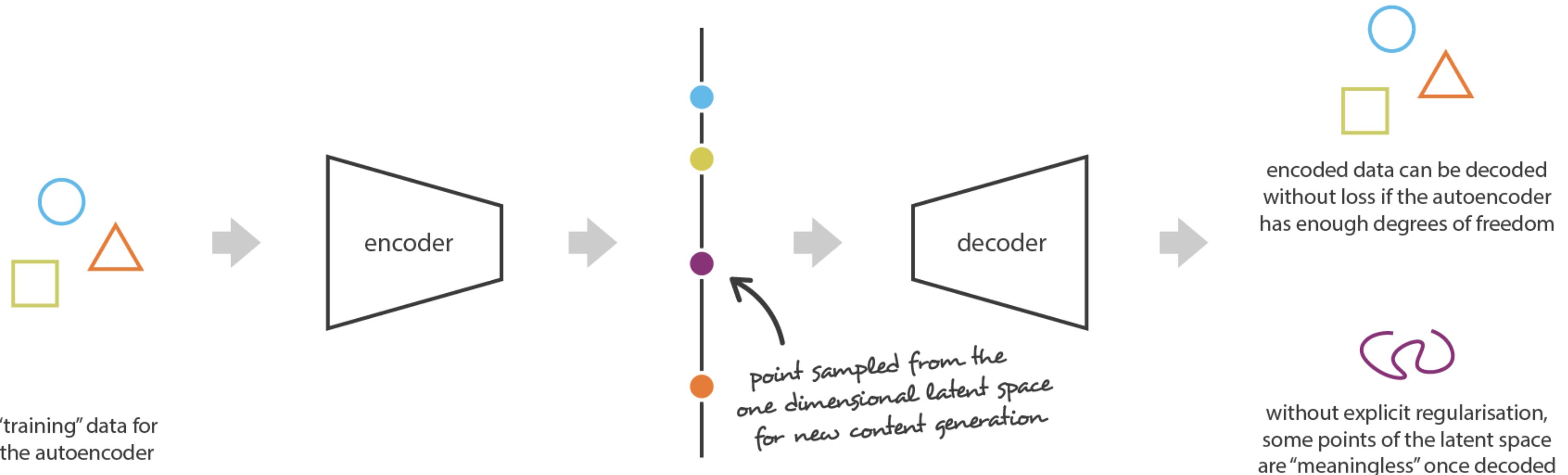


Source: doi:10.1007/978-3-030-32520-6_55

4 - Variational autoencoders (VAE)

Motivation

- Autoencoders are **deterministic**: after learning, the same input \mathbf{x} will generate the same latent code \mathbf{z} and the same reconstruction $\tilde{\mathbf{x}}$.
- Sampling the latent space generally generates non-sense reconstructions, because an autoencoder only learns data samples, it does not learn the underlying **probability distribution**.

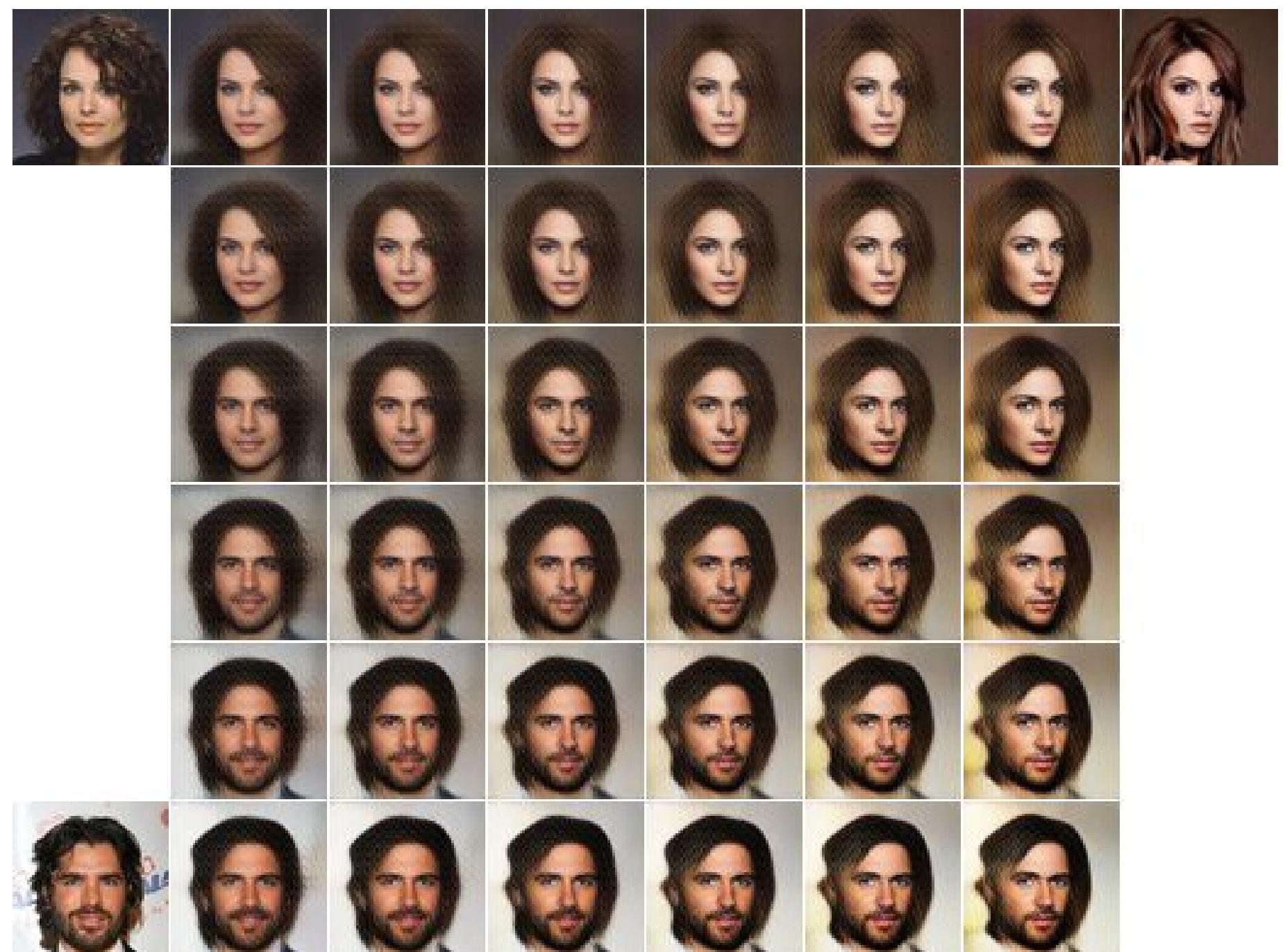


Source: <https://towardsdatascience.com/understanding-variational-autoencoders-vaes-f70510919f73>

Data augmentation with autoencoders

- The main problem of supervised learning is to get enough annotated data.
- Being able to generate **new** images similar to the training examples would be extremely useful (data augmentation).

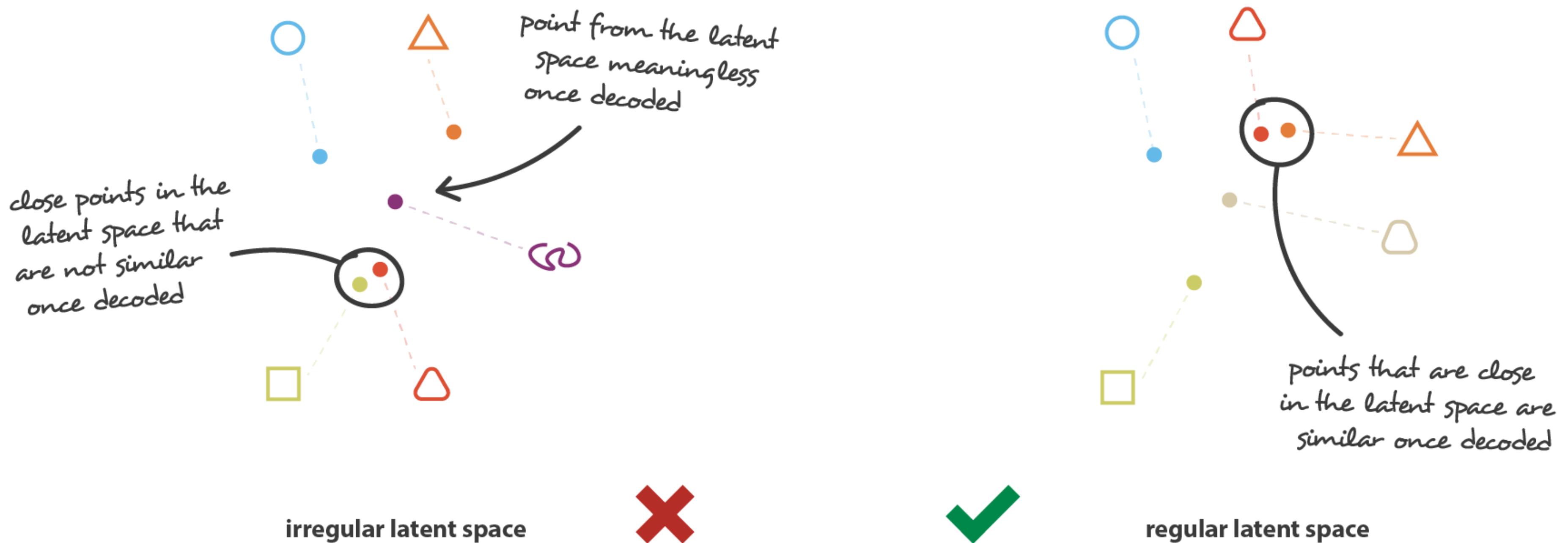
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Source: <https://hackernoon.com/latent-space-visualization-deep-learning-bits-2-bd09a46920df>

Regularized latent space

- In order for this to work, we need to **regularize** the latent space:
 - Close points in the latent space should correspond to close images.
- “Classical” L1 or L2 regularization does not ensure the regularity of the latent space.



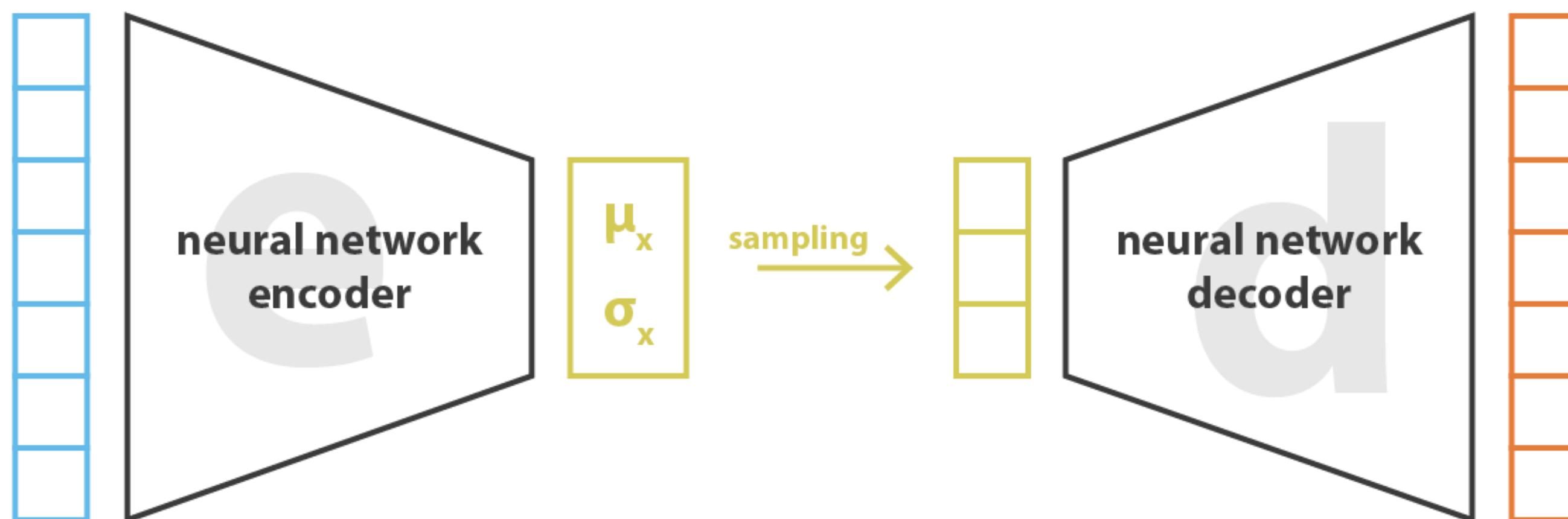
Source: <https://towardsdatascience.com/understanding-variational-autoencoders-vae-f70510919f73>

Variational autoencoder

- The **variational autoencoder** (VAE) (Kingma and Ba, 2013) solves this problem by having the encoder represent the **probability distribution** $q_\phi(\mathbf{z}|\mathbf{x})$ instead of a point \mathbf{z} in the latent space.
- This probability distribution is then **sampled** to obtain a vector \mathbf{z} that will be passed to the decoder $p_\theta(\mathbf{z})$.
- The strong hypothesis is that the latent space follows a **normal distribution** with mean μ_x and variance σ_x^2 .

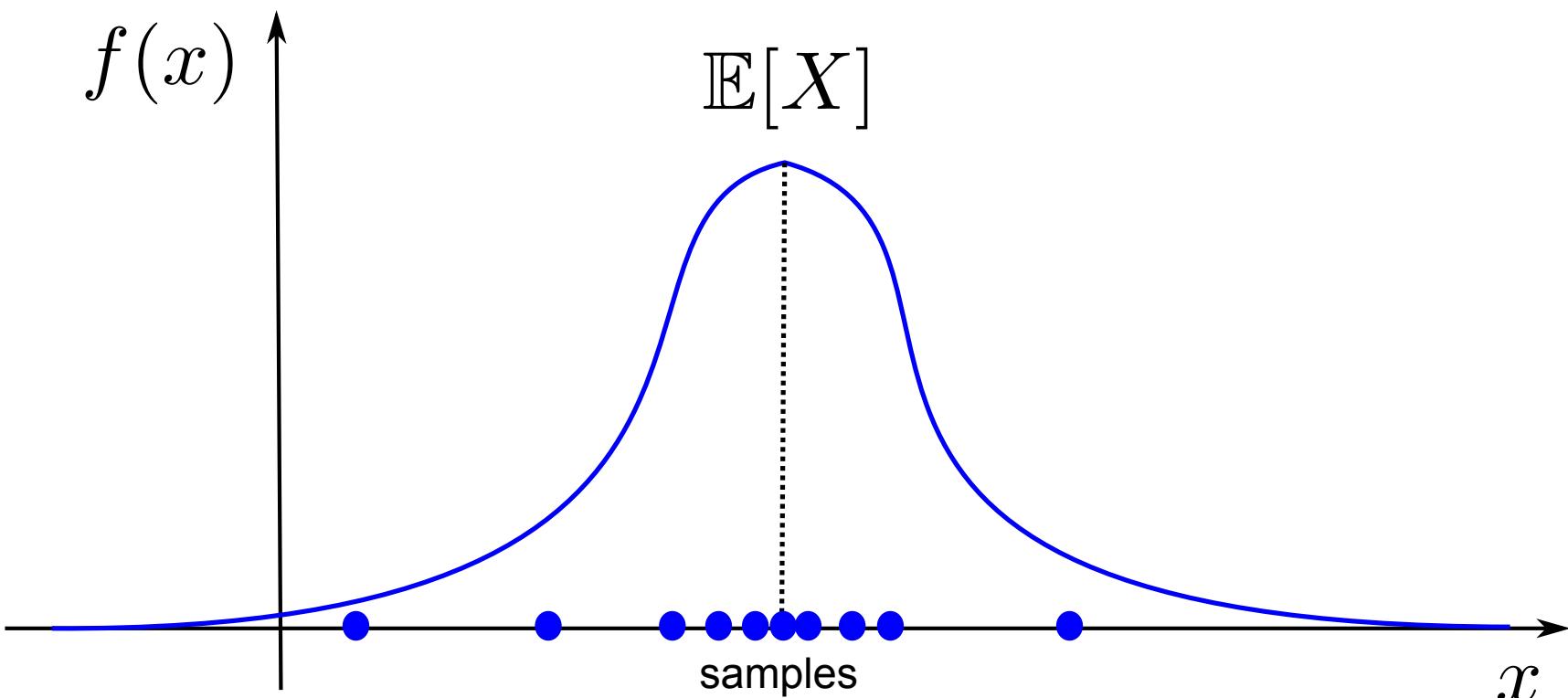
$$\mathbf{z} \sim \mathcal{N}(\mu_x, \sigma_x^2)$$

- The two vectors μ_x and σ_x^2 are the outputs of the encoder.



Source: <https://towardsdatascience.com/understanding-variational-autoencoders-vae-f70510919f73>

Sampling from a normal distribution



- The normal distribution $\mathcal{N}(\mu, \sigma^2)$ is fully defined by its two parameters:
 - μ is the mean of the distribution.
 - σ^2 is its variance.

- The **probability density function** (pdf) of the normal distribution is defined by the Gaussian function:

$$f(x; \mu, \sigma) = \frac{1}{\sqrt{2 \pi \sigma^2}} e^{-\frac{(x - \mu)^2}{2 \sigma^2}}$$

- A sample x will likely be close to μ , with a deviation defined by σ^2 .
- It can be obtained using a sample of the **standard normal distribution** $\mathcal{N}(0, 1)$:

$$x = \mu + \sigma \xi \text{ with } \xi \sim \mathcal{N}(0, 1)$$

Variational autoencoder

- Architecture of the VAE:
 1. The encoder $q_\phi(\mathbf{z}|\mathbf{x})$ outputs the parameters μ_x and σ_x^2 of a normal distribution $\mathcal{N}(\mu_x, \sigma_x^2)$.
 2. We sample one vector \mathbf{z} from this distribution: $\mathbf{z} \sim \mathcal{N}(\mu_x, \sigma_x^2)$.
 3. The decoder $p_\theta(\mathbf{x}|\mathbf{z})$ reconstructs the input.
- Open questions:
 1. Which loss should we use and how do we regularize?
 2. Does backpropagation still work?



Loss function of a VAE

- The **loss function** used in a VAE is of the form:

$$\mathcal{L}(\theta, \phi) = \mathcal{L}_{\text{reconstruction}}(\theta, \phi) + \mathcal{L}_{\text{regularization}}(\phi)$$

- The first term is the usual **reconstruction loss** of an autoencoder which depends on both the encoder and the decoder.
- One could simply compute the **mse** (summed over all pixels) between the input and the reconstruction:

$$\mathcal{L}_{\text{reconstruction}}(\theta, \phi) = \mathbb{E}_{\mathbf{x} \in \mathcal{D}, \mathbf{z} \sim q_{\phi}(\mathbf{z}|\mathbf{x})} [||p_{\theta}(\mathbf{z}) - \mathbf{x}||^2]$$

- In the expectation, \mathbf{x} is sampled from the dataset \mathcal{D} while \mathbf{z} is sampled from the encoder $q_{\phi}(\mathbf{z}|\mathbf{x})$.
- In (Kingma et al., 2013), pixels values are normalized between 0 and 1, the decoder uses the logistic activation function for its output layer and the binary cross-entropy loss function is used:

$$\mathcal{L}_{\text{reconstruction}}(\theta, \phi) = \mathbb{E}_{\mathbf{x} \in \mathcal{D}, \mathbf{z} \sim q_{\phi}(\mathbf{z}|\mathbf{x})} [-\log p_{\theta}(\mathbf{z})]$$

- The justification comes from variational inference and evidence lower-bound optimization (ELBO) but is out of the scope of this lecture.

Regularization term

- The second term is the **regularization term** for the latent space, which only depends on the encoder with weights ϕ :

$$\mathcal{L}_{\text{regularization}}(\phi) = \text{KL}(q_\phi(\mathbf{z}|\mathbf{x}) || \mathcal{N}(\mathbf{0}, \mathbf{1})) = \text{KL}(\mathcal{N}(\mu_{\mathbf{x}}, \sigma_{\mathbf{x}}^2) || \mathcal{N}(\mathbf{0}, \mathbf{1}))$$

- It is defined as the **Kullback-Leibler divergence** between the output of the encoder and the standard normal distribution $\mathcal{N}(\mathbf{0}, \mathbf{1})$.
- Think of it as a statistical “distance” between the distribution $q_\phi(\mathbf{z}|\mathbf{x})$ and the distribution $\mathcal{N}(\mathbf{0}, \mathbf{1})$.
- The principle is not very different from L2-regularization, where we want the weights to be as close as possible from 0.
- Here we want the encoder to be as close as possible from $\mathcal{N}(\mathbf{0}, \mathbf{1})$.

Regularization term

- Why do we want the latent distributions to be close from $\mathcal{N}(\mathbf{0}, \mathbf{1})$ for **all** inputs \mathbf{x} ?

$$\mathcal{L}(\theta, \phi) = \mathcal{L}_{\text{reconstruction}}(\theta, \phi) + \text{KL}(q_{\phi}(\mathbf{z}|\mathbf{x}) || \mathcal{N}(\mathbf{0}, \mathbf{1}))$$

- By forcing the distributions to be close, we avoid “holes” in the latent space: we can move smoothly from one distribution to another without generating **non-sense** reconstructions.



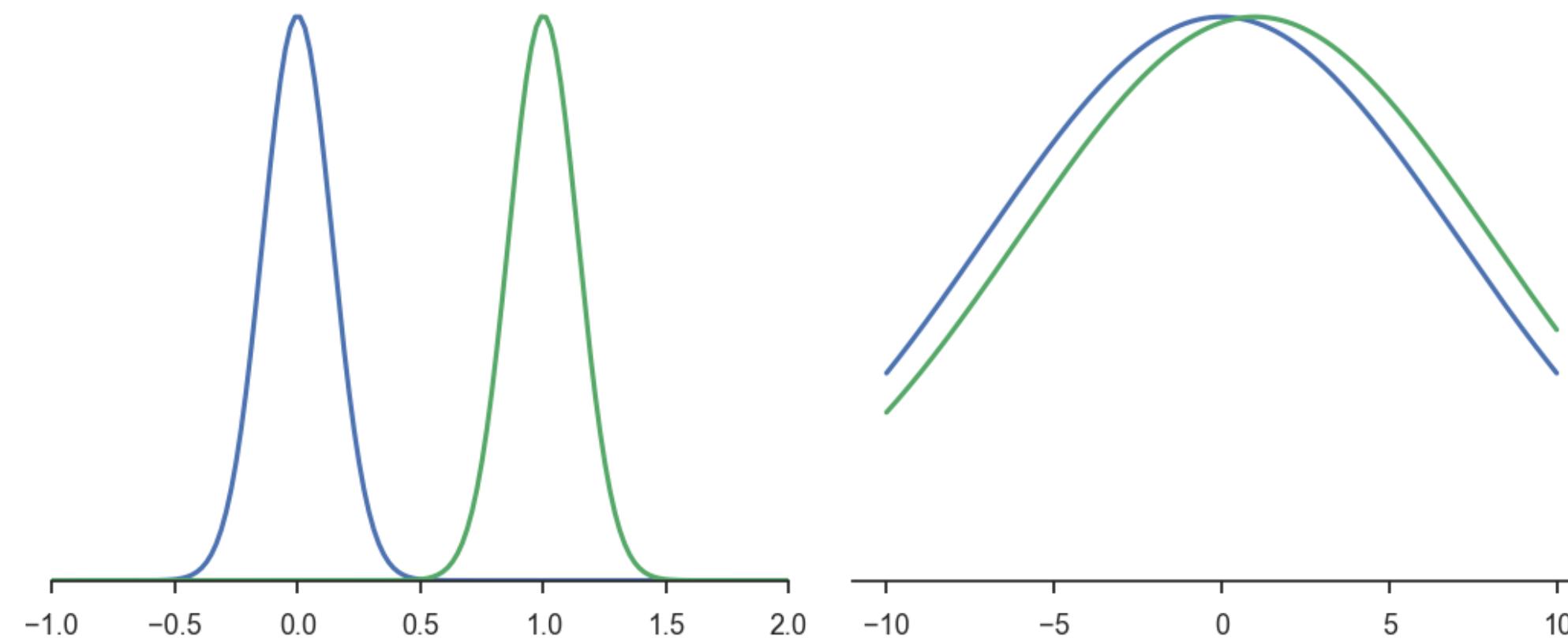
Source: <https://towardsdatascience.com/understanding-variational-autoencoders-vae-f70510919f73>

Why not regularize the mean and variance?

- To make $q_\phi(\mathbf{z}|\mathbf{x})$ close from $\mathcal{N}(\mathbf{0}, \mathbf{1})$, one could minimize the Euclidian distance in the **parameter space**:

$$\mathcal{L}(\theta, \phi) = \mathcal{L}_{\text{reconstruction}}(\theta, \phi) + (\|\mu_{\mathbf{x}}\|^2 + \|\sigma_{\mathbf{x}} - 1\|^2)$$

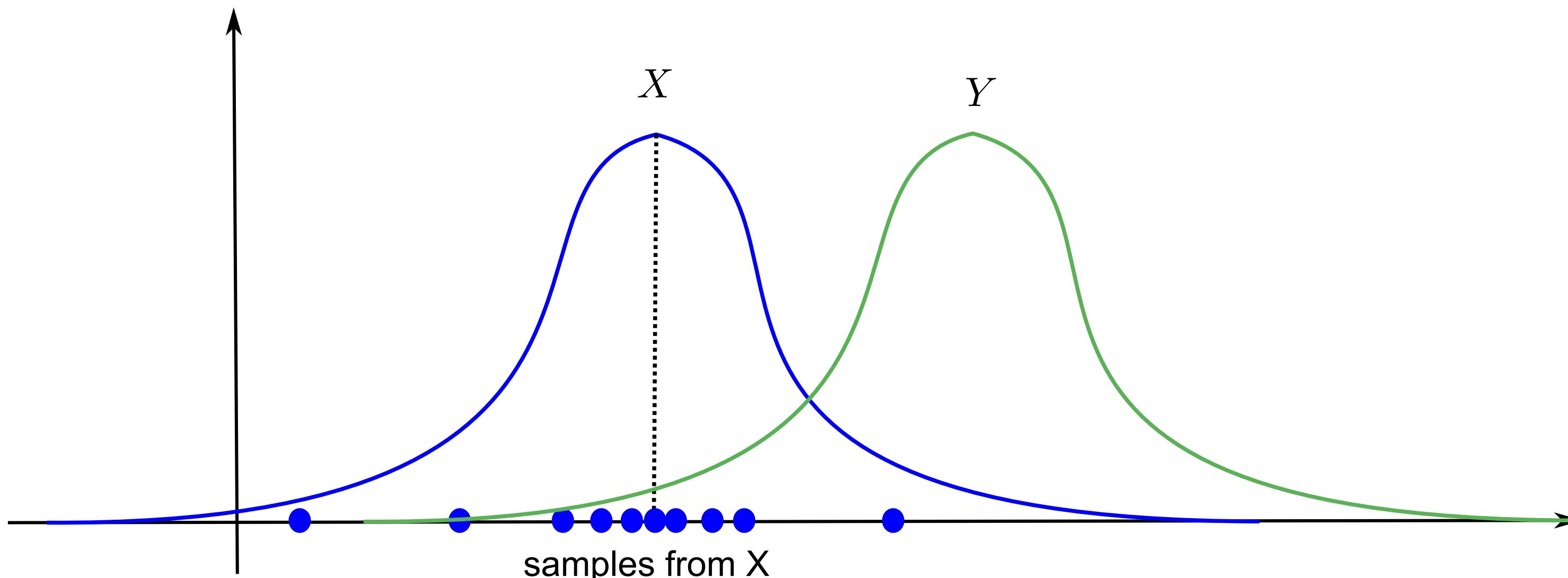
- However, this does not consider the **overlap** between the distributions.
- The two pairs of distributions below have the same distance between their means (0 and 1) and the same variance (1 and 10 respectively).
- The distributions on the left are very different from each other, but the distance in the parameter space is the same.



Kullback-Leibler divergence

- The **KL divergence** between two random distributions X and Y measures the **statistical distance** between them.
- It describes, on average, how likely a sample from X could come from Y :

$$\text{KL}(X||Y) = \mathbb{E}_{x \sim X}[-\log \frac{P(Y = x)}{P(X = x)}]$$



- When the two distributions are equal almost anywhere, the KL divergence is 0. Otherwise it is positive.
- **Minimizing the KL divergence between two distributions makes them close in the statistical sense.**

Kullback-Leibler divergence

- The advantage of minimizing the KL of $q_\phi(\mathbf{z}|\mathbf{x})$ with $\mathcal{N}(0, 1)$ is that the KL takes a **closed form** when the distributions are normal, i.e. there is no need to compute the expectation over all possible latent representations \mathbf{z} :

$$\mathcal{L}_{\text{regularization}}(\phi) = \text{KL}(q_\phi(\mathbf{z}|\mathbf{x}) || \mathcal{N}(\mathbf{0}, \mathbf{1})) = \mathbb{E}_{\mathbf{x} \in \mathcal{D}, \mathbf{z} \sim q_\phi(\mathbf{z}|\mathbf{x})} \left[-\log \frac{f_{0,1}(\mathbf{z}|\mathbf{x})}{q_\phi(\mathbf{z}|\mathbf{x})} \right]$$

- If $\mu_{\mathbf{x}}$ and $\sigma_{\mathbf{x}}$ have K elements (dimension of the latent space), the KL can be expressed as:

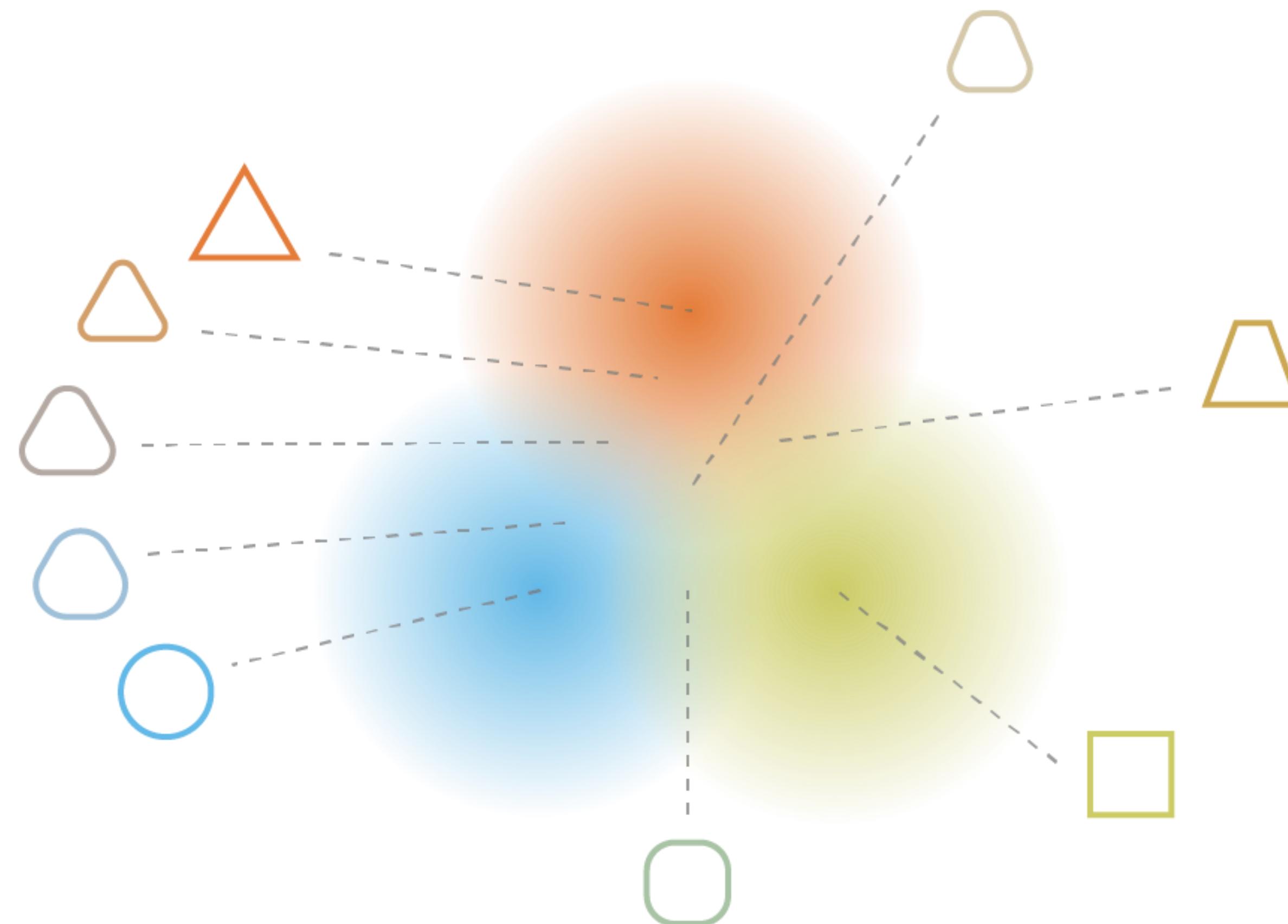
$$\mathcal{L}_{\text{regularization}}(\phi) = \mathbb{E}_{\mathbf{x} \in \mathcal{D}} \left[\frac{1}{2} \sum_{k=1}^K (\sigma_{\mathbf{x}}^2 + \mu_{\mathbf{x}}^2 - 1 - \log \sigma_{\mathbf{x}}^2) \right]$$

- The KL is very easy to differentiate w.r.t $\mu_{\mathbf{x}}$ and $\sigma_{\mathbf{x}}$, i.e. w.r.t ϕ !
- In practice, the encoder predicts the vectors $\mu_{\mathbf{x}}$ and $\Sigma_{\mathbf{x}} = \log \sigma_{\mathbf{x}}^2$, so the loss becomes:

$$\mathcal{L}_{\text{regularization}}(\phi) = \frac{1}{2} \sum_{k=1}^K (\exp \Sigma_{\mathbf{x}} + \mu_{\mathbf{x}}^2 - 1 - \Sigma_{\mathbf{x}})$$

Regularization

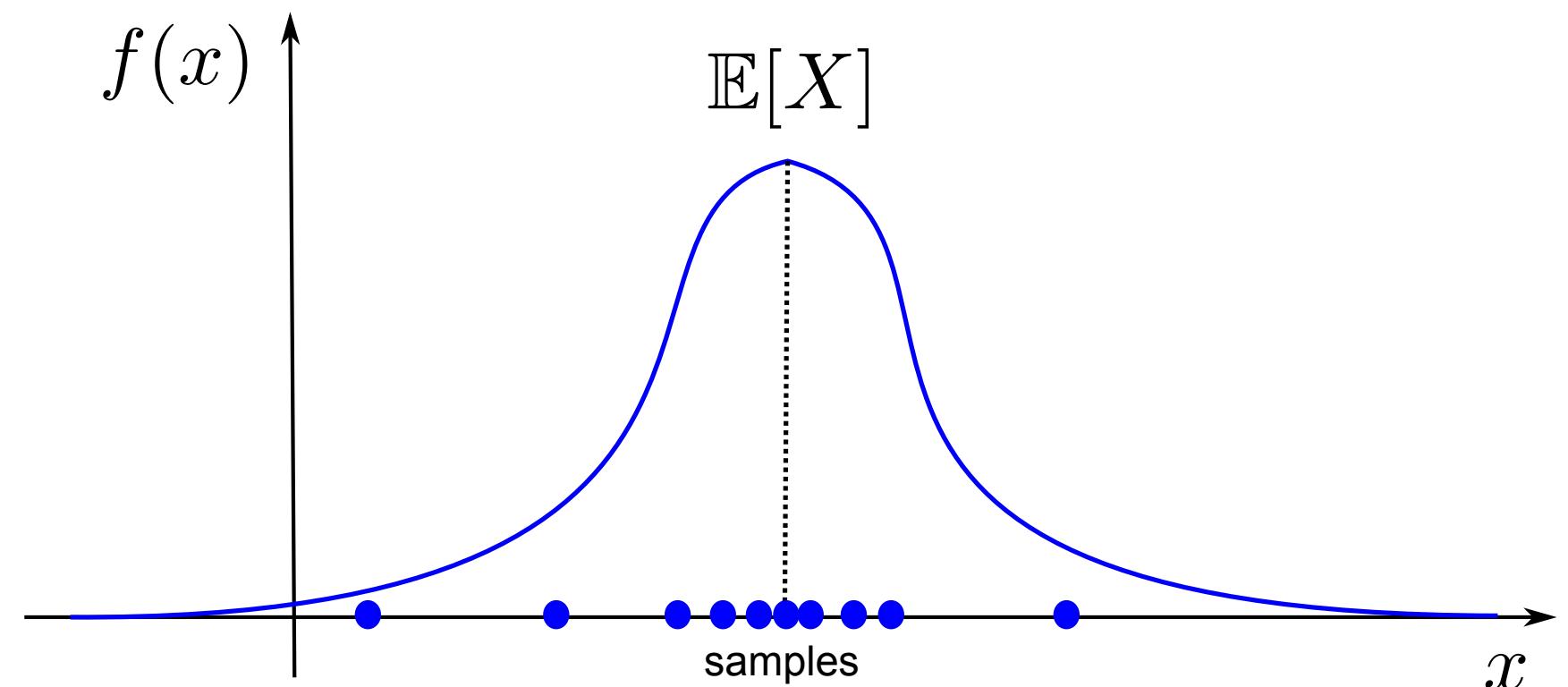
- Regularization tends to create a “gradient” over the information encoded in the latent space.
- A point of the latent space sampled between the means of two encoded distributions should be decoded in an image in between the two training images.



Reparameterization trick

- The second problem is that backpropagation does not work through the sampling operation.
- It is easy to backpropagate the gradient of the loss function through the decoder until the sample \mathbf{z} .
- But how do you backpropagate to the outputs of the encoder: μ_x and σ_x ?
- Modifying slightly μ_x or σ_x may not change at all the sample $\mathbf{z} \sim \mathcal{N}(\mu_x, \sigma_x^2)$, so you cannot estimate any gradient.

$$\frac{\partial \mathbf{z}}{\partial \mu_x} = ?$$



Reparameterization trick

- Backpropagation does not work through a **sampling** operation, because it is not differentiable.

$$\mathbf{z} \sim \mathcal{N}(\mu_{\mathbf{x}}, \sigma_{\mathbf{x}}^2)$$

- The **reparameterization trick** consists in taking a sample ξ out of $\mathcal{N}(0, 1)$ and reconstruct \mathbf{z} with:

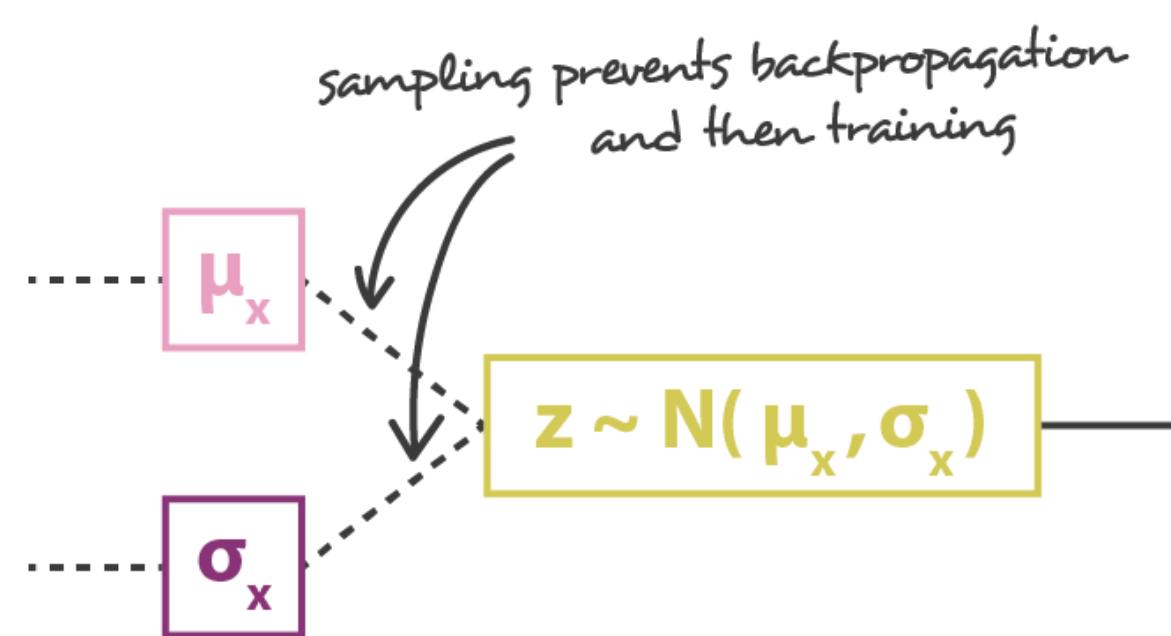
$$\mathbf{z} = \mu_{\mathbf{x}} + \sigma_{\mathbf{x}} \xi \quad \text{with} \quad \xi \sim \mathcal{N}(0, 1)$$



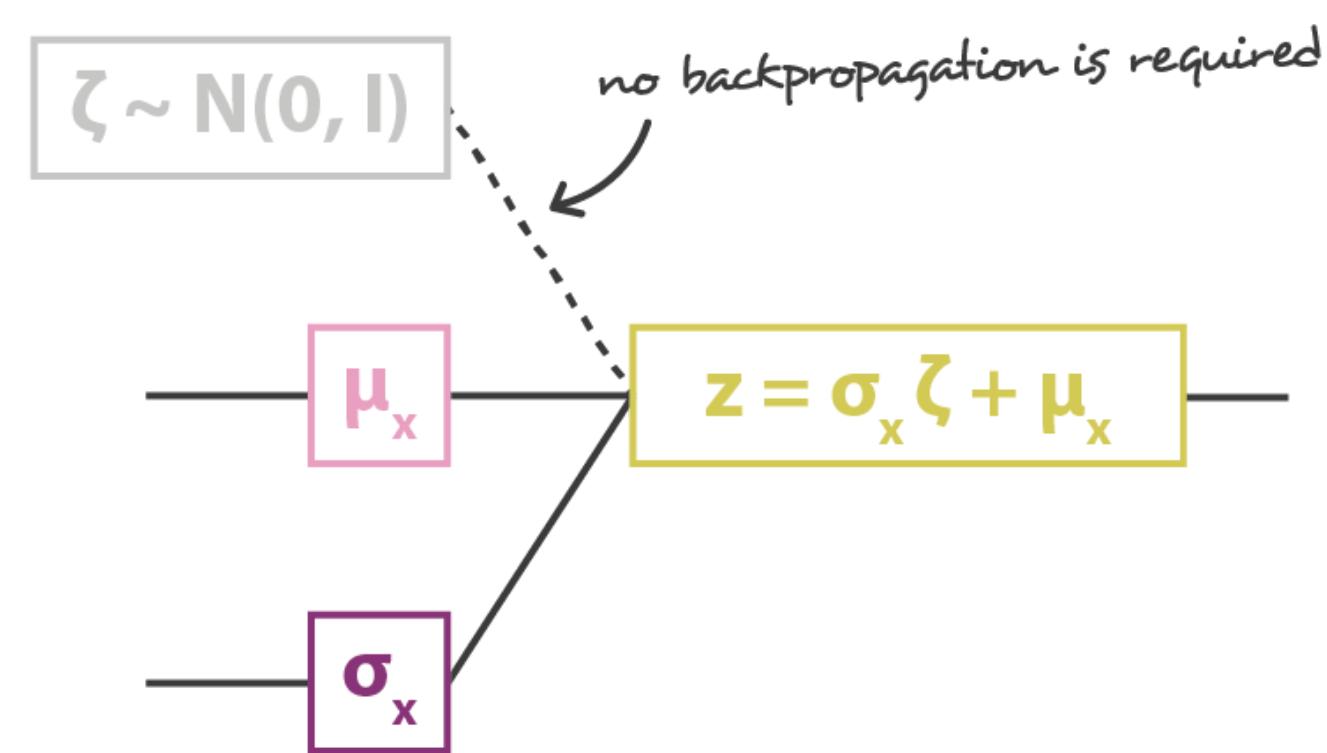
no problem for backpropagation



backpropagation is not possible due to sampling



sampling without reparametrisation trick

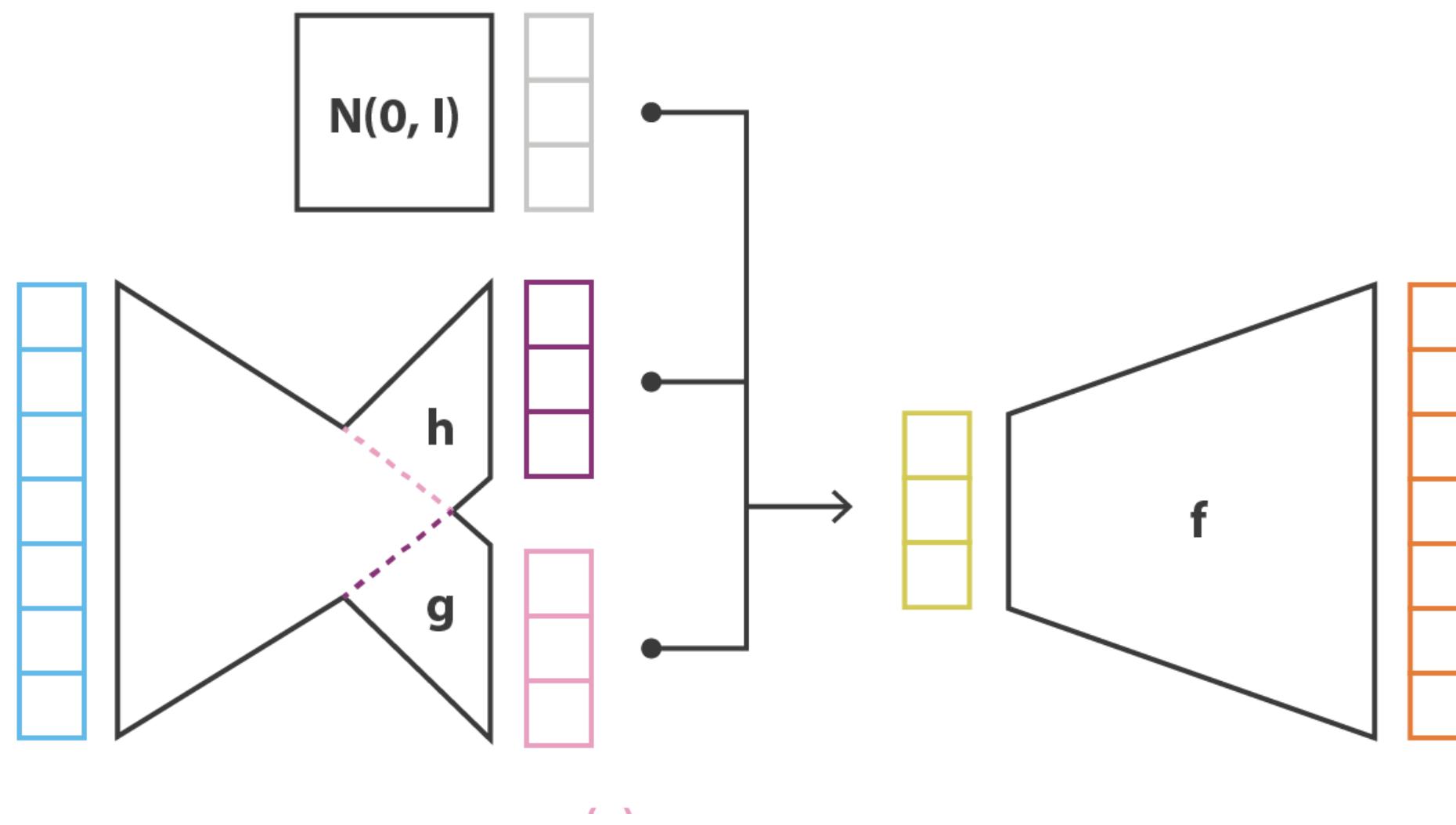


sampling with reparametrisation trick

Source: <https://towardsdatascience.com/understanding-variational-autoencoders-vae-f70510919f73>

Reparameterization trick

- The sampled value $\xi \sim \mathcal{N}(0, 1)$ becomes just another input to the neural network.



Source: <https://towardsdatascience.com/understanding-variational-autoencoders-vaes-f70510919f73>

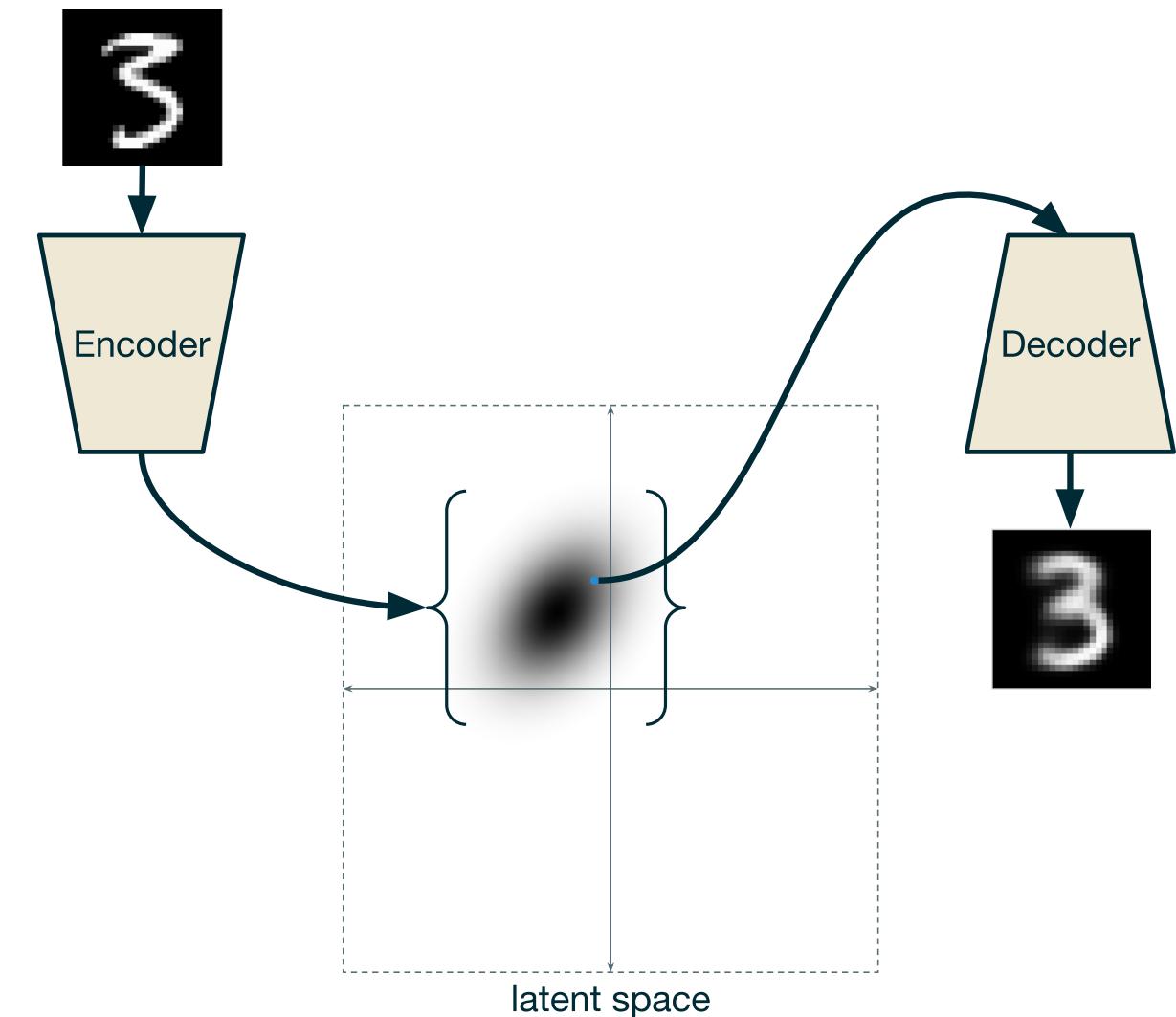
- It allows to transform μ_x and σ_x into a sample z of $\mathcal{N}(\mu_x, \sigma_x^2)$:

$$z = \mu_x + \sigma_x \xi$$

- We do not need to backpropagate through ξ , as there is no parameter to learn!
- The neural network becomes differentiable end-to-end, backpropagation will work.

Variational autoencoder

- A variational autoencoder is an autoencoder where the latent space represents a probability distribution $q_\phi(\mathbf{z}|\mathbf{x})$ using the mean μ_x and standard deviation σ_x of a normal distribution.
- The latent space can be sampled to generate new images using the decoder $p_\theta(\mathbf{z})$.
- KL regularization and the reparameterization trick are essential to VAE.



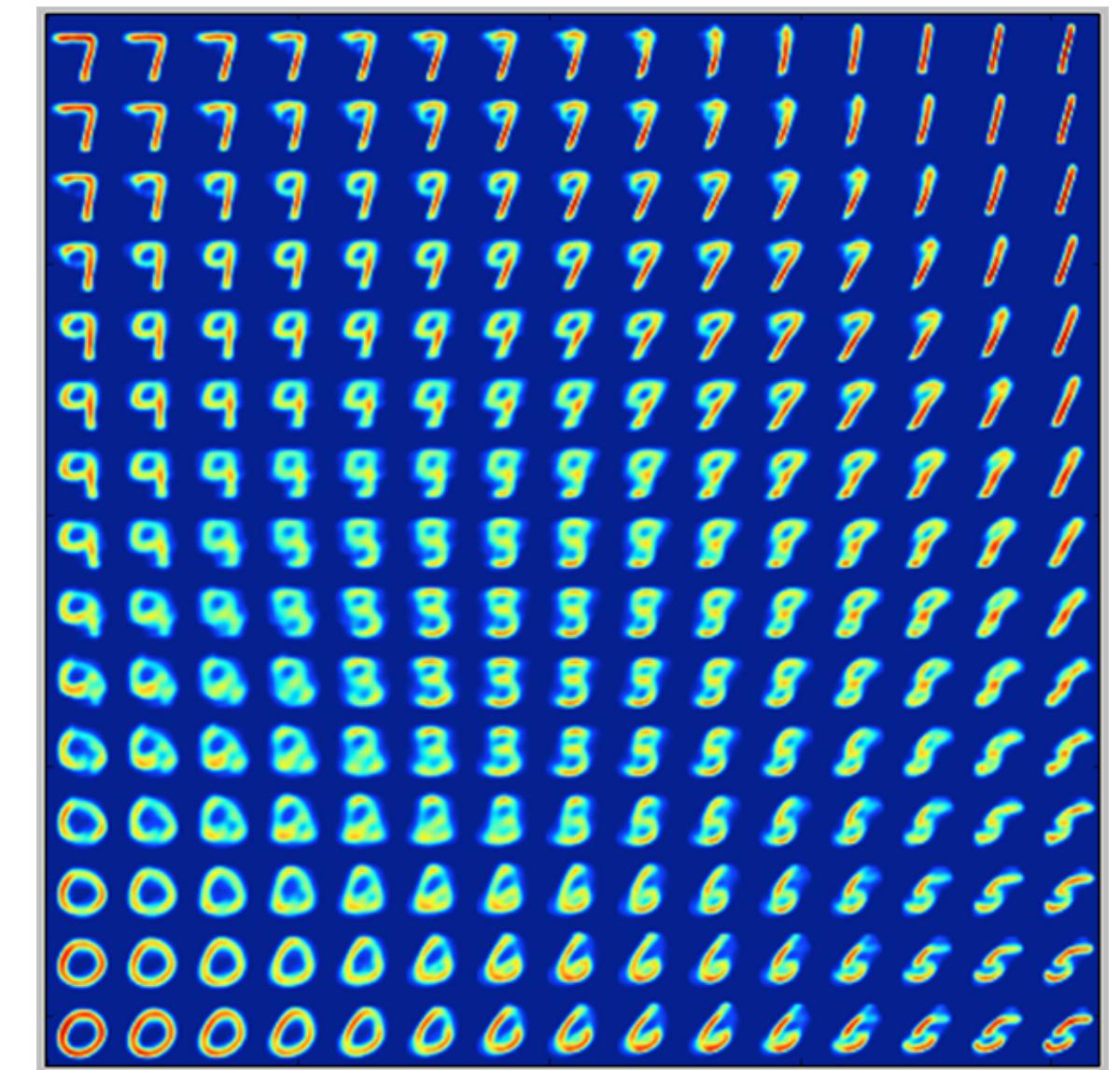
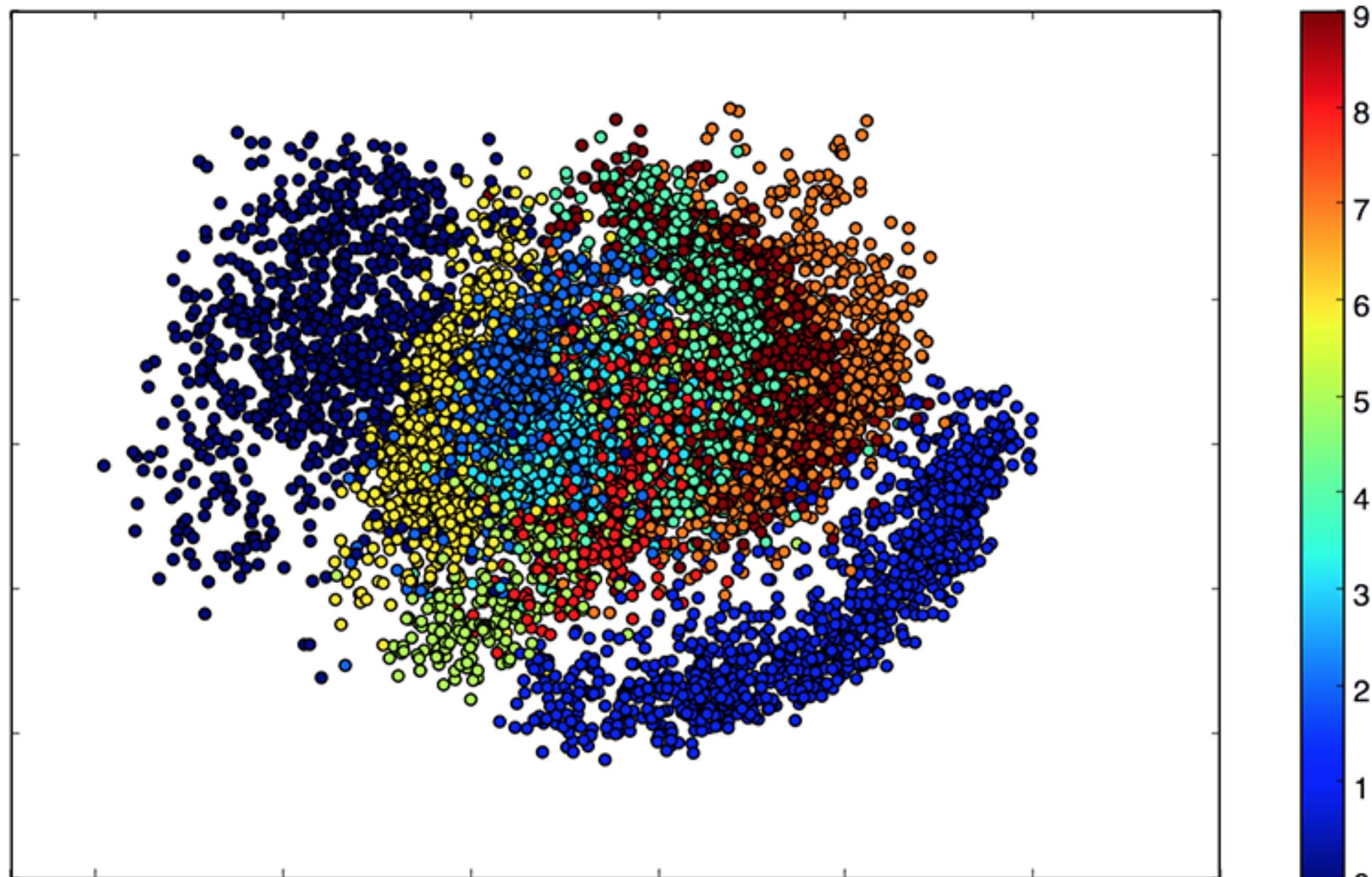
Source: <https://ijdykeman.github.io/ml/2016/12/21/cvae.html>

$$\mathcal{L}(\theta, \phi) = \mathcal{L}_{\text{reconstruction}}(\theta, \phi) + \mathcal{L}_{\text{regularization}}(\phi)$$

$$= \mathbb{E}_{\mathbf{x} \in \mathcal{D}, \xi \sim \mathcal{N}(0,1)} [-\log p_\theta(\mu_x + \sigma_x \xi) + \frac{1}{2} \sum_{k=1}^K (\sigma_x^2 + \mu_x^2 - 1 - \log \sigma_x^2)]$$

Variational autoencoder

- The two main applications of VAEs in **unsupervised learning** are:
 1. **Dimensionality reduction**: projecting high dimensional data (images) onto a smaller space, for example a 2D space for visualization.
 2. **Generative modeling**: generating samples from the same distribution as the training data (data augmentation, deep fakes) by sampling on the manifold.



Source: <https://blog.keras.io/building-autoencoders-in-keras.html>

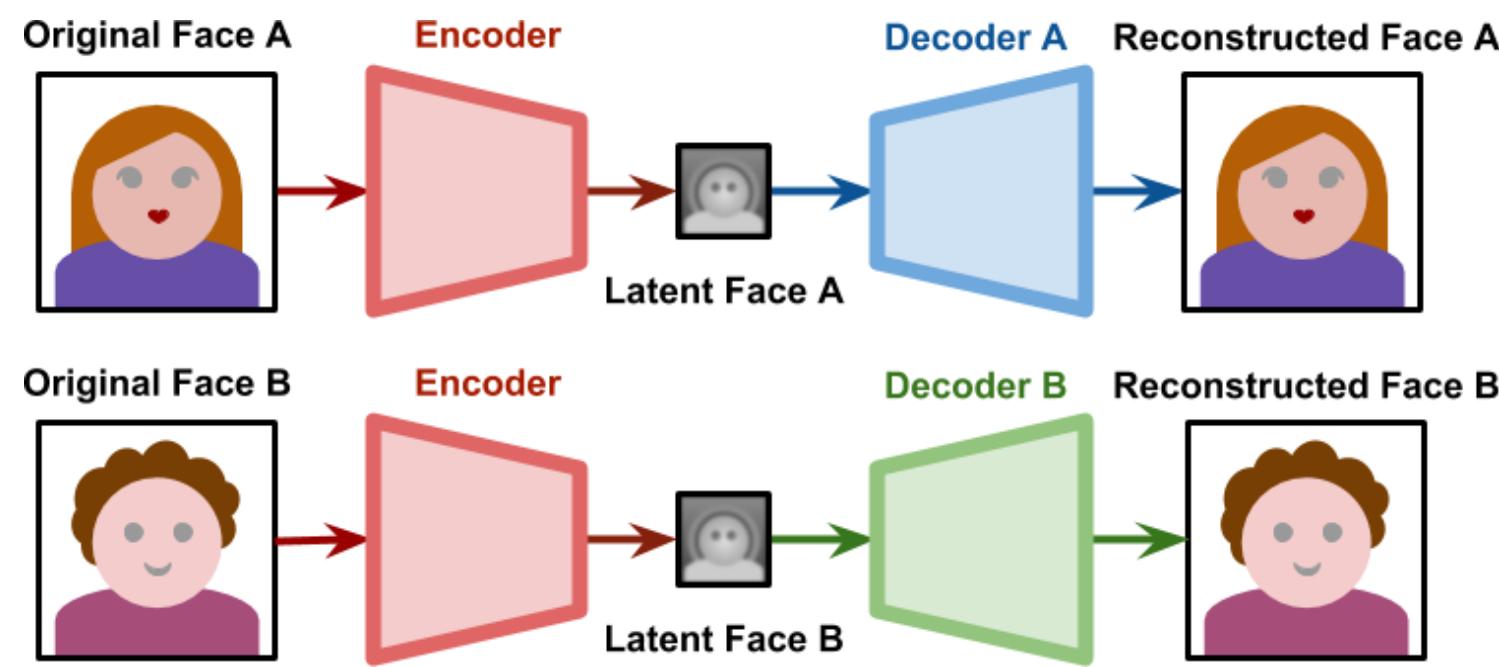
DeepFake



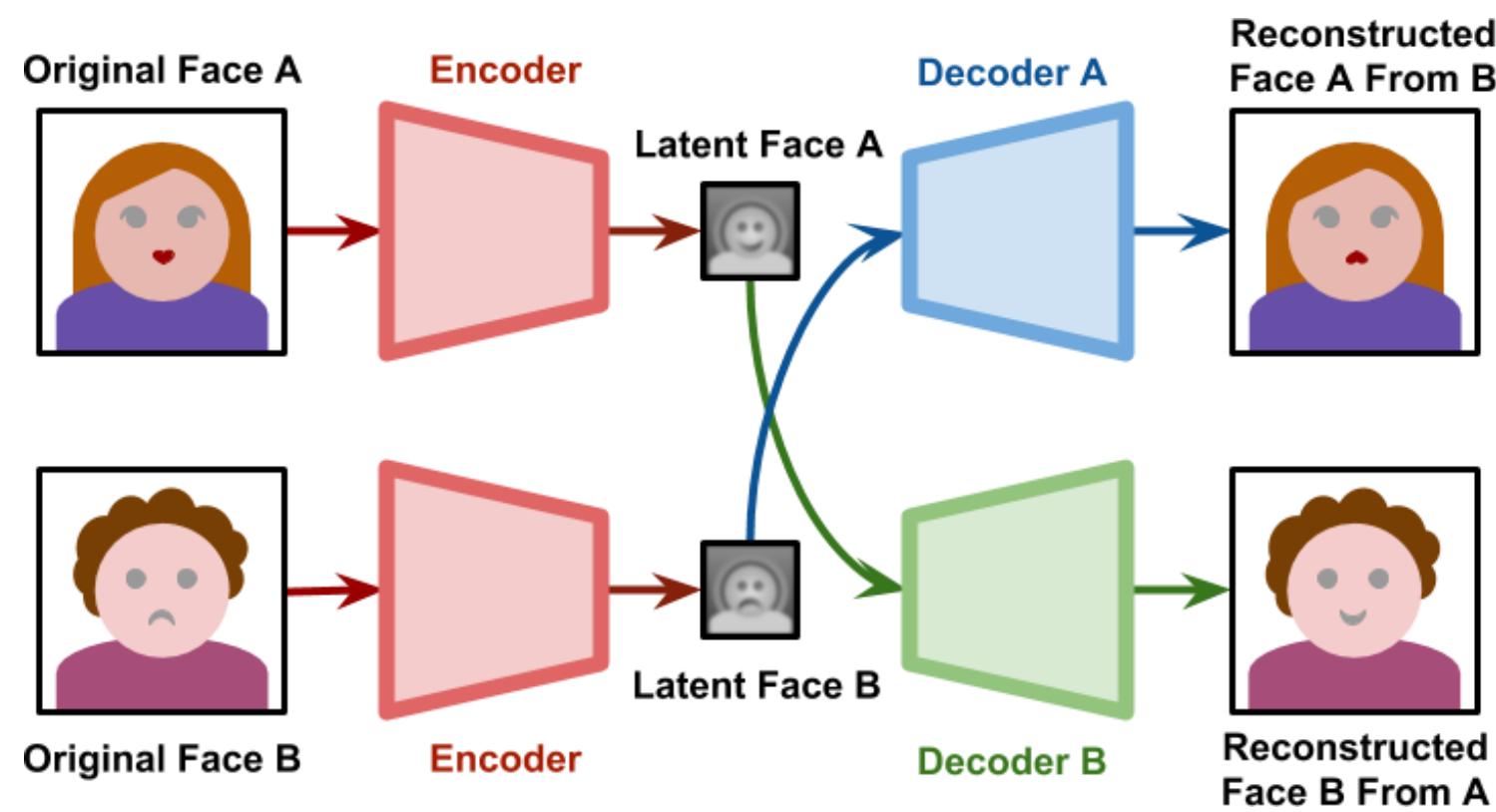
<https://github.com/iperov/DeepFaceLab>

DeepFake

- During training, **one** encoder and **two** decoders learns to reproduce the face of each person.



- When generating the deepfake, the decoder of person B is used on the latent representation of person A.

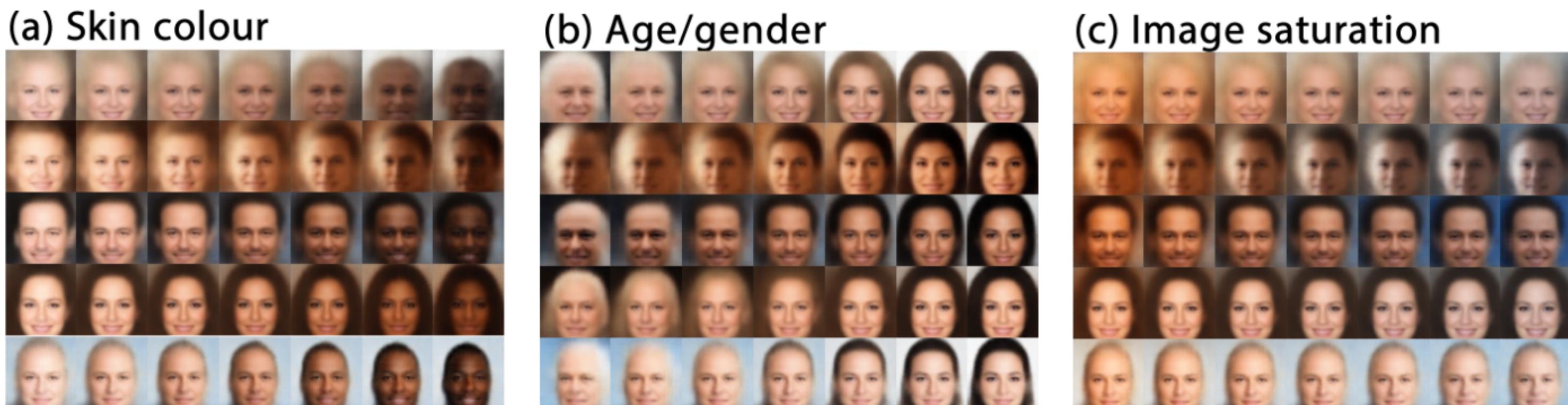


β -VAE

- VAE does not use a regularization parameter to balance the reconstruction and regularization losses.
What happens if you do?

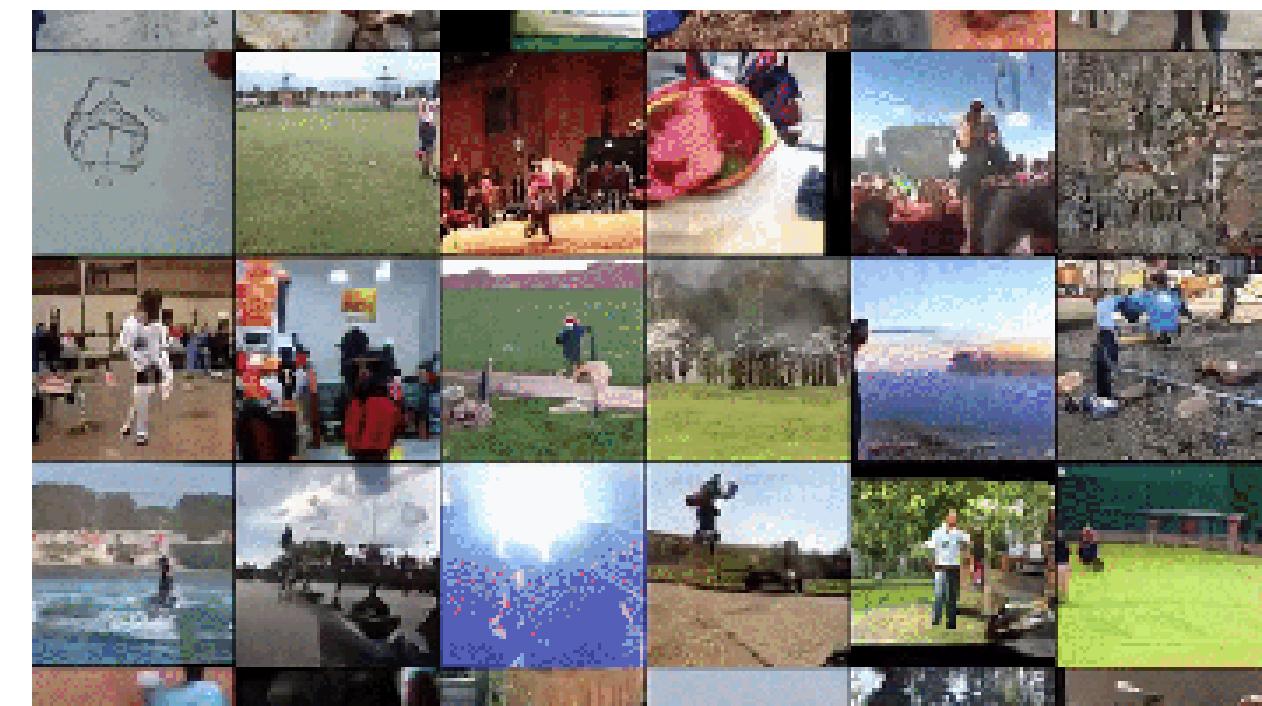
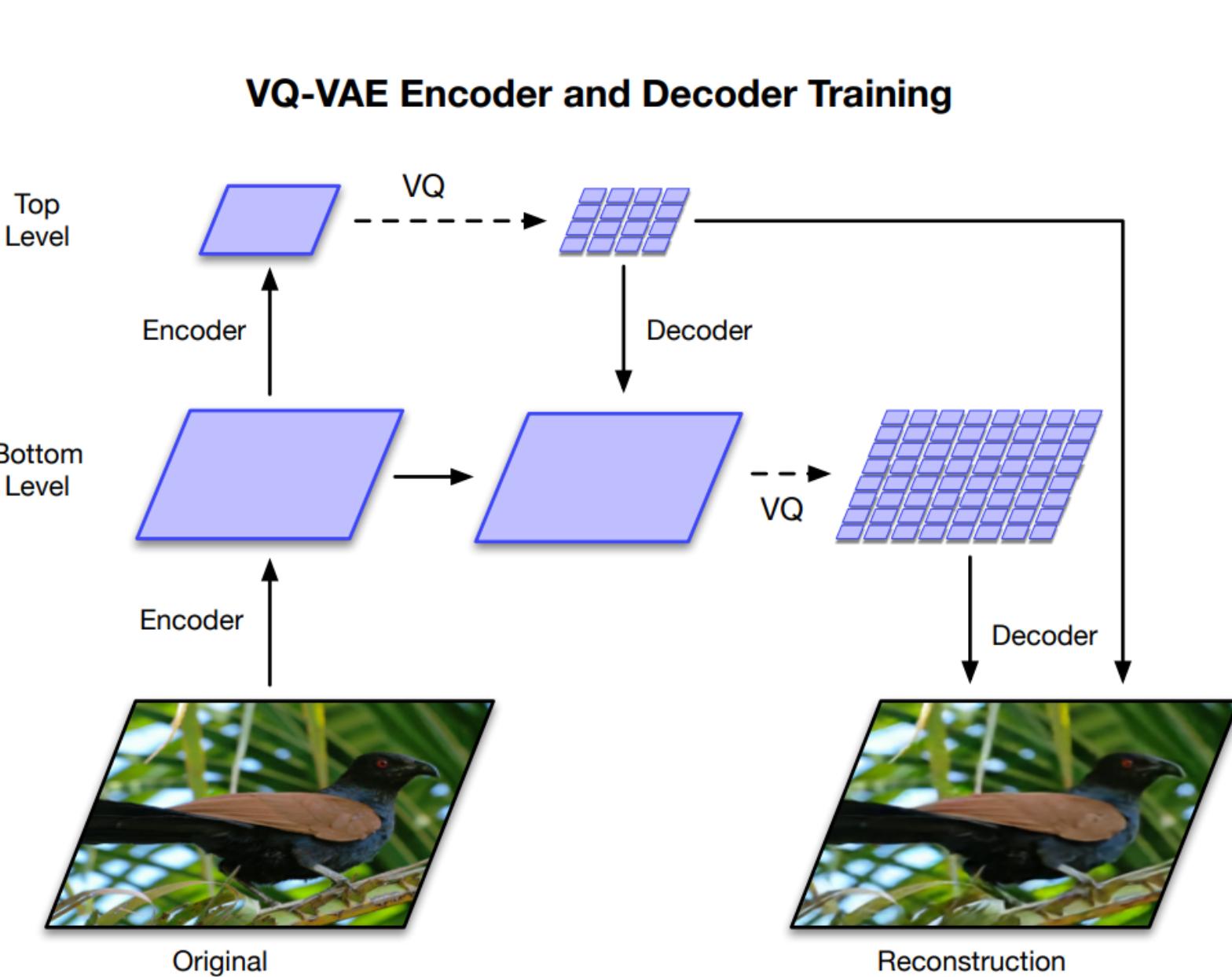
$$\begin{aligned}\mathcal{L}(\theta, \phi) &= \mathcal{L}_{\text{reconstruction}}(\theta, \phi) + \beta \mathcal{L}_{\text{regularization}}(\phi) \\ &= \mathbb{E}_{\mathbf{x} \in \mathcal{D}, \xi \sim \mathcal{N}(0,1)} [-\log p_{\theta}(\mu_{\mathbf{x}} + \sigma_{\mathbf{x}} \xi) + \frac{\beta}{2} \sum_{k=1}^K (\sigma_{\mathbf{x}}^2 + \mu_{\mathbf{x}}^2 - 1 - \log \sigma_{\mathbf{x}}^2)]\end{aligned}$$

- Using $\beta > 1$ puts emphasis on learning statistically independent latent factors.
- The β -VAE allows to **disentangle** the latent variables, i.e. manipulate them individually to vary only one aspect of the image (pose, color, gender, etc.).



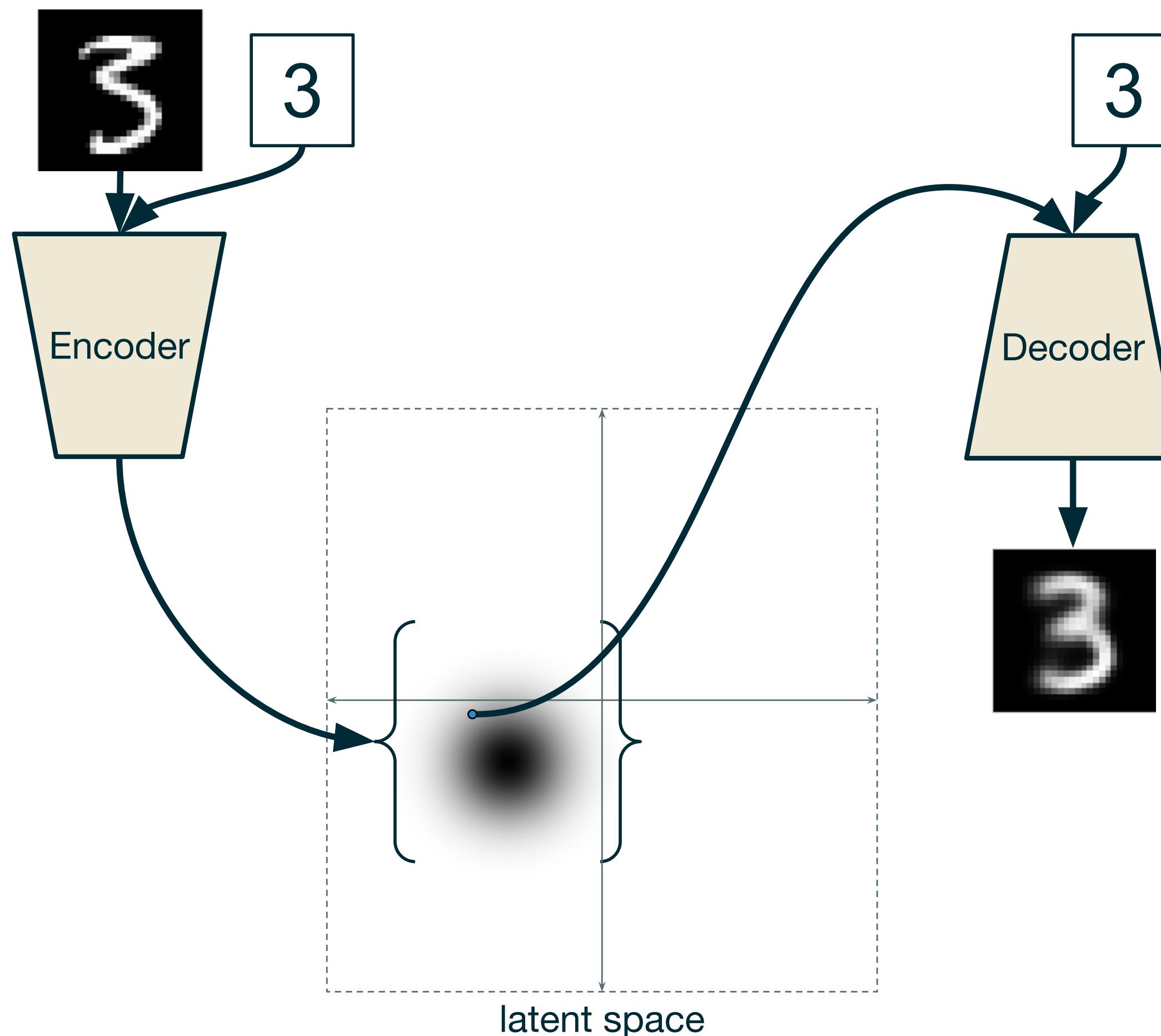
VQ-VAE

- Deepmind researchers proposed VQ-VAE-2, a hierarchical VAE using vector-quantized priors able to generate high-resolution images.



Conditional variational autoencoder (CVAE)

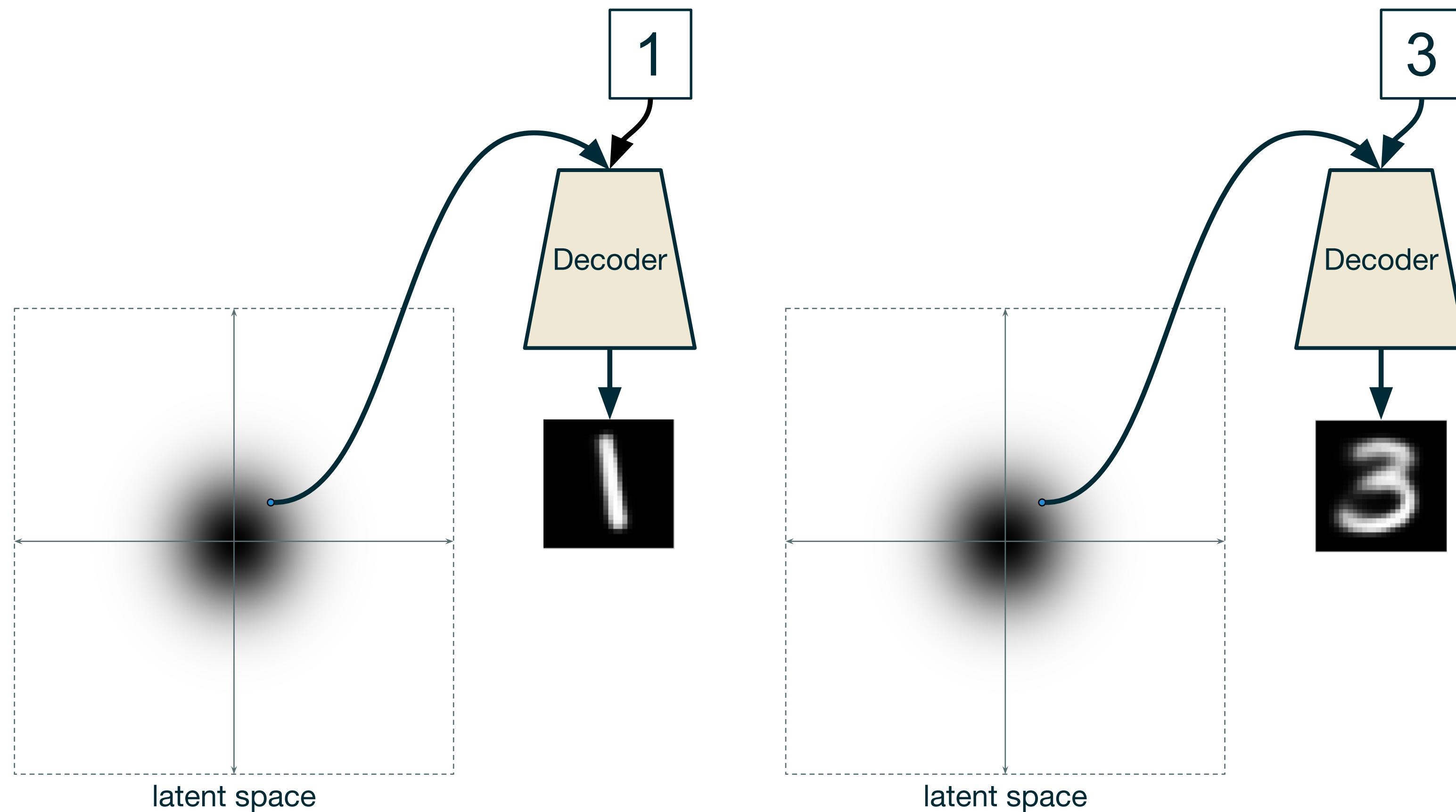
- What if we provide the labels to the encoder and the decoder during training?



Source: <https://ijdykeman.github.io/ml/2016/12/21/cvae.html>

Conditional variational autoencoder (CVAE)

- When trained with labels, the **conditional variational autoencoder** (CVAE) becomes able to sample many images of the same class.



Source: <https://ijdykeman.github.io/ml/2016/12/21/cvae.html>

CVAE on MNIST

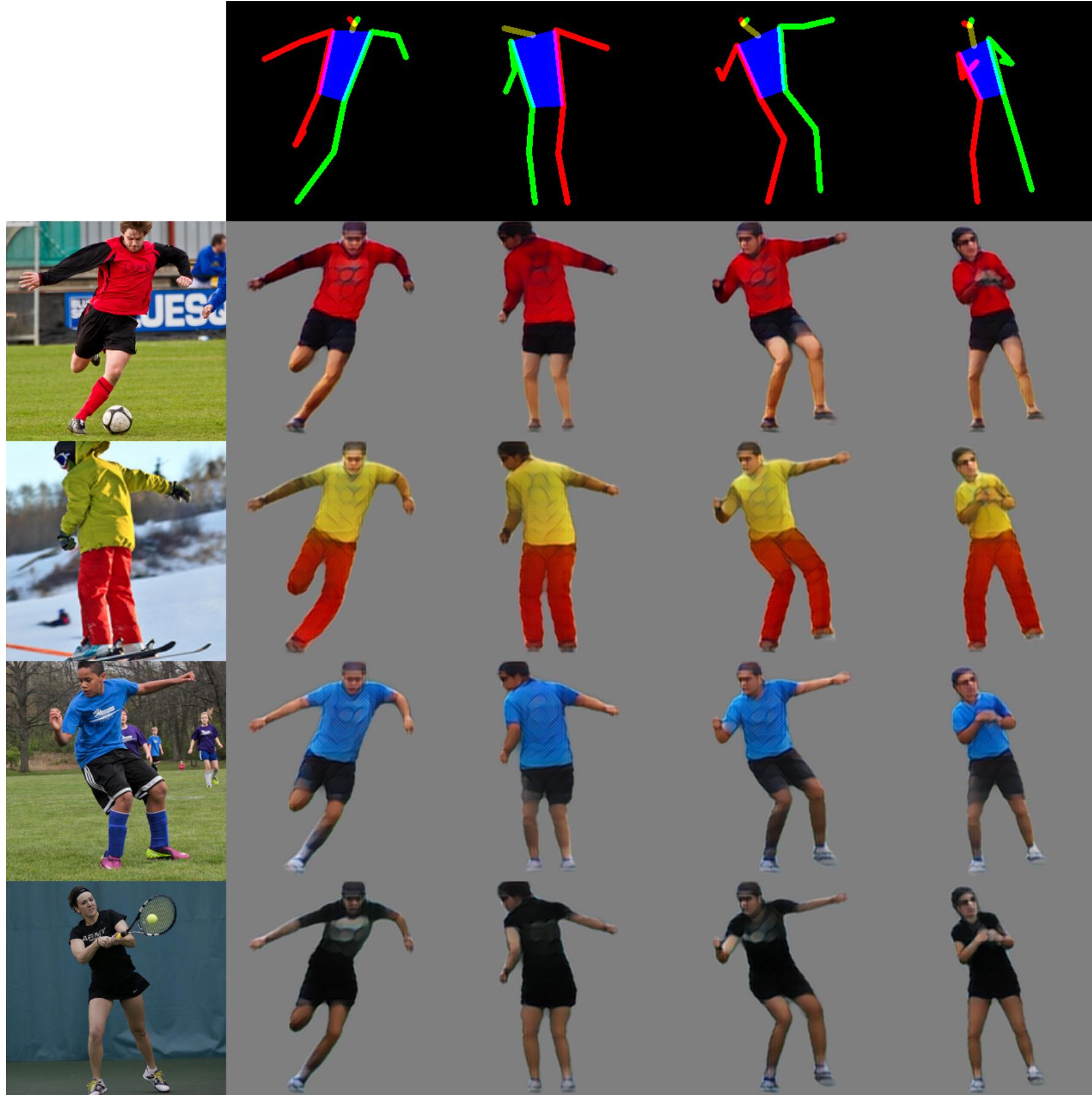
- CVAE allows to sample as many samples of a given class as we want: **data augmentation**.

0 0 0 0 0 0 0 0 0 0
1 1 1 1 1 1 1 1 1 1
2 2 2 2 2 2 2 2 2 2
3 3 3 3 3 3 3 3 3 3
4 4 4 4 4 4 4 4 4 4
5 5 5 5 5 5 5 5 5 5
6 6 6 6 6 6 6 6 6 6
7 7 7 7 7 7 7 7 7 7
8 8 8 8 8 8 8 8 8 8
9 9 9 9 9 9 9 9 9 9

Source: <https://ijdykeman.github.io/ml/2016/12/21/cvae.html>

CVAE on shapes

- The condition does not need to be a label, it can be a shape or another image (passed through another encoder).

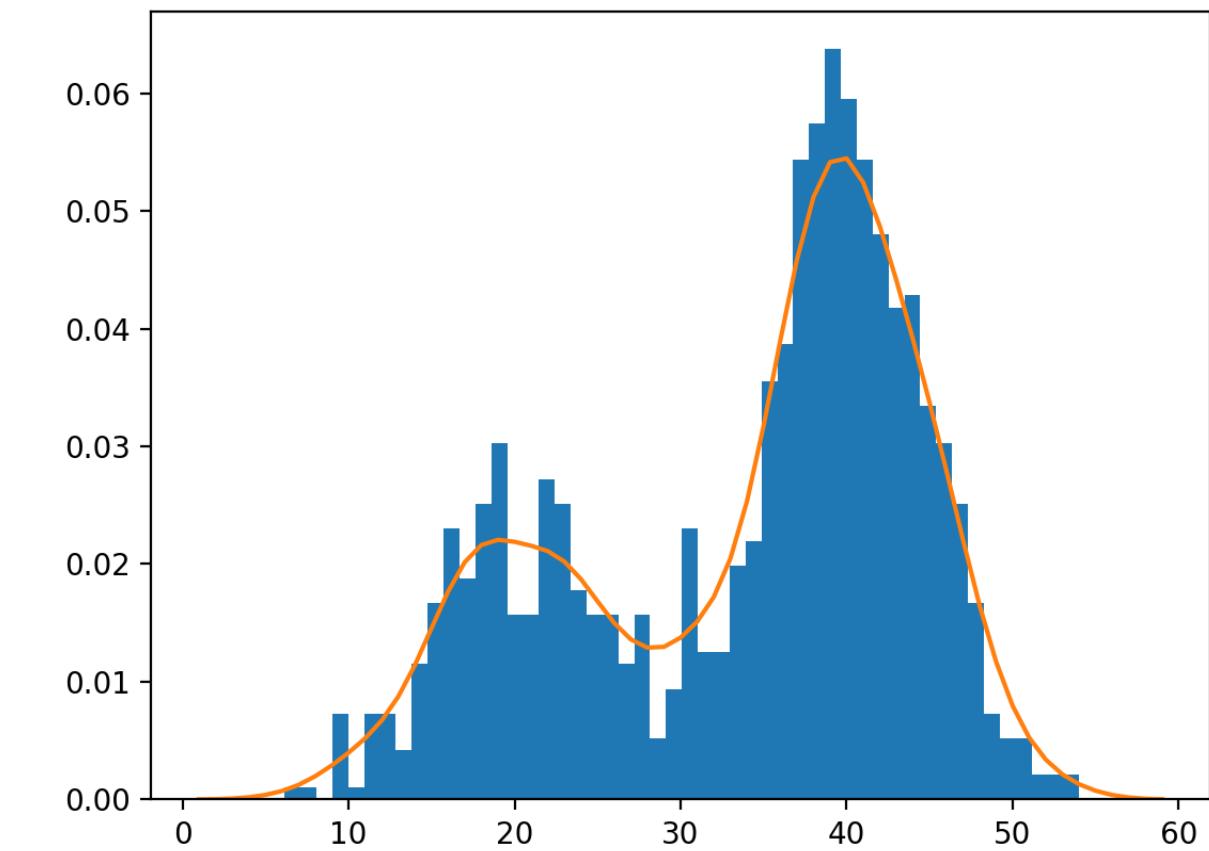


Source: <https://hci.iwr.uni-heidelberg.de/content/variational-u-net-conditional-appearance-and-shape-generation>

5 - Variational inference (optional)

Learning probability distributions from samples

- The input data X comes from an unknown distribution $P(X)$
 - . The training set \mathcal{D} is formed by **samples** of that distribution.
- Learning the distribution of the data means learning a **parameterized distribution** $p_\theta(X)$ that is as close as possible from the true distribution $P(X)$.
- The parameterized distribution could be a family of known distributions (e.g. normal) or a neural network with a softmax output layer.



Source: <https://machinelearningmastery.com/probability-density-estimation/>

- This means that we want to minimize the KL between the two distributions:

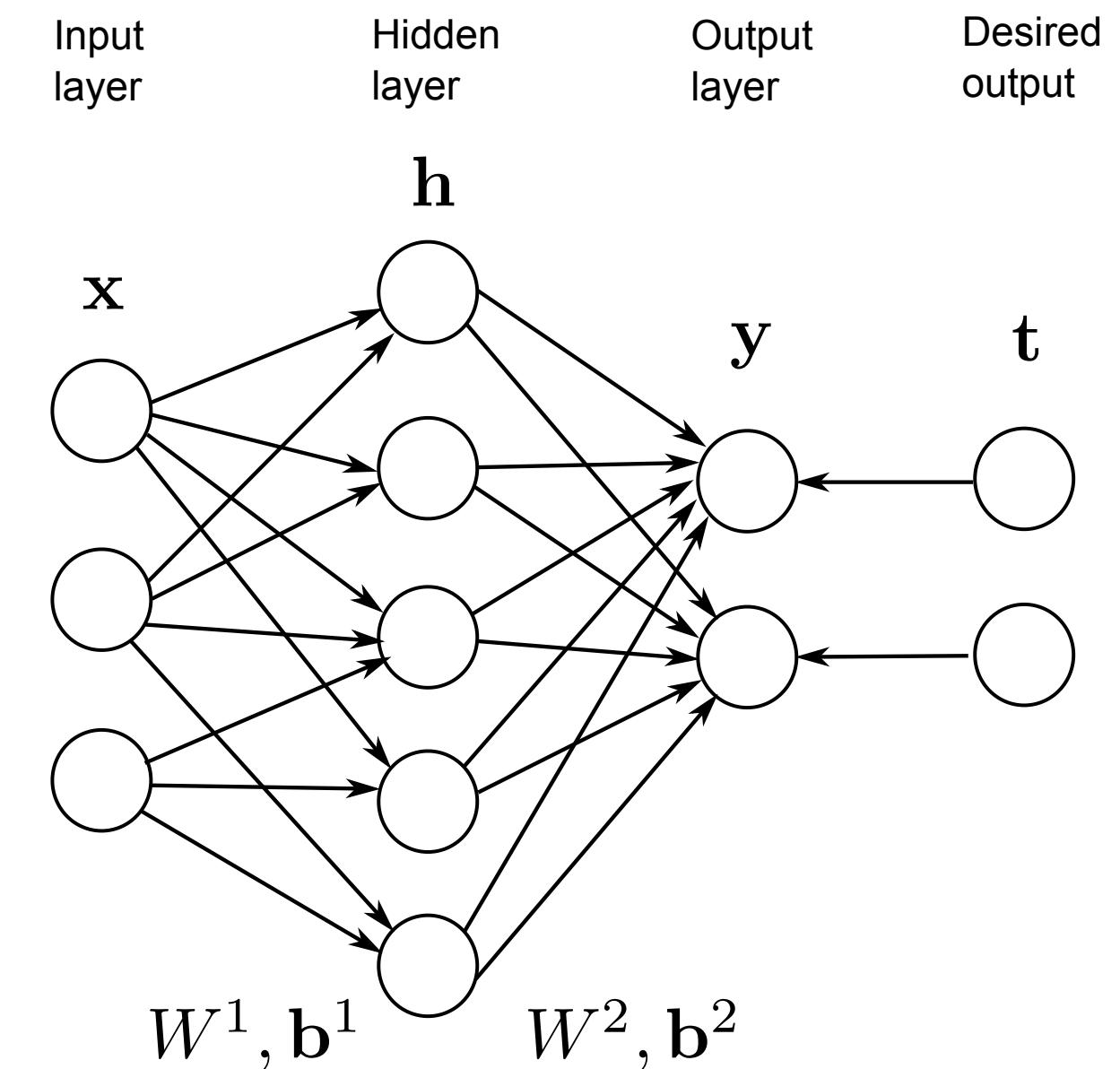
$$\min_{\theta} \text{KL}(P(X) || p_\theta(X)) = \mathbb{E}_{x \sim P(X)} \left[-\log \frac{p_\theta(X = x)}{P(X = x)} \right]$$

- The problem is that we do not know $P(X)$ as it is what we want to learn, so we cannot estimate the KL directly.

Supervised learning

- In supervised learning, we are learning the **conditional probability** $P(T|X)$ of the targets given the inputs, i.e. what is the probability of having the label $T = t$ given the input $X = x$.
- A NN with a softmax output layer represents the parameterized distribution $p_\theta(T|X)$.
- The KL between the two distributions is:

$$\text{KL}(P(T|X) || p_\theta(T|X)) = \mathbb{E}_{x,t \sim \mathcal{D}} \left[-\log \frac{p_\theta(T = t|X = x)}{P(T = t|X = x)} \right]$$



- With the properties of the log, we know that the KL is the cross-entropy minus the entropy of the data:

$$\begin{aligned} \text{KL}(P(T|X) || p_\theta(T|X)) &= \mathbb{E}_{x,t \sim \mathcal{D}} [-\log p_\theta(T = t|X = x)] - \mathbb{E}_{x,t \sim \mathcal{D}} [-\log P(T = t|X = x)] \\ &= H(P(T|X), p_\theta(T|X)) - H(P(T|X)) \end{aligned}$$

Supervised learning

- Kullback-Leibler divergence between the model and the data:

$$\text{KL}(P(T|X) || p_\theta(T|X)) = H(P(T|X), p_\theta(T|X)) - H(P(T|X))$$

- When we minimize the KL by applying gradient descent on the parameters θ , only the cross-entropy will change, as the data does not depends on the model:

$$\nabla_\theta \text{KL}(P(T|X) || p_\theta(T|X)) = \nabla_\theta H(P(T|X), p_\theta(T|X)) - \nabla_\theta H(P(T|X))$$

$$= \nabla_\theta H(P(T|X), p_\theta(T|X))$$

$$= \nabla_\theta \mathbb{E}_{x,t \sim \mathcal{D}}[-\log p_\theta(T = t | X = x)]$$

- Minimizing the cross-entropy (negative log likelihood) of the model on the data is the same as minimizing the KL between the two distributions in supervised learning!
- We were actually minimizing the KL all along.

Maximum likelihood estimation

- When trying to learn the distribution $P(X)$ of the data directly, we could use the same trick:

$$\nabla_{\theta} \text{KL}(P(X) || p_{\theta}(X)) = \nabla_{\theta} H(P(X), p_{\theta}(X)) = \nabla_{\theta} \mathbb{E}_{x \sim X}[-\log p_{\theta}(X = x)]$$

i.e. maximize the log-likelihood of the model on the data X .

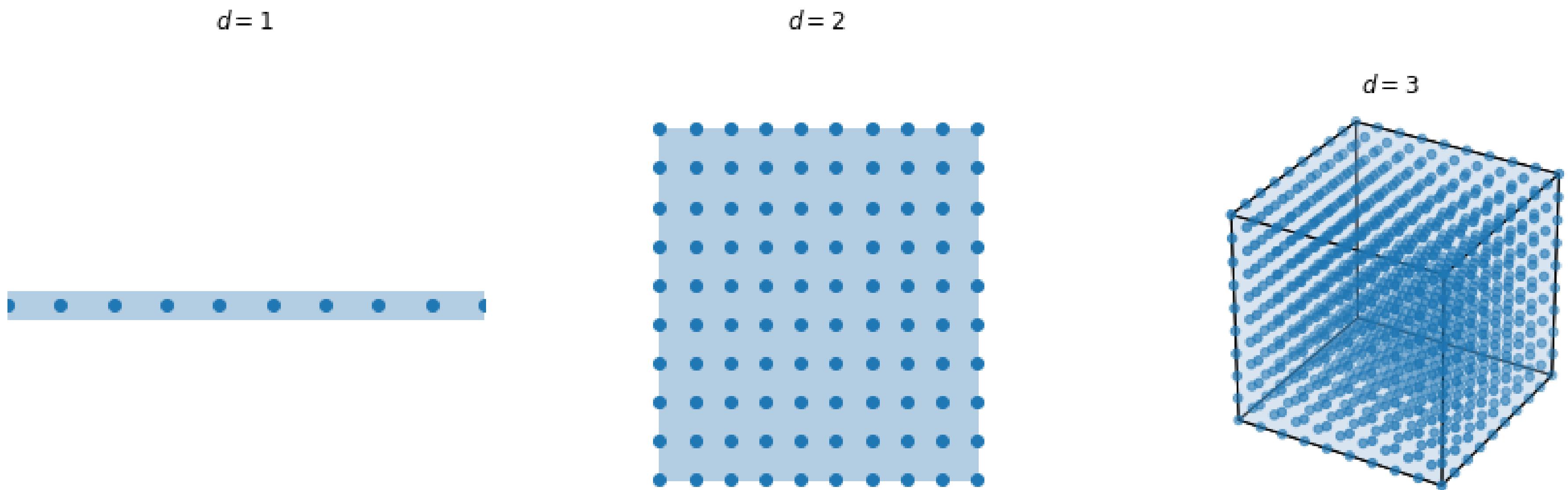
- If we use N data samples to estimate the expectation, we notice that:

$$\mathbb{E}_{x \sim X}[\log p_{\theta}(X = x)] \approx \frac{1}{N} \sum_{i=1}^N \log p_{\theta}(X = x_i) = \frac{1}{N} \log \prod_{i=1}^N p_{\theta}(X = x_i) = \frac{1}{N} \log L(\theta)$$

is indeed the log-likelihood of the model on the data that we maximized in **maximum likelihood estimation**.

Curse of dimensionality

- The problem is that images are **highly-dimensional** (one dimension per pixel), so we would need astronomical numbers of samples to estimate the gradient (once): **curse of dimensionality**.

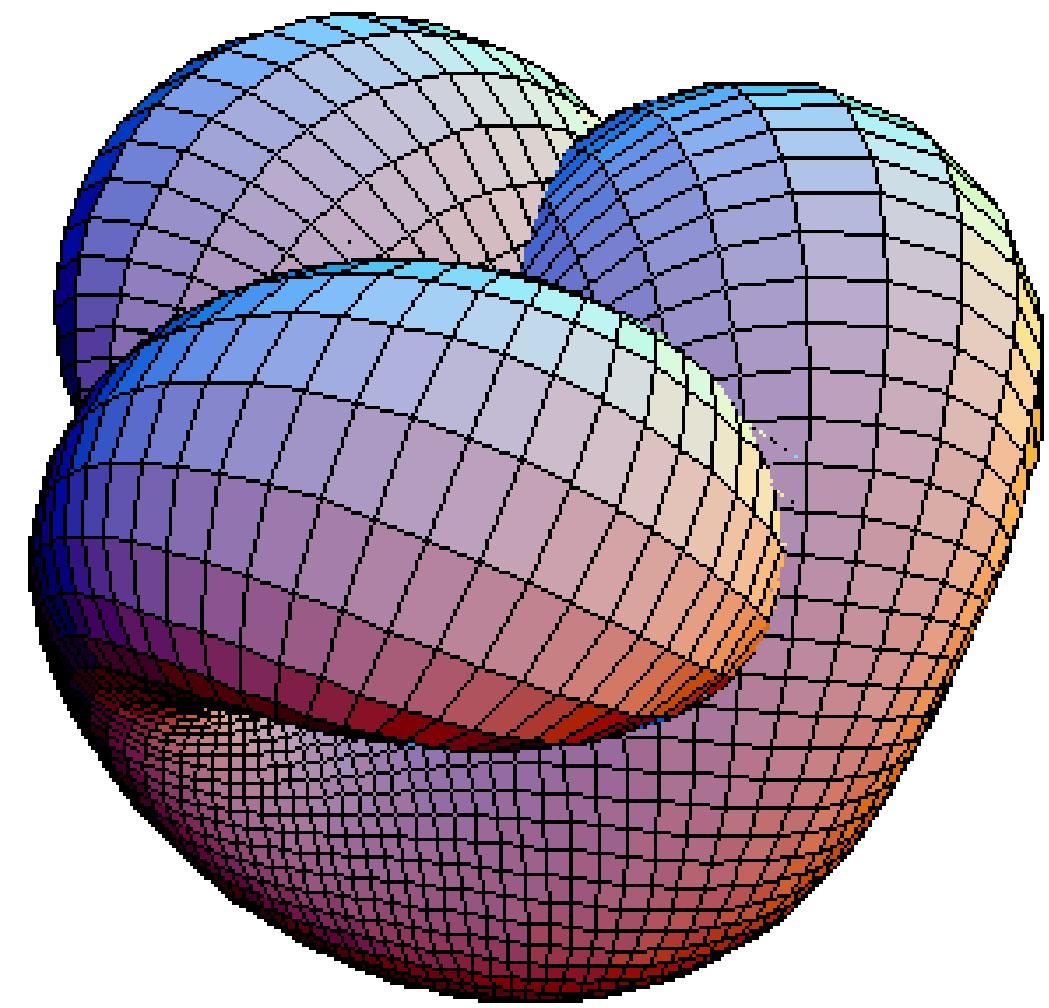


Source: <https://dibyaghosh.com/blog/probability/highdimensionalgeometry.html>

- MLE does not work well in high-dimensional spaces.
- We need to work in a much lower-dimensional space.

Manifolds

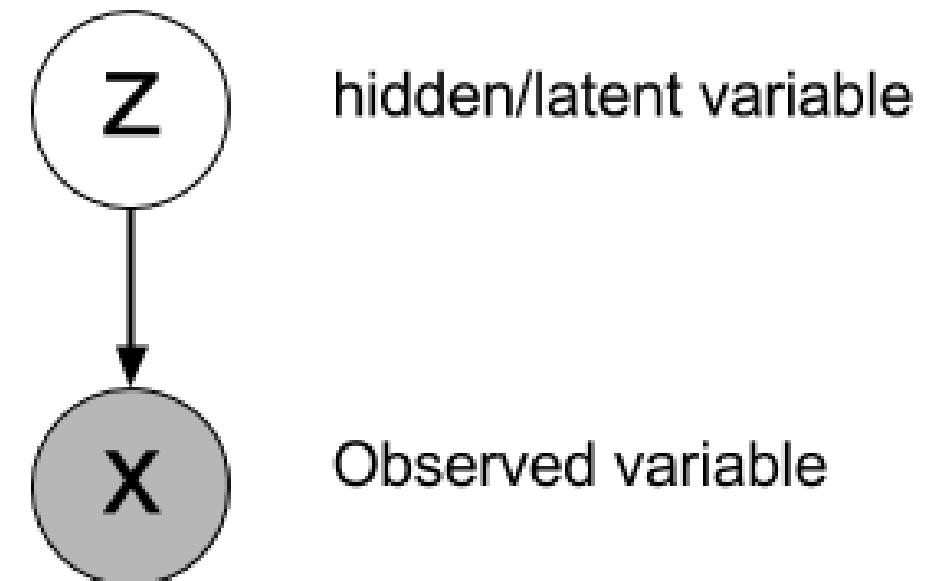
- Images are not random samples of the pixel space: **natural images** are embedded in a much lower-dimensional space called a **manifold**.
- A manifold is a **locally Euclidian** topological space of lower dimension.
- The surface of the earth is locally flat and 2D, but globally spherical and 3D.
- If we have a **generative model** telling us how a point on the manifold z maps to the image space ($P(X|z)$), we would only need to learn the distribution of the data in the lower-dimensional **latent space**.



Source: <https://en.wikipedia.org/wiki/Manifold>

Generative model

- The low-dimensional **latent variables** z are the actual cause for the observations X .
- Given a sample z on the manifold, we can train a **generative model** $p_\theta(X|z)$ to recreate the input X .
- $p_\theta(X|z)$ is the **decoder**: given a latent representation z , what is the corresponding observation X ?



Source:
<https://blog.evjang.com/2016/08/variational-bayes.html>

- If we learn the distribution $p_\theta(z)$ of the manifold (latent space), we can infer the distribution of the data $p_\theta(X)$ using that model:

$$p_\theta(X) = \mathbb{E}_{z \sim p_\theta(z)}[p_\theta(X|z)] = \int_z p_\theta(X|z) p_\theta(z) dz$$

- Problem: we do not know $p_\theta(z)$, as the only data we see is X : z is called a **latent variable** because it explains the data but is hidden.

Variational inference

- To estimate $p_\theta(z)$, we could again marginalize over X :

$$p_\theta(z) = \mathbb{E}_{x \sim p_\theta(X)} [p_\theta(z|x)] = \int_x p_\theta(z|x) p_\theta(x) dx$$

- $p_\theta(z|x)$ is the **encoder**: given an input $x \sim p_\theta(X)$, what is its latent representation z ?
- The Bayes rule tells us:

$$p_\theta(z|x) = p_\theta(x|z) \frac{p_\theta(z)}{p_\theta(x)}$$

- The posterior probability (encoder) $p_\theta(z|X)$ depends on the model (decoder) $p_\theta(X|z)$, the prior (assumption) $p_\theta(z)$ and the evidence (data) $p_\theta(X)$.
- We get:

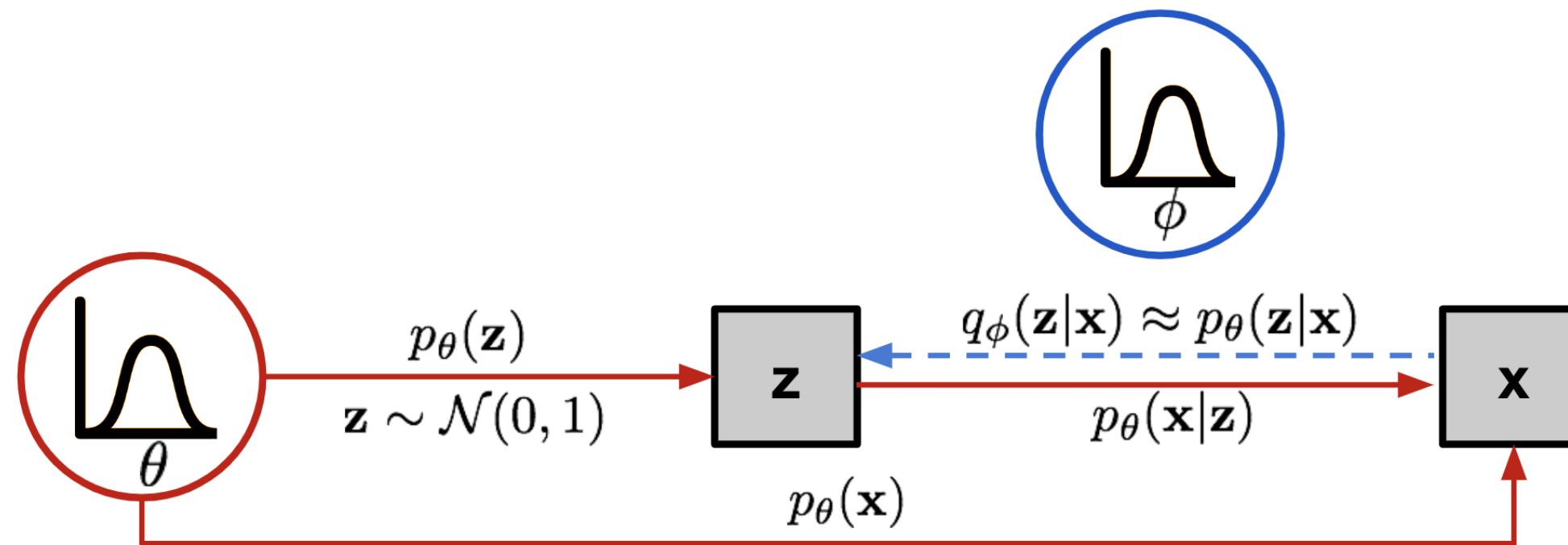
$$p_\theta(z) = \mathbb{E}_{x \sim p_\theta(X)} [p_\theta(x|z) \frac{p_\theta(z)}{p_\theta(x)}]$$

Variational inference

- The posterior is **untractable** as it would require to integrate over all possible inputs $x \sim p_\theta(X)$:

$$p_\theta(z) = \mathbb{E}_{x \sim p_\theta(X)} [p_\theta(x|z) \frac{p_\theta(z)}{p_\theta(x)}] = \int_x p_\theta(x|z) p_\theta(z) dx$$

- Variational inference** proposes to approximate the true encoder $p_\theta(z|x)$ by another parameterized distribution $q_\phi(z|x)$.



Source: <https://lilianweng.github.io/lil-log/2018/08/12/from-autoencoder-to-beta-vae.html>

- The decoder $p_\theta(x|z)$ generates observations x from a latent representation z with parameters θ .
- The encoder $q_\phi(z|x)$ estimates the latent representation z of a generated observation x . It should approximate $p_\theta(z|x)$ with parameters ϕ .

Variational inference

- To make $q_\phi(z|X)$ close from $p_\theta(z|X)$, we minimize their KL divergence:

$$\text{KL}(q_\phi(z|X) || p_\theta(z|X)) = \mathbb{E}_{z \sim q_\phi(z|X)} \left[-\log \frac{p_\theta(z|X)}{q_\phi(z|X)} \right]$$

- Note that we sample the latent representations from the learned encoder $q_\phi(z|X)$ (imagination).
- As $p_\theta(z|X) = p_\theta(X|z) \frac{p_\theta(z)}{p_\theta(X)}$, we get:

$$\begin{aligned} \text{KL}(q_\phi(z|X) || p_\theta(z|X)) &= \mathbb{E}_{z \sim q_\phi(z|X)} \left[-\log \frac{p_\theta(X|z) p_\theta(z)}{q_\phi(z|X) p_\theta(X)} \right] \\ &= \mathbb{E}_{z \sim q_\phi(z|X)} \left[-\log \frac{p_\theta(z)}{q_\phi(z|X)} \right] - \mathbb{E}_{z \sim q_\phi(z|X)} \left[-\log p_\theta(X) \right] \\ &\quad + \mathbb{E}_{z \sim q_\phi(z|X)} \left[-\log p_\theta(X|z) \right] \end{aligned}$$

- $p_\theta(X)$ does not depend on z , so its expectation w.r.t z is constant:

$$\text{KL}(q_\phi(z|X) || p_\theta(z|X)) = \text{KL}(q_\phi(z|X) || p_\theta(z)) + \log p_\theta(X) + \mathbb{E}_{z \sim q_\phi(z|X)} \left[-\log p_\theta(X|z) \right]$$

Evidence lower bound

- We rearrange the terms:

$$\log p_\theta(X) - \text{KL}(q_\phi(z|X) || p_\theta(z|X)) = -\mathbb{E}_{z \sim q_\phi(z|X)}[-\log p_\theta(X|z)] - \text{KL}(q_\phi(z|X) || p_\theta(z))$$

- Training the **encoder** means that we **minimize** $\text{KL}(q_\phi(z|X) || p_\theta(z|X))$.
- Training the **decoder** means that we **maximize** $\log p_\theta(X)$ (log-likelihood of the model).
- Training the encoder and decoder together means that we **maximize**:

$$\text{ELBO}(\theta, \phi) = \log p_\theta(X) - \text{KL}(q_\phi(z|X) || p_\theta(z|X))$$

- The KL divergence is always positive or equal to 0, so we have:

$$\text{ELBO}(\theta, \phi) \leq \log p_\theta(X)$$

- This term is called the **evidence lower bound** (ELBO): by maximizing it, we also maximize the untractable evidence $\log p_\theta(X)$, which is what we want to do.

Variational inference

- The trick is that the right-hand term of the equation gives us a tractable definition of the ELBO term:

$$\begin{aligned}\text{ELBO}(\theta, \phi) &= \log p_\theta(X) - \text{KL}(q_\phi(z|X) || p_\theta(z|X)) \\ &= -\mathbb{E}_{z \sim q_\phi(z|X)}[-\log p_\theta(X|z)] - \text{KL}(q_\phi(z|X) || p_\theta(z))\end{aligned}$$

- What happens when we **minimize** the negative ELBO?

$$\mathcal{L}(\theta, \phi) = -\text{ELBO}(\theta, \phi) = \mathbb{E}_{z \sim q_\phi(z|X)}[-\log p_\theta(X|z)] + \text{KL}(q_\phi(z|X) || p_\theta(z))$$

- $\mathbb{E}_{z \sim q_\phi(z|X)}[-\log p_\theta(X|z)]$ is the **reconstruction loss** of the decoder $p_\theta(X|z)$:
 - Given a sample z of the encoder $q_\phi(z|X)$, minimize the negative log-likelihood of the reconstruction $p_\theta(X|z)$.
- $\text{KL}(q_\phi(z|X) || p_\theta(z))$ is the **regularization loss** for the encoder:
 - The latent distribution $q_\phi(z|X)$ should be too far from the **prior** $p_\theta(z)$.

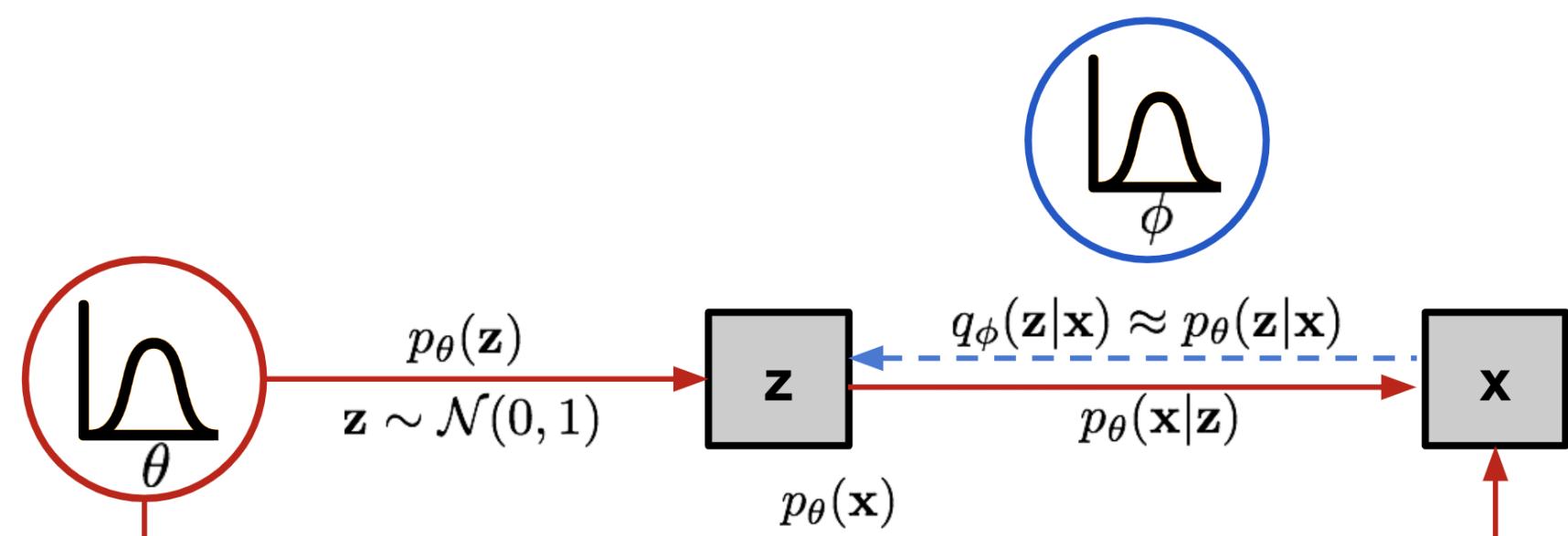
Variational autoencoders

- **Variational autoencoders** use $\mathcal{N}(0, 1)$ as a prior for the latent space, but any other prior could be used.

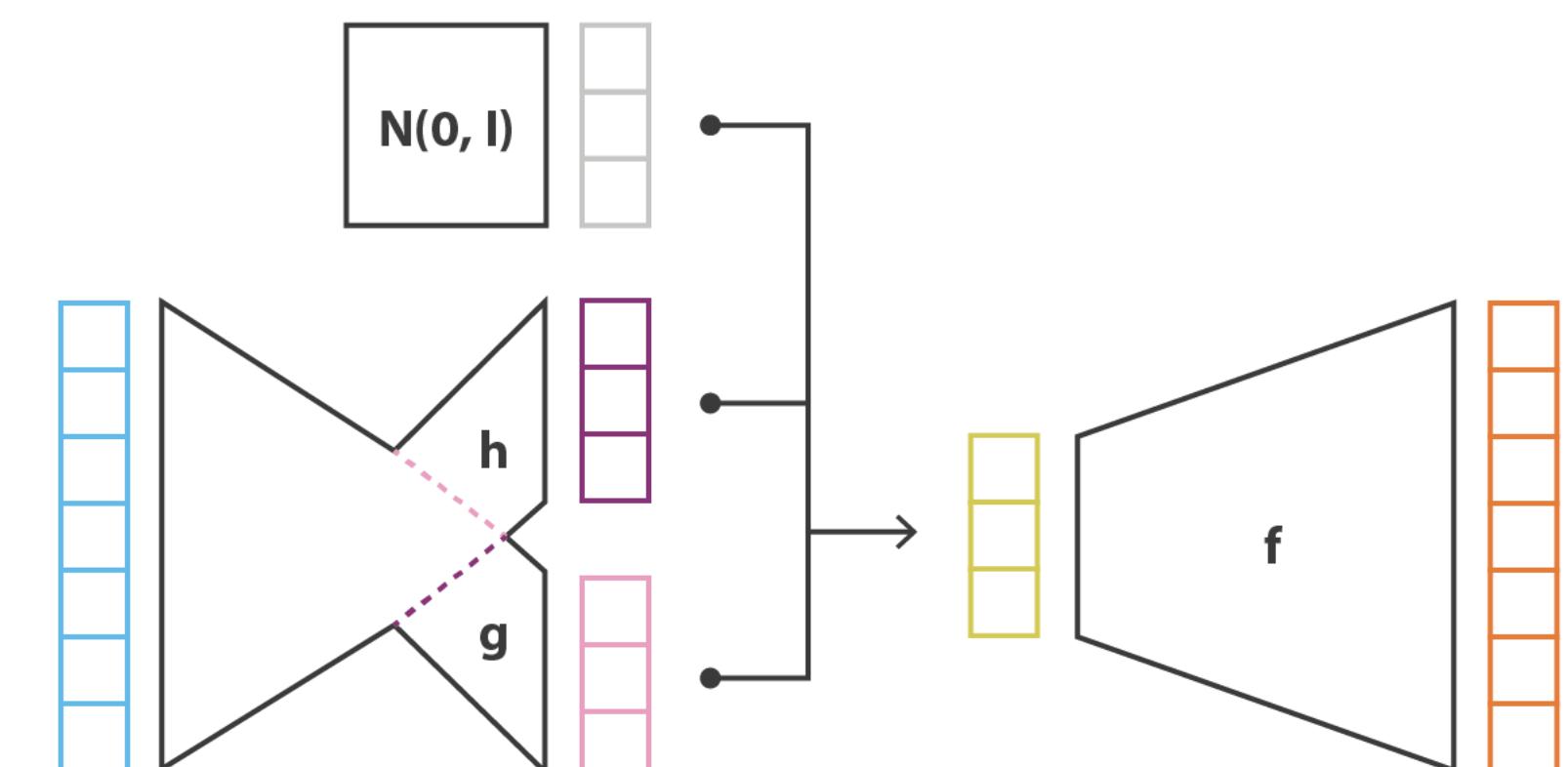
$$\mathcal{L}(\theta, \phi) = \mathcal{L}_{\text{reconstruction}}(\theta, \phi) + \mathcal{L}_{\text{regularization}}(\phi)$$

$$= \mathbb{E}_{\mathbf{x} \in \mathcal{D}, \mathbf{z} \sim q_\phi(\mathbf{z}|\mathbf{x})} [-\log p_\theta(\mathbf{z})] + \text{KL}(q_\phi(\mathbf{z}|\mathbf{x}) || \mathcal{N}(0, 1))$$

- The reparameterization trick and the fact that the KL between normal distributions has a closed form allow us to use backpropagation end-to-end.
- The encoder $q_\phi(z|X)$ and decoder $p_\theta(X|z)$ are neural networks in a VAE, but other parametrized distributions can be used (e.g. in physics).



Source: <https://lilianweng.github.io/lil-log/2018/08/12/from-autoencoder-to-beta-vae.html>



Source: <https://ijdykeman.github.io/ml/2016/12/21/cvae.html>