Deep Learning & Applied AI

PCA and VAEs

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SAPIENZA
UNIVERSITÀ DI ROMA

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Generative models

Overall idea:

Learn a distribution from some given training samples, and generate new samples from the same distribution.

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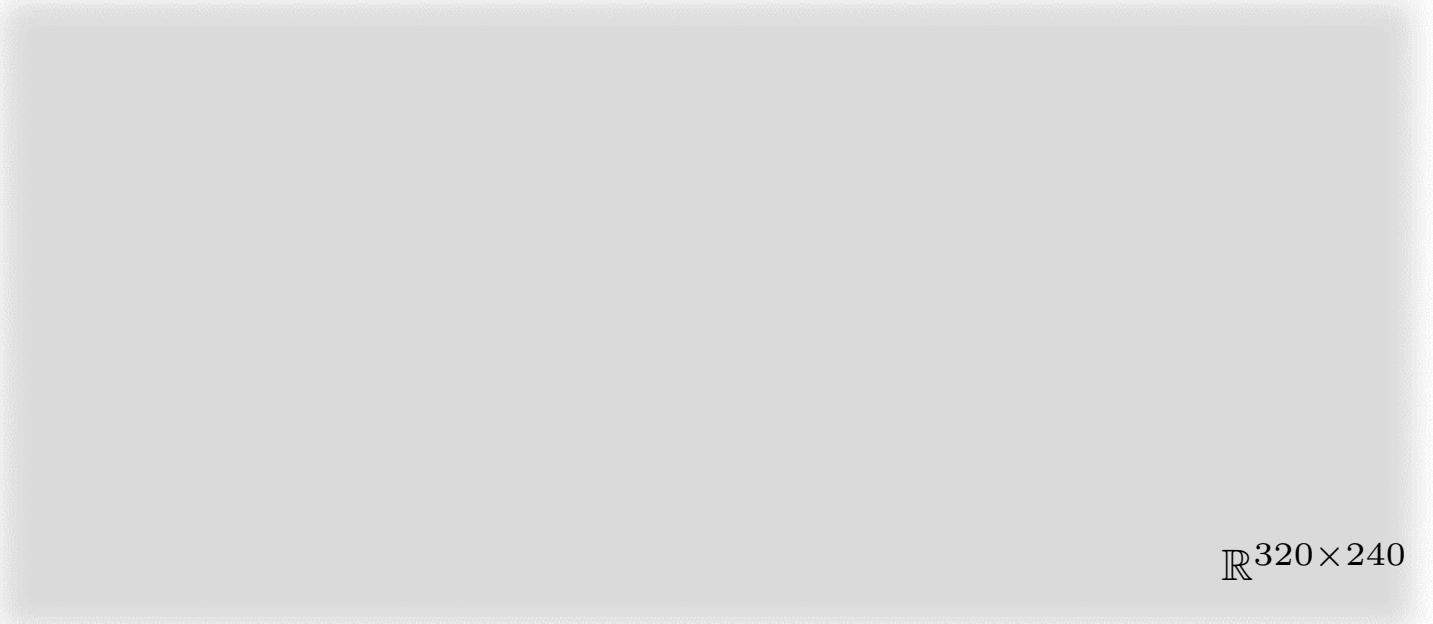
https://this-person-does-not-exist.com/

Generative models

What does it mean to learn a distribution?



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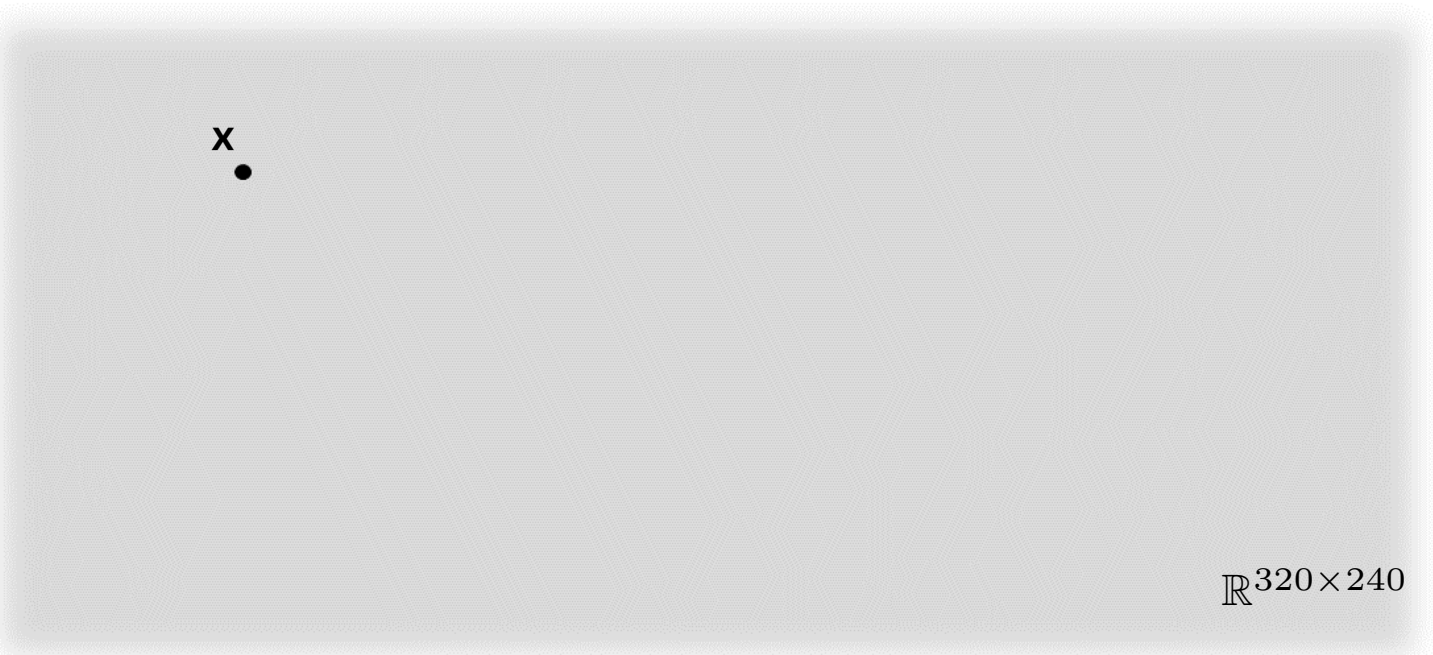

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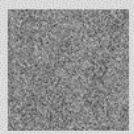

$\mathbb{R}^{320 \times 240}$

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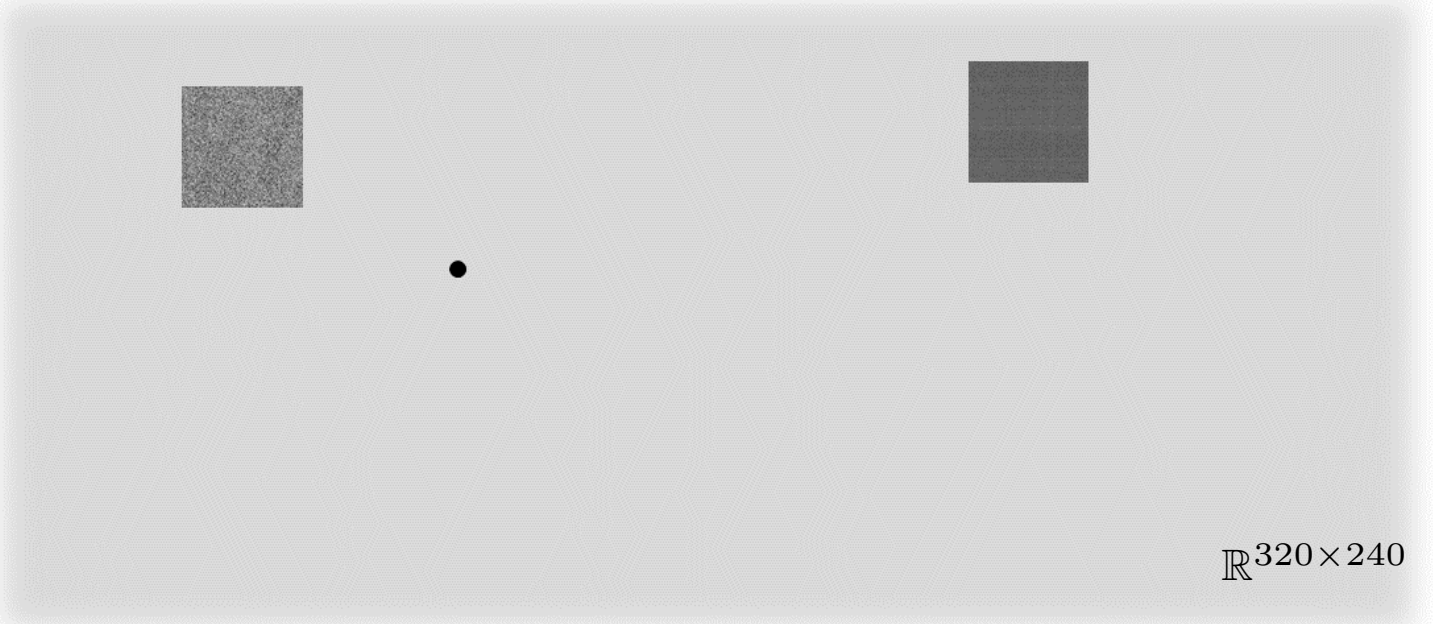

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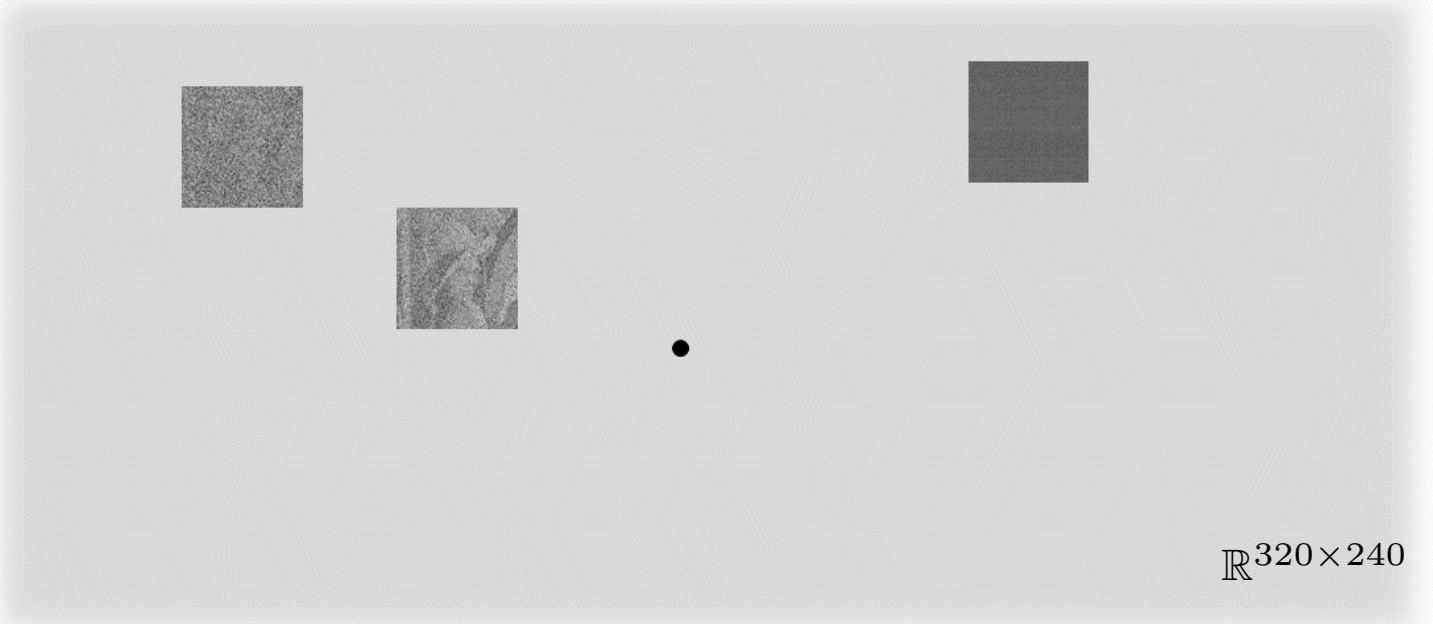

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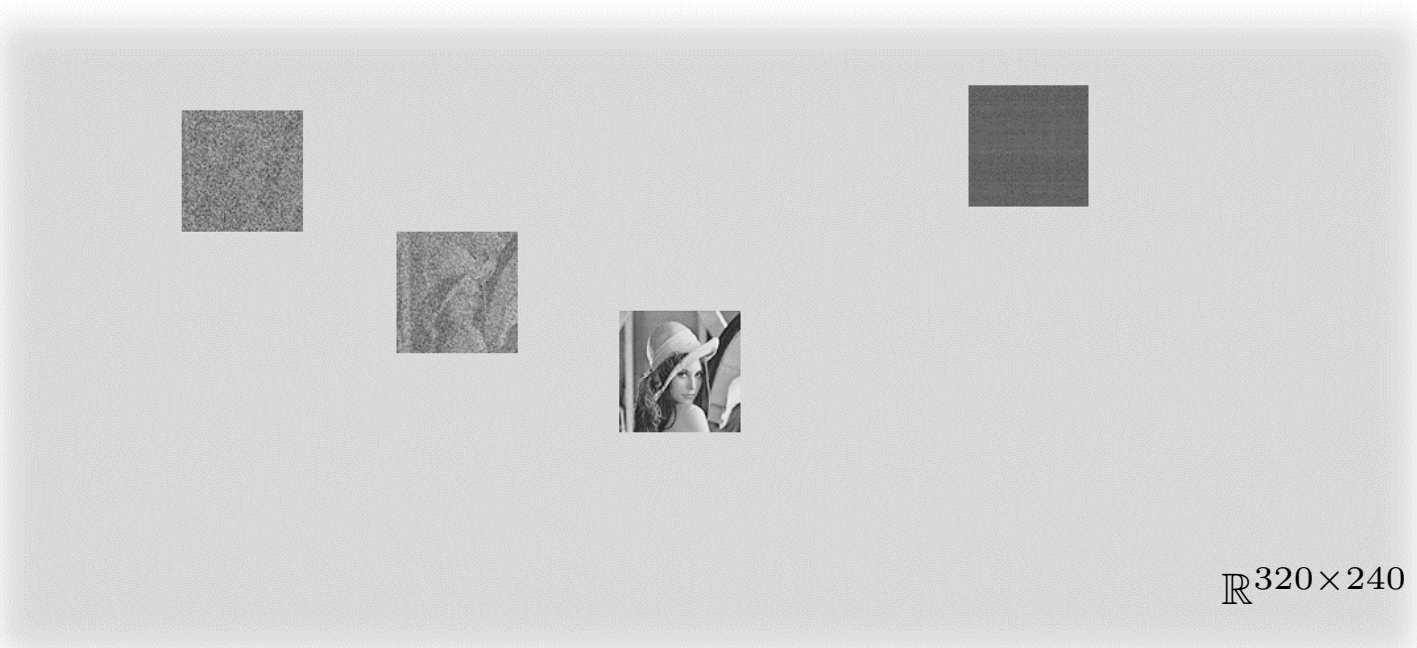

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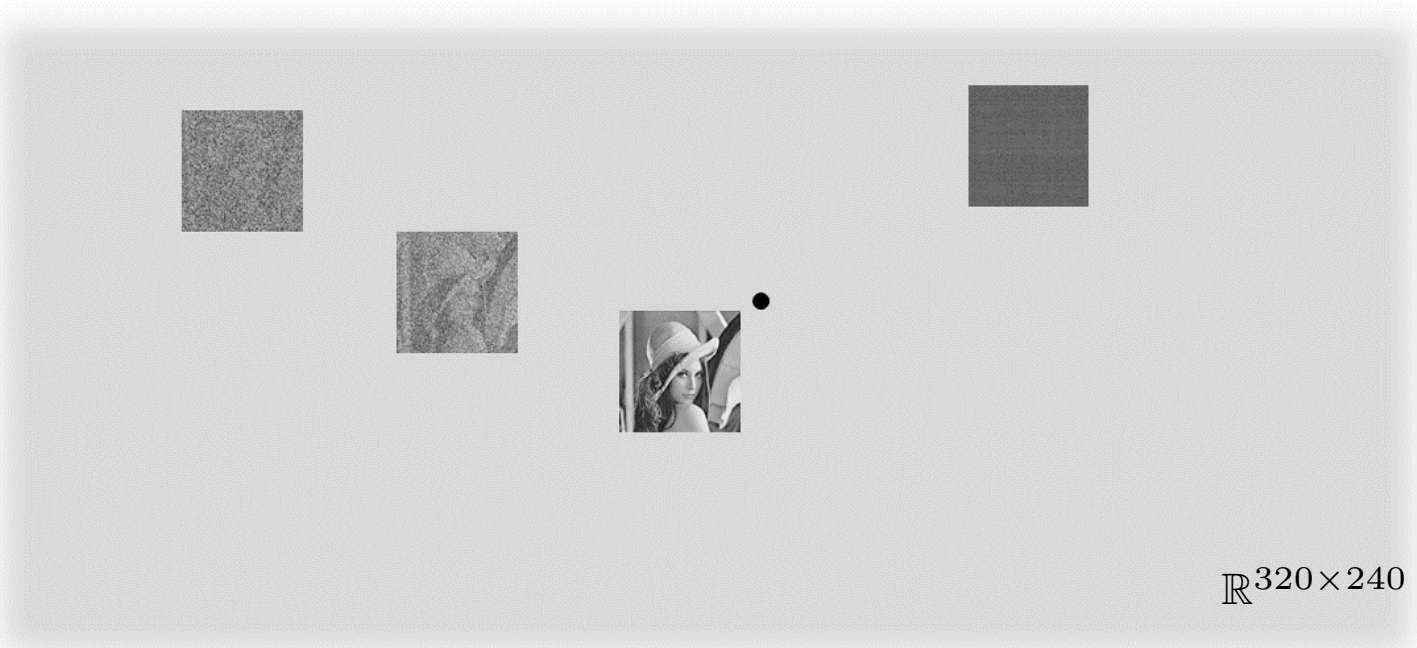

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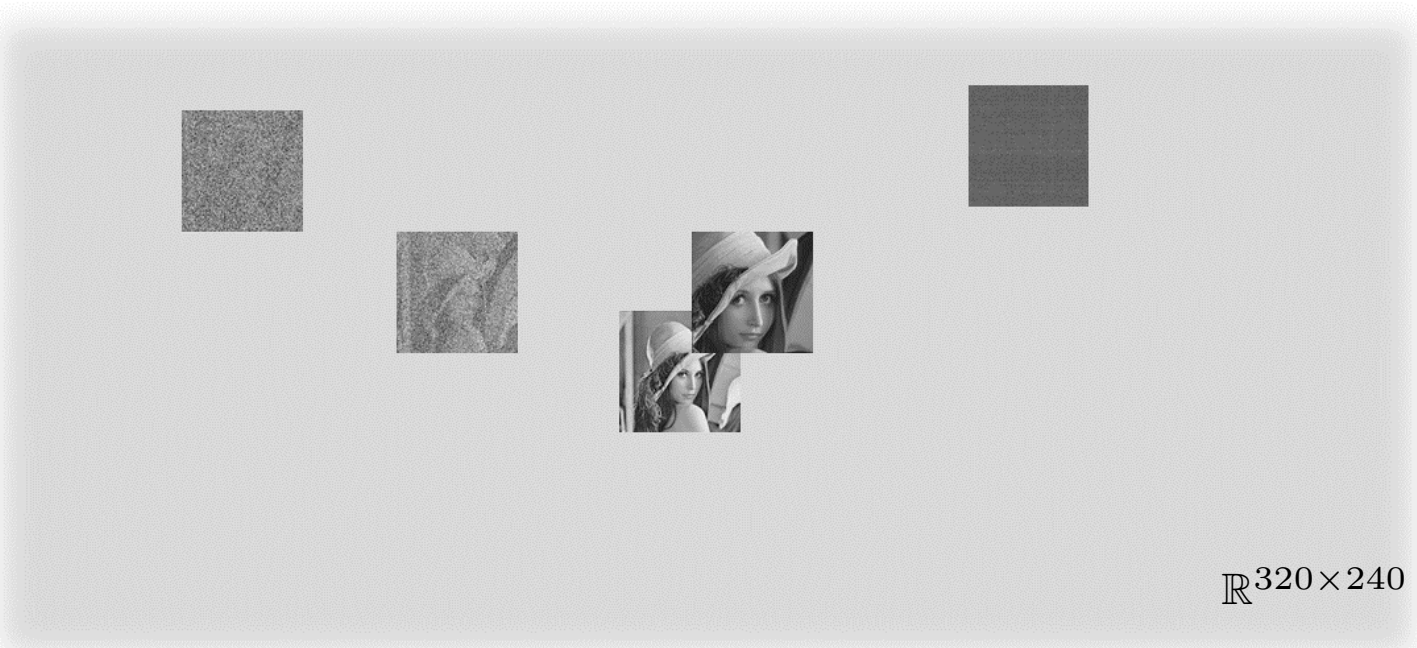

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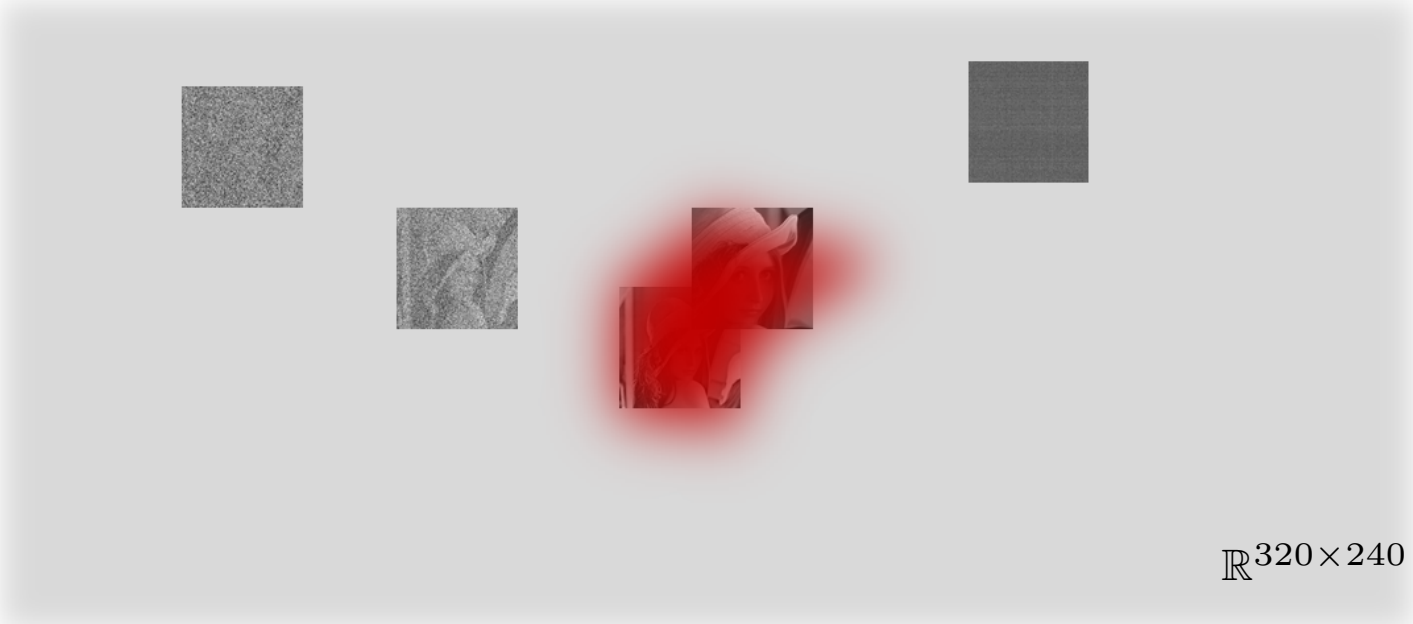

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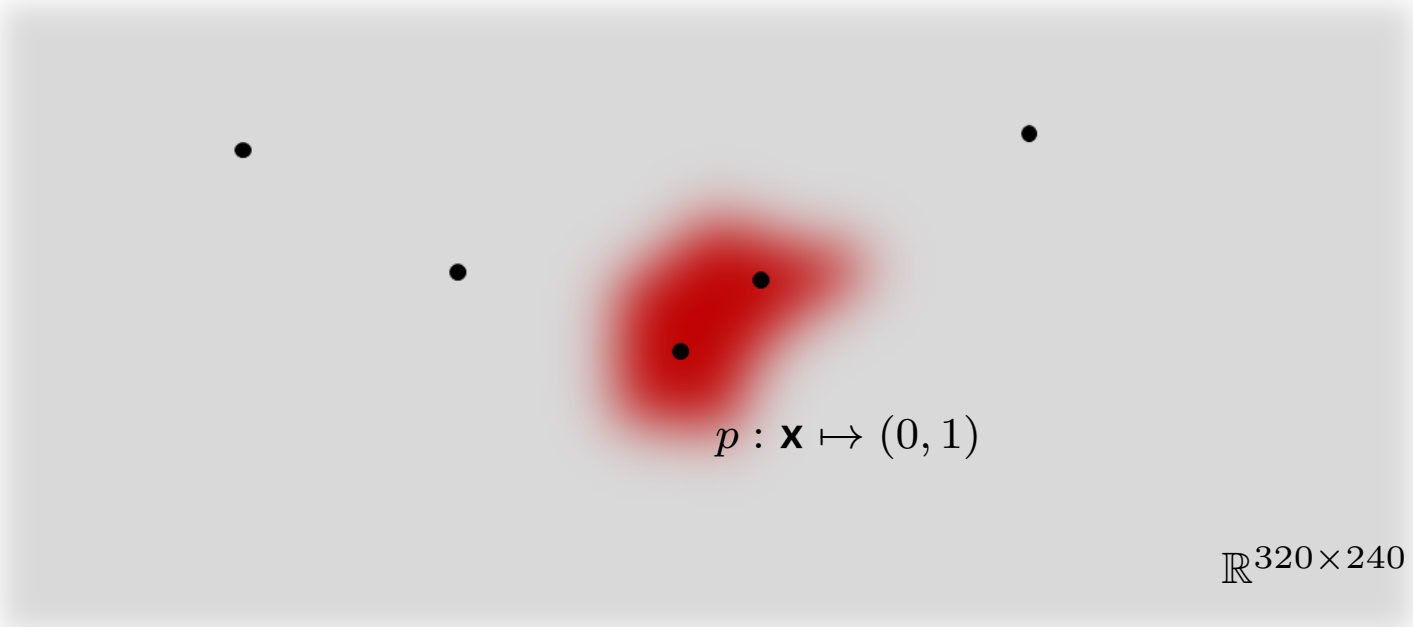
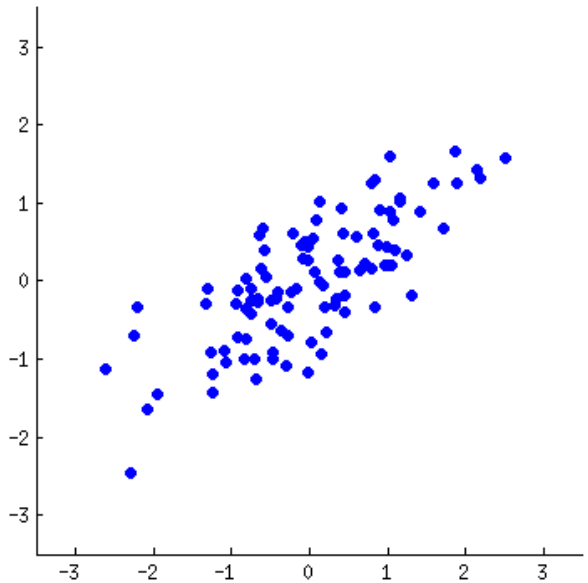


Probability distribution p defined on the entire data space.

Principal component analysis (PCA)

Regard our data as n points in $\mathbb{R}^d$:



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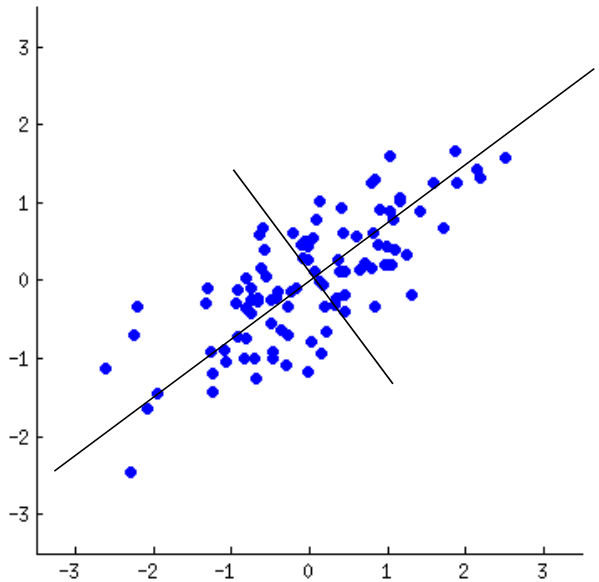

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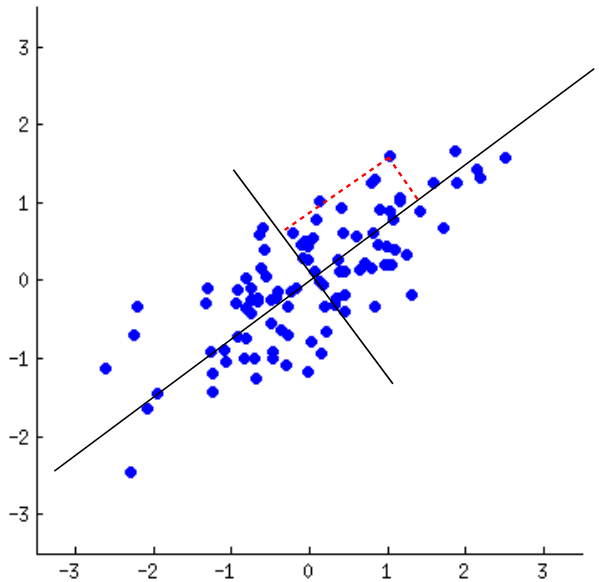

Overall idea:

- Find $k \leq d$ orthogonal directions with the most variance.
- Project all the data points onto these directions.

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In matrix notation:

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We call the columns of $\mathbf{W}$ principal components.

They are unknown and must be computed.

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We seek the direction $\mathbf{w}$ (a column of $\mathbf{W}$) that:

- Minimizes the projection/reconstruction error.
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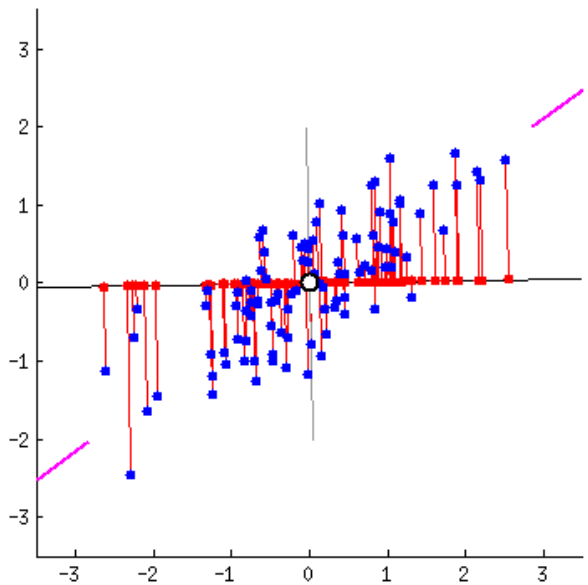

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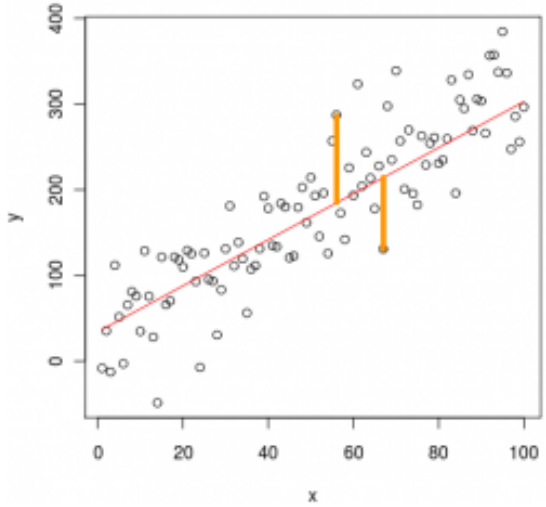
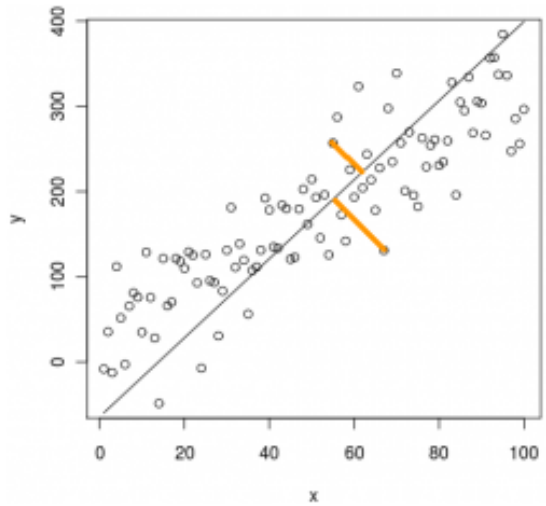
Solution: $\mathbf{w} =$ principal eigenvector of $\mathbf{C}$

PCA is not linear regression

Linear regression: measure along the y coordinate:



PCA: measure orthogonal to the principal direction:



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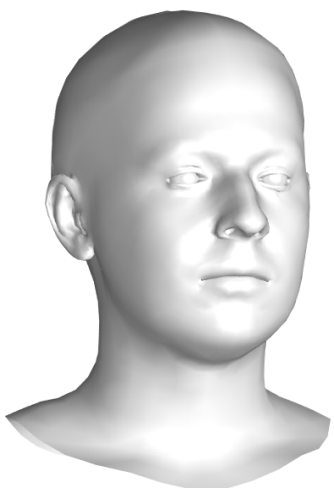
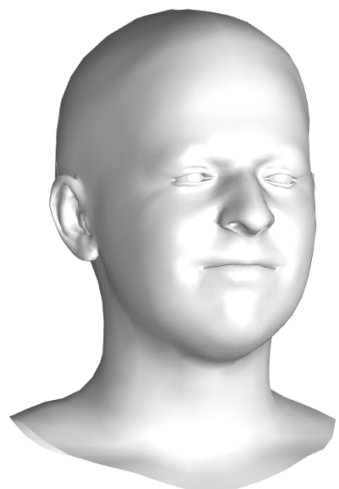
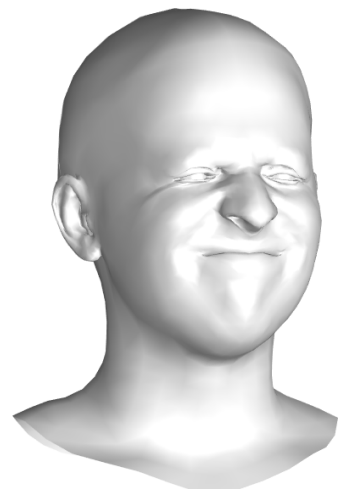
Example:



Data point $\mathbf{x}_1$



Generated
$\mathbf{x}_{\text{new}} = \frac{1}{2}\mathbf{W}(\mathbf{z}_1 + \mathbf{z}_2)$



Data point $\mathbf{x}_2$

Codes

Consider again the relations:

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New perspective: PCA as a parametric model.

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Each data point $\mathbf{x}$ is transformed into a low-dimensional code $\mathbf{z} \in \mathbb{R}^k$, where the dimension $k < d$ is fixed.

Encoding and decoding are linear.

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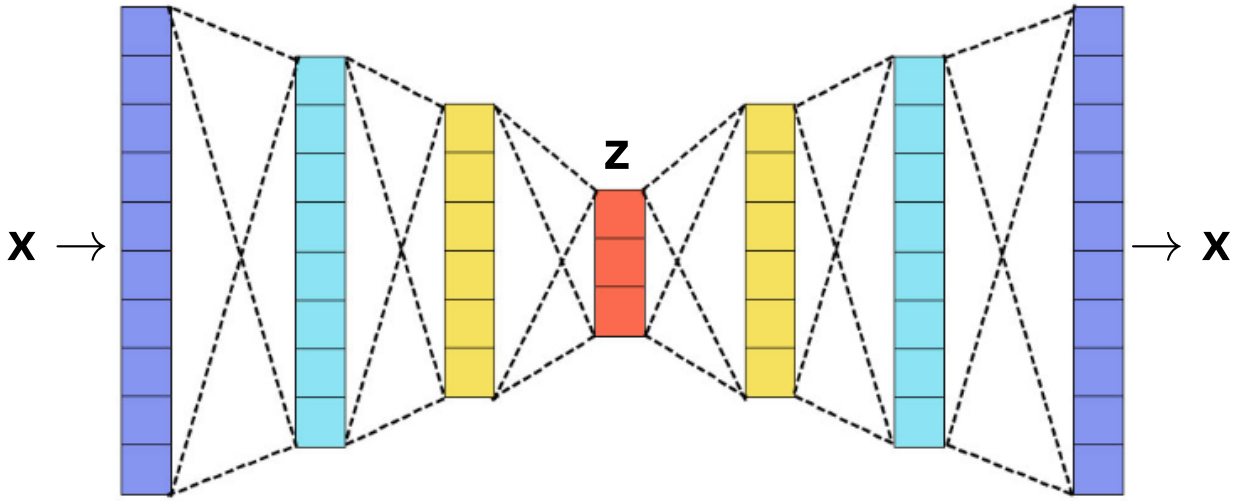
How to generalize this idea?

Autoencoders (AE)

Implement encoding and decoding via deep nets.



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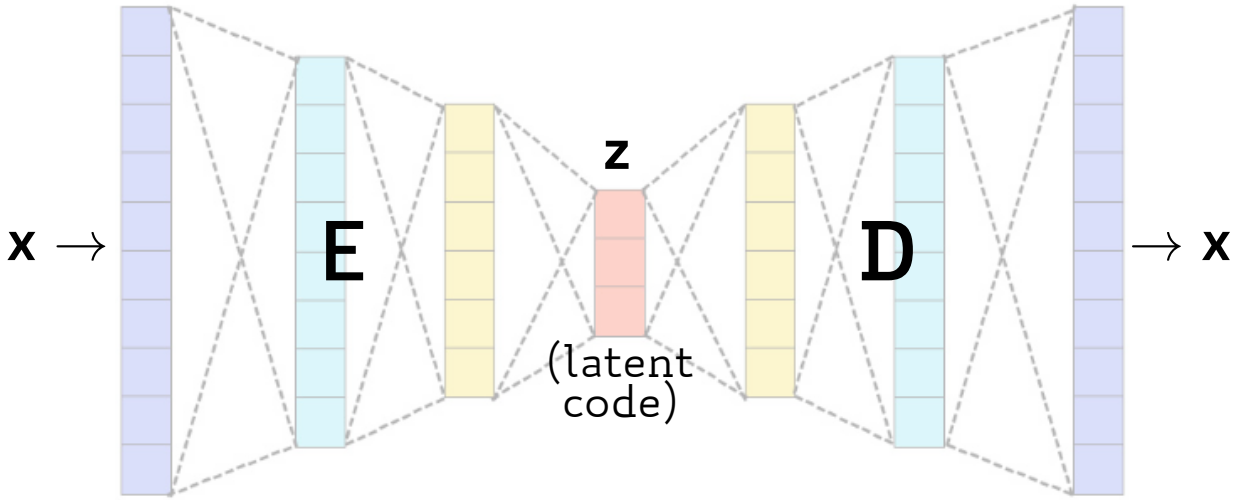

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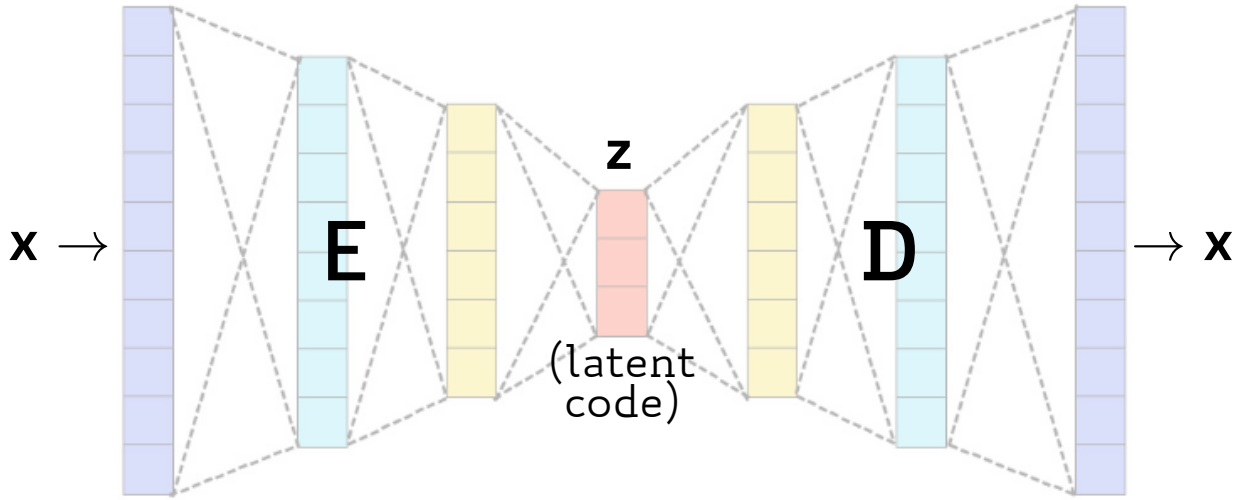

Given a dataset $\{\mathbf{x}_i\}$, require encoder E and decoder (or generator) D to minimize the reconstruction loss:

$$\ell_\Theta = \sum_i \|\mathbf{x}_i - D_\Theta(E_\Theta(\mathbf{x}_i))\|$$

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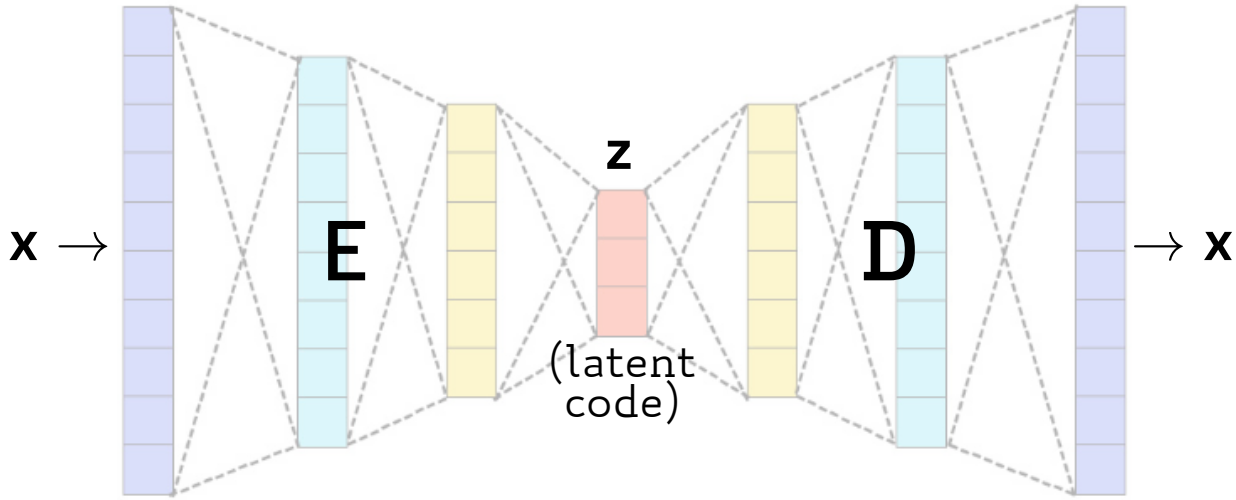

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The choice of the metric depends on the data.

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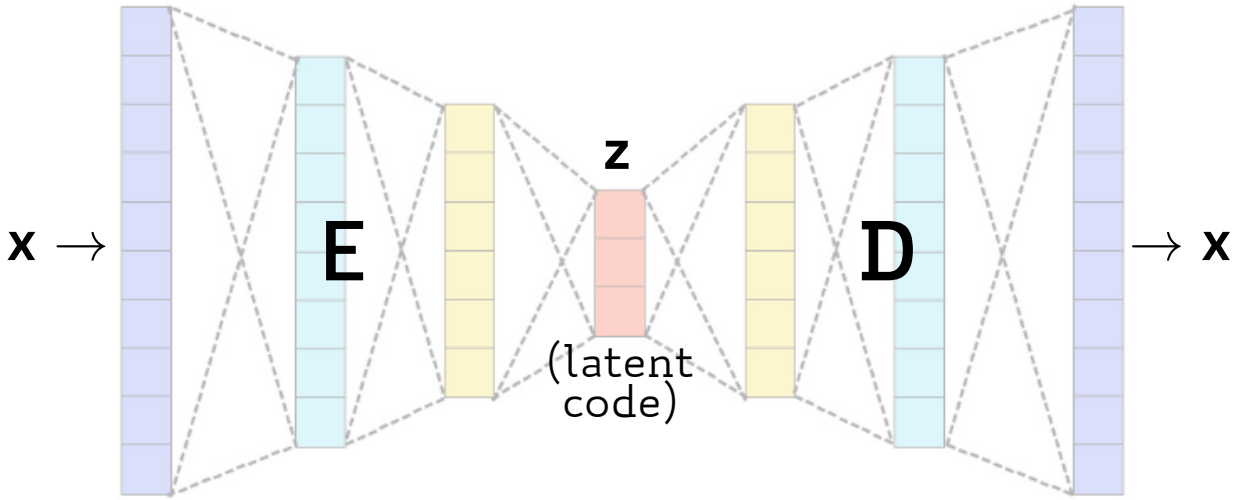

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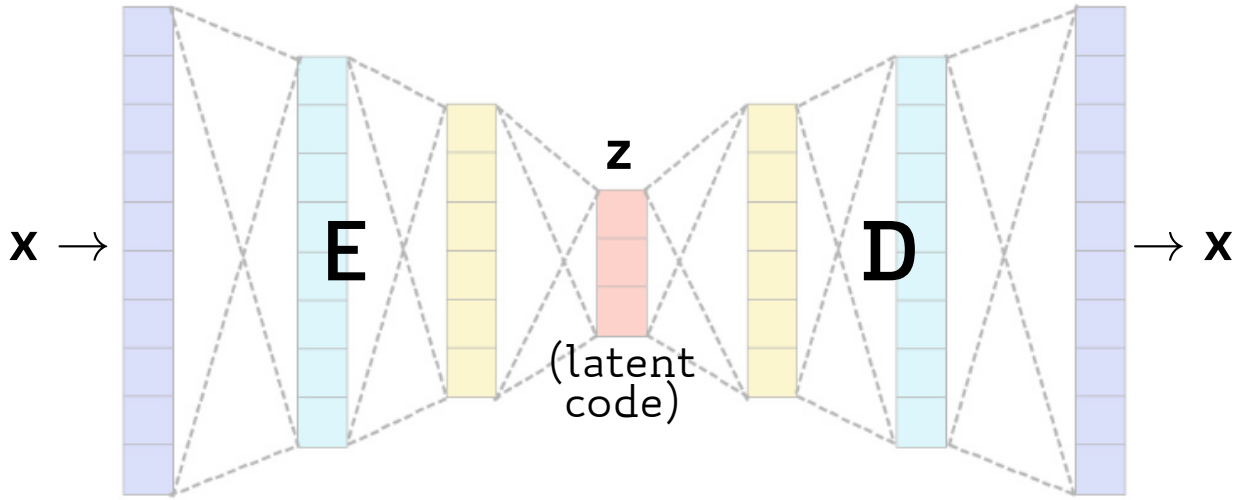
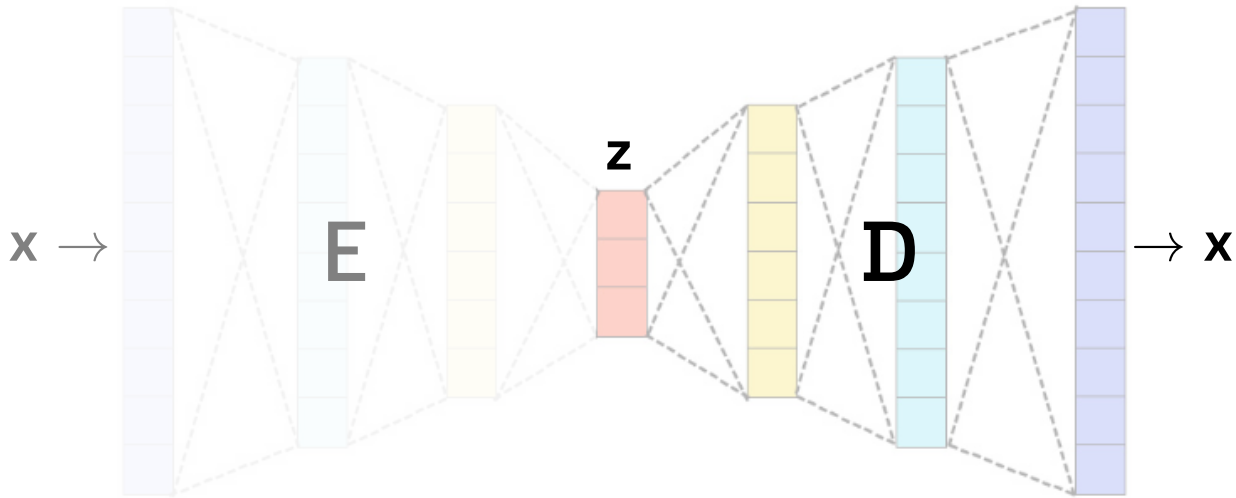


- The bottleneck prevents trivial solutions.
- Task: reconstruction.

  Once the AE is trained, study the structure of the latent space and use E, D for new tasks.

Manifold hypothesis



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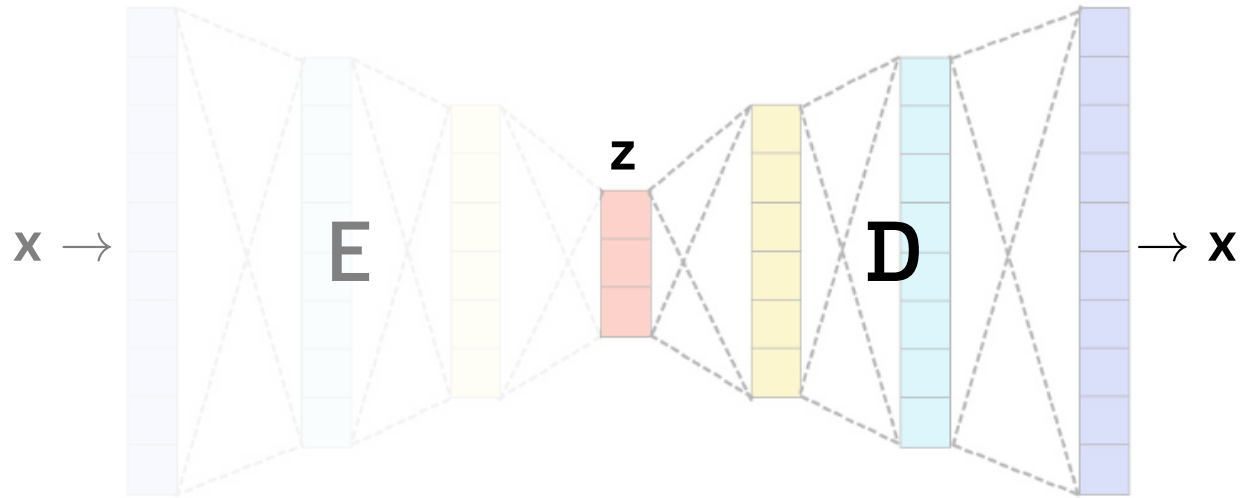

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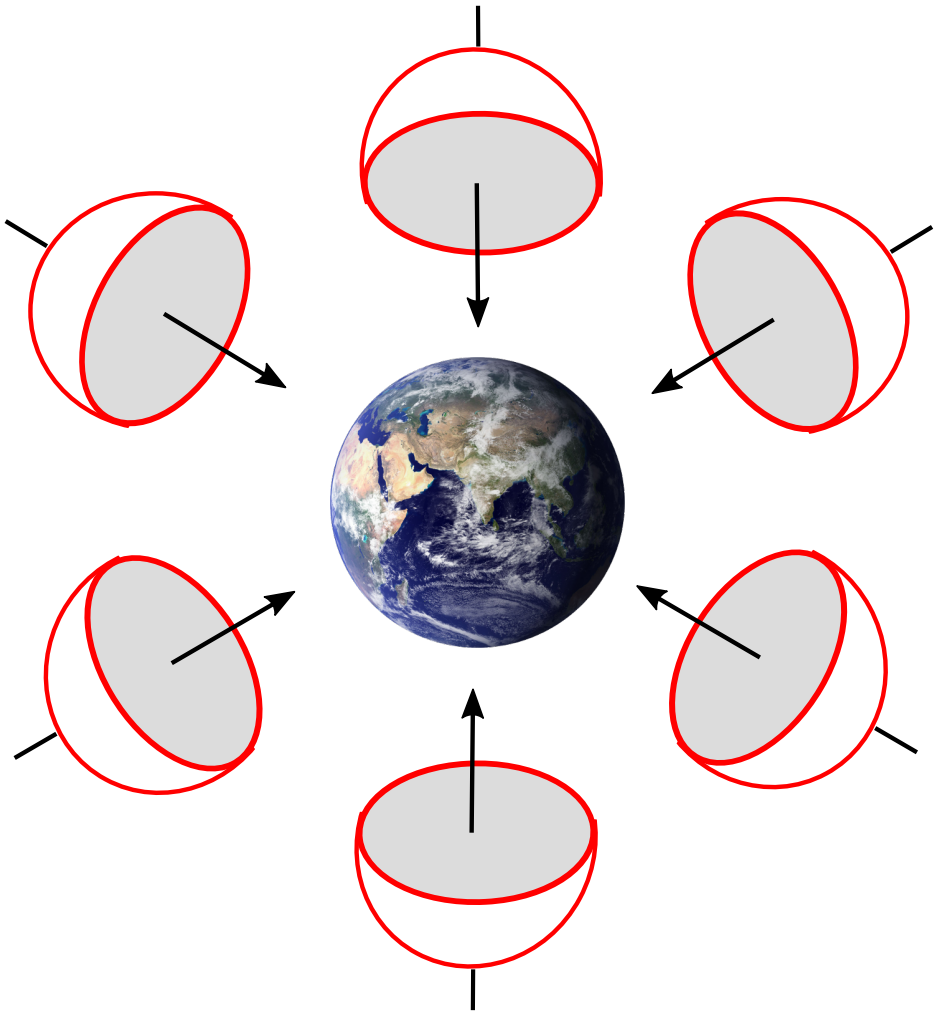
The latent space is Euclidean.

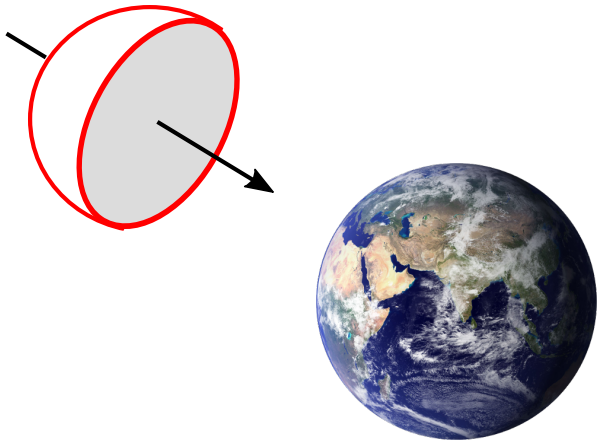
The data embedding space is curved (manifold hypothesis).

Manifolds

Manifolds are unions of charts:



2D manifolds (surfaces)



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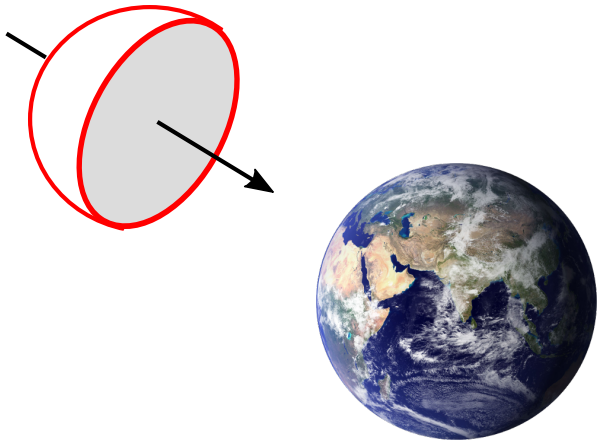

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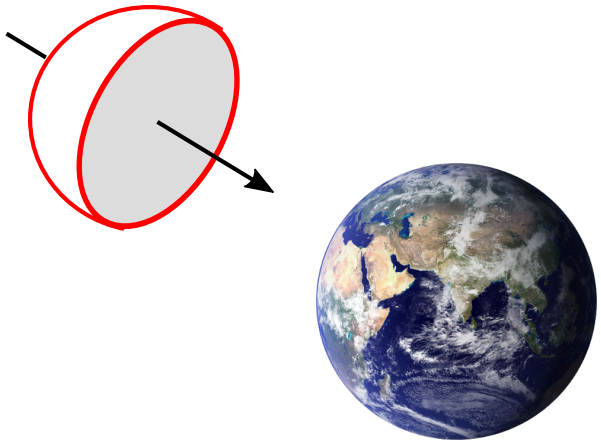

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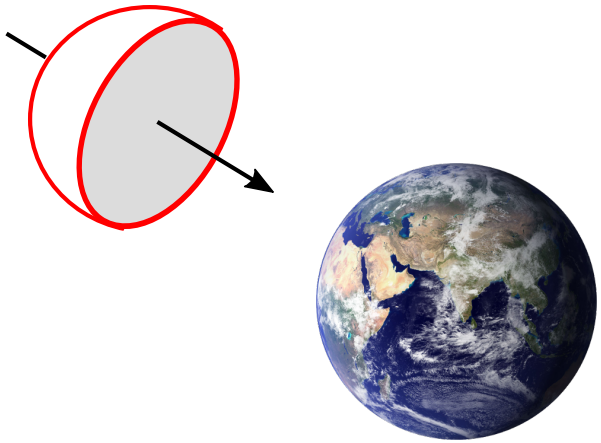

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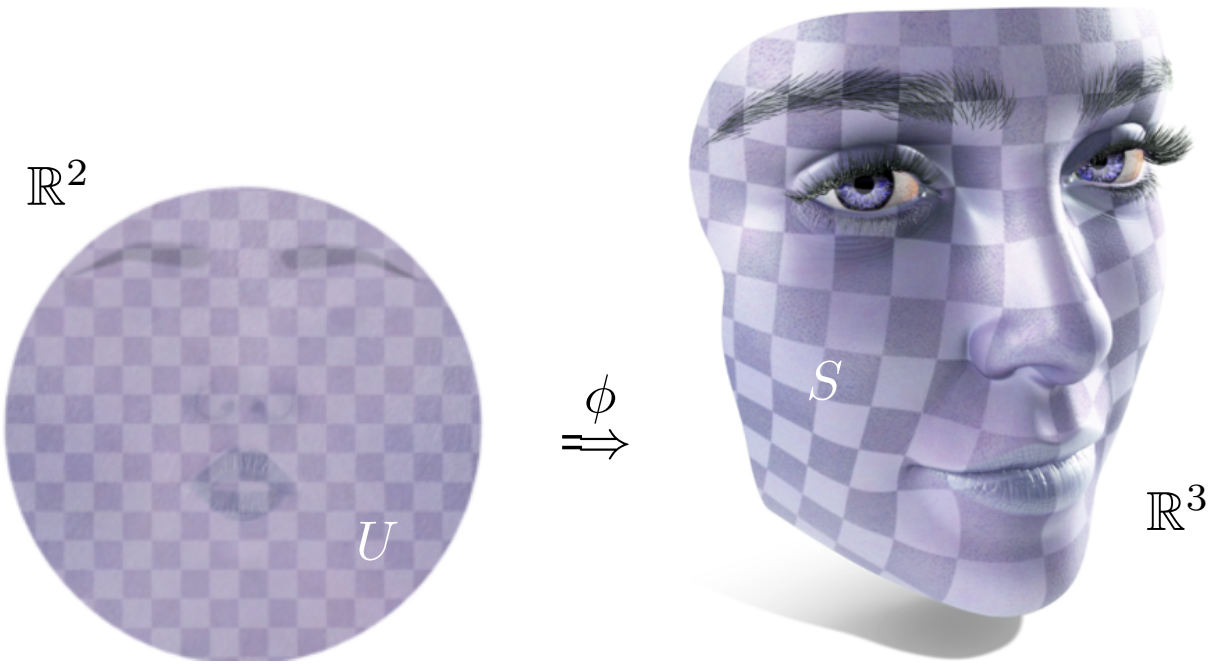

Figure by Keenan Crane

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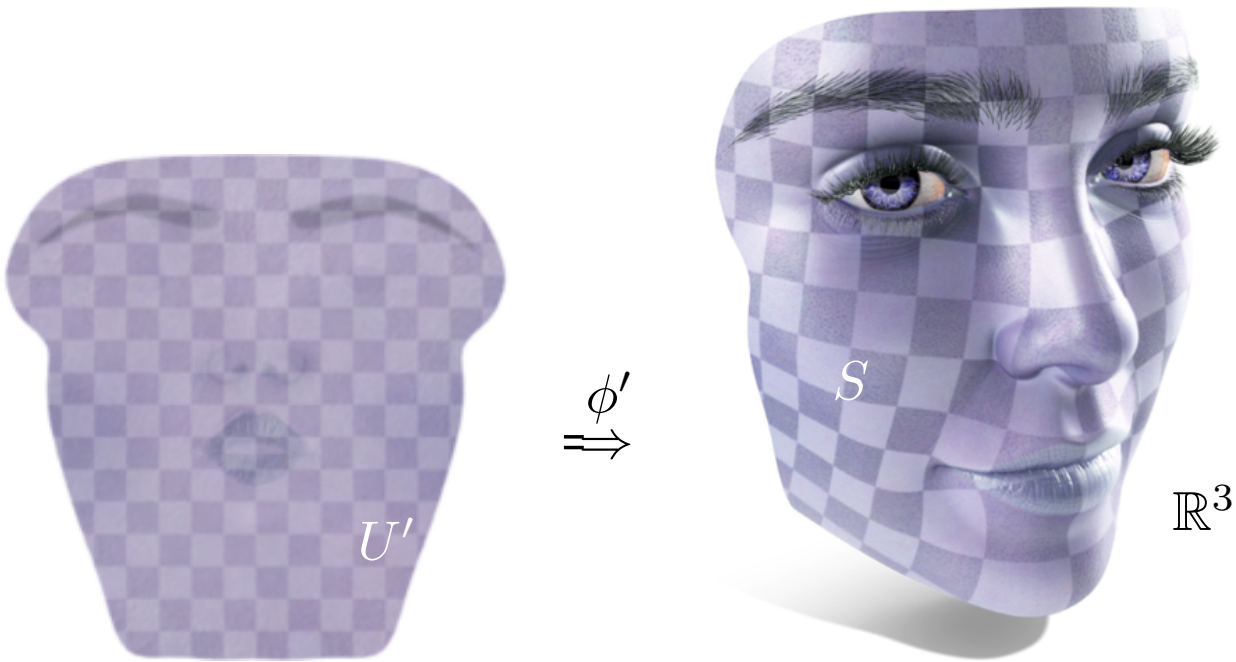

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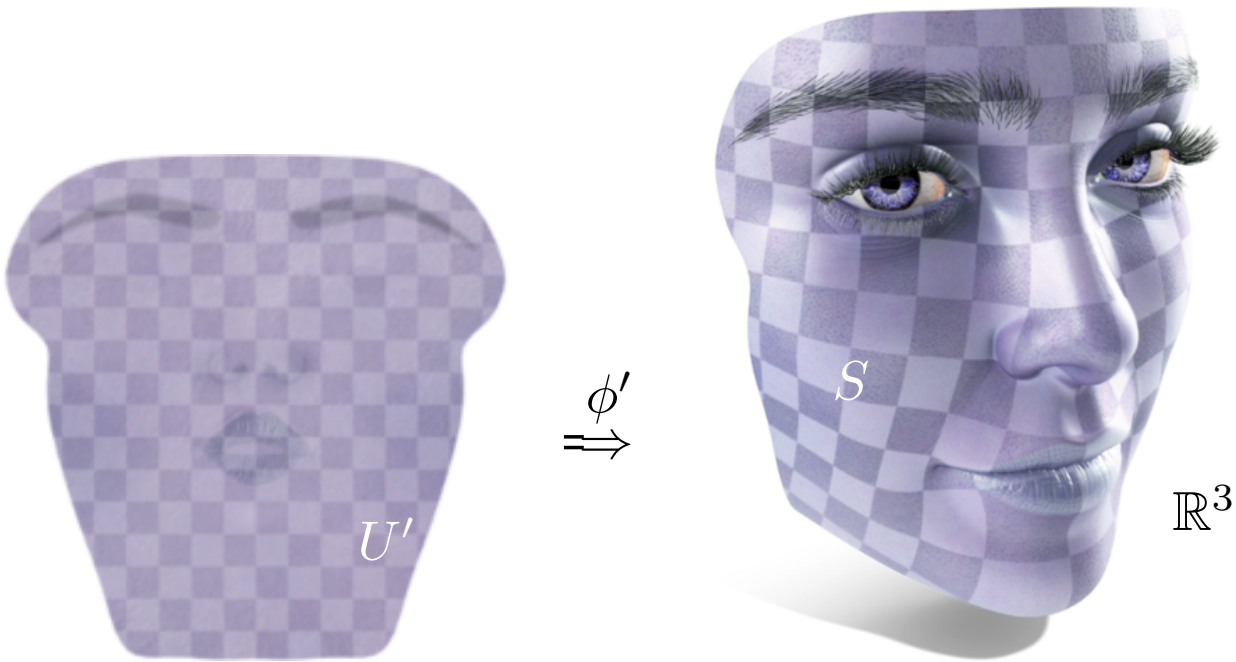
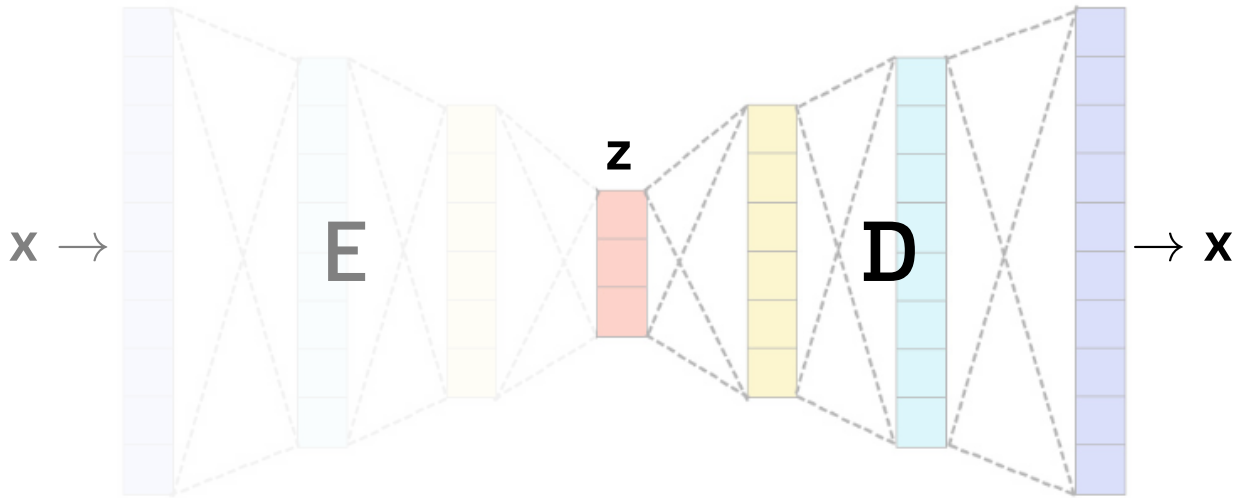


They all encode the same geometric information.

Figure by Keenan Crane

Manifolds and generative models



The decoder $D : \mathbb{R}^k \to \mathbb{R}^d$ is a chart from the latent space spanned by the codes **z** to the data space of the inputs **x**.

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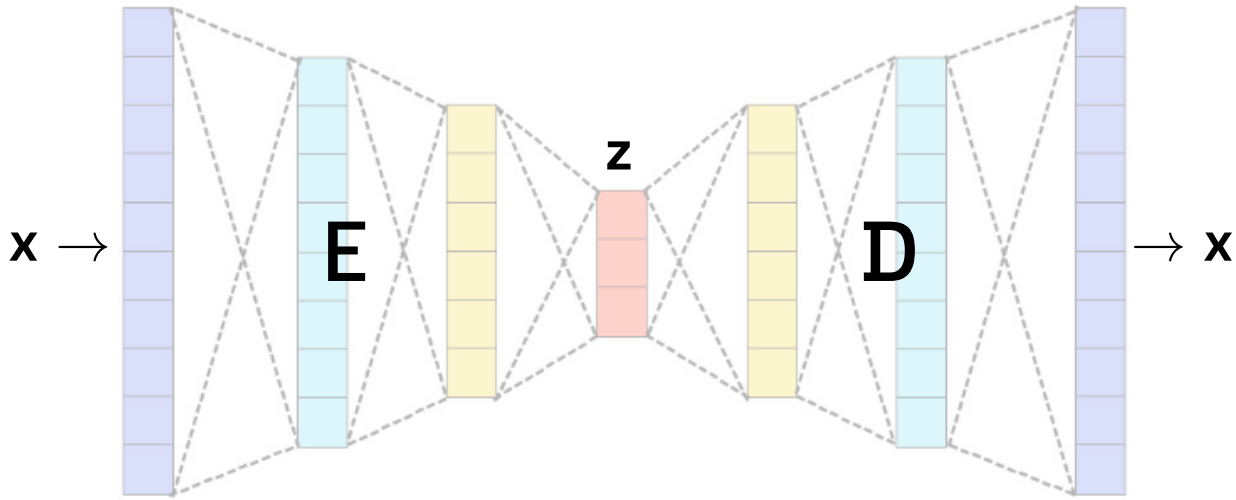

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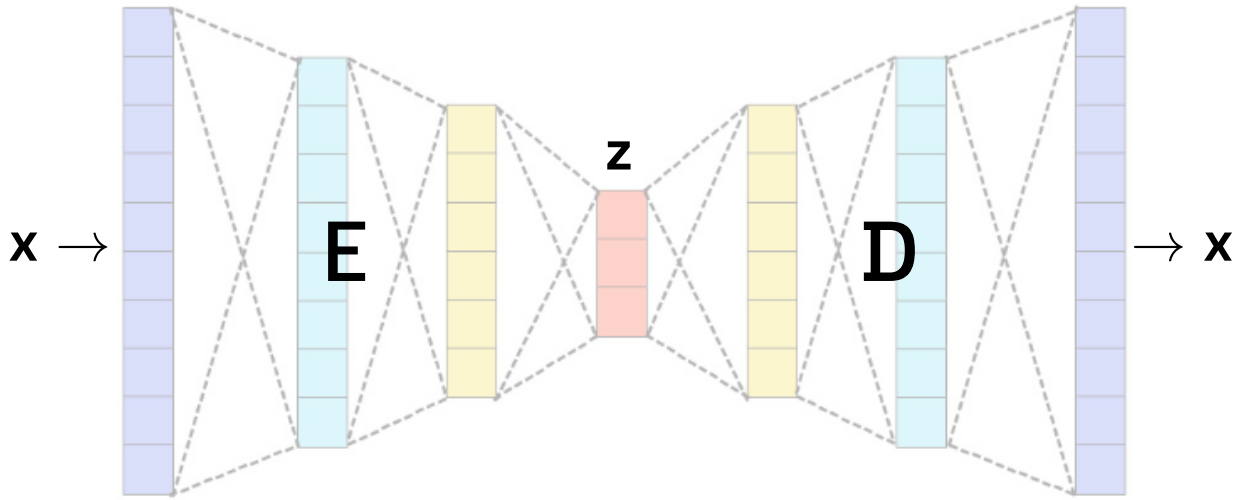

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PCA puts the data on a linear (flat) manifold, since D simply performs a linear combination of orthogonal vectors.

Shao et al, "The Riemannian geometry of deep generative models", 2018

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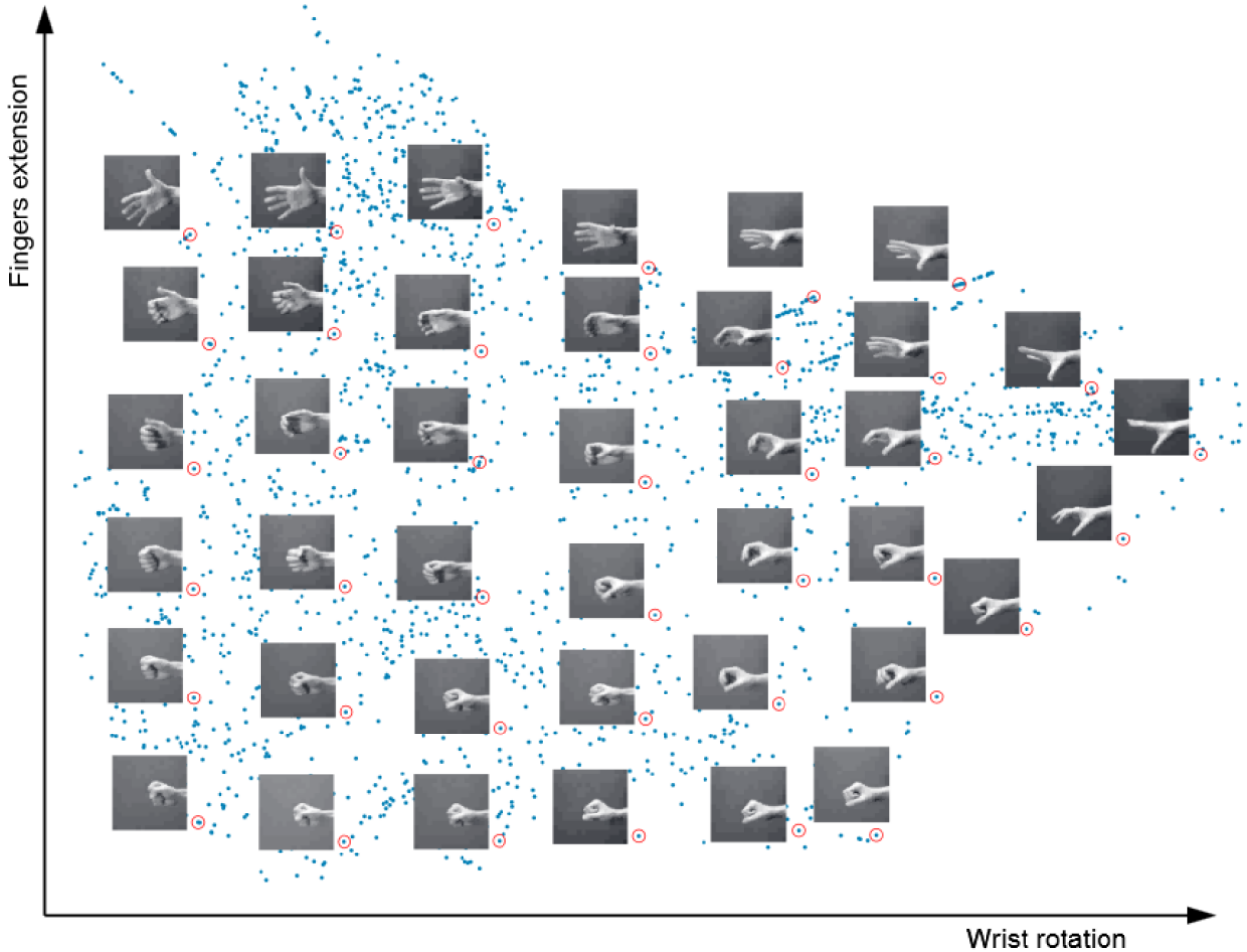

Have a look at the notebook:
https://colab.research.google.com/github/erodola/ML-s2-2025/blob/main/labs/05_PCA.ipynb

Variational autoencoders (VAE)

AEs can map similar inputs to dissimilar latent codes.

Kingma and Welling, "Auto-Encoding Variational Bayes", 2013

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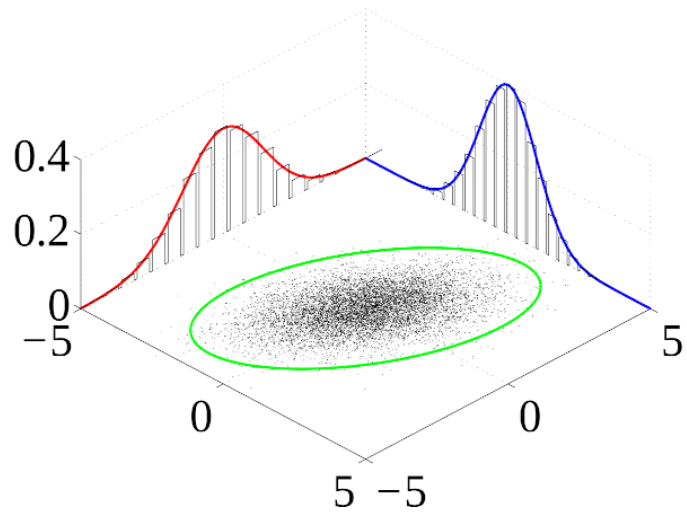
A variational AE learns a probability distribution on the latent space.

- The data is seen as a sampling of the distribution.
- The distribution is fixed and decided a priori (e.g. Gaussian).



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Entropy and divergence

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In our scenario: **x** is a data point, and **z** is a latent code.

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However, this integral:

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is intractable over the entire latent space.

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$$\boldsymbol{\phi}^* = \arg\max_{\boldsymbol{\phi},\boldsymbol{\theta}} \sum_{\mathbf{z}} q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x}) \log \frac{p_{\boldsymbol{\theta}}(\mathbf{x},\mathbf{z})}{q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})} - \cancel{\log p_{\boldsymbol{\theta}}(\mathbf{x})} \quad \text{relax}$$

where $q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})$ is a neural network with weights $\boldsymbol{\phi}$.

Kingma and Welling, "Auto-Encoding Variational Bayes", 2013

Variational inference

In our scenario: $\mathbf{x}$ is a data point, and $\mathbf{z}$ is a latent code.

Define a parametric probabilistic encoder:

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

Instead, compute an approximation $q_{\boldsymbol{\phi}^*}(\mathbf{z}|\mathbf{x}) \approx p_{\boldsymbol{\theta}}(\mathbf{z}|\mathbf{x})$ with:

$$\boldsymbol{\phi}^* = \arg\max_{\boldsymbol{\phi},\boldsymbol{\theta}} \; ELBO_{\boldsymbol{\phi},\boldsymbol{\theta}}(\mathbf{x}) - \cancel{\log p_{\boldsymbol{\theta}}(\mathbf{x})} \quad \text{relax}$$

where $q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})$ is a neural network with weights $\boldsymbol{\phi}$ and:

$$ELBO_{\boldsymbol{\phi},\boldsymbol{\theta}}(\mathbf{x}) = \sum_{\mathbf{z}} q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x}) \log \frac{p_{\boldsymbol{\theta}}(\mathbf{x},\mathbf{z})}{q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})} \leq \log p_{\boldsymbol{\theta}}(\mathbf{x})$$

is called the Evidence variational Lower BOund.

Kingma and Welling, "Auto-Encoding Variational Bayes", 2013

Variational autoencoder (VAE)

$$\max_{\boldsymbol{\phi},\boldsymbol{\theta}} \; ELBO_{\boldsymbol{\phi},\boldsymbol{\theta}}(\mathbf{x})$$

Kingma and Welling, "Auto-Encoding Variational Bayes", 2013

Variational autoencoder (VAE)

$$\max_{\phi,\theta} \sum_{\mathbf{z}} q_\phi(\mathbf{z}|\mathbf{x}) \log \frac{p_\theta(\mathbf{x},\mathbf{z})}{q_\phi(\mathbf{z}|\mathbf{x})}$$

Kingma and Welling, "Auto-Encoding Variational Bayes", 2013

Variational autoencoder (VAE)

$$\max_{\phi,\theta} \sum_{\mathbf{z}} q_\phi(\mathbf{z}|\mathbf{x}) \log \frac{p_\theta(\mathbf{x}|\mathbf{z}) p_\theta(\mathbf{z})}{q_\phi(\mathbf{z}|\mathbf{x})}$$

Kingma and Welling, "Auto-Encoding Variational Bayes", 2013

Variational autoencoder (VAE)

$$\max_{\phi,\theta} \sum_{\mathbf{z}} q_\phi(\mathbf{z}|\mathbf{x}) \left(\log p_\theta(\mathbf{x}|\mathbf{z}) + \log \frac{p_\theta(\mathbf{z})}{q_\phi(\mathbf{z}|\mathbf{x})} \right)$$

Kingma and Welling, "Auto-Encoding Variational Bayes", 2013

Variational autoencoder (VAE)

$$\max_{\phi,\theta} \sum_{\mathbf{z}} q_\phi(\mathbf{z}|\mathbf{x}) \log p_\theta(\mathbf{x}|\mathbf{z}) + \sum_{\mathbf{z}} q_\phi(\mathbf{z}|\mathbf{x}) \log \frac{p_\theta(\mathbf{z})}{q_\phi(\mathbf{z}|\mathbf{x})}$$

Kingma and Welling, "Auto-Encoding Variational Bayes", 2013

Variational autoencoder (VAE)

$$\max_{\boldsymbol{\phi},\boldsymbol{\theta}} \; \mathbb{E}_{q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})} \log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}) - KL(q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x}) \| p_{\boldsymbol{\theta}}(\mathbf{z}))$$

Kingma and Welling, "Auto-Encoding Variational Bayes", 2013

Variational autoencoder (VAE)

$$\max_{\phi,\theta} \underbrace{\mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})} \log p_\theta(\mathbf{x}|\mathbf{z})}_{\text{likelihood of observing } \mathbf{x} \text{ given } \mathbf{z}} - KL(q_\phi(\mathbf{z}|\mathbf{x}) \| p_\theta(\mathbf{z}))$$

Kingma and Welling, "Auto-Encoding Variational Bayes", 2013

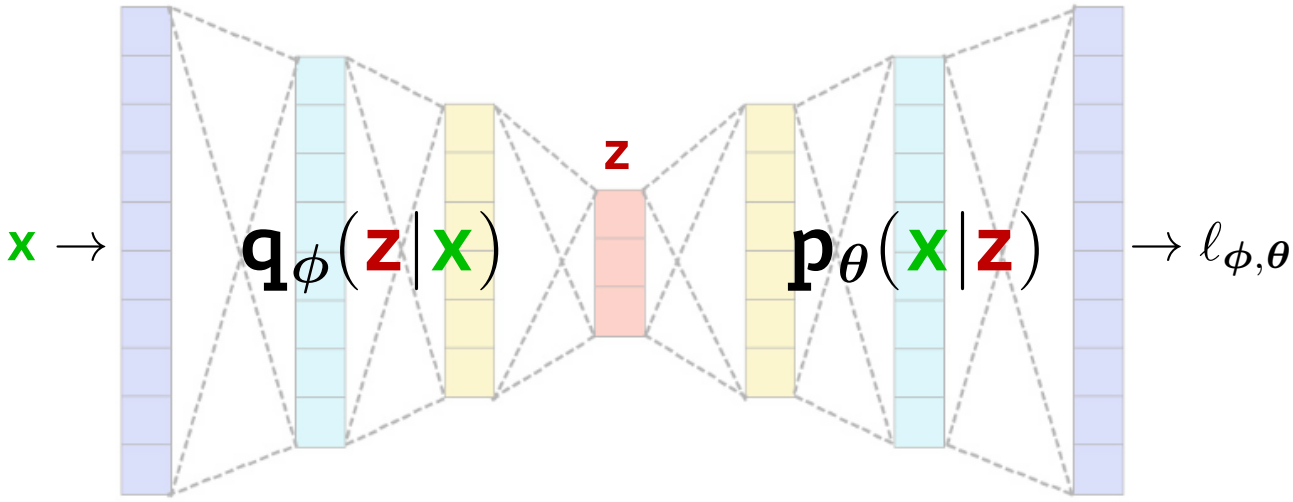
Variational autoencoder (VAE)

$$\max_{\phi,\theta} \underbrace{\mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})} \log p_\theta(\mathbf{x}|\mathbf{z})}_{\text{likelihood of observing } \mathbf{x} \text{ given } \mathbf{z}} \underbrace{-KL(q_\phi(\mathbf{z}|\mathbf{x})\|p_\theta(\mathbf{z}))}_{\text{ensures } q_\phi(\mathbf{z}|\mathbf{x}) \approx p_\theta(\mathbf{z})}$$

Kingma and Welling, "Auto-Encoding Variational Bayes", 2013

Variational autoencoder (VAE)

$$\ell_{\boldsymbol{\phi},\boldsymbol{\theta}} = \underbrace{-\mathbb{E}_{q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})} \log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z})}_{\text{likelihood of observing } \mathbf{x} \text{ given } \mathbf{z}} \underbrace{+KL(q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})\|p_{\boldsymbol{\theta}}(\mathbf{z}))}_{\text{ensures } q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x}) \approx p_{\boldsymbol{\theta}}(\mathbf{z})}$$



Kingma and Welling, "Auto-Encoding Variational Bayes", 2013

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Fixed Gaussian prior over the latent variables:

$$p(\mathbf{z}) = \mathcal{N}_{\mathbf{0},\mathbf{I}}(\mathbf{z})$$

Kingma and Welling, "Auto-Encoding Variational Bayes", 2013

Variational autoencoder (VAE)

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The probabilistic encoder also generates a Gaussian distribution:

$$q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x}) = \mathcal{N}_{\boldsymbol{\mu},\boldsymbol{\sigma}}(\mathbf{z})$$

Kingma and Welling, "Auto-Encoding Variational Bayes", 2013

Variational autoencoder (VAE)

$$\ell_{\boldsymbol{\phi},\boldsymbol{\theta}} = \underbrace{-\mathbb{E}_{q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})} \log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z})}_{\text{likelihood of observing } \mathbf{x} \text{ given } \mathbf{z}} \underbrace{+KL(q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})\|p_{\boldsymbol{\theta}}(\mathbf{z}))}_{\text{ensures } q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x}) \approx p_{\boldsymbol{\theta}}(\mathbf{z})}$$

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$\boldsymbol{\mu}, \boldsymbol{\sigma}$ are functions of the input $\mathbf{x}$ and the network parameters $\boldsymbol{\phi}$.

The probabilistic encoder outputs $\boldsymbol{\mu}, \boldsymbol{\sigma}$, not $\mathbf{z}$.

Kingma and Welling, "Auto-Encoding Variational Bayes", 2013

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$$\ell_{\boldsymbol{\phi},\boldsymbol{\theta}} = \underbrace{-\mathbb{E}_{q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})} \log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z})}_{\substack{\text{likelihood of observing} \\ \mathbf{x} \text{ given } \mathbf{z}}} \underbrace{+KL(q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})\|p_{\boldsymbol{\theta}}(\mathbf{z}))}_{\text{ensures } q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x}) \approx p_{\boldsymbol{\theta}}(\mathbf{z})}$$

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$\boldsymbol{\mu}, \boldsymbol{\sigma}$ are functions of the input $\mathbf{x}$ and the network parameters $\boldsymbol{\phi}$.

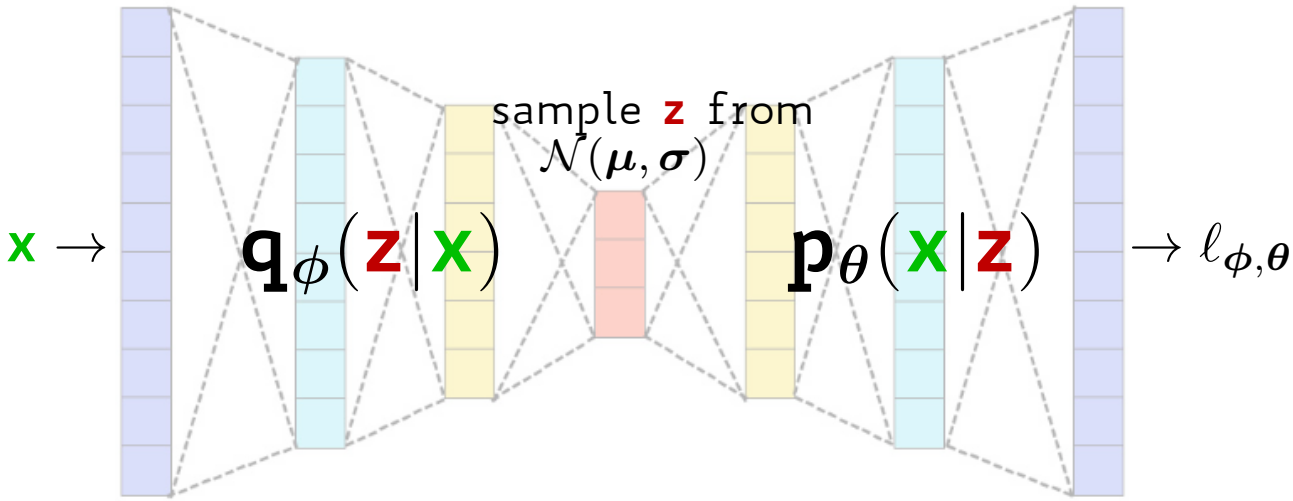
The probabilistic encoder outputs $\boldsymbol{\mu}, \boldsymbol{\sigma}$, not $\mathbf{z}$.

Using Gaussians, the KL term has a closed form.

Kingma and Welling, "Auto-Encoding Variational Bayes", 2013

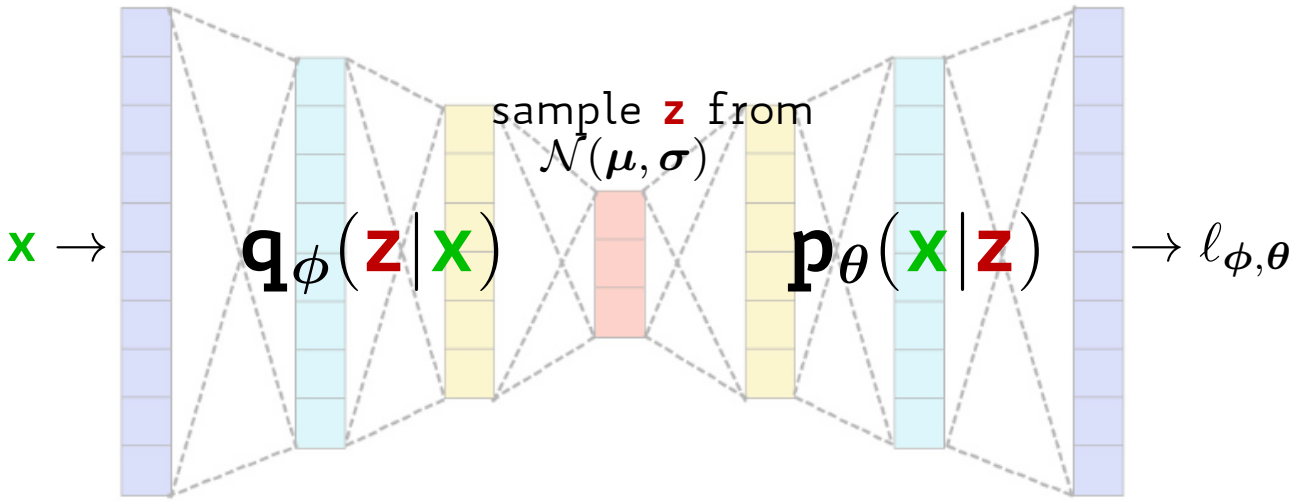
Variational autoencoder (VAE)

$$\ell_{\phi,\theta} = \underbrace{-\mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})} \log p_\theta(\mathbf{x}|\mathbf{z})}_{\text{likelihood of observing } \mathbf{x} \text{ given } \mathbf{z}} \underbrace{+KL(q_\phi(\mathbf{z}|\mathbf{x})\|p_\theta(\mathbf{z}))}_{\text{ensures } q_\phi(\mathbf{z}|\mathbf{x}) \approx p_\theta(\mathbf{z})}$$



Variational autoencoder (VAE)

$$\ell_{\phi,\theta} = \underbrace{-\mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})} \log p_\theta(\mathbf{x}|\mathbf{z})}_{\text{reconstruction loss (choose your own)}} \underbrace{+KL(q_\phi(\mathbf{z}|\mathbf{x})\|p_\theta(\mathbf{z}))}_{\text{regularizer}}$$



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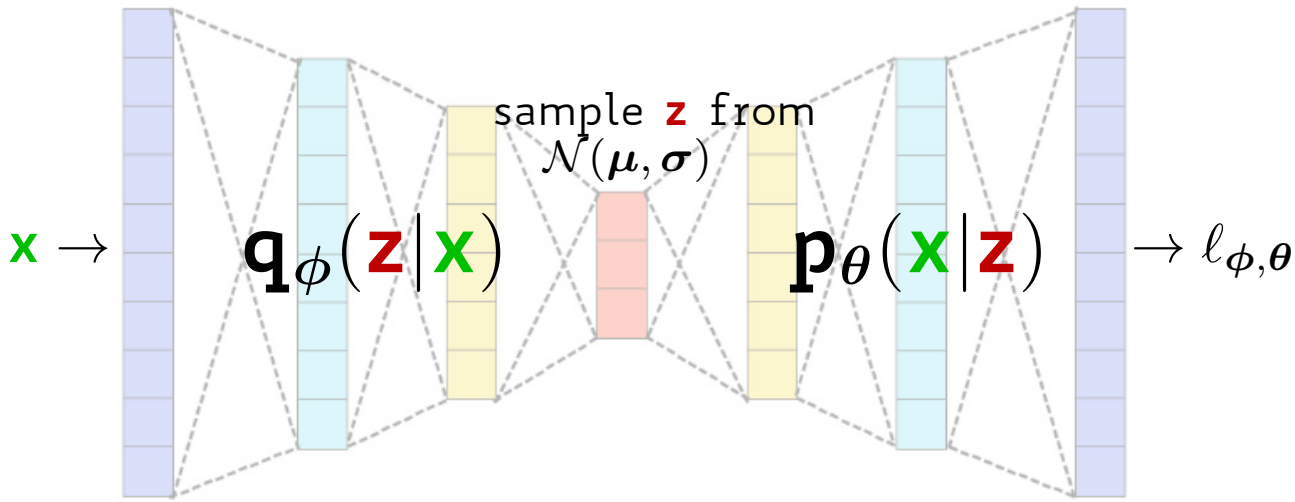
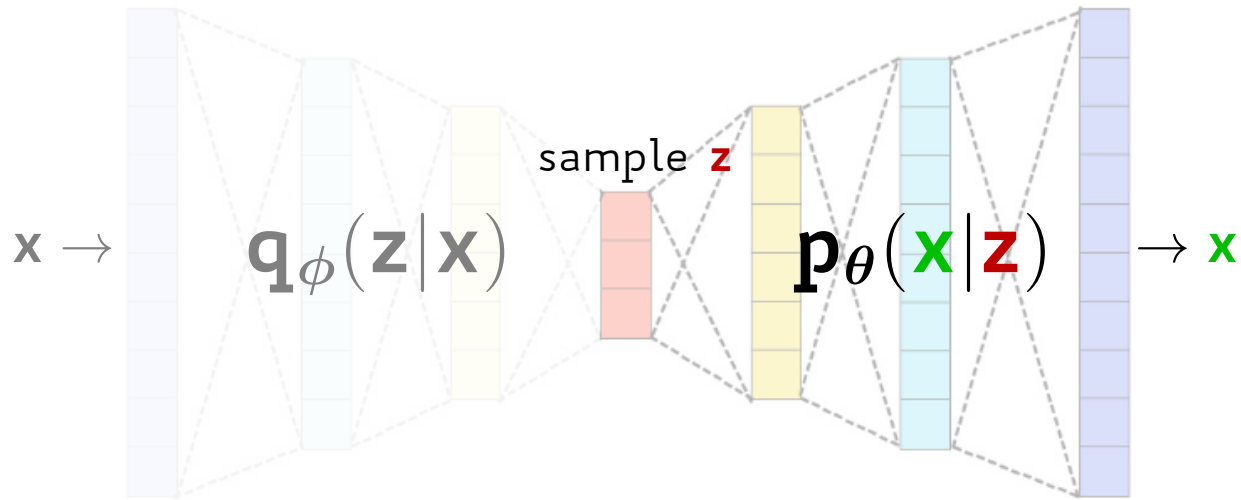


For clarity, classical AEs are called deterministic AEs.

Variational autoencoder (VAE)

$$\ell_{\boldsymbol{\phi},\boldsymbol{\theta}} = \underbrace{-\mathbb{E}_{q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})} \log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z})}_{\text{reconstruction loss (choose your own)}} \underbrace{+KL(q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})\|p_{\boldsymbol{\theta}}(\mathbf{z}))}_{\text{regularizer}}$$



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Generation: Sample $\mathbf{z}$ according to the learned distribution.

Variational autoencoder (VAE)

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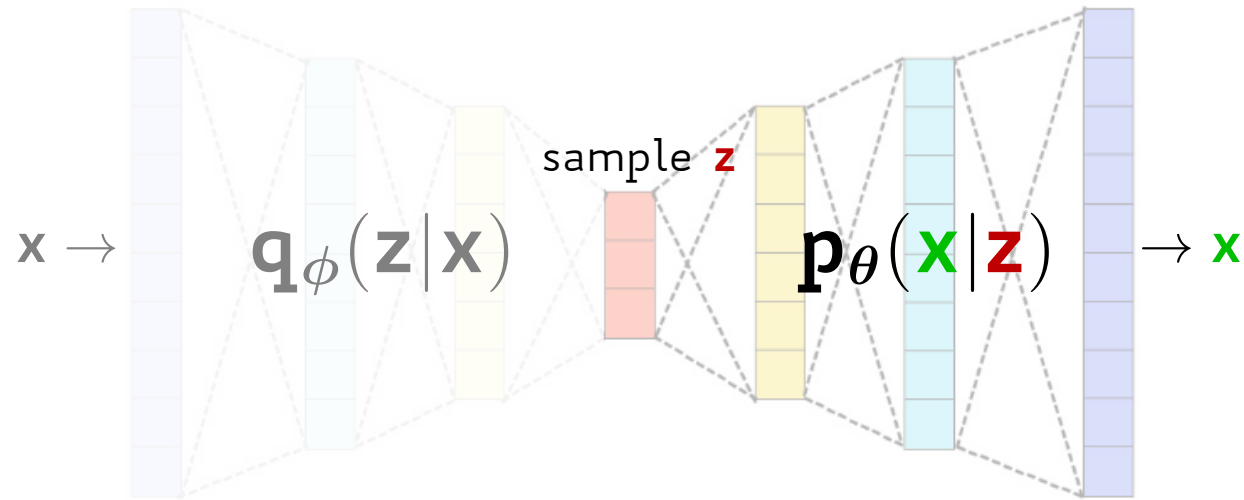
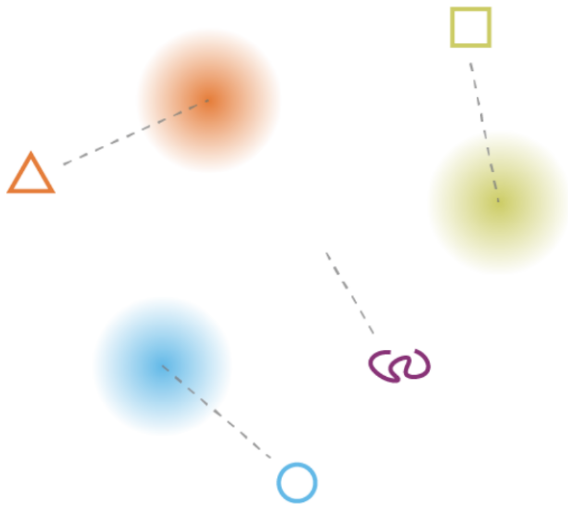


For clarity, classical AEs are called deterministic AEs.

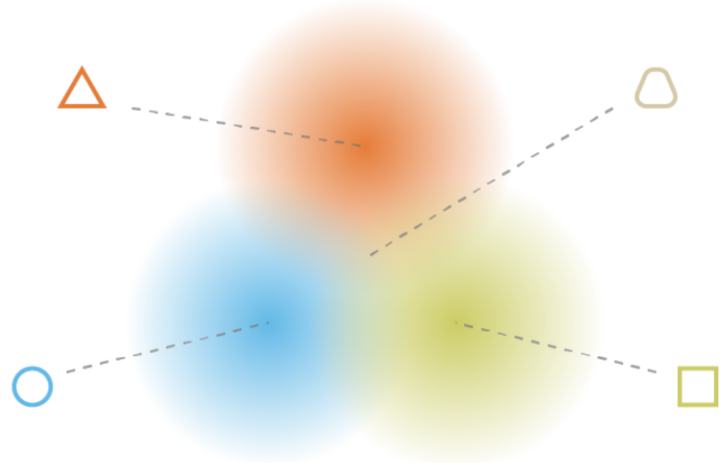
Generation: Sample $\mathbf{z}$ according to the learned distribution.

Note: also the decoder outputs a probability distribution.
If the reconstruction loss does not need a distribution, take $\mathbf{x} := \mu$.

Regularizing effect



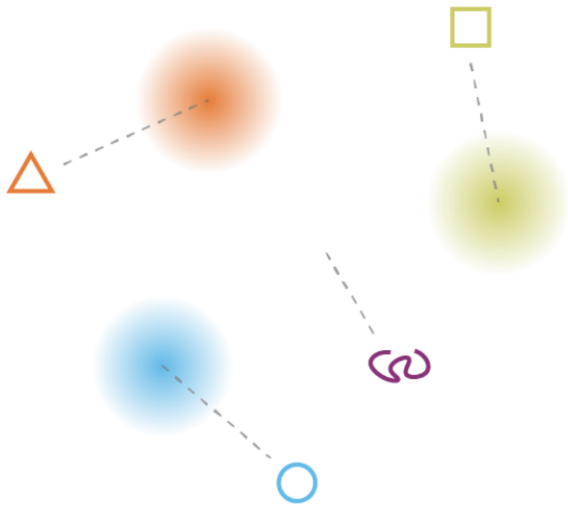
latent space of deterministic AE



latent space of variational AE

The requirement $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ leads to a compact latent space.
Small distances $\|\mathbf{z}_1 - \mathbf{z}_2\| \Rightarrow$ small changes in the decodings.

Regularizing effect



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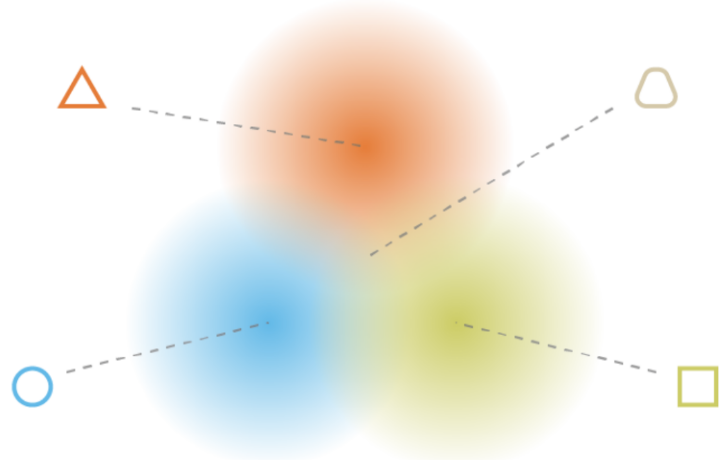

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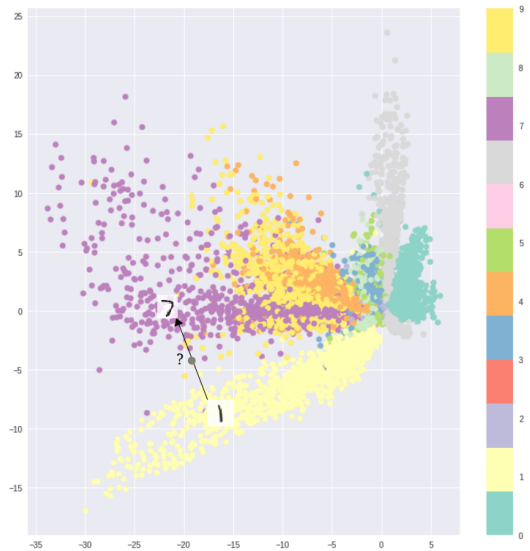
The requirement $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ leads to a compact latent space.
Small distances $\|\mathbf{z}_1 - \mathbf{z}_2\| \Rightarrow$ small changes in the decodings.

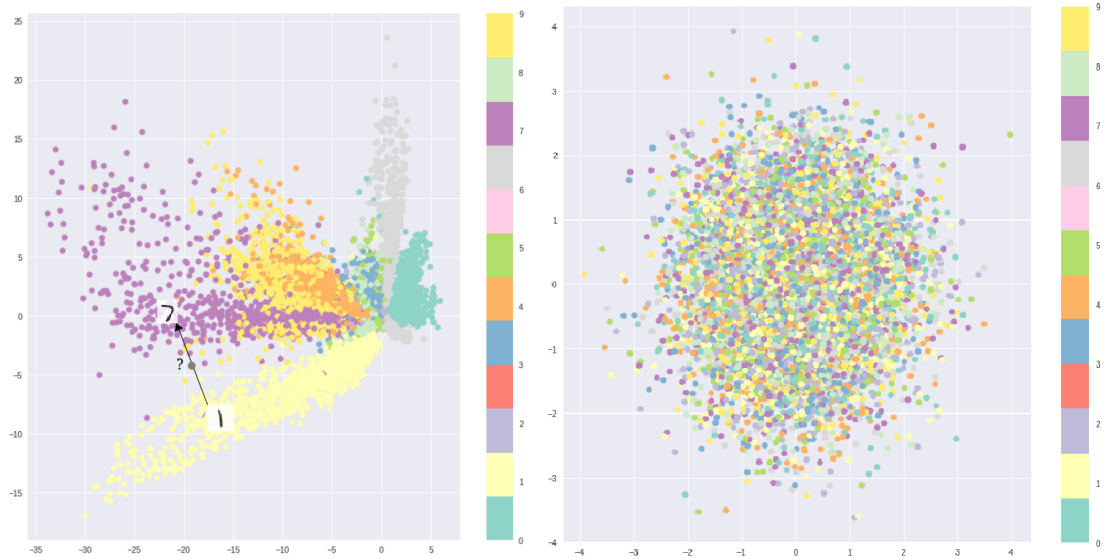
A deterministic AE might generate arbitrary noise.

Regularizing effect



Only reconstruction loss (BCE)

Regularizing effect



Only reconstruction loss (BCE)

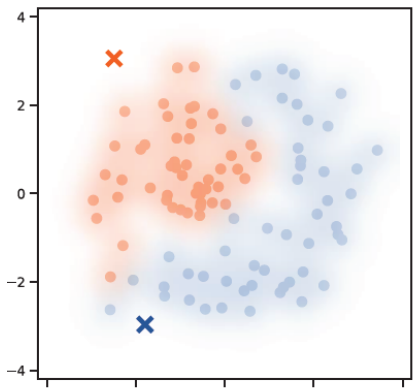
Only continuity loss (KLD)

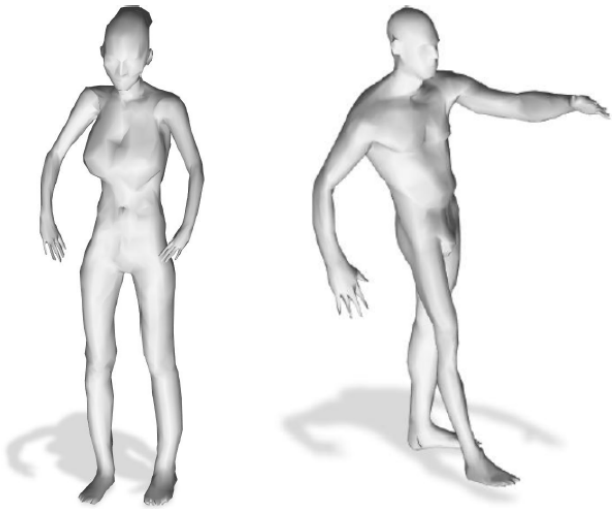
Regularizing effect

The distributional regularizer brings smoothness in the learned space.

Unlikely samples

Sampling on the boundaries of the learned distribution leads to the generation of unlikely samples:





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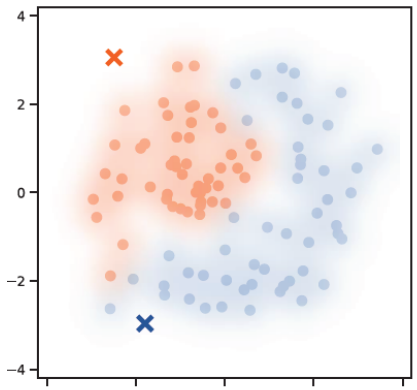
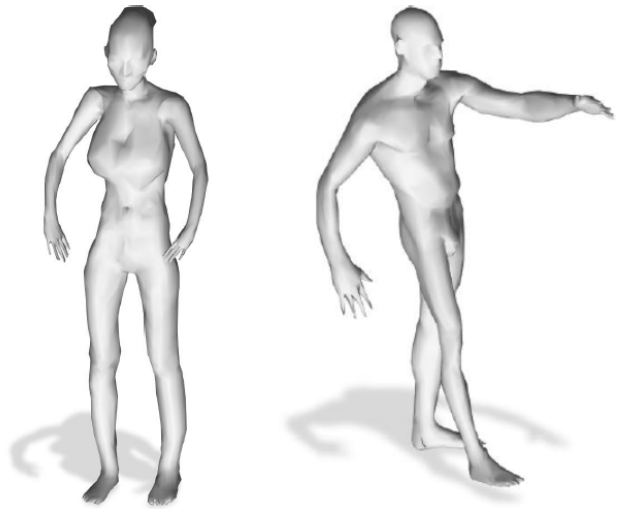


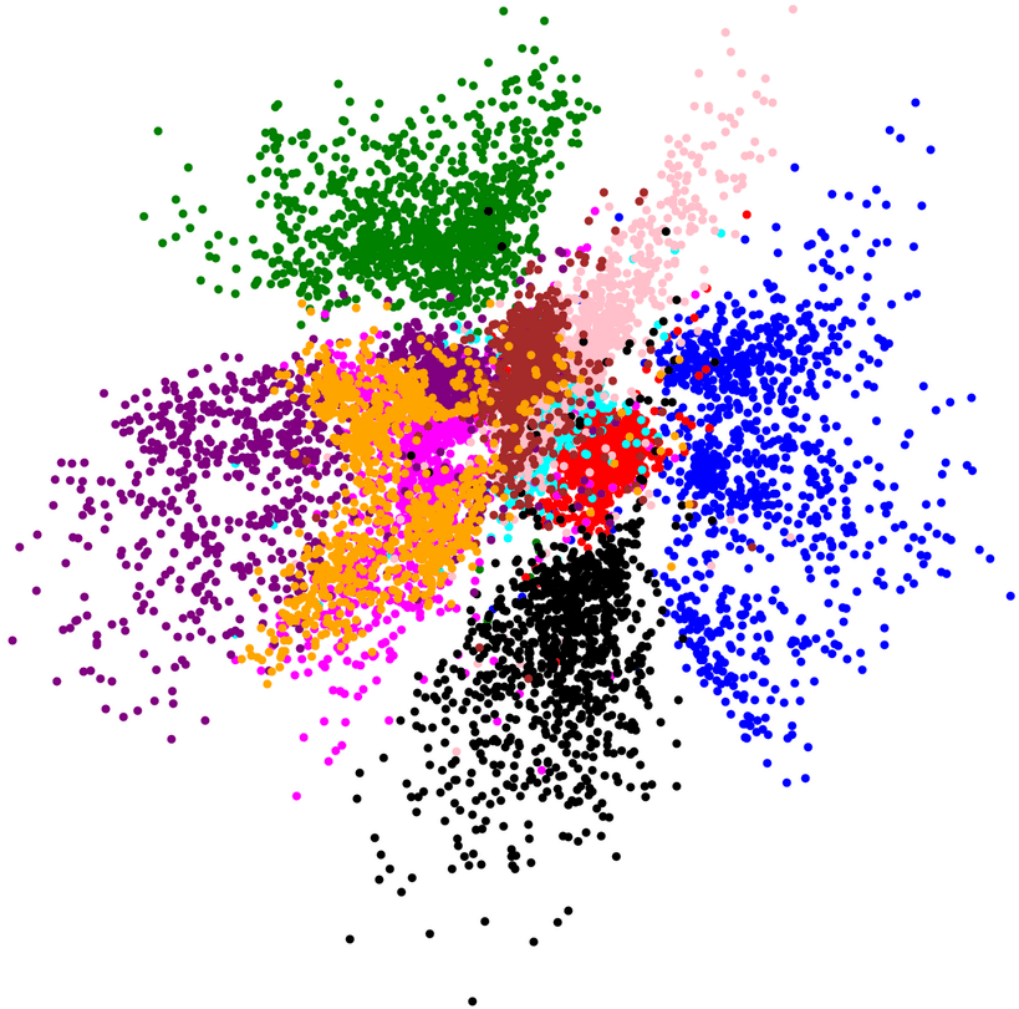


Posterior collapse: the latents are ignored if the decoder is powerful enough to model the data perfectly!

Razavi et al, "Preventing Posterior Collapse with delta-VAEs", 2019

VAE interpolation

Assume we have a trained VAE, colors correspond to different classes:



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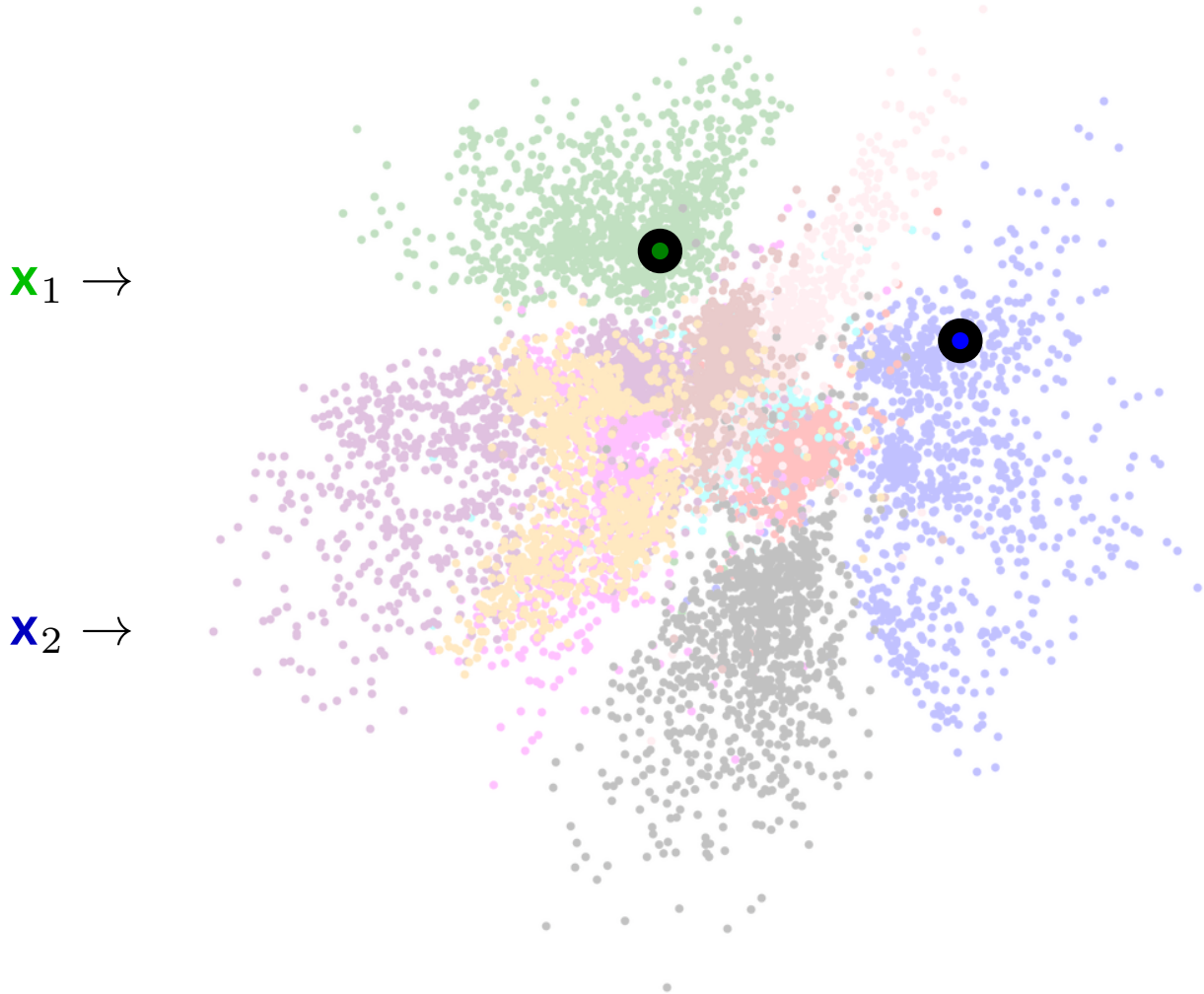

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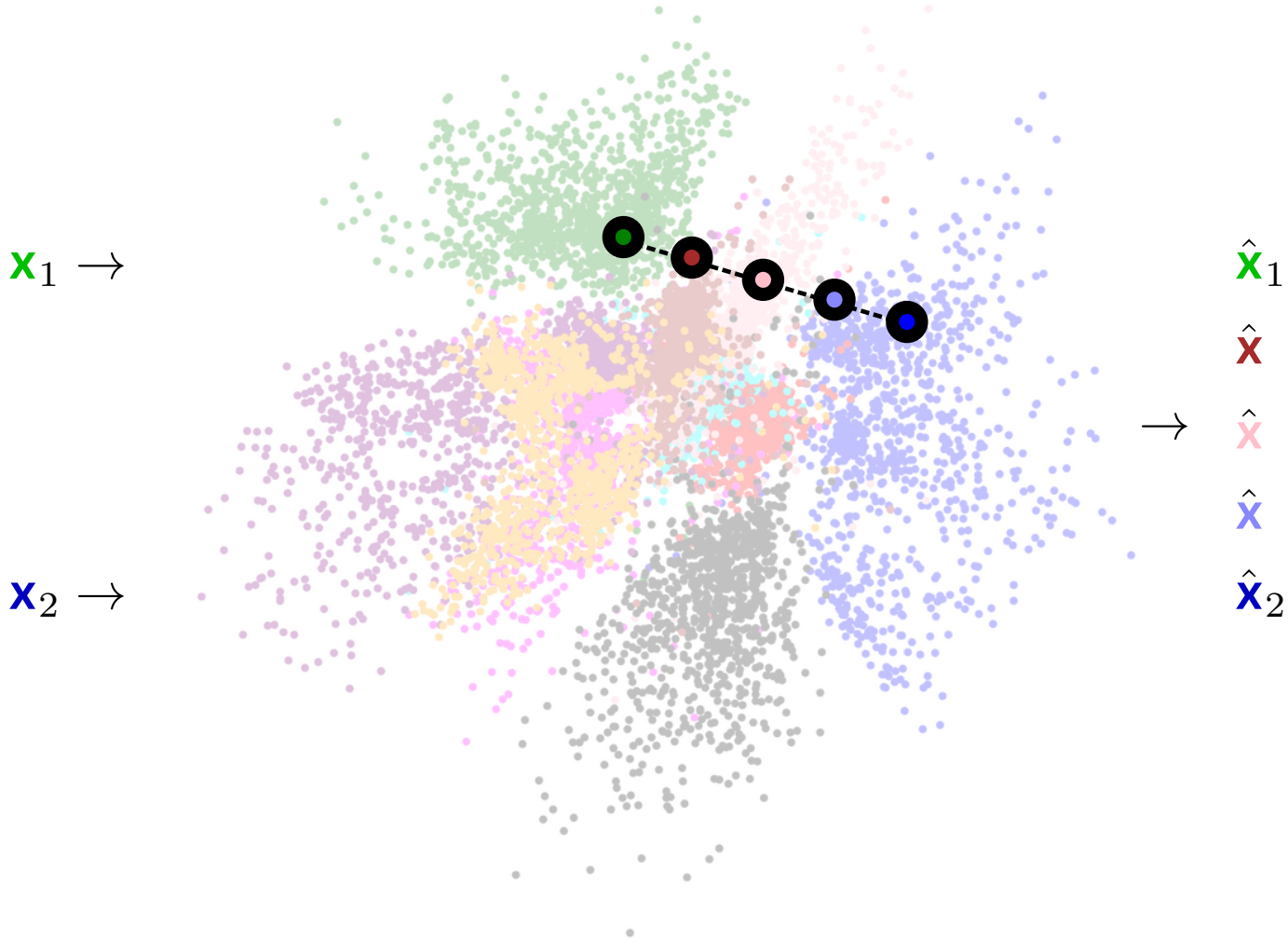


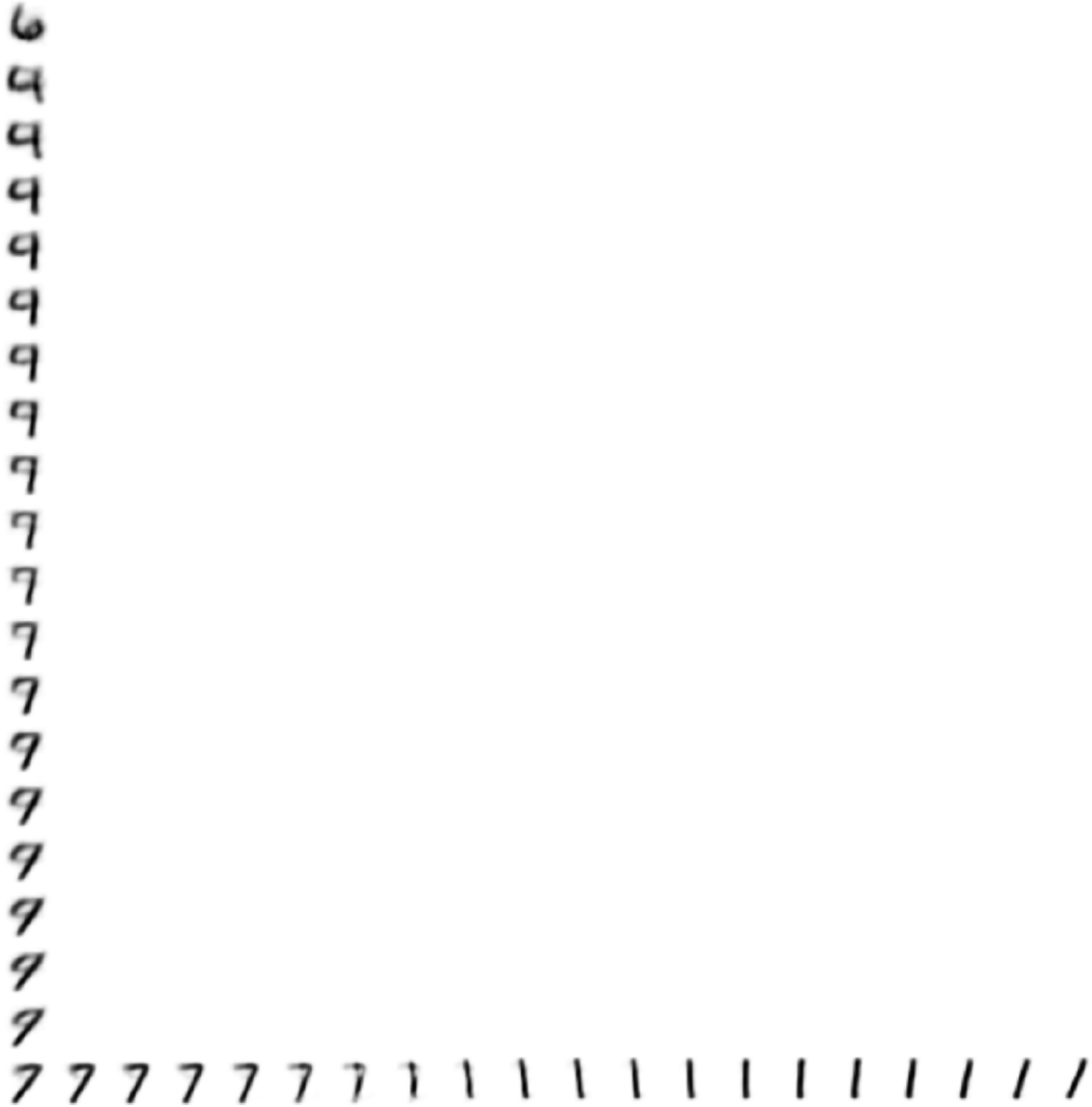
The interpolated samples are **not** part of the training set.

VAE interpolation

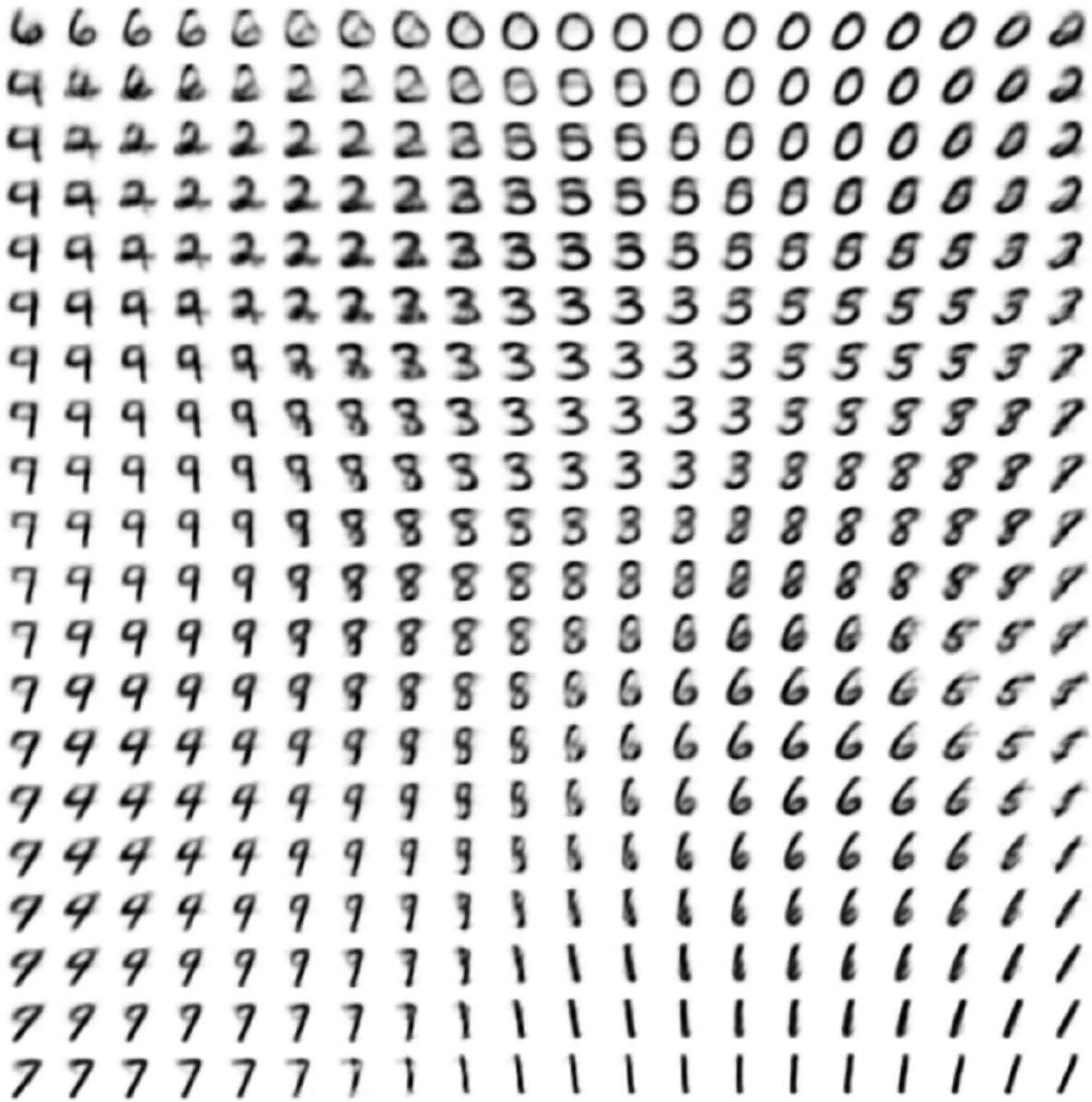
VAE interpolation

VAE interpolation

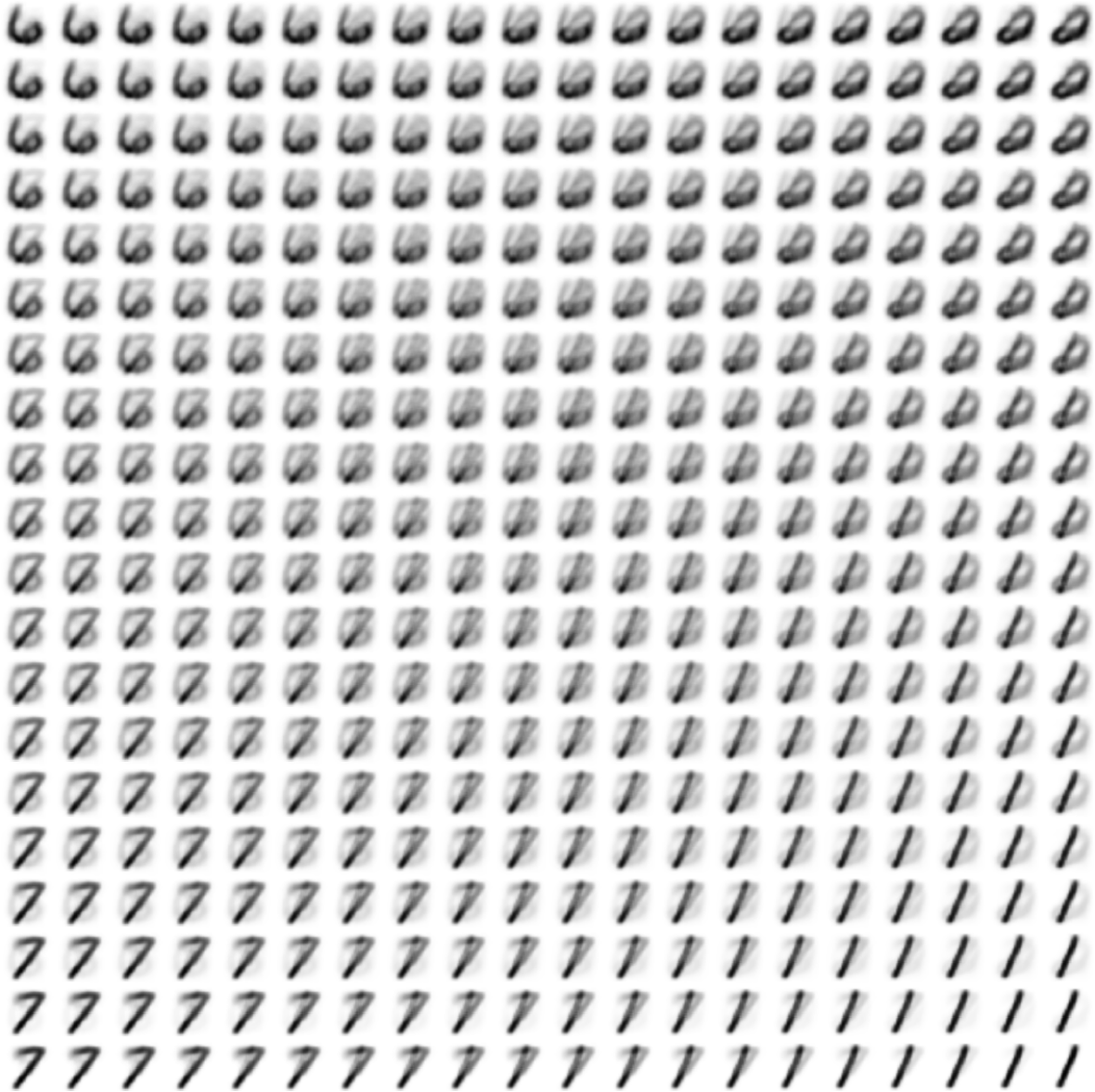
VAE interpolation



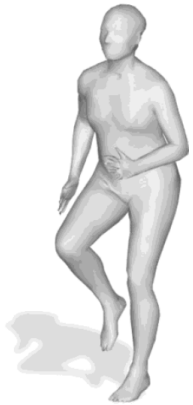
VAE interpolation



Euclidean interpolation

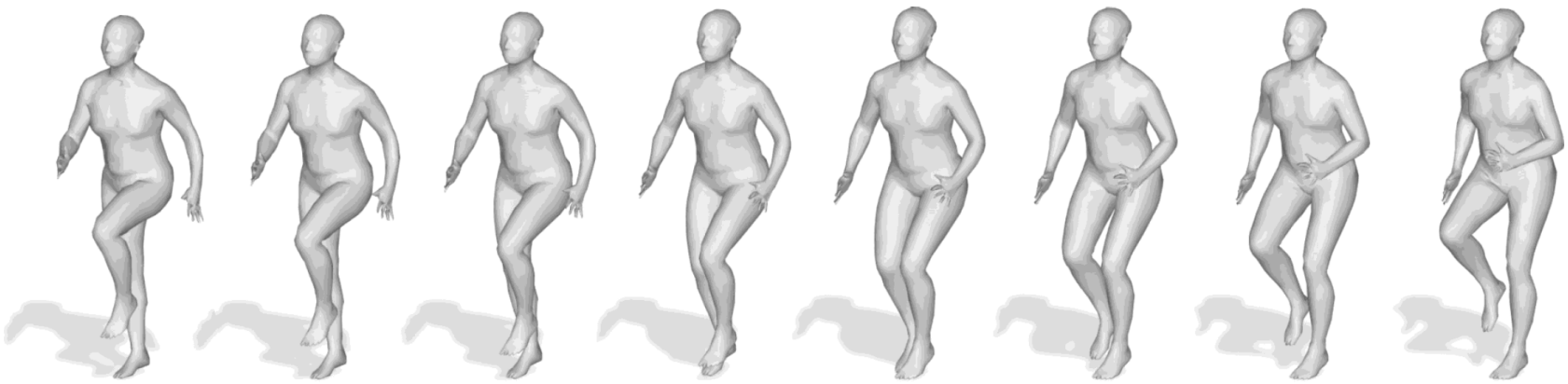


Example: Deformable 3D shapes



Cosmo, Norelli, Halimi, Kimmel, Rodolà, "LIMP: Learning Latent Shape Representations with Metric Preservation Priors", 2020

Example: Deformable 3D shapes



Cosmo, Norelli, Halimi, Kimmel, Rodolà, "LIMP: Learning Latent Shape Representations with Metric Preservation Priors", 2020

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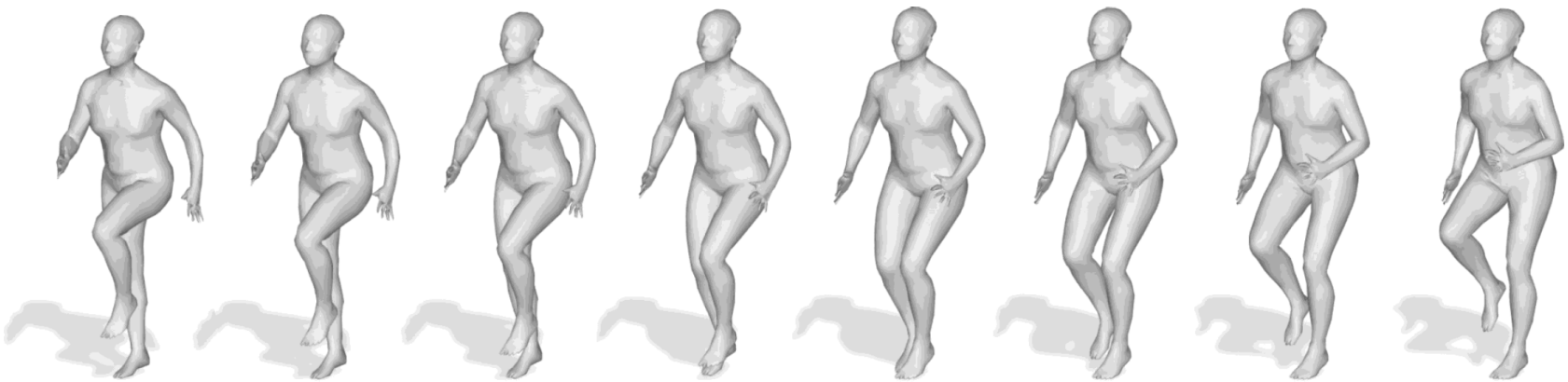
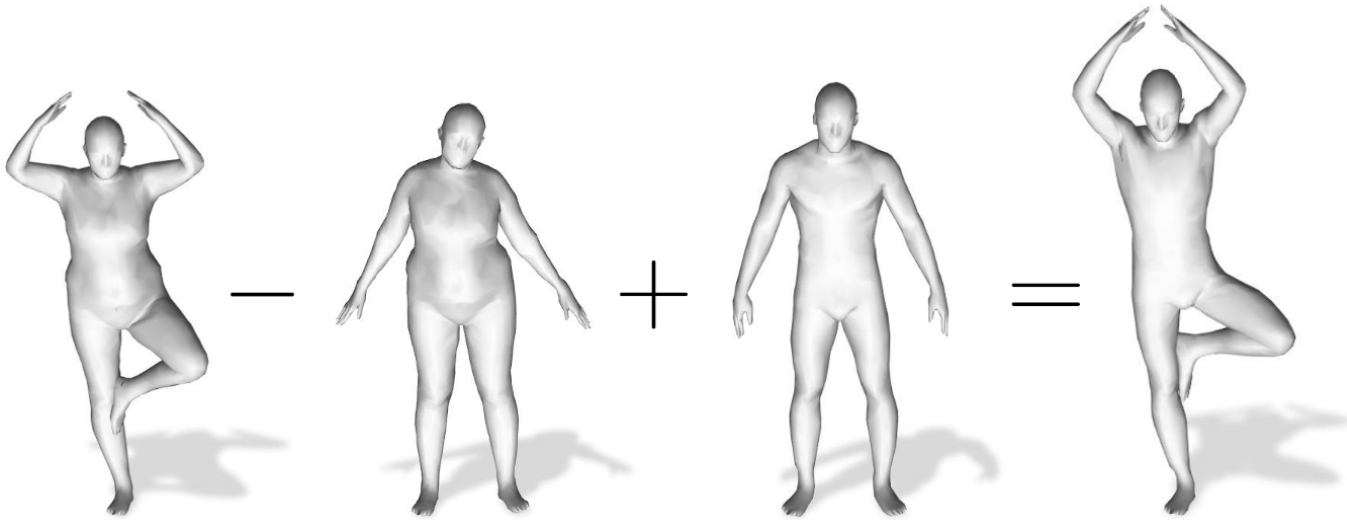


The latent space can be explored along different dimensions (disentanglement):

Cosmo, Norelli, Halimi, Kimmel, Rodolà, "LIMP: Learning Latent Shape Representations with Metric Preservation Priors", 2020

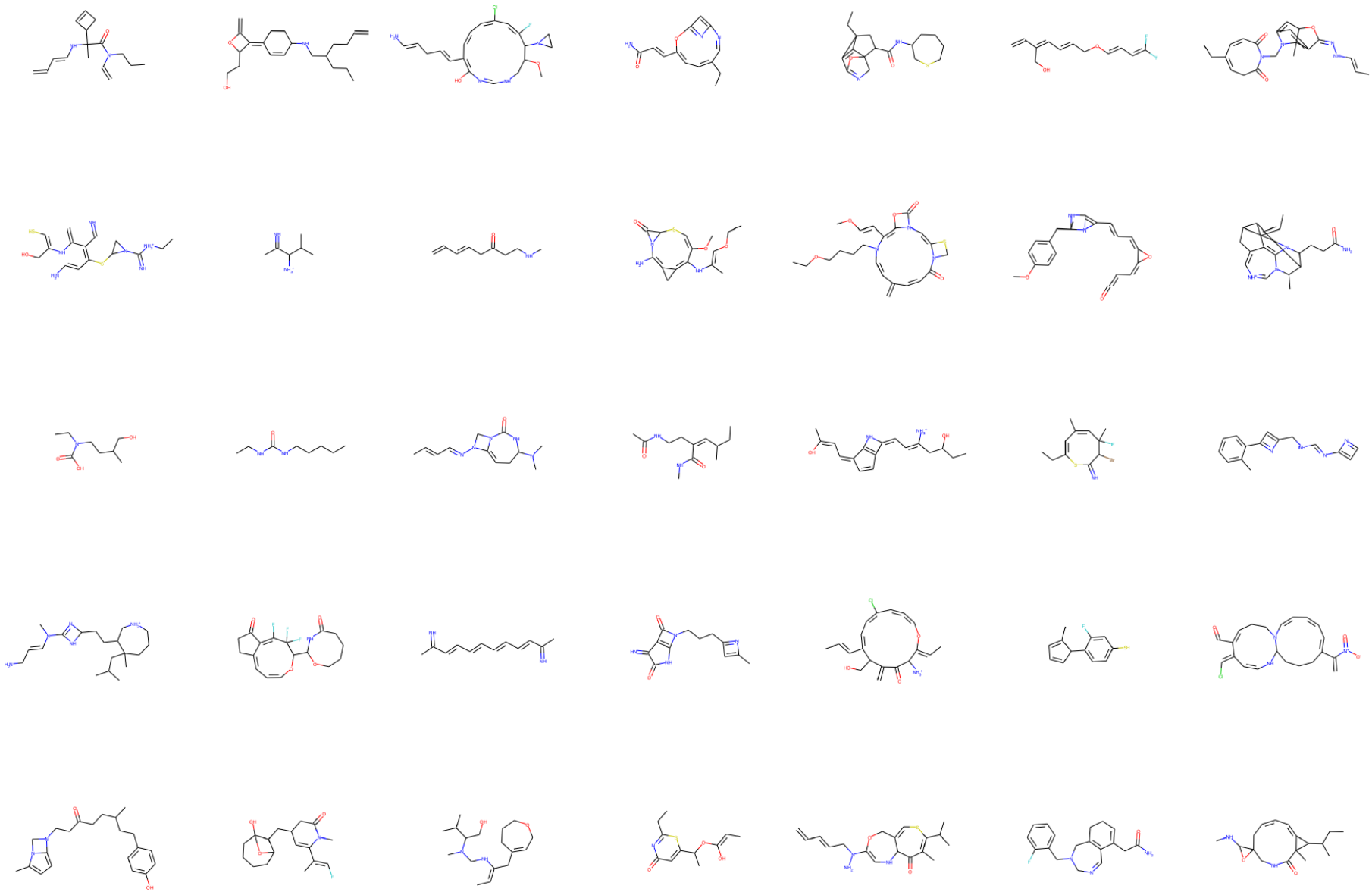
Analogies

Algebraic manipulation of codes leads to the following:



In NLP this is done by manipulating word embeddings:

King – Man + Woman = Queen



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