Deep Learning & Applied AI

Deep generative models

Emanuele Rodolà
rodola@di.uniroma1.it

SAPIENZA
UNIVERSITÀ DI ROMA

2nd semester a.y. 2020/2021 · May 05, 2021

Generative models

Overall idea:

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

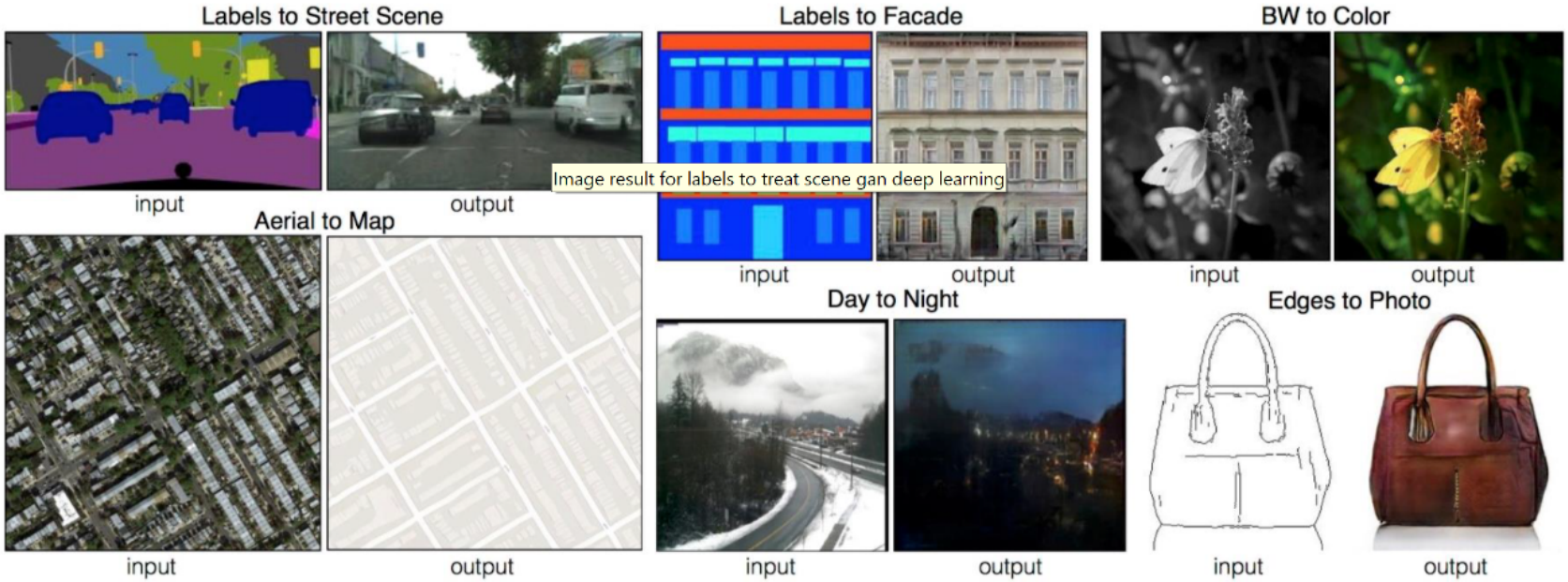
Generative models

Overall idea:

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

https://thispersondoesnotexist.com/

Generative models

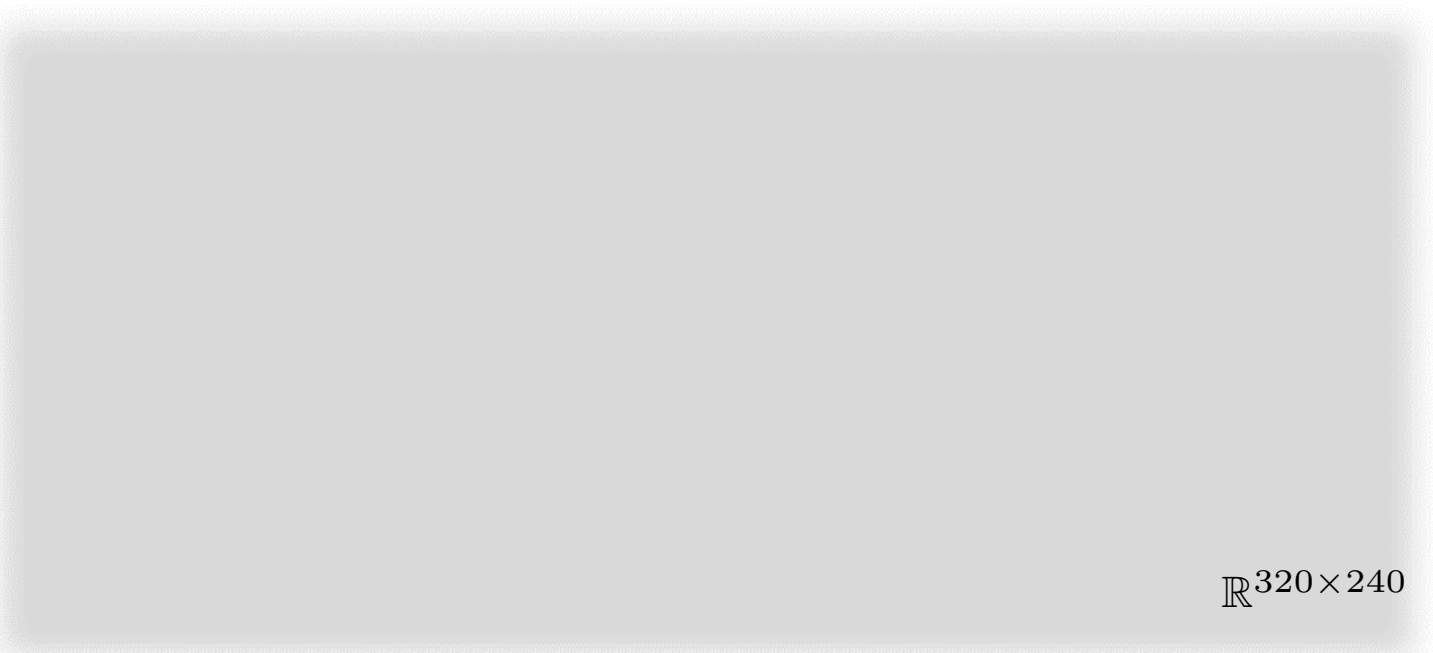


Generative models

Caption	Image
this flower has white petals and a yellow stamen	
the center is yellow surrounded by wavy dark purple petals	
this flower has lots of small round pink petals	

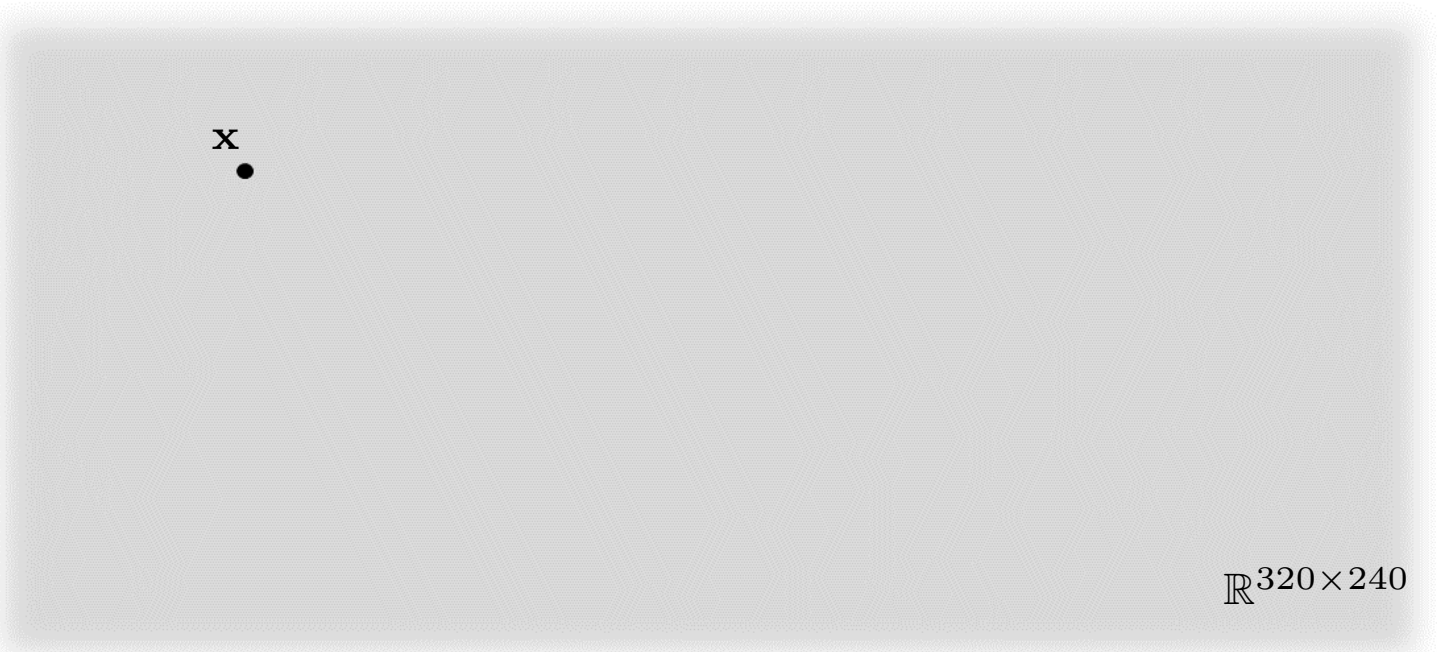
Generative models

What does it mean to learn a distribution?



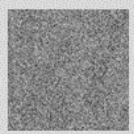
Generative models

What does it mean to learn a distribution?



Generative models

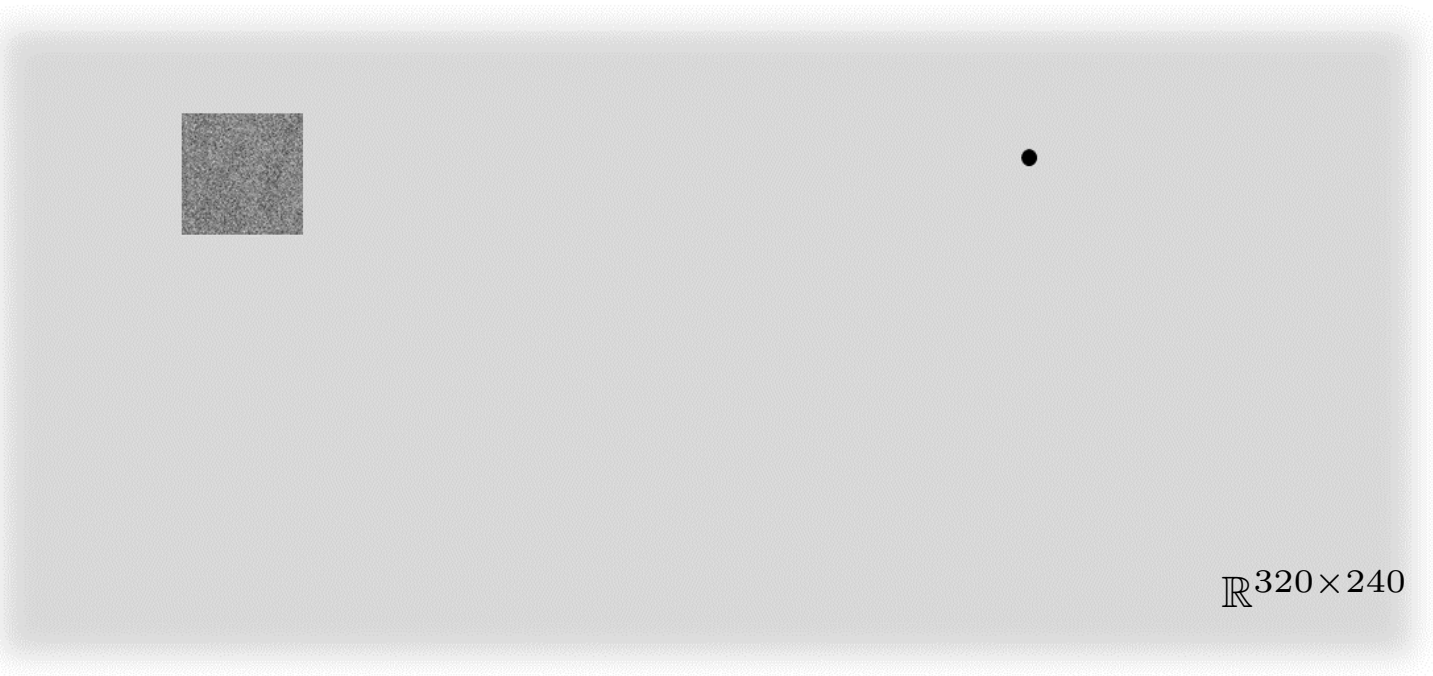
What does it mean to learn a distribution?



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

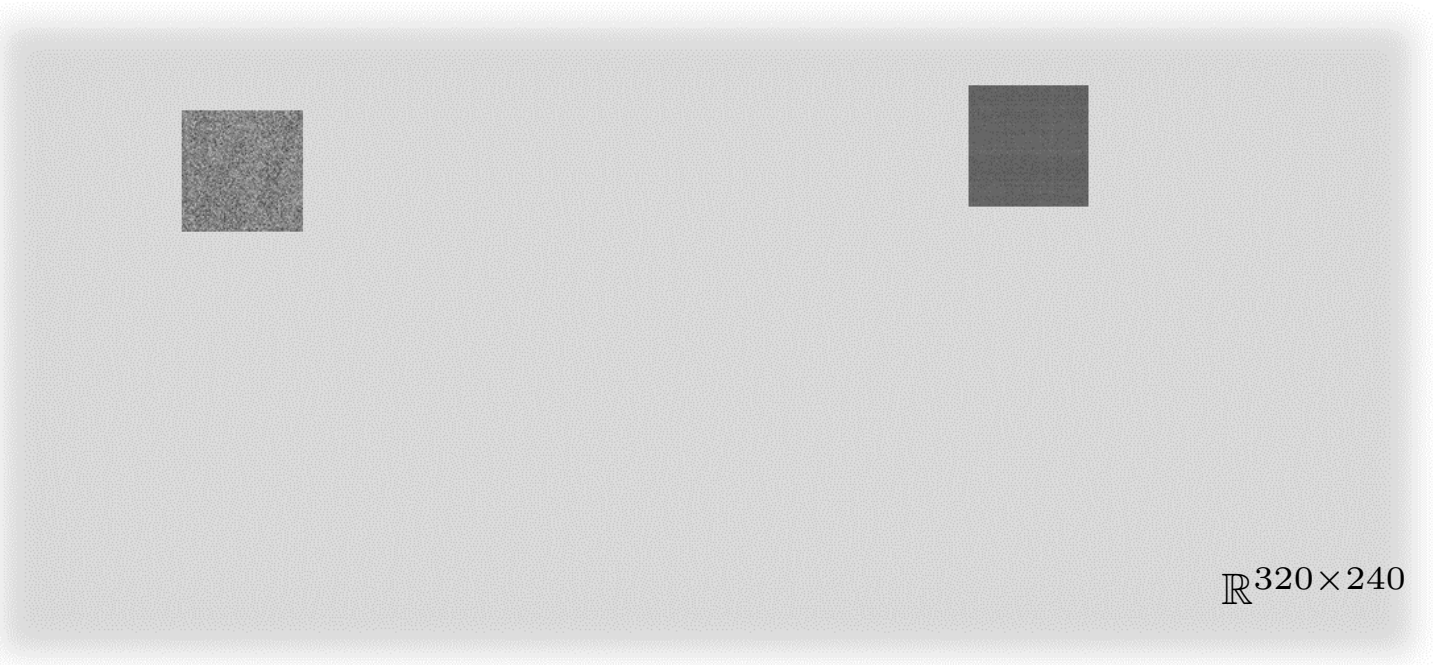
Generative models

What does it mean to learn a distribution?



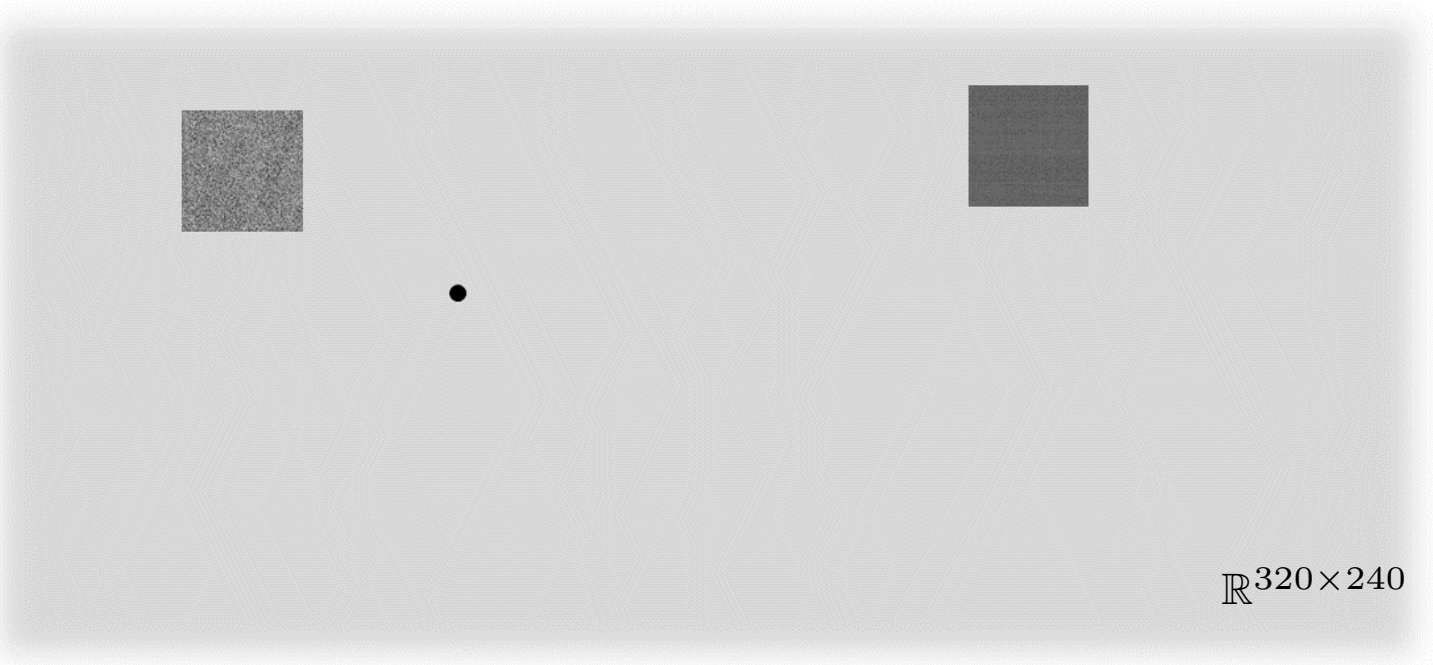
Generative models

What does it mean to learn a distribution?



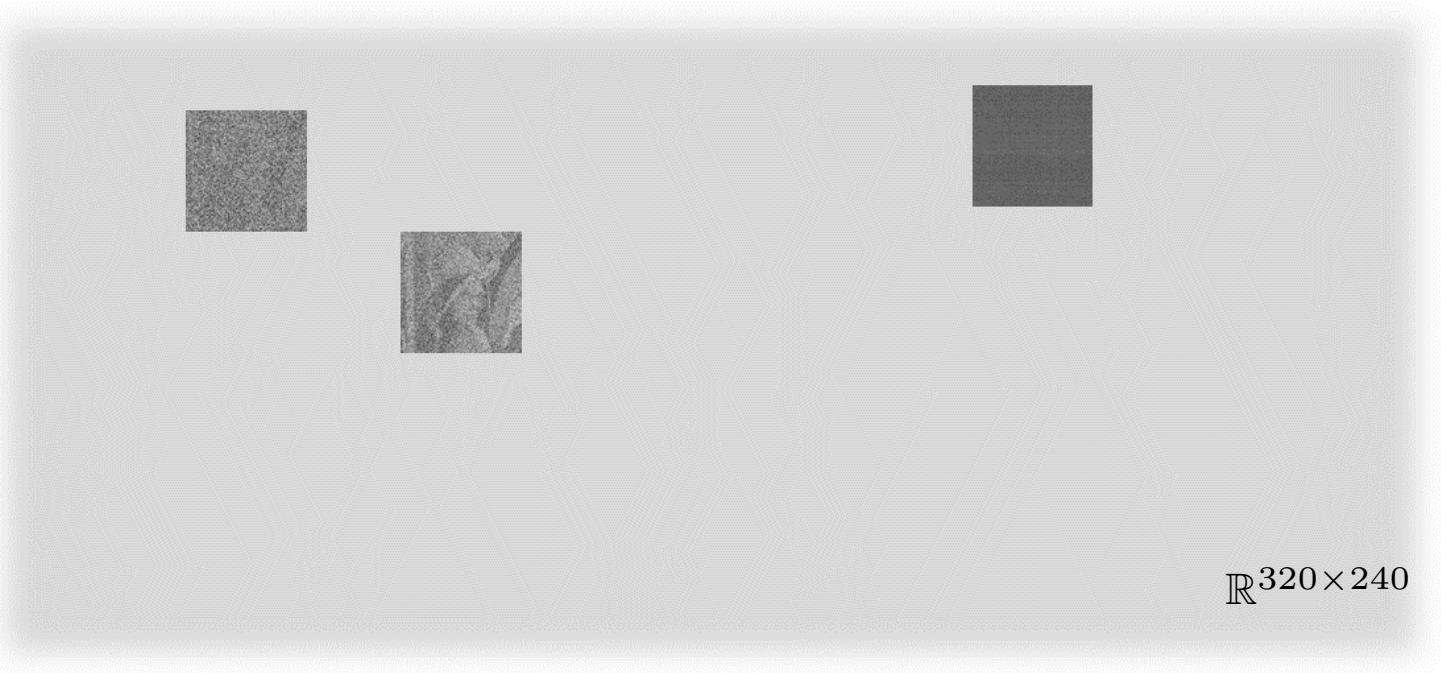
Generative models

What does it mean to learn a distribution?



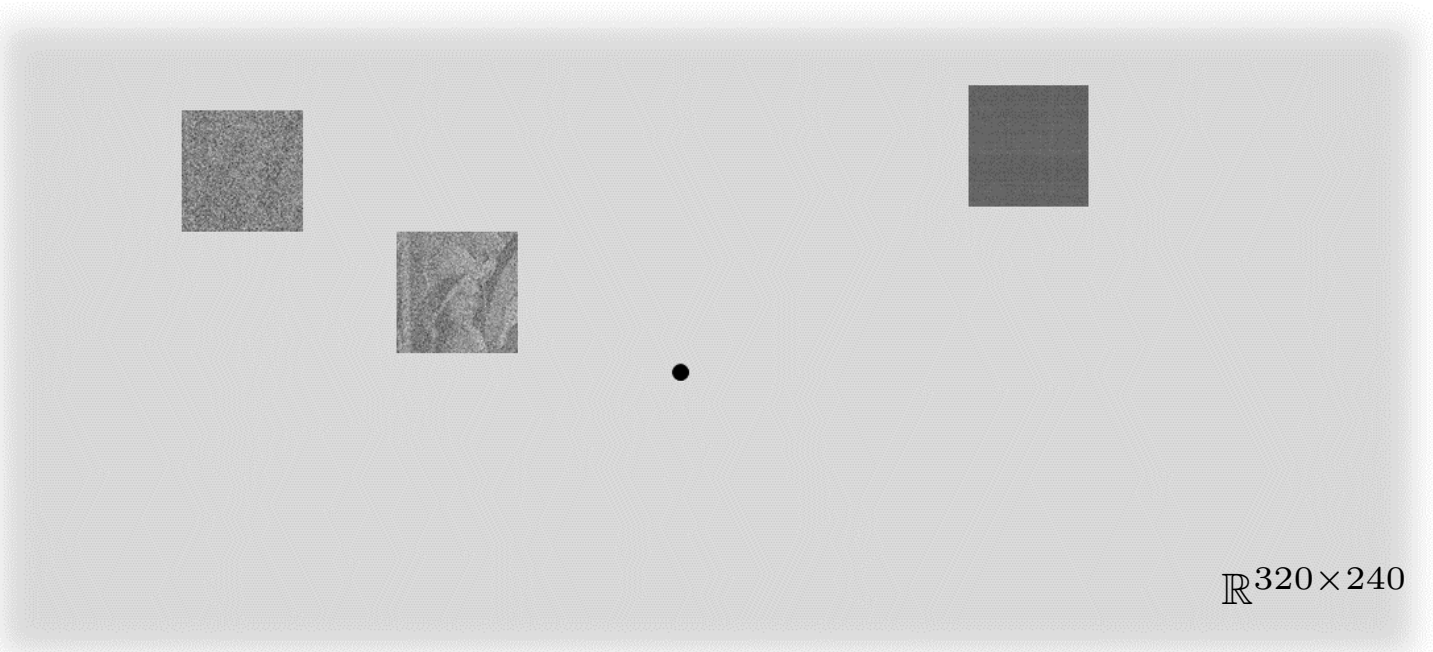
Generative models

What does it mean to learn a distribution?



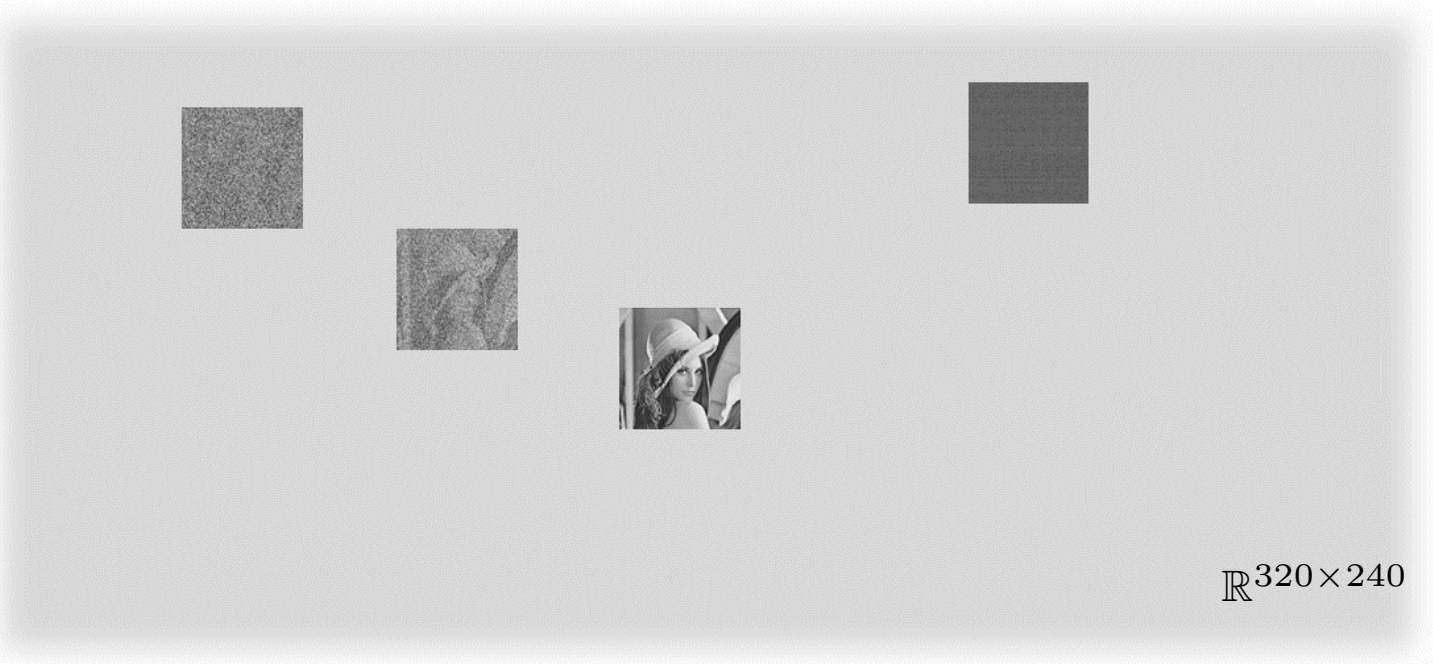
Generative models

What does it mean to learn a distribution?



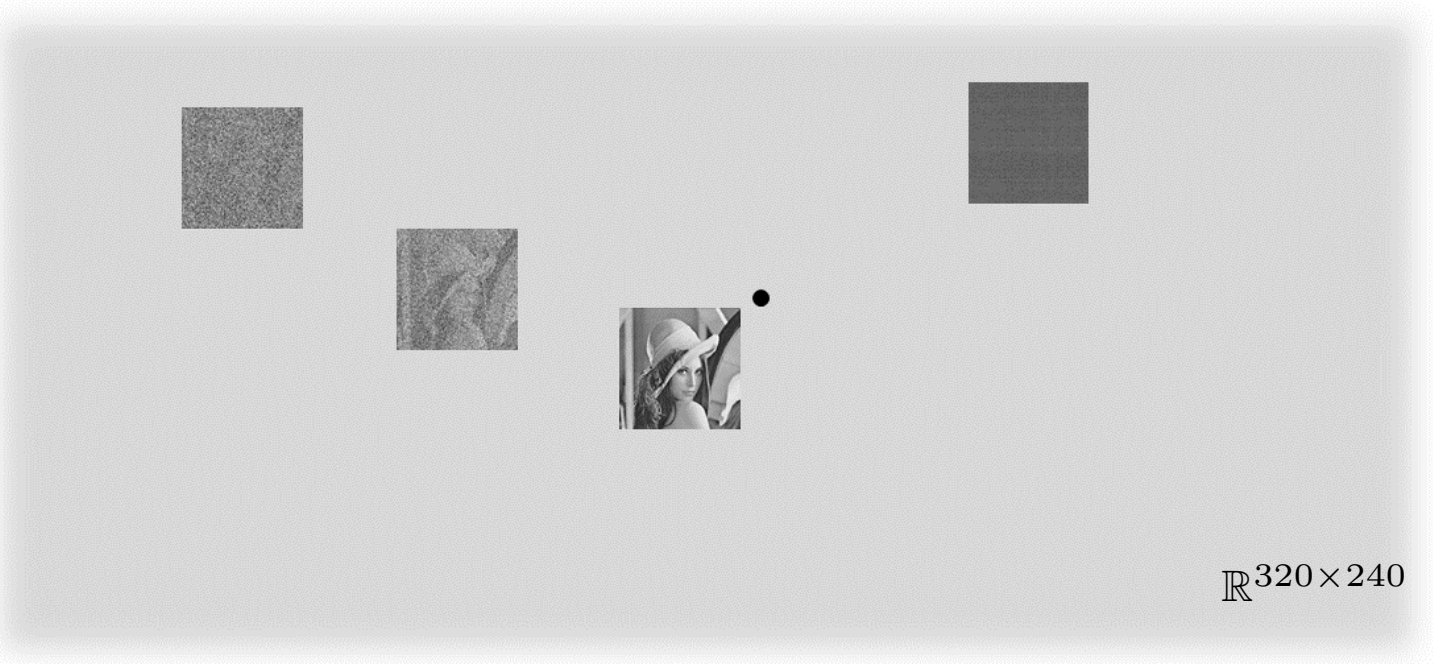
Generative models

What does it mean to learn a distribution?



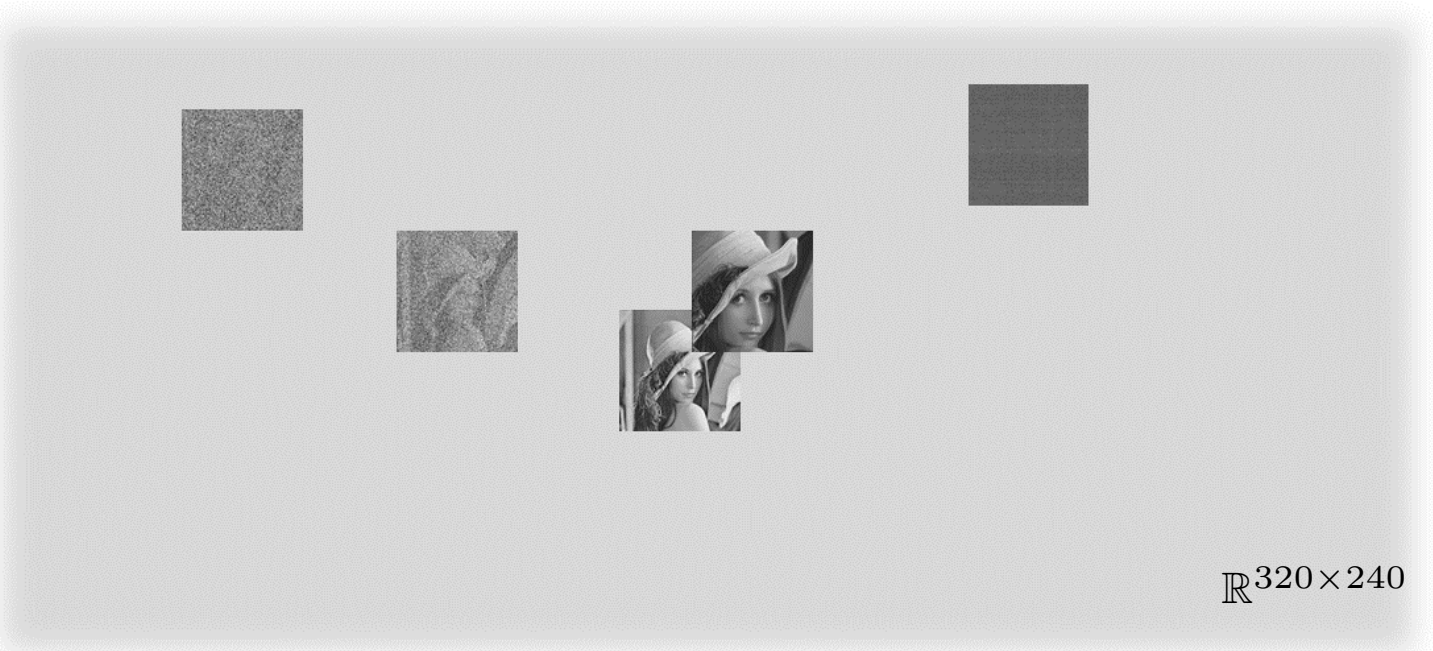
Generative models

What does it mean to learn a distribution?



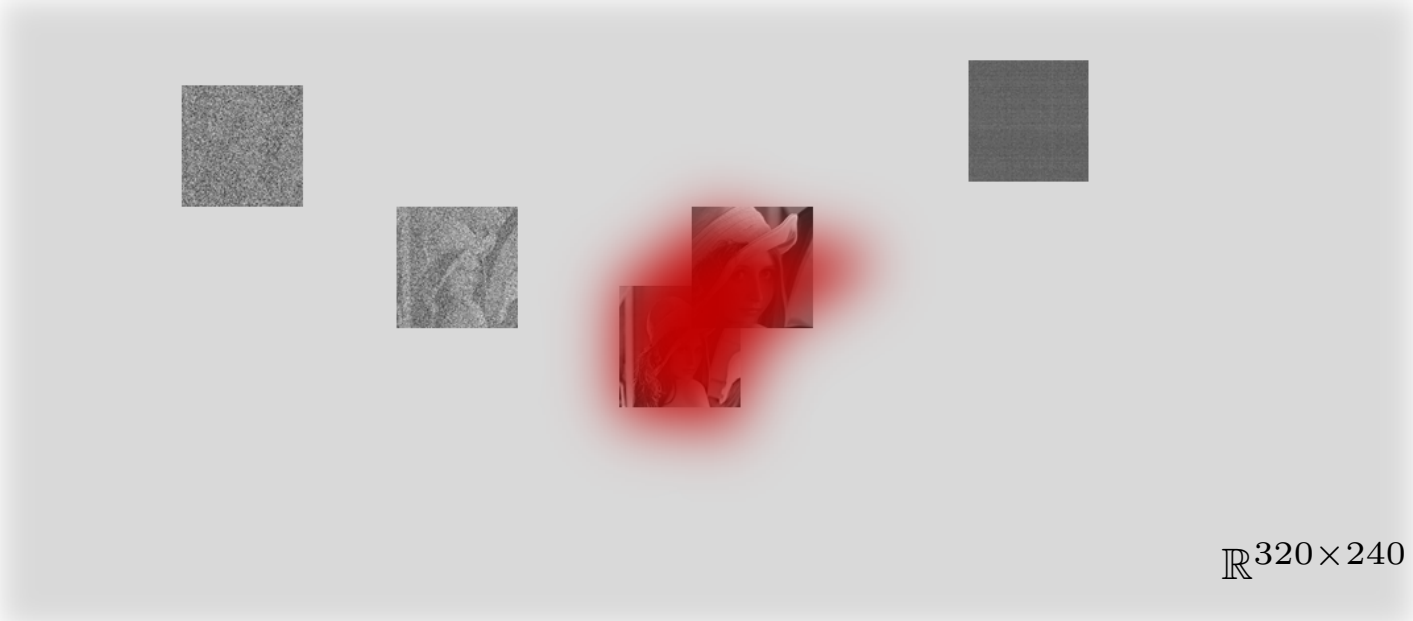
Generative models

What does it mean to learn a distribution?



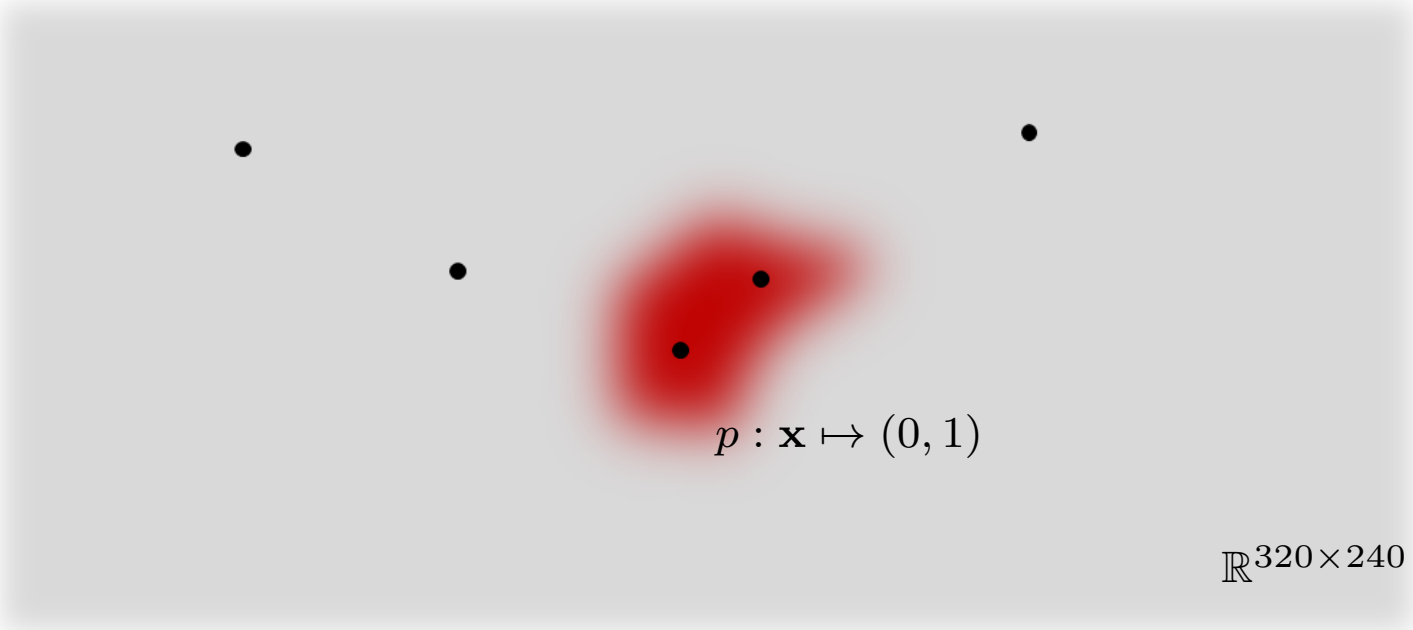
Generative models

What does it mean to learn a distribution?



Generative models

What does it mean to learn a distribution?



The probability distribution p is defined on the entire data space.

Dimensionality reduction

Let us be given n data points stored in matrix $\mathbf{X} \in \mathbb{R}^{d \times n}$:

$$\mathbf{X}^\top = \begin{pmatrix} — & \mathbf{x}_1^\top & — \\ & \vdots & \\ — & \mathbf{x}_n^\top & — \end{pmatrix}$$

Dimensionality reduction

Let us be given n data points stored in matrix $\mathbf{X} \in \mathbb{R}^{d \times n}$:

$$\mathbf{X}^\top = \begin{pmatrix} — & \mathbf{x}_1^\top & — \\ & \vdots & \\ — & \mathbf{x}_n^\top & — \end{pmatrix} \approx \begin{pmatrix} - & \tilde{\mathbf{x}}_1^\top & - \\ & \vdots & \\ - & \tilde{\mathbf{x}}_n^\top & - \end{pmatrix} = \tilde{\mathbf{X}}^\top$$

We want to replace them with a lower-dimensional approximation $\tilde{\mathbf{X}} \in \mathbb{R}^{k \times n}$, with $k \ll d$

Dimensionality reduction

Let us be given n data points stored in matrix $\mathbf{X} \in \mathbb{R}^{d \times n}$:

$$\mathbf{X}^\top = \begin{pmatrix} — & \mathbf{x}_1^\top & — \\ & \vdots & \\ — & \mathbf{x}_n^\top & — \end{pmatrix} \approx \begin{pmatrix} - & \tilde{\mathbf{x}}_1^\top & - \\ & \vdots & \\ - & \tilde{\mathbf{x}}_n^\top & - \end{pmatrix} = \tilde{\mathbf{X}}^\top$$

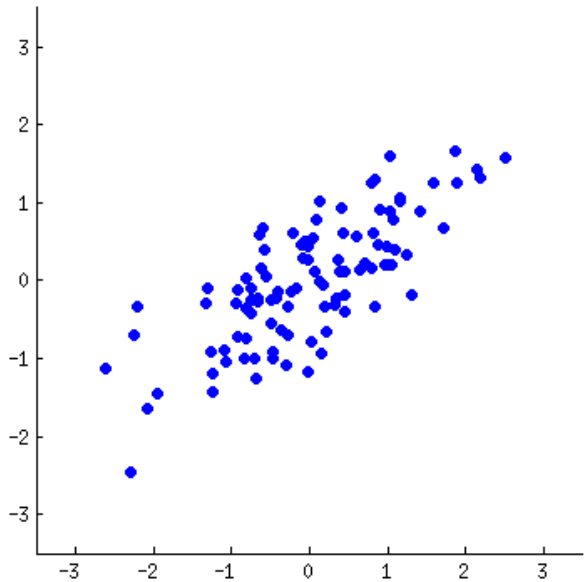
We want to replace them with a lower-dimensional approximation $\tilde{\mathbf{X}} \in \mathbb{R}^{k \times n}$, with $k \ll d$

This can be useful for many other tasks:

- Outlier detection
- Visualization
- Denoising
- As a generative model

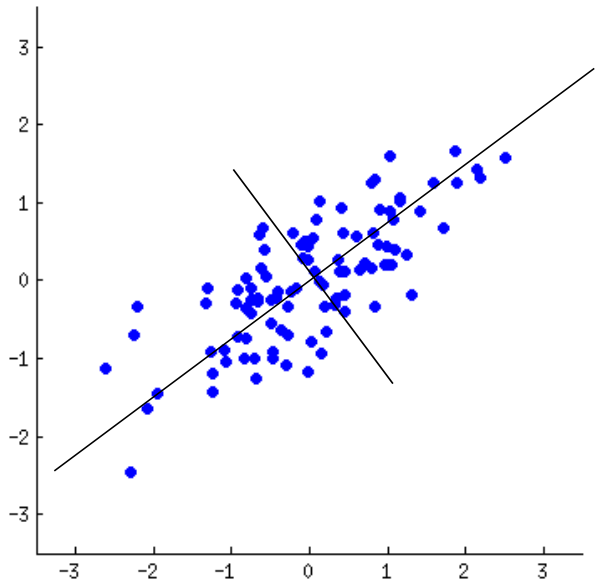
Principal component analysis (PCA)

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



Principal component analysis (PCA)

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

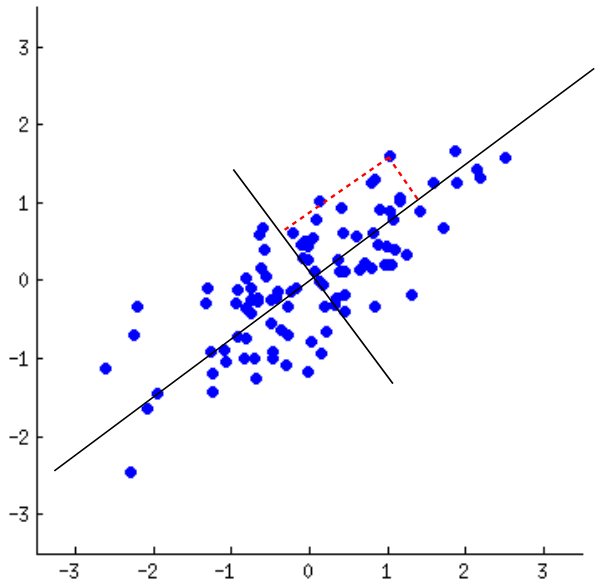


Overall idea:

- Find $k \leq d$ orthogonal directions with the most variance.
  These span a k-dimensional subspace of the data.

Principal component analysis (PCA)

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



Overall idea:

- Find $k \leq d$ orthogonal directions with the most variance.
  These span a k-dimensional subspace of the data.
- Project all the data points onto these directions.
  This is lossy, but can be done with the smallest possible error.

Principal component analysis (PCA)

In matrix notation:

$$\underbrace{\begin{pmatrix} — & \mathbf{x}_1^\top & — \\ & \vdots & \\ — & \mathbf{x}_n^\top & — \end{pmatrix}}_{n \times d}$$

Principal component analysis (PCA)

In matrix notation:

$$\underbrace{\begin{pmatrix} — & \mathbf{x}_1^\top & — \\ & \vdots & \\ — & \mathbf{x}_n^\top & — \end{pmatrix}}_{n \times d} \underbrace{\begin{pmatrix} | & & | \\ \mathbf{w}_1 & \cdots & \mathbf{w}_k \\ | & & | \end{pmatrix}}_{d \times k}$$

Principal component analysis (PCA)

In matrix notation:

$$\underbrace{\begin{pmatrix} — & \mathbf{x}_1^\top & — \\ & \vdots & \\ — & \mathbf{x}_n^\top & — \end{pmatrix}}_{n \times d} \underbrace{\begin{pmatrix} | & & | \\ \mathbf{w}_1 & \cdots & \mathbf{w}_k \\ | & & | \end{pmatrix}}_{d \times k} = \underbrace{\begin{pmatrix} — & \mathbf{z}_1^\top & — \\ & \vdots & \\ — & \mathbf{z}_n^\top & — \end{pmatrix}}_{n \times k}$$

Principal component analysis (PCA)

In matrix notation:

$$\underbrace{\begin{pmatrix} — & \mathbf{x}_1^\top & — \\ & \vdots & \\ — & \mathbf{x}_n^\top & — \end{pmatrix}}_{n \times d} \underbrace{\begin{pmatrix} | & & | \\ \mathbf{w}_1 & \cdots & \mathbf{w}_k \\ | & & | \end{pmatrix}}_{d \times k} = \underbrace{\begin{pmatrix} — & \mathbf{z}_1^\top & — \\ & \vdots & \\ — & \mathbf{z}_n^\top & — \end{pmatrix}}_{n \times k}$$

Assuming $\mathbf{W}^\top \mathbf{W} = \mathbf{I}$, for $k = d$ we get:

$$\mathbf{X}^\top \mathbf{W} = \mathbf{Z}^\top$$
$$\mathbf{X} = \mathbf{W}\mathbf{Z}$$

Principal component analysis (PCA)

In matrix notation:

$$\underbrace{\begin{pmatrix} — & \mathbf{x}_1^\top & — \\ & \vdots & \\ — & \mathbf{x}_n^\top & — \end{pmatrix}}_{n \times d} \underbrace{\begin{pmatrix} | & & | \\ \mathbf{w}_1 & \cdots & \mathbf{w}_k \\ | & & | \end{pmatrix}}_{d \times k} = \underbrace{\begin{pmatrix} — & \mathbf{z}_1^\top & — \\ & \vdots & \\ — & \mathbf{z}_n^\top & — \end{pmatrix}}_{n \times k}$$

Assuming $\mathbf{W}^\top \mathbf{W} = \mathbf{I}$, for $k < d$ we get:

$$\mathbf{X}^\top \mathbf{W} = \mathbf{Z}^\top$$
$$\mathbf{X} \approx \mathbf{W}\mathbf{Z}$$

Principal component analysis (PCA)

In matrix notation:

$$\underbrace{\begin{pmatrix} — & \mathbf{x}_1^\top & — \\ & \vdots & \\ — & \mathbf{x}_n^\top & — \end{pmatrix}}_{n \times d} \underbrace{\begin{pmatrix} | & & | \\ \mathbf{w}_1 & \cdots & \mathbf{w}_k \\ | & & | \end{pmatrix}}_{d \times k} = \underbrace{\begin{pmatrix} — & \mathbf{z}_1^\top & — \\ & \vdots & \\ — & \mathbf{z}_n^\top & — \end{pmatrix}}_{n \times k}$$

Assuming $\mathbf{W}^\top \mathbf{W} = \mathbf{I}$, for $k < d$ we get:

$$\mathbf{X}^\top \mathbf{W} = \mathbf{Z}^\top \quad \text{projection}$$
$$\mathbf{X} \approx \mathbf{W}\mathbf{Z} \quad \text{reconstruction}$$

Principal component analysis (PCA)

In matrix notation:

$$\underbrace{\begin{pmatrix} — & \mathbf{x}_1^\top & — \\ & \vdots & \\ — & \mathbf{x}_n^\top & — \end{pmatrix}}_{n \times d} \underbrace{\begin{pmatrix} | & & | \\ \mathbf{w}_1 & \cdots & \mathbf{w}_k \\ | & & | \end{pmatrix}}_{d \times k} = \underbrace{\begin{pmatrix} — & \mathbf{z}_1^\top & — \\ & \vdots & \\ — & \mathbf{z}_n^\top & — \end{pmatrix}}_{n \times k}$$

Assuming $\mathbf{W}^\top \mathbf{W} = \mathbf{I}$, for $k < d$ we get:

$$\mathbf{X}^\top \mathbf{W} = \mathbf{Z}^\top \quad \text{projection}$$
$$\mathbf{X} \approx \mathbf{W}\mathbf{Z} \quad \text{reconstruction}$$

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

They are unknown and must be computed.

Principal component analysis (PCA)

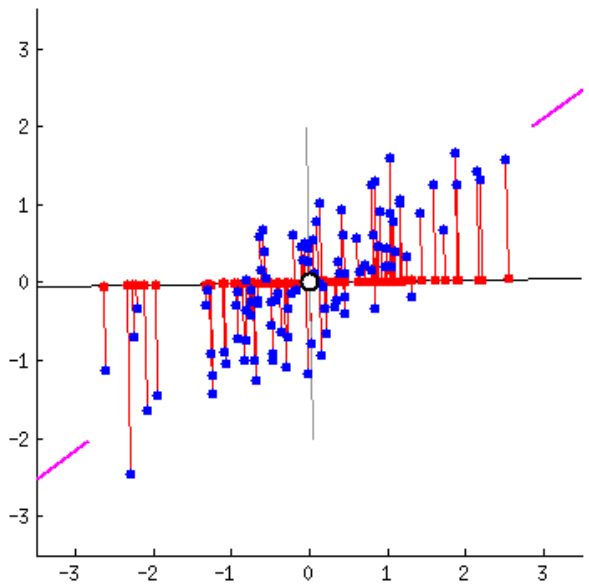
We seek the direction $\mathbf{w}$ (a column of $\mathbf{W}$) that:

- Minimizes the projection/reconstruction error.
- Maximizes the variance of the projected data.

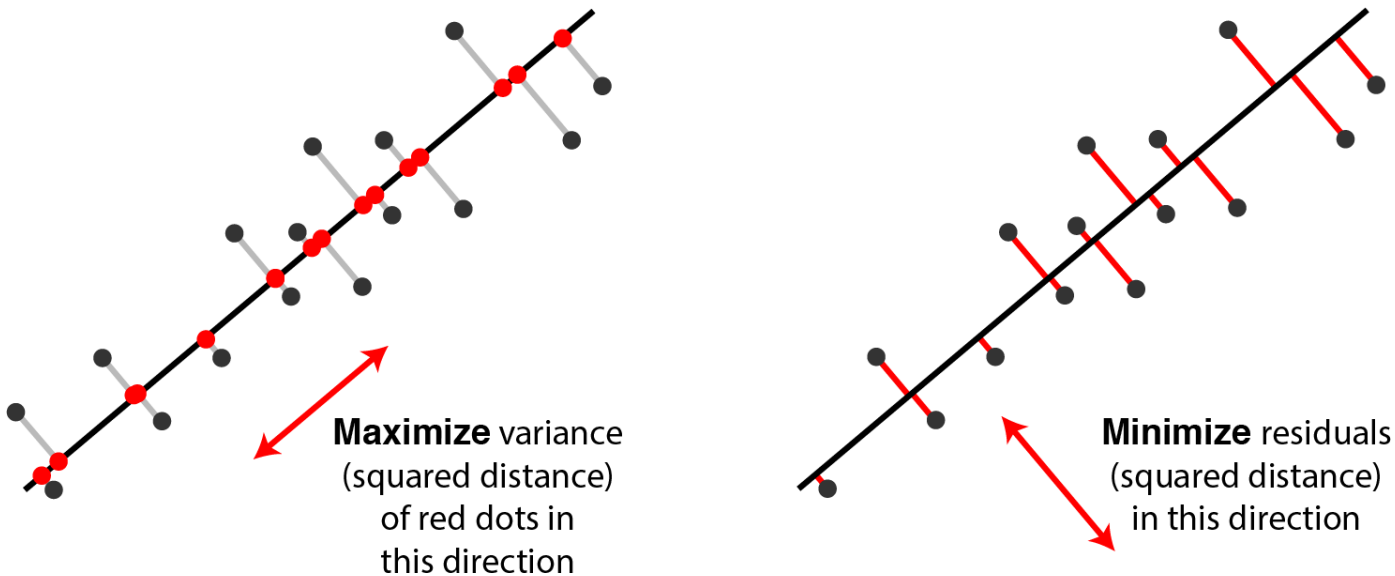
Principal component analysis (PCA)

We seek the direction $\mathbf{w}$ that:

- Minimizes the projection/reconstruction error.
- Maximizes the variance of the projected data.



Principal component analysis (PCA)



Principal component analysis (PCA)

Assume the data points $\mathbf{X}$ are centered at zero.

For a given $\mathbf{w}$, the projection of all n points onto $\mathbf{w}$ is $\mathbf{X}^\top \mathbf{w}$.

Principal component analysis (PCA)

Assume the data points $\mathbf{X}$ are centered at zero.

For a given $\mathbf{w}$, the projection of all n points onto $\mathbf{w}$ is $\mathbf{X}^\top \mathbf{w}$.

The variance to maximize is $\|\mathbf{X}^\top \mathbf{w}\|_2^2$:

$$(\mathbf{X}^\top \mathbf{w})^\top (\mathbf{X}^\top \mathbf{w})$$

Principal component analysis (PCA)

Assume the data points $\mathbf{X}$ are centered at zero.

For a given $\mathbf{w}$, the projection of all n points onto $\mathbf{w}$ is $\mathbf{X}^\top \mathbf{w}$.

The variance to maximize is $\|\mathbf{X}^\top \mathbf{w}\|_2^2$:

$$(\mathbf{X}^\top \mathbf{w})^\top (\mathbf{X}^\top \mathbf{w}) = \mathbf{w}^\top (\mathbf{X}\mathbf{X}^\top)\mathbf{w}$$

Principal component analysis (PCA)

Assume the data points $\mathbf{X}$ are centered at zero.

For a given $\mathbf{w}$, the projection of all n points onto $\mathbf{w}$ is $\mathbf{X}^\top \mathbf{w}$.

The variance to maximize is $\|\mathbf{X}^\top \mathbf{w}\|_2^2$:

$$(\mathbf{X}^\top \mathbf{w})^\top (\mathbf{X}^\top \mathbf{w}) = \mathbf{w}^\top \underbrace{(\mathbf{X}\mathbf{X}^\top)}_{\mathbf{C}} \mathbf{w}$$

where $\mathbf{C} \in \mathbb{R}^{d \times d}$ is the symmetric covariance matrix.

Principal component analysis (PCA)

Assume the data points $\mathbf{X}$ are centered at zero.

For a given $\mathbf{w}$, the projection of all n points onto $\mathbf{w}$ is $\mathbf{X}^\top \mathbf{w}$.

The variance to maximize is $\|\mathbf{X}^\top \mathbf{w}\|_2^2$:

$$(\mathbf{X}^\top \mathbf{w})^\top (\mathbf{X}^\top \mathbf{w}) = \mathbf{w}^\top \underbrace{(\mathbf{X}\mathbf{X}^\top)}_{\mathbf{C}} \mathbf{w}$$

where $\mathbf{C} \in \mathbb{R}^{d \times d}$ is the symmetric covariance matrix.

We want to solve the problem:

$$\max_{\mathbf{w}} \mathbf{w}^\top \mathbf{C}\mathbf{w} \quad \text{s.t. } \|\mathbf{w}\|_2 = 1$$

Principal component analysis (PCA)

Assume the data points $\mathbf{X}$ are centered at zero.

For a given $\mathbf{w}$, the projection of all n points onto $\mathbf{w}$ is $\mathbf{X}^\top \mathbf{w}$.

The variance to maximize is $\|\mathbf{X}^\top \mathbf{w}\|_2^2$:

$$(\mathbf{X}^\top \mathbf{w})^\top (\mathbf{X}^\top \mathbf{w}) = \mathbf{w}^\top \underbrace{(\mathbf{X}\mathbf{X}^\top)}_{\mathbf{C}} \mathbf{w}$$

where $\mathbf{C} \in \mathbb{R}^{d \times d}$ is the symmetric covariance matrix.

We want to solve the problem:

$$\max_{\mathbf{w}} \mathbf{w}^\top \mathbf{C}\mathbf{w} \quad \text{s.t. } \|\mathbf{w}\|_2 = 1$$

The solution is $\mathbf{w} =$ principal eigenvector of $\mathbf{C}$ (Courant minmax principle), and the value $\mathbf{w}^\top \mathbf{C}\mathbf{w}$ is the corresponding eigenvalue.

Principal component analysis (PCA)

After solving the problem:

$$\mathbf{w}_1 = \arg\max_{\mathbf{w}} \mathbf{w}^\top \mathbf{C}\mathbf{w}$$
$$\text{s.t. } \|\mathbf{w}\|_2 = 1$$

Principal component analysis (PCA)

After solving the problem:

$$\mathbf{w}_1 = \arg\max_{\mathbf{w}} \mathbf{w}^\top \mathbf{C}\mathbf{w}$$
$$\text{s.t. } \|\mathbf{w}\|_2 = 1$$

The successive orthogonal direction can be found by solving:

$$\mathbf{w}_2 = \arg\max_{\mathbf{w}} \mathbf{w}^\top \mathbf{C}\mathbf{w}$$
$$\text{s.t. } \|\mathbf{w}\|_2 = 1$$
$$\mathbf{w}_1^\top \mathbf{w} = 0$$

Principal component analysis (PCA)

After solving the problem:

$$\mathbf{w}_1 = \arg\max_{\mathbf{w}} \mathbf{w}^\top \mathbf{C}\mathbf{w}$$
$$\text{s.t. } \|\mathbf{w}\|_2 = 1$$

The successive orthogonal direction can be found by solving:

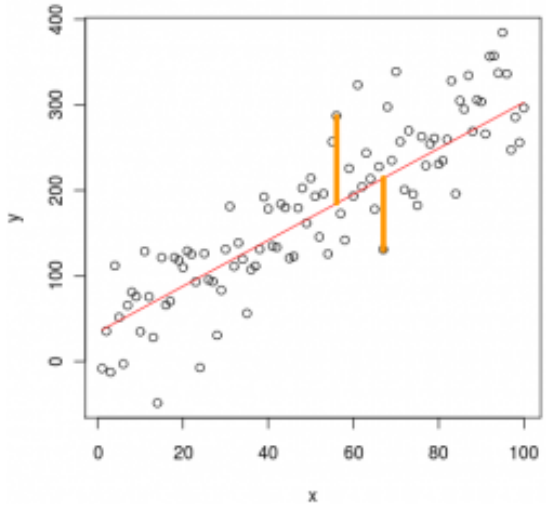
$$\mathbf{w}_2 = \arg\max_{\mathbf{w}} \mathbf{w}^\top \mathbf{C}\mathbf{w}$$
$$\text{s.t. } \|\mathbf{w}\|_2 = 1$$
$$\mathbf{w}_1^\top \mathbf{w} = 0$$

which is the second eigenvector of $\mathbf{C}$, and so on for all $\mathbf{w}_{i=2\ldots k}$.

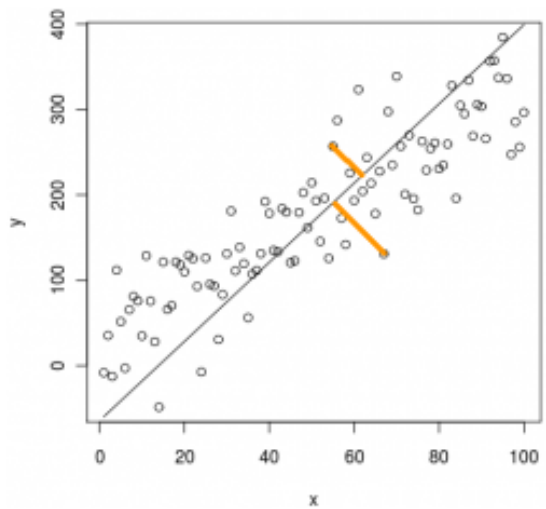
The principal components are thus the first $k \ll d$ eigenvectors of $\mathbf{C}$, sorted by decreasing eigenvalue.

PCA is not linear regression

With linear regression we measure the error along the y coordinate:



With PCA we measure the error orthogonal to the principal direction:



PCA as a generative model

Given the $\mathbf{W}$ satisfying, for the observations $\mathbf{X}$:

$$\mathbf{X}^\top \mathbf{W} = \mathbf{Z}^\top \quad \text{projection}$$
$$\mathbf{X} \approx \mathbf{W}\mathbf{Z} \quad \text{reconstruction}$$

We can generate new data just by sampling $\mathbf{z}_{\text{new}} \in \mathbb{R}^k$ and computing:

$$\mathbf{x}_{\text{new}} = \mathbf{W}\mathbf{z}_{\text{new}}$$

PCA as a generative model

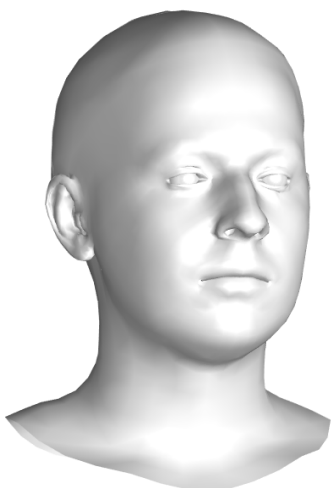
Given the $\mathbf{W}$ satisfying, for the observations $\mathbf{X}$:

$$\mathbf{X}^\top \mathbf{W} = \mathbf{Z}^\top \quad \text{projection}$$
$$\mathbf{X} \approx \mathbf{W}\mathbf{Z} \quad \text{reconstruction}$$

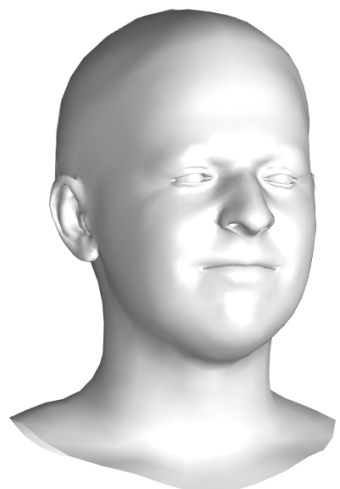
We can generate new data just by sampling $\mathbf{z}_{\text{new}} \in \mathbb{R}^k$ and computing:

$$\mathbf{x}_{\text{new}} = \mathbf{W}\mathbf{z}_{\text{new}}$$

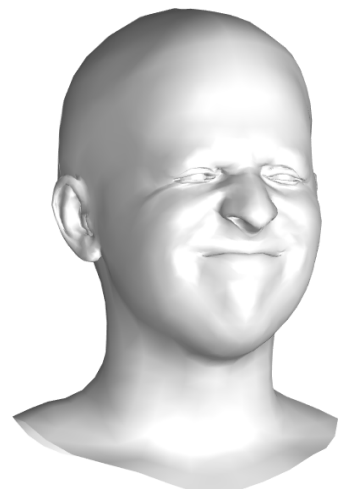
Example:



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:

$$\mathbf{W}^\top \mathbf{x} = \mathbf{z} \qquad \text{projection}$$
$$\mathbf{x} \approx \mathbf{W}\mathbf{z} \qquad \text{reconstruction}$$

From a different perspective, PCA gives us a parametric model.

Codes

Consider again the relations:

$$\mathbf{W}^\top \mathbf{x} = \mathbf{z} \qquad \text{encoding}$$
$$\mathbf{x} \approx \mathbf{W}\mathbf{z} \qquad \text{decoding}$$

From a different perspective, PCA gives us a parametric model.

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.

The encoding and decoding procedures are linear.

Codes

Consider again the relations:

$$\mathbf{W}^\top \mathbf{x} = \mathbf{z} \qquad \text{encoding}$$
$$\mathbf{x} \approx \mathbf{W}\mathbf{z} \qquad \text{decoding}$$

From a different perspective, PCA gives us a parametric model.

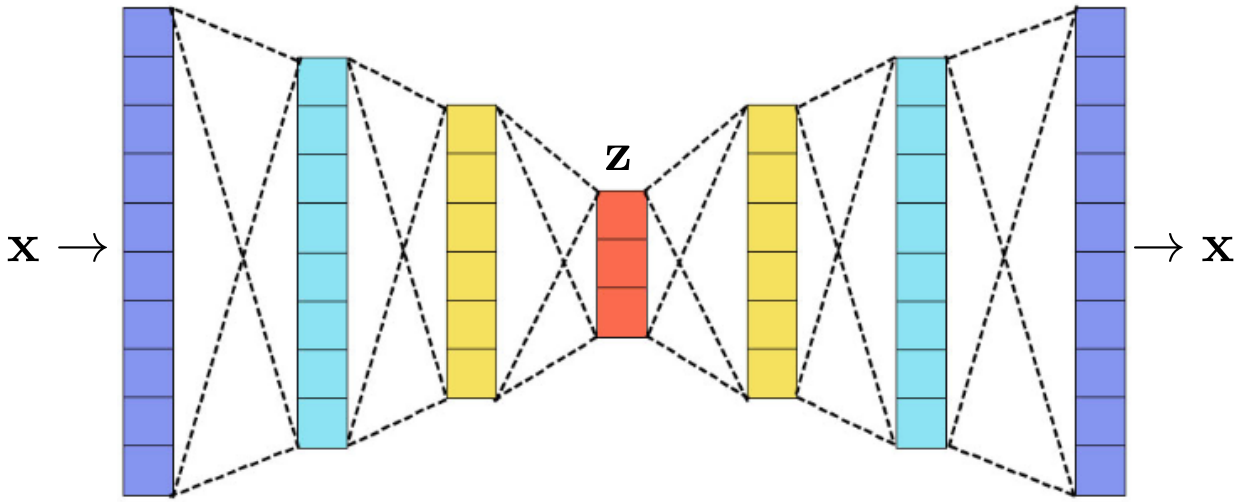
Each data point $\mathbf{x}$ is transformed into a low-dimensional code $\mathbf{z} \in \mathbb{R}^k$, where the dimension $k < d$ is fixed.

The encoding and decoding procedures are linear.

How to generalize this idea?

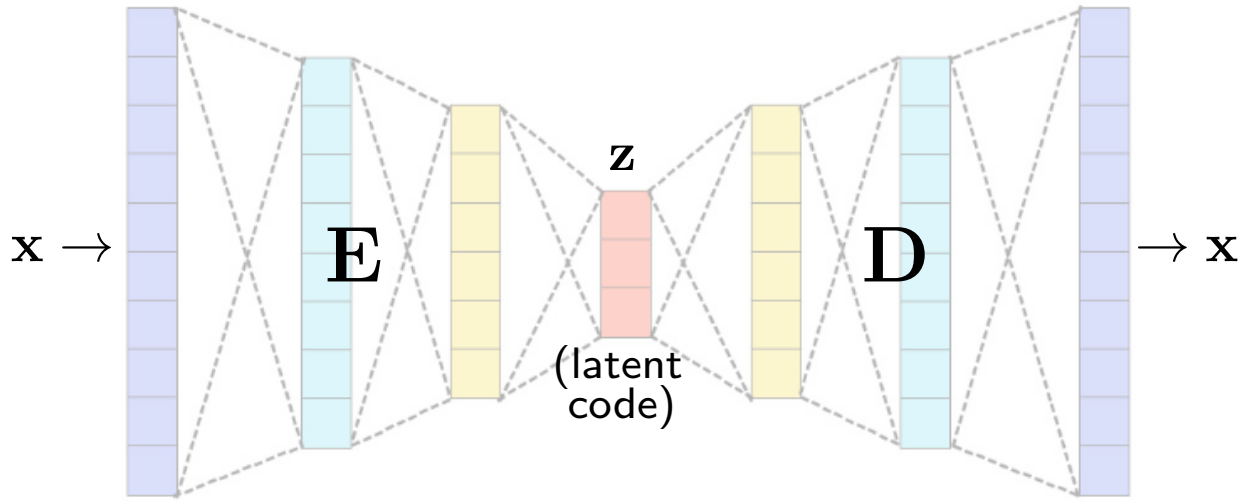
Autoencoders (AE)

We can construct powerful parametric models using deep nets.



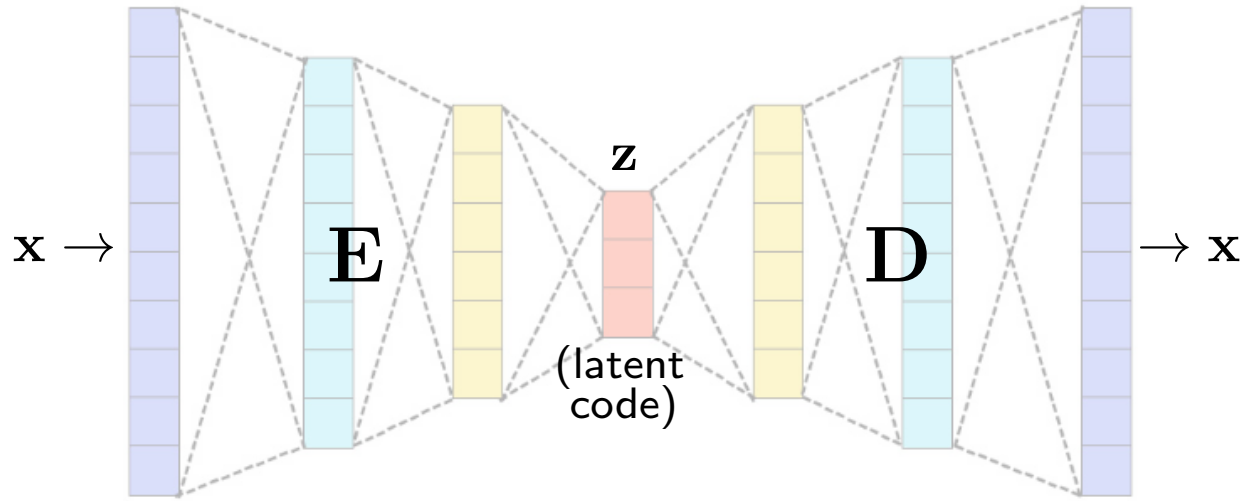
Autoencoders (AE)

We can construct powerful parametric models using deep nets.



Autoencoders (AE)

We can construct powerful parametric models using deep nets.

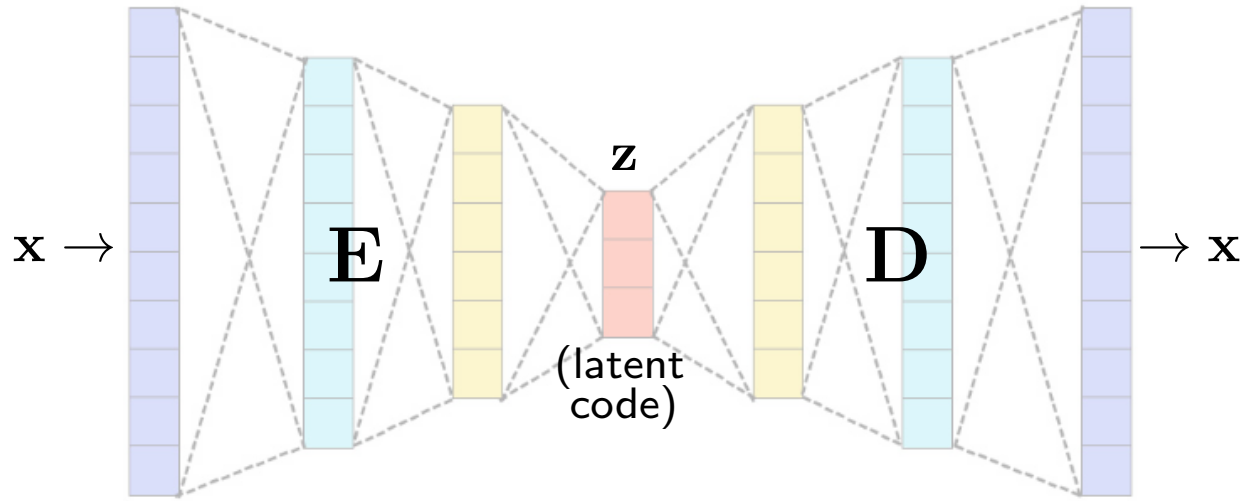


For a given dataset $\{\mathbf{x}_i\}$, we require the encoder E and decoder (or generator) D to minimize the reconstruction loss:

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

Autoencoders (AE)

We can construct powerful parametric models using deep nets.



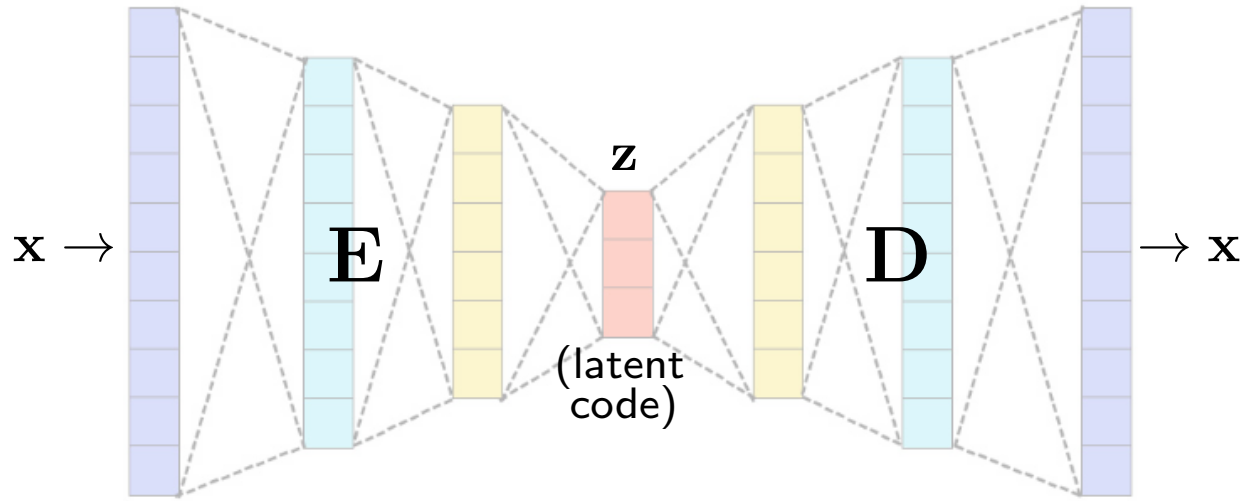
For a given dataset $\{\mathbf{x}_i\}$, we require the encoder E and decoder (or generator) D to minimize the reconstruction loss:

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

The choice of the metric depends on the data and on the task.

Autoencoders (AE)

We can construct powerful parametric models using deep nets.



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

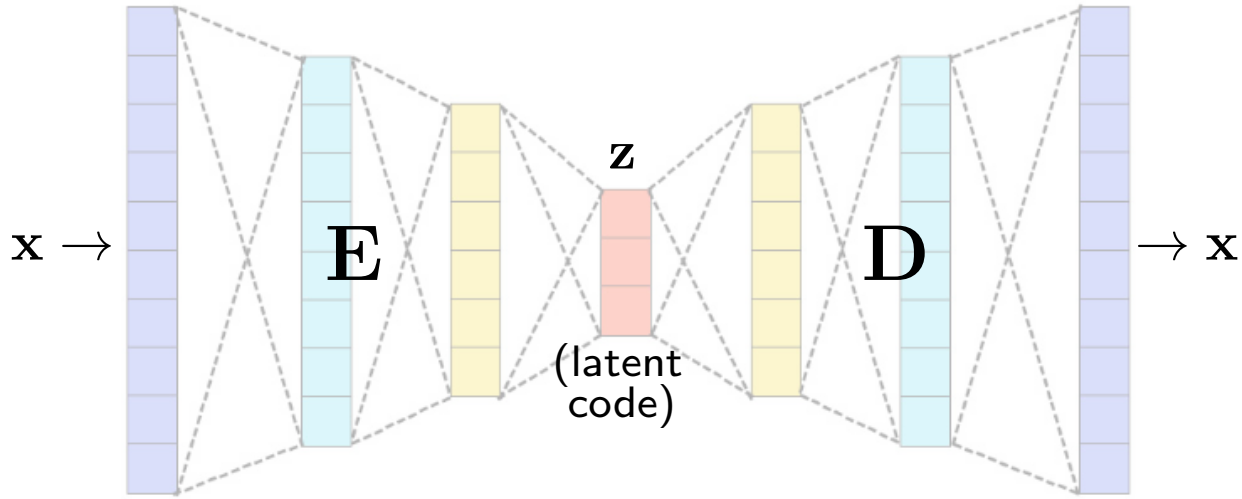
$$\ell_\Theta = \sum_i \|\mathbf{x}_i - D_\Theta(E_\Theta(\mathbf{x}_i))\|$$

The choice of the metric depends on the data and on the task.

If the layers are linear, the codes $\mathbf{z}_i$ span exactly the same space as PCA.

Autoencoders (AE)

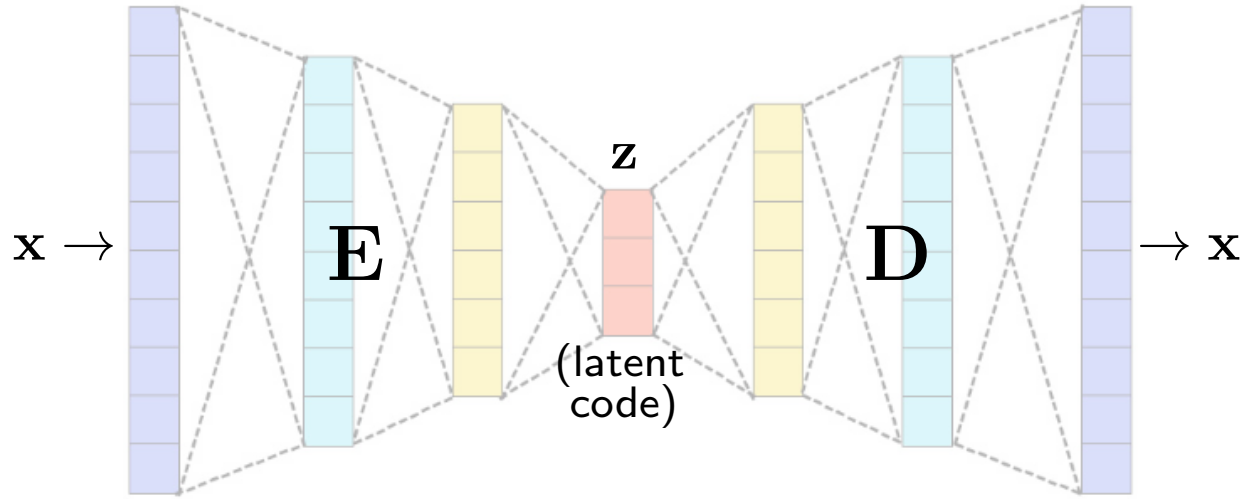
We can construct powerful parametric models using deep nets.



- The bottleneck prevents trivial solutions.

Autoencoders (AE)

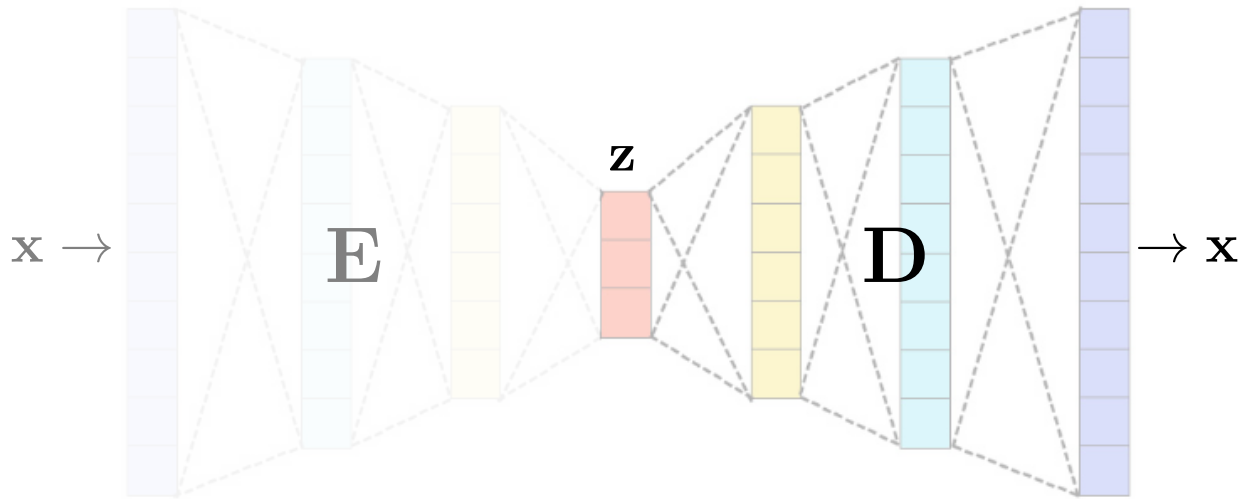
We can construct powerful parametric models using deep nets.



- The bottleneck prevents trivial solutions.
- The task is not important here: it is always reconstruction.

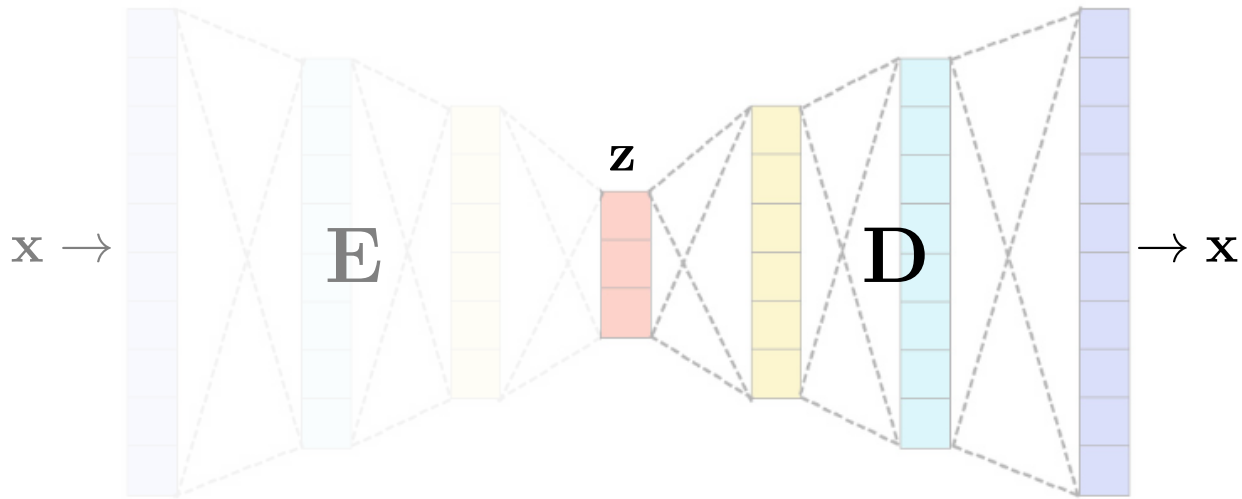
  Once the AE is trained, we are interested in the structure of the latent space and in the adoption of E, D for new tasks.

Manifold hypothesis



The decoder performs a mapping from a low-dimensional latent space to a high-dimensional embedding of observed data.

Manifold hypothesis

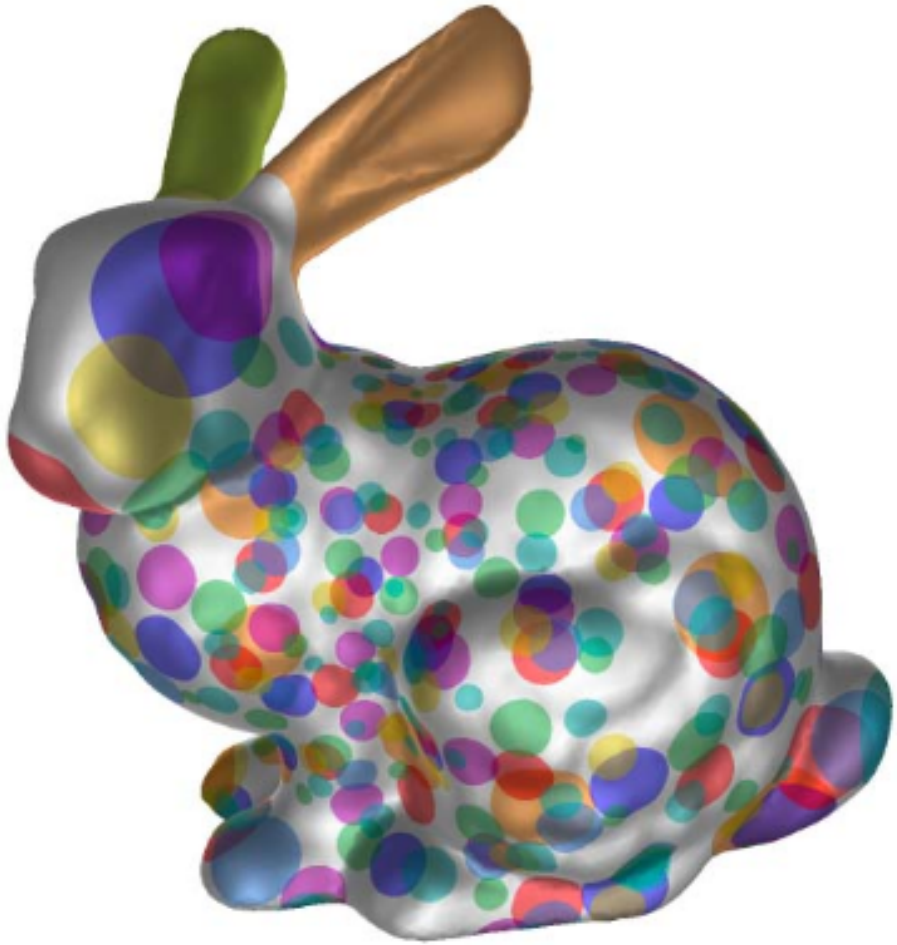


The decoder performs a mapping from a low-dimensional latent space to a high-dimensional embedding of observed data.

The latent space is Euclidean.

The data embedding space is curved (manifold hypothesis).

Differential geometry

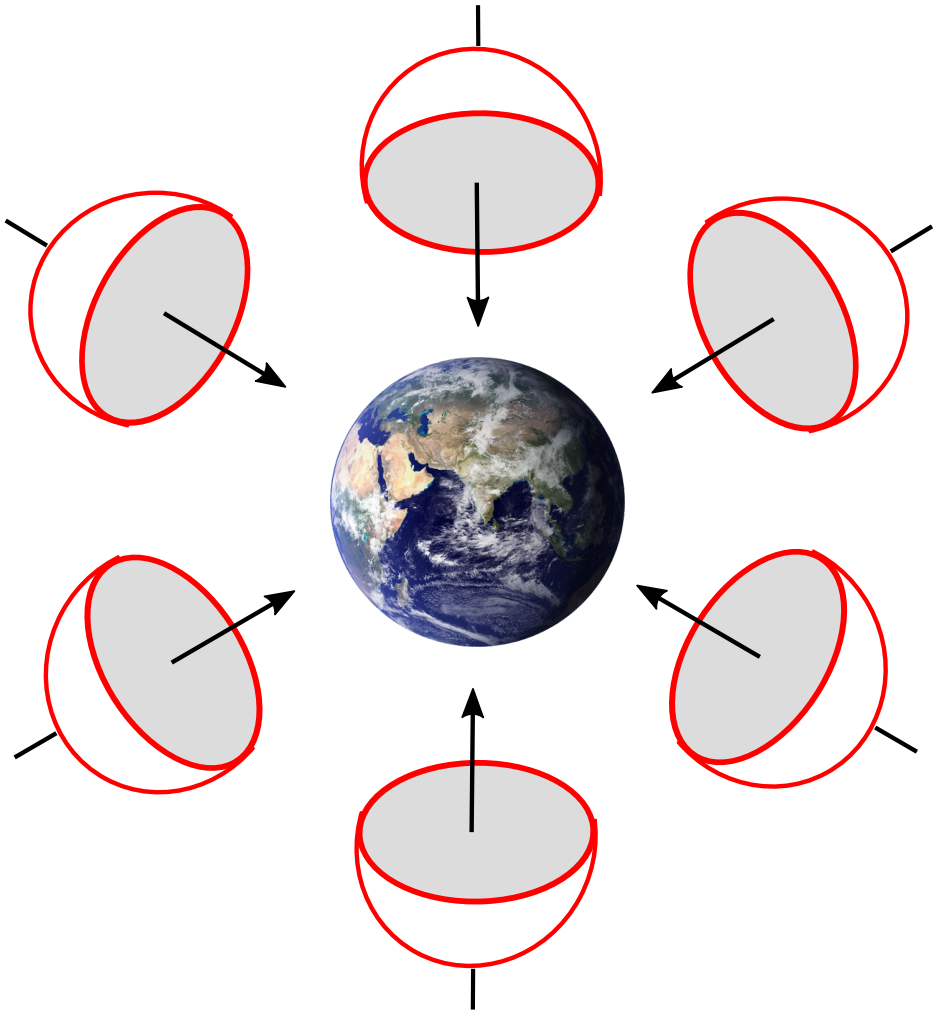


The study of local properties of curves and surfaces.

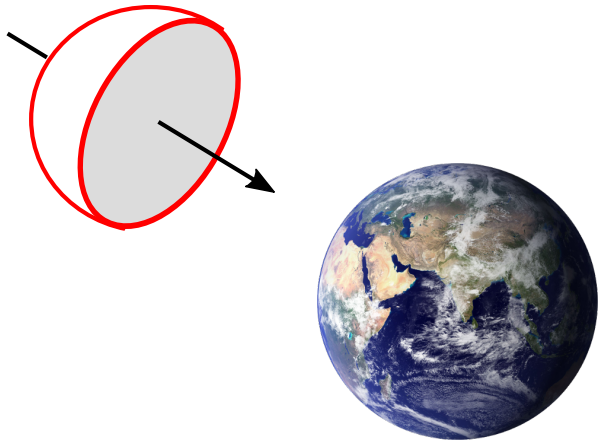
Each neighborhood has a well-behaved mapping to some subset $U \subset \mathbb{R}^2$.

Manifolds

Manifolds are unions of charts:



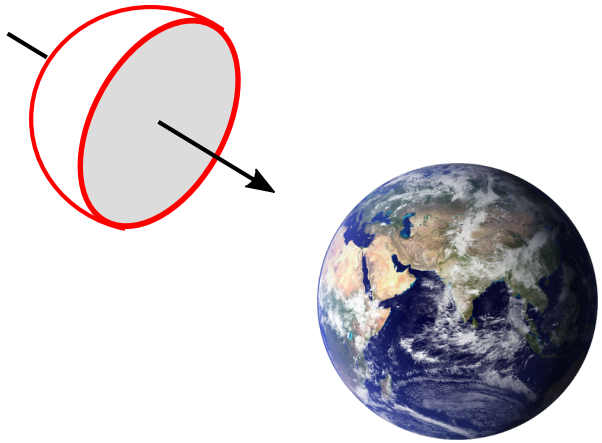
2D manifolds (surfaces)



chart

Each chart can be seen as a mapping $\phi : \mathbb{R}^2 \to \mathcal{S} \subset \mathbb{R}^3$.

2D manifolds (surfaces)

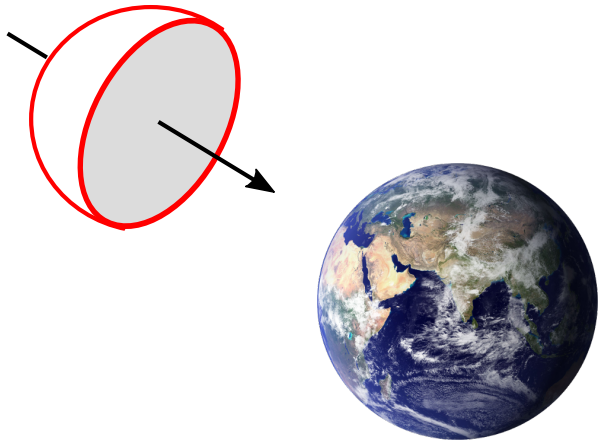


chart

Each chart can be seen as a mapping $\phi : \mathbb{R}^2 \to \mathcal{S} \subset \mathbb{R}^3$.

We require ϕ to be smooth and invertible (diffeomorphism).

2D manifolds (surfaces)



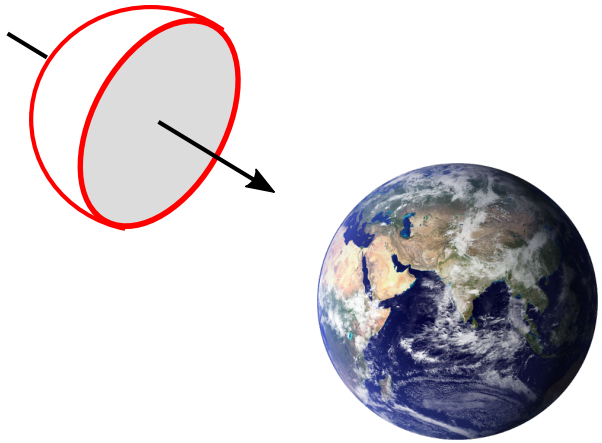
chart

Each chart can be seen as a mapping $\phi : \mathbb{R}^2 \to \mathcal{S} \subset \mathbb{R}^3$.

We require ϕ to be smooth and invertible (diffeomorphism).

- The domain of ϕ is the parametric space and is Euclidean.

2D manifolds (surfaces)



chart

Each chart can be seen as a mapping $\phi : \mathbb{R}^2 \to \mathcal{S} \subset \mathbb{R}^3$.

We require ϕ to be smooth and invertible (diffeomorphism).

- The domain of ϕ is the parametric space and is Euclidean.
- The image of ϕ is the embedding and is a surface.

2D manifolds (surfaces)

- Cut pieces of a plane.

2D manifolds (surfaces)

- Cut pieces of a plane.
- Deform these pieces.

2D manifolds (surfaces)

- Cut pieces of a plane.
- Deform these pieces.
- Glue them together.

2D manifolds (surfaces)

- Cut pieces of a plane.
- Deform these pieces.
- Glue them together.

Manifolds

Manifolds can be k-dimensional, meaning that we have charts:

$$\phi : \mathbb{R}^k \to \mathcal{M} \subset \mathbb{R}^d \quad \text{with } k < d$$

Manifolds

Manifolds can be k-dimensional, meaning that we have charts:

$$\phi : \mathbb{R}^k \to \mathcal{M} \subset \mathbb{R}^d \quad \text{with } k < d$$

The parametrization is not unique:

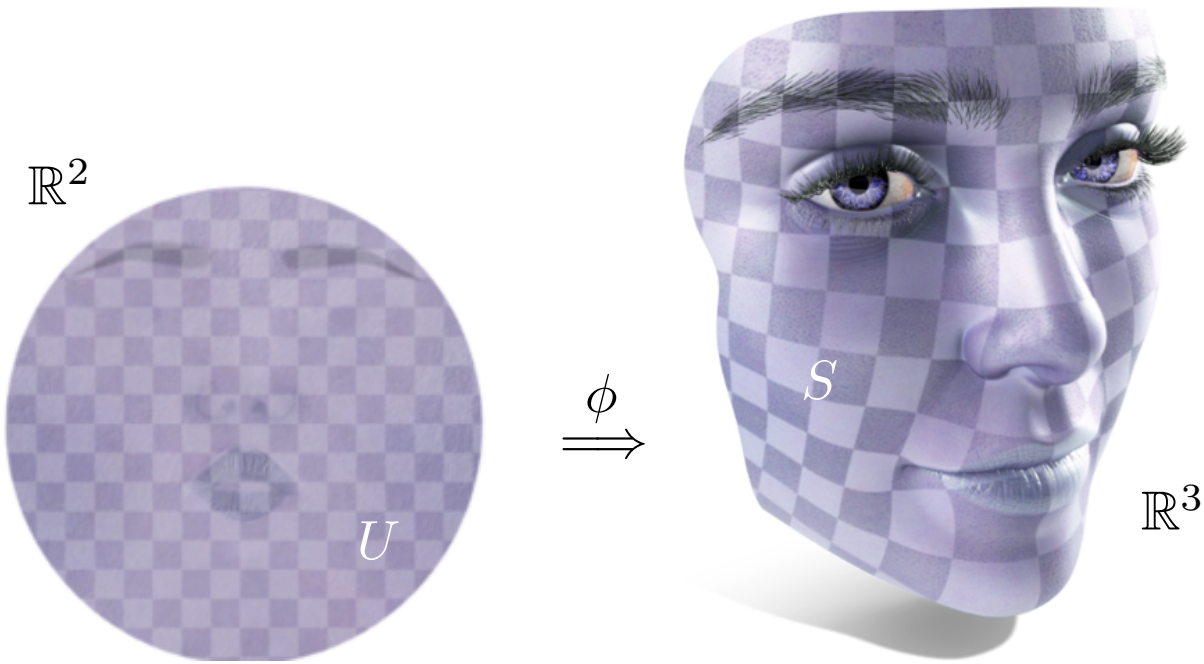


Figure by Keenan Crane

Manifolds

Manifolds can be k-dimensional, meaning that we have charts:

$$\phi : \mathbb{R}^k \to \mathcal{M} \subset \mathbb{R}^d \quad \text{with } k < d$$

The parametrization is not unique:

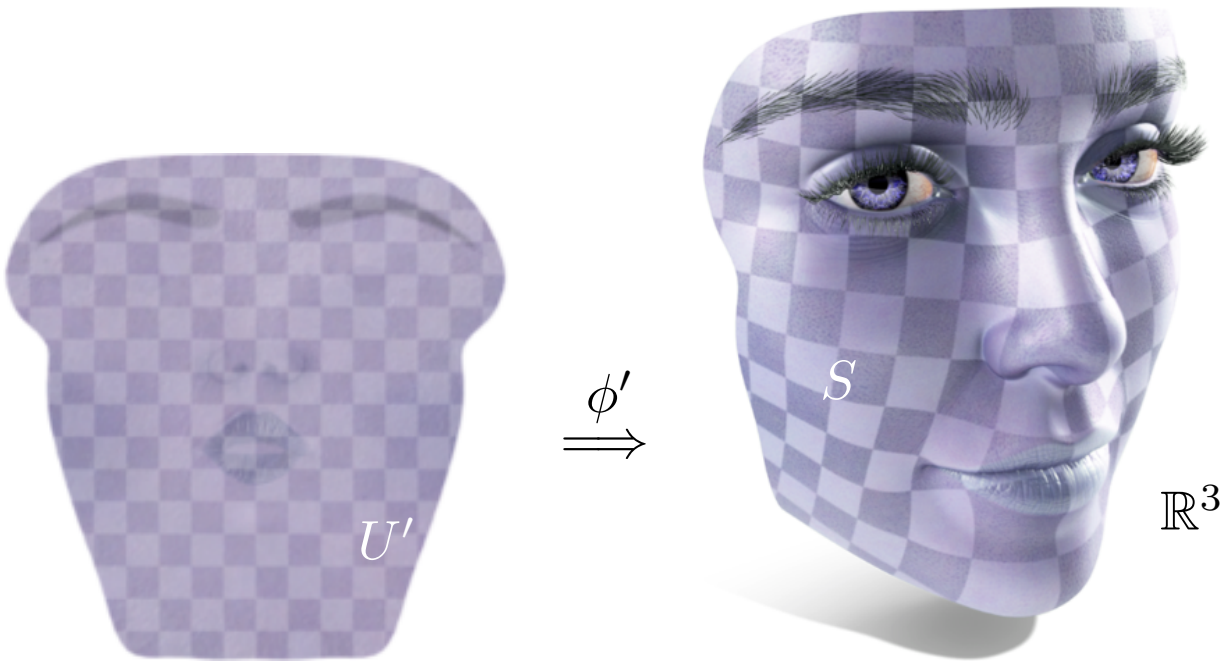


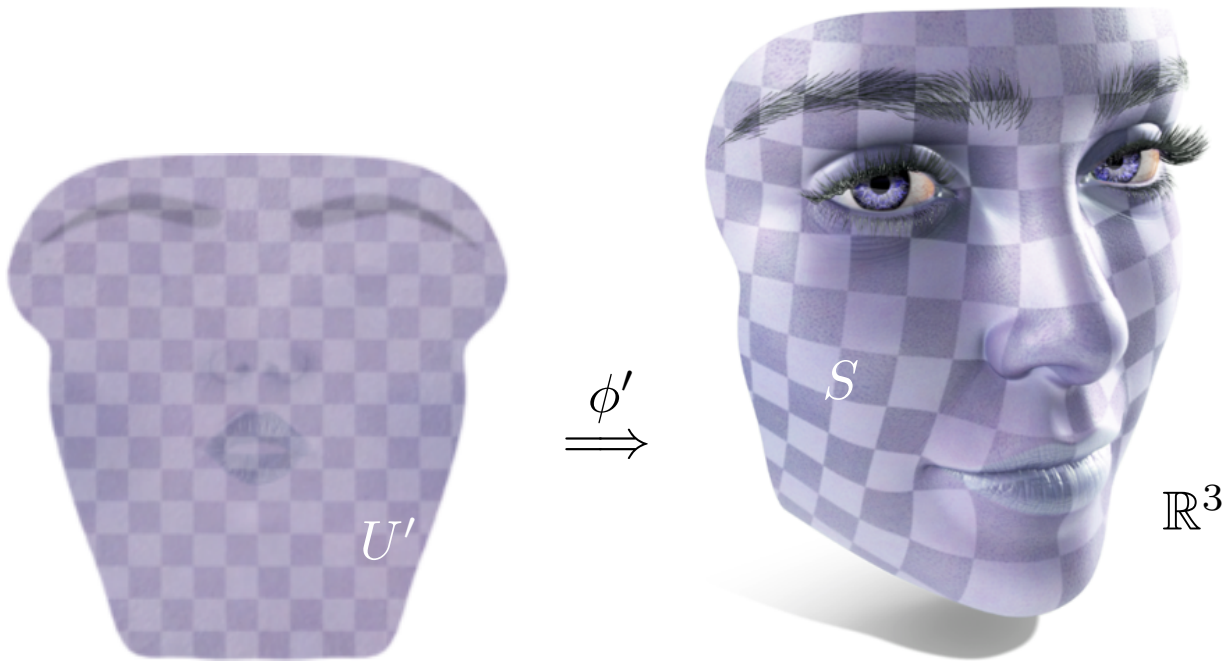
Figure by Keenan Crane

Manifolds

Manifolds can be k-dimensional, meaning that we have charts:

$$\phi : \mathbb{R}^k \to \mathcal{M} \subset \mathbb{R}^d \quad \text{with } k < d$$

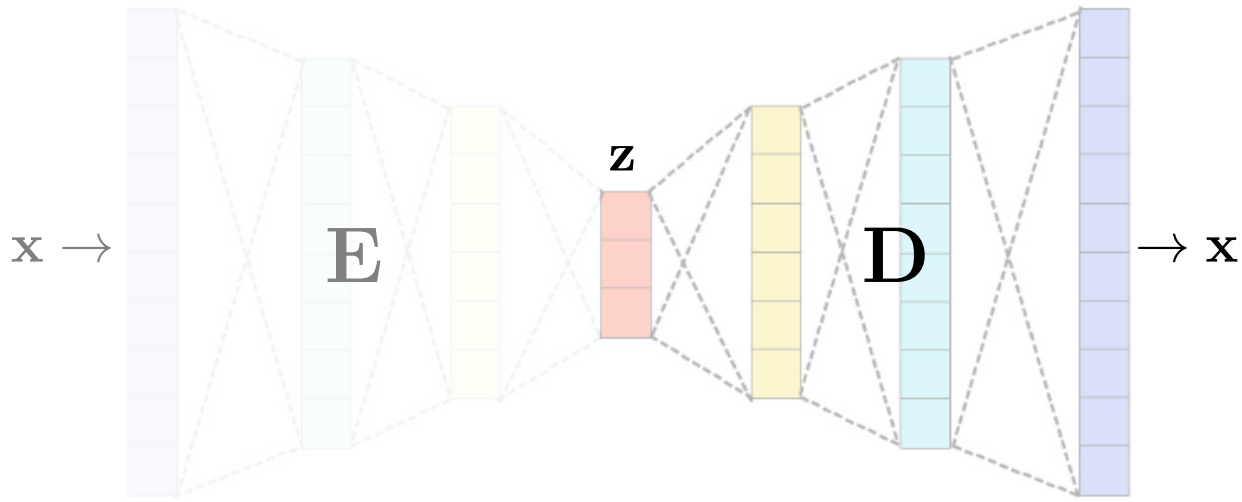
The parametrization is not unique:



However, all encode exactly the same geometric information.

Figure by Keenan Crane

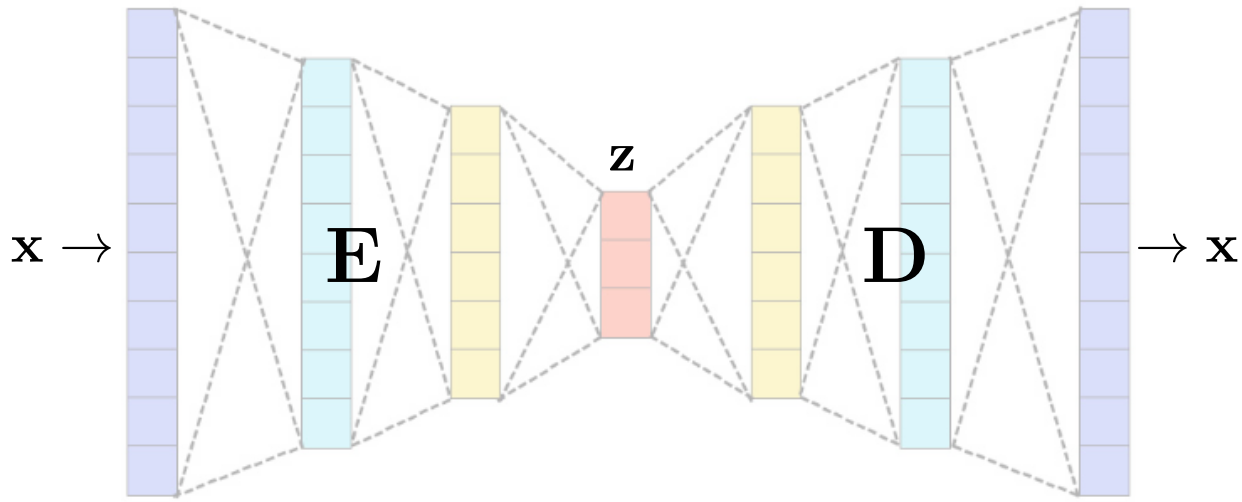
Manifolds and generative models



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

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

Manifolds and generative models



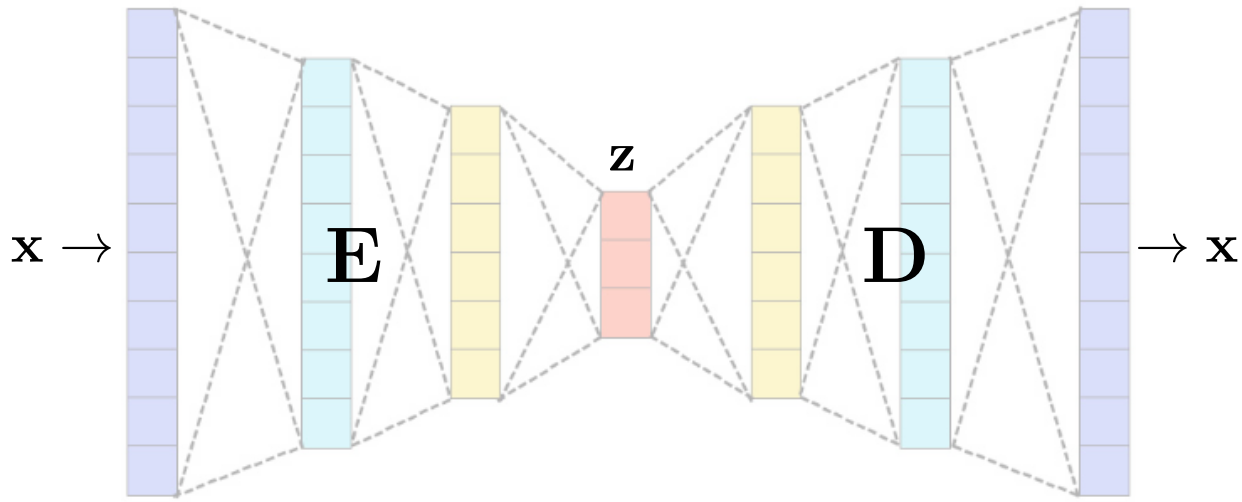
The decoder $D : \mathbb{R}^k \rightarrow \mathbb{R}^d$ is a chart from the latent space spanned by the codes $\mathbf{z}$ to the data space of the inputs $\mathbf{x}$.

It is differentiable.

It is invertible via the encoder E.

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

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 $\mathbf{z}$ to the data space of the inputs $\mathbf{x}$.

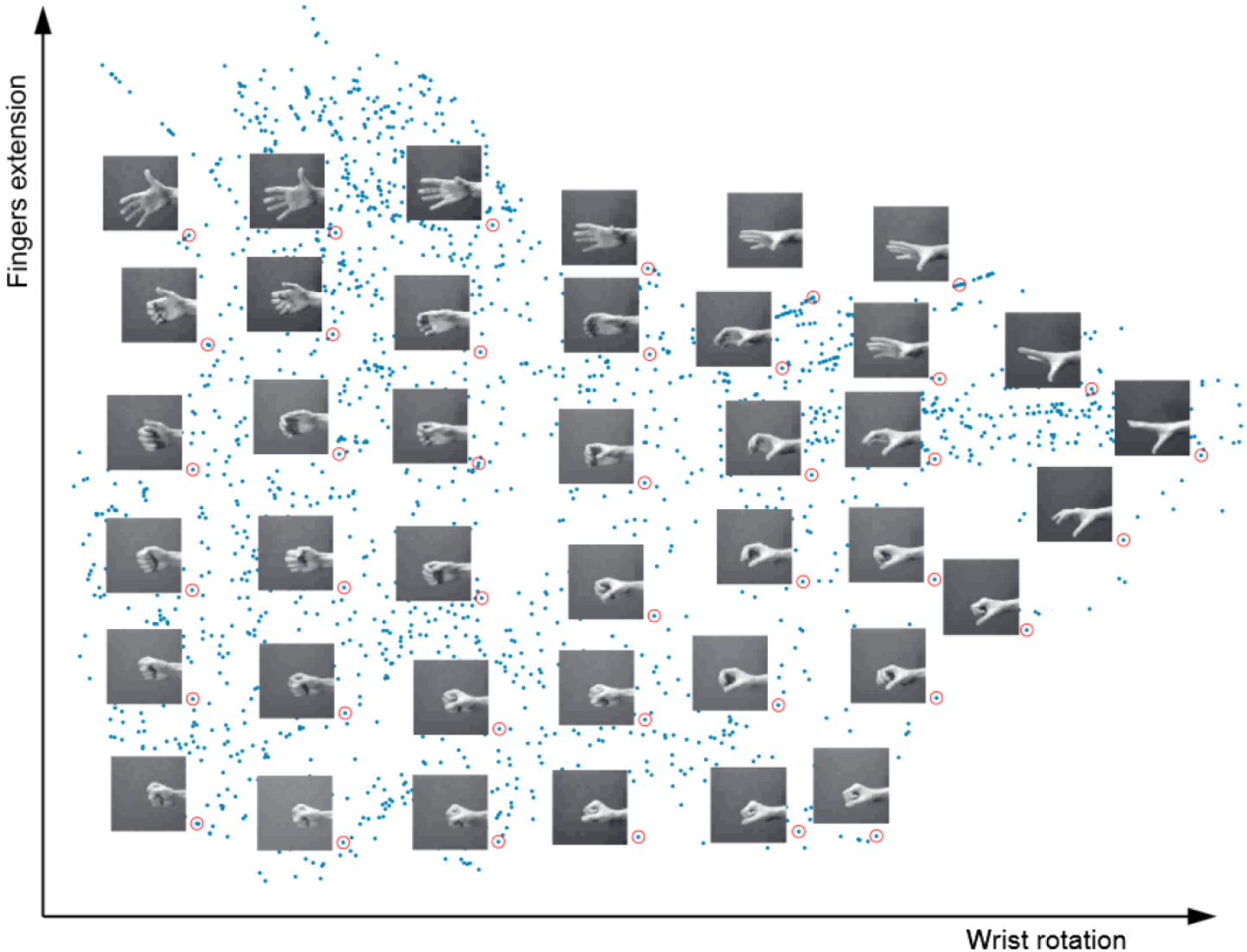
It is differentiable.

It is invertible via the encoder E.

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

Manifolds and generative models



The intrinsic/latent dimension k of the manifold is not known a priori.

AE Variants

Many possible variations are possible, acting as extra regularization.

Examples:

- Denoising AE

  Set random values of the input to zero, require exact reconstruction.

  The AE is forced to capture correlations between inputs.

Vincent et al, "Extracting and composing robust features with denoising autoencoders", ICML 2008

AE Variants

Many possible variations are possible, acting as extra regularization.

Examples:

- Denoising AE

  Set random values of the input to zero, require exact reconstruction.

  The AE is forced to capture correlations between inputs.

- Contractive AE

  Penalize the gradient of the latent code w.r.t the input.

  The latent code becomes robust to small variations in the input.

Vincent et al, "Extracting and composing robust features with denoising autoencoders", ICML 2008; Rifai et al, "Contractive auto-encoders: Explicit invariance during feature extraction", 2011

AE Variants

Many possible variations are possible, acting as extra regularization.

Examples:

- Denoising AE

  Set random values of the input to zero, require exact reconstruction.

  The AE is forced to capture correlations between inputs.

- Contractive AE

  Penalize the gradient of the latent code w.r.t the input.

  The latent code becomes robust to small variations in the input.

Adding constraints on the latent codes (es. sparsity), optimizing for the dimension, etc.

Vincent et al, "Extracting and composing robust features with denoising autoencoders", ICML 2008; Rifai et al, "Contractive auto-encoders: Explicit invariance during feature extraction", 2011

Variational autoencoders (VAE)

Autoencoders can map similar inputs to arbitrarily distant regions of the latent space. But we want to make sure to learn a distribution.

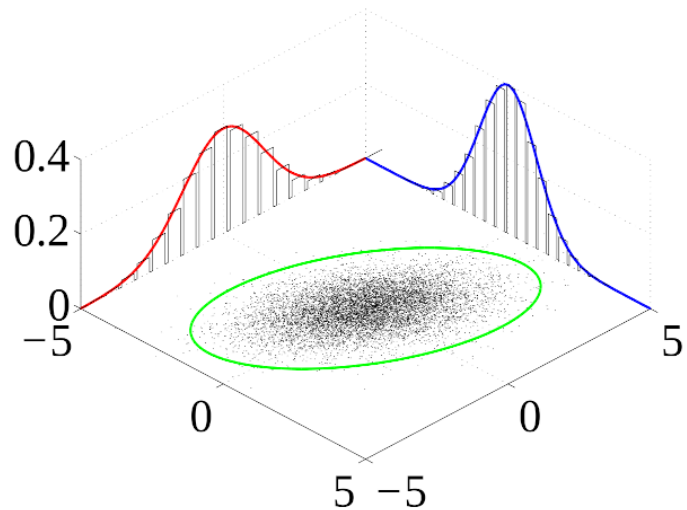
Kingma and Welling, "Auto-Encoding Variational Bayes", 2013

Variational autoencoders (VAE)

Autoencoders can map similar inputs to arbitrarily distant regions of the latent space. But we want to make sure to learn a distribution.

A variational autoencoder constructs the parameters of a probability distribution on the latent space.

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



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

Entropy and divergence

The information carried by an event $\mathbf{x}$ can be quantified as:

$$I(\mathbf{x}) = -\log p(\mathbf{x})$$

Entropy and divergence

The information carried by an event $\mathbf{x}$ can be quantified as:

$$I(\mathbf{x}) = -\log p(\mathbf{x})$$

The average information encoded in p is its entropy:

$$H(p) = -\sum_{\mathbf{x}} p(\mathbf{x}) \log p(\mathbf{x})$$

Entropy and divergence

The information carried by an event $\mathbf{x}$ can be quantified as:

$$I(\mathbf{x}) = -\log p(\mathbf{x})$$

The average information encoded in p is its entropy:

$$H(p) = -\sum_{\mathbf{x}} p(\mathbf{x}) \log p(\mathbf{x})$$

Given two distributions p and q, the Kullback-Leibler divergence:

$$KL(p\|q) \approx H(q) - H(p)$$

measures their dissimilarity in terms of their entropy.

Entropy and divergence

The information carried by an event $\mathbf{x}$ can be quantified as:

$$I(\mathbf{x}) = -\log p(\mathbf{x})$$

The average information encoded in p is its entropy:

$$H(p) = -\sum_{\mathbf{x}} p(\mathbf{x}) \log p(\mathbf{x})$$

Given two distributions p and q, the Kullback-Leibler divergence:

$$KL(p\|q) \approx -\sum q(\mathbf{x}) \log q(\mathbf{x}) + \sum p(\mathbf{x}) \log p(\mathbf{x})$$

measures their dissimilarity in terms of their entropy.

Entropy and divergence

The information carried by an event $\mathbf{x}$ can be quantified as:

$$I(\mathbf{x}) = -\log p(\mathbf{x})$$

The average information encoded in p is its entropy:

$$H(p) = -\sum_{\mathbf{x}} p(\mathbf{x}) \log p(\mathbf{x})$$

Given two distributions p and q, the Kullback-Leibler divergence:

$$KL(p\|q) = -\sum p(\mathbf{x}) \log q(\mathbf{x}) + \sum p(\mathbf{x}) \log p(\mathbf{x}) \geq 0$$

measures their dissimilarity in terms of their entropy.

Entropy and divergence

The information carried by an event $\mathbf{x}$ can be quantified as:

$$I(\mathbf{x}) = -\log p(\mathbf{x})$$

The average information encoded in p is its entropy:

$$H(p) = -\sum_{\mathbf{x}} p(\mathbf{x}) \log p(\mathbf{x})$$

Given two distributions p and q, the Kullback-Leibler divergence:

$$KL(p\|q) = \sum p(\mathbf{x}) \log \frac{p(\mathbf{x})}{q(\mathbf{x})} \geq 0$$

measures their dissimilarity in terms of their entropy.

Entropy and divergence

The information carried by an event $\mathbf{x}$ can be quantified as:

$$I(\mathbf{x}) = -\log p(\mathbf{x})$$

The average information encoded in p is its entropy:

$$H(p) = -\sum_{\mathbf{x}} p(\mathbf{x}) \log p(\mathbf{x})$$

Given two distributions p and q, the Kullback-Leibler divergence:

$$KL(p\|q) = -\sum p(\mathbf{x}) \log \frac{q(\mathbf{x})}{p(\mathbf{x})} \geq 0$$

measures their dissimilarity in terms of their entropy.

Variational inference

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

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

Variational inference

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

We define a parametric probabilistic encoder as the distribution:

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

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

Variational inference

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

We define a parametric probabilistic encoder as the distribution:

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

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

Variational inference

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

We define a parametric probabilistic encoder as the distribution:

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

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

Variational inference

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

We define a parametric probabilistic encoder as the distribution:

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

However, computing:

$$p_{\boldsymbol{\theta}}(\mathbf{x}) = \int p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z})p_{\boldsymbol{\theta}}(\mathbf{z})d\mathbf{z}$$

is a high-dimensional intractable integral over the entire latent space.

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

Variational inference

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

The encoder is modeled as the parametric posterior distribution:

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

Instead, compute an approximation:

$$q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x}) \approx p_{\boldsymbol{\theta}}(\mathbf{z}|\mathbf{x})$$

where $q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})$ has a fixed parametric form w.r.t. $\boldsymbol{\phi}$.

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

Variational inference

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

The encoder is modeled as the parametric posterior distribution:

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

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

$$\boldsymbol{\phi}^* = \arg\min_{\boldsymbol{\phi},\boldsymbol{\theta}} \; KL(q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})\|p_{\boldsymbol{\theta}}(\mathbf{z}|\mathbf{x}))$$

where $q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})$ has a fixed parametric form w.r.t. $\boldsymbol{\phi}$.

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

Variational inference

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

The encoder is modeled as the parametric posterior distribution:

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

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

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

where $q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})$ has a fixed parametric form w.r.t. $\boldsymbol{\phi}$.

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

Variational inference

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

The encoder is modeled as the parametric posterior distribution:

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

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

$$\boldsymbol{\phi}^* = \arg\min_{\boldsymbol{\phi},\boldsymbol{\theta}} -\sum_{\mathbf{z}} q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x}) \log \frac{p_{\boldsymbol{\theta}}(\mathbf{x},\mathbf{z})/p_{\boldsymbol{\theta}}(\mathbf{x})}{q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})}$$

where $q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})$ has a fixed parametric form w.r.t. $\boldsymbol{\phi}$.

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

Variational inference

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

The encoder is modeled as the parametric posterior distribution:

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

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

$$\boldsymbol{\phi}^* = \arg\min_{\boldsymbol{\phi},\boldsymbol{\theta}} -\sum_{\mathbf{z}} q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x}) \log \frac{p_{\boldsymbol{\theta}}(\mathbf{x},\mathbf{z})}{q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})} \frac{1}{p_{\boldsymbol{\theta}}(\mathbf{x})}$$

where $q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})$ has a fixed parametric form w.r.t. $\boldsymbol{\phi}$.

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

Variational inference

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

The encoder is modeled as the parametric posterior distribution:

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

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

$$\boldsymbol{\phi}^* = \arg\min_{\boldsymbol{\phi},\boldsymbol{\theta}} -\sum_{\mathbf{z}} q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x}) \left(\log \frac{p_{\boldsymbol{\theta}}(\mathbf{x},\mathbf{z})}{q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})} + \log \frac{1}{p_{\boldsymbol{\theta}}(\mathbf{x})} \right)$$

where $q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})$ has a fixed parametric form w.r.t. $\boldsymbol{\phi}$.

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

Variational inference

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

The encoder is modeled as the parametric posterior distribution:

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

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

$$\boldsymbol{\phi}^* = \arg\min_{\boldsymbol{\phi},\boldsymbol{\theta}} -\sum_{\mathbf{z}} q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x}) \left(\log \frac{p_{\boldsymbol{\theta}}(\mathbf{x},\mathbf{z})}{q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})} - \log p_{\boldsymbol{\theta}}(\mathbf{x}) \right)$$

where $q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})$ has a fixed parametric form w.r.t. $\boldsymbol{\phi}$.

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

Variational inference

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

The encoder is modeled as the parametric posterior distribution:

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

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

$$\boldsymbol{\phi}^* = \arg\min_{\boldsymbol{\phi},\boldsymbol{\theta}} -\sum_{\mathbf{z}} q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x}) \log \frac{p_{\boldsymbol{\theta}}(\mathbf{x},\mathbf{z})}{q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})} + \sum_{\mathbf{z}} q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x}) \log p_{\boldsymbol{\theta}}(\mathbf{x})$$

where $q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})$ has a fixed parametric form w.r.t. $\boldsymbol{\phi}$.

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

Variational inference

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

The encoder is modeled as the parametric posterior distribution:

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

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

$$\boldsymbol{\phi}^* = \arg\min_{\boldsymbol{\phi},\boldsymbol{\theta}} -\sum_{\mathbf{z}} q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x}) \log \frac{p_{\boldsymbol{\theta}}(\mathbf{x},\mathbf{z})}{q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})} + \log p_{\boldsymbol{\theta}}(\mathbf{x}) \sum_{\mathbf{z}} q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})$$

where $q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})$ has a fixed parametric form w.r.t. $\boldsymbol{\phi}$.

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

Variational inference

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

The encoder is modeled as the parametric posterior distribution:

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

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

$$\boldsymbol{\phi}^* = \arg\min_{\boldsymbol{\phi},\boldsymbol{\theta}} -\sum_{\mathbf{z}} q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x}) \log \frac{p_{\boldsymbol{\theta}}(\mathbf{x},\mathbf{z})}{q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})} + \log p_{\boldsymbol{\theta}}(\mathbf{x}) \sum_{\mathbf{z}} q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})$$

$\sum_{\mathbf{z}} q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x}) = 1$

where $q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})$ has a fixed parametric form w.r.t. $\boldsymbol{\phi}$.

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

Variational inference

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

The encoder is modeled as the parametric posterior distribution:

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

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

$$\boldsymbol{\phi}^* = \arg\min_{\boldsymbol{\phi},\boldsymbol{\theta}} -\sum_{\mathbf{z}} q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x}) \log \frac{p_{\boldsymbol{\theta}}(\mathbf{x},\mathbf{z})}{q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})} + \log p_{\boldsymbol{\theta}}(\mathbf{x})$$

where $q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})$ has a fixed parametric form w.r.t. $\boldsymbol{\phi}$.

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

Variational inference

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

The encoder is modeled as the parametric posterior distribution:

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

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

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

where $q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})$ has a fixed parametric form w.r.t. $\boldsymbol{\phi}$.

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

Variational inference

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

The encoder is modeled as the parametric posterior distribution:

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

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

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

where $q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})$ has a fixed parametric form w.r.t. $\boldsymbol{\phi}$.

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

Variational inference

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

The encoder is modeled as the parametric posterior distribution:

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

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

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

where $q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})$ has a fixed parametric form w.r.t. $\boldsymbol{\phi}$ 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)

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

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

Variational autoencoder (VAE)

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

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

Variational autoencoder (VAE)

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

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

Variational autoencoder (VAE)

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

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)

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

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

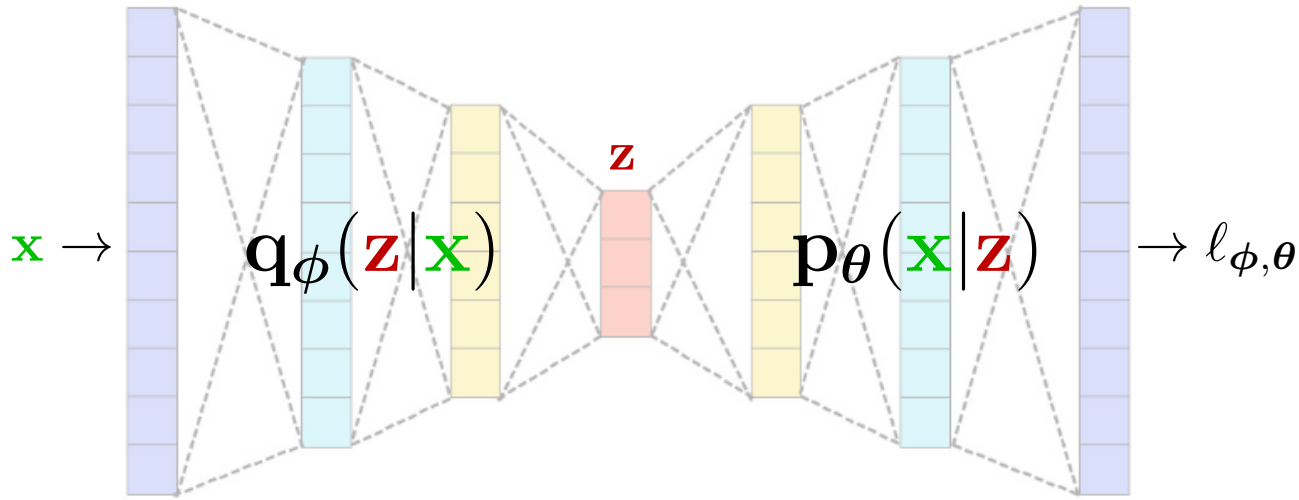
Variational autoencoder (VAE)

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

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

Variational autoencoder (VAE)

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

The prior over the latent variables is Gaussian and has no free parameters:

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

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

Variational autoencoder (VAE)

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

The prior over the latent variables is Gaussian and has no free parameters:

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

The probabilistic encoder also generates a Gaussian distribution:

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

where $\boldsymbol{\mu}, \boldsymbol{\sigma}$ 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

Variational autoencoder (VAE)

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

The prior over the latent variables is Gaussian and has no free parameters:

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

The probabilistic encoder also generates a Gaussian distribution:

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

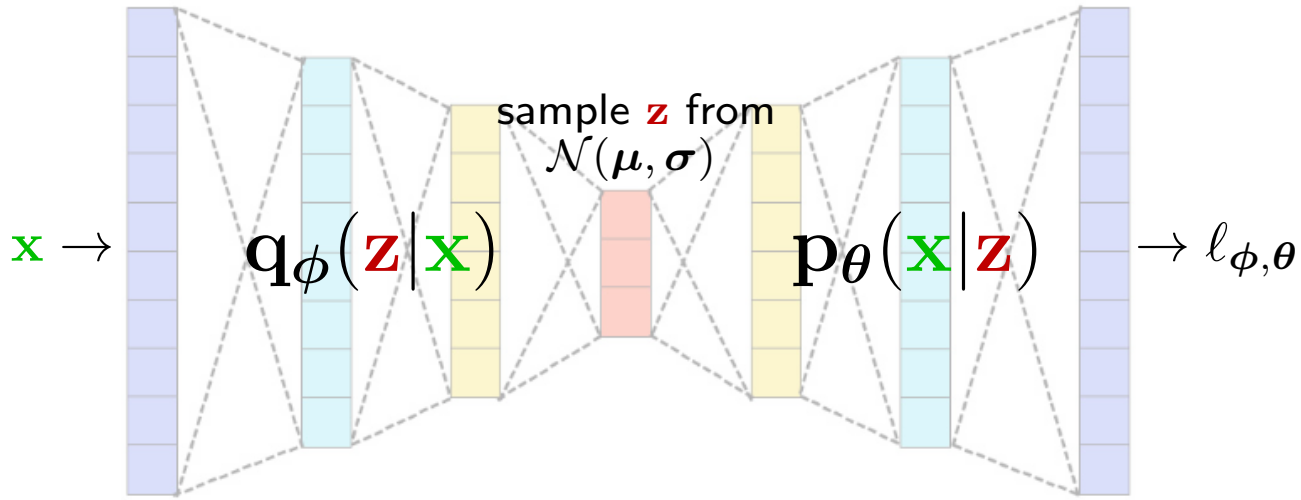
where $\boldsymbol{\mu}, \boldsymbol{\sigma}$ are functions of the input $\mathbf{x}$ and the network parameters $\boldsymbol{\phi}$.
The probabilistic encoder outputs $\boldsymbol{\mu}, \boldsymbol{\sigma}$, not $\mathbf{z}$.

Using Gaussians, the KL term has a closed form.

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

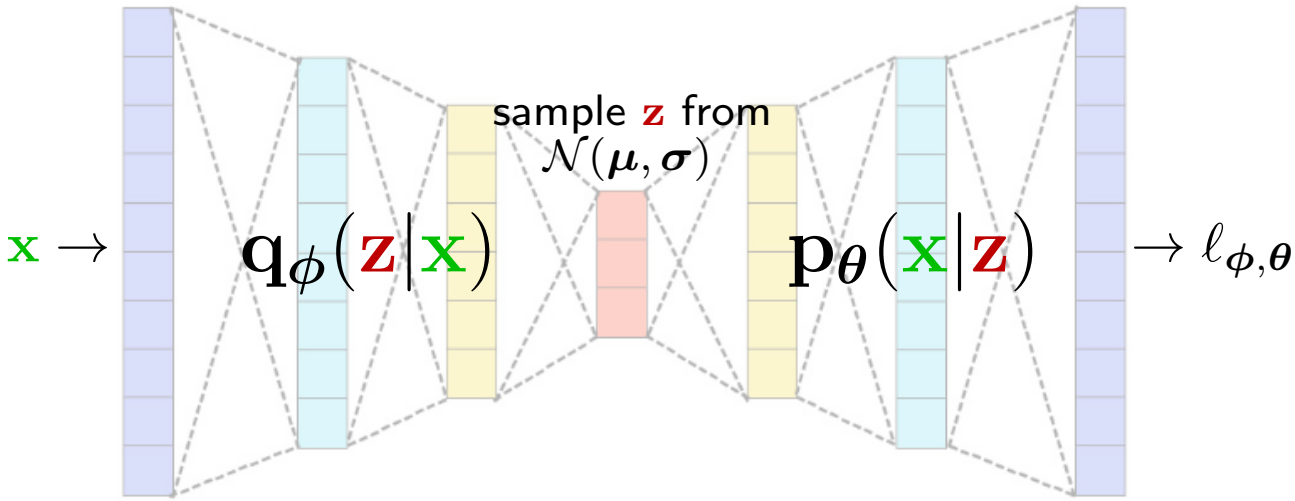
Variational autoencoder (VAE)

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



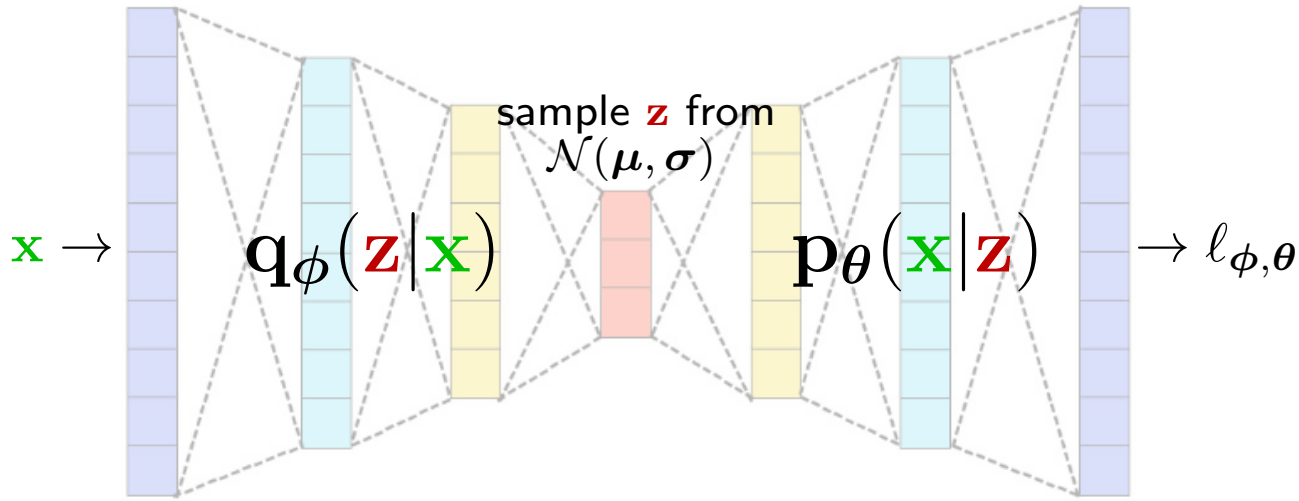
Variational autoencoder (VAE)

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



Variational autoencoder (VAE)

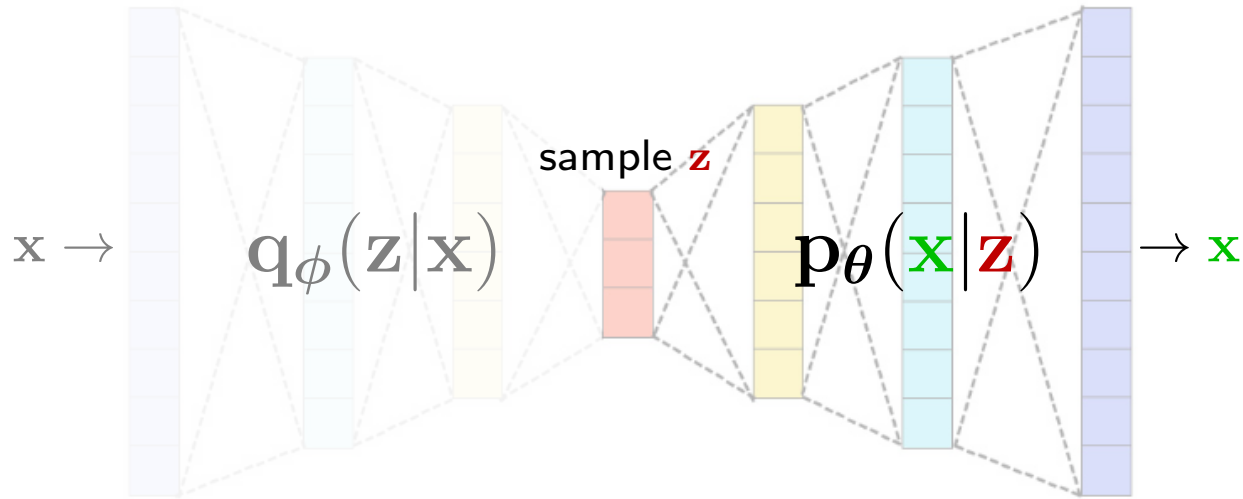
$$\ell_{\boldsymbol{\phi},\boldsymbol{\theta}} = \underbrace{-\mathbb{E}_{q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})} \log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z})}_{\text{reconstruction loss (choose your own)}} \underbrace{+KL(q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})\|p_{\boldsymbol{\theta}}(\mathbf{z}))}_{\text{regularizer}}$$



To distinguish from VAE, classical AE are also called deterministic AE.

Variational autoencoder (VAE)

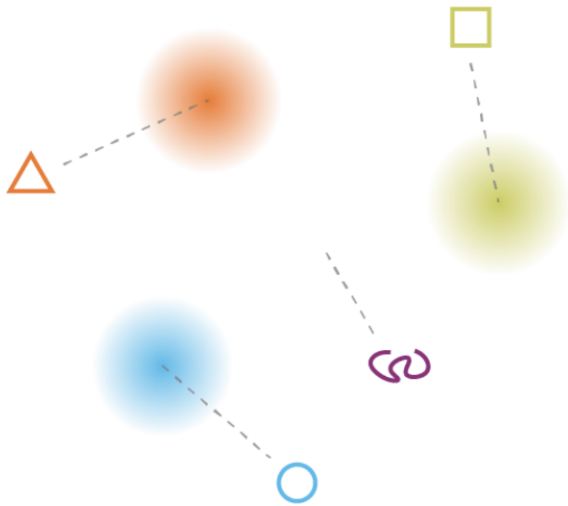
$$\ell_{\boldsymbol{\phi},\boldsymbol{\theta}} = \underbrace{-\mathbb{E}_{q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})} \log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z})}_{\substack{\text{reconstruction loss} \\ \text{(choose your own)}}} \underbrace{+KL(q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})\|p_{\boldsymbol{\theta}}(\mathbf{z}))}_{\text{regularizer}}$$



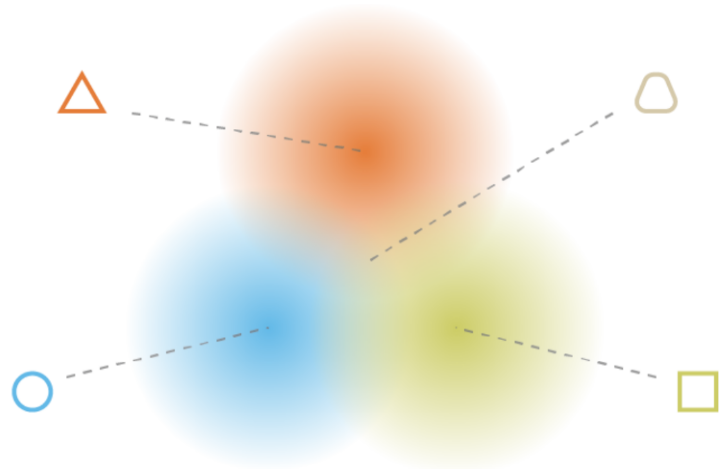
To distinguish from VAE, classical AE are also called deterministic AE.

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

Regularizing effect



latent space of deterministic AE

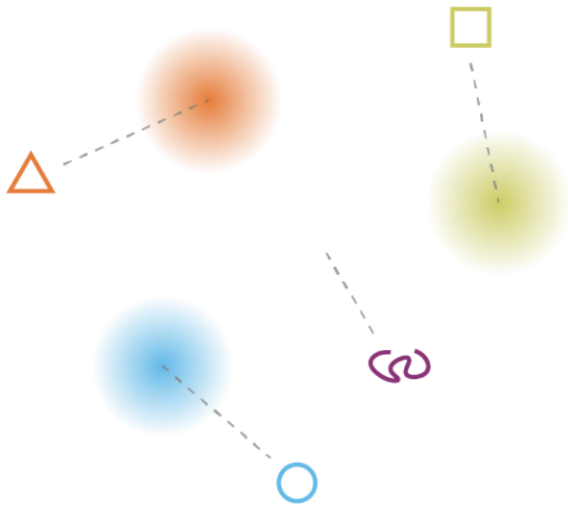


latent space of variational AE

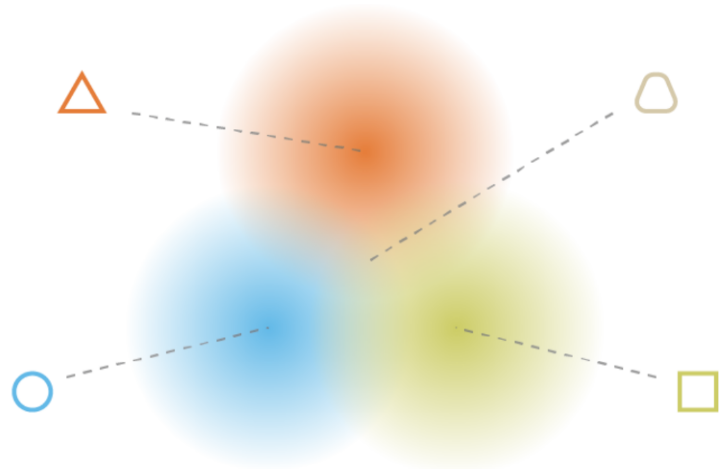
The requirement $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ leads to a compact latent space.

Small distances $\|\mathbf{z}_1 - \mathbf{z}_2\|_2 \Rightarrow$ small changes in the decoded output.

Regularizing effect



latent space of deterministic AE



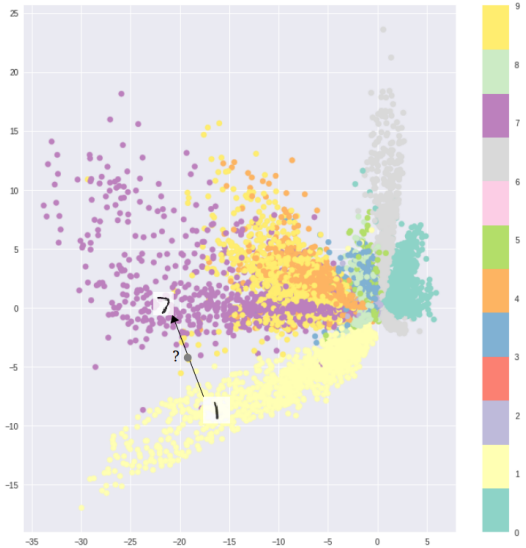
latent space of variational AE

The requirement $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ leads to a compact latent space.

Small distances $\|\mathbf{z}_1 - \mathbf{z}_2\|_2 \Rightarrow$ small changes in the decoded output.

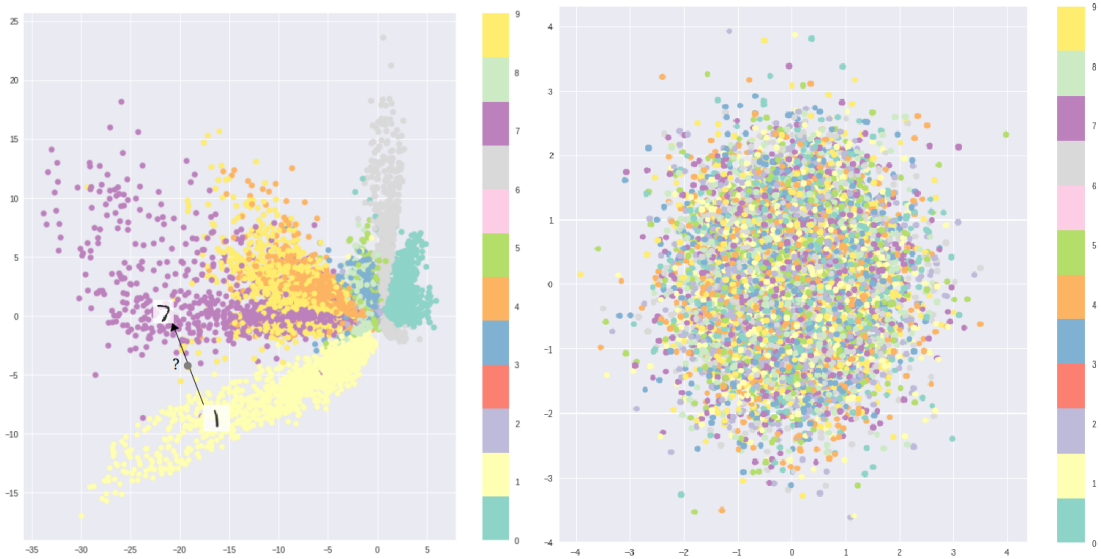
A deterministic AE might generate arbitrary noise.

Regularizing effect



Only reconstruction loss (BCE)

Regularizing effect



Only reconstruction loss (BCE)

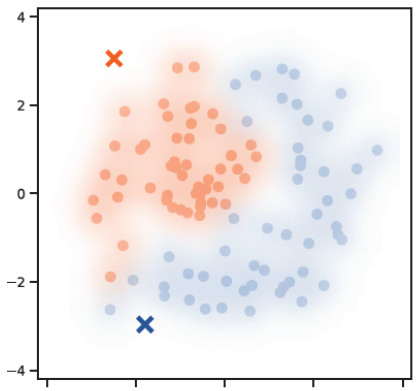
Only continuity loss (KLD)

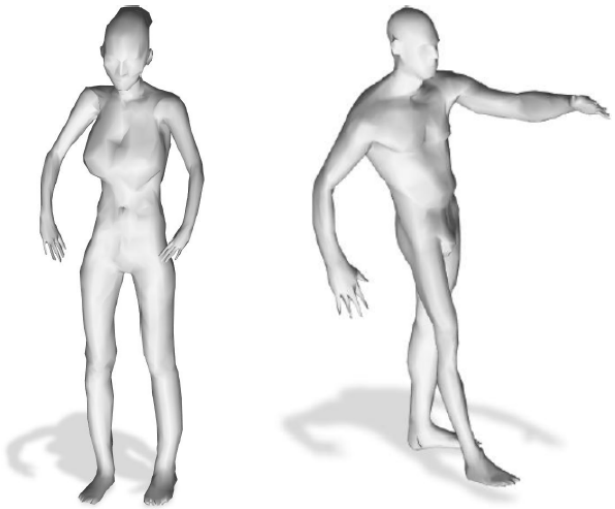
Regularizing effect

The distributional regularizer brings smoothness in the learned space.

Unlikely samples

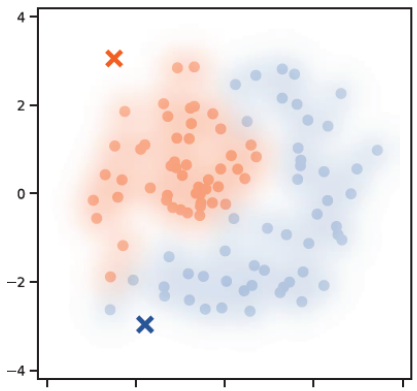
Sampling on the boundaries of the learned distribution leads to the generation of unlikely samples:

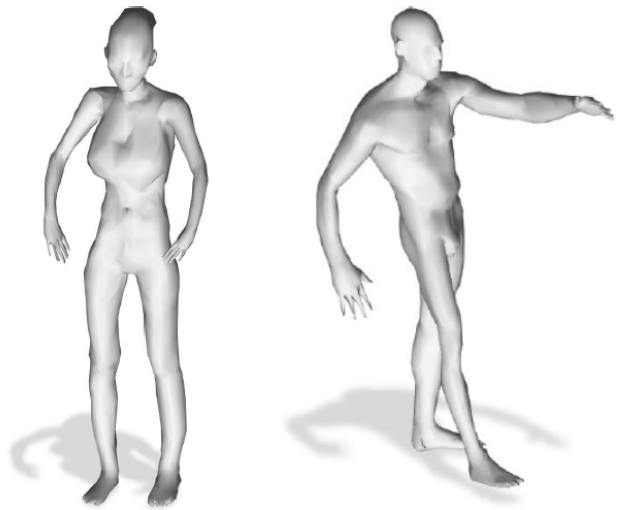




Unlikely samples

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



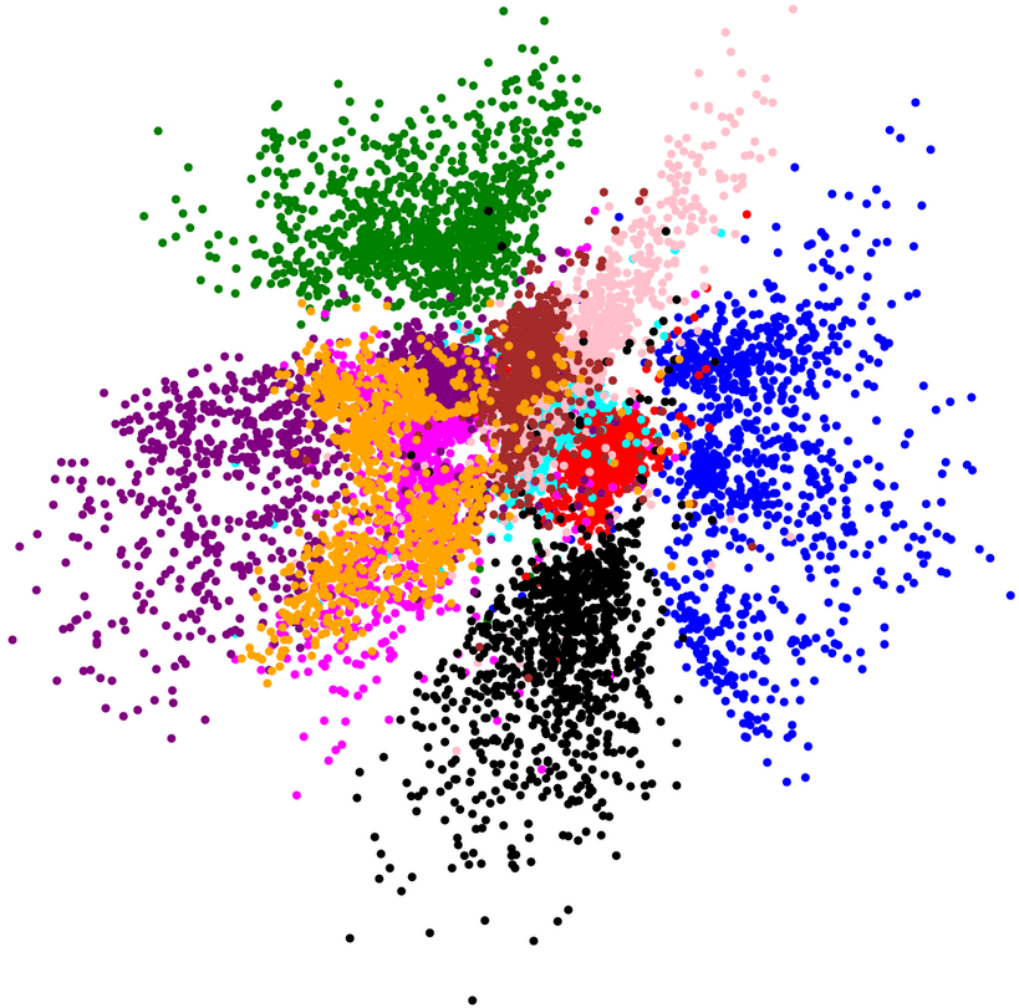


Another relevant phenomenon is posterior collapse, where the latents are ignored if the decoder is powerful enough to model the data perfectly.

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

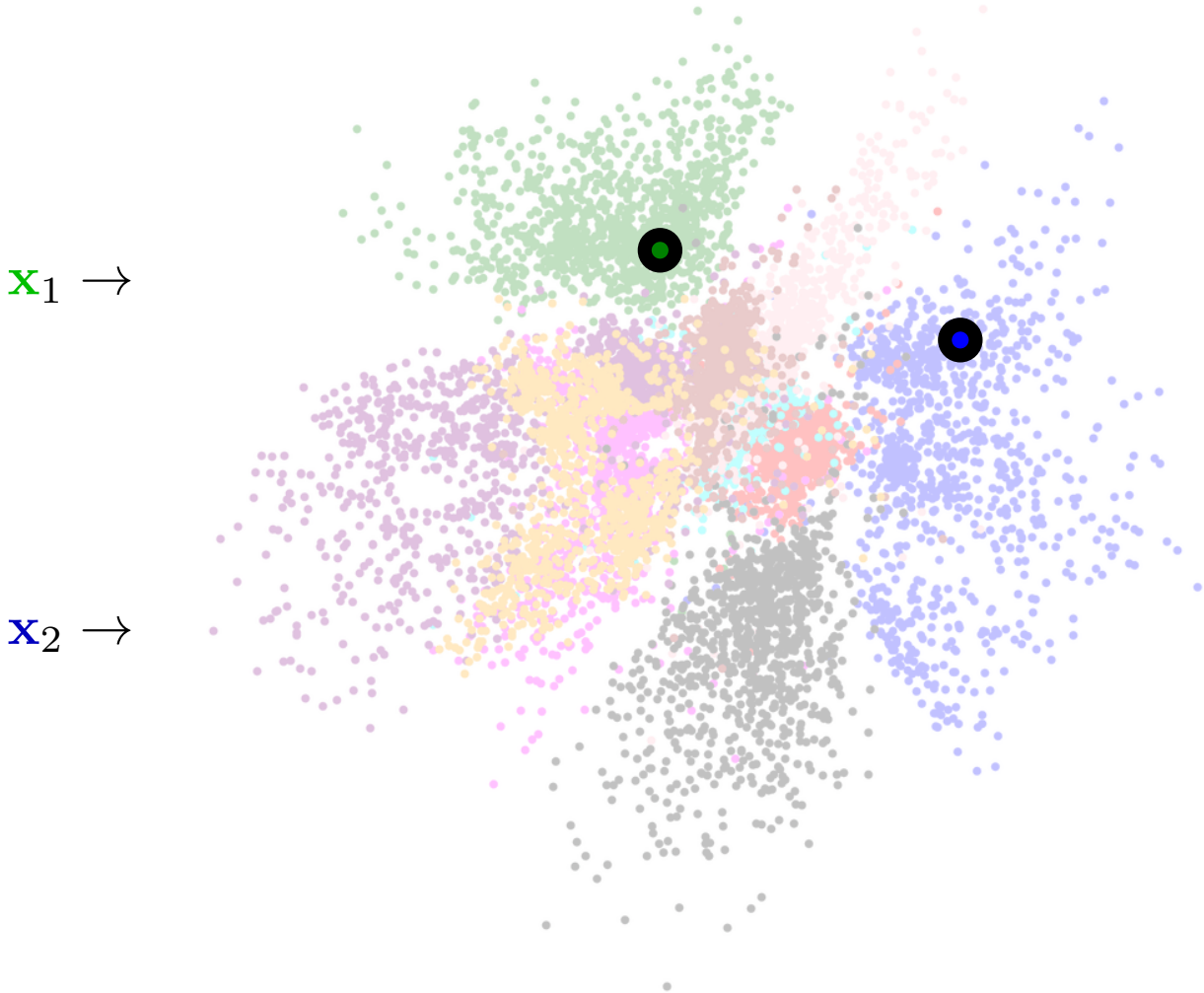
VAE interpolation

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



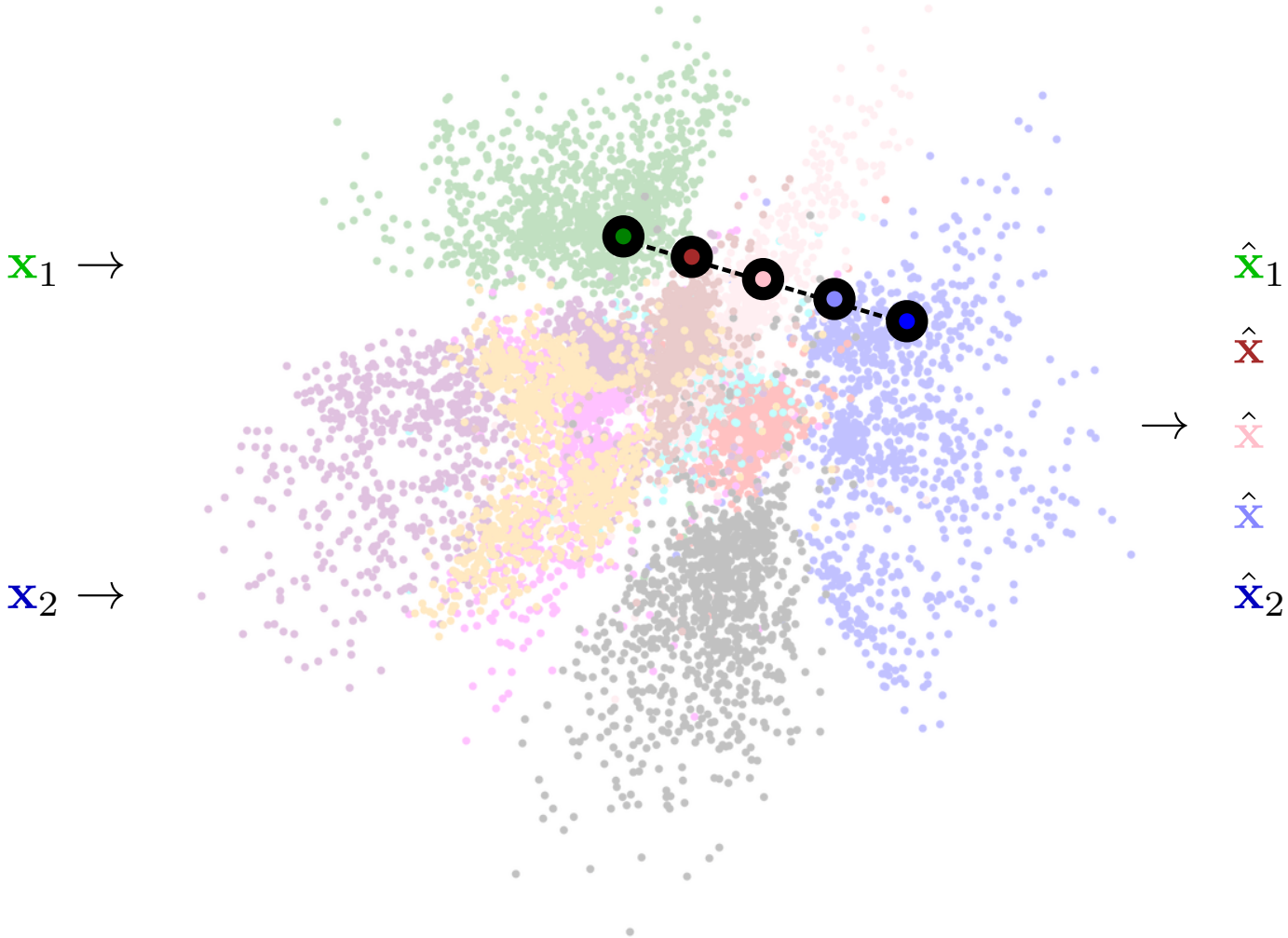
VAE interpolation

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



VAE interpolation

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



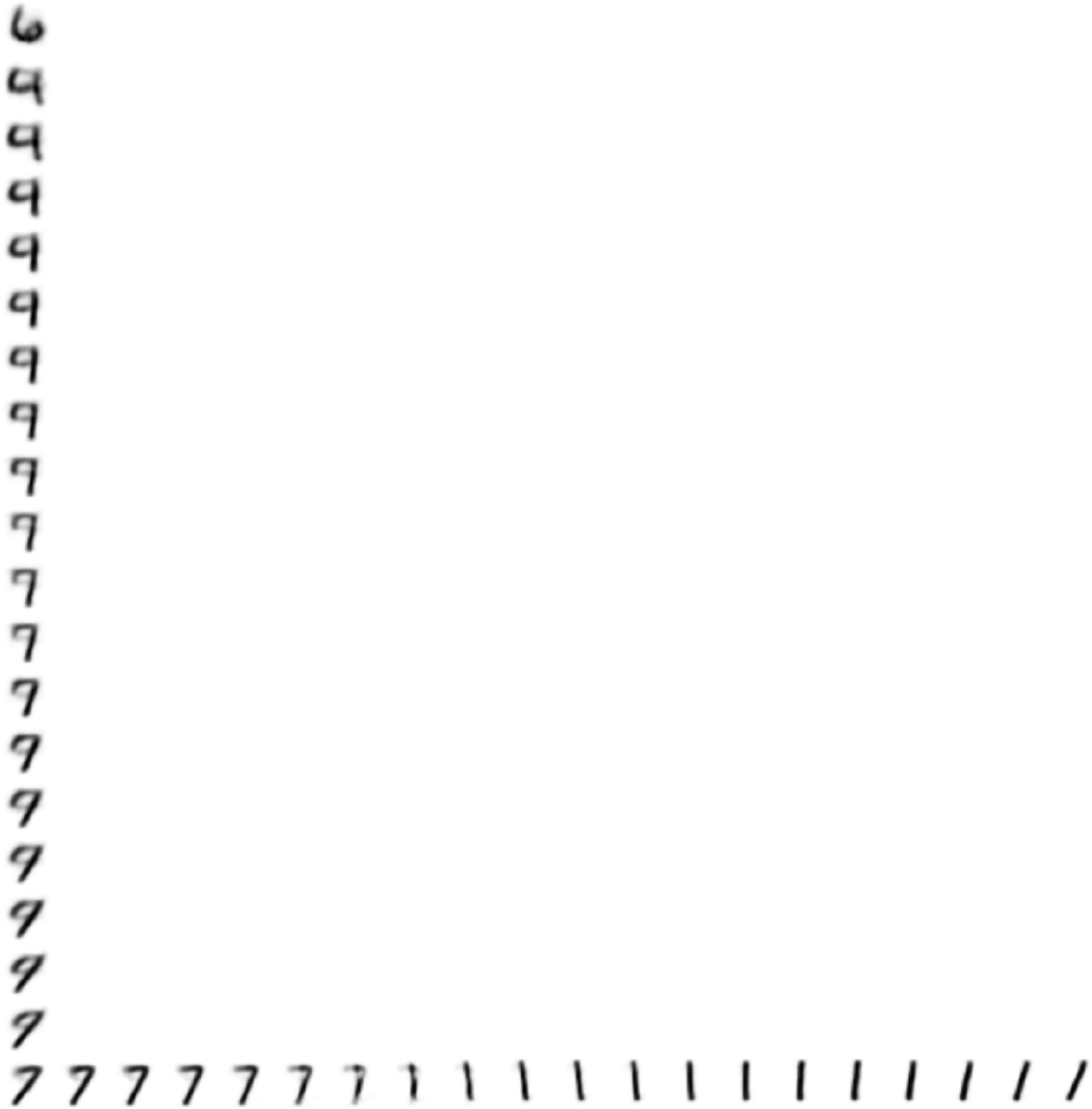
The interpolated samples are **not** part of the training set.

VAE interpolation

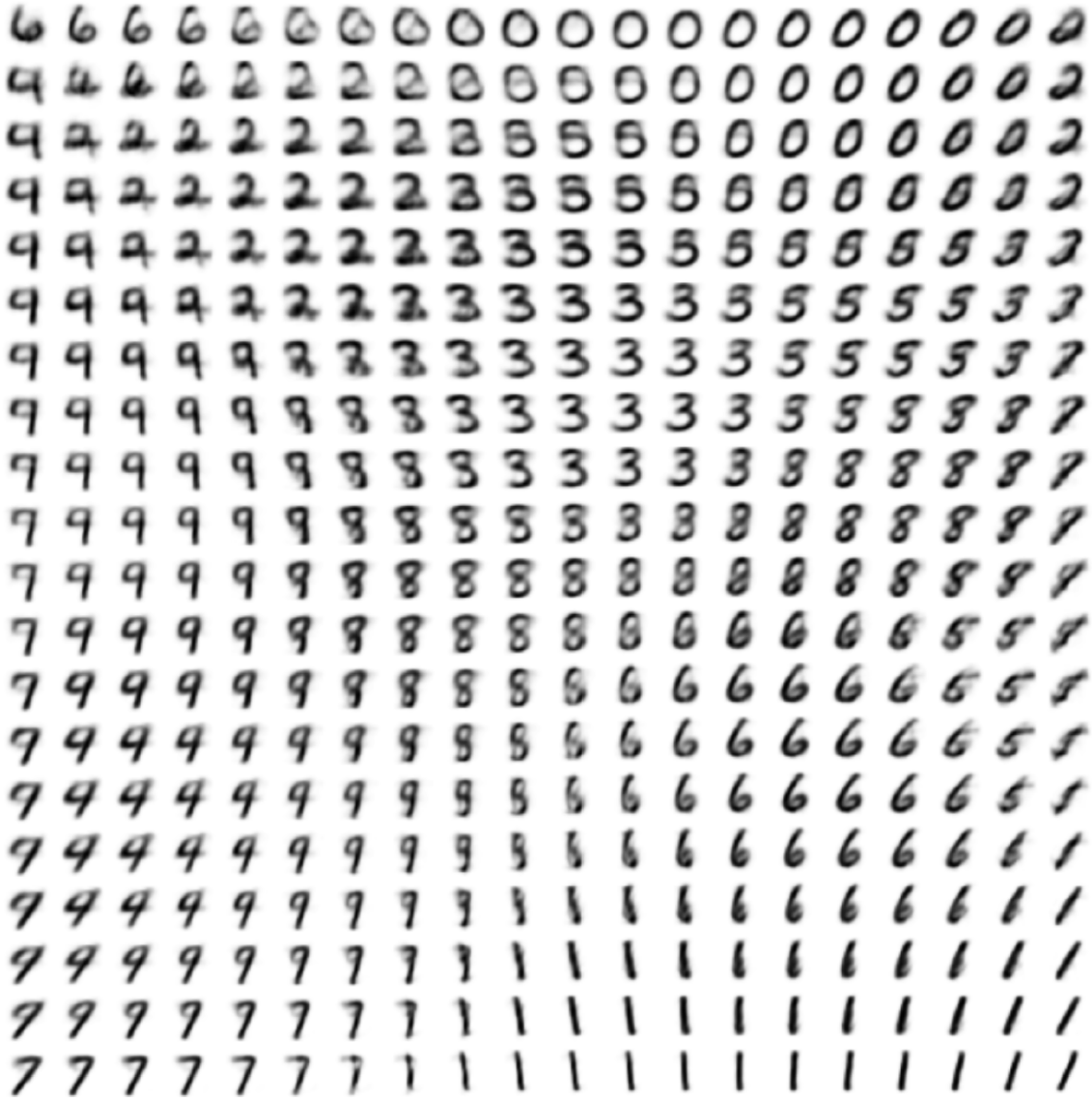
VAE interpolation

VAE interpolation

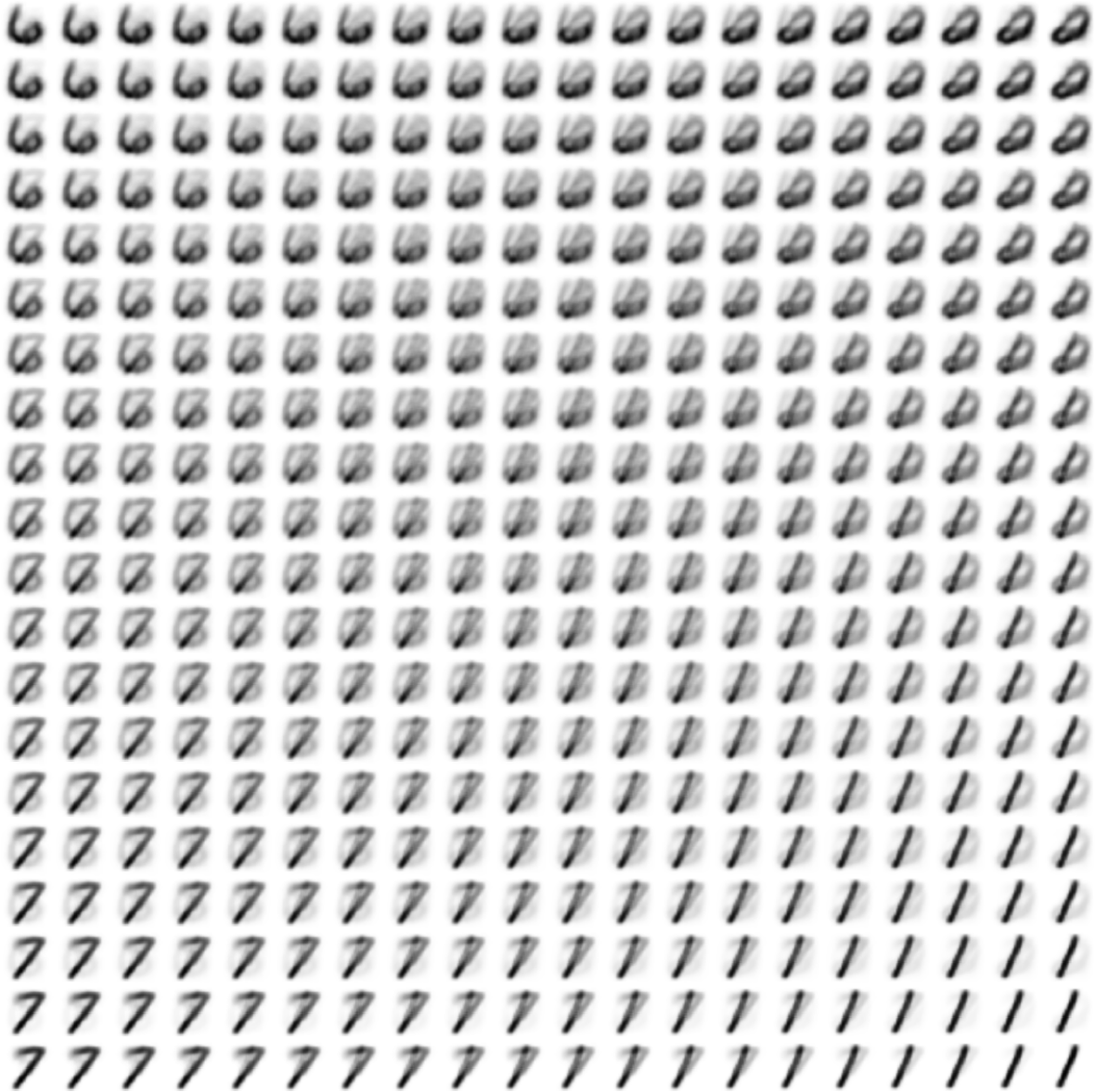
VAE interpolation



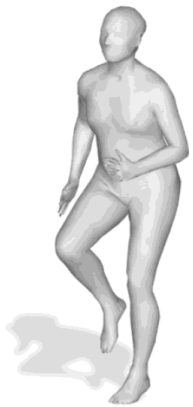
VAE interpolation



Euclidean interpolation

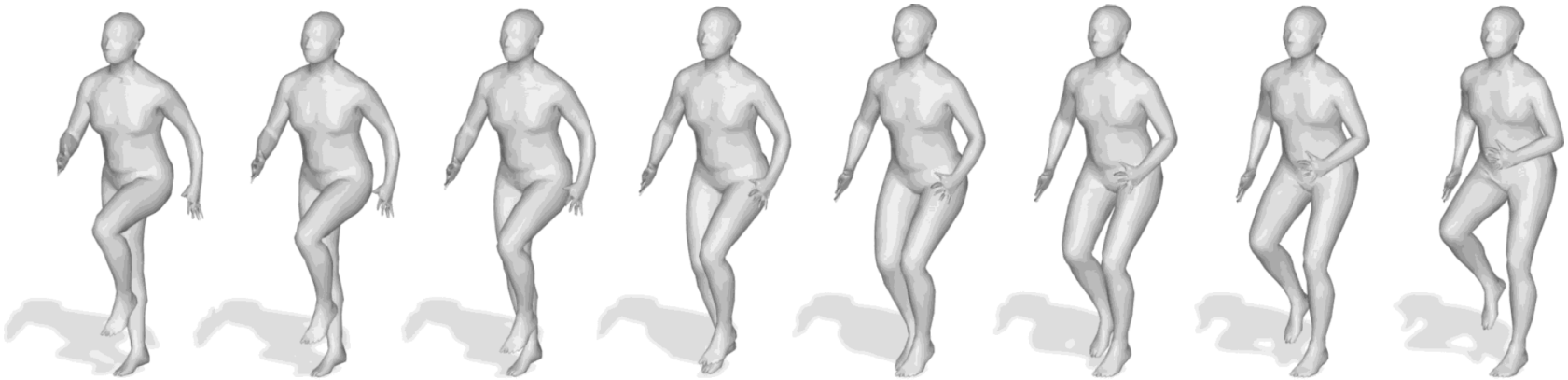


Example: Deformable 3D shapes



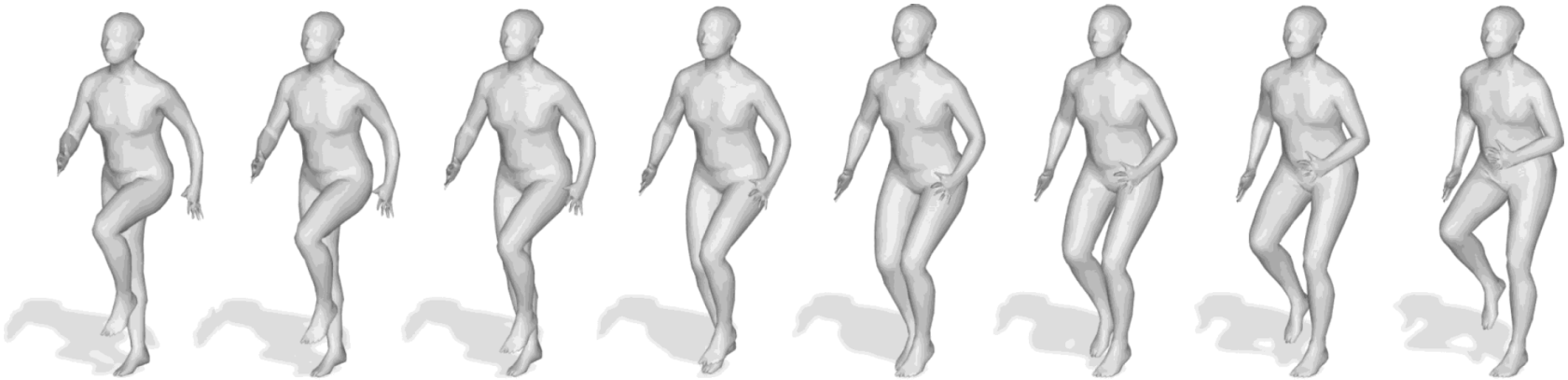
Cosmo, Norelli, Halimi, Kimmel, Rodolà, "LIMP: Learning Latent Shape Representations with Metric Preservation Priors", 2020

Example: Deformable 3D shapes



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

Example: Deformable 3D shapes

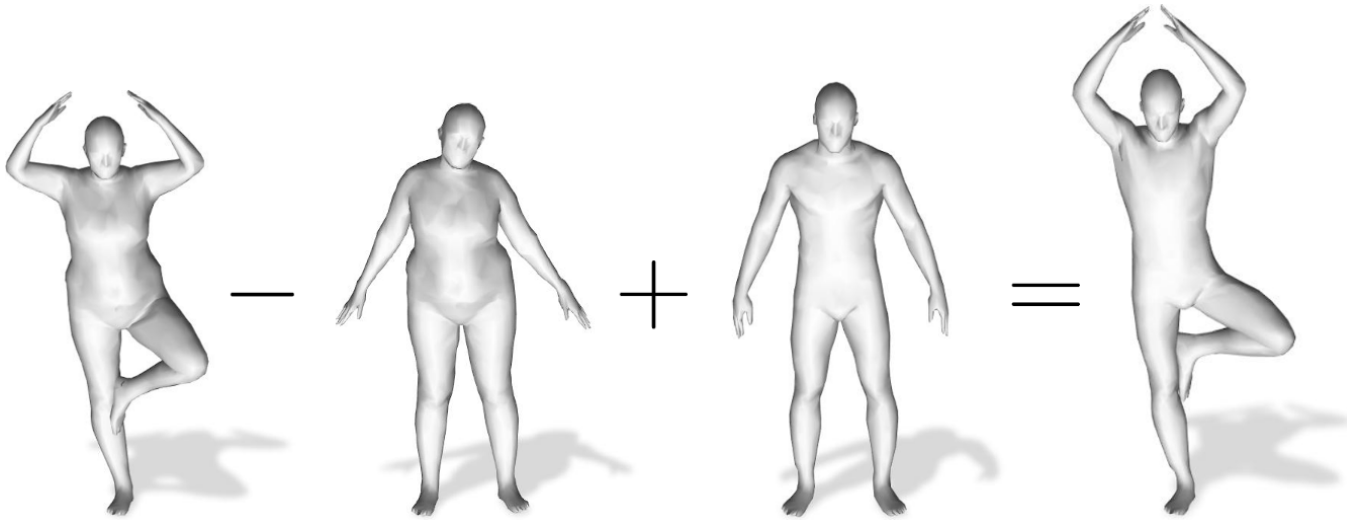


The latent space can be explored along different dimensions (disentanglement):

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

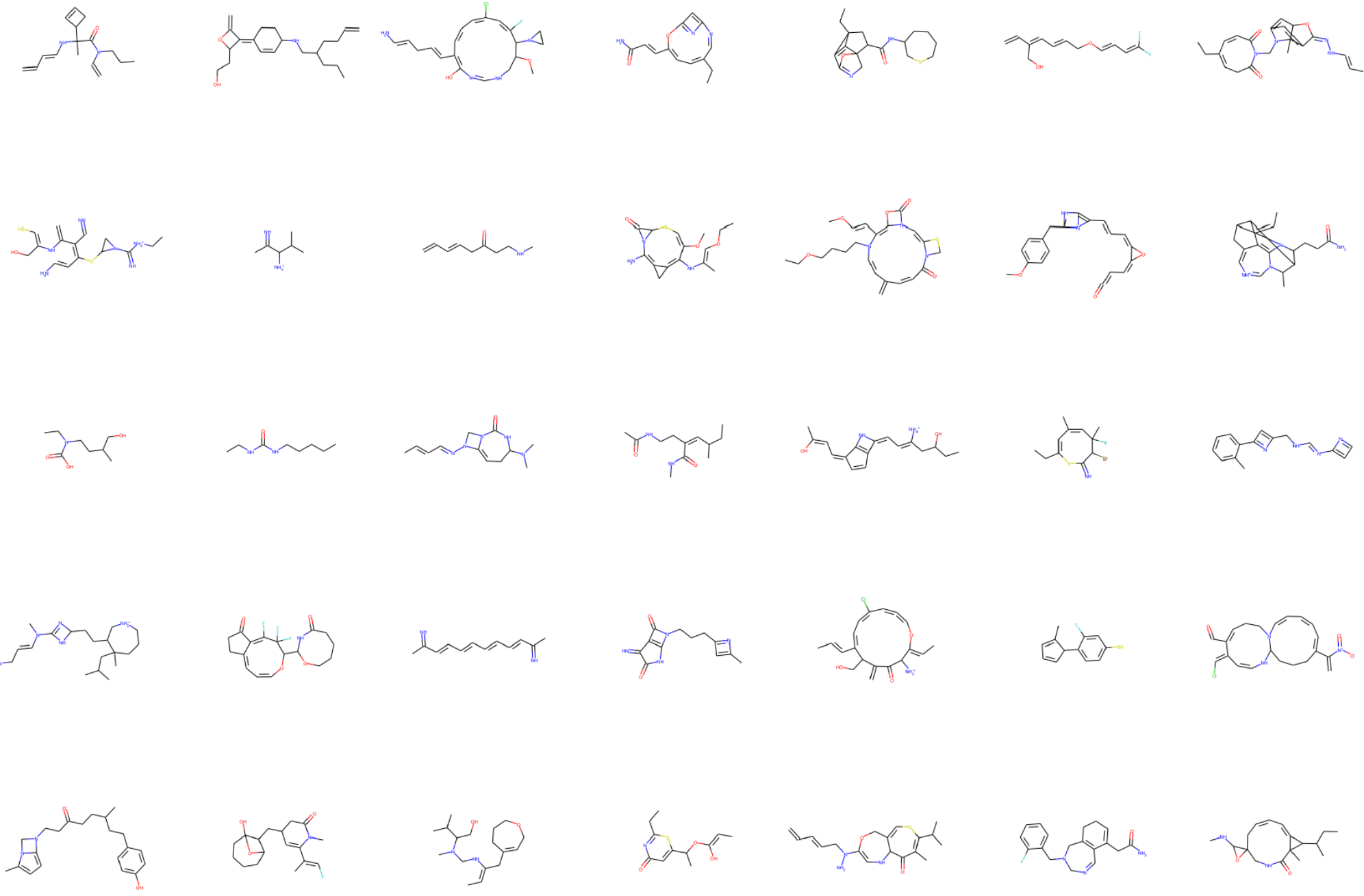
Analogies

Algebraic manipulation of codes leads to the following:



In NLP this is done by manipulating word embeddings:

$$\text{King} - \text{Man} + \text{Woman} = \text{Queen}$$



Bresson, “A Two-Step Graph Convolutional Decoder for Molecule Generation”, 2019

Razavi et al, “Generating Diverse High-Fidelity Images with VQ-VAE-2”, 2019