

Deep Learning & Applied AI

Deep generative models

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SAPIENZA
UNIVERSITÀ DI ROMA

Generative models

Overall idea:

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

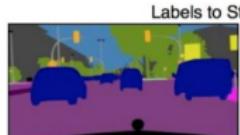
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Generative models



input



output

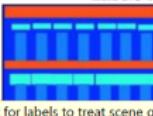


Image result for labels to treat scene gan deep learning

input



output

BW to Color



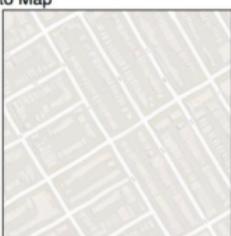
input



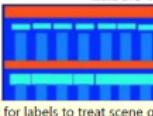
output



input



output



input



output

Day to Night



input



output

Edges to Photo

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**?

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

Generative models

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x
•

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

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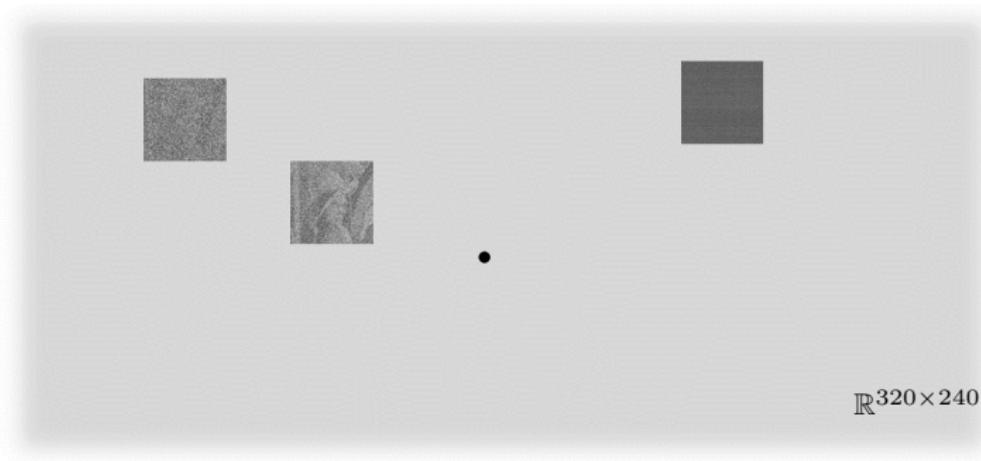
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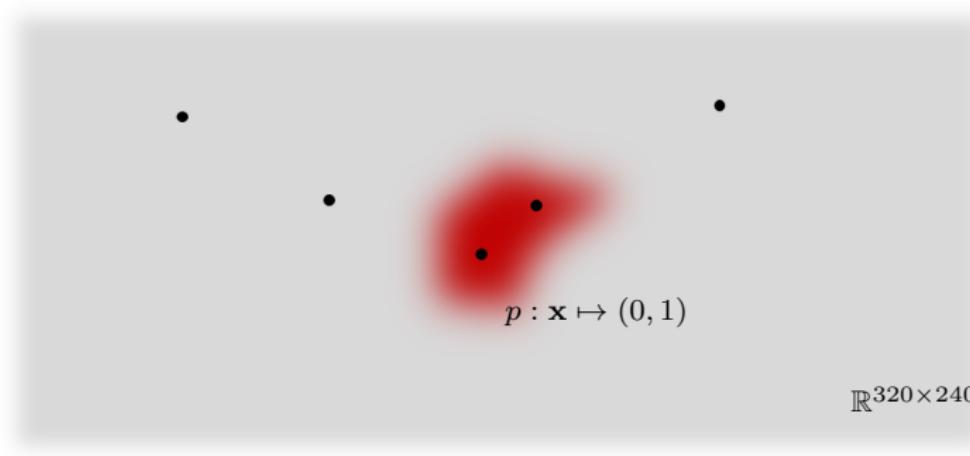
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Generative models

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 $\mathbf{X} \in \mathbb{R}^{d \times n}$:

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

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

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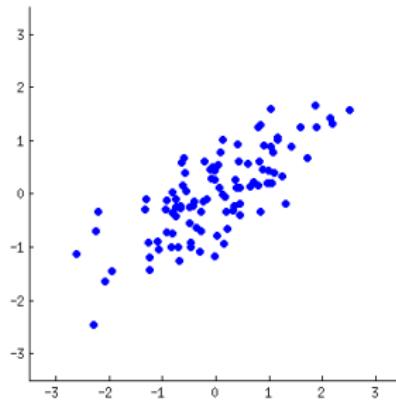
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This can be useful for many other tasks:

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

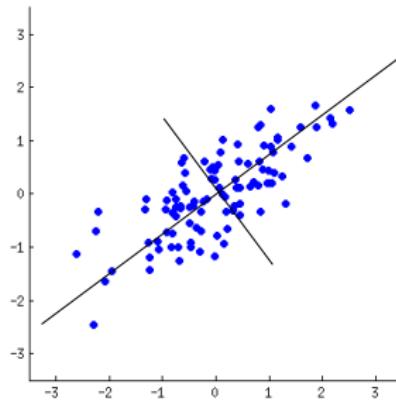
Principal component analysis (PCA)

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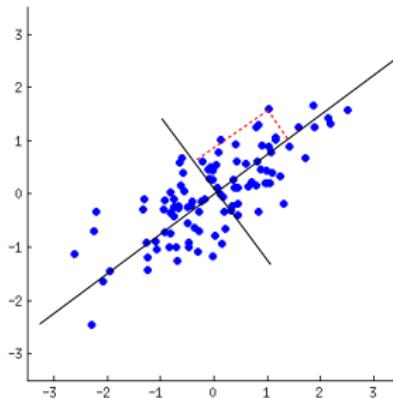


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- Find $k \leq d$ orthogonal directions with the most variance.
These span a k -dimensional subspace of the data.

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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:

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

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

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

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

They are unknown and must be computed.

Principal component analysis (PCA)

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

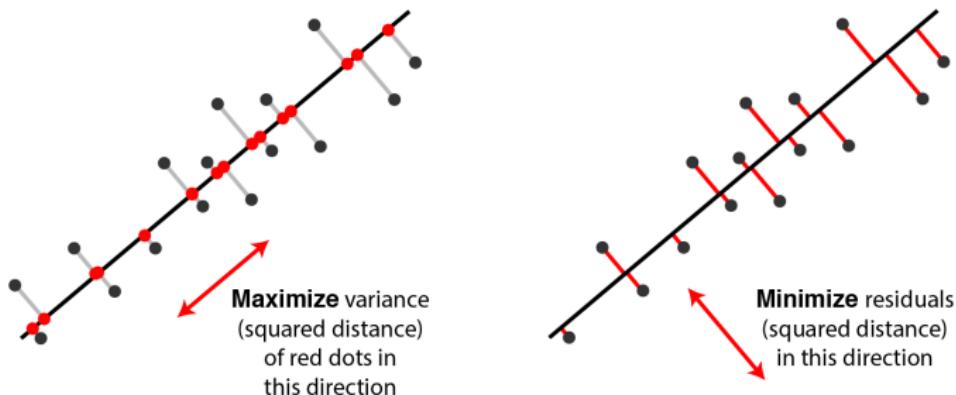
- Minimizes the **projection/reconstruction error**.
- Maximizes the **variance** of the projected data.

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

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

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

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

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The solution is $\mathbf{w} = \text{principal eigenvector of } \mathbf{C}$ ([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:

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

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The successive orthogonal direction can be found by solving:

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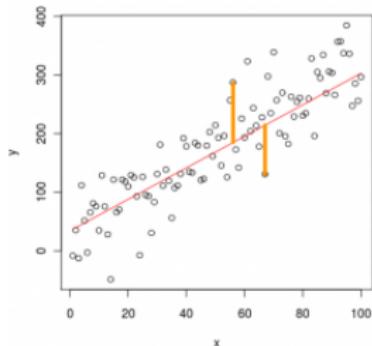
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which is the second eigenvector of \mathbf{C} , and so on for all $\mathbf{w}_{i=2\dots k}$.

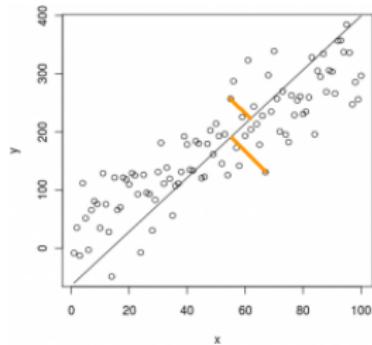
The **principal components** are thus the first $k \ll d$ eigenvectors of \mathbf{C} , sorted by decreasing eigenvalue.

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} :

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

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

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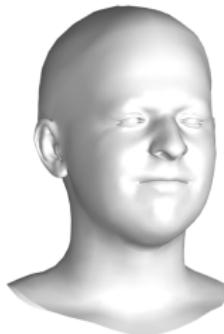
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Example:

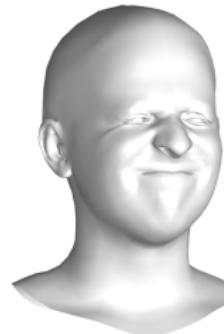


Data point \mathbf{x}_1



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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From a different perspective, PCA gives us 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.

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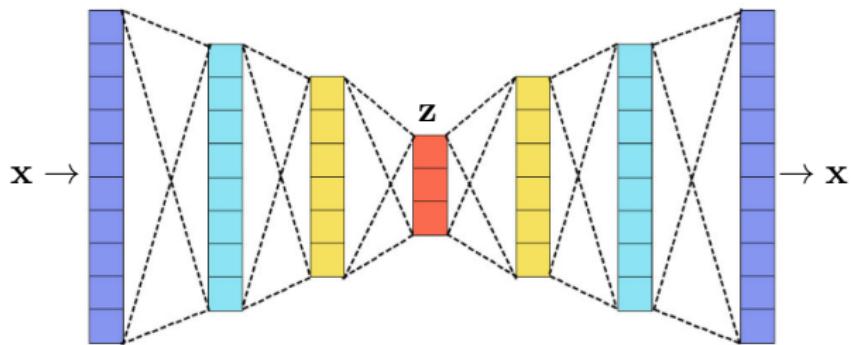
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How to generalize this idea?

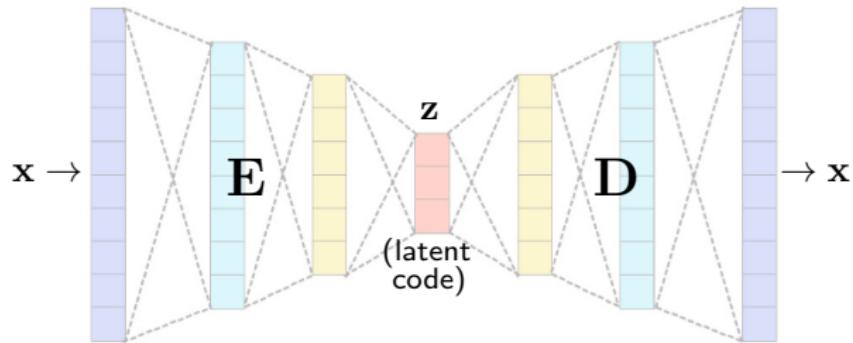
Autoencoders (AE)

We can construct powerful parametric models using deep nets.



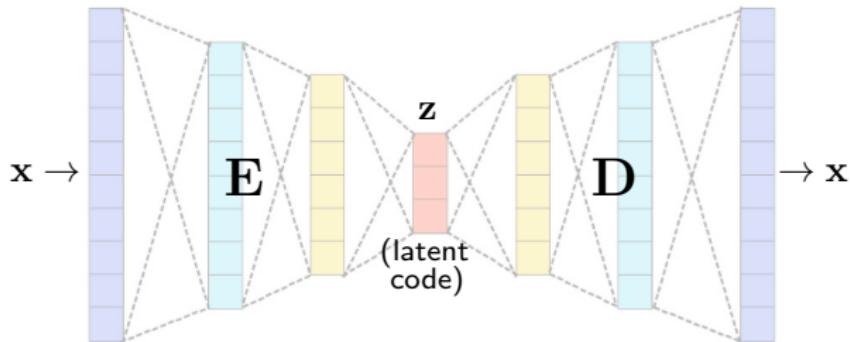
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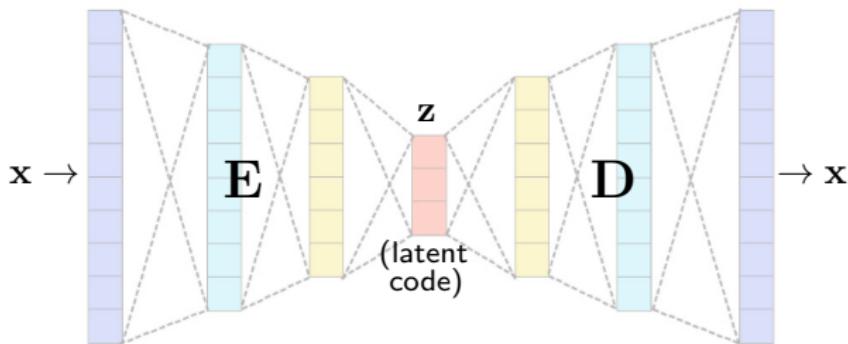


For a given dataset $\{\mathbf{x}_i\}$, we require the encoder E and decoder (or generator) D to minimize the **reconstruction loss**:

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

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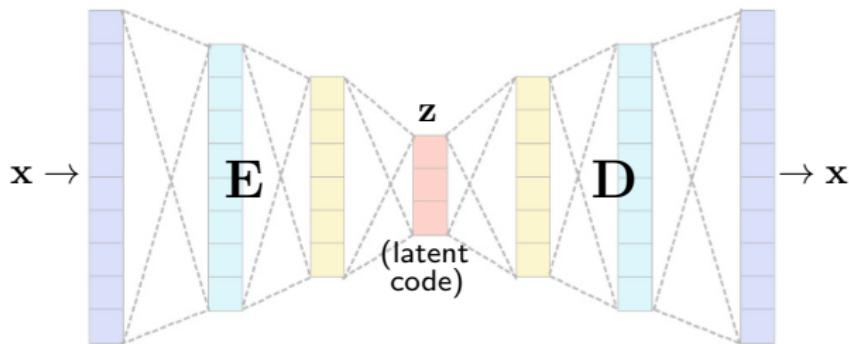
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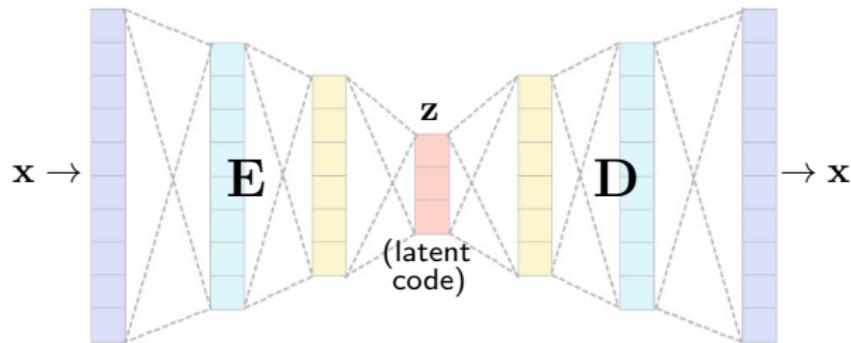
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If the layers are **linear**, the codes \mathbf{z}_i span exactly the same space as PCA.

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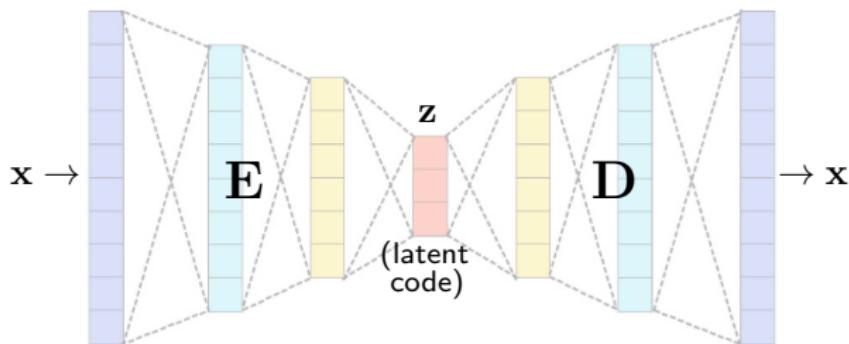
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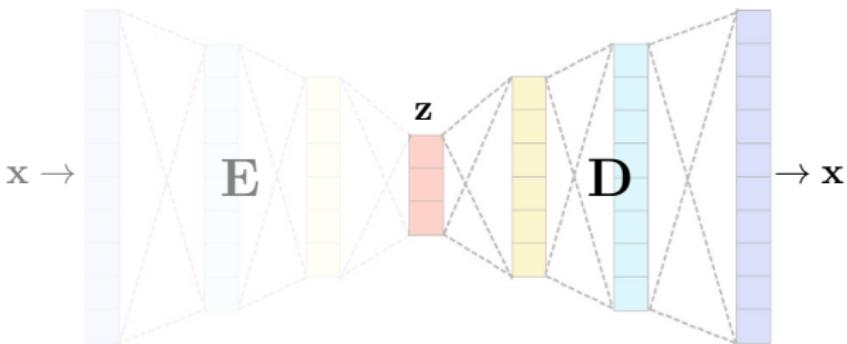
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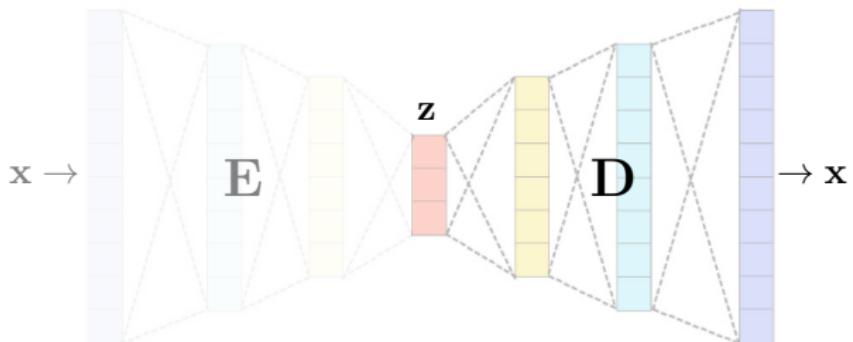
- The **bottleneck** prevents trivial solutions.
- The **task** is not important here: it is always reconstruction.
Once the AE is trained, we are interested in the structure of the **latent space** and in the adoption of E, D for new tasks.

Manifold hypothesis



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

Manifold hypothesis

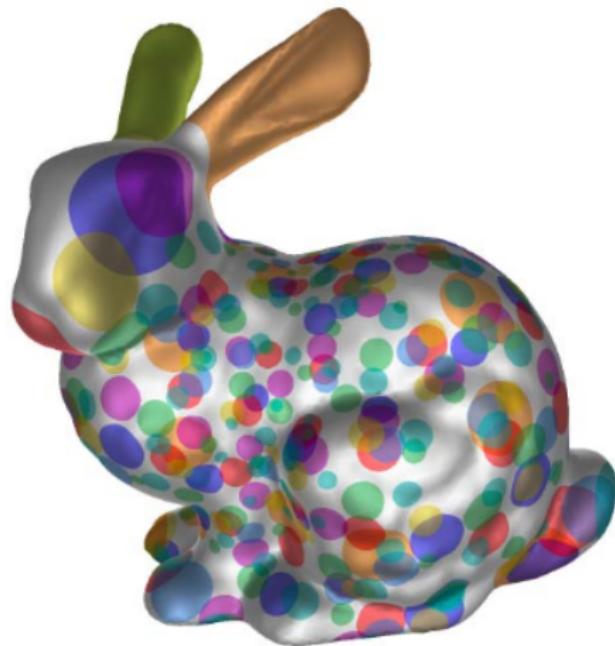


The decoder performs a mapping from a low-dimensional **latent space** to a high-dimensional **embedding** of observed data.

The latent space is Euclidean.

The data embedding space is curved (**manifold hypothesis**).

Differential geometry

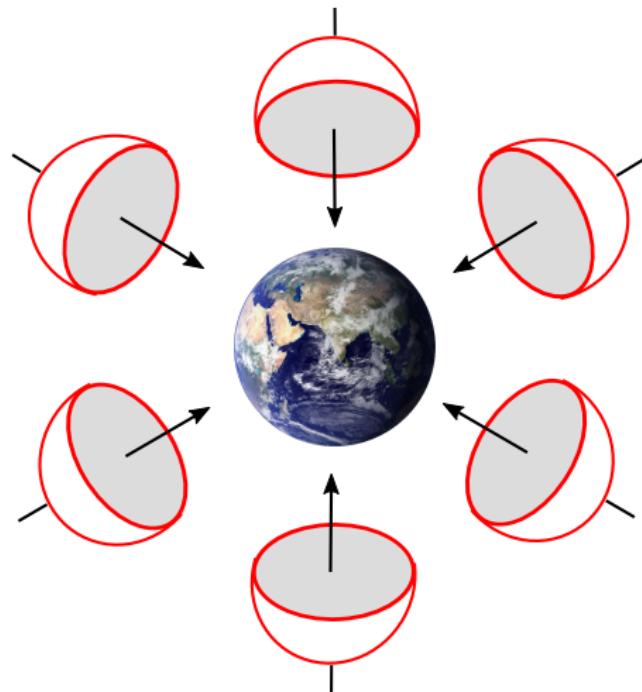


The study of local properties of curves and **surfaces**.

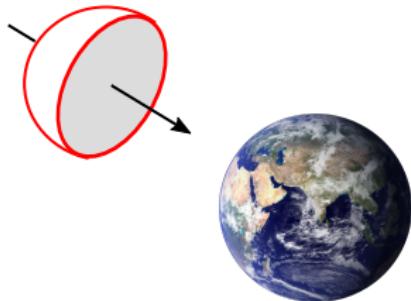
Each neighborhood has a well-behaved mapping to some subset $U \subset \mathbb{R}^2$.

Manifolds

Manifolds are unions of **charts**:



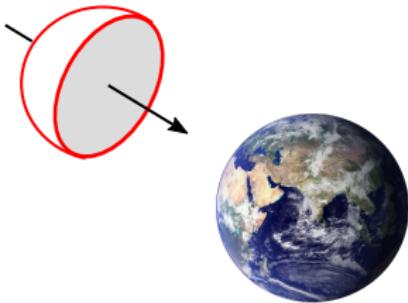
2D manifolds (surfaces)



chart

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

2D manifolds (surfaces)

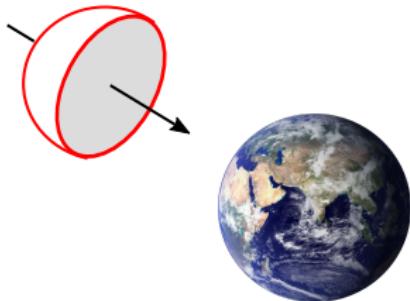


chart

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

2D manifolds (surfaces)



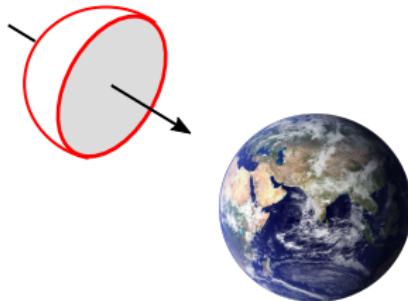
chart

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

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2D manifolds (surfaces)



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2D manifolds (surfaces)

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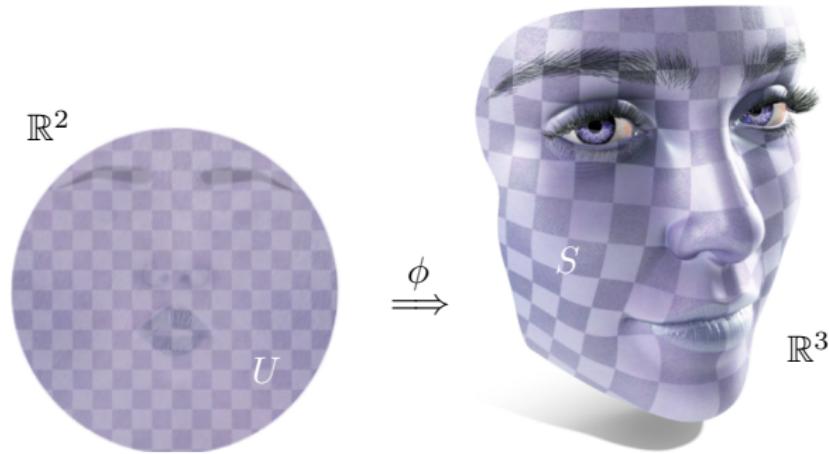


Figure by Keenan Crane

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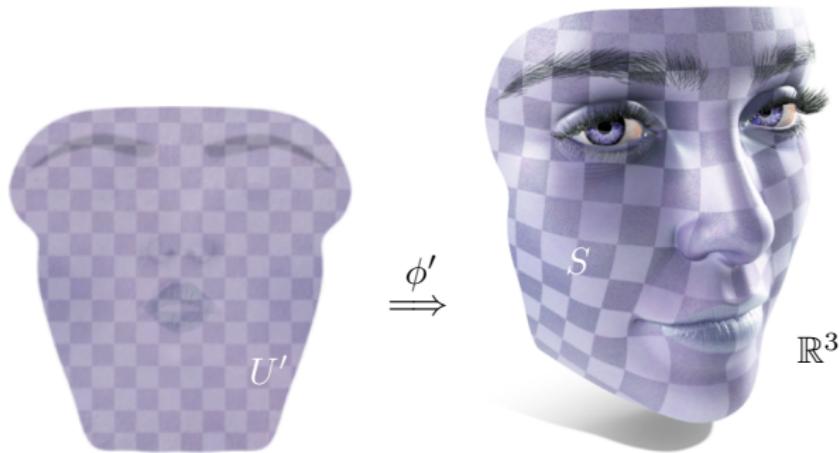


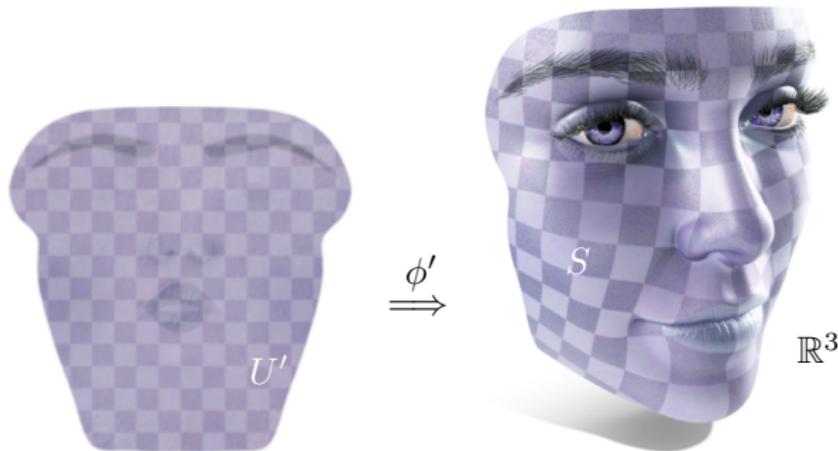
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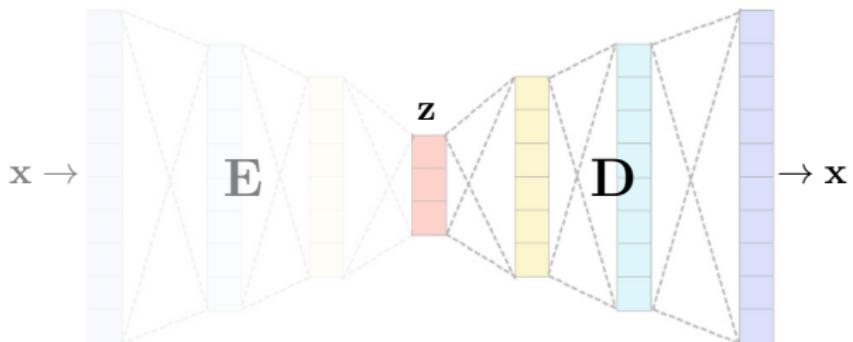
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However, all encode exactly **the same** geometric information.

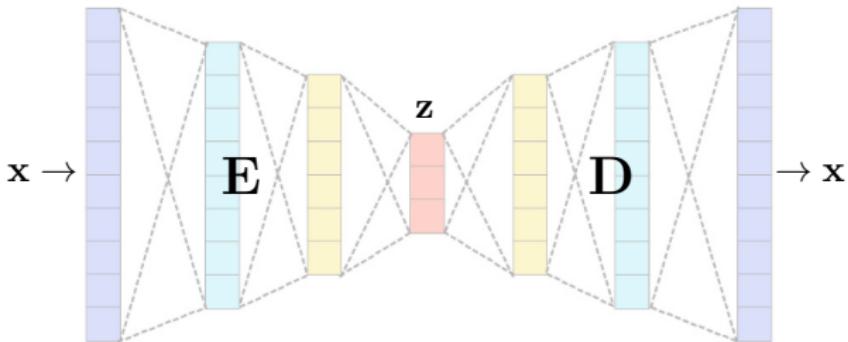
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Manifolds and generative models



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Manifolds and generative models

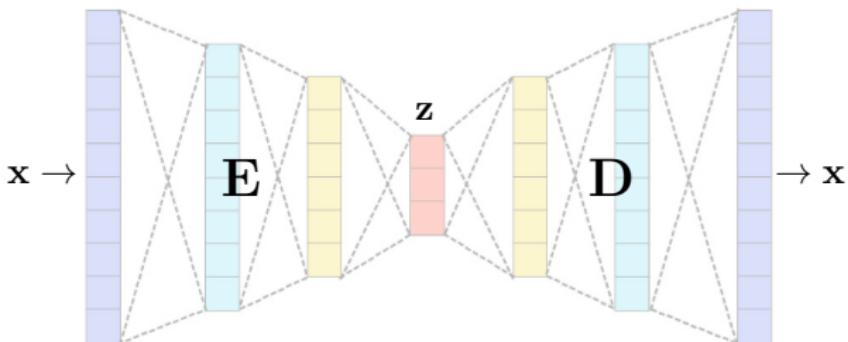


The decoder $D : \mathbb{R}^k \rightarrow \mathbb{R}^d$ is a chart from the latent space spanned by the codes \mathbf{z} to the data space of the inputs \mathbf{x} .

It is differentiable.

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Manifolds and generative models



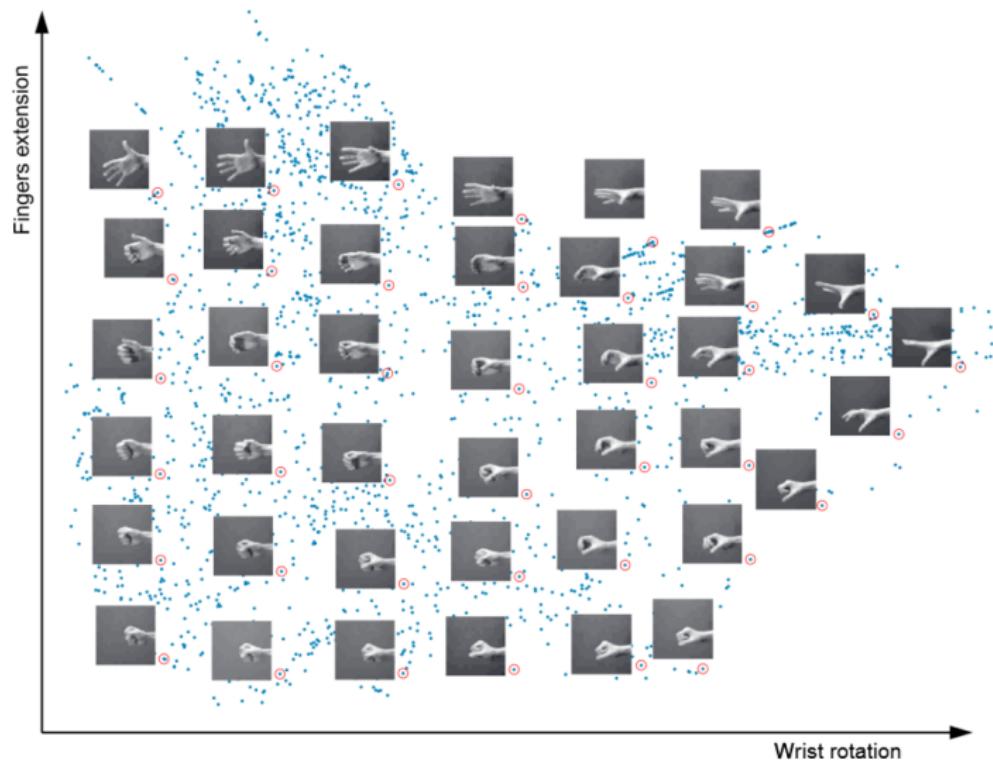
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PCA puts the data on a **linear** (flat) manifold, since D simply performs a linear combination of orthogonal vectors.

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.

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

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Variational autoencoders (VAE)

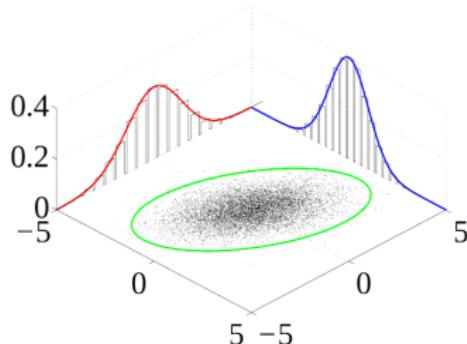
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Autoencoders can map similar inputs to arbitrarily distant regions of the latent space. But we want to make sure to learn a **distribution**.

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).



Entropy and divergence

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However, computing:

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

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

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

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

is called the Evidence variational Lower BOund.

Variational autoencoder (VAE)

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

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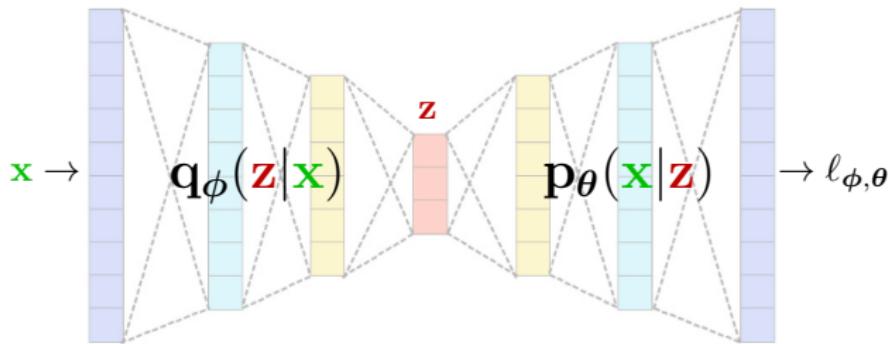
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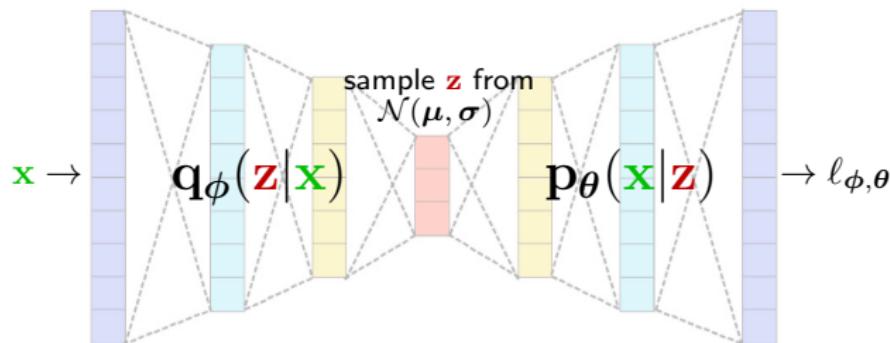
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Using Gaussians, the KL term has a closed form.

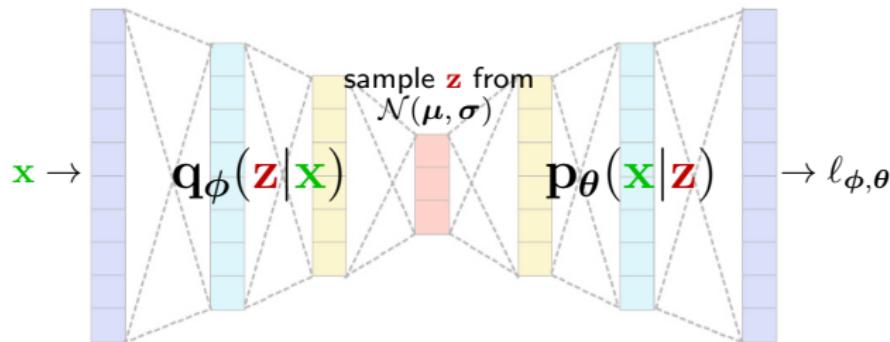
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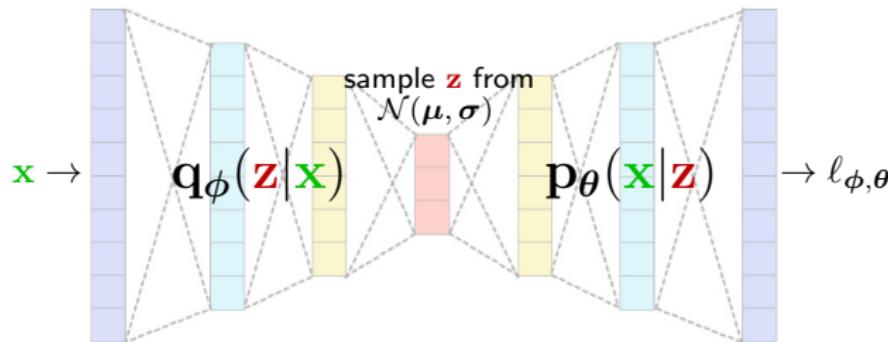
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Variational autoencoder (VAE)

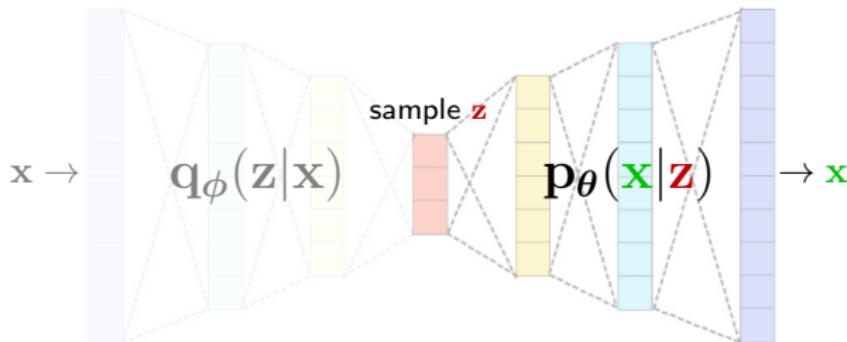
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To distinguish from VAE, classical AE are also called [deterministic AE](#).

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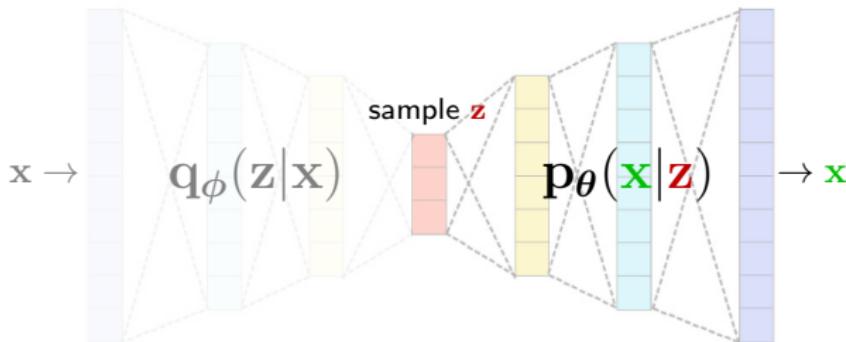


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Generation: Sample \mathbf{z} according to the learned distribution.

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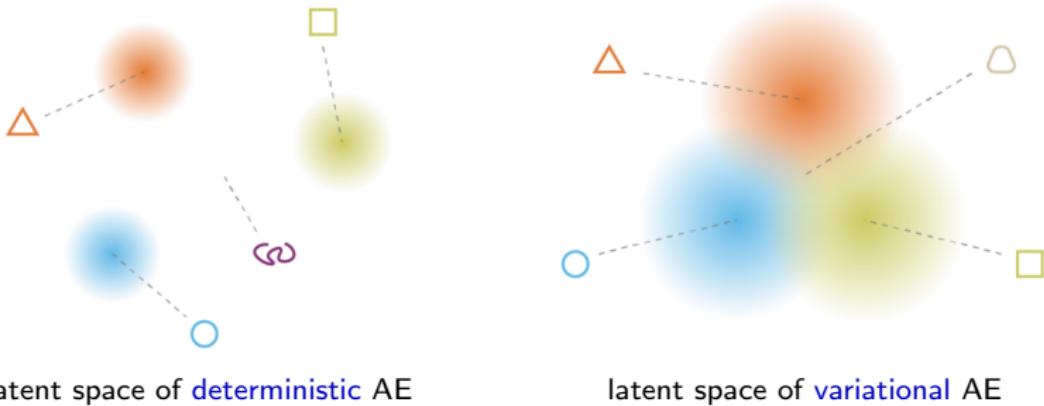
To distinguish from VAE, classical AE are also called **deterministic AE**.

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

In principle, **also the decoder outputs a probability distribution**.

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

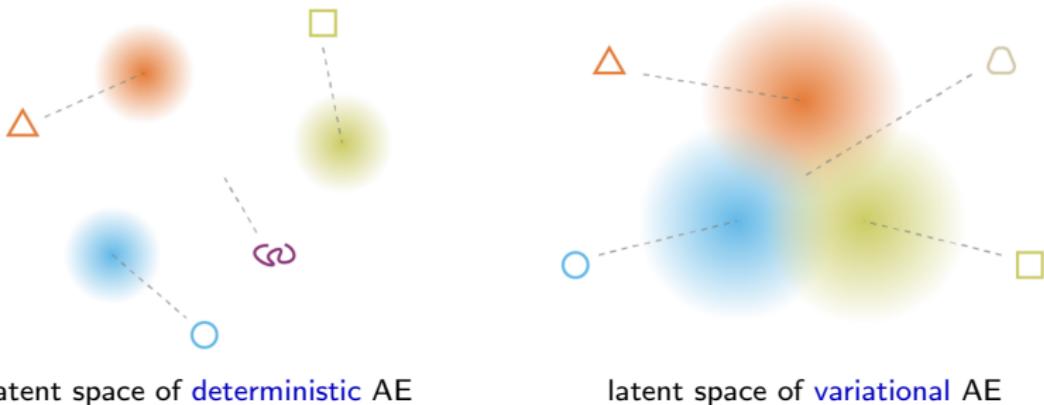
Regularizing effect



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

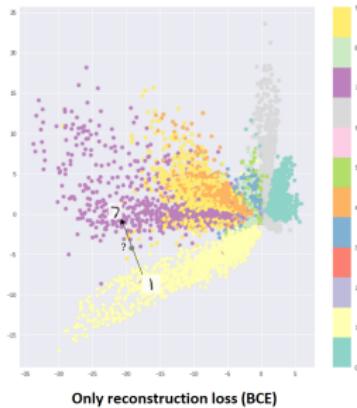
latent space of variational AE

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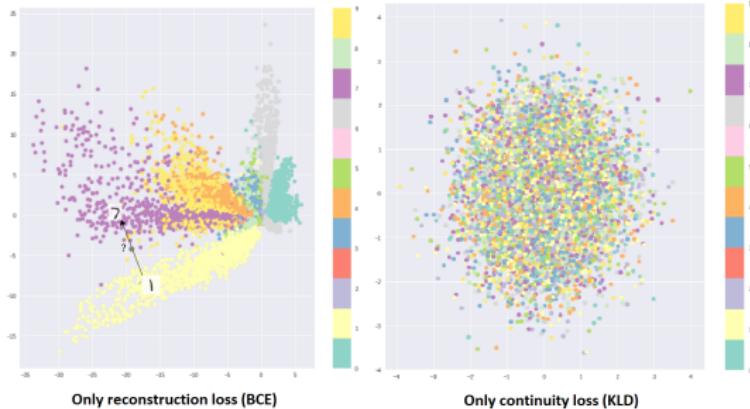
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A deterministic AE might generate arbitrary noise.

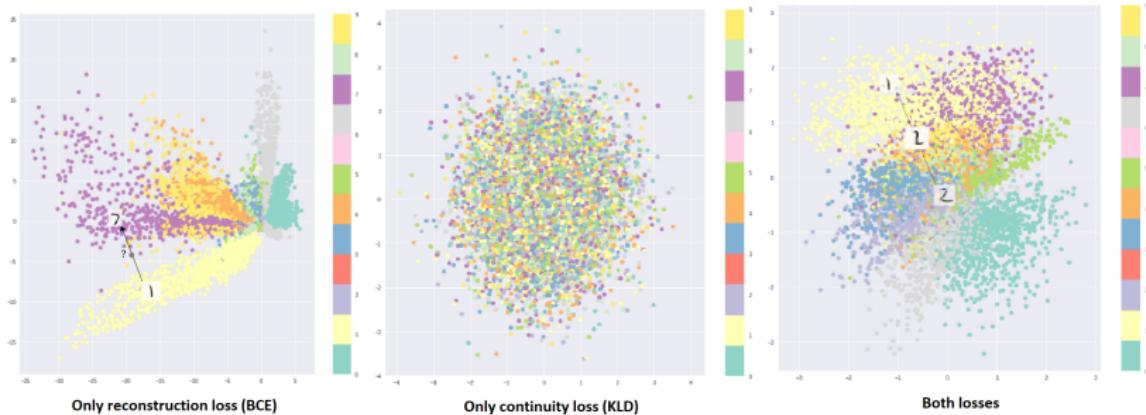
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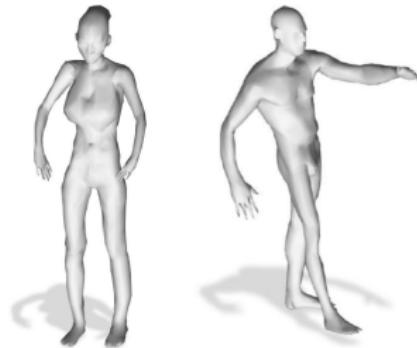
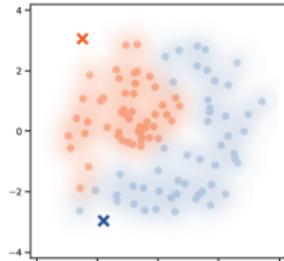
Regularizing effect



The distributional regularizer brings **smoothness** in the learned space.

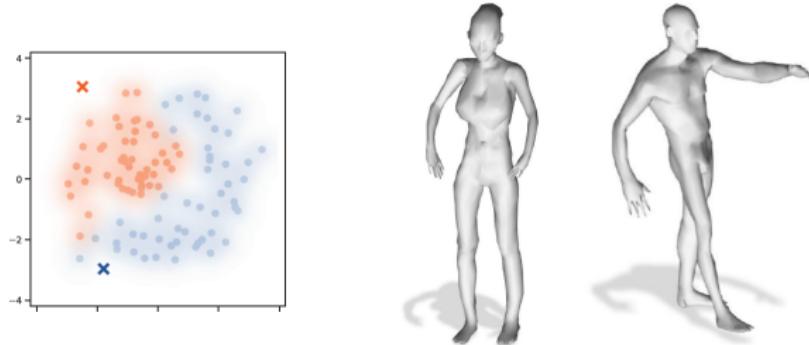
Unlikely samples

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



Unlikely samples

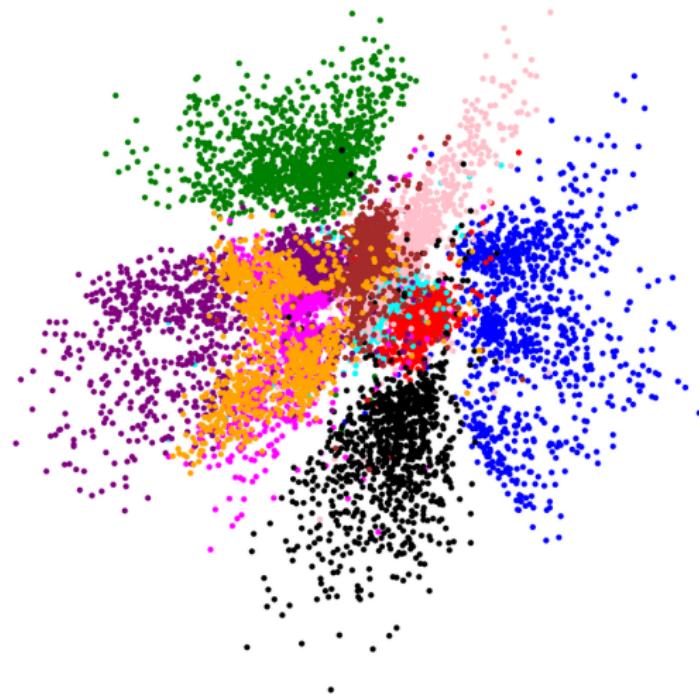
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Another relevant phenomenon is **posterior collapse**, where the latents are ignored if the decoder is powerful enough to model the data perfectly.

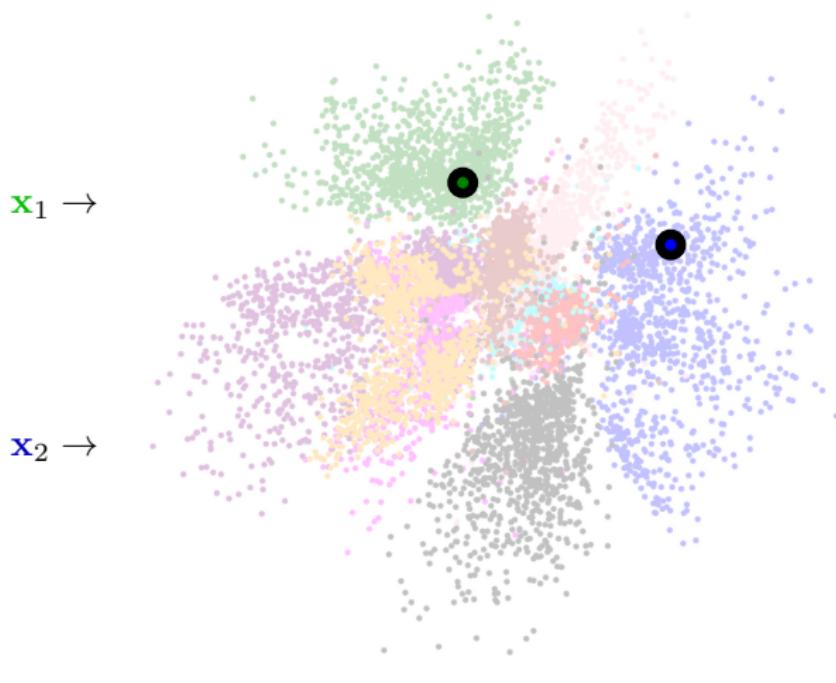
VAE interpolation

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



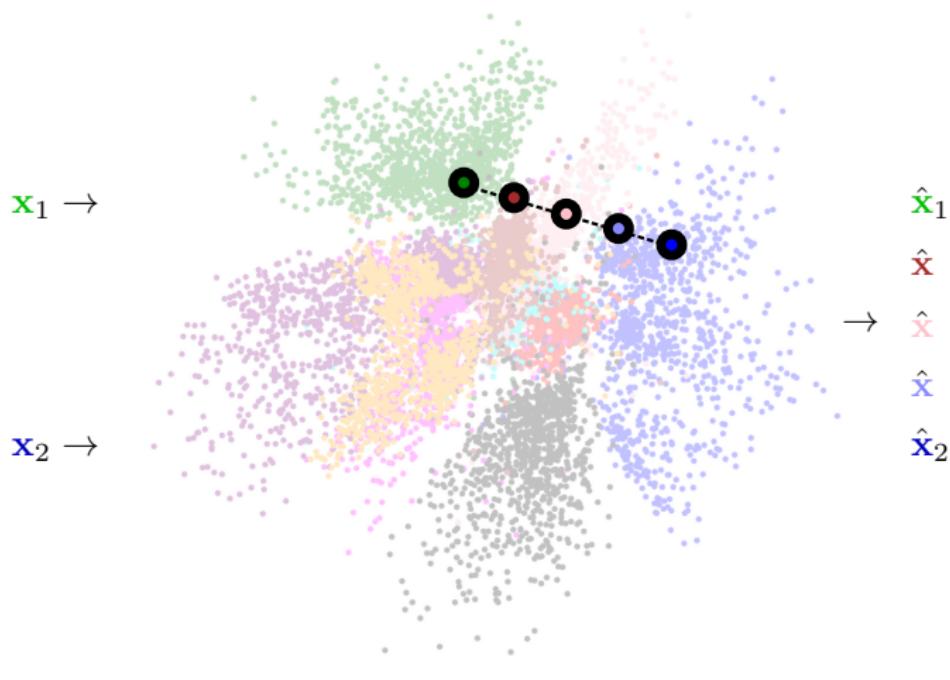
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VAE interpolation

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

VAE interpolation

7

1

VAE interpolation

7 7 7 7 7 7 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1

VAE interpolation

6

7 7 7 7 7 7 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1

VAE interpolation

六四九九九九九九

777777771111111111111111

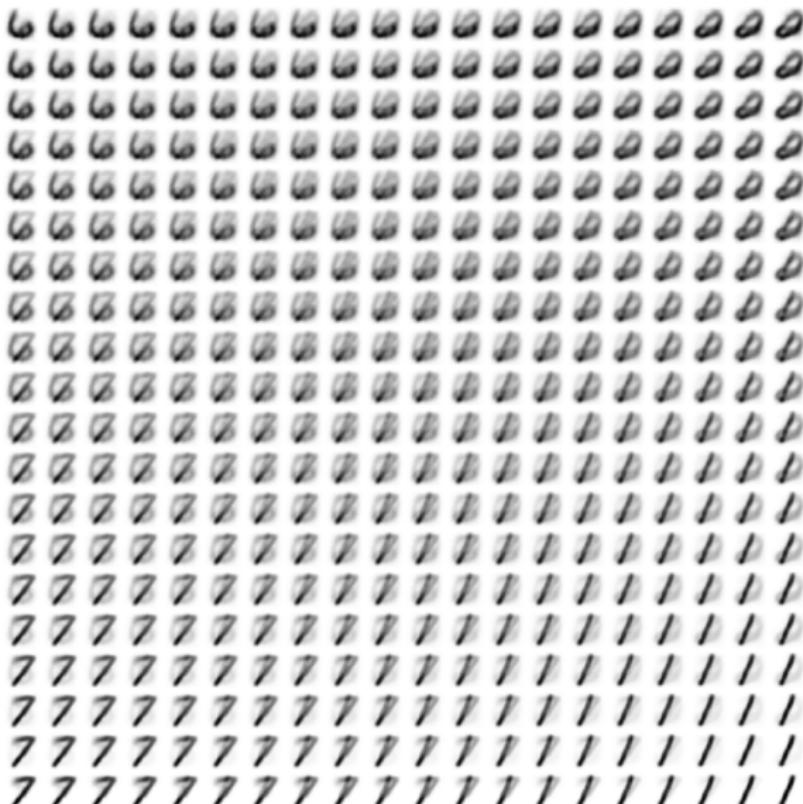
VAE interpolation

A 10x10 grid of handwritten digits, likely generated by a Variational Autoencoder (VAE) during an interpolation process. The digits transition smoothly from a '6' at the top-left to a '7' at the bottom-right, illustrating the latent space manifold.

The digits are arranged in a grid:

- Row 1: 6 6 6 6 6 6 6 6 6 6
- Row 2: 9 4 4 2 2 2 2 2 2 2
- Row 3: 9 2 2 2 2 2 2 2 2 2
- Row 4: 9 9 2 2 2 2 2 2 2 2
- Row 5: 9 9 4 2 2 2 2 2 2 3
- Row 6: 9 9 4 2 2 2 2 2 3 3
- Row 7: 9 9 9 9 2 2 2 3 3 3
- Row 8: 9 9 9 9 9 3 3 3 3 3
- Row 9: 9 9 9 9 9 8 3 3 3 3
- Row 10: 7 9 9 9 9 9 8 8 8 8
- Row 11: 7 9 9 9 9 9 8 8 8 8
- Row 12: 7 9 9 9 9 9 8 8 8 8
- Row 13: 7 9 9 9 9 9 8 8 8 8
- Row 14: 7 9 9 9 9 9 9 8 8 8
- Row 15: 7 9 9 9 9 9 9 9 8 8
- Row 16: 7 9 9 9 9 9 9 9 9 8
- Row 17: 7 9 9 9 9 9 9 9 9 9
- Row 18: 7 9 9 9 9 9 9 9 9 9
- Row 19: 7 9 9 9 9 9 9 9 9 9
- Row 20: 7 7 7 7 7 7 7 7 7 7

Euclidean interpolation

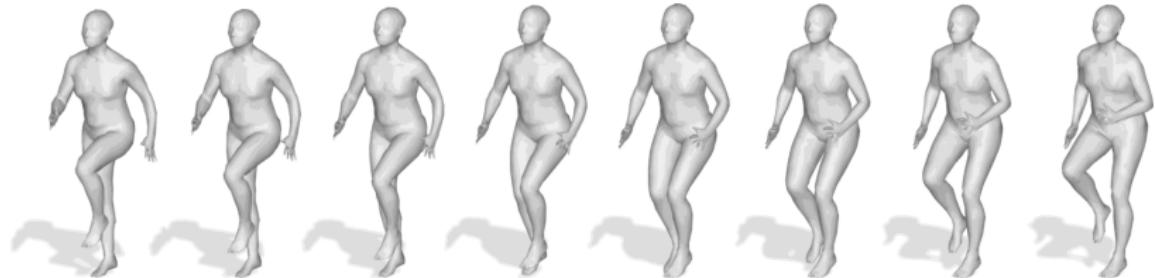


Example: Deformable 3D shapes



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

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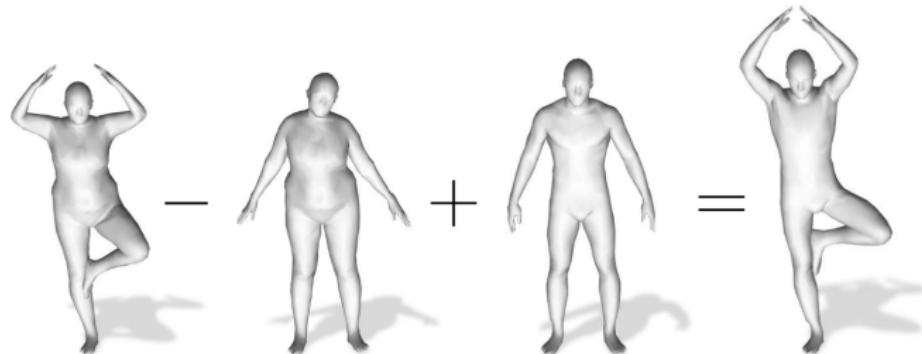
The latent space can be explored along different dimensions
(disentanglement):



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

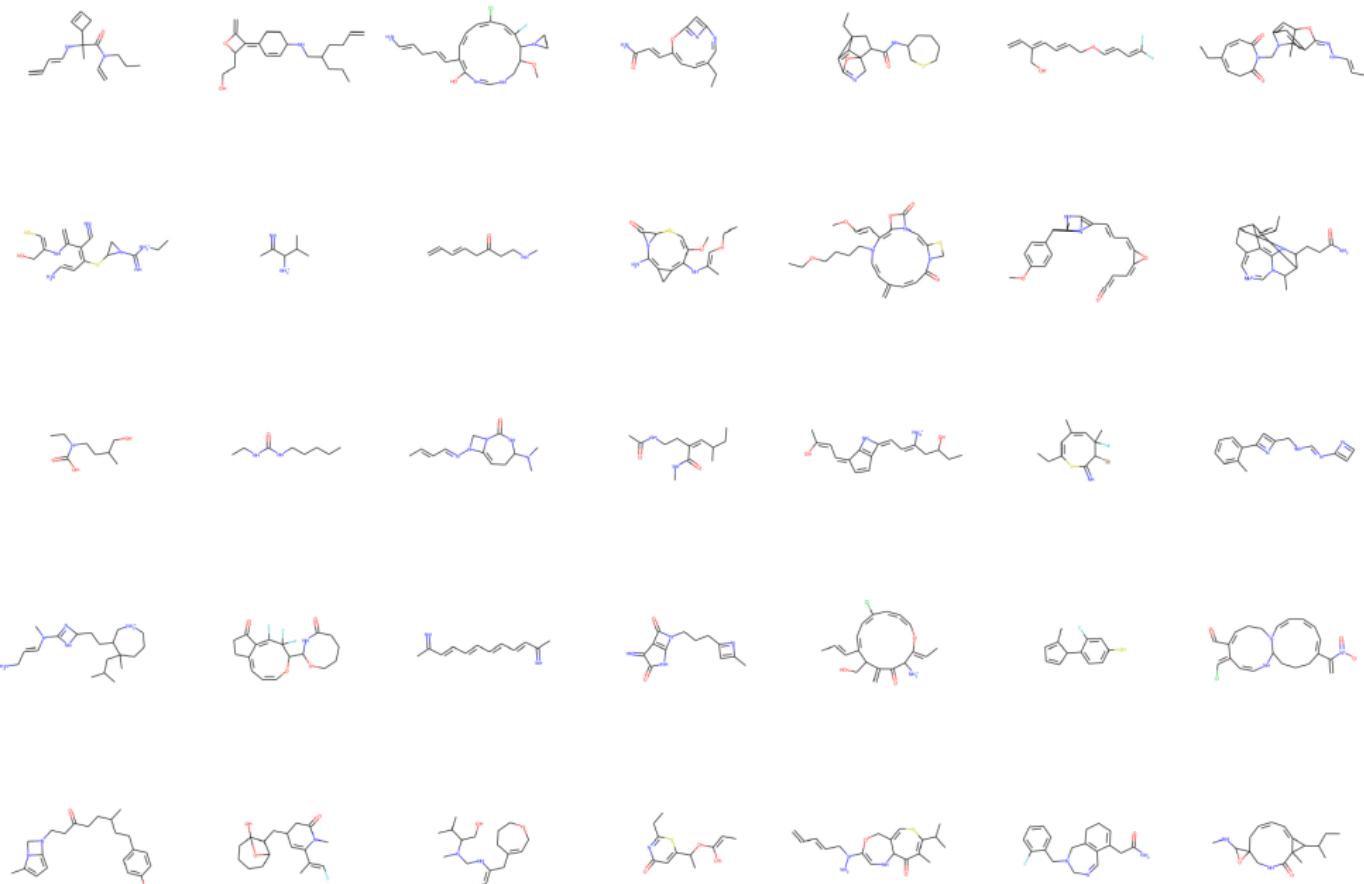
Analogies

Algebraic manipulation of codes leads to the following:

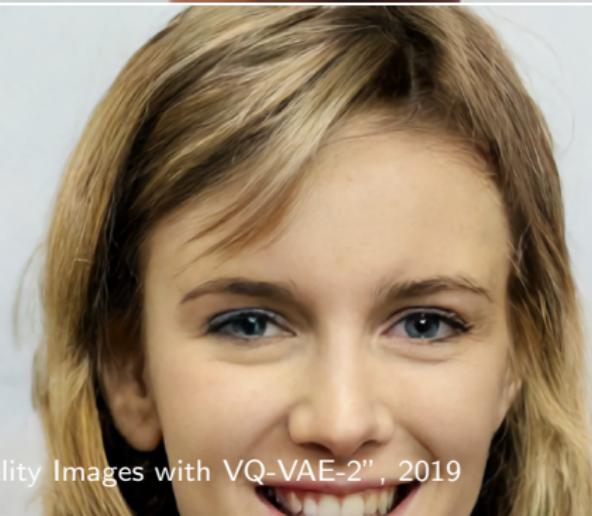


In NLP this is done by manipulating [word embeddings](#):

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



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



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