Deep learning workshop
Alan Turing Institute

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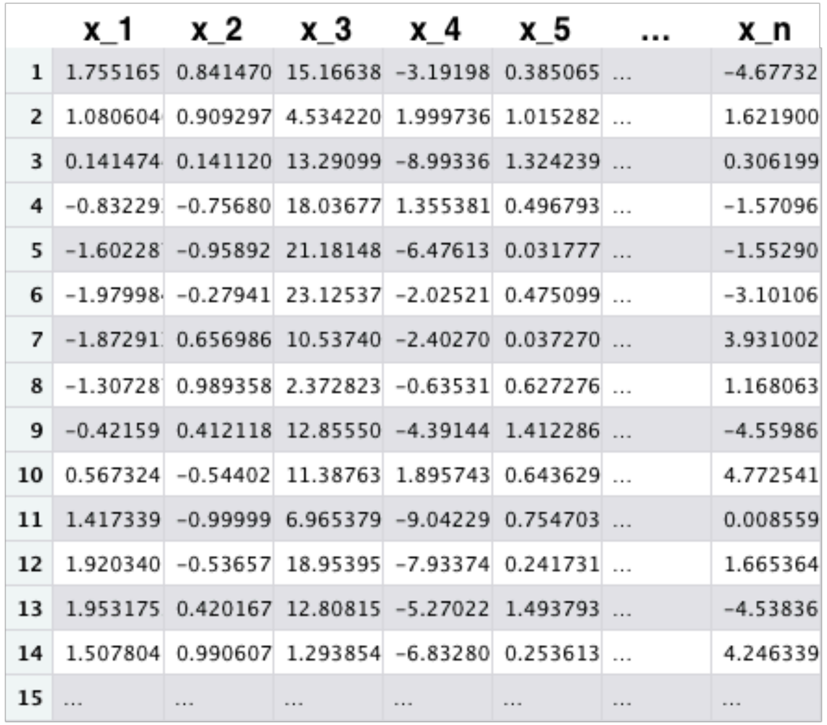
25th February 2020

Topics in dimensionality reduction

Why dimensionality reduction? (1)

- **Multi-dimensional data visualisation**

data frame



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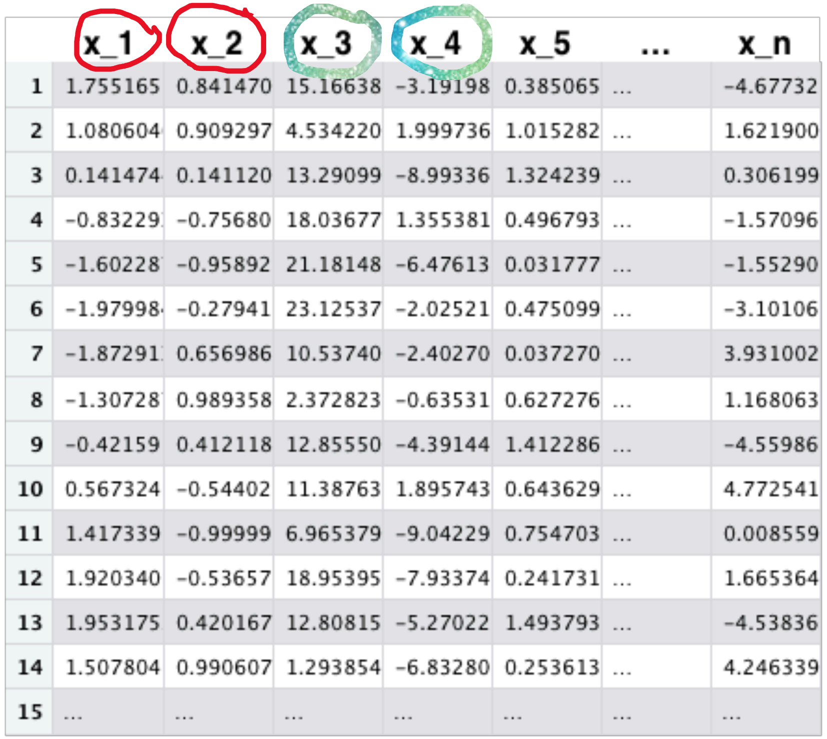

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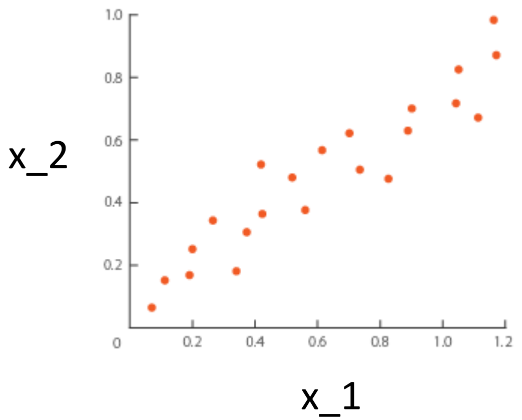
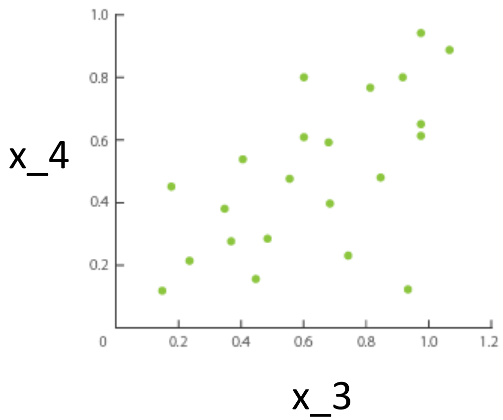
- Want to discover structure in the data
- Can plot variables pairwise:





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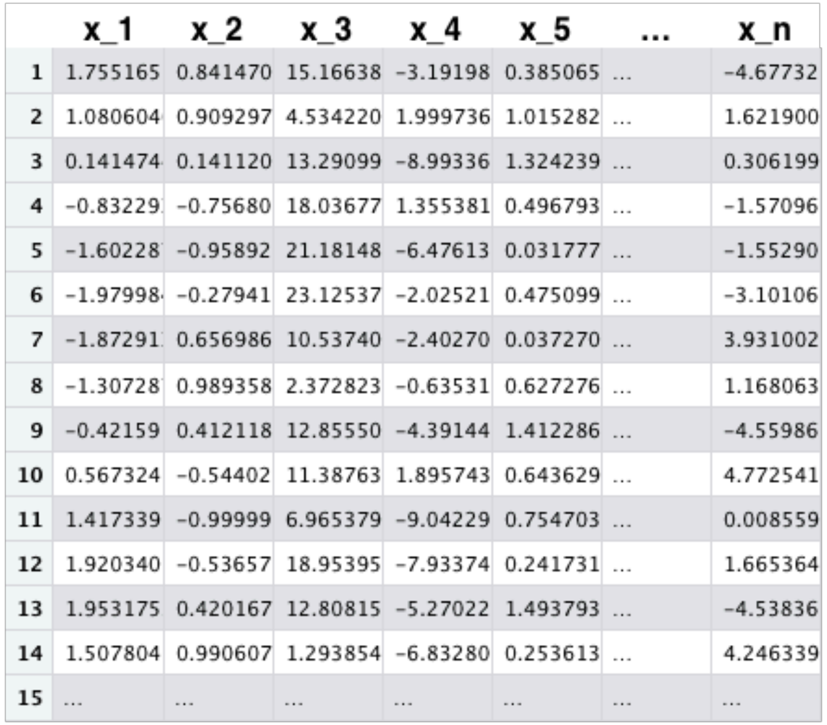

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- Want to discover structure in the data
- Can plot variables pairwise
- This won't uncover higher order structure in complex data
- E.g. $x_n = f(x_1, ..., x_{n-1})$

Why dimensionality reduction? (2)

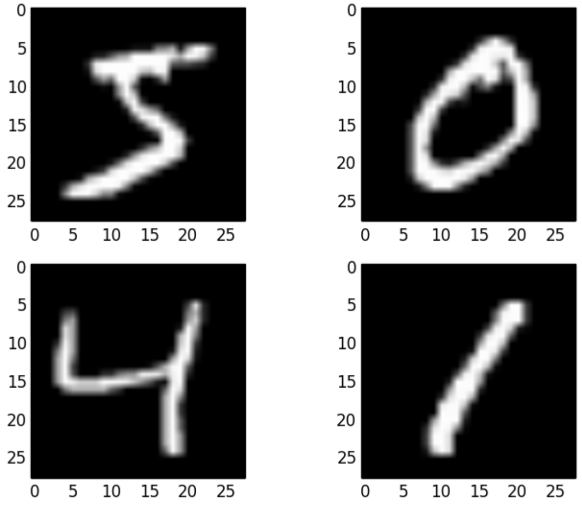
- Data compression

- JPEG:

- MP3

Why dimensionality reduction? (3)

- Noise filtering / informative feature extraction



- Can we get rid of the uninformative components of the data?
- Machine learning on compressed representations:
  - Slimmer models
  - Faster training
  - Less overfitting

Outline

- Principal component analysis
- Autoencoders
- Persistent homology
- Mapper
- Variational autoencoders

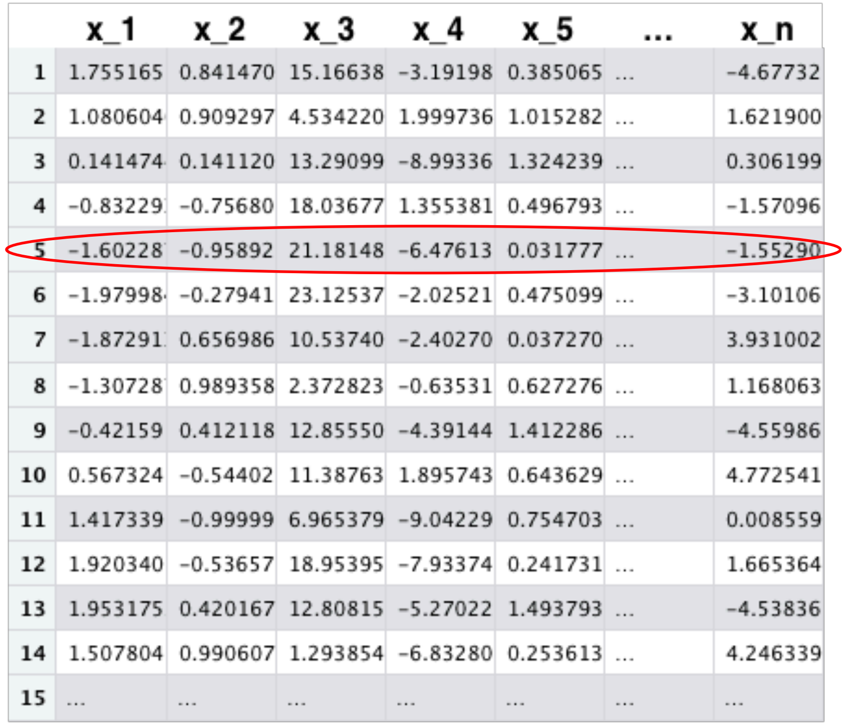
Principal Component Analysis

- Canonical dimension reduction technique

Principal Component Analysis

- Canonical dimension reduction technique

data frame



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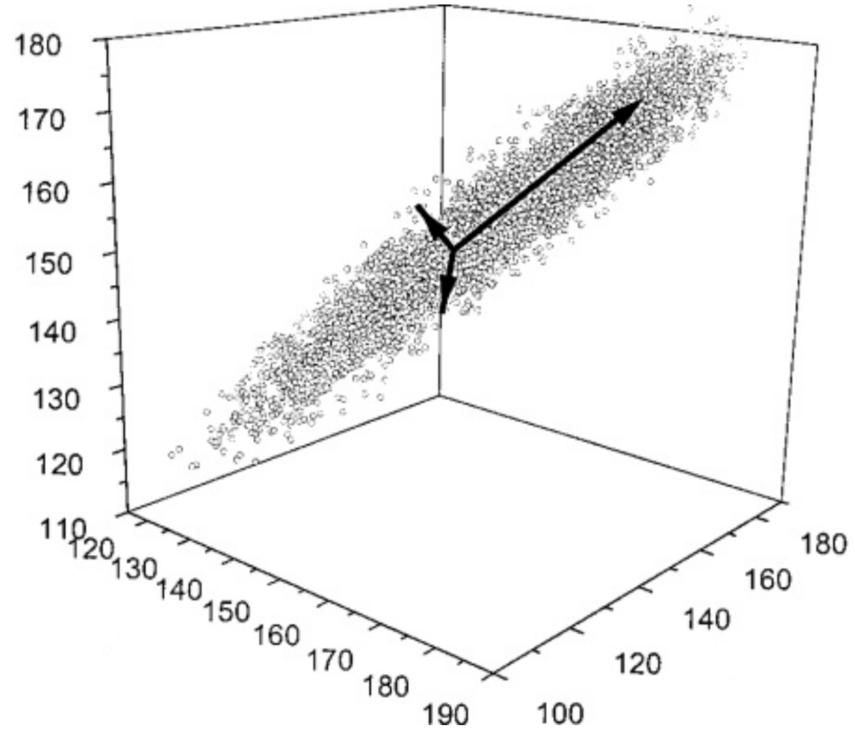
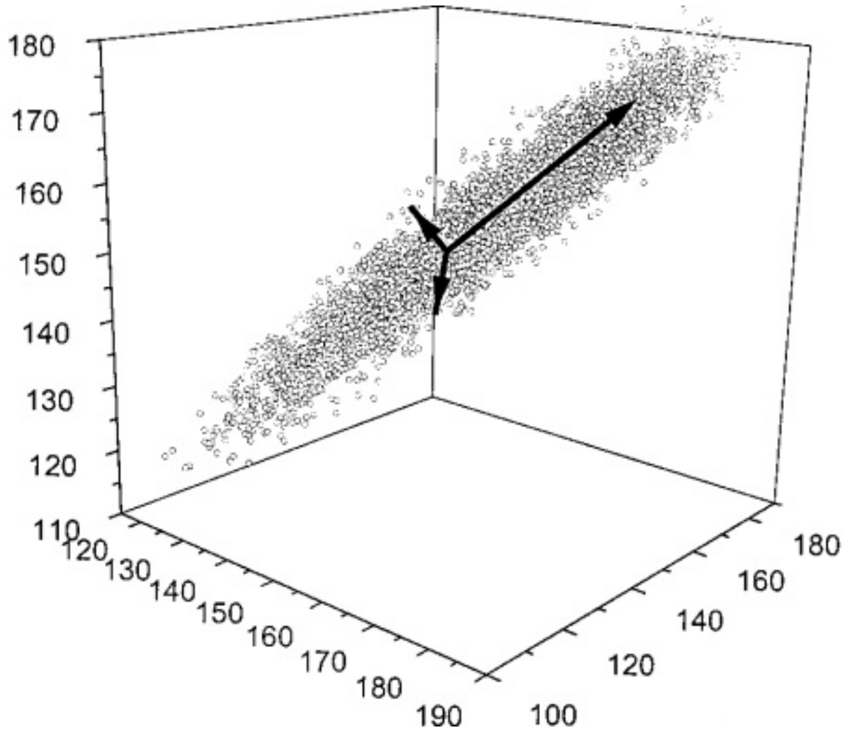
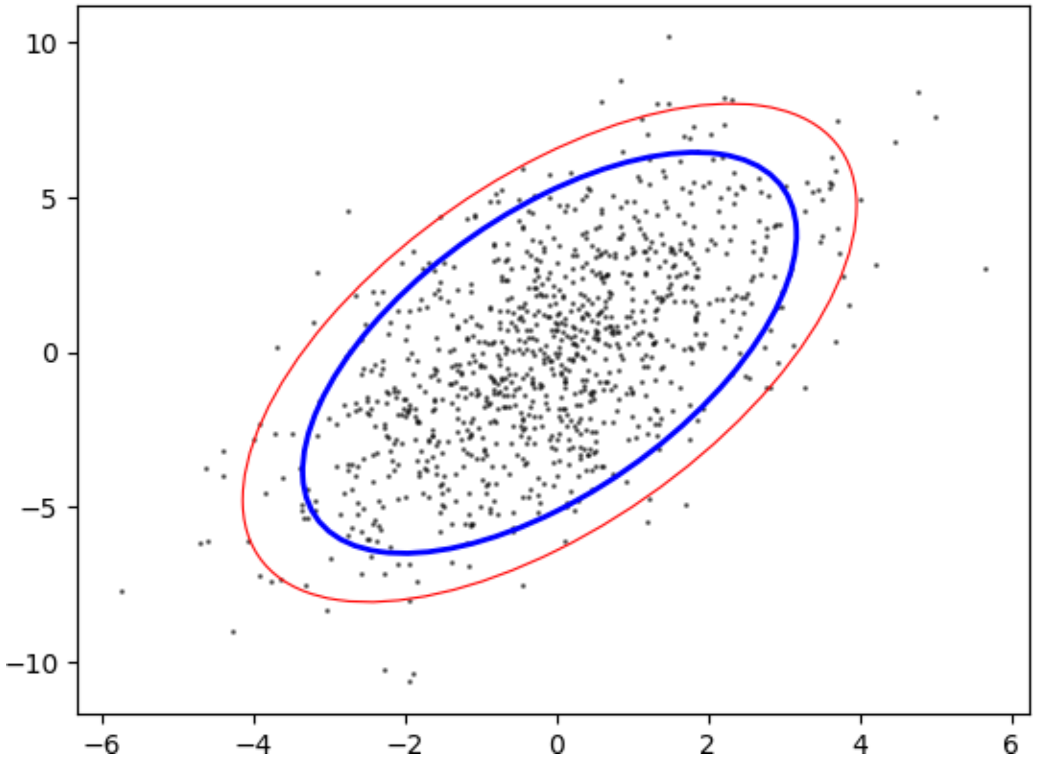
$\in \mathbb{R}^n$



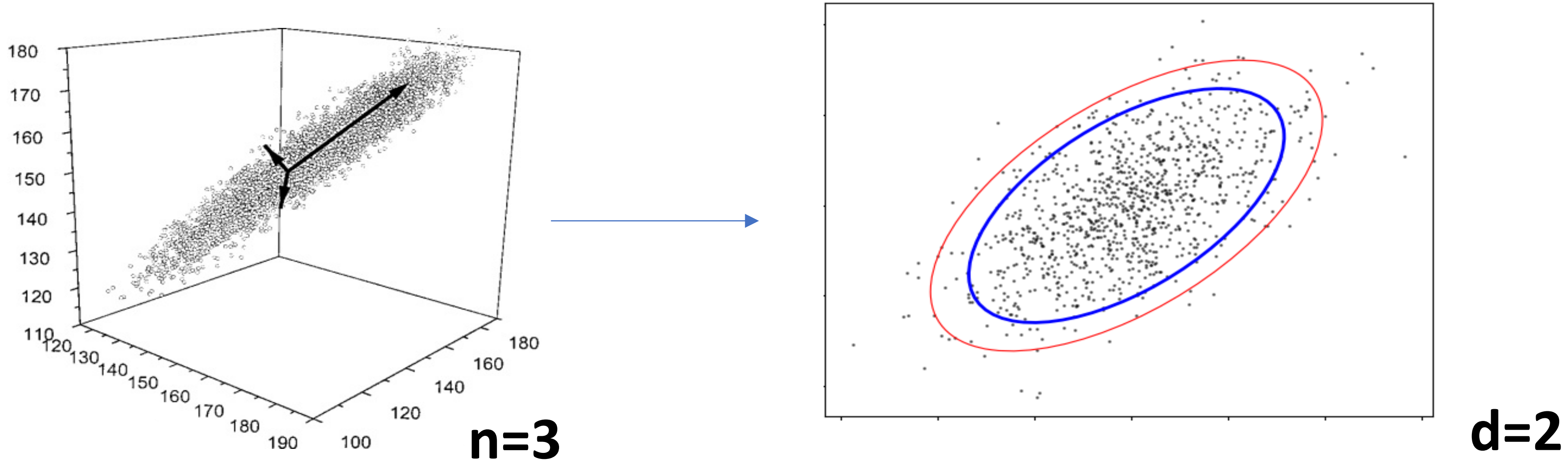
Principal Component Analysis





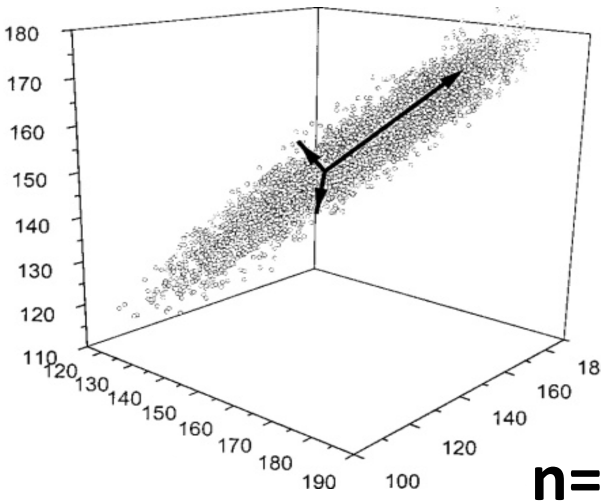
Principal Component Analysis

- **Input**: dimension *d* < *n*
- Projects the data onto a *d* dimensional plane (aka *d* coordinates)
    - Maximise the variance of output data
    - Minimise the distance of original datapoints to the plane
    - These two characterisations of PCA are equivalent!

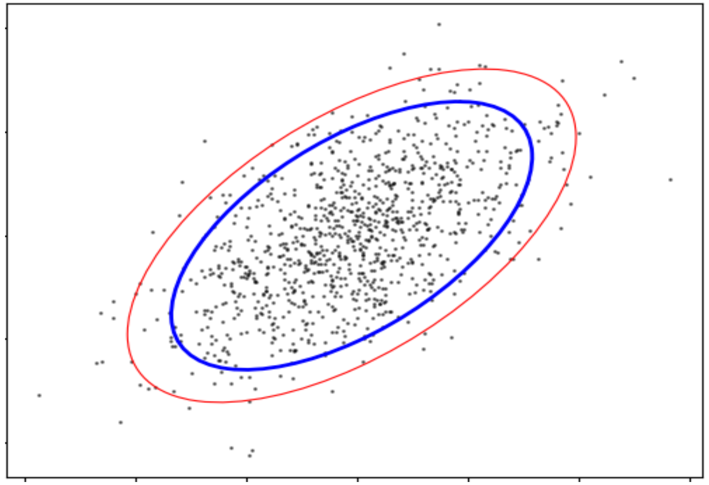


PCA: technicalities

- Uses singular value decomposition (SVD)
  - A generalisation of eigenvectors for non-square matrices
- Problem can be reduced to linear algebra



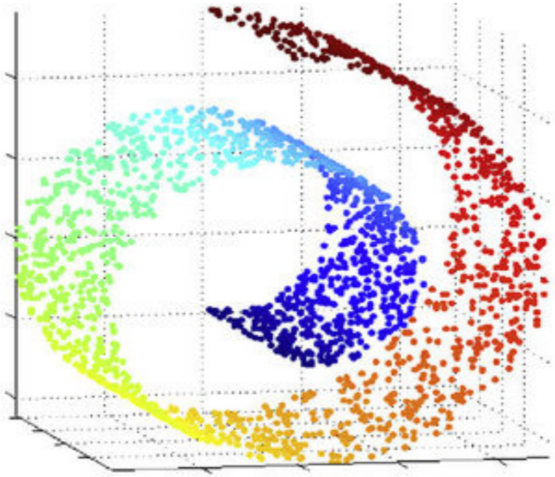
n=3

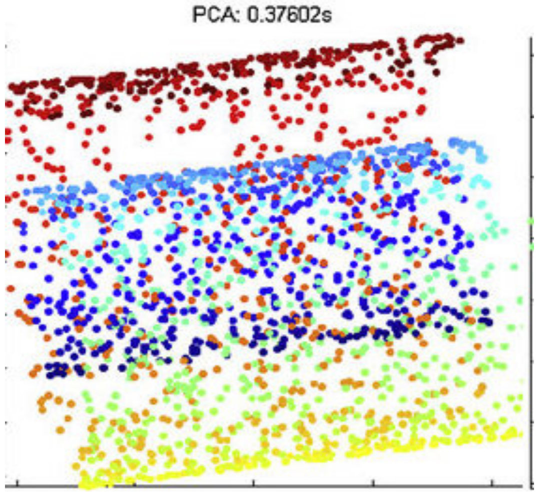


d=2

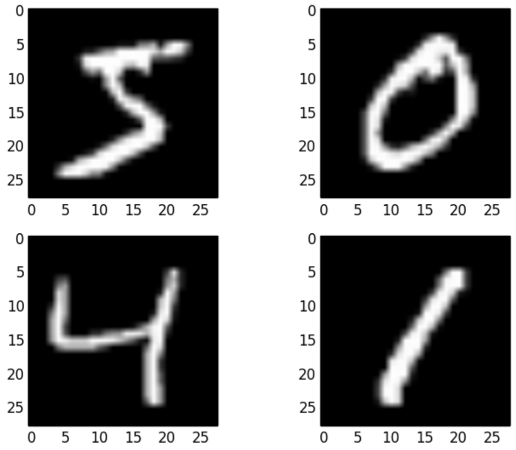
PCA: limitations

- The ‘Swiss’ roll





- MNIST digits



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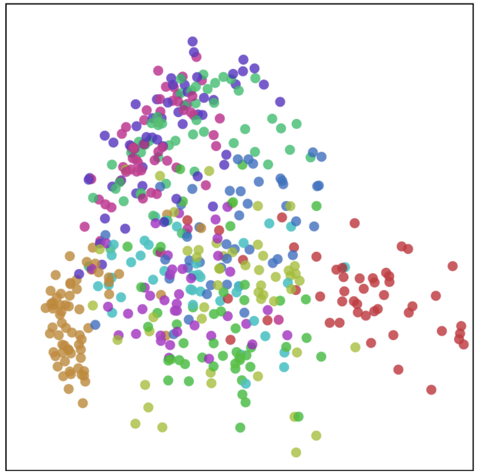


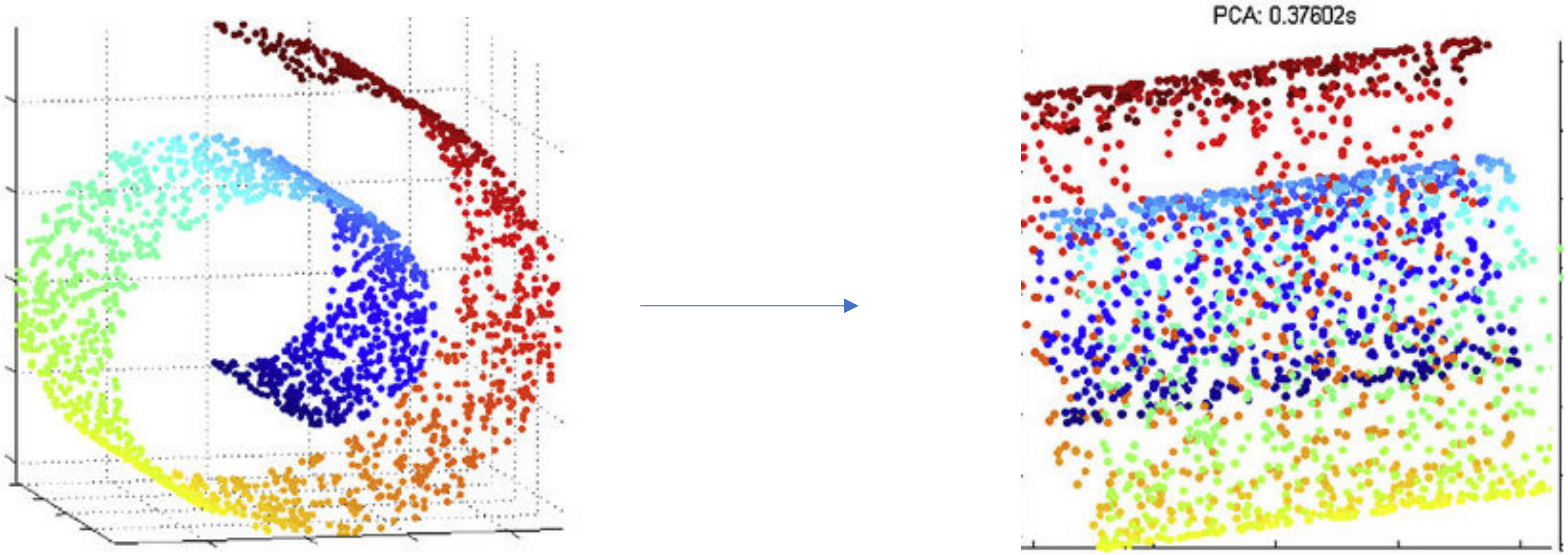
1 colour

= 1 digit

http://colah.github.io/posts/2014-10-Visualizing-MNIST/

PCA: Summary

- Runs fast (problem can be reduced to linear algebra)
- Result is easy to interpret
- Does not preserve the overall ‘shape’ of the data
- Dimension reduction is purely linear

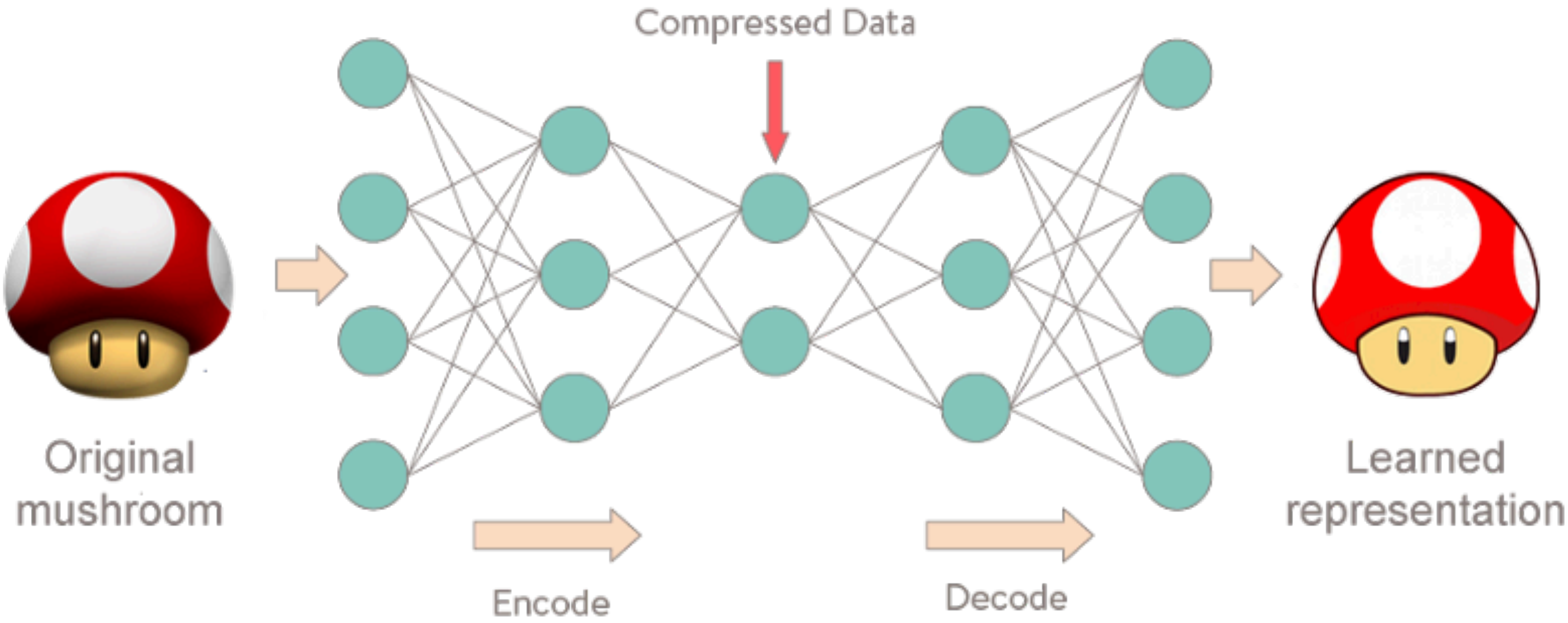


- In Python scikit-learn: see sklearn.decomposition.PCA

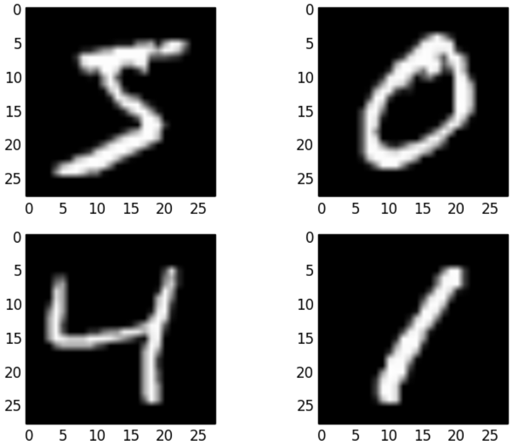
Autoencoders

- Neural network trained to approximate the identity function

$$f(x) = x \qquad dist(f(x), x) \searrow 0$$

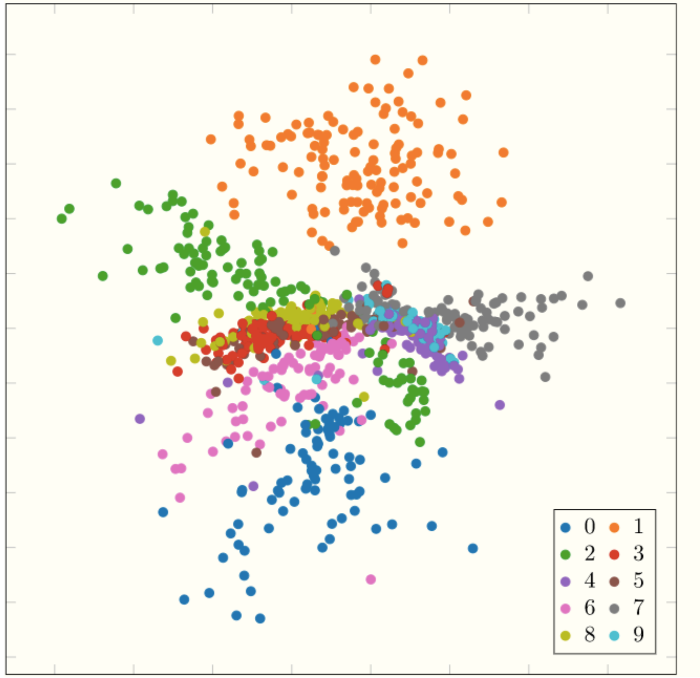


Autoencoder VS PCA: example

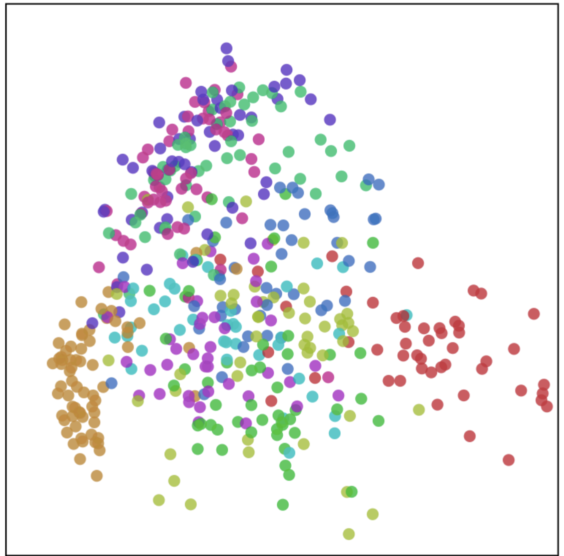


...

Autoencoder

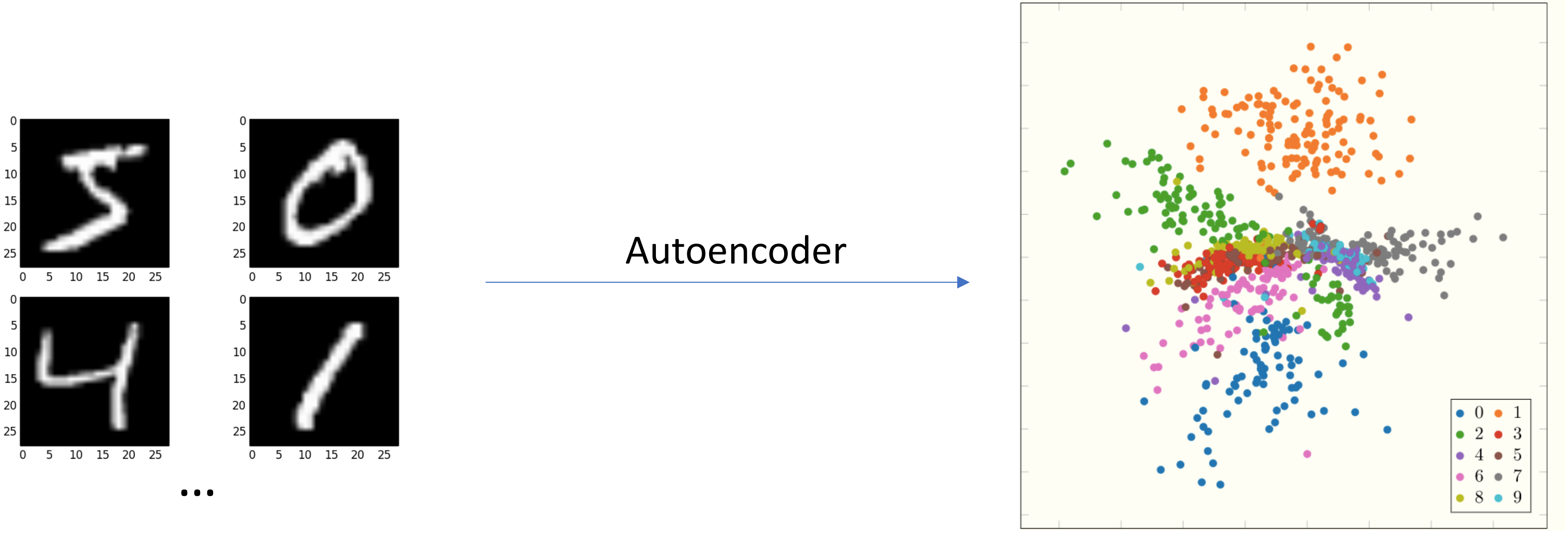


PCA



https://gertjanvandenburg.com/blog/autoencoder/

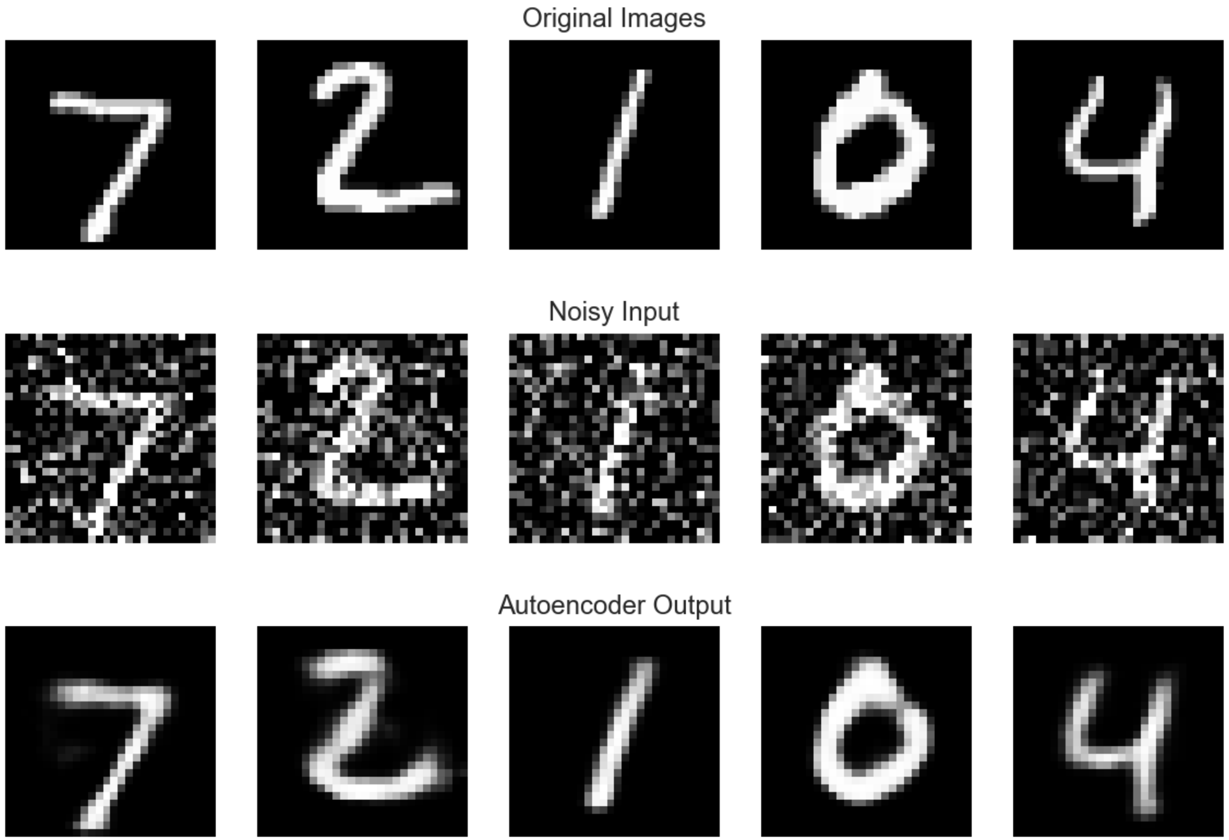
Autoencoder: feature extraction



- Resulting features can be used in machine learning, e.g.,
  - Classification
  - Regression
  - etc

https://gertjanvandenburg.com/blog/autoencoder/

Denoising autoencoder



For state of the art see:

- Generative adversarial denoising
- Variational autoencoder denoising

https://towardsdatascience.com/applied-deep-learning-part-3-autoencoders-1c083af4d798

Autencoders

+ Data compression

+ Data denoising

+ Informative feature extraction

- Usually latent representation is not useful for visualisation

The topology of data

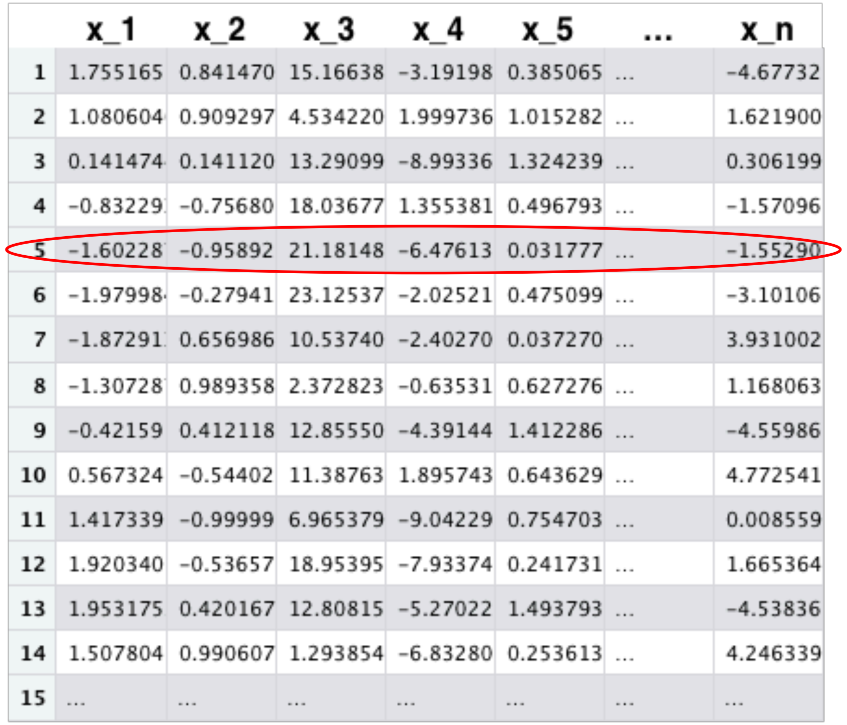
Idea: real world data is often noisy, therefore one must look at its global structure.

Topology enables to analyse the structure of data, by using methods that are resistant to noise perturbations.

Setup

- Complex multidimensional data

data frame



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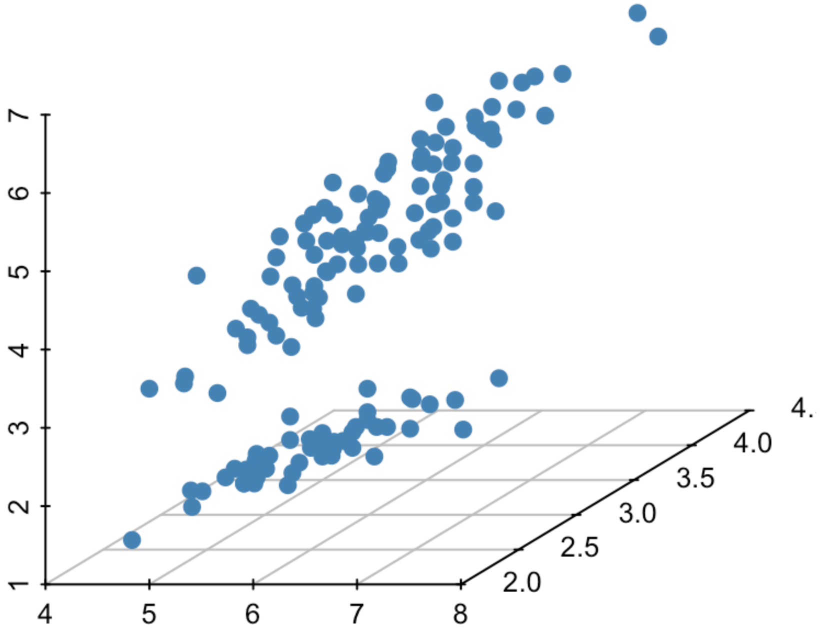
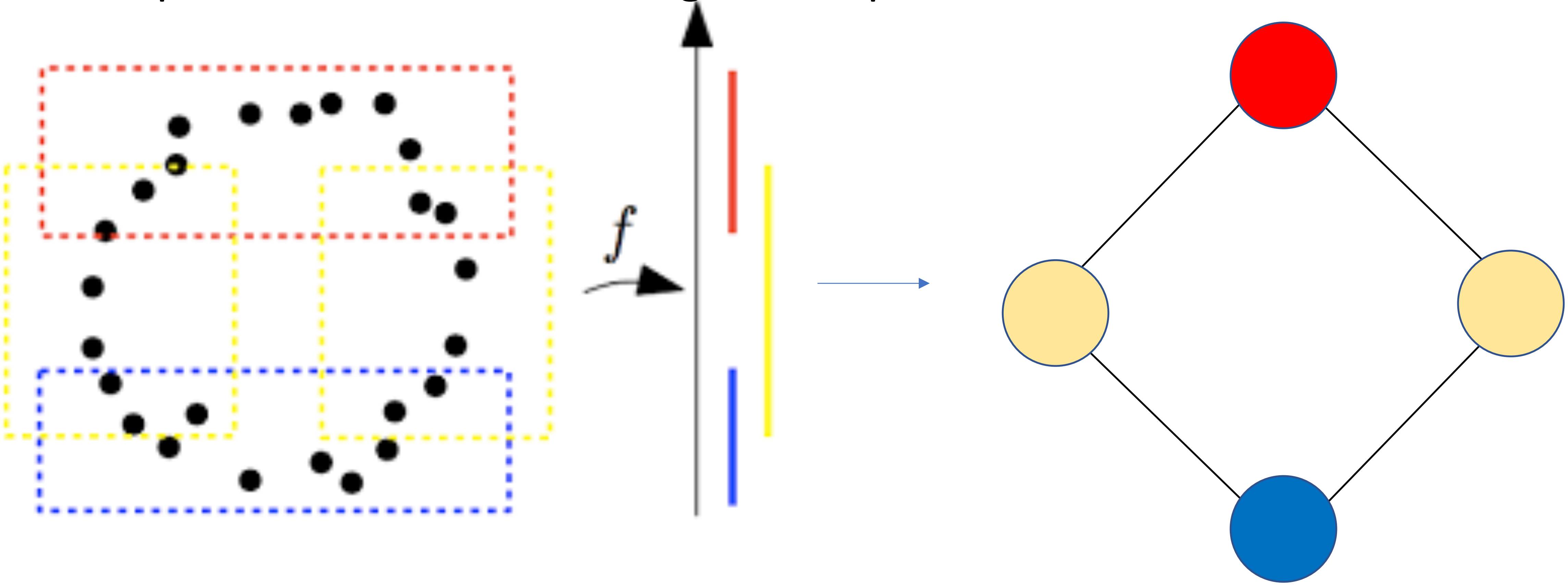
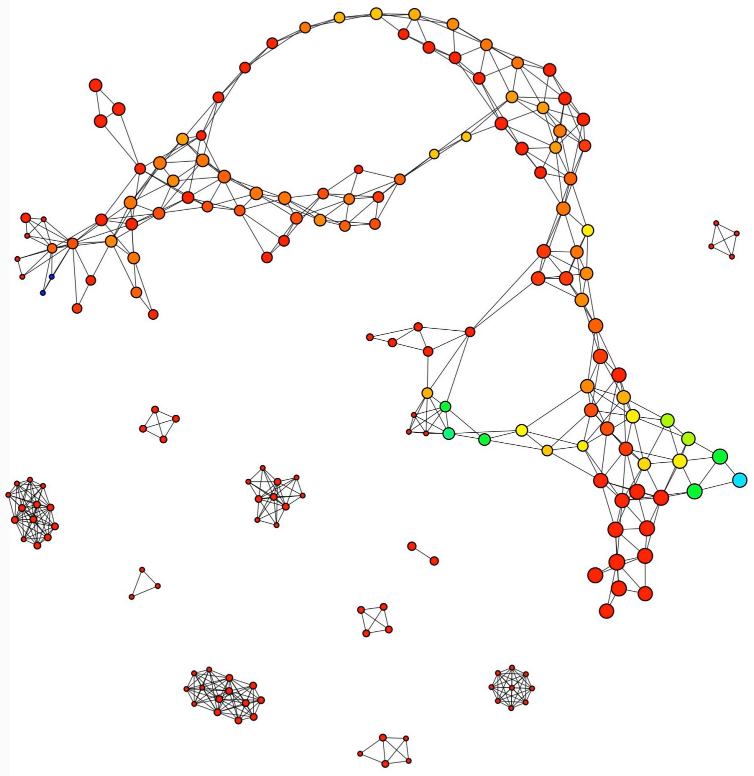


Mapper

- Visualising the ‘shape’ of data
- Output: network summarising the shape of the data



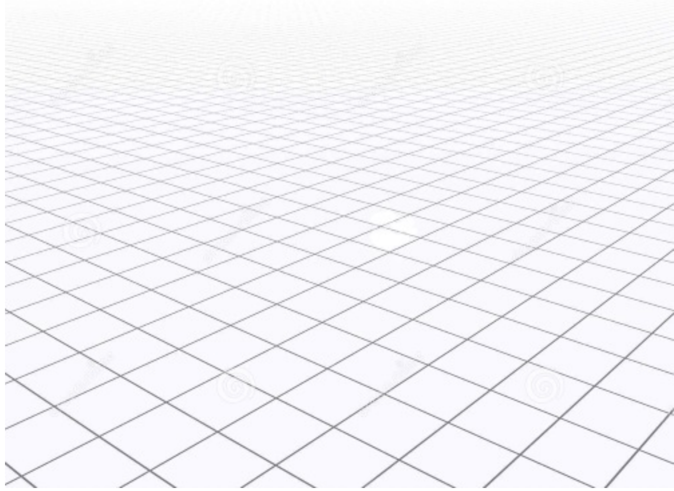
Mapper: algorithm



- Input:
  - Function of data *f (lens)*
  - Bin size
  - Bin percentage % overlap
- For each bin
  - Take the datapoints with get mapped into the bin by *f*
  - Perform clustering algorithm on such data
  - Create a node for each cluster
  - Link node to other existing nodes if they share at least a datapoint
- Output: network summarising the shape
- Geometric structure of visual output doesn't matter – connections only

Mapper: lens functions of data

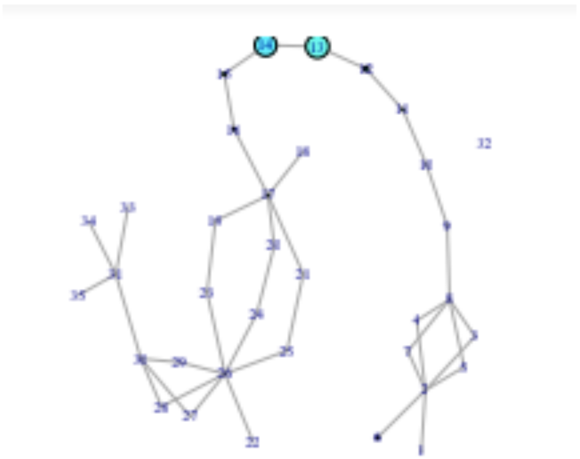
- Note: this algorithm works for non-scalar functions *f*!
  - Need to bin target space and perform algorithm
  - Curse of dimensionality
- There are many possible (and natural choices) for *f*
  - Projection onto an important variable
  - Distance to the center of mass
  - PCA
  - Autoencoder
  - …
- Intuitively, *f* must disentangle the data well



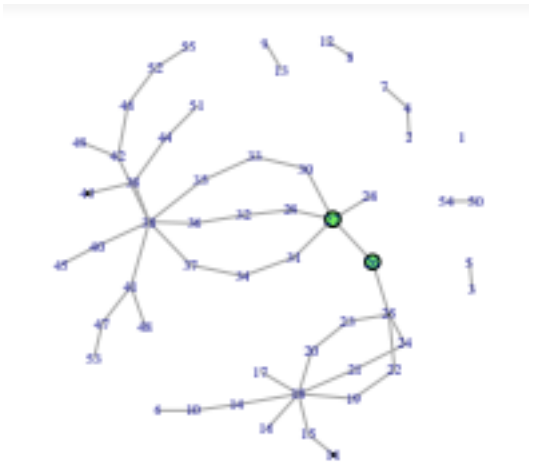
If target space is the plane

Mapper: example

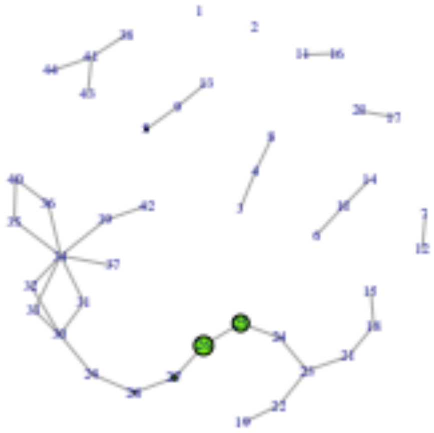
- Patterns in tree growth and meteorological data



Lens 1



Lens 2



Lens 3

- Conclusion: there is no network that rules them all!

Mapper: summary

+ Visualise data through different facets

+ Resistant to noise in data

- Computationally intensive
- Output may vary greatly with respect to input variables
  - One has to run in many different ways and interpret the globality of outputs

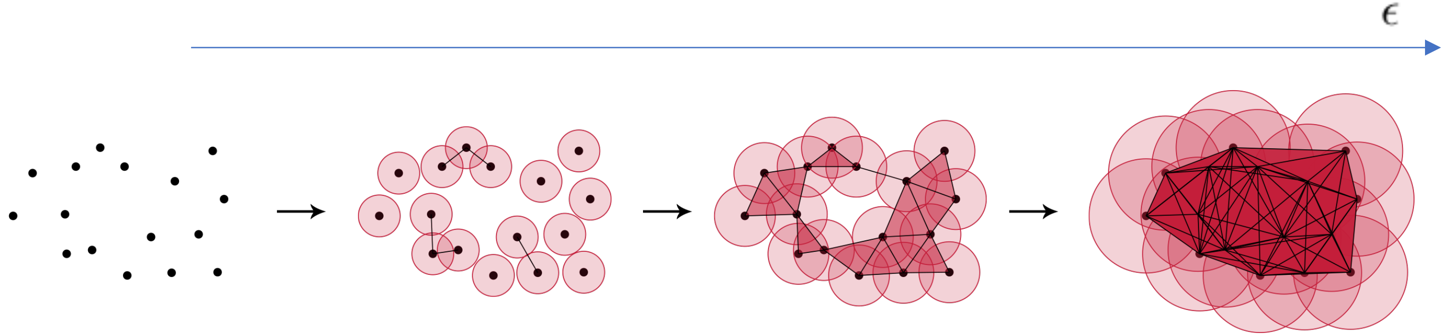
Python: see module Giotto

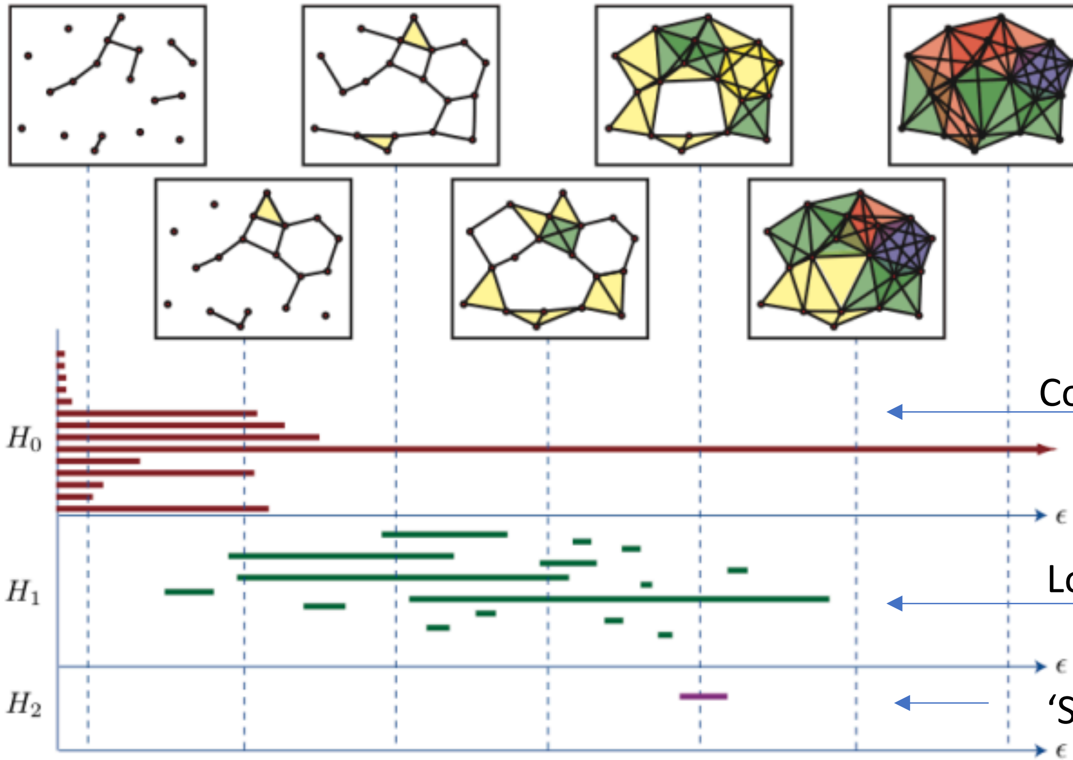
R: see package TDAmapper

Persistent homology

ϵ = diameter

Illustrations:





Persistence barcodes

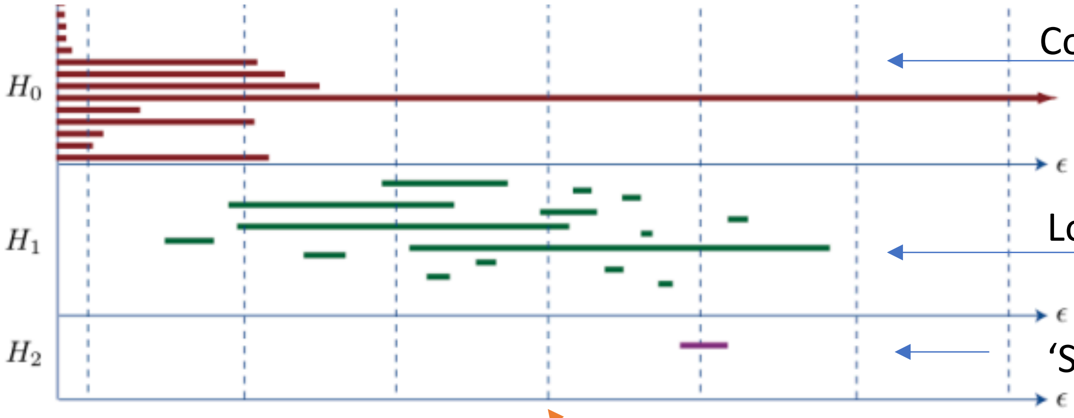
Connected components

Loops

‘Spheres’

Persistence diagram

Persistence barcodes



Connected components

Loops

‘Spheres’

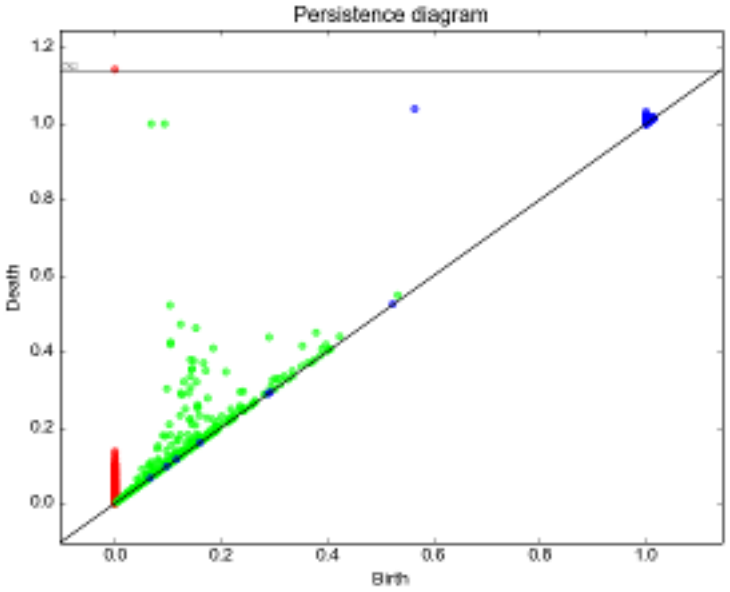
Persistence diagram:

Each dot is (birth, death)

Of a:

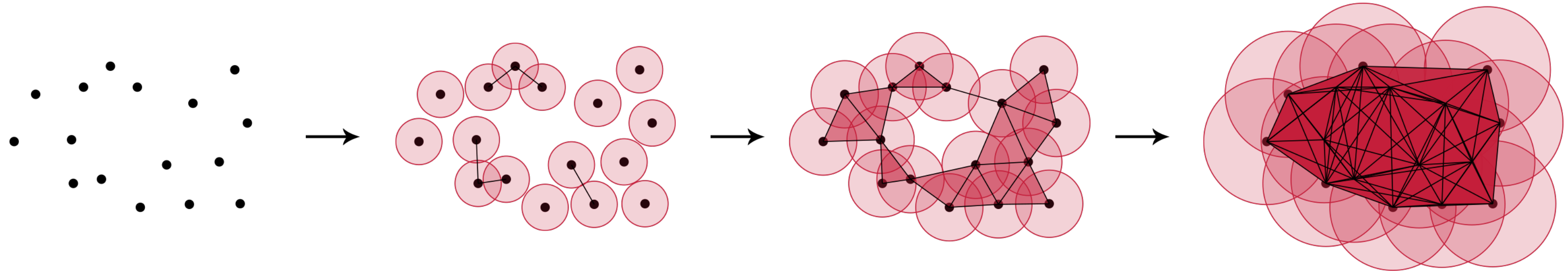
- Connected component
- Loop
- Sphere

Depending on colour



Beware these are not from the same dataset!

Persistence homology: algorithm



```
From $\epsilon$ = 0 to D
        Draw spheres around each datapoint of diameter $\epsilon$
        Link datapoints when spheres intersect
        Let a k-clique be a fully connected set of k+1 points that is not within a k+2 fully connected set of points
        For each k from 0 to N: record the number of k-cliques
Output: birth and death of each k-clique as a function of epsilon
```

Persistence homology: summary

+ Informative feature extraction

+ Easy to interpret

+ Useful exploratory data analysis technique

+ Resistant to noise in data

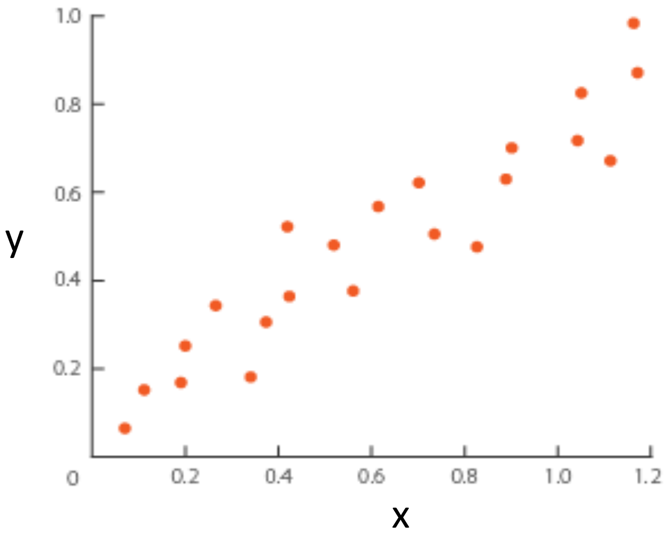
- Computationally intensive

Implementations: see Python module Giotto

Toy examples: predicting y from x

- Pearson corr. ≈1

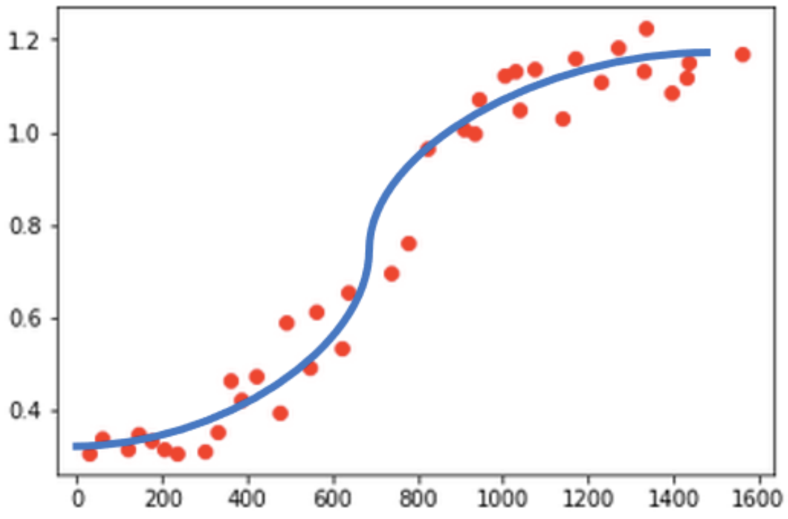
-> Linear regression



- Pearson corr. ≪1
- Spearman corr. ≈1

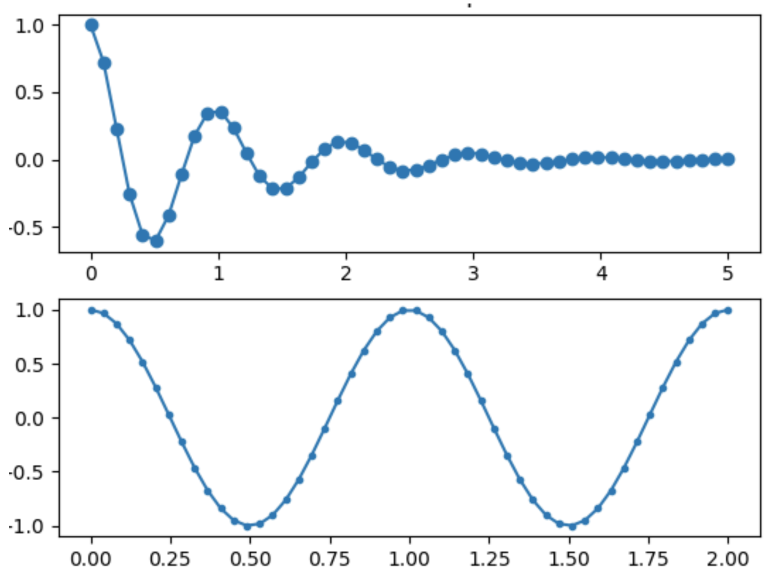
-> Non-linear regression

e.g., logistic regression

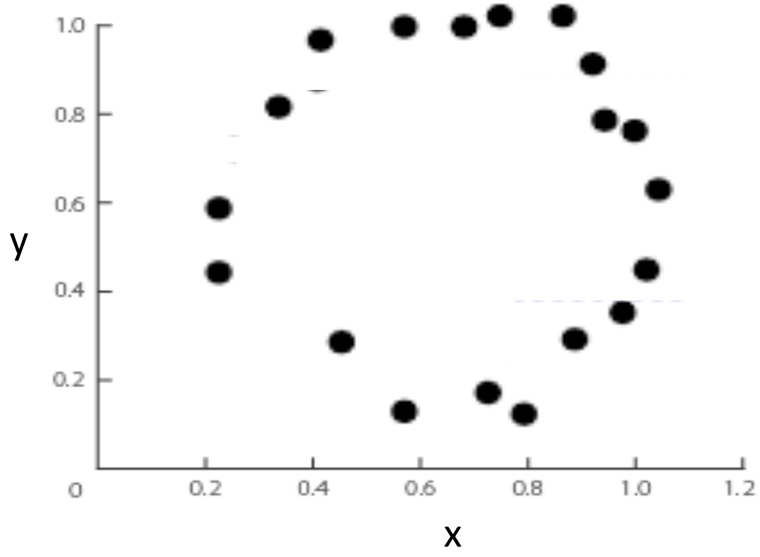


- Pearson corr. ≪1
- Spearman corr. ≪1
- PH detects no topological features

-> Neural network or non-parametric regression regression techniques



Toy examples: predicting y from x



- Pearson corr. ≈ 0
- Spearman corr. ≈ 0
- PH detects a loop

-> No functional relationship x -> y

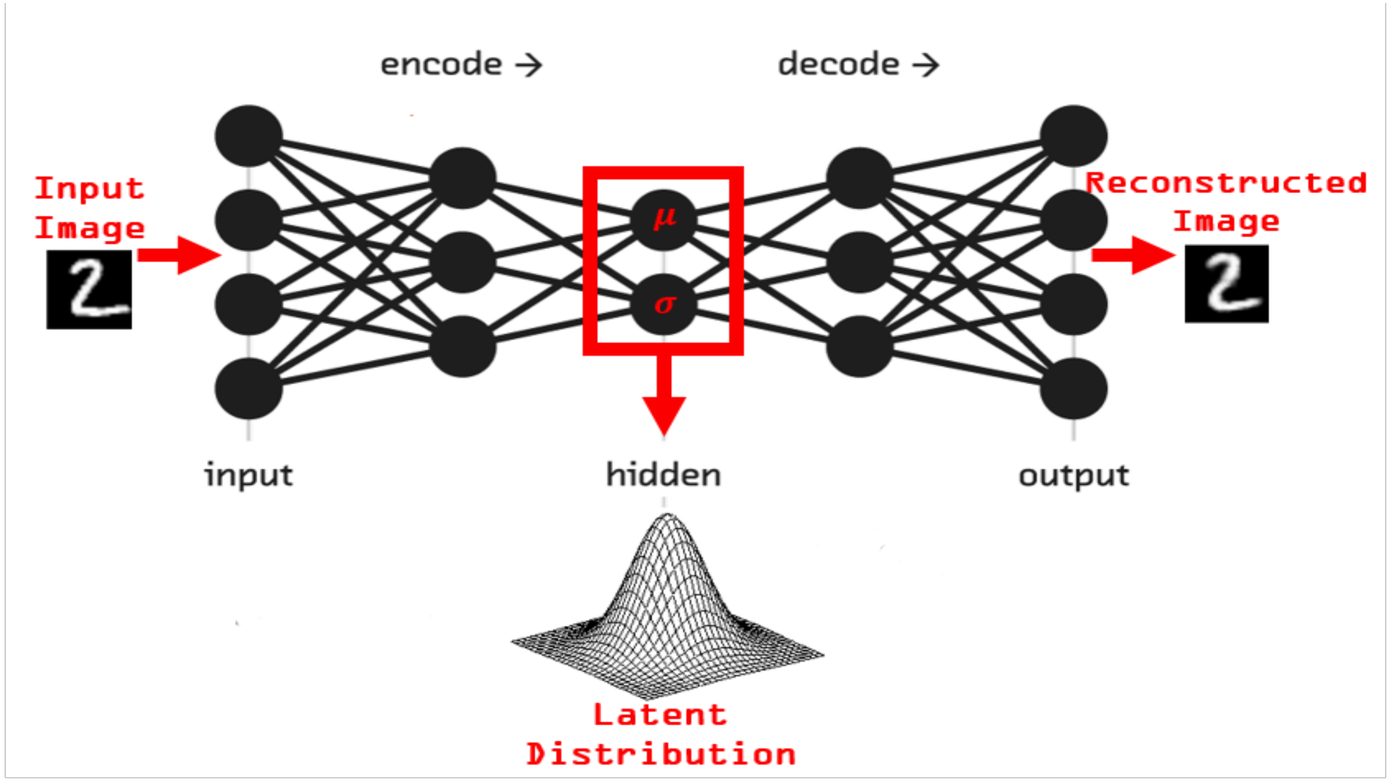
- Neural networks and regression techniques **will fail**
- Find what causes y to exhibit two different behaviours with respect to x
- Once the cause found, add it to the data set, and return to the cases beforehand

The intrinsic dimension of data

“You only truly understand some data, when you can capture the hidden causes that generated it, and generate the data yourself”.

VAE intuition

VAE Motto: “An autoencoder, which does not overfit!”

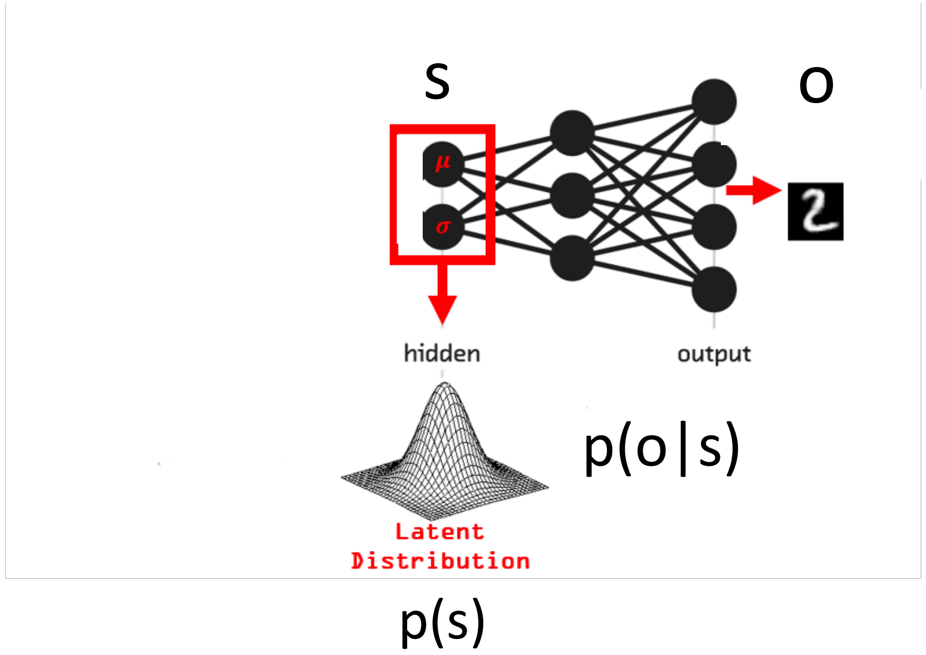


Compresses each datapoint onto a Gaussian distribution

VAE intuition

- Build probability distribution over ‘hidden’ states and how these give rise to outcomes:

$$p(o|s)p(s)$$



- This allows to:
  - Create new data by sampling from *p(s)*
  - Compressing data via Bayes rule:

$$p(s|o) = \frac{p(o|s)p(s)}{p(o)}$$

VAE intuition

- There are ‘few’ important variables in observable data *o*
- Let us call these ‘hidden’ variables. E.g.,
  - Orientation, depth, colour.
- Want to determine what these hidden states *s* are
- More generally, want to build a good model of the data

$$p(o|s)p(s)$$

A probability distribution over ‘hidden’ states and how these give rise to outcomes.

Model evidence

The best model maximises model evidence *p(o)*

$$p(o) = \int p(o \mid s) p(s) \, ds$$

Problems:

- Model evidence is intractable to compute
- This means that we can’t compress our data via

$$p(s|o) = \frac{p(o|s)p(s)}{p(o)}$$

*very important in advanced Bayesian machine learning

Workaround: Variational Bayes

The KL divergence measures the discrepancy between probability distributions.

$$0 \leq \mathrm{KL}(q(s)\,||\,p(s\,|\,o)) := \int_S q(s)\,\ln\frac{q(s)}{p(s\,|\,o)}\,ds$$

q= arbitrary distribution

$$= \int_S q(s)\,\ln\frac{q(s)p(o)}{p(o,s)}ds = \underbrace{\int_S q(s)\,\ln\frac{q(s)}{p(o,s)}ds}_{\text{-ELBO(q)}} + \underset{= \ln p(o)}{\int_S q(s)\,\cancel{\ln}\,p(o)\,ds}$$

Compression ⇔ Minimising KL ⇔ maximising ELBO

Optimal *q* = compressed representation

Maximising ELBO => good model

ELBO(q) $\leq$ ln *p(o)* (Jensen's inequality)

Moral of the story:

By maximising ELBO(q) = $\int_S q(s)\ \ln \frac{q(s)}{p(o,s)} ds$

- one obtains a good model of the data that captures the hidden dimensions
- efficient data compression.

Since Model evidence = Model Accuracy – Complexity => no-overfitting!

VAE Caveats

One fixes:

p(s) standard gaussian

p(o|s), q(s) gaussians parameterised by a neural network

This means that we optimise ELBO wrt the network parameters!

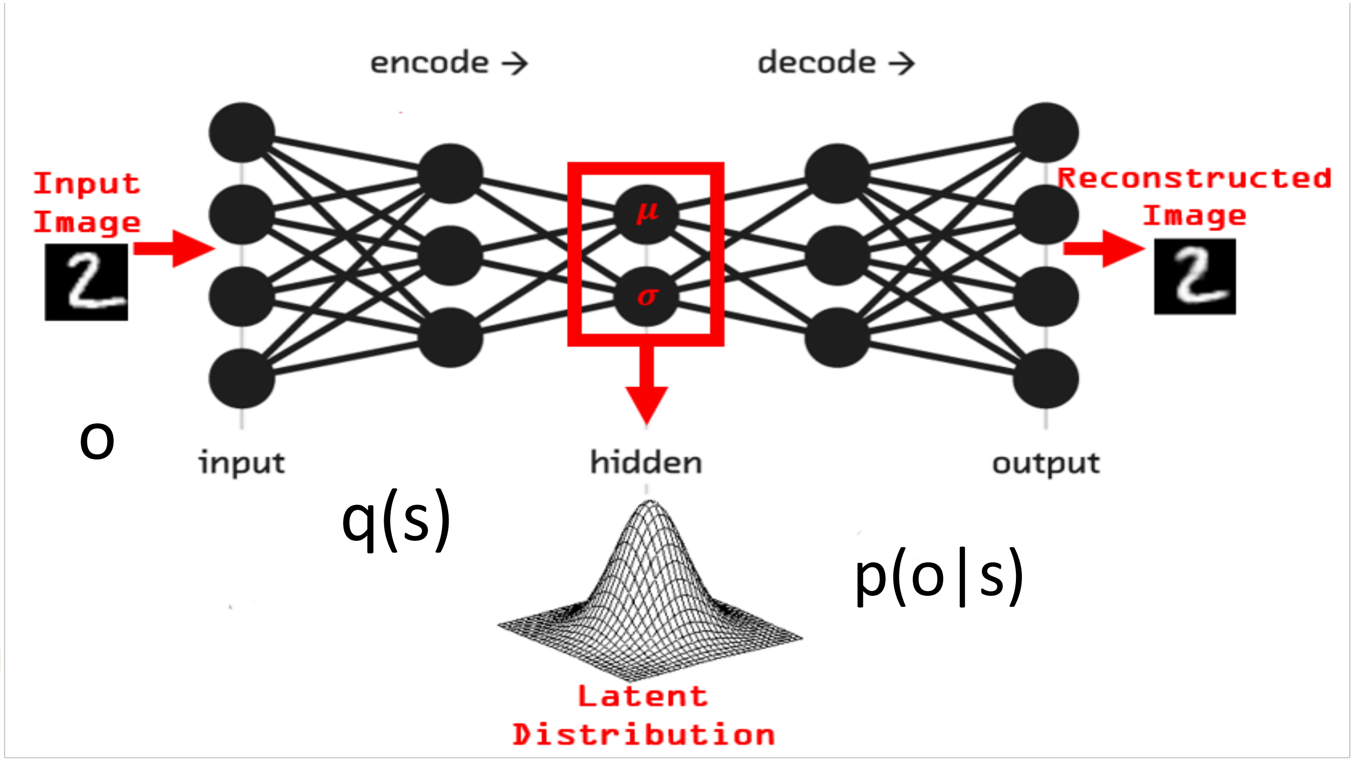
ELBO(q) = $$\int_S q(s) \ \ln \frac{q(s)}{p(o,s)} ds$$

Caveat: with these choices, ELBO is also intractable to compute.

One uses the ‘reparameterization trick’ to approximate it

… et voilà!

Variational autoencoders



+ Data compression
+ Data denoising
+ Informative feature extraction
+ Does not overfit
+ Data generation

- Usually latent representation is not useful for visualisation
- Technically more involved

Thank you for your attention