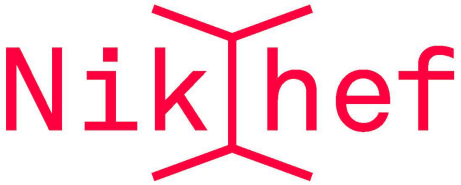

Machine Learning for Physics and Astronomy

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VU Amsterdam & Theory group, Nikhef

Natuur- en Sterrenkunde BSc (Joint Degree), Honours Track

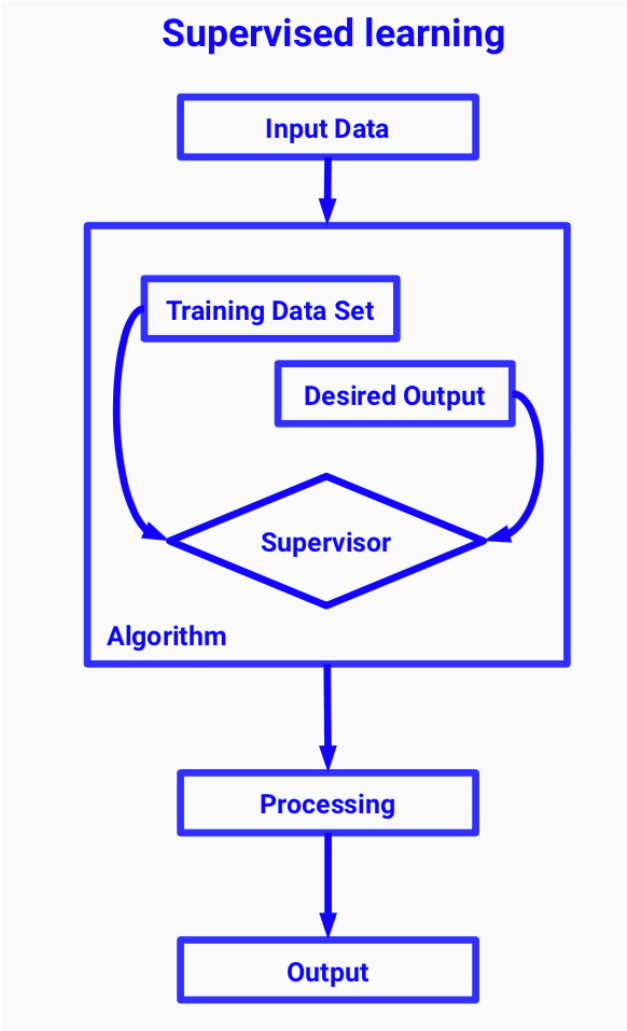
Lecture 3, 14/09/2020

Today's lecture

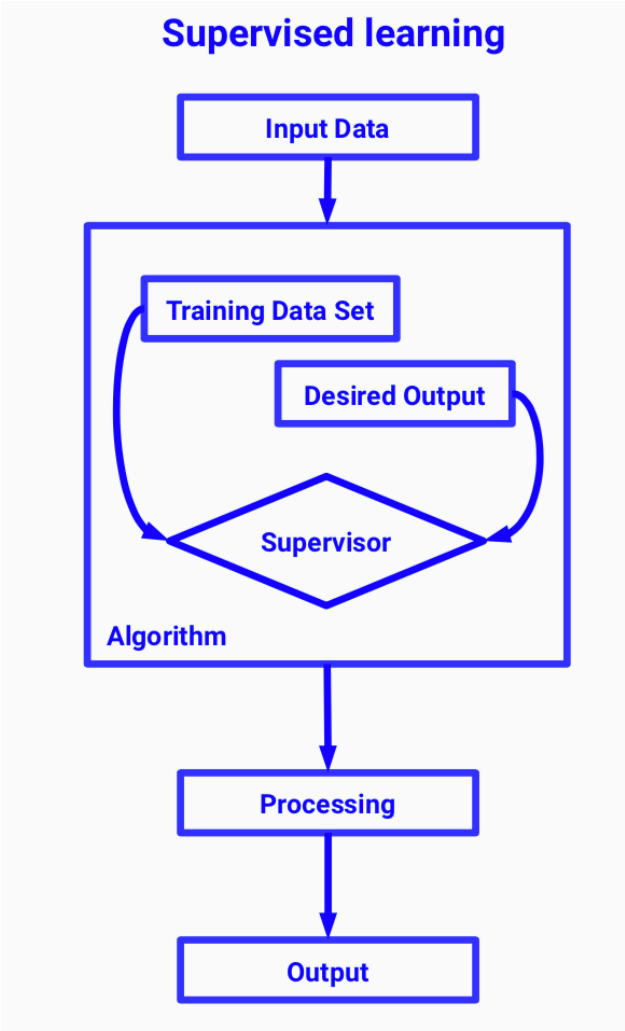
- Unsupervised Learning & Clustering
- Data visualisation and dimensional reduction
- Ensemble methods and Bootstrapping
- Random Forests and Decision Trees

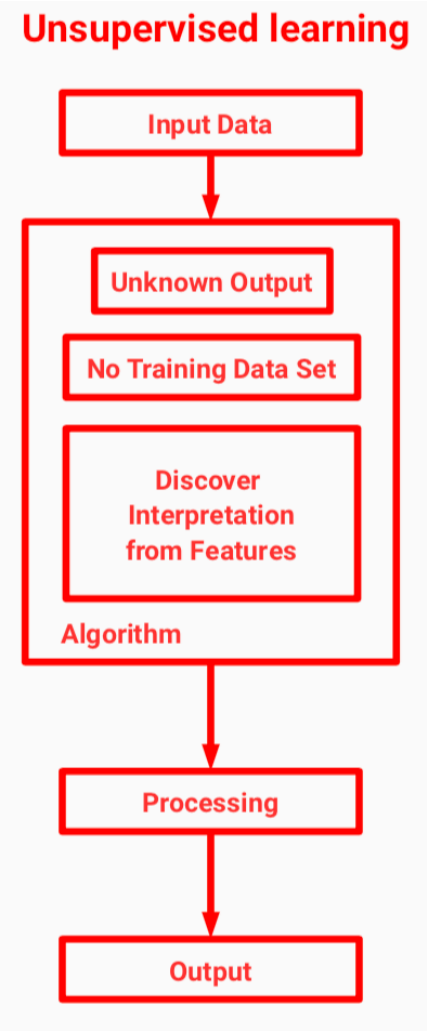
Unsupervised Learning

Supervised vs Unsupervised Learning

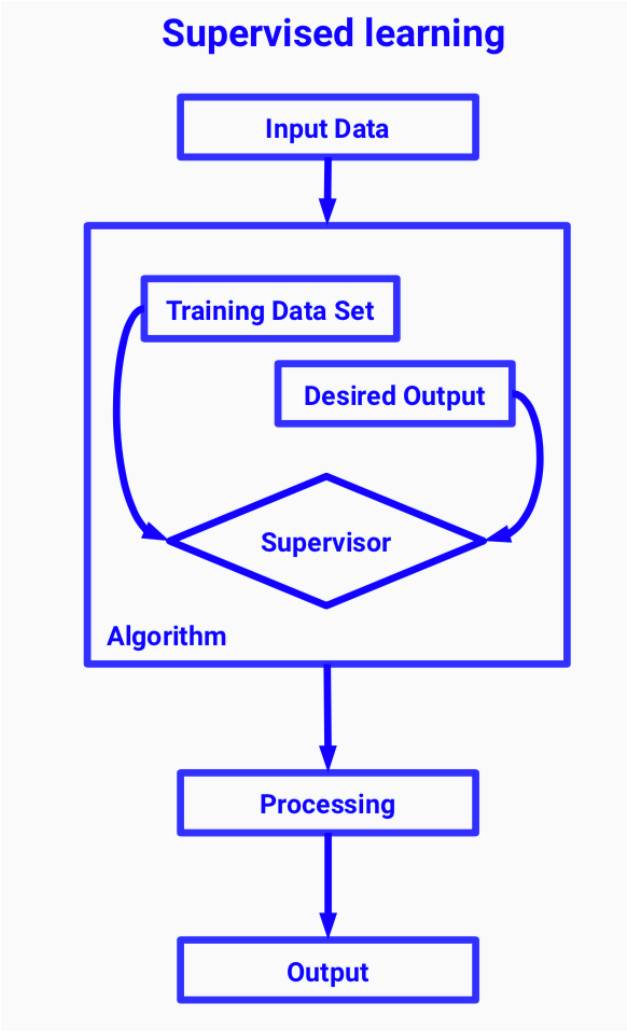


Supervised vs Unsupervised Learning



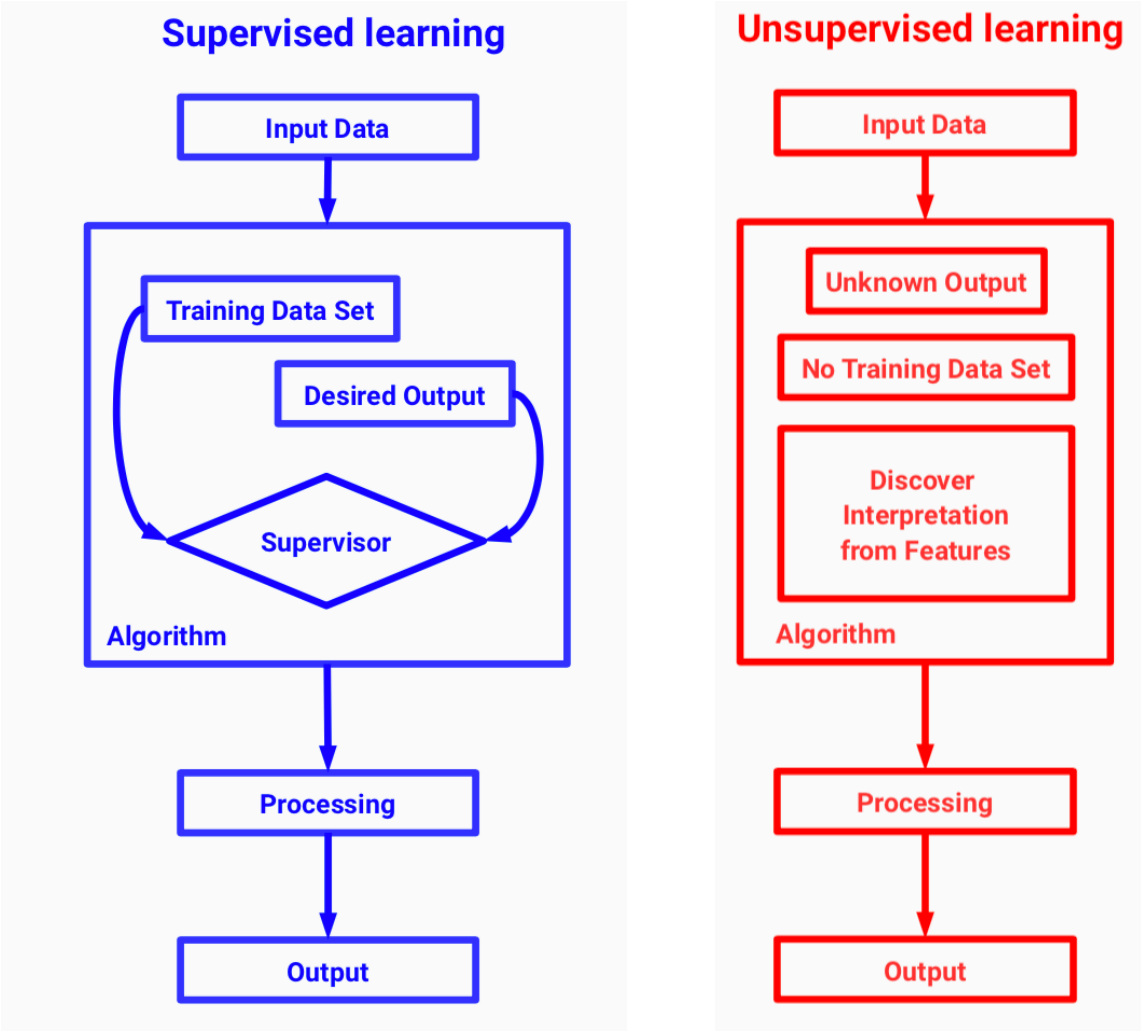


Supervised vs Unsupervised Learning



Supervised Learning: find a **model** that reproduces the underlying law of a set of **labelled input/output patterns**

Supervised vs Unsupervised Learning



Unsupervised Learning: there are no labels and our **aim is to identify underlying structures and connections** present in the data

Clustering

In ML context, **unsupervised learning** is concerned with discovering underlying structures in **unlabelled data**

an important example of unsupervised learning is **clustering:** the aim is to group unlabelled data into clusters using some **distance or similarity measure**

let us illustrate these ideas with ***K*-means clustering**

$$\{\boldsymbol{x}_n\}_{n=1}^{N} \qquad \boldsymbol{x}_n = (x_{n,1}, x_{n,2}, \ldots, x_{n,p})$$

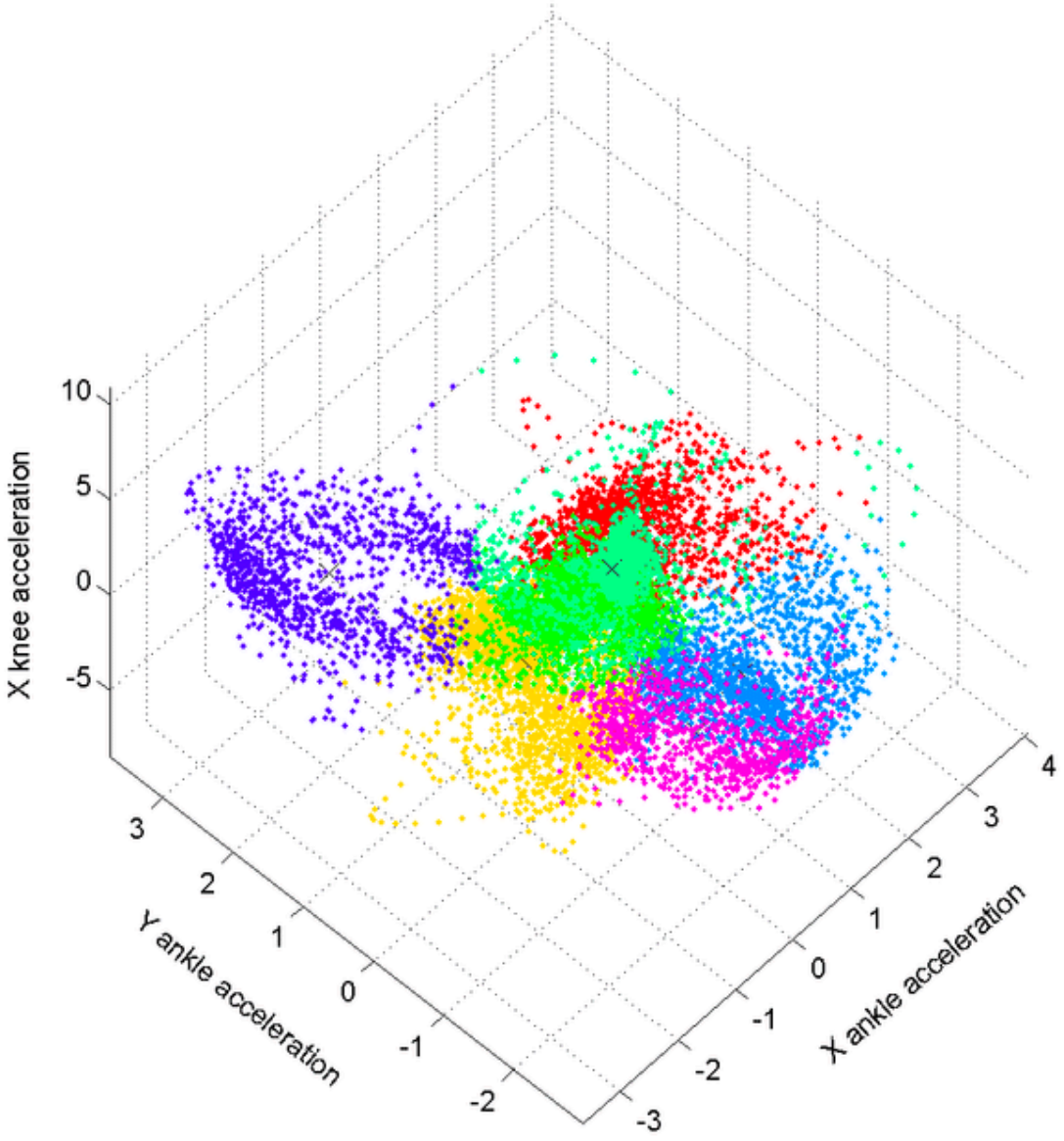
unlabelled dataset: N points with p features each

$$\{\boldsymbol{\mu}_k\}_{k=1}^{K} \qquad \boldsymbol{\mu}_k = (\mu_{k,1}, \mu_{k,2}, \ldots, \mu_{k,p})$$

***cluster means**: K clusters with p features each*

the intuitive idea is that the cluster means represent the **main features of each cluster**, to which the data points will be assigned in the clustering procedure

Unsupervised Learning



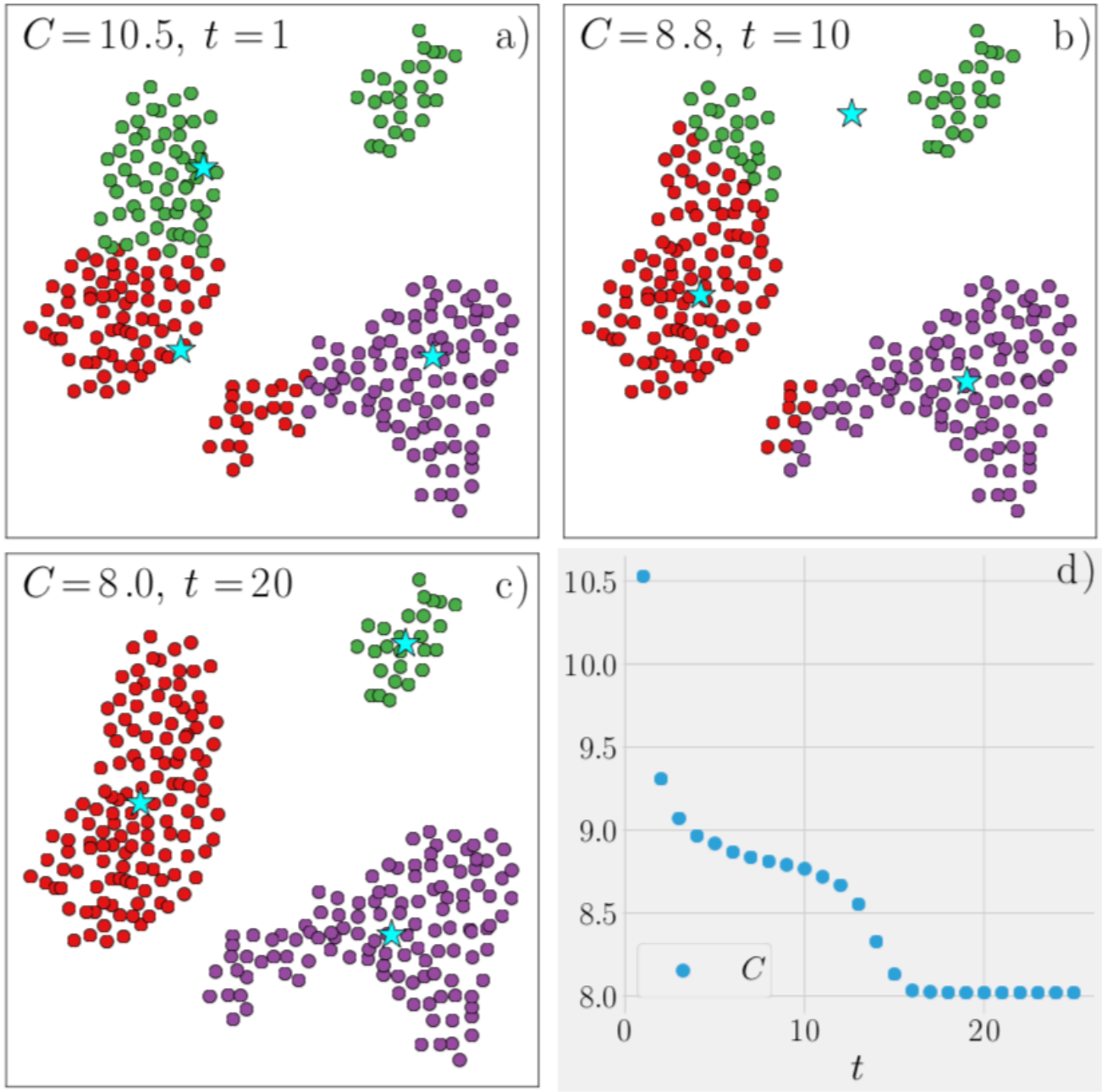
nb color here for visualisation, but not this info not available in real applications!

how many ``**groups of samples"** do we have have in our dataset?

Clustering

2D example of clustering: each colour represents a cluster, with stars indicating their **centers**

how is this clustering achieved **in practice?**



Clustering

in *K*-means clustering, the **cluster means** and the **data point assignments** are determined from the minimisation of a cost function:

$$C\left(\boldsymbol{x};\boldsymbol{\mu}\right) = \sum_{n=1}^{N}\sum_{k=1}^{K} r_{nk}\left(\boldsymbol{x}_n - \boldsymbol{\mu}_k\right)^2$$

other distances possible: the user needs to define what ``closeness" means!

binary assignment variable

Euclidean distance between n-th data point and k-th cluster centre

$r_{nk} = 1$ ⟶ *the n-th point is assigned to the k-th cluster*

$r_{nk} = 0$ ⟶ *the n-th point is not assigned to the k-th cluster*

furthermore since **clustering is exclusive** one needs to impose: $\sum_{k=1}^{K} r_{nk} = 1 \quad \forall n$

one sees that *K*-means clustering aims to **minimise the variance within each cluster**

Clustering

Let's describe an algorithm that implements *K*-means clustering by minimising the cost function

$$C\left(\boldsymbol{x};\boldsymbol{\mu}\right)=\sum_{n=1}^{N}\sum_{k=1}^{K}r_{nk}\left(\boldsymbol{x}_n-\boldsymbol{\mu}_k\right)^2$$

this algorithm alternates iteratively between two main steps:

- ***(1) Expectation***: starting from set of cluster assignments ***{r_{nk}}*** minimise *C* wrt cluster means

$$\frac{\partial}{\partial\boldsymbol{\mu}_k}C\left(\boldsymbol{x};\boldsymbol{\mu}\right)=0\quad\rightarrow\quad\boldsymbol{\mu}_k=\frac{1}{N_k}\sum_{n=1}^{N}r_{nk}\boldsymbol{x}_n\qquad N_k=\sum_{n=1}^{N}r_{nk}$$

number of points in k-th cluster

- ***(2) Maximization***: given the *K* cluster centers, the assignments ***{r_{nk}}*** should minimise *C*. This can be achieved by assigning each data point to its closest cluster-mean

$$r_{nk}=1\quad\text{if}\quad k=\arg\min_{k'}(\boldsymbol{x}_n-\boldsymbol{\mu}_{k'})$$
$$r_{nk}=0\quad\text{if}\quad k\neq\arg\min_{k'}(\boldsymbol{x}_n-\boldsymbol{\mu}_{k'})$$

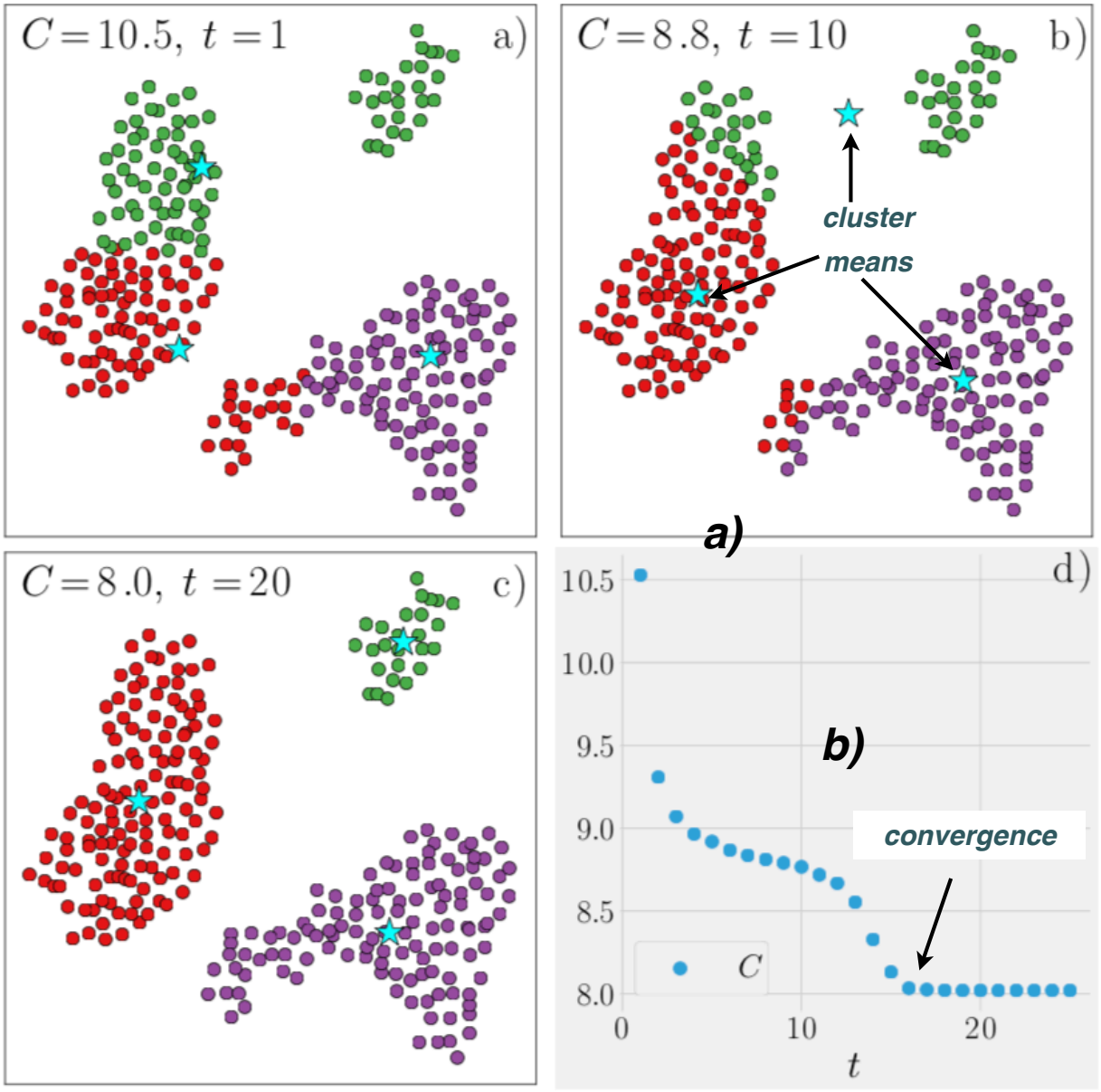
iterate until convergence achieved!

note that here GD not required, optimisation is semi-analytical

Clustering

these two steps are iterated until some **convergence criterion** is achieved, *e.g.* when the change in the cost function between two iterations is below some threshold

each colour: different cluster

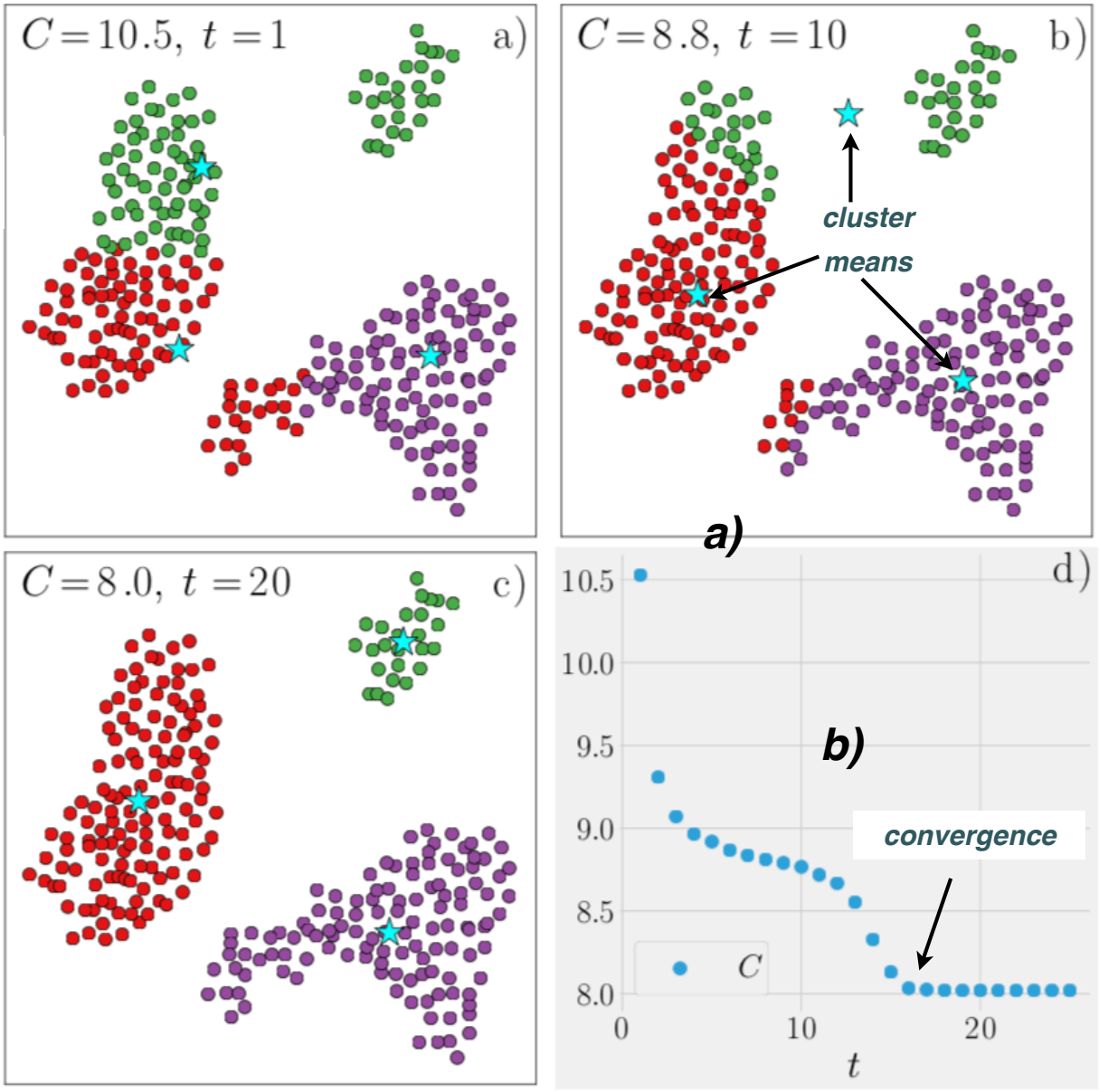


here overfitting not possible: there exists a unique assignment that minimises the cost function

Clustering

these two steps are iterated until some **convergence criterion** is achieved, *e.g.* when the change in the cost function between two iterations is below some threshold

each colour: different cluster

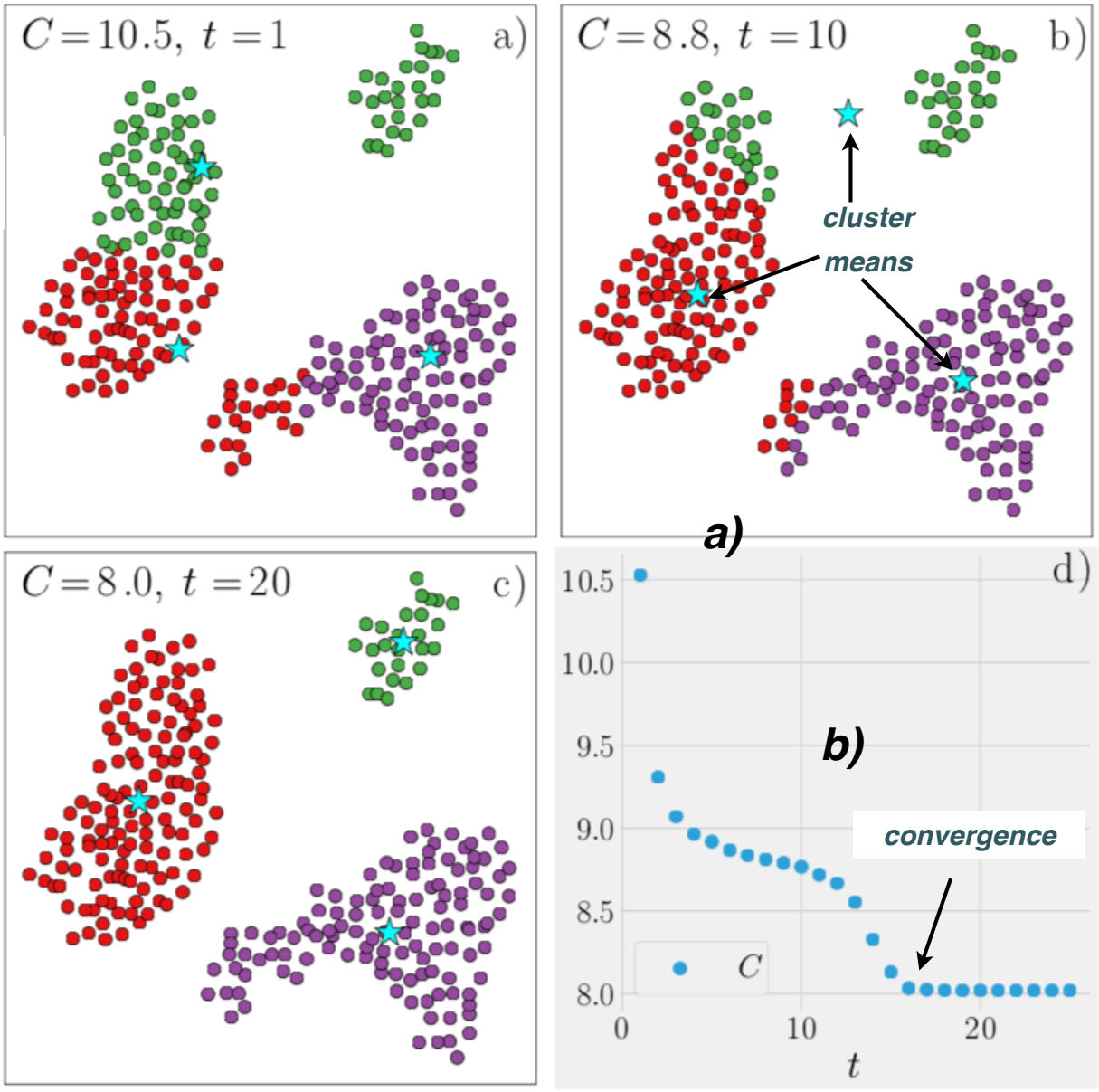


what is the underlying assumption in K-means clustering? And when it would not be justified?

Clustering

these two steps are iterated until some **convergence criterion** is achieved, *e.g.* when the change in the cost function between two iterations is below some threshold

each colour: different cluster



*K-means clustering can lead to spurious results since the **underlying assumption** is that the latent model has uniform variances*

fails if the underlying clusters have different variances!

Hierarchical clustering

- Another approach to clustering is based on **agglomerative methods**, where one starts from small clusters which are progressively **merged into bigger clusters**

- This hierarchical structure provides information on the relations between clusters and the **subcomponents of individual clusters**

- As before, we need to specify a **distance**, this time between two clusters *X, Y*

$$d(X, Y) \in \mathscr{R}$$

- At each iteration, the two clusters closer to each other (quantified by *d*) are *merged*

the **agglomerative cluster algorithm** works as follows:

- ***(1)*** Assign **each data point to be its own cluster**

- ***(2)*** Given the resulting set of K clusters, find the closest pair

$$(X_i, X_j) \quad \text{such that} \quad (i, j) = \arg\min_{i'j'} d(X_{i'}, X_{j'})$$

- ***(3)*** Merge the pair into a single cluster. Iterate ***(2)*** and ***(3)*** until a single cluster remains

Hierarchical clustering

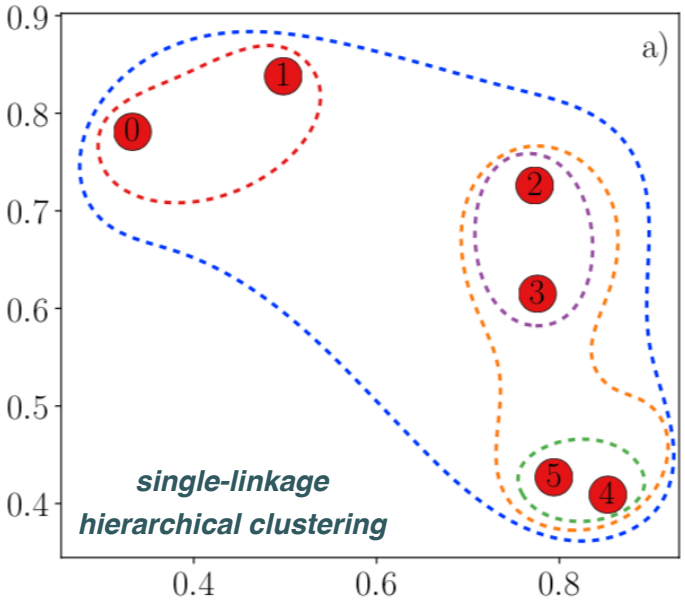
Clearly the results of hierarchical clustering depend on the **choice of distance**

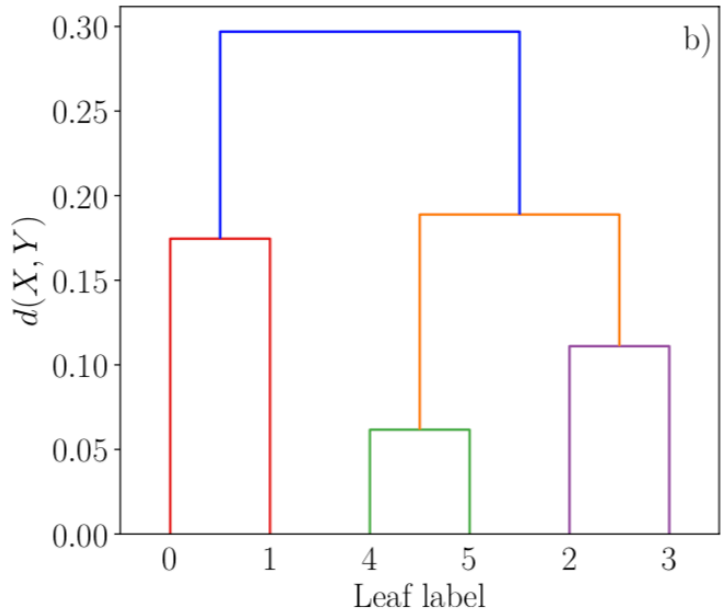
distance between clusters

single linkage → $d(X_i, X_j) = \min_{\boldsymbol{x}_i \in X_i, \boldsymbol{x}_j \in X_j} ||\boldsymbol{x}_i - \boldsymbol{x}_j||_2$

complete linkage → $d(X_i, X_j) = \max_{\boldsymbol{x}_i \in X_i, \boldsymbol{x}_j \in X_j} ||\boldsymbol{x}_i - \boldsymbol{x}_j||_2$

Euclidean distance





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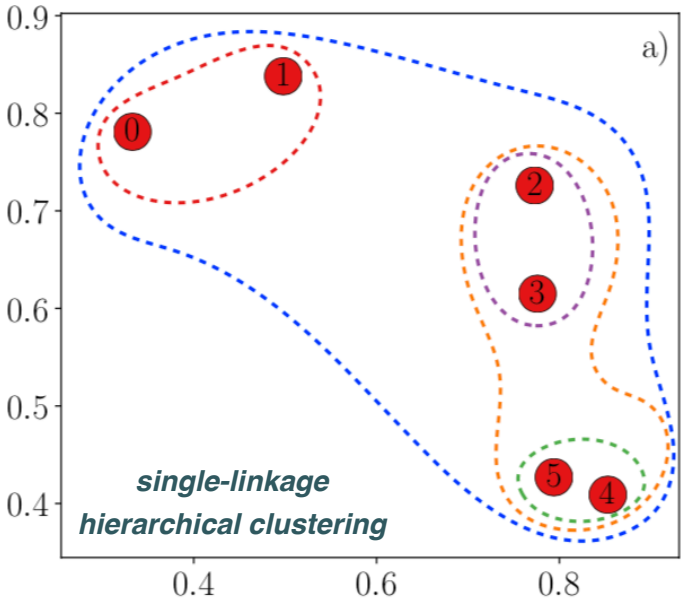
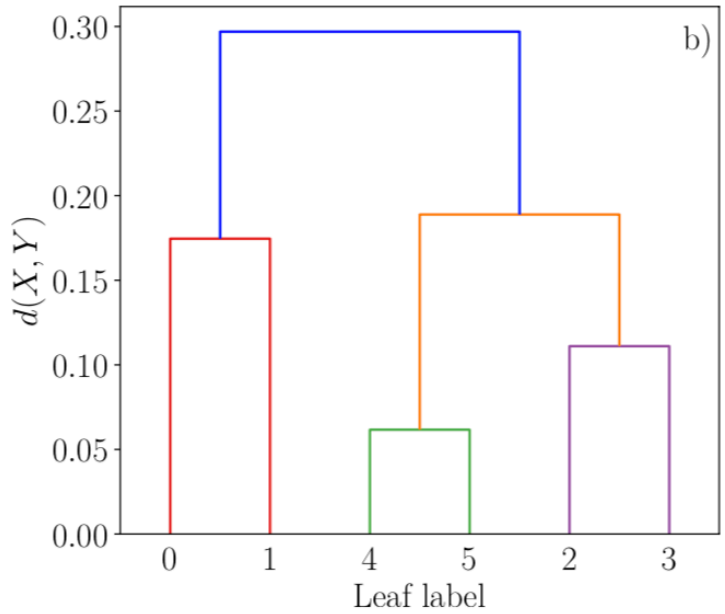




hierarchical clustering methods do not scale well for large *N*, so they are typically **combined with *K*-means clustering** in the initial steps to define small clusters

Clustering and Latent variables

A central concept in **Unsupervised Learning** is that of a **latent or hidden variable**: not directly observable, but still they influence visible structure of data

e.g. in clustering, a latent variable is the cluster identity of each datapoint

One can think of clustering as an algorithm to learn **the most probable value of a latent variable**

a common feature of all Unsupervised Learning algorithms is the need for assumptions about the underlying probability distribution of the data: the **generative model**

e.g. in K-means clustering, we assume that the points of each cluster are generated Gaussianly with respect to its mean (center)

$$C\left(\boldsymbol{x};\boldsymbol{\mu}\right) = \sum_{n=1}^{N}\sum_{k=1}^{K} r_{nk}\left(\boldsymbol{x}_n - \boldsymbol{\mu}_k\right)^2$$

different **generative models** lead to different types of clustering algorithms

Gaussian Mixture Models

in **Gaussian Mixture Models (GMM)**, a generative model used in clustering applications, points are drawn from *K* gaussians with different means and covariances

$$\mathcal{N}\left(\boldsymbol{x};\boldsymbol{\mu},\boldsymbol{\Sigma}\right) \sim \exp\left[-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})\boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu})^{T}\right]$$

one of the K gaussians

The probability of generating a point ***x*** in a GMM is given by

$$p(\boldsymbol{x}, \{\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k, \pi_k\}) = \sum_{k=1}^{K} \mathcal{N}\left(\boldsymbol{x};\boldsymbol{\mu}_k,\boldsymbol{\Sigma}_k\right)\pi_k$$

probability of drawing a point from mixture k

$$\boldsymbol{\theta} = \{\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k, \pi_k\}$$

GMM parameters

the probability that a data point ***x*** is associated to the *k-th* cluster is

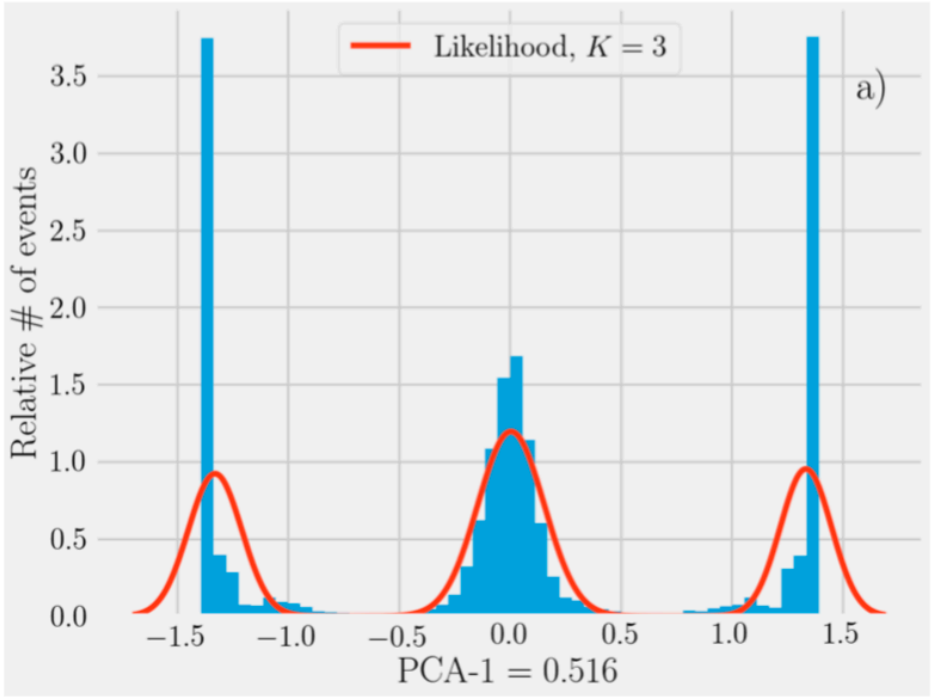
$$\gamma_k(\boldsymbol{x}) \sim \mathcal{N}\left(\boldsymbol{x}\,|\,\boldsymbol{\mu}_k,\boldsymbol{\Sigma}_k\right)\pi_k$$

model parameters found my maximising likelihood using SGD

$$\hat{\boldsymbol{\theta}} = \arg\max_{\theta} \log p(\boldsymbol{X}\,|\,\boldsymbol{\theta})$$

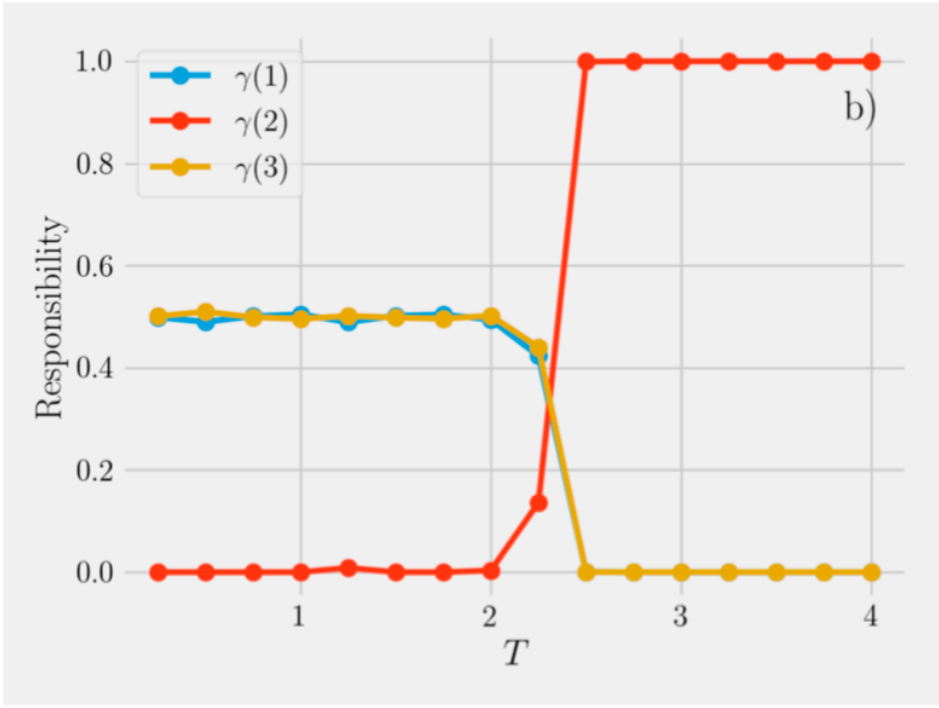
Gaussian Mixture Models

Ising dataset fitted to 3-component GGM



1st principal component (magnetisation)

Probability of being on each phase



probability coincide at critical point

recall that this model has been trained only on examples: **no knowledge of the underlying physical mechanisms** whatsoever

Dimensional Reduction & Data Visualisation

Dimensional reduction

ML problems often deal with samples of **very high dimensionality!**

Dimensional reduction

Efficient **data visualisation techniques** are essential to construct better models in ML applications eg by **identifying correlated, redundant, or irrelevant features**

Traditional data visualisation methods are not practical when the datasets involve a large number of features (such as images) and we need to project the data onto a lower-dimensional space, called the **latent space,** using **dimensional reduction**

A good data visualisation strategy is very useful to identify the most suitable strategy to approach a ML problem

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This is easier said that done: many pitfalls associated to **high-dimensionality datasets**

``the curse of dimensionality'

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- *High-dimensional data lives near the edge of the sample space*

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This is easier said that done: many pitfalls associated to **high-dimensionality datasets**

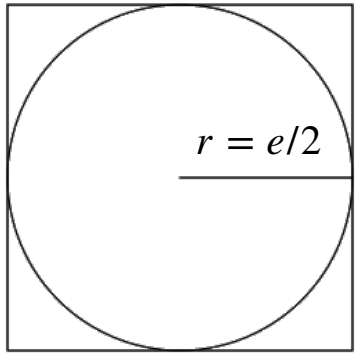
- *High-dimensional data lives near the edge of the sample space*

consider data distributed at random in a *D*-dimensional hypercube $C = [-e/2, e/2]^D$

consider a *D*-dimensional sphere *S* of radius *e/2* entered at origin

probability that random point from *C* is sampled inside the sphere *S* is

$$P\left(\boldsymbol{x}_i \in \mathcal{S}\right) \simeq \frac{\pi^{D/2}(e/2)^D/\Gamma(D/2+1)}{e^D} = \simeq \frac{\pi^{D/2}}{2^D D^D} \to 0$$



so most of the data lies close to the hypercube **edge**!

Dimensional reduction

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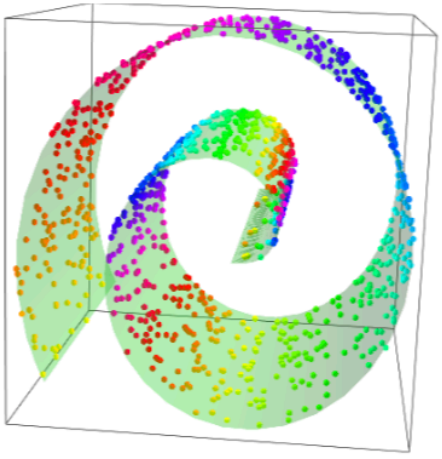
This is easier said that done: many pitfalls associated to high-dimensionality datasets

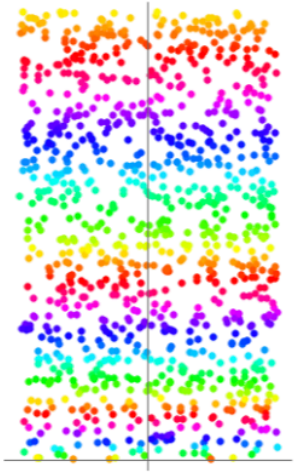
- *High-dimensional data lives near the edge of the sample space*
- *We need to conserve information on original pair-wise distances or similarities when transforming to the latent space*

the minimum number of parameters needed to capture the original patters is the **intrinsic dimensionally of the data**

a) ***original data space: 3D***



b) ***latent space: 2D***



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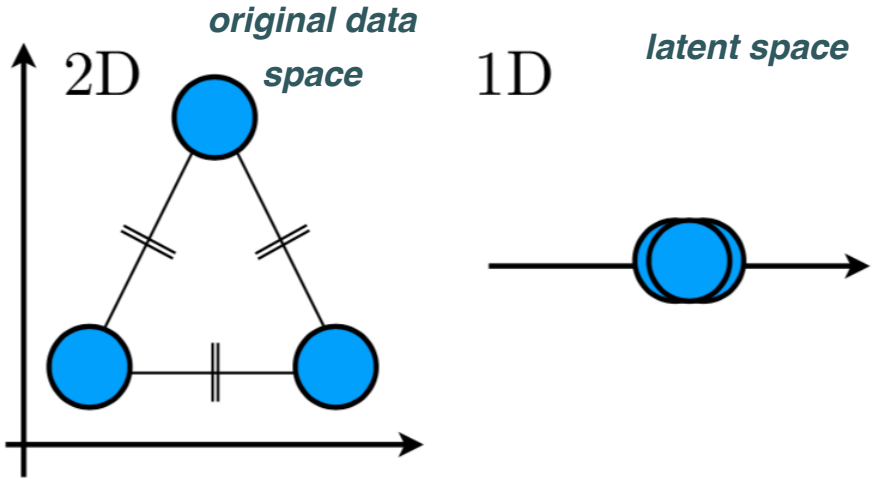
This is easier said that done: many pitfalls associated to high-dimensionality datasets

- *High-dimensional data lives near the edge of the sample space*
- *We need to conserve information on original pair-wise distances or similarities when transforming to the latent space*
- *Dimensional reduction cannot be such to destroy info on original patterns in the data*

``the crowding problem"



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there are two main classes of **dimensional reduction methods**

linear methods, based on linear transformations

e.g. Principal Component Analysis (PCA)

non-linear methods, based on non-linear transformations

e.g. Stochastic Neighbour Embedding (SNE)

Principal Component Analysis

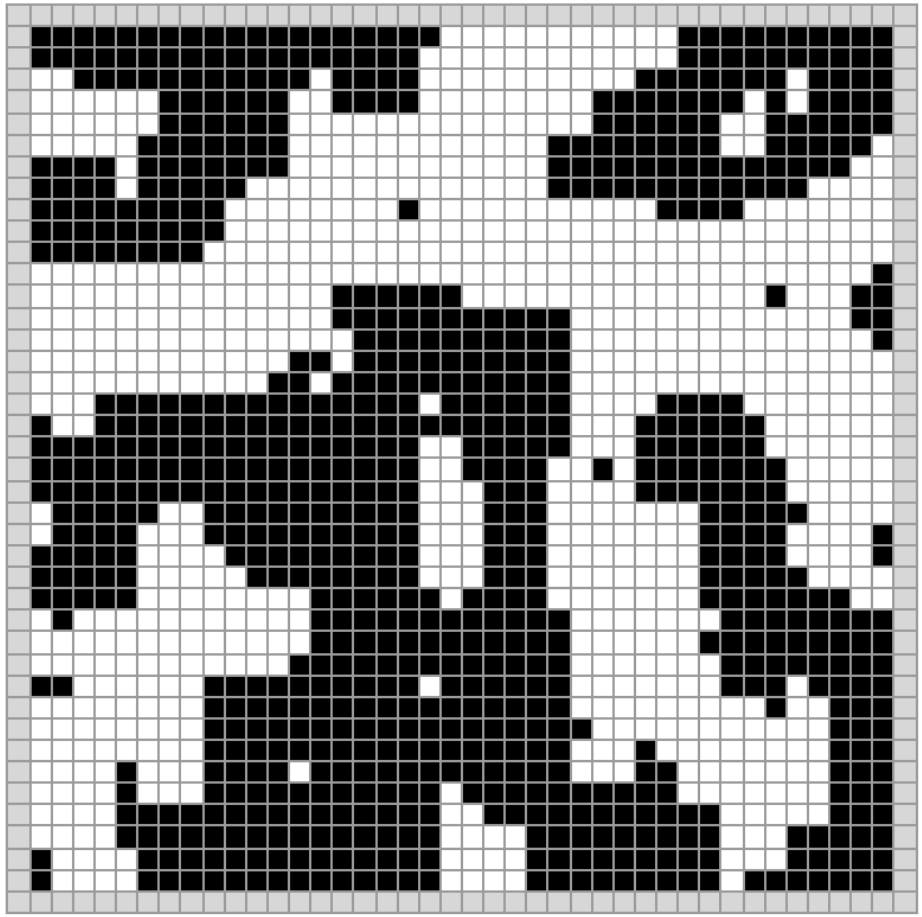
PCA projections often capture the **large-scale structure** of high-dimensional datasets

consider for example the **Ising Model in 2D** with 40 spins: 1600-dimensional space

can we **measure ``order''** with few parameters?

disordered (random) phase

ordered phase



https://demonstrations.wolfram.com/The2DIsingModelMonteCarloSimulationUsingTheMetropolisAlgorit/

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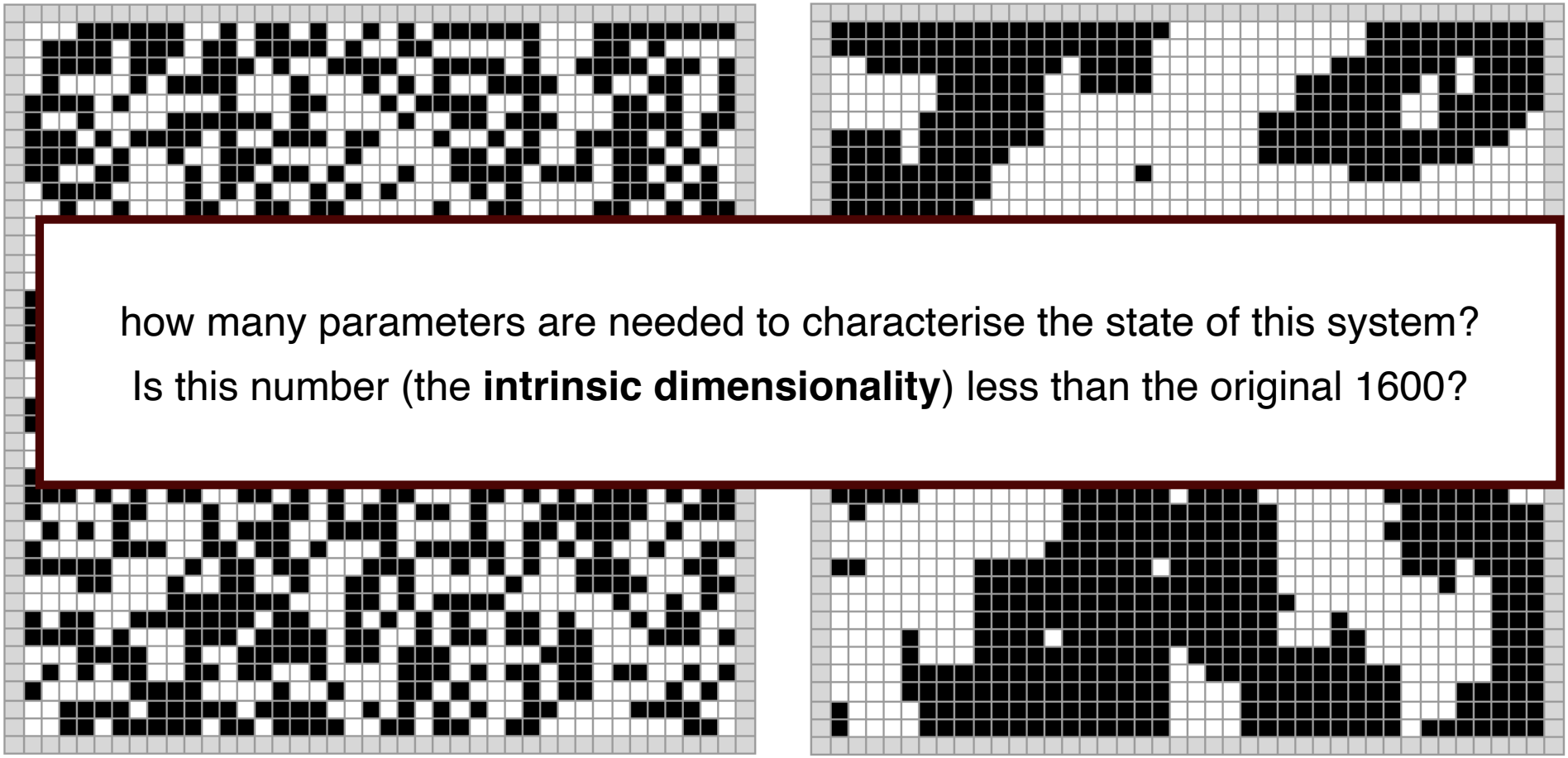

how many parameters are needed to characterise the state of this system?

Is this number (the **intrinsic dimensionality**) less than the original 1600?

https://demonstrations.wolfram.com/The2DIsingModelMonteCarloSimulationUsingTheMetropolisAlgorit/

Principal Component Analysis

consider *n* data points that live in a *p*-dimensional feature space

$$\{\boldsymbol{x}_i\}_{i=1}^{n} \qquad \boldsymbol{x}_i = (x_{i,1}, x_{i,2}, \ldots, x_{i,p})$$

assume for simplicity that the mean of these points vanishes

$$\bar{\boldsymbol{x}} = \frac{1}{n}\sum_{i=1}^{n} \boldsymbol{x}_i = 0$$

Now denote the **design matrix** as

$$\boldsymbol{X} = [\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n]^T$$

In a design matrix, each row represents an individual data point and each each columns one of the data features

where rows are the data points and columns are features

$$\boldsymbol{X} = \begin{pmatrix} x_{1,1} & x_{1,2} & \cdots & x_{1,p} \\ x_{2,1} & x_{2,2} & \cdots & x_{2,p} \\ \cdots & \cdots & \cdots & \cdots \\ x_{n,1} & x_{n,2} & \cdots & x_{n,p} \end{pmatrix}$$

data points

features

Principal Component Analysis

the associated (symmetric) *p*-dimensional **covariance matrix** is then

$$\boldsymbol{\Sigma}(X) = \frac{1}{n-1} X^T X \quad \rightarrow \quad \boldsymbol{\Sigma}_{lm} = \frac{1}{n-1} \sum_{i=1}^{n} X_{li} X_{im}$$

p-dimensional in space of features

sum over data points

from where we see that $\boldsymbol{\Sigma}_{lm}$ measures the correlation between **features *l* and *m***

The goal of PCA is to rotate this matrix to a **new feature-basis** (different from the one present in the original data) that emphasises high-variability directions. This can be done by a linear transformation that **reduces the covariance between features**

recall the **eigenvalue decomposition** for a square matrix

$$A = Q \Lambda Q^T$$

columns are eigenvectors of A

diagonal matrix of eigenvalues

columns are eigenvectors of A

Principal Component Analysis

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sum over data points

from where we see that $\boldsymbol{\Sigma}_{lm}$ measures the correlation between **features *l* and *m***

The goal of PCA is to rotate this matrix to a **new feature-basis** (different from the one present in the original data) that emphasises high-variability directions. This can be done by a linear transformation that **reduces the covariance between features**

for this we will use **Singular Value Decomposition** (SVD), a factorisation of a real or complex matrix that generalizes the eigendecomposition of a positive semidefinite matrix

$$X = USV^T$$

left (right) singular vectors of X: orthonormal eigenvectors of XX^* (X^*X)

columns are left singular vectors of X

diagonal matrix of singular values

columns are right singular vectors of X

Principal Component Analysis

Using SVD we can express the data covariance matrix as

$$\boldsymbol{\Sigma}(X) = \frac{1}{n-1}\boldsymbol{VSU}^T\boldsymbol{USV}^T = \boldsymbol{V}\left(\frac{S^2}{n-1}\right)\boldsymbol{V}^T \equiv \boldsymbol{V}\Lambda\boldsymbol{V}^T$$

U,V are unitary matrices

diagonal matrix with eigenvalues in decreasing order along diagonal

columns of $\boldsymbol{V}$ → principal directions of $\boldsymbol{\Sigma}$

at this point we are ready to use PCA to reduce the dimensionality of data **from *p* to *p'* < *p***

$$\widetilde{\boldsymbol{Y}} = \boldsymbol{X}\widetilde{\boldsymbol{V}}_{p'}$$

reduced dataset: n points with p' < p features each in the rotated-feature matrix

original dataset: n points with p features each

projection matrix: select the p' largest eigenvectors

with PCA only the ***p'* directions with higher variability** remain

Principal Component Analysis

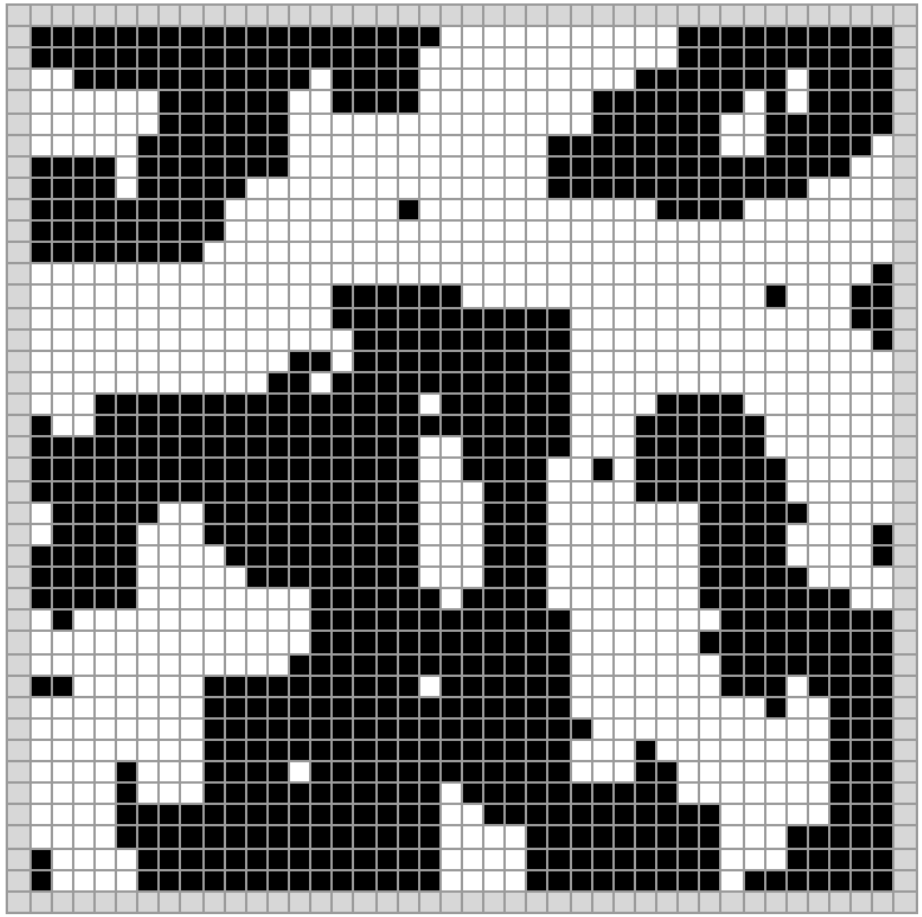
PCA projections often capture the **large-scale structure** of high-dimensional datasets

consider for example the **Ising Model in 2D** with 40 spins: 1600-dimensional space

can we **measure ``order''** with few parameters?

disordered (random) phase

ordered phase



https://demonstrations.wolfram.com/The2DIsingModelMonteCarloSimulationUsingTheMetropolisAlgorit/

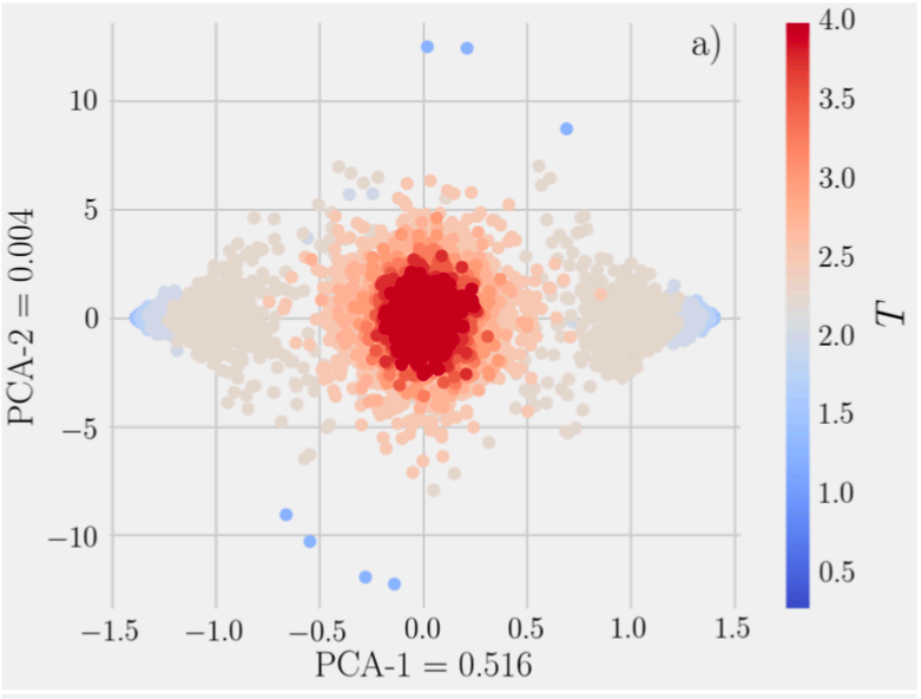
Principal Component Analysis

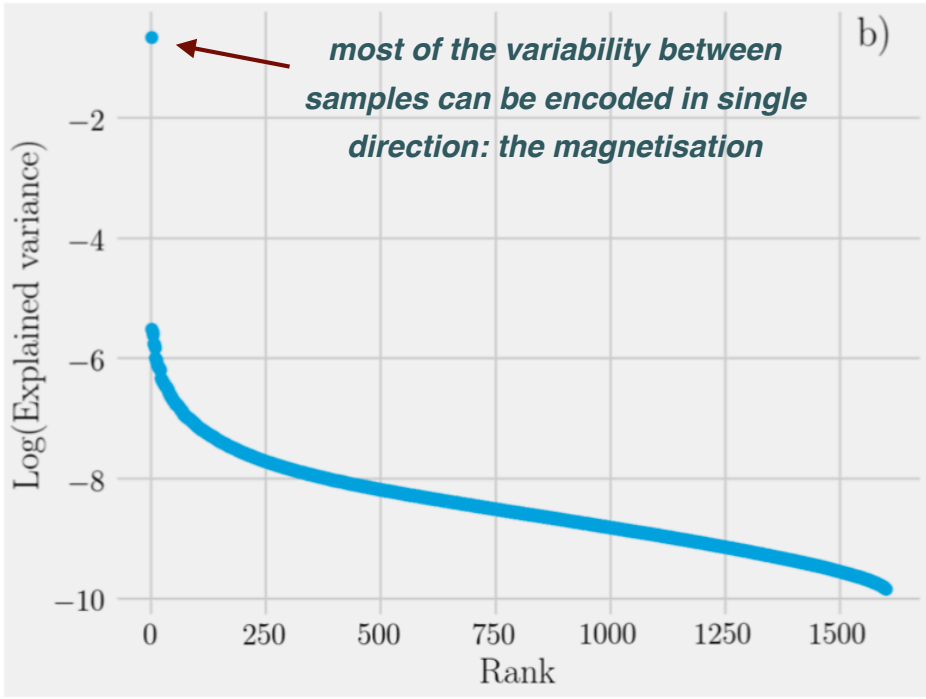
PCA projections often capture the **large-scale structure** of high-dimensional datasets

consider for example the **Ising Model in 2D** with 40 spins: 1600-dimensional space

can we **measure ``order''** with few parameters?

1000 samples for each T



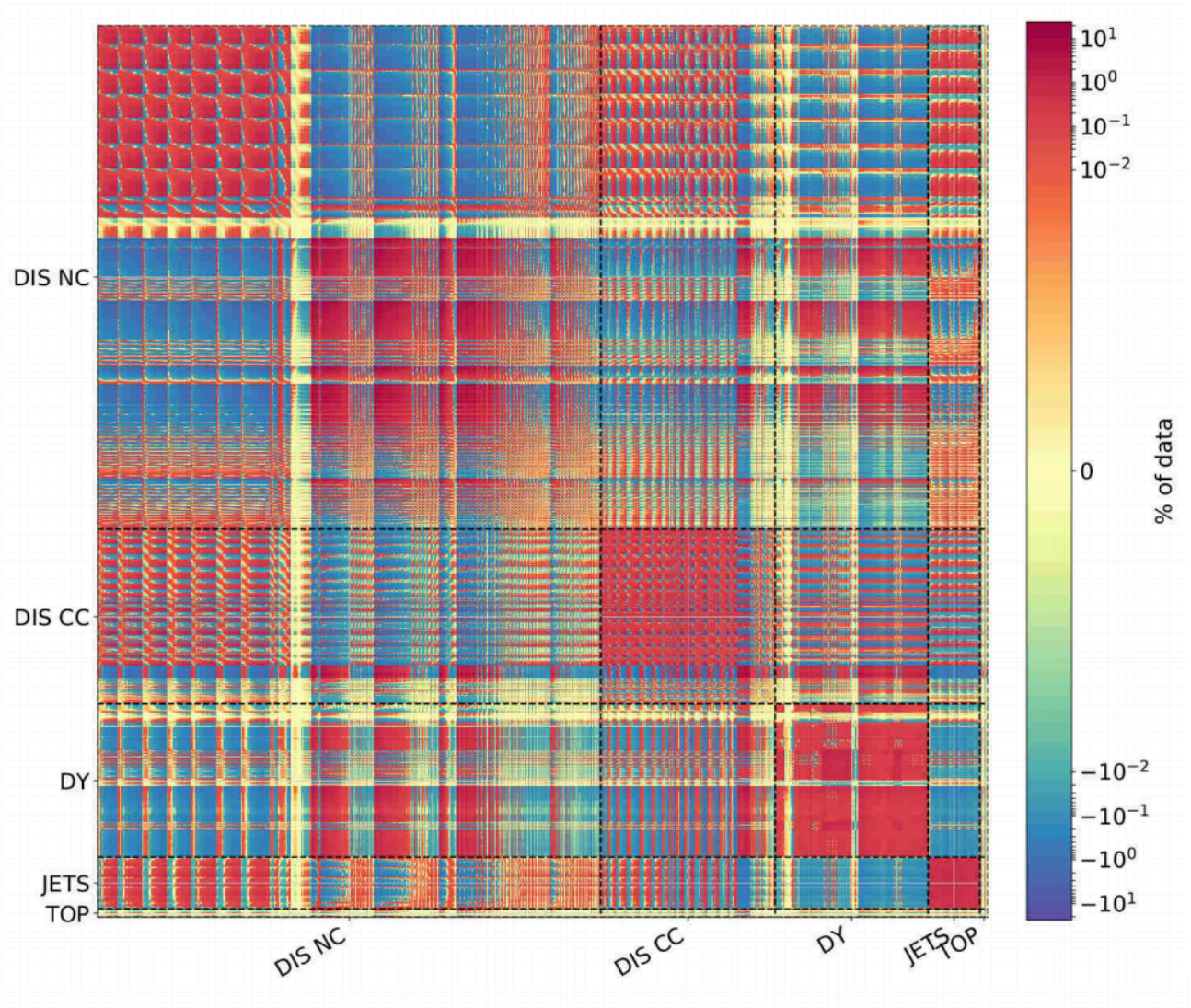


The first principal component accounts for > 50% of total variability!

This first PCA component corresponds to the **magnetisation order parameter**, which we have thus identified without any prior physical knowledge of the system

PCA for propagation of theory errors

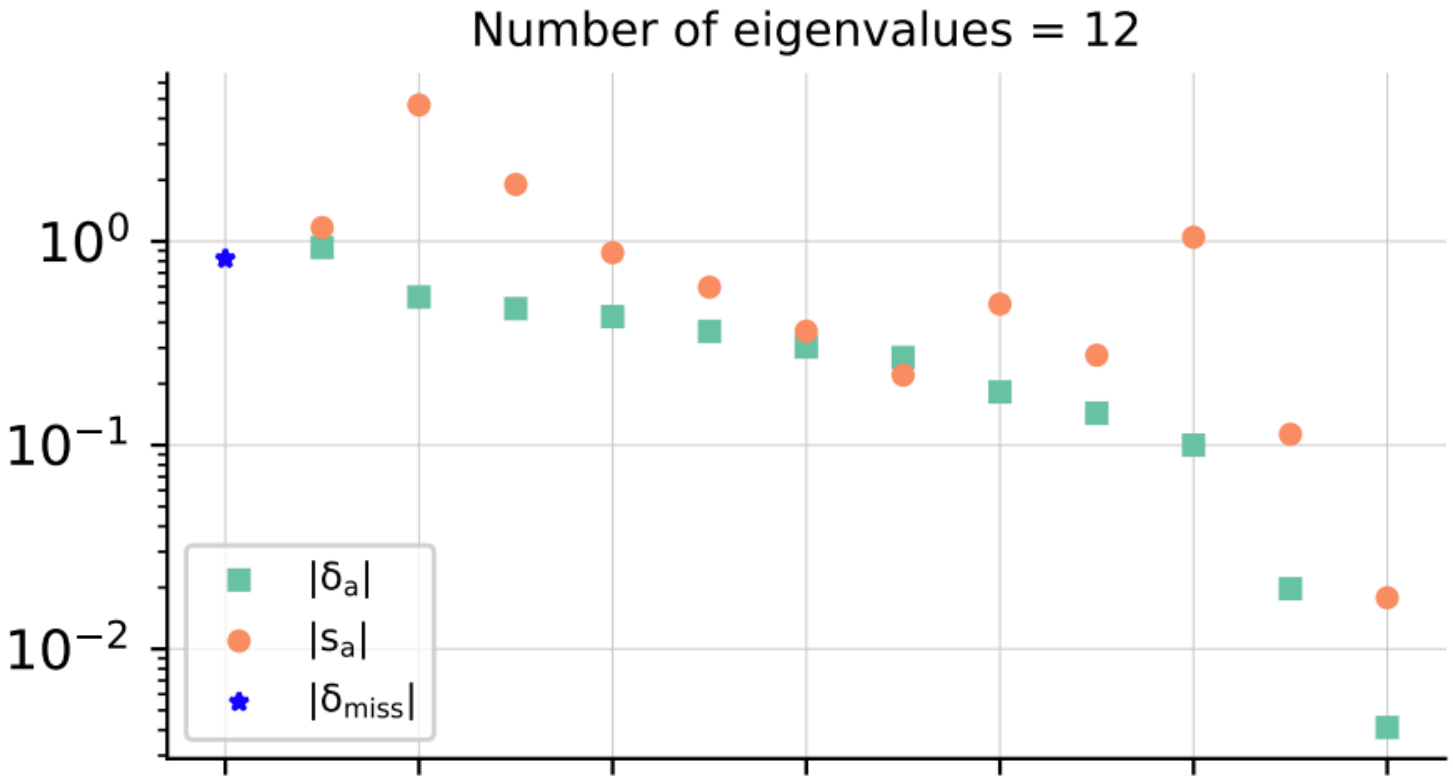
assume that some gives you the **covariance matrix of theory errors** of a global PDF fit (3000-dimensional space!). What are the **relevant components**?



Process Type	Dataset	Reference	$N_{\rm dat}$	$N_{\rm dat}$ (total)
DIS NC	NMC	[28,29]	134	1593
	SLAC	[30]	12	
	BCDMS	[31,32]	530	
	HERA σ^p_{NC}	[36]	886	
	HERA σ^c_{NC}	[37]	31	
DIS CC	NuTeV dimuon	[33,34]	41	552
	CHORUS	[35]	430	
	HERA σ^p_{CC}	[36]	81	
DY	ATLAS W,Z, 7 TeV 2010	[42]	30	484
	ATLAS W,Z, 7 TeV 2011	[43]	34	
	ATLAS low-mass DY 2011	[44]	4	
	ATLAS high-mass DY 2011	[45]	5	
	ATLAS Z p_T 8 TeV (p_T^{ll}, M_{ll})	[46]	44	
	ATLAS Z p_T 8 TeV (p_T^{ll}, y_Z)	[46]	48	
	CMS Drell-Yan 2D 2011	[51]	88	
	CMS W asy 840 pb	[52]	11	
	CMS W asy 4.7 pb	[53]	11	
	CMS W rap 8 TeV	[54]	22	
	CMS Z p_T 8 TeV (p_T^{ll}, M_{ll})	[55]	28	
	LHCb Z 940 pb	[60]	9	
	LHCb $Z \to ee$ 2 fb	[61]	17	
	LHCb $W,Z \to \mu$ 7 TeV	[62]	29	
	LHCb $W,Z \to \mu$ 8 TeV	[63]	30	
	CDF Z rap	[38]	29	
	D0 Z rap	[39]	28	
	D0 $W \to e\nu$ asy	[40]	8	
	D0 $W \to \mu\nu$ asy	[41]	9	
JET	ATLAS jets 2011 7 TeV	[47]	31	164
	CMS jets 7 TeV 2011	[56]	133	
TOP	ATLAS $\sigma^{\rm top}_{tt}$	[48,49]	3	26
	ATLAS $t\bar{t}$ rap	[50]	10	
	CMS $\sigma^{\rm top}_{tt}$	[57,58]	3	
	CMS $t\bar{t}$ rap	[59]	10	
Total			2819	2819

PCA for propagation of theory errors

assume that some gives you the **covariance matrix of theory errors** of a global PDF fit (3000-dimensional space!). What are the **relevant components**?



no knowledge of underlying physics required

only **O(10) directions** encode all the variability of **3000-dimensional covmat**

physical reason: theory errors are **highly correlated** among processes

t-SNE

- In dimensional reduction and data visualisation techniques, it is often desirable to **preserve local structures** in high-dimensional datasets
- In many cases **non-linear methods** (unlike PCA, which is linear) are required
- On of these is ***t*-stochastic neighbour embedding** (t-SNE), where each high-dimensional training point is mapped to low-dimensional embedding coordinates optimized to preserve the local structures in the data

the main idea is to **associate a probability distribution** to the neighbour of each data point

Data Space

$$p_{i|j} = \frac{\exp\left(-||\boldsymbol{x}_i - \boldsymbol{x}_j||^2/2\sigma_i\right)}{\sum_{k\neq i}\exp\left(-||\boldsymbol{x}_i - \boldsymbol{x}_k||^2/2\sigma_i\right)} \qquad \boldsymbol{x}_i \in \mathbb{R}^p$$

probability that j is neighbour of I

model parameter

t-SNE

the main idea is to **associate a probability distribution** to the neighbour of each data point

Data Space

$$p_{i|j} = \frac{\exp\left(-||\boldsymbol{x}_i - \boldsymbol{x}_j||^2/2\sigma_i\right)}{\sum_{k\neq i}\exp\left(-||\boldsymbol{x}_i - \boldsymbol{x}_k||^2/2\sigma_i\right)} \qquad \boldsymbol{x}_i \in \mathbb{R}^p$$

and then **constructing a similar probability** in the **lower-dimensional latent space**

Latent Space

$$q_{i|j} = \frac{\left(1 + ||\boldsymbol{y}_i - \boldsymbol{y}_j||^2\right)^{-1}}{\sum_{k\neq i}\left(1 + ||\boldsymbol{y}_i - \boldsymbol{y}_k||^2\right)^{-1}} \qquad \boldsymbol{y}_i \in \mathbb{R}^{p'}, \quad p' < p$$

the latent space coordinates are determined by minimising the **Kullback-Leibler divergence** between the two probability distributions

cost function: $$C(Y) = D_{\mathrm{KL}}(p\,||\,q) \equiv \sum_{ij} p_{i|j}\log\frac{p_{i|j}}{q_{i|j}}$$

minimisation using e.g. Gradient Descent

output of minimisation: latent-space coordinates $\{y_i\}$ of each data point $\{x_i\}$

The Kullback-Leibler divergence

The KL divergence, a measure of the similarity between two probability distributions *p(**x**)* and *q(**x**)* plays an important role in machine learning applications

$$D_{KL}\left(p\,||\,q\right) = \int d\boldsymbol{x}\, p(\boldsymbol{x}) \log \frac{p(\boldsymbol{x})}{q(\boldsymbol{x})} \qquad D_{KL}\left(q\,||\,p\right) = \int d\boldsymbol{x}\, q(\boldsymbol{x}) \log \frac{q(\boldsymbol{x})}{p(\boldsymbol{x})}$$

which can be symmetrised to construct a **squared metric** (distance)

$$D_{JS}\left(p\,||\,q\right) = \frac{1}{2}\left(D_{KL}\left(p\,\middle|\middle|\,\frac{p+q}{2}\right) + D_{KL}\left(q\,\middle|\middle|\,\frac{p+q}{2}\right)\right)$$

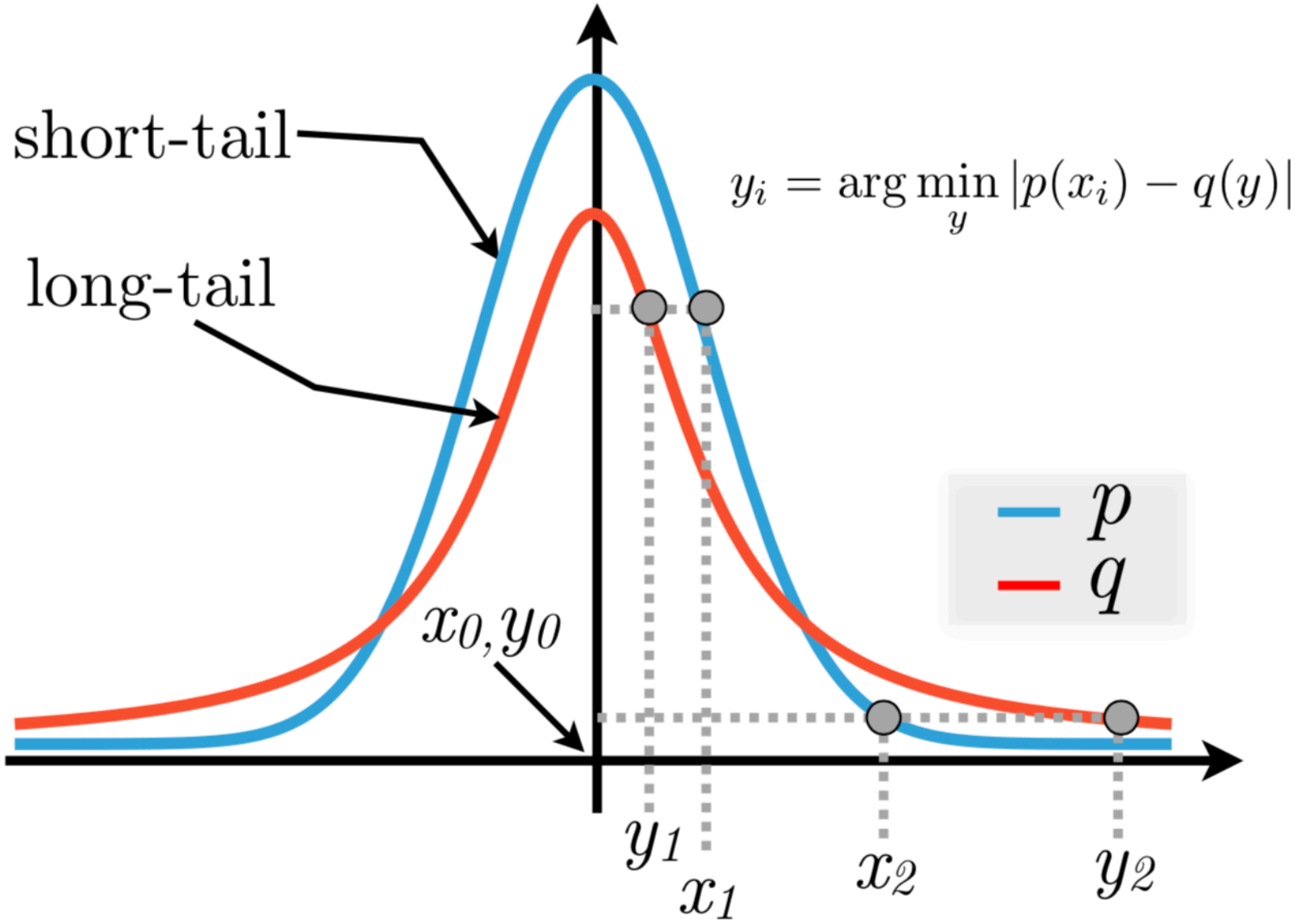
Jensen-Shannon divergence

The KL-divergence is **positive-definite**, and only vanishes when *p(**x**)*= q*(**x**)*

$$D_{KL}\left(p\,||\,q\right) \geq 0$$

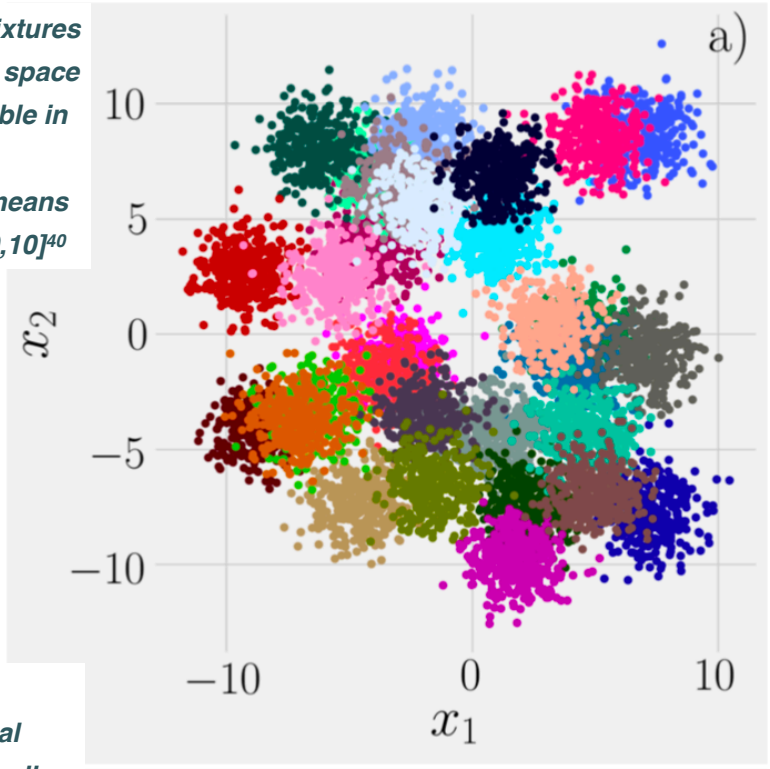
in general the integral cannot be computed and one needs to sample the two probability distributions by means of a suitable binning

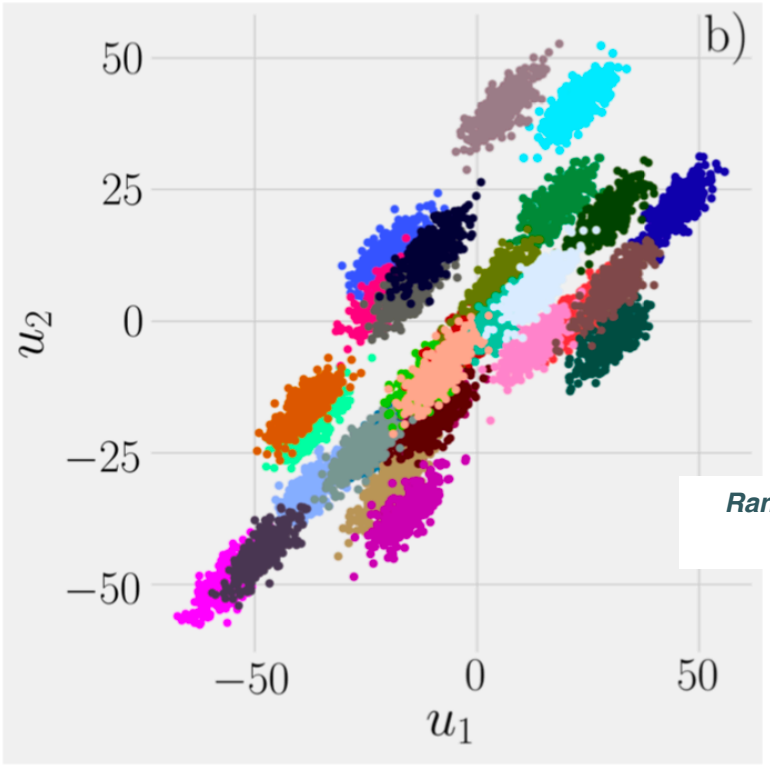
t-SNE



Note that *q* is a **long-tail distribution** (Cauchy): this preserves short distance information while repelling two points that are far apart in the original space

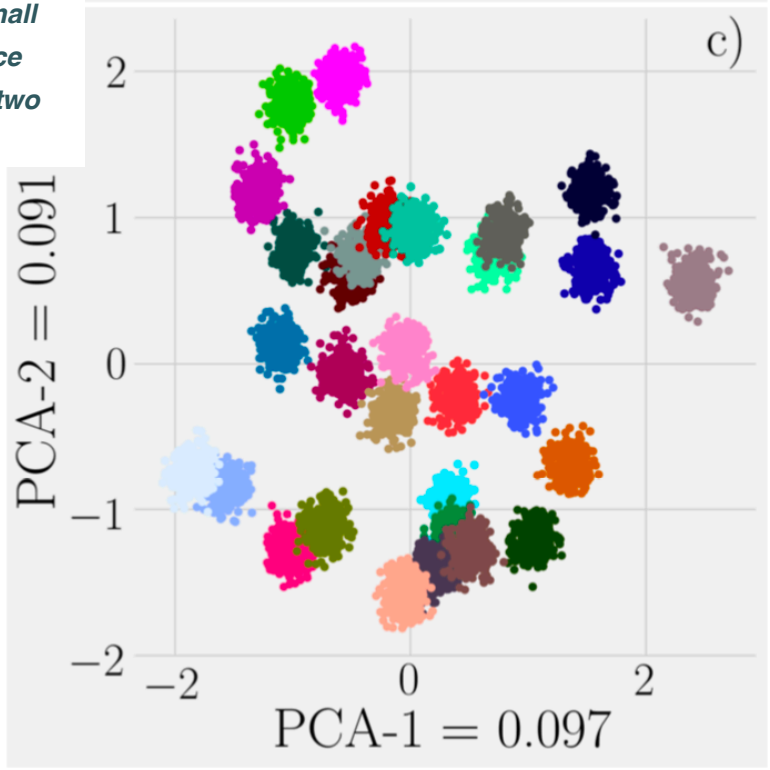
K=30 Gaussian mixtures in 40-dimensional space (labels not available in real case!)
Same variance, means at random in $[-10,10]^{40}$

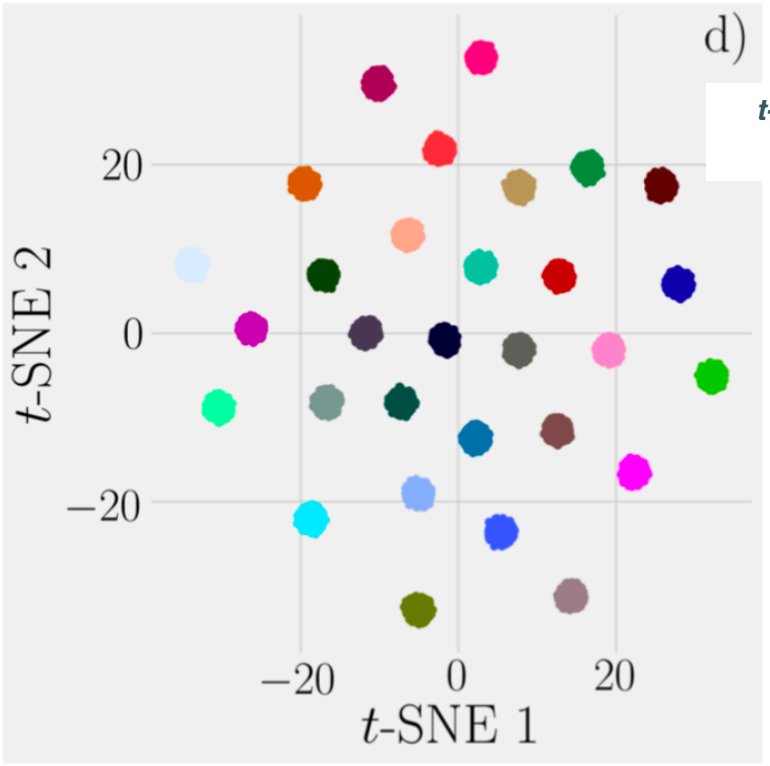




Random projection to 2D space

PCA projection (linear dimensional reduction): only small fraction of variance accounted by first two components





t-SNE embedding to 2D latent space

Ensemble Methods & Bootstrapping

Combining models

a powerful strategy in machine learning is that of **ensemble methods** that **combine predictions from multiple statistical models** to improve predictive performance

- Key aspect: assess the **degree of correlation** between the models of the ensemble
- The reason is that **combining correlated models reduces the overall variance less** than in the uncorrelated case
- Also these correlations can **increase the bias of the combined model**, offsetting potential reductions in variance from ensemble averaging

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e. g. assume that your model predicts *X,* and you have *n* models. If each of these models has variance σ, then the variance of their sum is

$$\mathrm{Var}\left(\sum_{i=1}^{n} X_i\right) = \sum_{i=1}^{n} \mathrm{Var}(X_i) + 2 \sum_{1 \le i \le j \le n} \mathrm{Cov}(X_i, X_j)$$

$$\mathrm{Var}\left(\overline{X}\right) = \mathrm{Var}\left(\frac{1}{n}\sum_{i=1}^{n} X_i\right) = \frac{1}{n^2}\sum_{i=1}^{n} \mathrm{Var}(X_i)$$

$$\mathrm{Var}\left(\overline{X}\right) = \frac{\sigma^2}{n} + \frac{n-1}{n}\rho\sigma^2$$

reduction as n increased — *correlations increase variance*

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$$\mathrm{Var}\left(\overline{X}\right) = \frac{\sigma^2}{n} + \frac{n-1}{n}\rho\sigma^2$$

for fully correlated models →

$$\mathrm{Var}\left(\overline{X}\right) = \frac{\sigma^2}{n} + \frac{n-1}{n}\sigma^2 \to \sigma^2$$

no reduction of variance in the combination

Bagging

Bootstrap AGGgregation (Bagging) is a popular **ensemble combination method**

we start from a large dataset that is **partitioned** into *M* smaller datasets:

$$\mathcal{L} \quad \rightarrow \quad \{\mathcal{L}_1, \mathcal{L}_2, \ldots, \mathcal{L}_M\} \qquad \sum_{m=1}^{M} \mathcal{L}_m = \mathcal{L}$$

so that each of the *M* datasets is large enough to train a predictor. The **aggregate predictor** is then constructed from those trained in each separate dataset

$$\hat{g}^A_{\mathcal{L}}(\boldsymbol{x}) = \frac{1}{M} \sum_{i=1}^{M} g^A_{\mathcal{L}_i}(\boldsymbol{x})$$

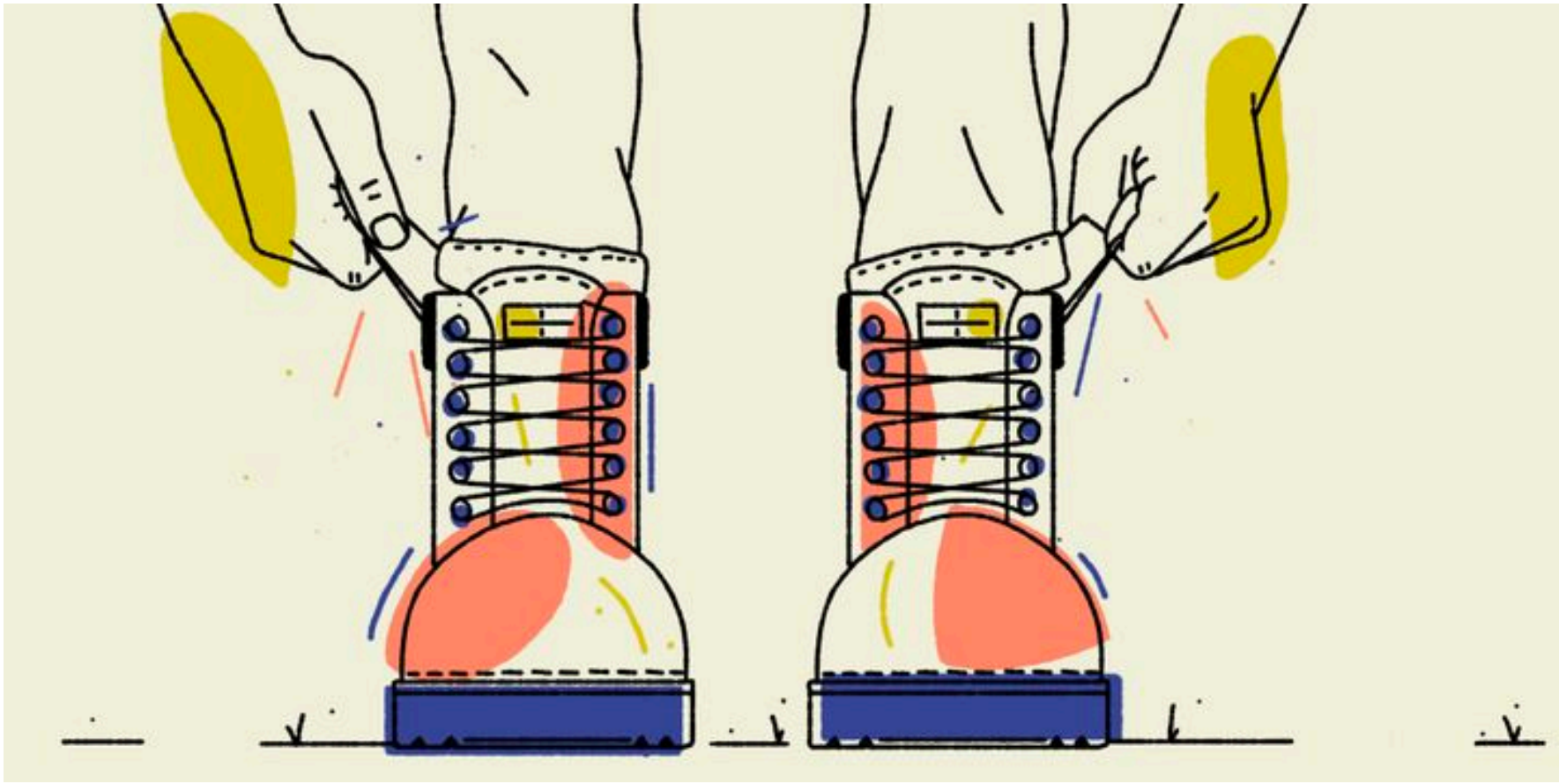
for continuous datasets, analogous expressions for discrete classifiers

such aggregation can **reduce the variance without increasing the bias**

But what should we do if we don't have a very large dataset? If each partitioned set one has few data points then the prediction will be poor …

and if using more data/examples is not possible?

Bootstrapping



Bootstrapping quantifies properties of an estimator by measuring those properties when **sampling from an approximating distribution** (*e.g.* a subset of the original data)

Bootstrapping

- Assume we are given a training dataset and we want to compute *e.g.* confidence intervals

$$\mathscr{D} = \{X_1, \ldots, X_n\}$$

- This can be done by **sampling *n* points with replacement** to get ***B* new datasets**

$$\mathscr{D}^{*(1)} = \{X_1^{*(1)}, \ldots, X_n^{*(1)}\}$$

$$\vdots$$

$$\mathscr{D}^{*(B} = \{X_1^{*(B)}, \ldots, X_n^{*(B)}\}$$

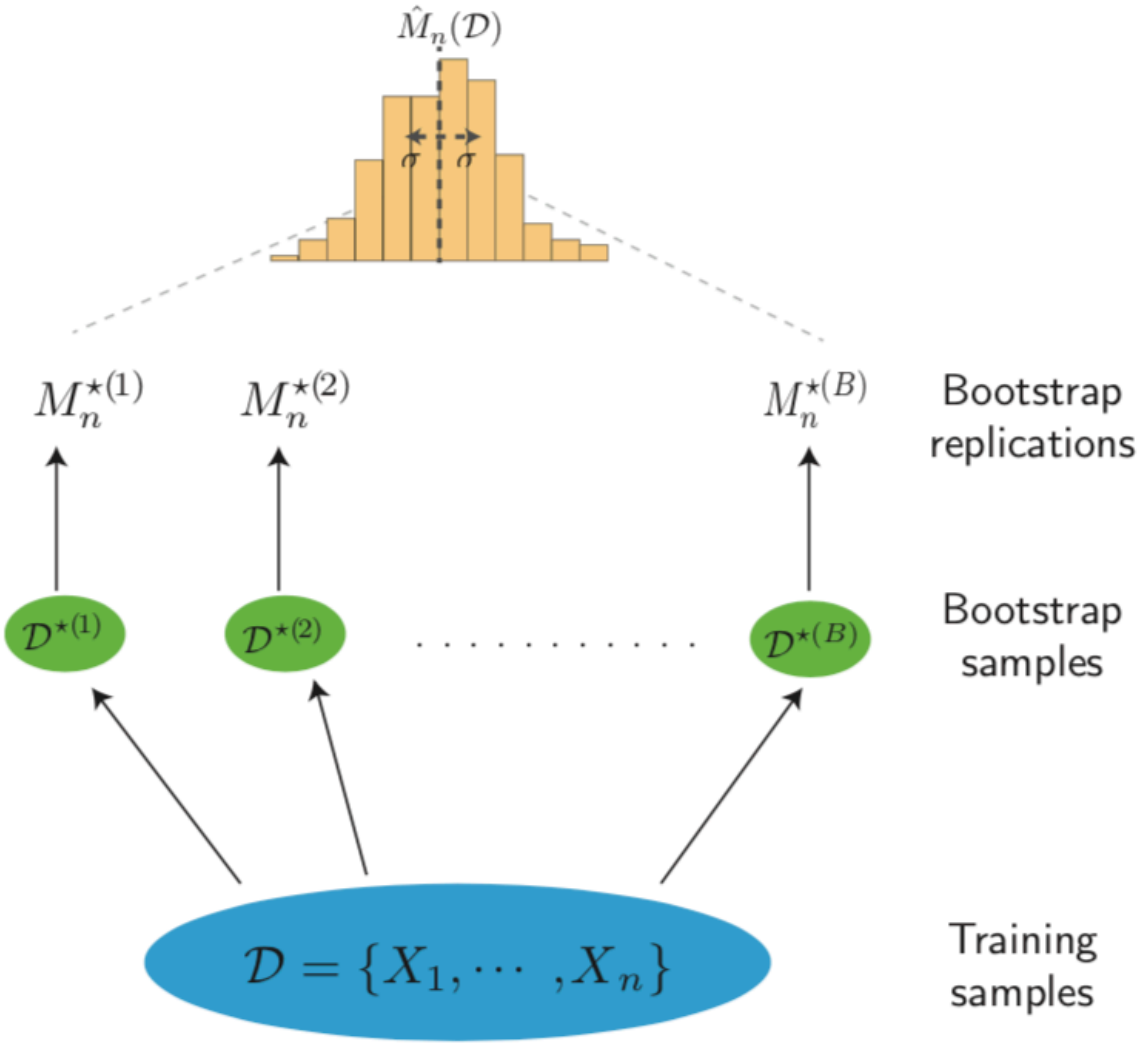
bootstrap samples (with repeated elements)

- With the **bootstrapped samples** we can construct statistical quantities of interest:

$$\widehat{\mathrm{Var}}_B(M_n) = \frac{1}{B-1}\sum_{k=1}^{B}\left(M_n^{*(k)} - \overline{M}_n^*\right)^2 \qquad \overline{M}_n^* = \frac{1}{B}\sum_{k=1}^{B} M_n^{*(k)}$$

it can be shown that in the large *n* limit the **bootstrap distributions** approximate well the **sampling distributions** from which the training dataset was obtained

Bootstrapping



In ML applications, bootstrapping is frequently used to **assign measures of accuracy** (defined in terms of bias, variance, correlations etc to sample estimates

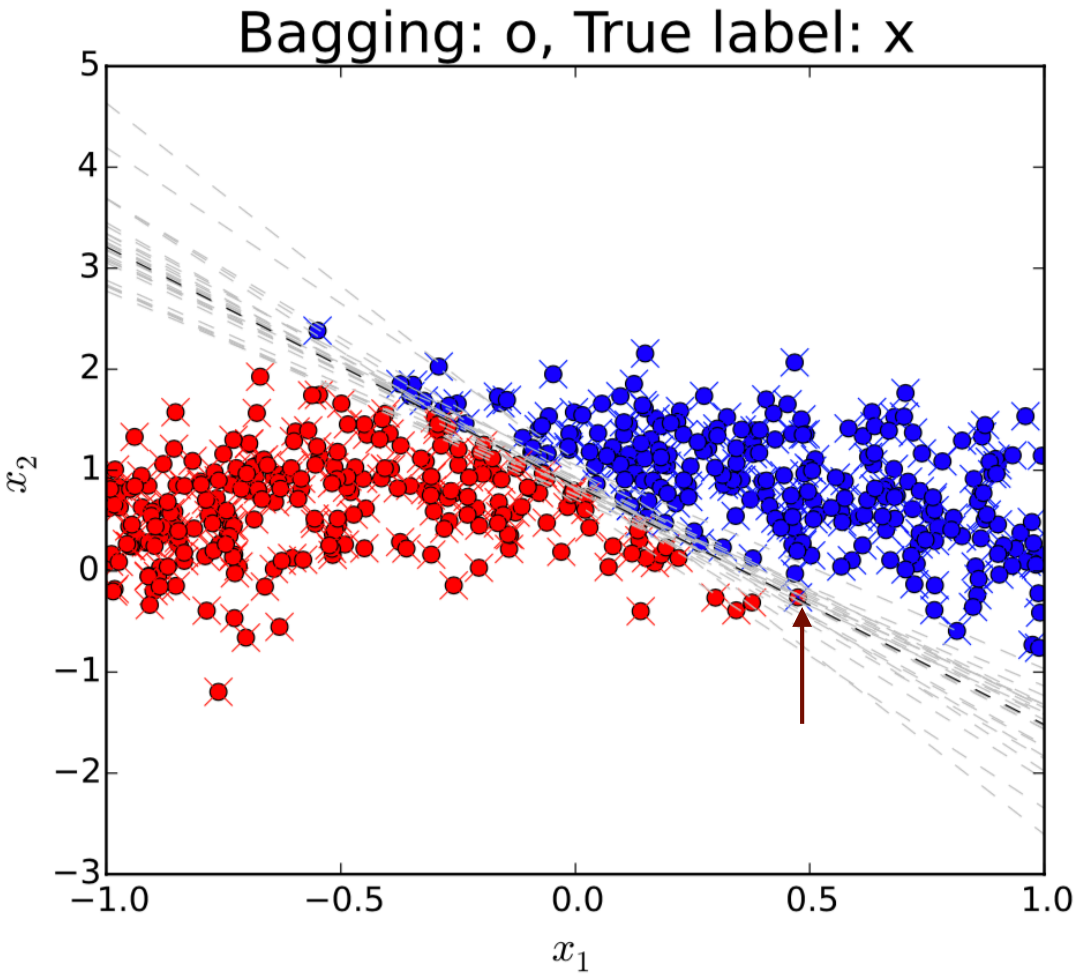
It can be shown that in the large *n* limit the **bootstrap distributions** approximate well the **sampling distributions** from which the training dataset was obtained

Bagging with bootstrap

same as before, but now the datasets have been partitioned with bootstrapping

$$\hat{g}^{\mathrm{BS}}_{\mathscr{L}}(\boldsymbol{x}) = \frac{1}{M}\sum_{i=1}^{M} g^{A}_{\mathscr{L}^{\mathrm{BS}}_{i}}(\boldsymbol{x})$$

which can lead to a **variance reduction** to the price of an **increase in the bias**



ex: bagging with bootstrap ***(2D classification)***

n=500, *B*=25 (50 points each)

grey dashed: bootstrap predictions

black dahed: bagging average

individual predictors poor, bagging much better!

bagging is specially useful for **unstable learning algorithms** where small changes in the training dataset result in large changes in the prediction

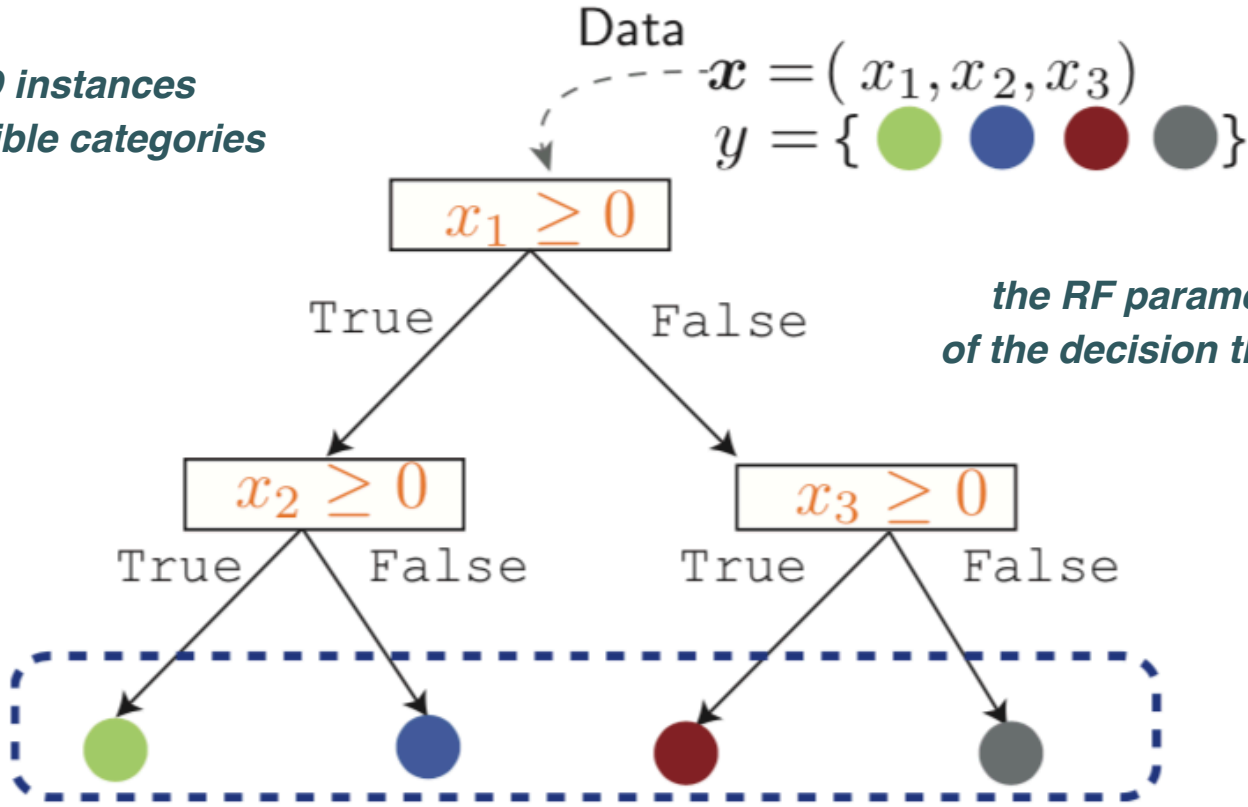
Decision Trees and Random Forests

more on ML for classification in the lecture 4!

Random Forests

Ensemble method widely used in complex classification tasks constructed from **randomised tree-based classifier decision trees**

classify 3D instances into four possible categories



the RF parameters are the values of the decision threshold at each node

In ML, a **decision tree** is an algorithm which uses a series of questions to hierarchically partition the data, where each branch of the tree splits the data into smaller subsets

Random Forests

individual trees have often **high variance** and are weak classifiers:
we can improve by incorporating them in an ensemble method

→ We need an ensemble of **randomised decision trees** (minimised correlations)

- ***(1)*** train each decision tree on a different bootstrapped dataset: **bagged decision tree**
- ***(2)*** use different random subset of features at each split: **random forest**

reduces correlations between trees that arise
when only few features are strongly predictive

as other ML learning classifiers also Random Forests require some **regularisation**, for example a maximum depth of the tree, to control complexity and prevent overfitting

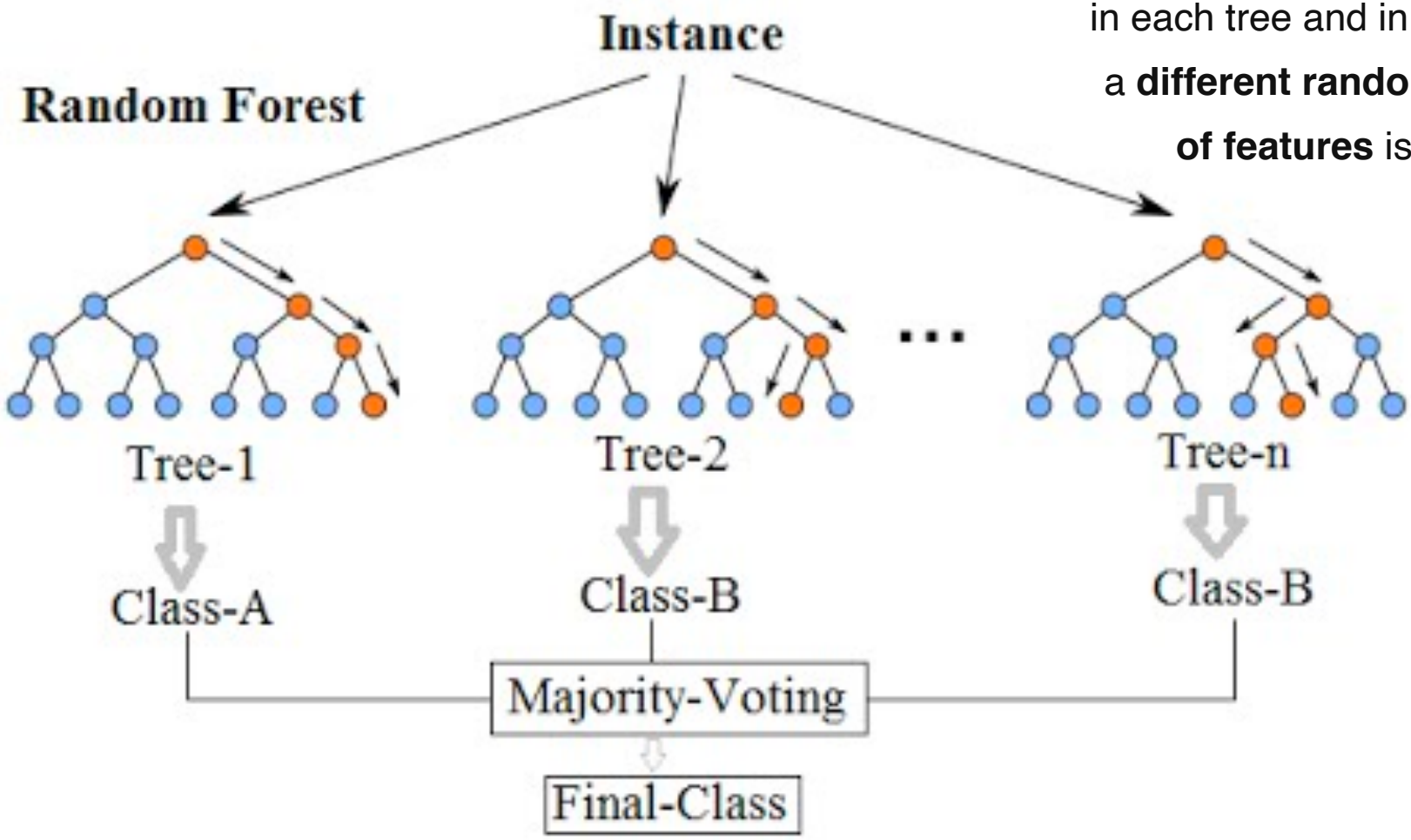
typically, a classification problem with p features, in RFs only $p^{1/2}$ features are used in each split

Random forests have other attractive features, for example, they can be used to **rank the importance of variables** in a regression or classification problem in a natural way

Random Forests

each decision tree in the ensemble is built upon a **random bootstrap sample** of the original data

in each tree and in each split, a **different random subset of features** is used



the final categorisation is assigned *e.g.* from **majority voting**