Machine Learning:

A new toolbox for Theoretical Physics

Juan Rojo

VU Amsterdam & Theory group, Nikhef

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Recap from Lecture 1

Supervised Learning

problems in **Supervised Machine Learning** are defined by the following ingredients:

(1) Input dataset: $\mathscr{D} = (\boldsymbol{X}, \boldsymbol{Y})$

(2) Model: $f\left(\boldsymbol{X}, \boldsymbol{\theta}\right)$

models can be simple (polynomials) or very complex (deep networks)

(3) Cost function: $C\left(\boldsymbol{Y}; f(\boldsymbol{X}; \boldsymbol{\theta}\right)$

The cost function measures how well the model (for a specific choice of its parameters) is able to **describe the input dataset**

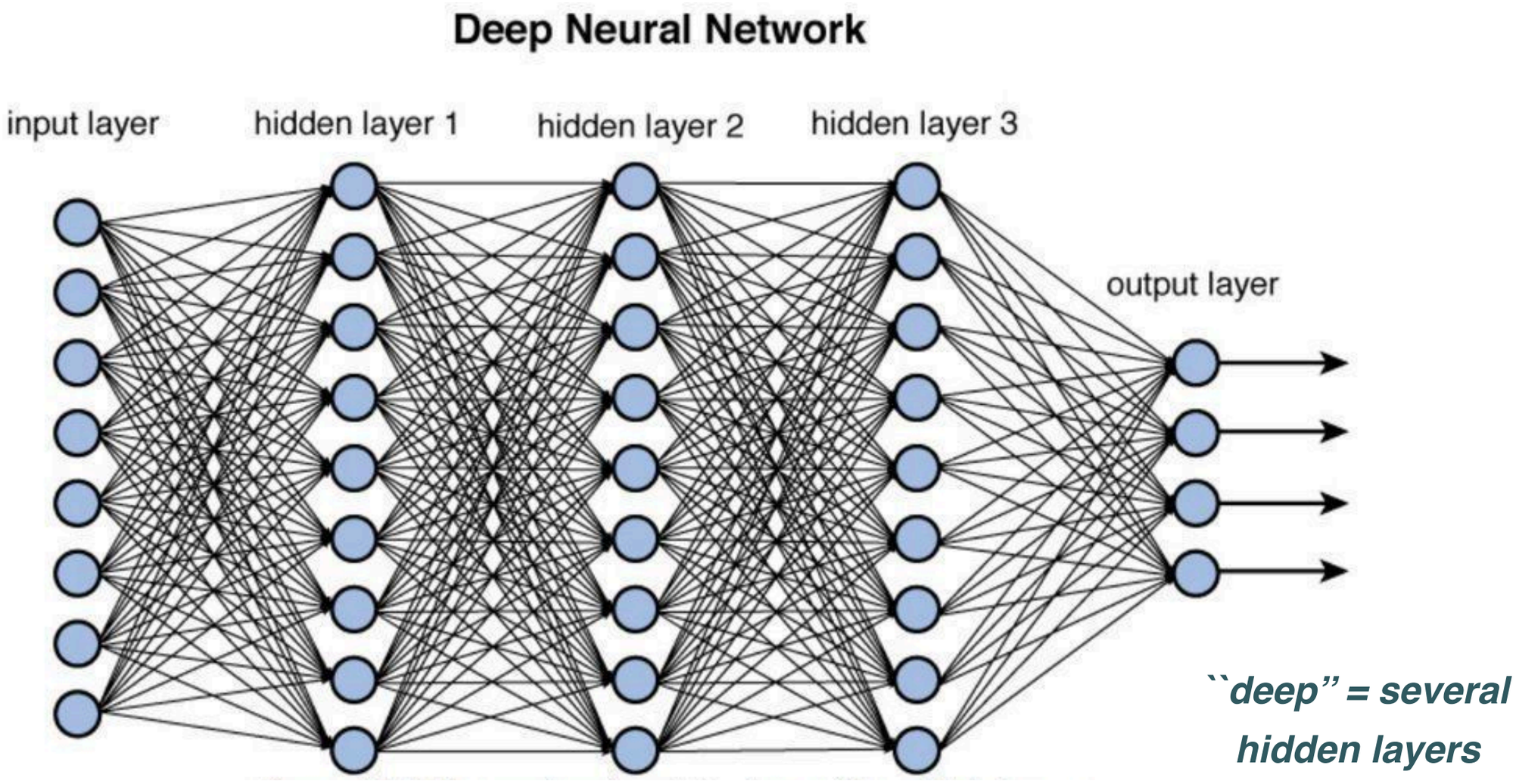
example of cost function for single dependent variable: sum of residuals squared

$$C\left(\boldsymbol{Y}; f(\boldsymbol{X}; \boldsymbol{\theta}\right) = \frac{1}{n} \sum \left(y_i - f(\boldsymbol{x}_i, \boldsymbol{\theta})\right)^2$$

Deep Networks

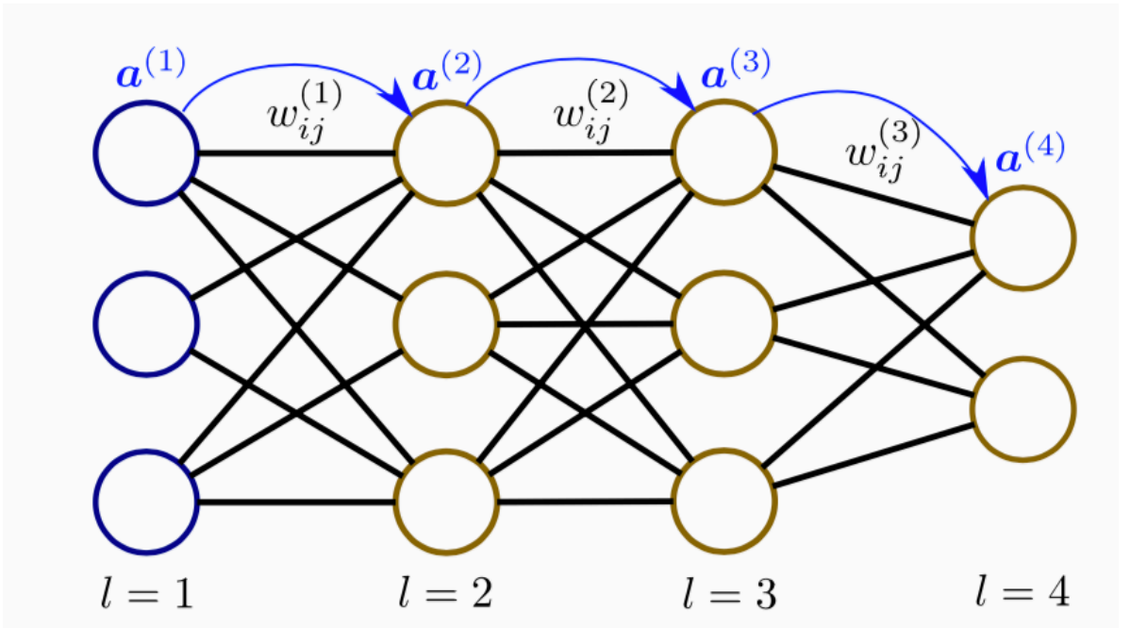
A neural network can thus be thought of a **complicated non-linear mapping** between the inputs and the outputs that depends on the parameters (weights and bias) of each neuron

We can make a NN **deep** by adding hidden layers, which greatly expands their **representational power**, also known as **expressivity**

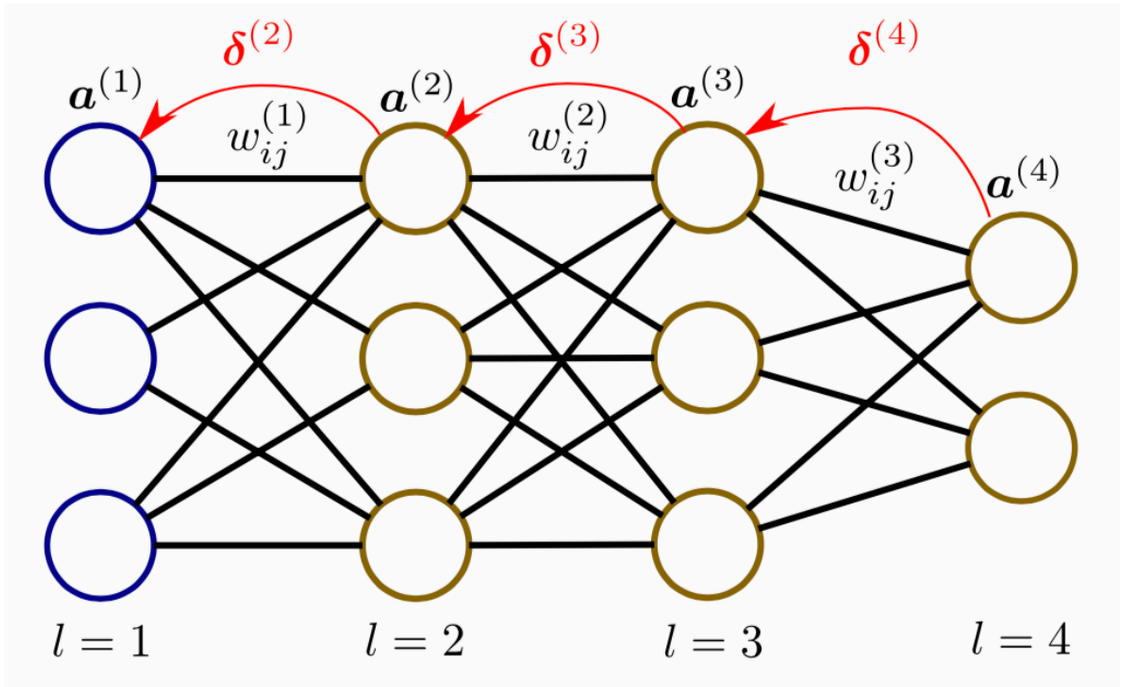


Backpropagation

first evaluate the activation states of all neurons using **forward propagation …**



then **backpropagate** to evaluate the **errors Δ** and thus the gradients over model parameters



Tutorial 2 Exercise 2a

starting point is the **Python script** that you will find in

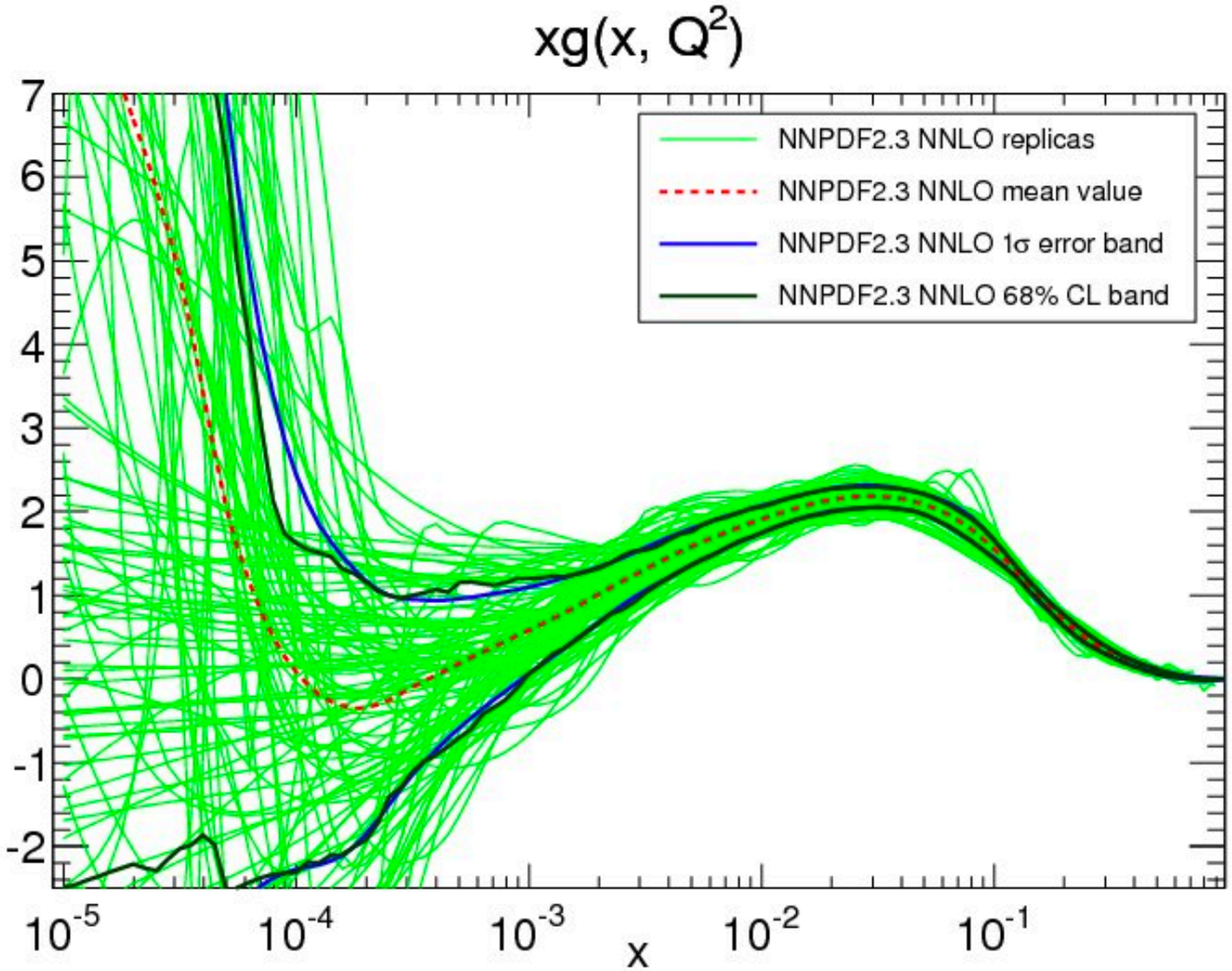
https://github.com/juanrojochacon/ml-ditp-attp/blob/master/Tutorials/Tutorial2/

- Train a **deep neural network** on pseudo-data for Parton Distribution Functions

- Study the dependence of the results with the choice of architecture

- Which minimiser settings lead to the fastest convergence?

- What happens if you change the random seed? How to you interpret the results?



Logistic regression

cost function for logistic regression from **Maximum Likelihood Estimation** (MLE):
choose parameters that maximise the probability of seeing the observed data

$$P(y_i \,|\, \boldsymbol{x}_i, \boldsymbol{\theta}) = \Big(P(y_i = 1 \,|\, \boldsymbol{x}_i, \boldsymbol{\theta})\Big)^{y_i} \times \Big(P(y_i = 0 \,|\, \boldsymbol{x}_i, \boldsymbol{\theta})\Big)^{1-y_i}$$

recovers limits when y_i=0, y_i=1

$$P(y_i \,|\, \boldsymbol{x}_i, \boldsymbol{\theta}) = \Big(\sigma(\boldsymbol{x}_i^T \boldsymbol{\theta})\Big)^{y_i} \times \Big(1 - \sigma(\boldsymbol{x}_i^T \boldsymbol{\theta})\Big)^{1-y_i}$$

assuming that all observations are Bernoulli **independent**, the total likelihood is

$$\mathscr{L}(\boldsymbol{\theta} \,|\, \mathscr{D}) = \prod_{i=1}^{n} P(y_i \,|\, \boldsymbol{x}_i, \boldsymbol{\theta}) = \prod_{i=1}^{n} \Big(\sigma(\boldsymbol{x}_i^T \boldsymbol{\theta})\Big)^{y_i} \times \Big(1 - \sigma(\boldsymbol{x}_i^T \boldsymbol{\theta})\Big)^{1-y_i}$$

the model for the classification probabilities can be either very simple (linear model) of very complex (Deep neural networks)

Today's lecture

- Unsupervised Learning: clustering
- Data visualisation and dimensional reduction
- Reinforcement Learning
- Ensemble methods and bootstrapping

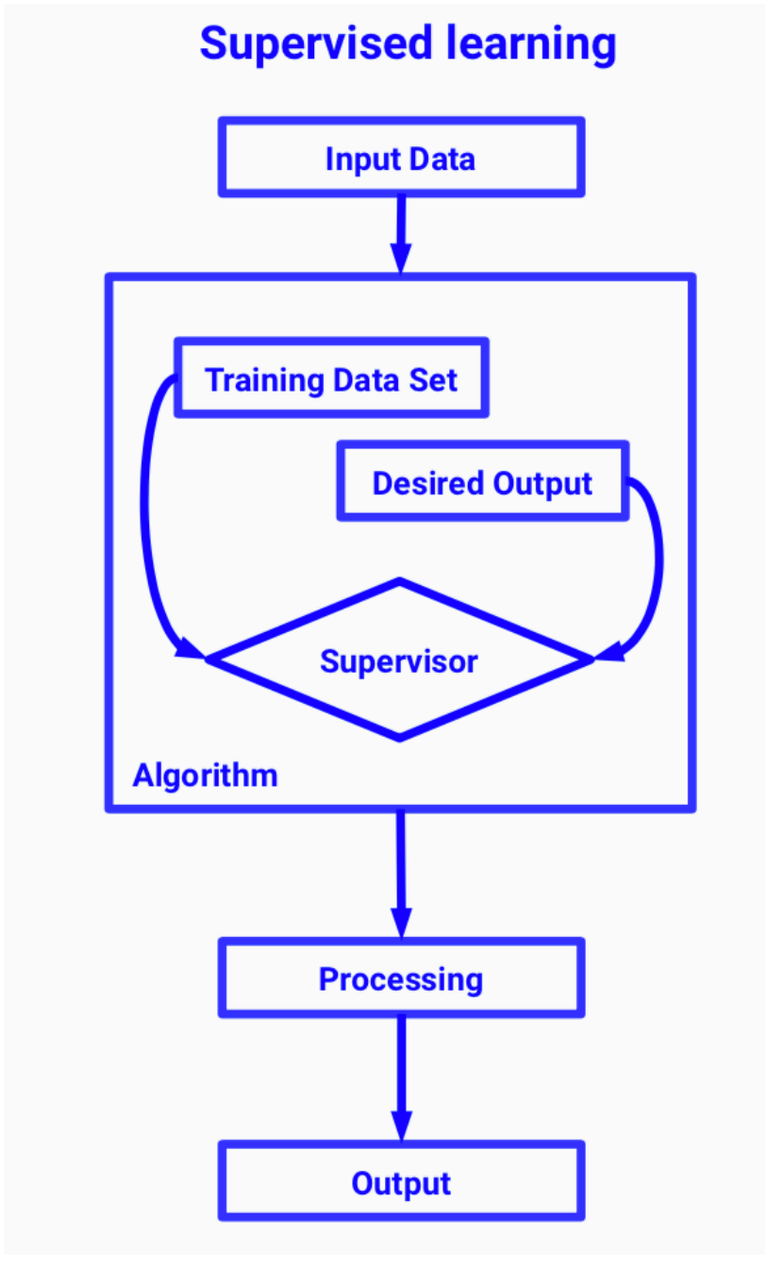
Tutorial 3:

(a) Clustering with Unsupervised Learning

(b) Bagging and Random Forests for classification in the Ising Model

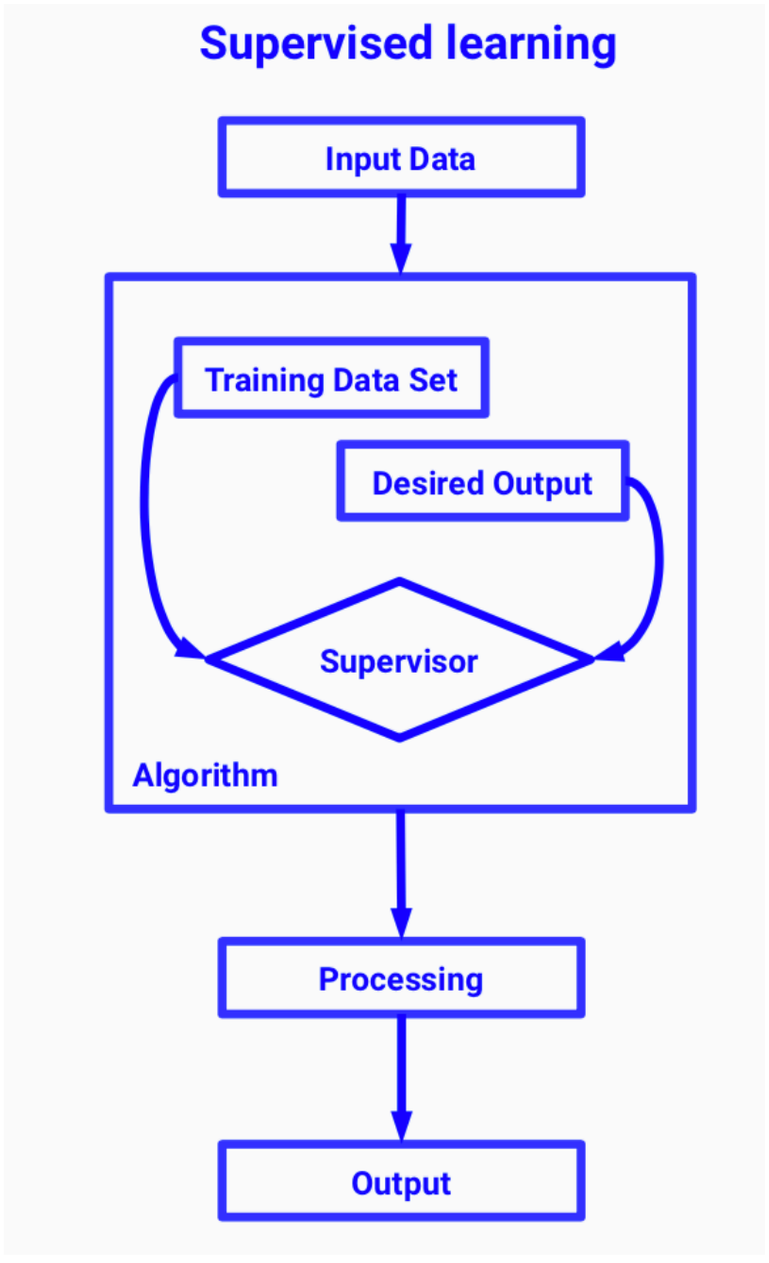
Unsupervised Learning

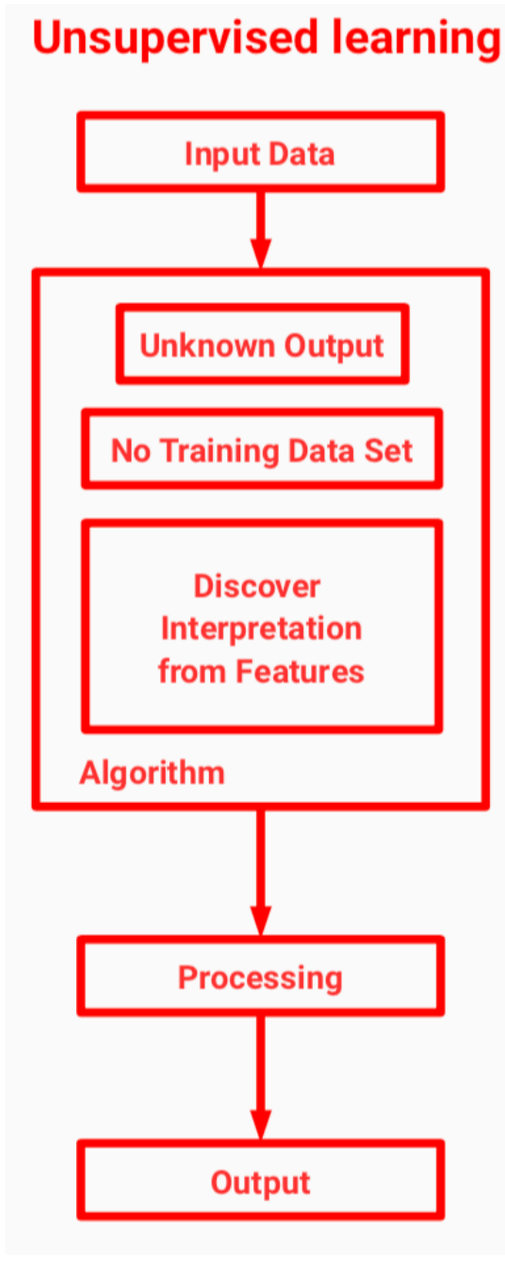
Supervised vs Unsupervised Learning

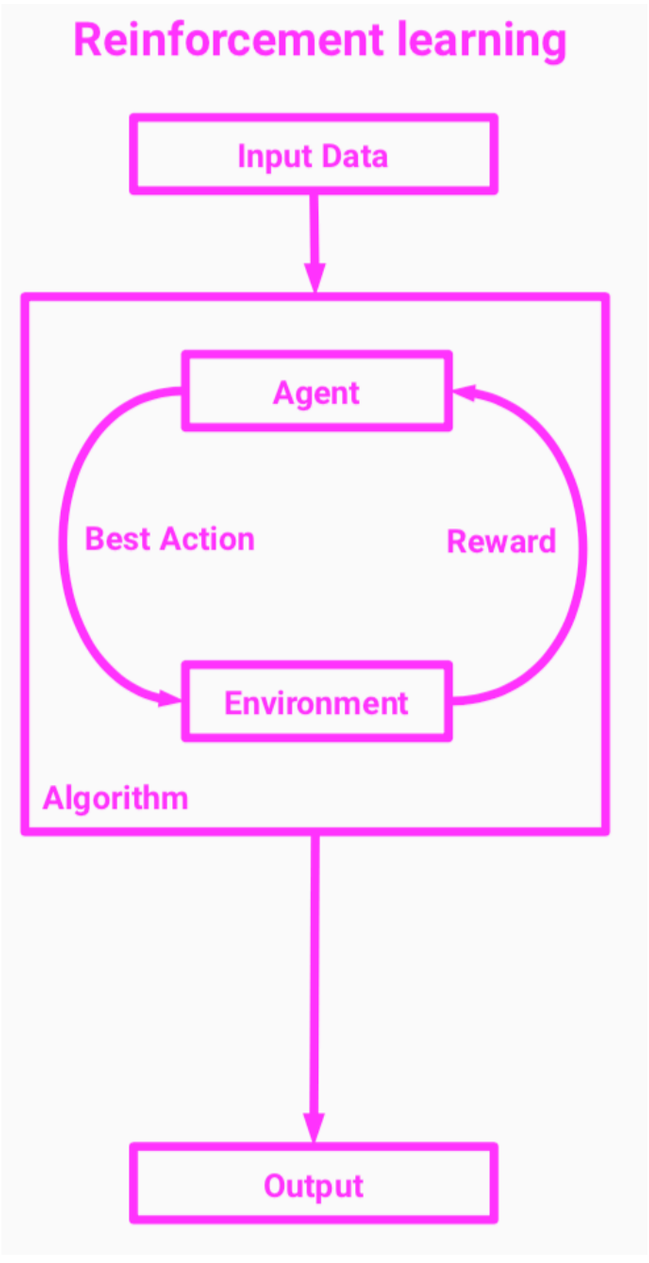


Lectures 1+2

Supervised vs Unsupervised Learning



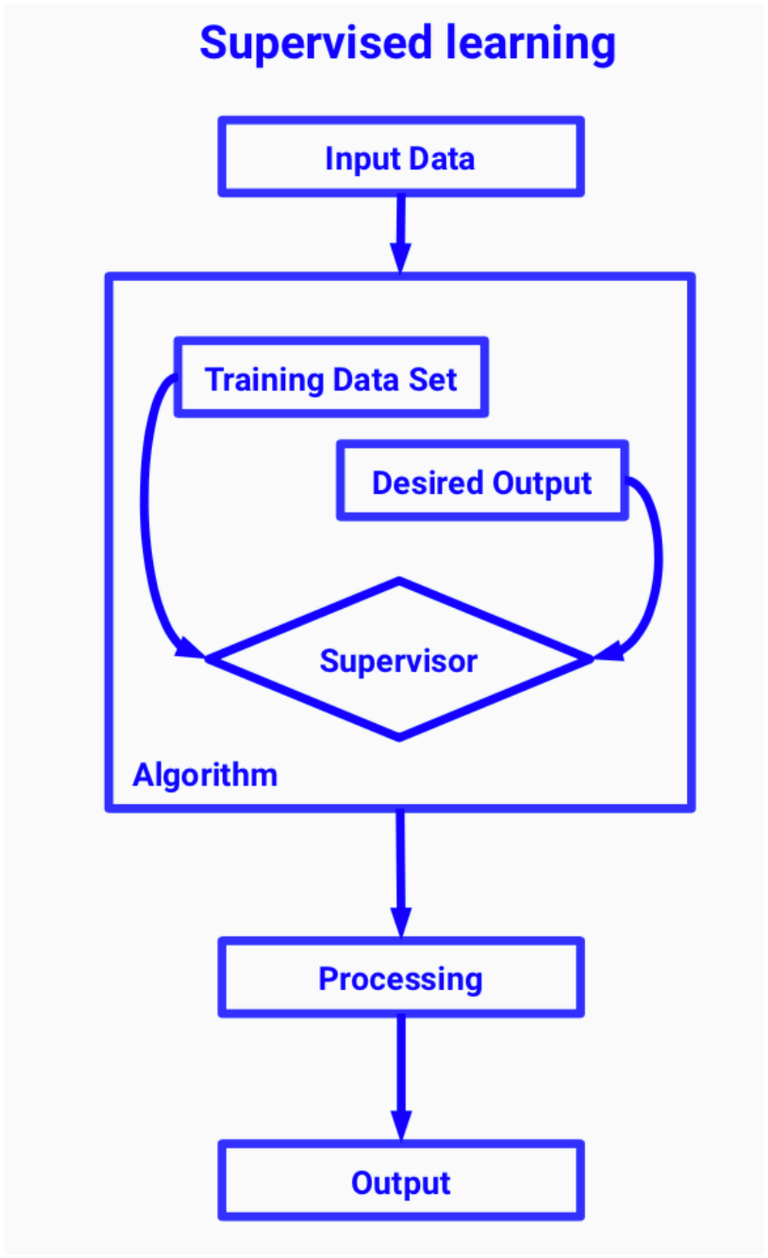




Lectures 1+2

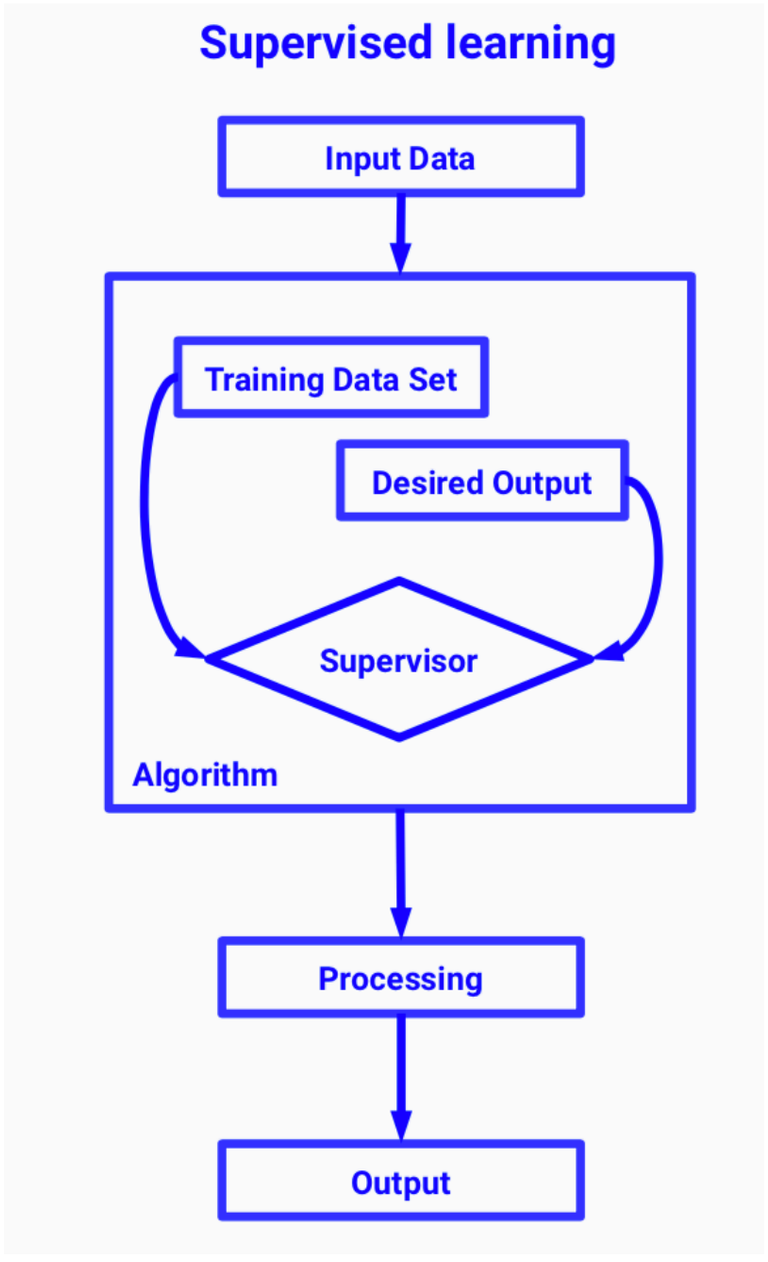
Lecture 3

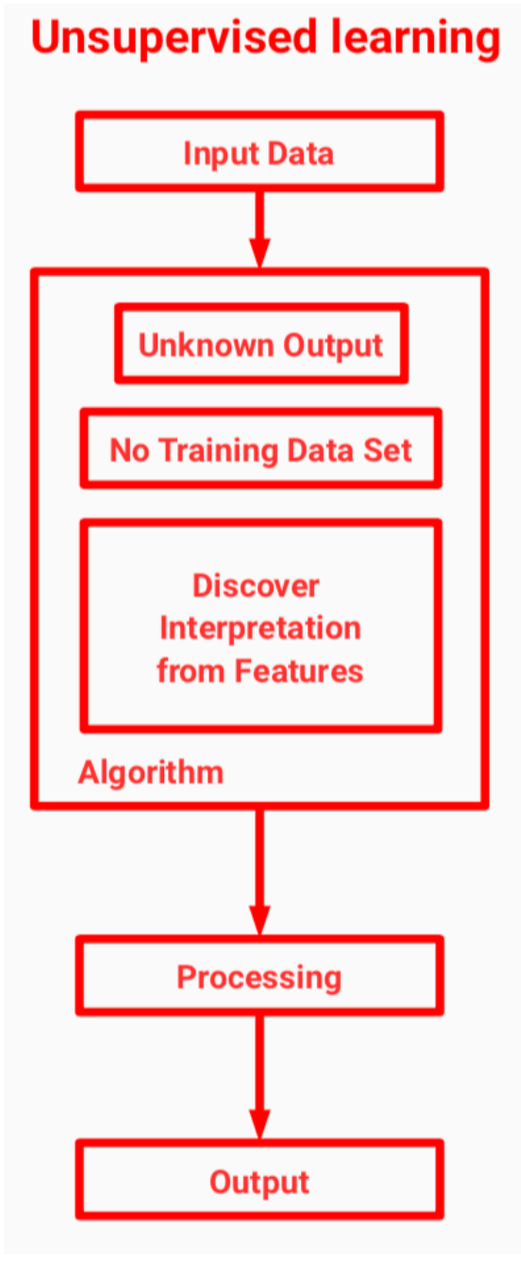
Supervised vs Unsupervised Learning



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

Unsupervised Learning

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**

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

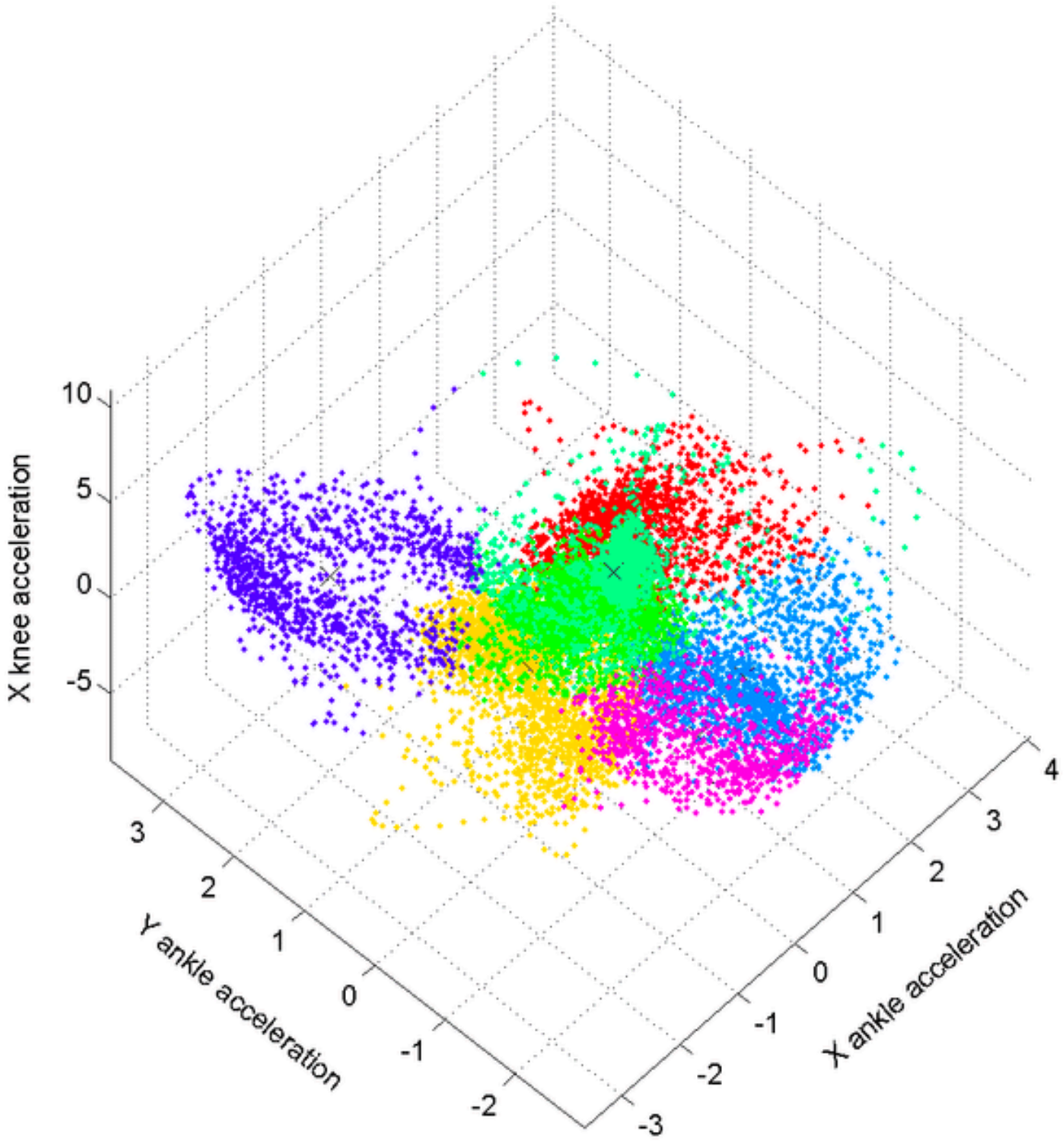
unlabelled dataset: N points with p features each

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

***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



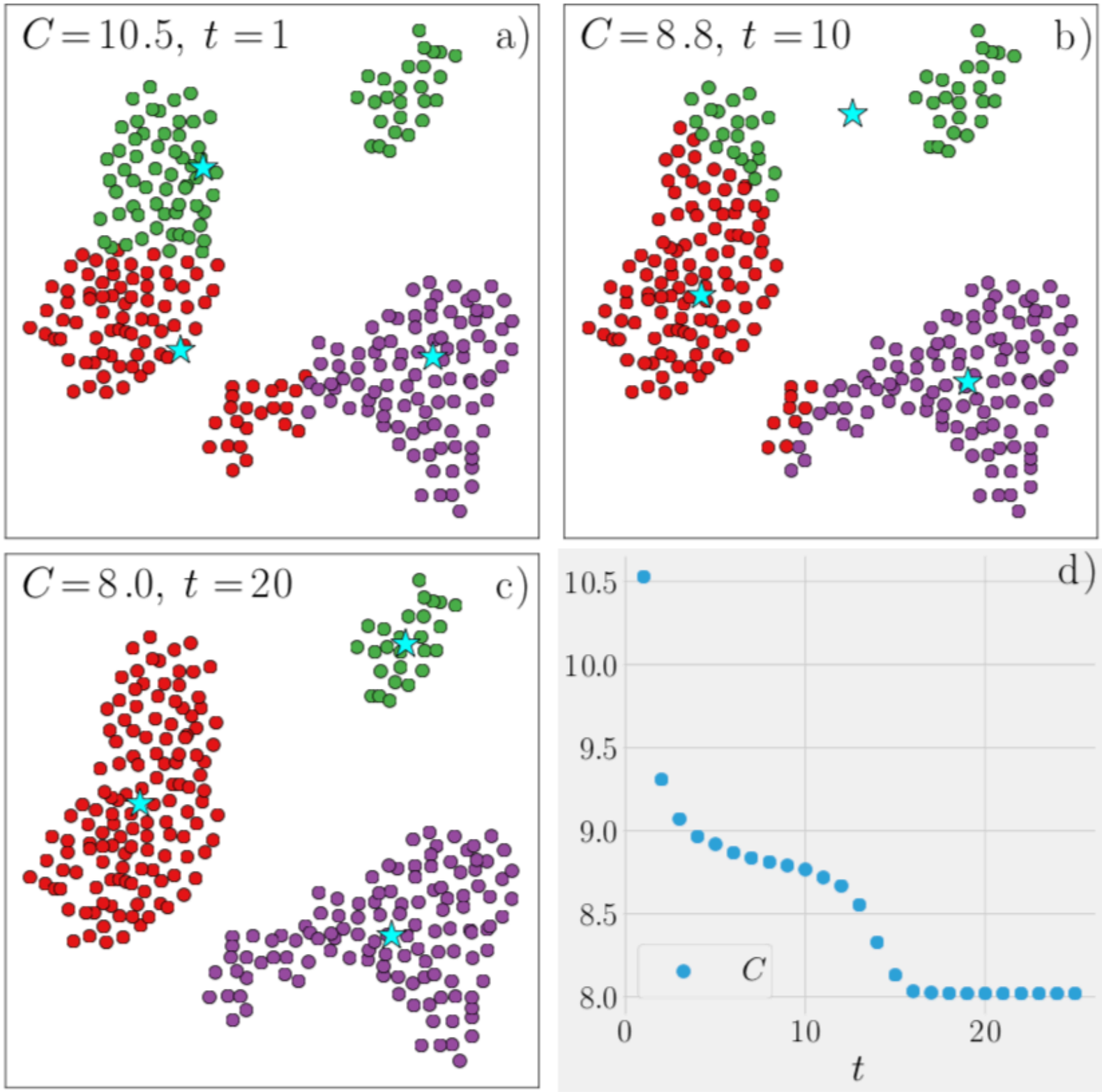
nb color here for visualisation, but not this info not available in real applications!

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

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

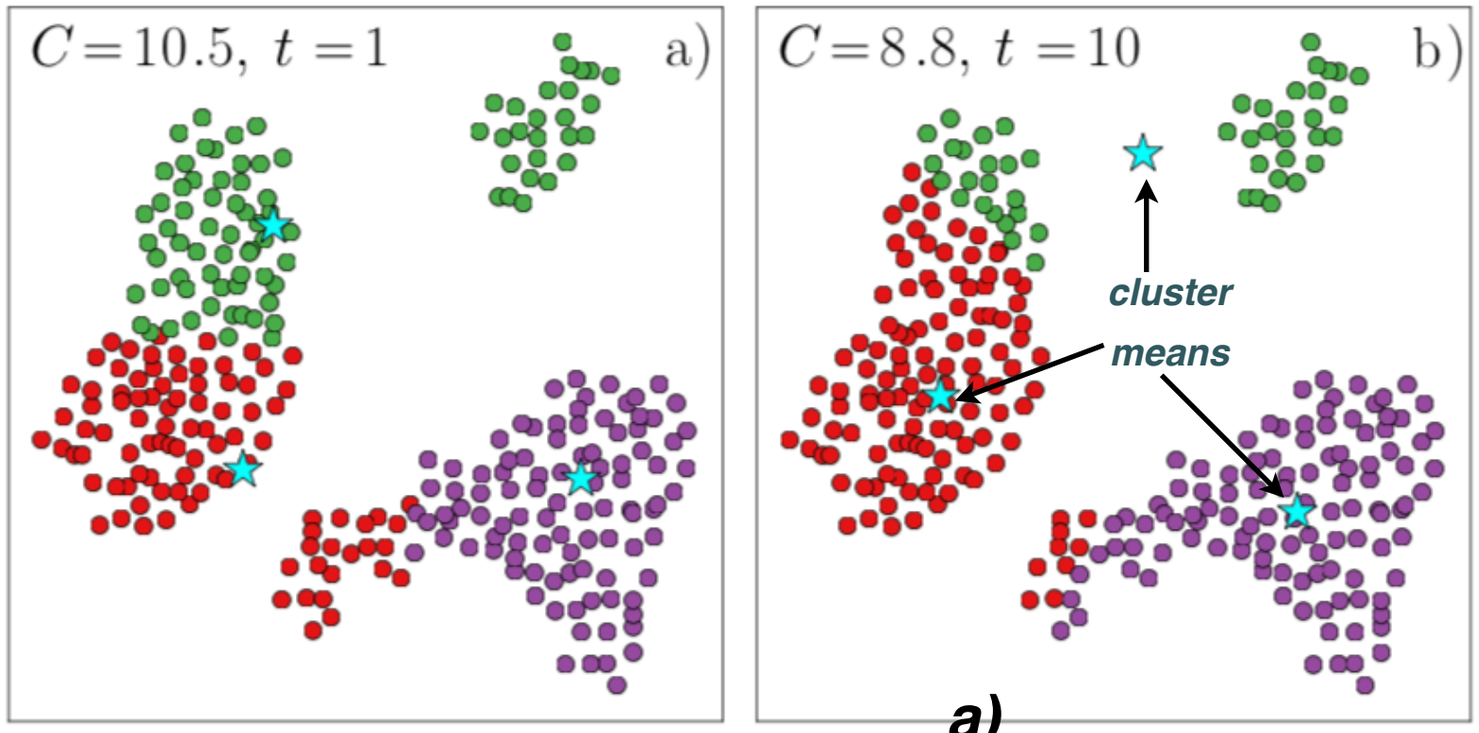
iterate until convergence achieved!

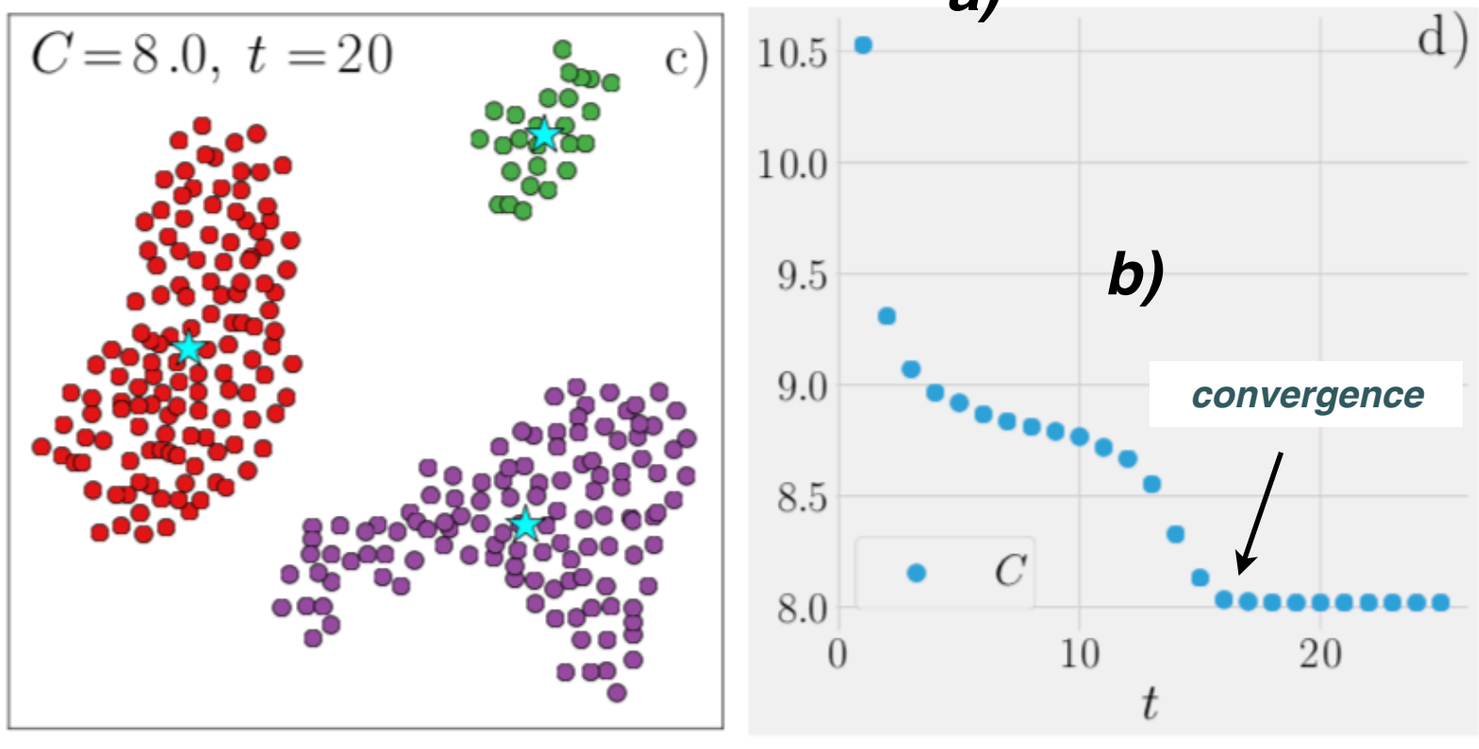
note that here GD not required, optimisation is semi-analytical

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

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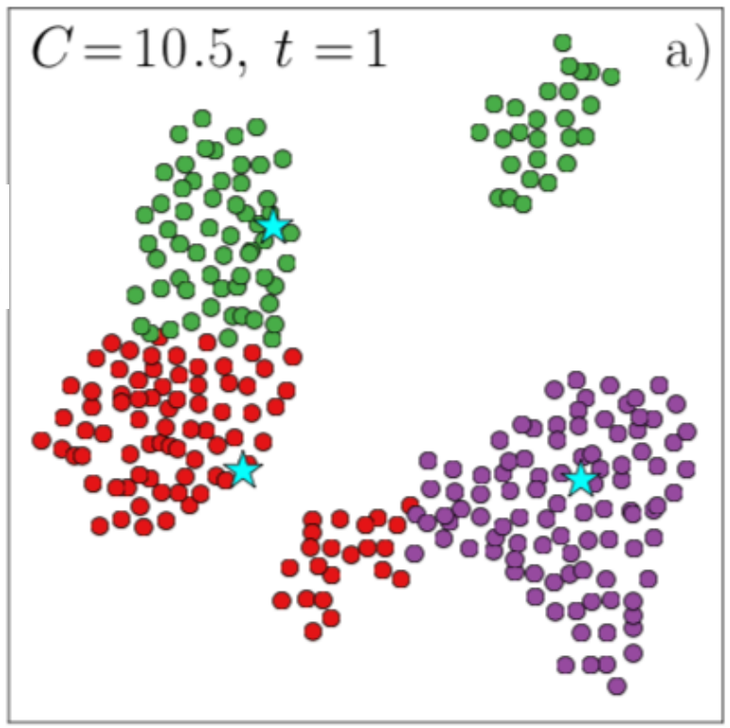
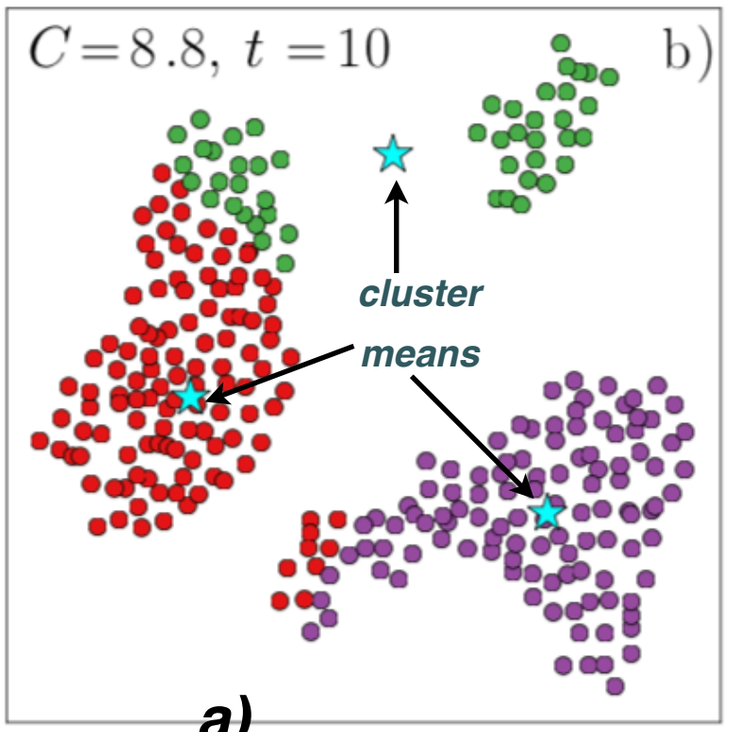
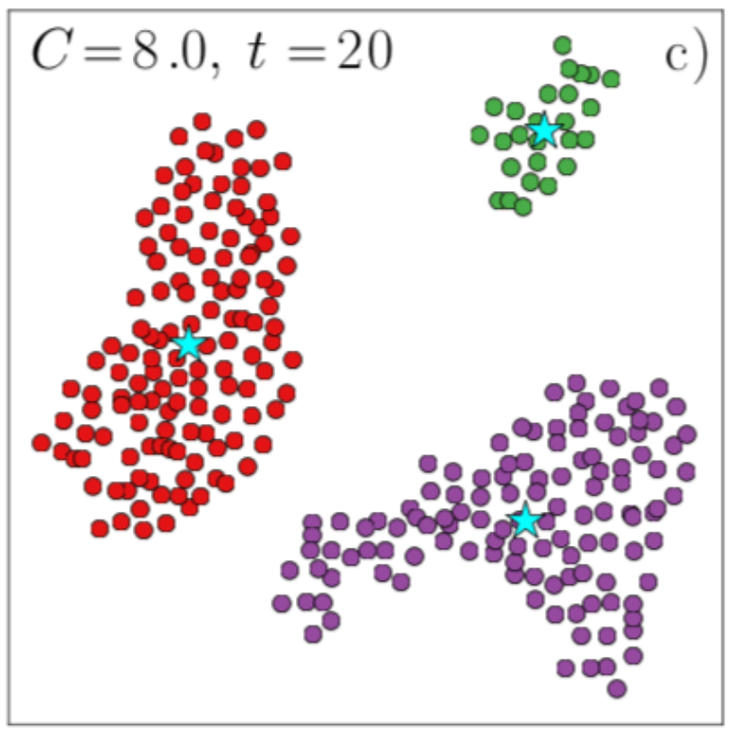
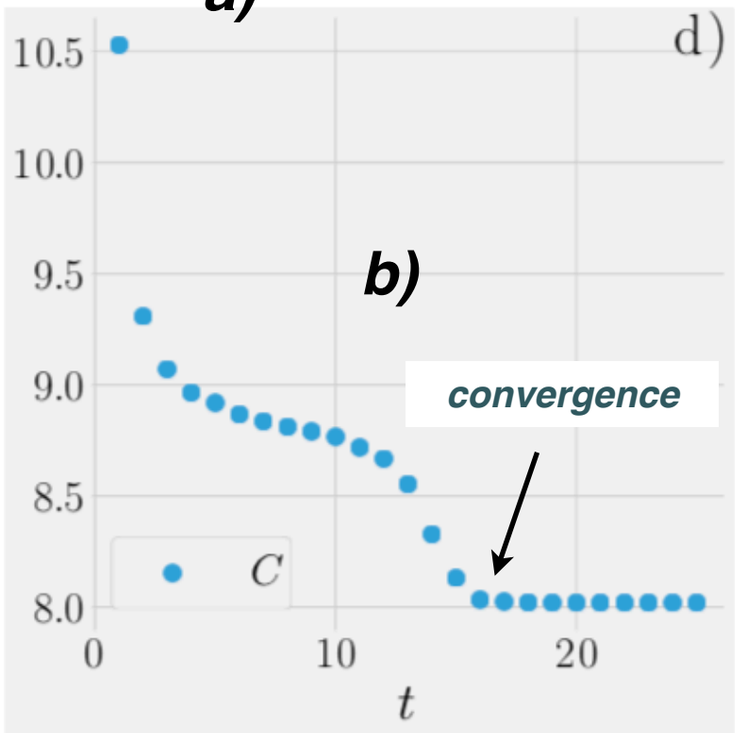




what is the underlying assumption in K-means clustering? And when it would not be justified?



a)



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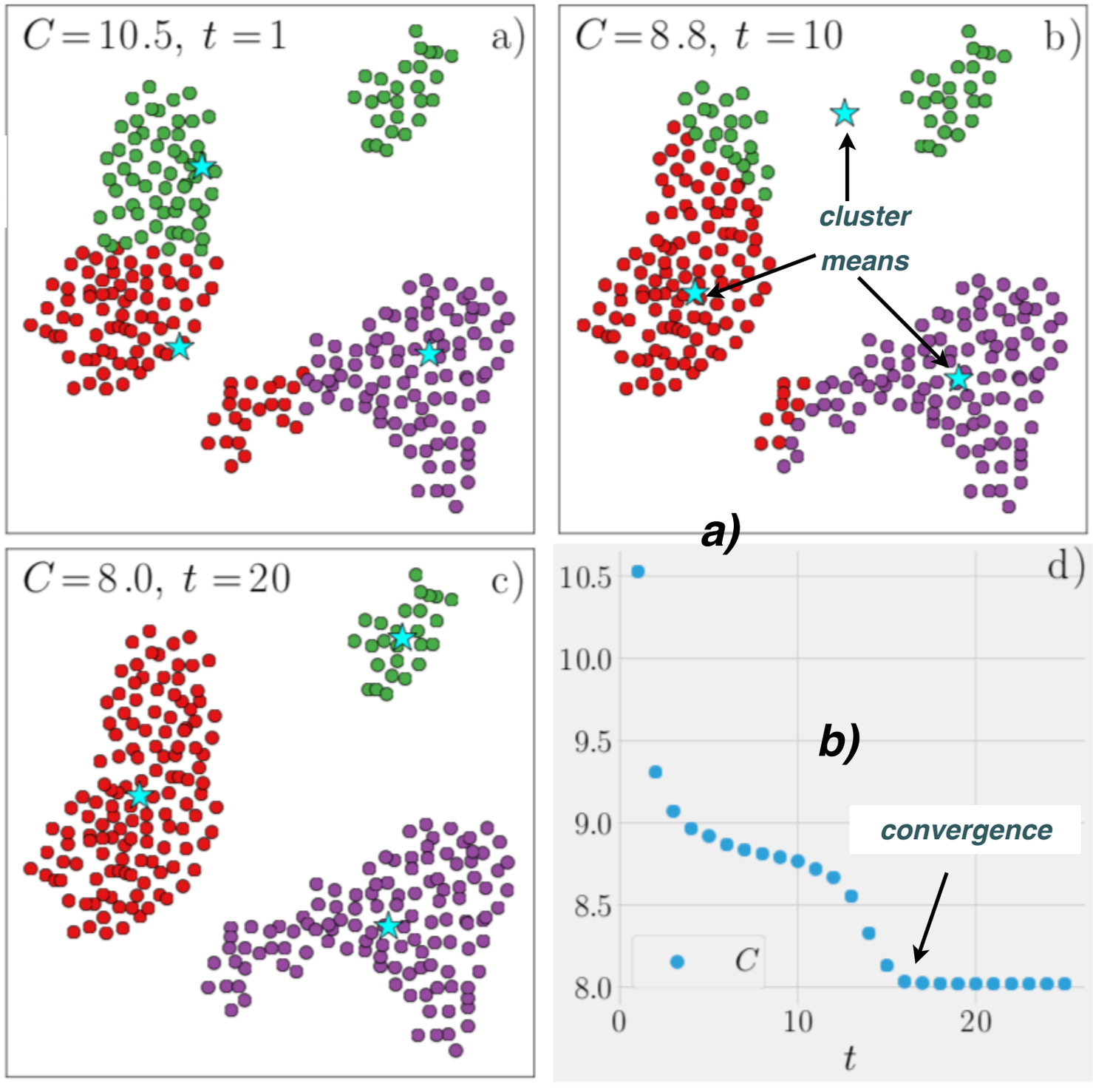


each colour: different cluster

cluster means

a)

b)

*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

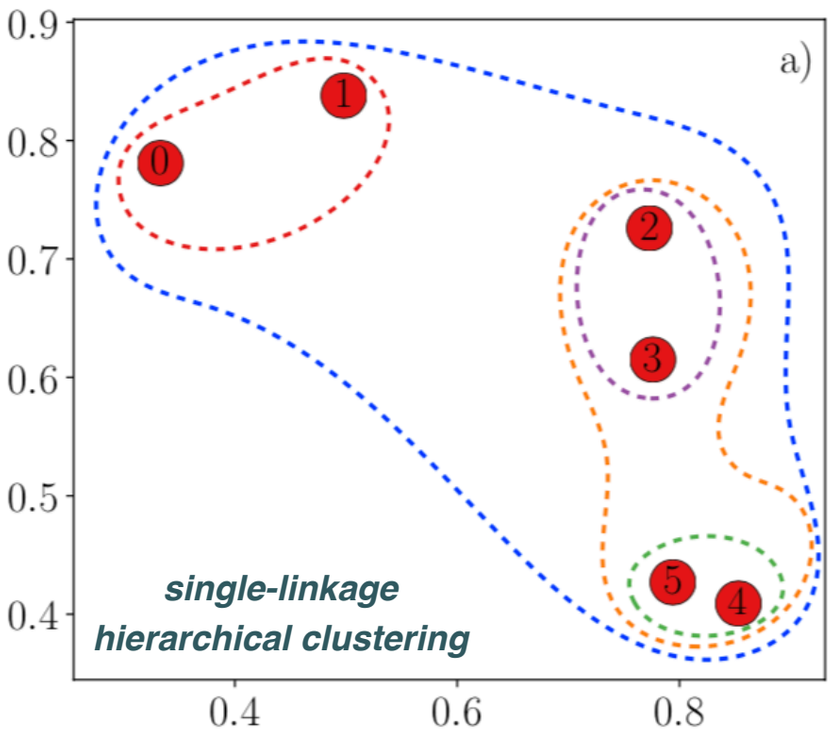
Clearly the results of hierarchical clustering depend on the **choice of distance**

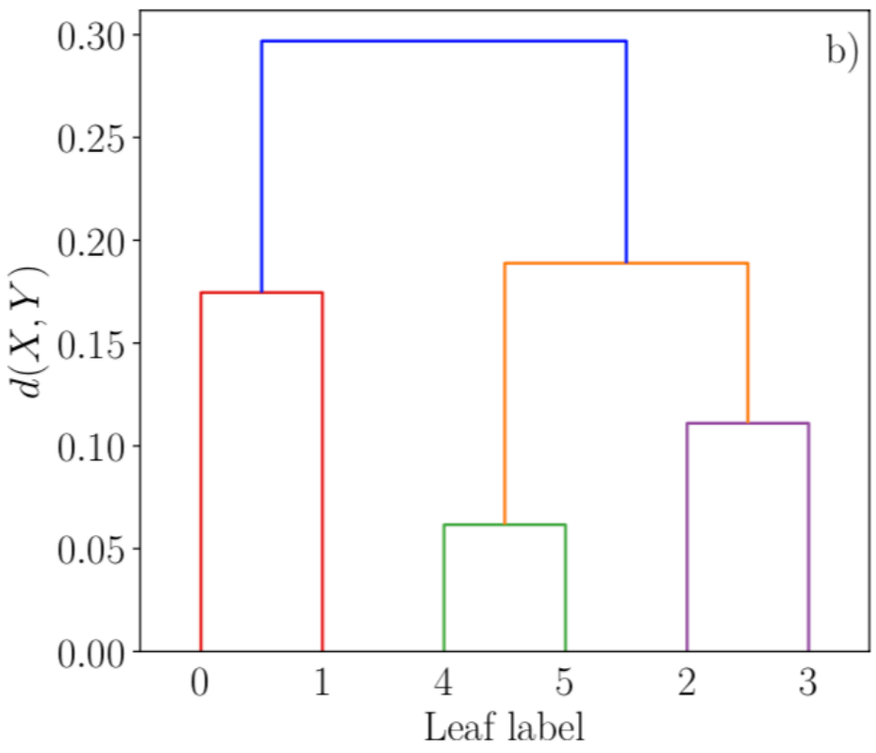
distance between clusters

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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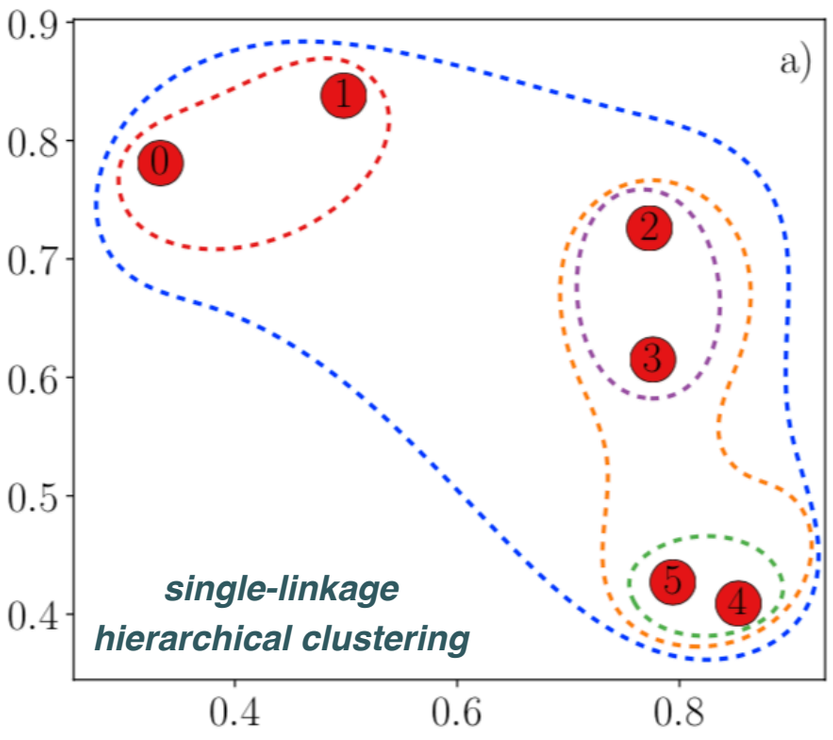
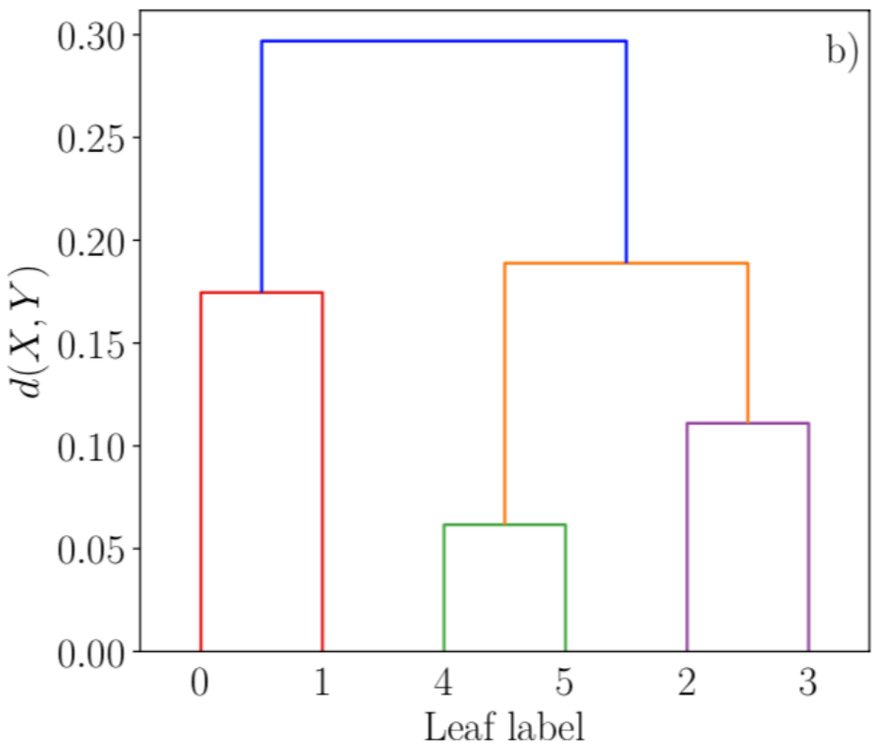




hierarchical clustering methods do not scale well for large *N*, so they are typically **combined with *K*-means clustering** in the initial steps to define small clusters

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 $\boldsymbol{x}$ 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 $\boldsymbol{x}$ is associated to the *k-th* cluster is

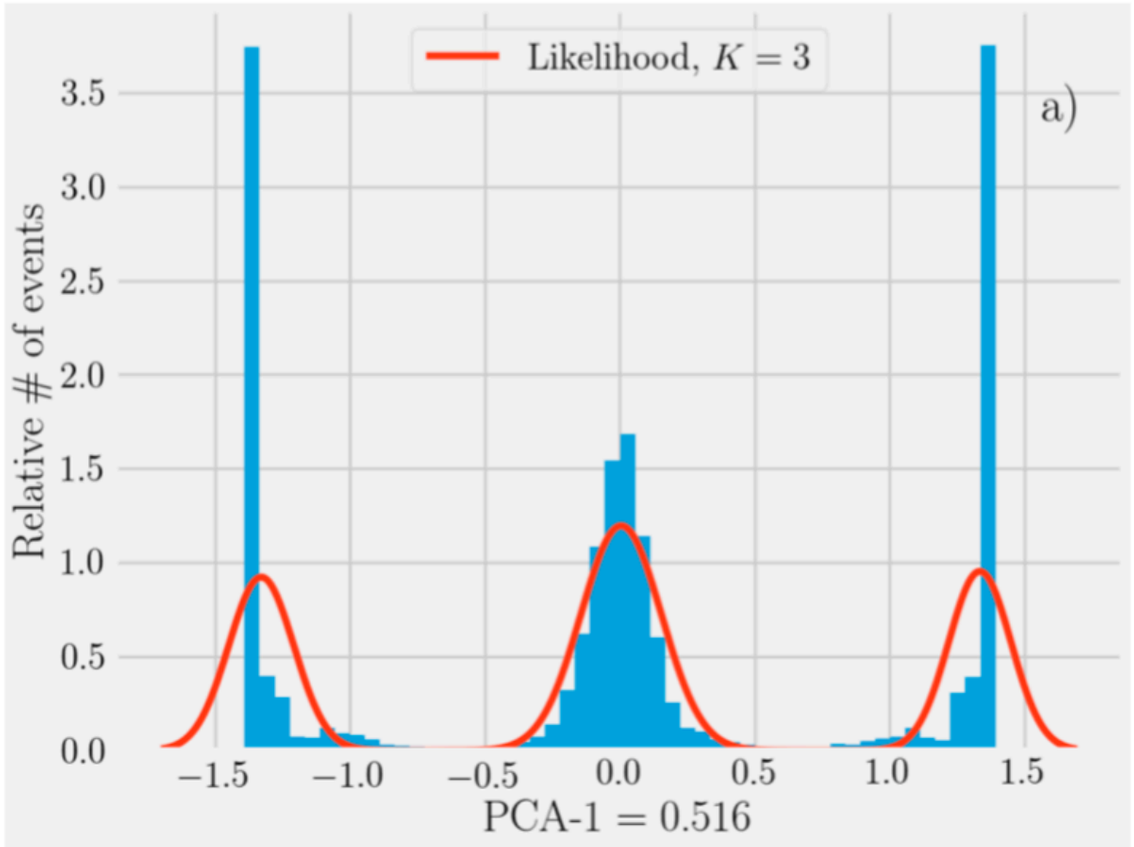
$$\gamma_k(\boldsymbol{x}) \sim \mathcal{N}\left(\boldsymbol{x}\,|\,\boldsymbol{\mu}_k,\boldsymbol{\Sigma}_k\right)\pi_k$$

model parameters found my maximising likelihood using SGD

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

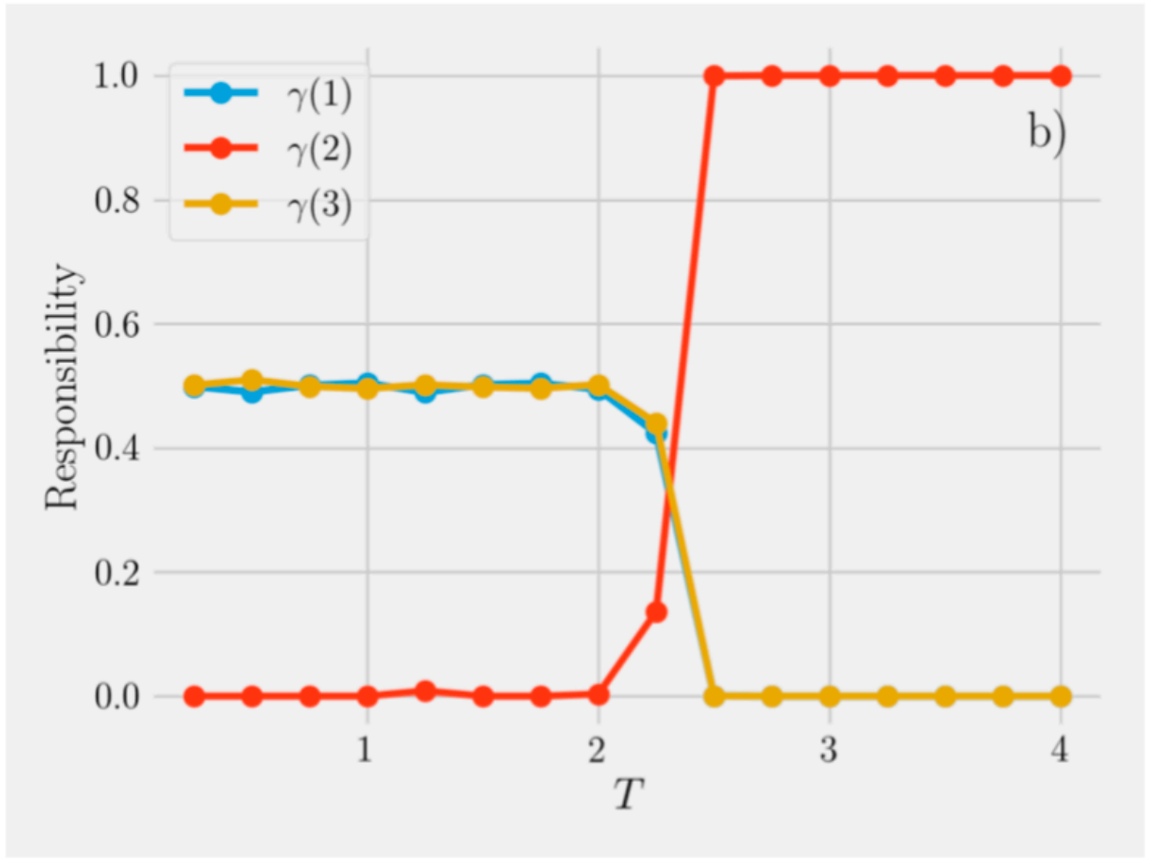
Gaussian Mixture Models

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

Tutorial 3 Exercise 3a

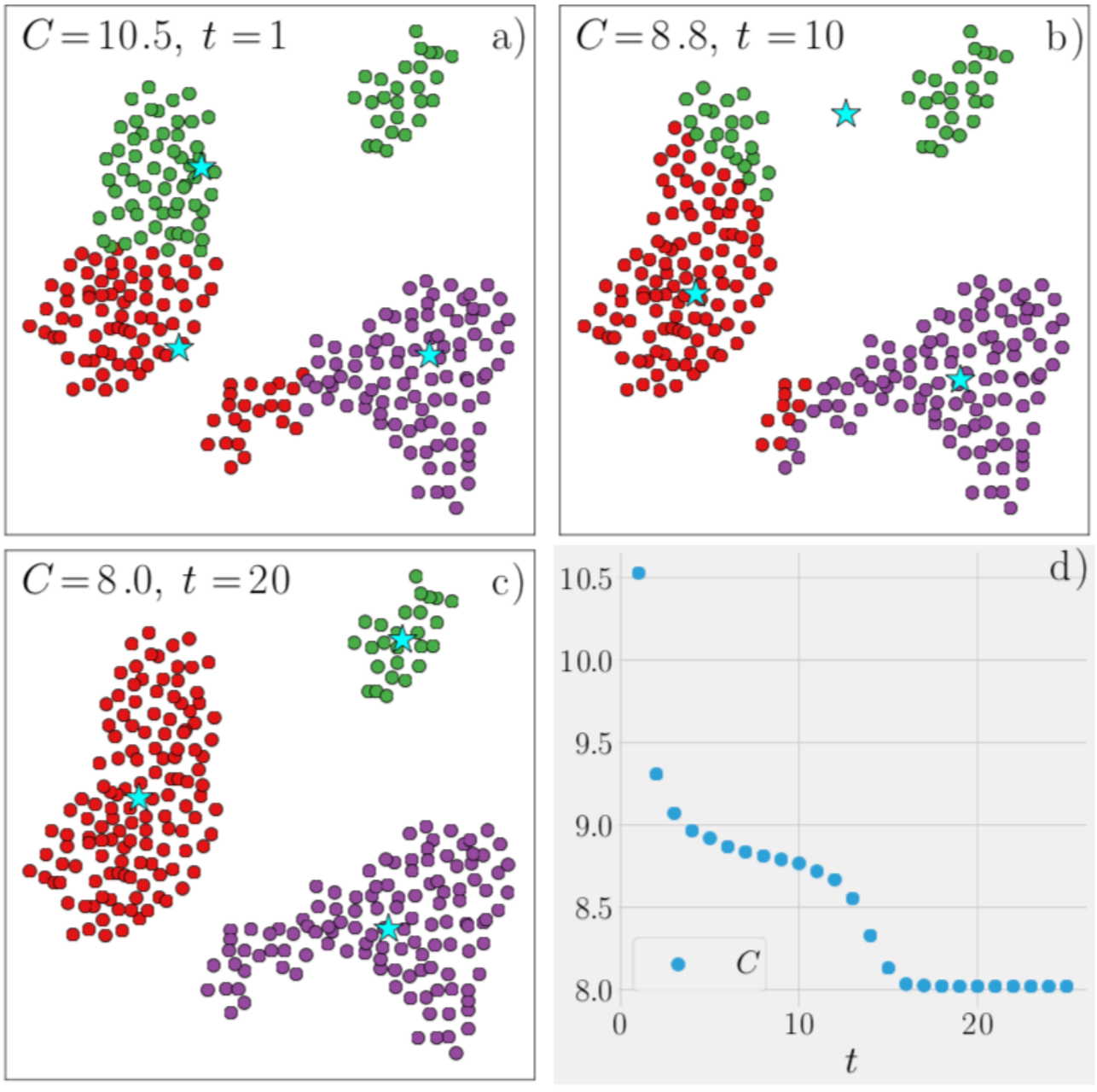
starting point is the **Python script** that you will find in

https://github.com/juanrojochacon/ml-ditp-attp/blob/master/Tutorials/Tutorial3/

- Become familiar with the ideas underlying Unsupervised Learning with their application to **clustering**

- Compare the performance of different clustering algorithms, and study different ways of representing the training data

- How do results depend on your assumptions concerning the definition of the distance between points



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

Dimensional reduction

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

``the curse of dimensionality'

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*

Dimensional reduction

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

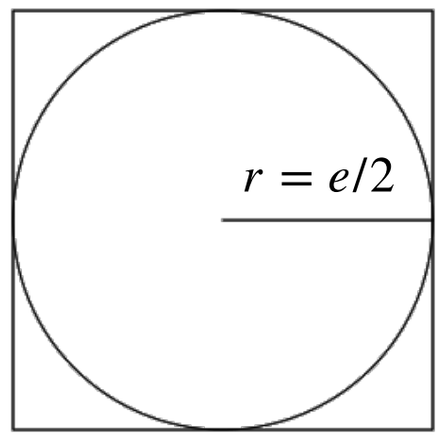
High-dimensional data lives near the edge of the sample space

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

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

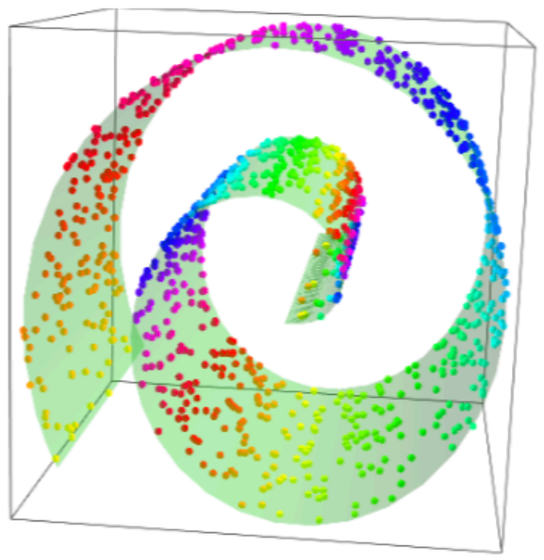
Traditional data visualisation methods are not practical when the datasets involve a large number of features (such as images) and we need to project the data onto a lower-dimensional space, called the **latent space,** using **dimensional reduction**

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

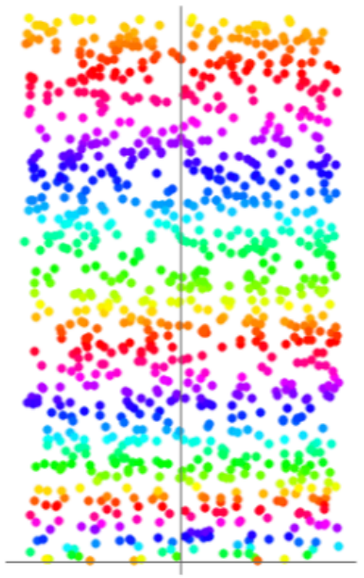
- *High-dimensional data lives near the edge of the sample space*
- *We need to conserve information on original pair-wise distances or similarities when transforming to the latent space*

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***



Dimensional reduction

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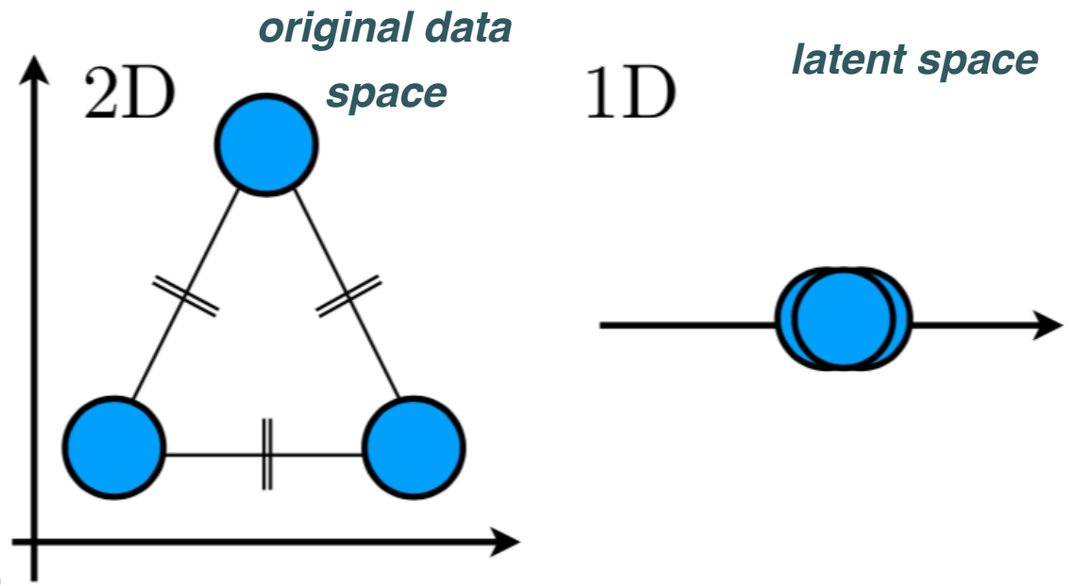
This is easier said that done: many pitfalls associated to high-dimensionality datasets

- *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*
- *Dimensional reduction cannot be such to destroy info on original patterns in the data*

``the crowding problem"



Dimensional reduction

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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**

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

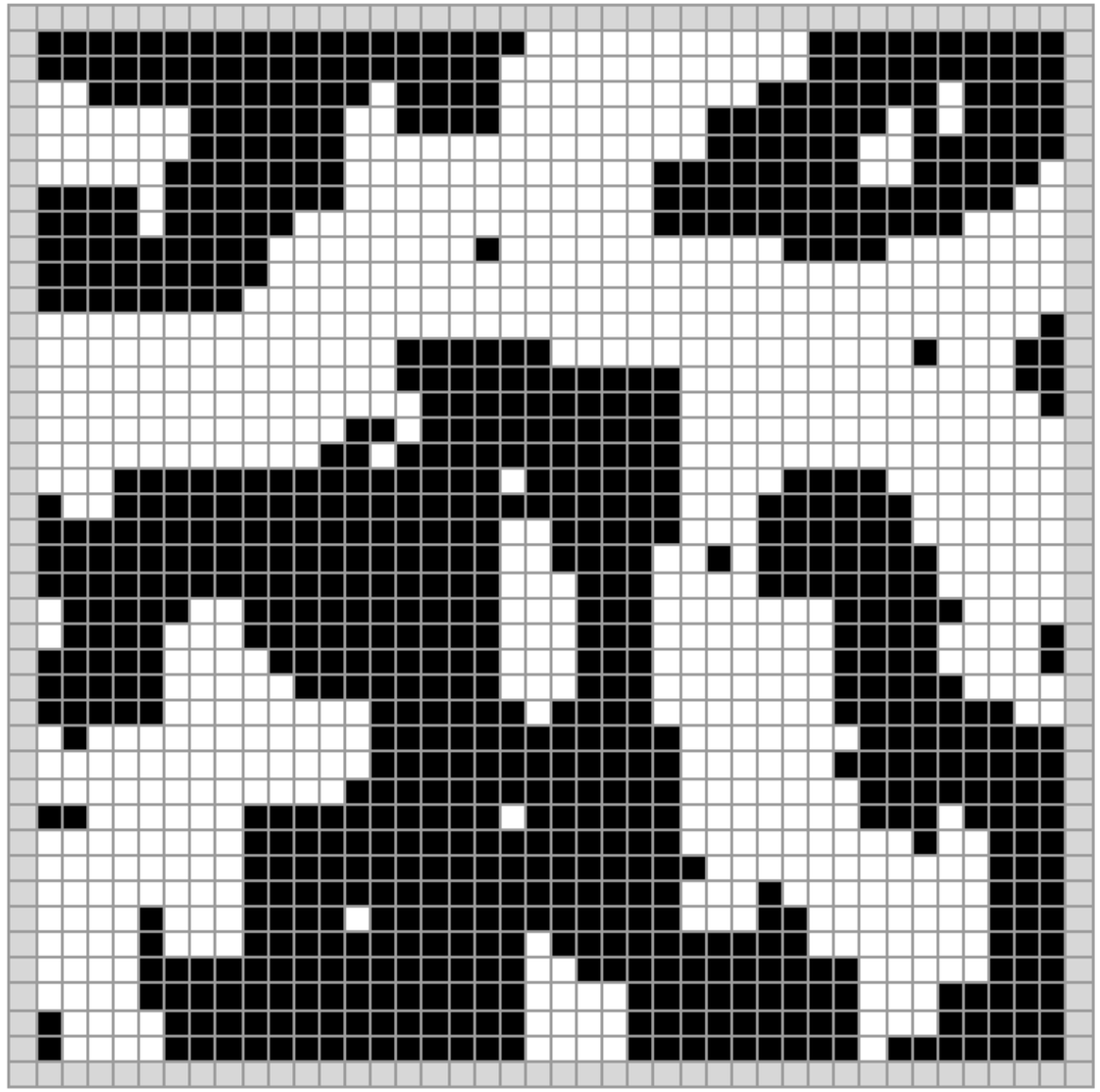
PCA projections often capture the **large-scale structure** of high-dimensional datasets

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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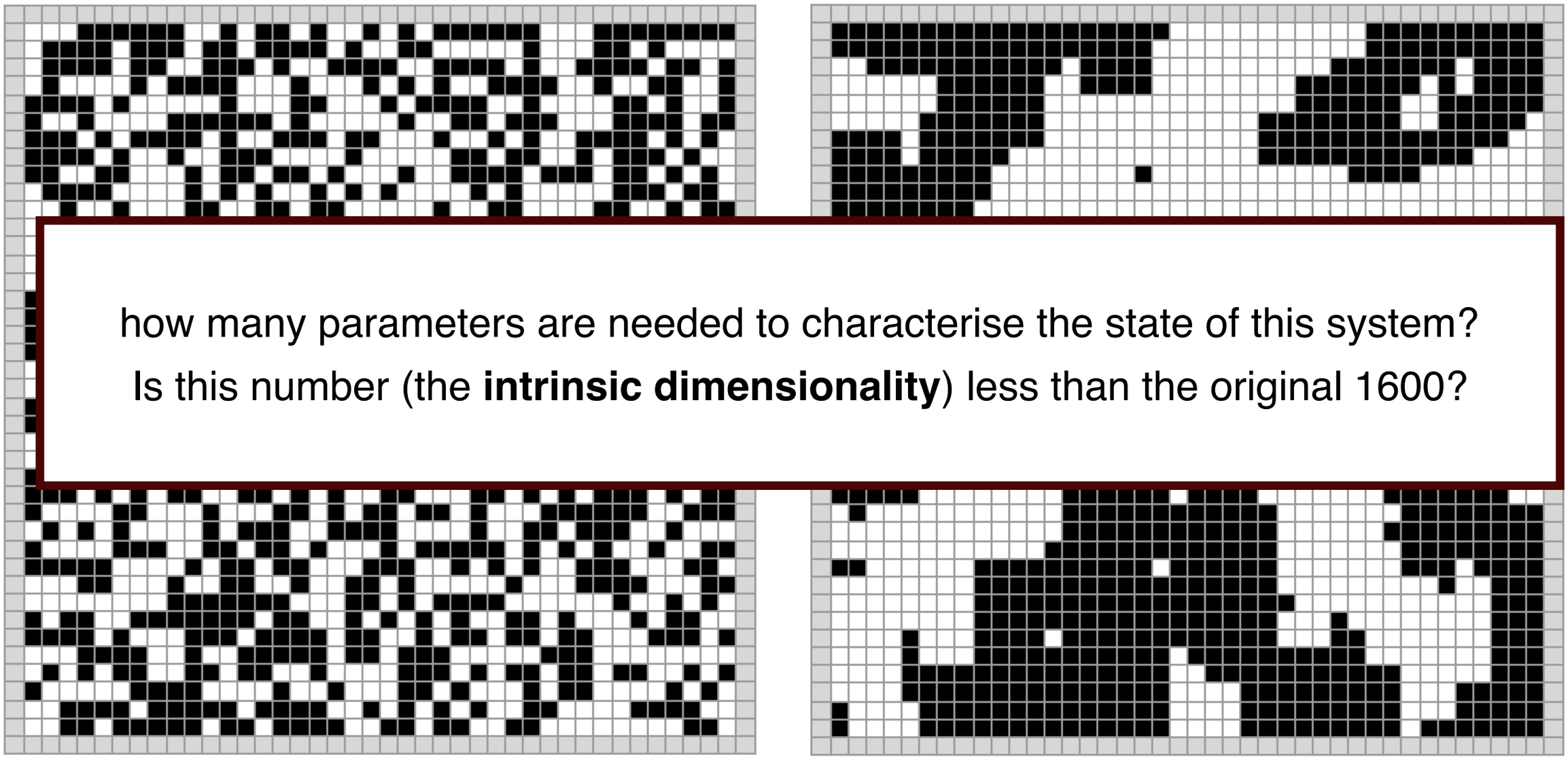

how many parameters are needed to characterise the state of this system?

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

$$\boldsymbol{\Sigma}(X) = \frac{1}{n-1} X^T X \quad \rightarrow \quad \underset{\substack{\textit{p-dimensional} \\ \textit{in space of features}}}{\boldsymbol{\Sigma}_{lm}} = \frac{1}{n-1} \overset{\textit{sum over data points}}{\sum_{i=1}^{n}} X_{li} X_{im}$$

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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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

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

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

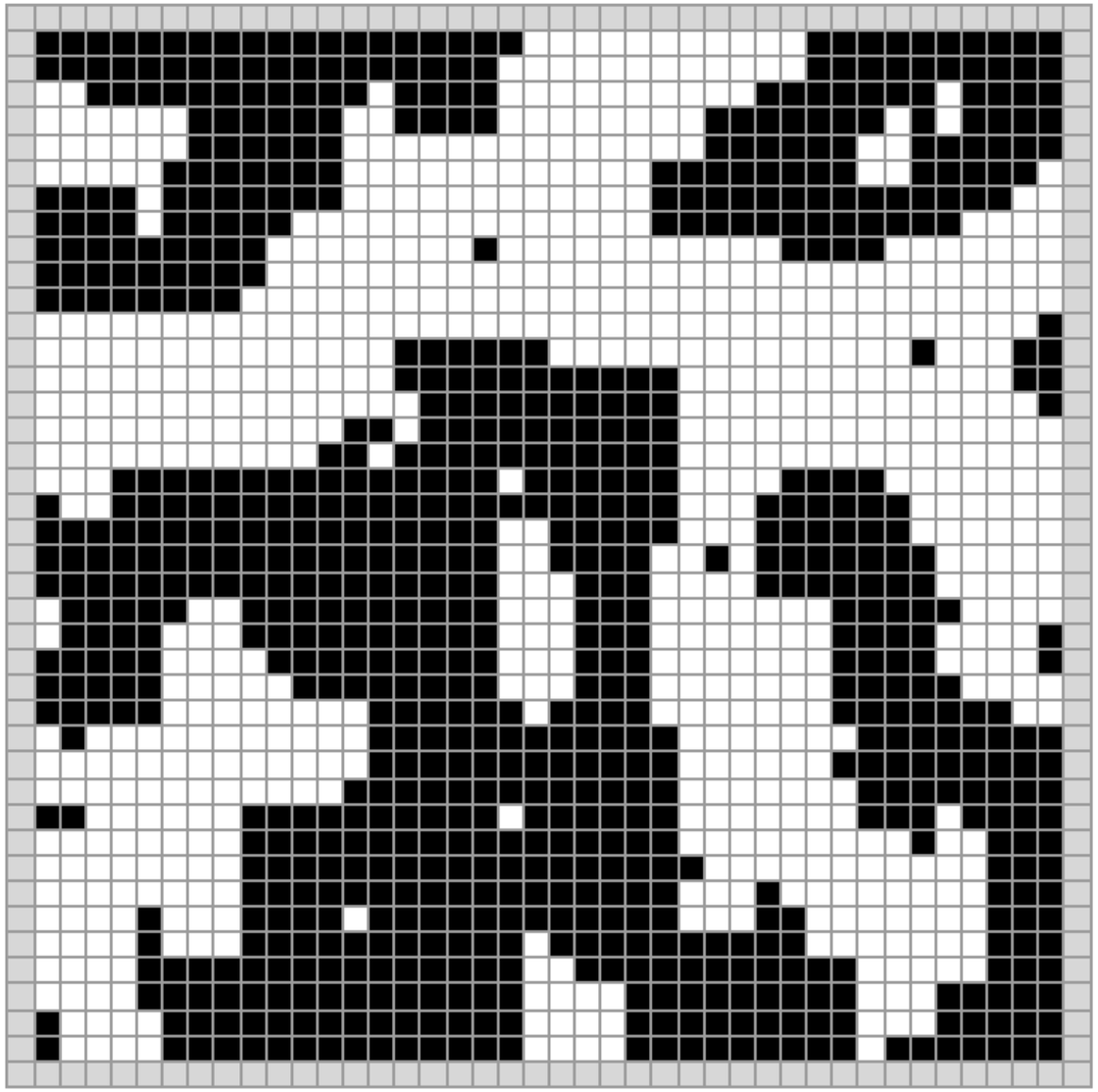
PCA projections often capture the **large-scale structure** of high-dimensional datasets

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



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Principal Component Analysis

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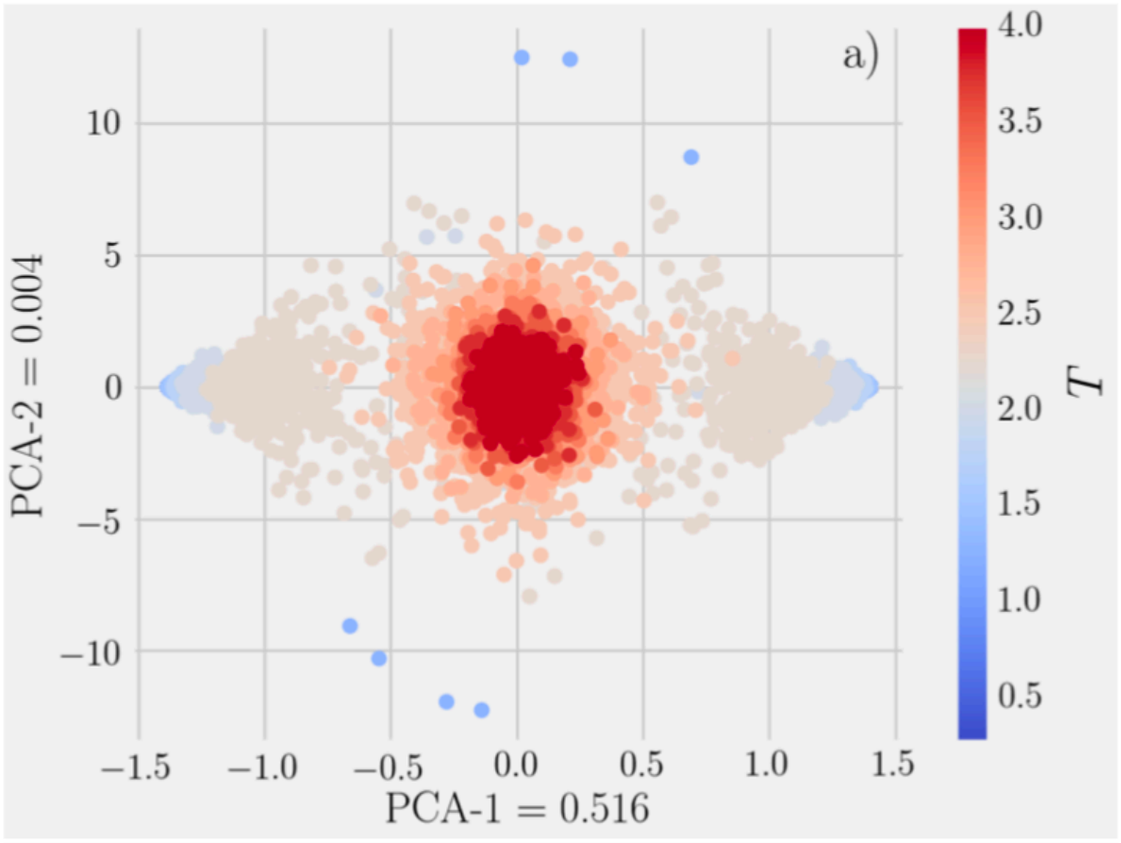
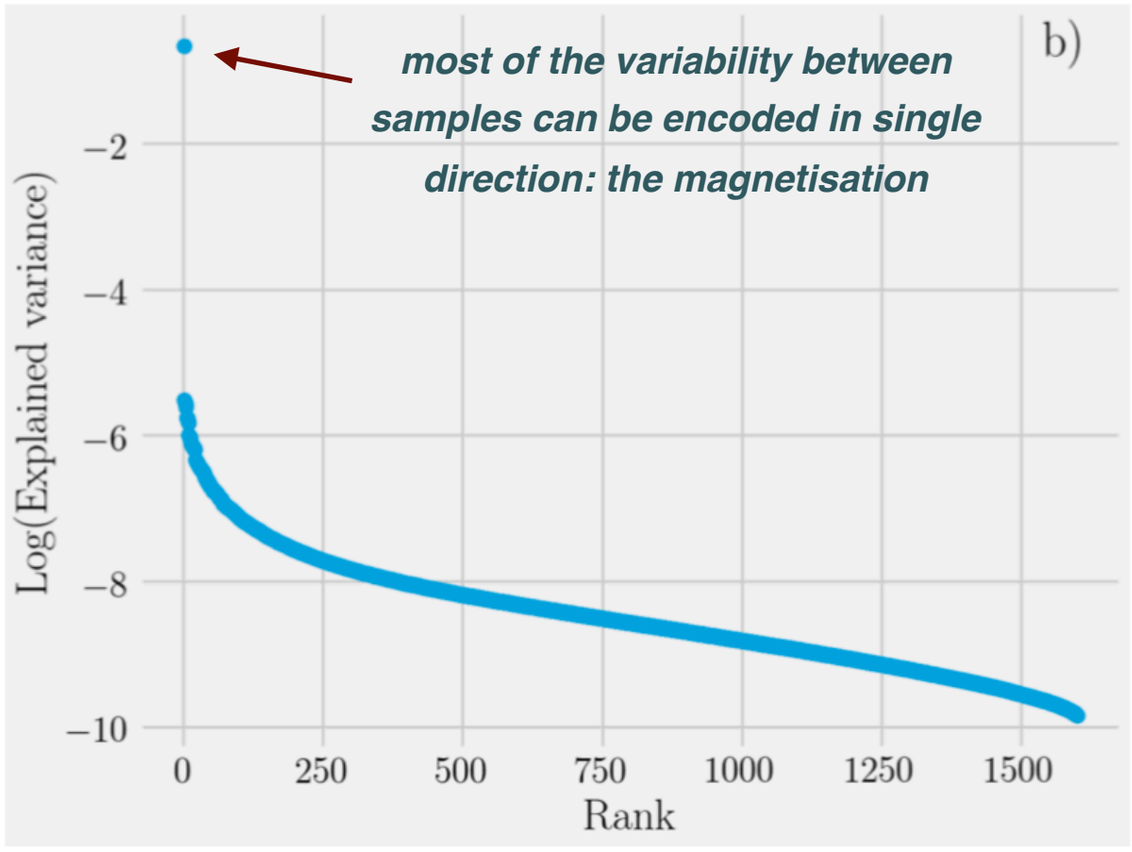
1000 samples for each T



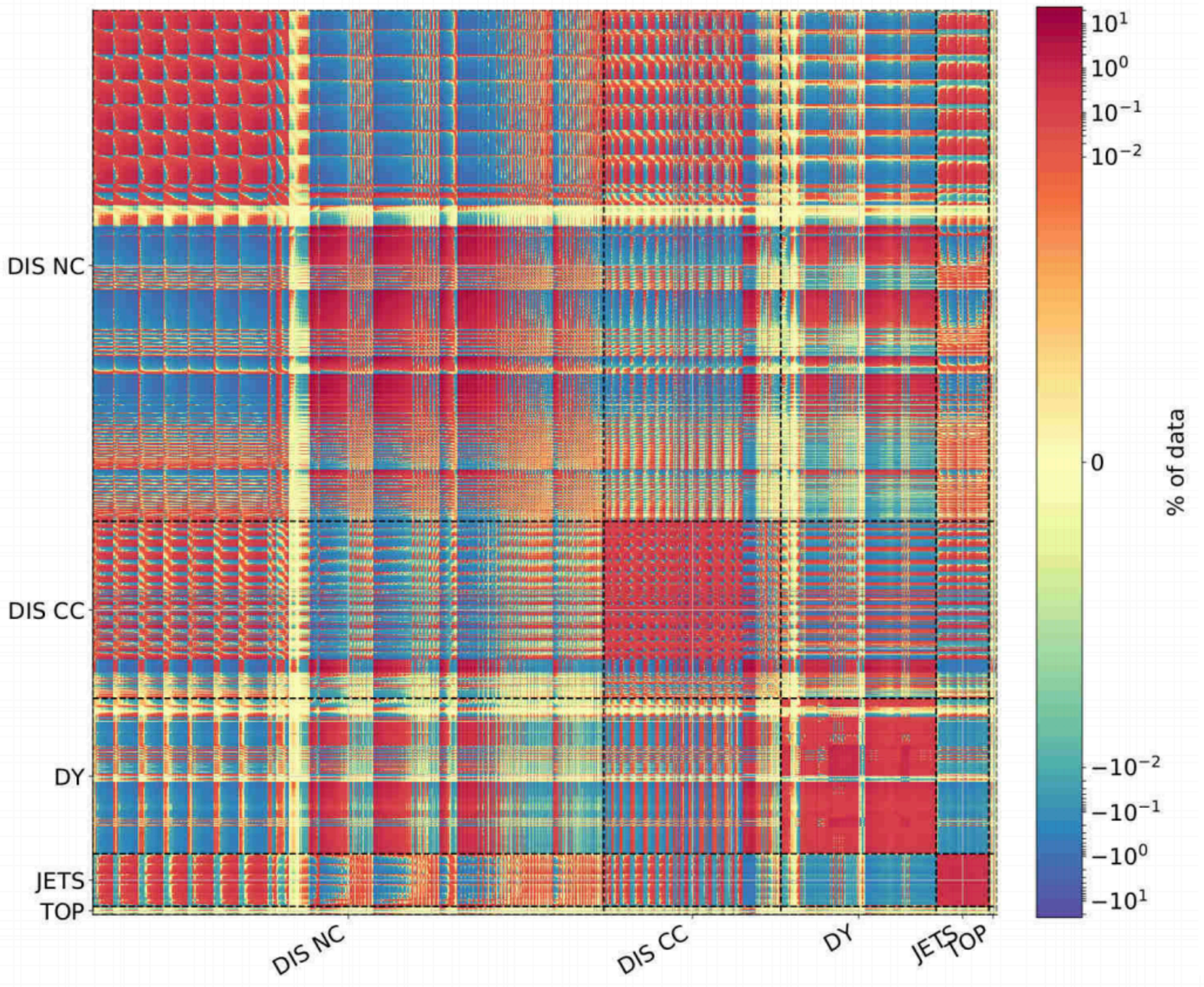


The first principal component accounts for > 50% of total variability!

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

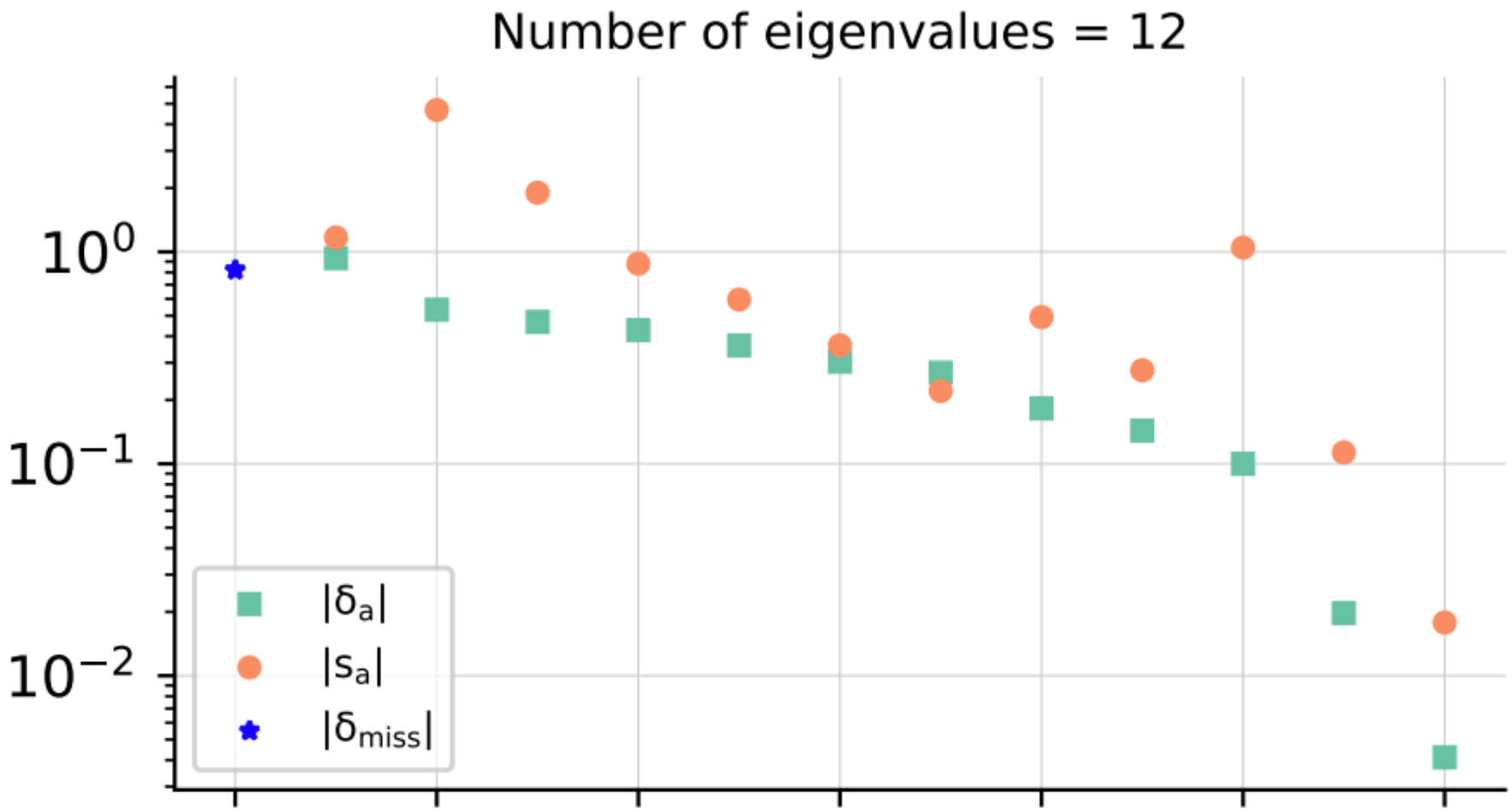
assume that some gives you the **covariance matrix of theory errors** of a global PDF fit (3000-dimensional space!). What are the **relevant components**?



Process Type	Dataset	Reference	N_{dat}	N_{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^{ll}_T, M_{ll})	[46]	44	
	ATLAS Z p_T 8 TeV (p^{ll}_T, 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^{ll}_T, 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 σ^{top}_{tt}	[48,49]	3	26
	ATLAS $t\bar{t}$ rap	[50]	10	
	CMS σ^{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)

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

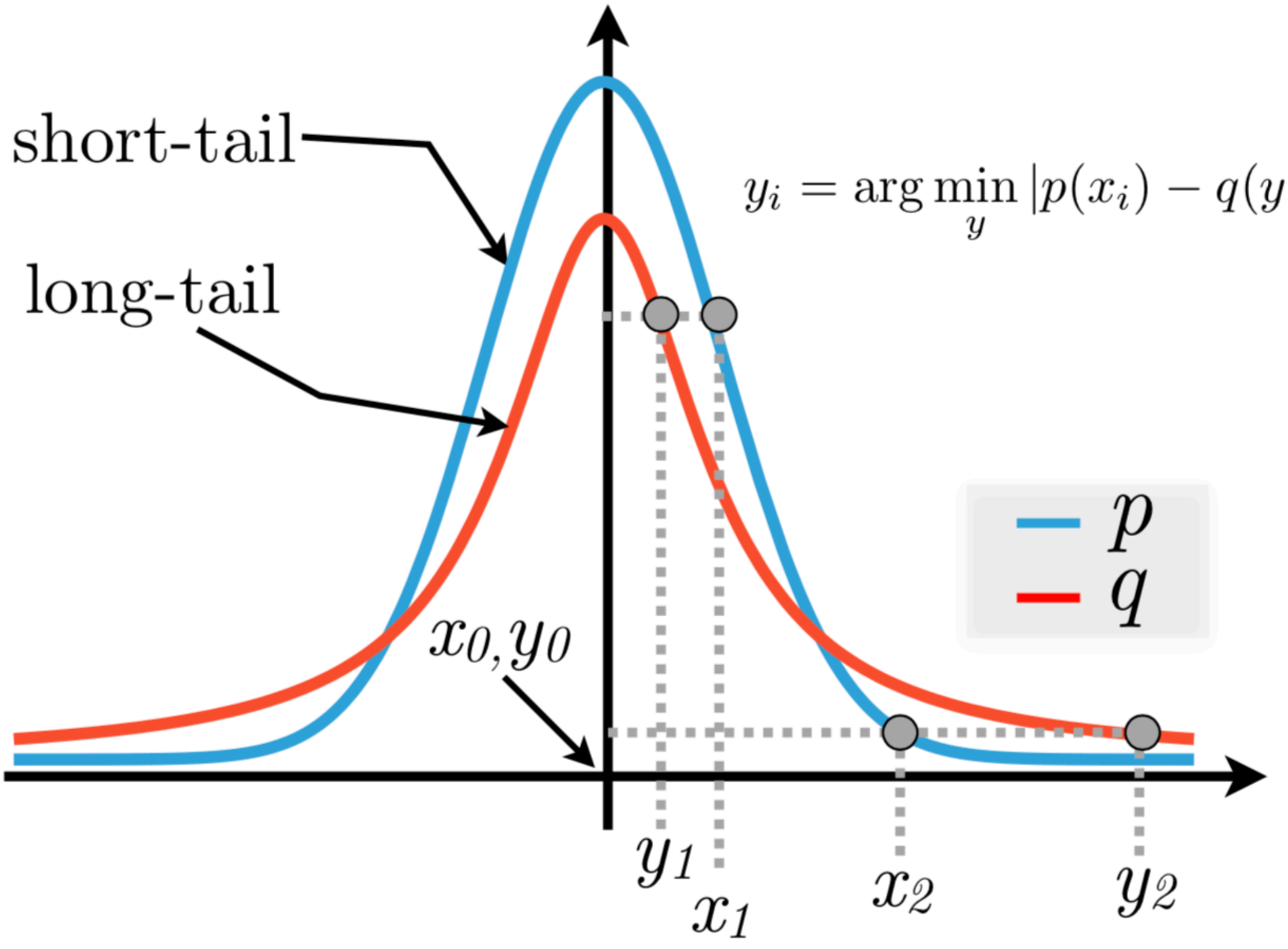
Jensen-Shannon divergence

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

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

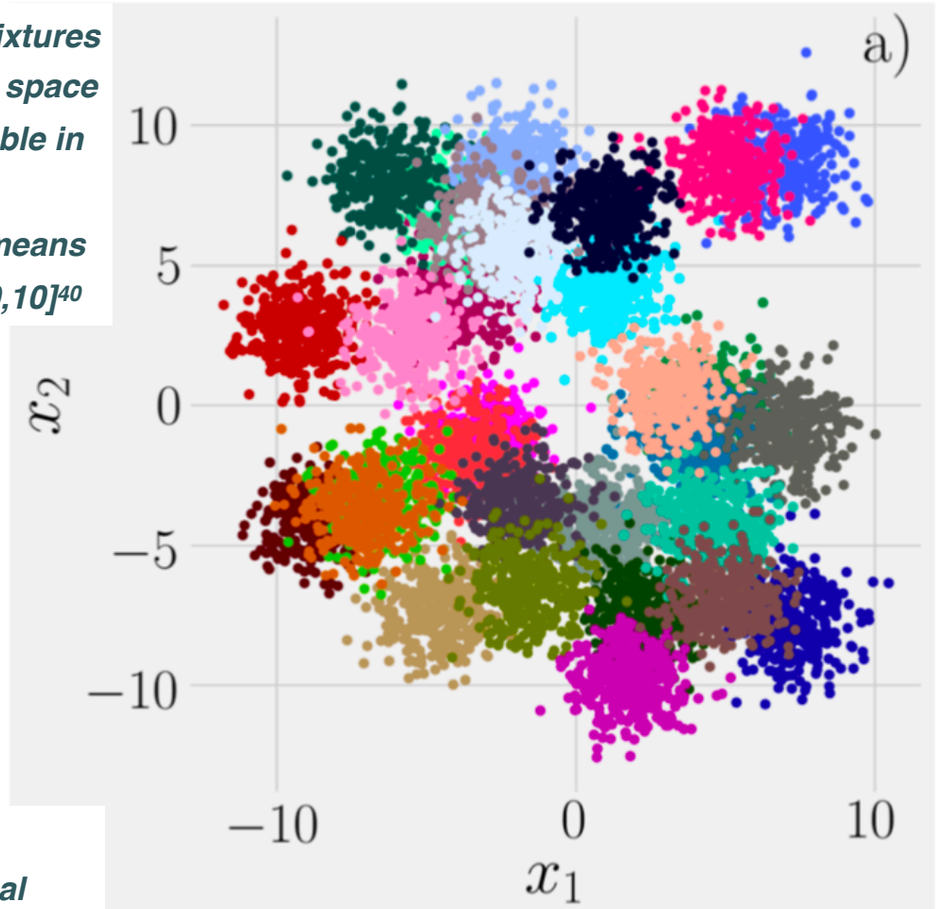
in general the integral cannot be computed and one needs to sample the two probability distributions by means of a suitable binning

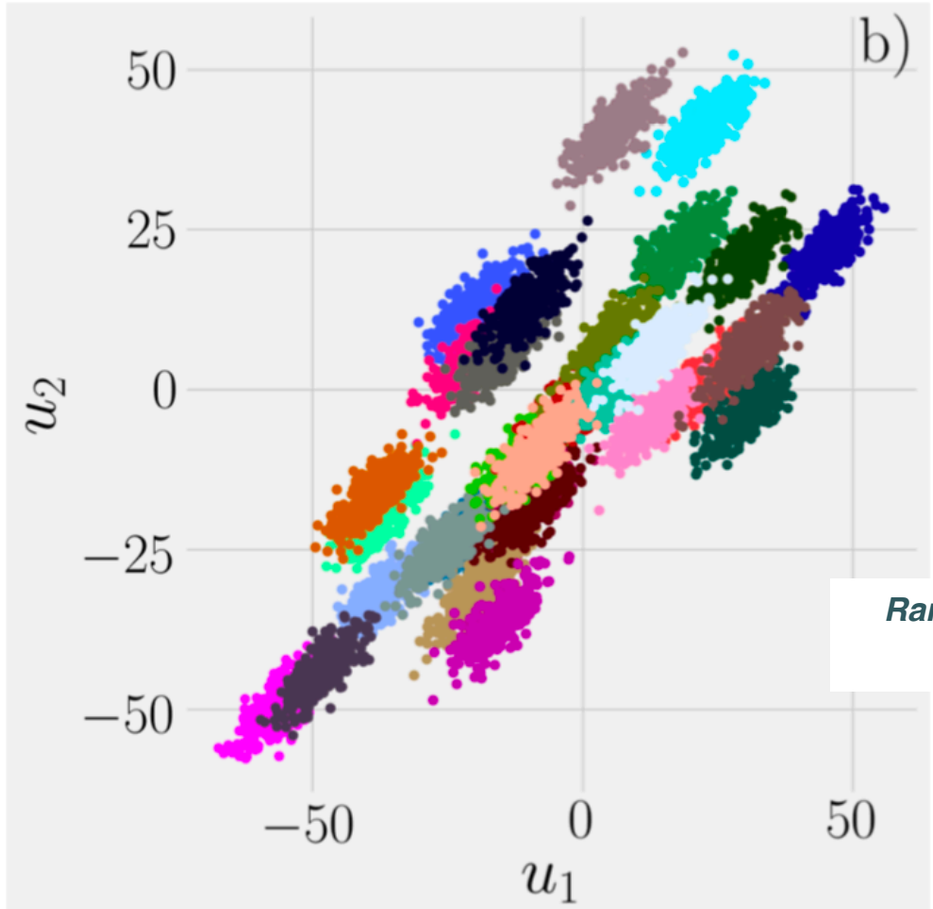
t-SNE



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

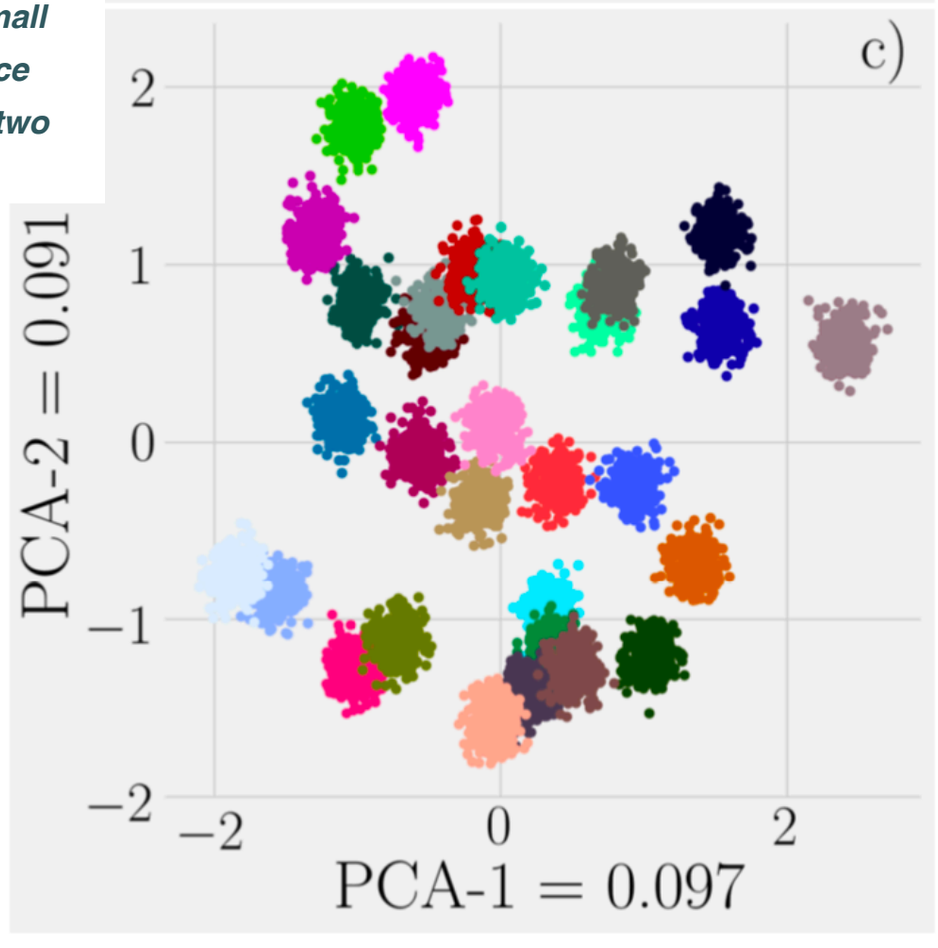
K=30 Gaussian mixtures in 40-dimensional space (labels not available in real case!)
Same variance, means at random in $[-10,10]^{40}$

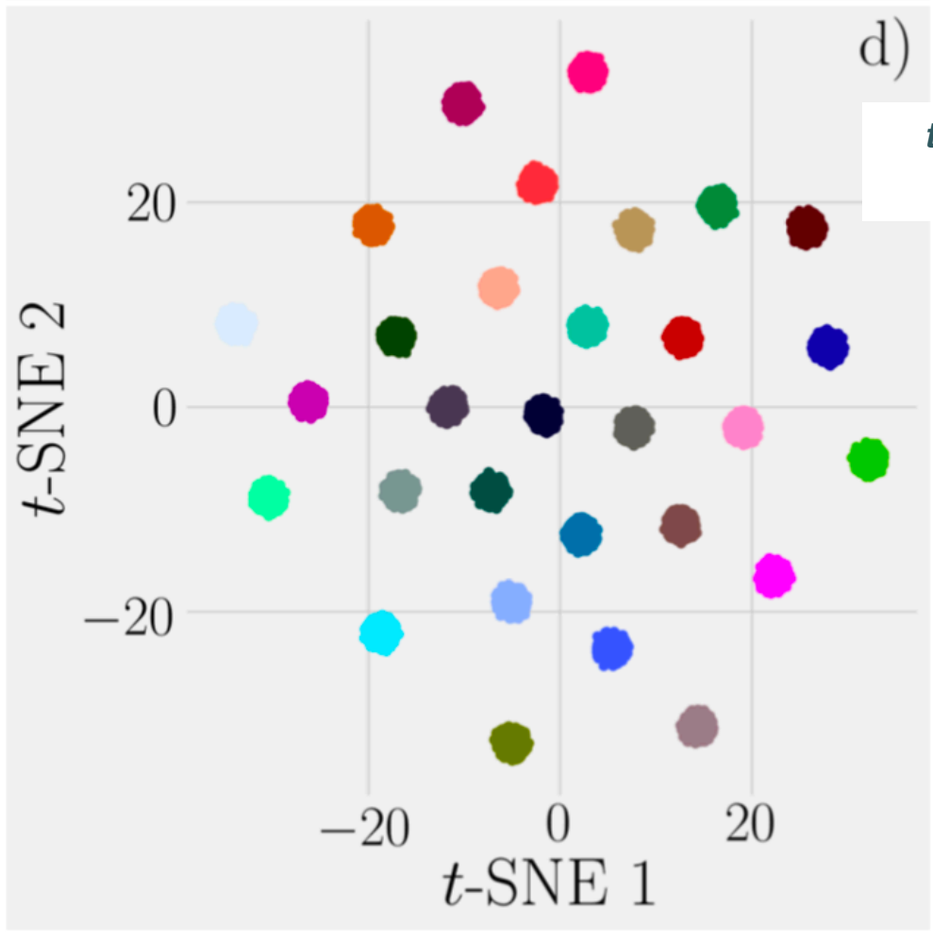




Random projection to 2D space

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





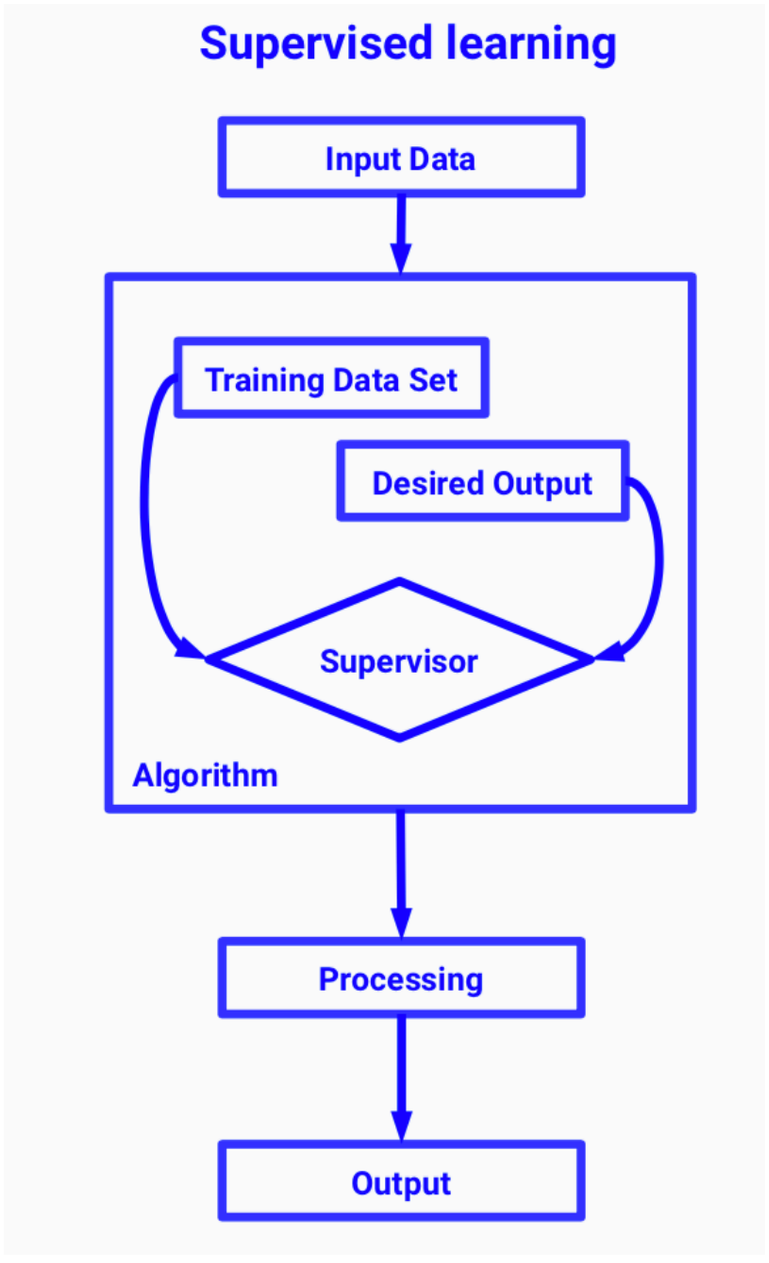
t-SNE embedding to 2D latent space

rning

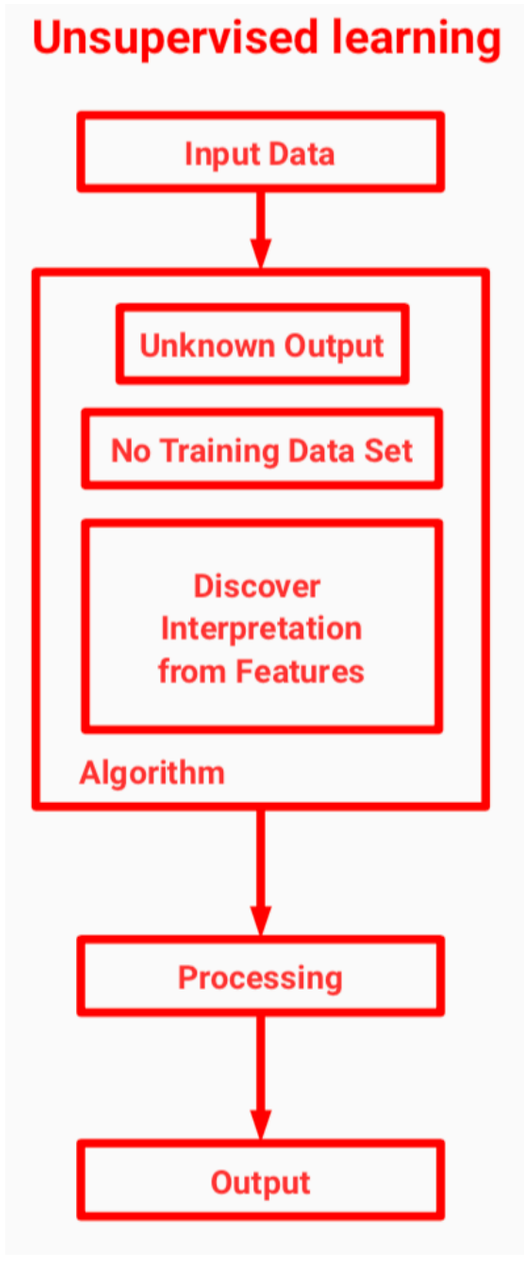
Reinforcement Learning

with input from A*n overview of Reinforcement Learning and Multi-Agent Systems,* Alberto Guffanti, NNPDF meeting August 2019, https://indico.cern.ch/event/825705/

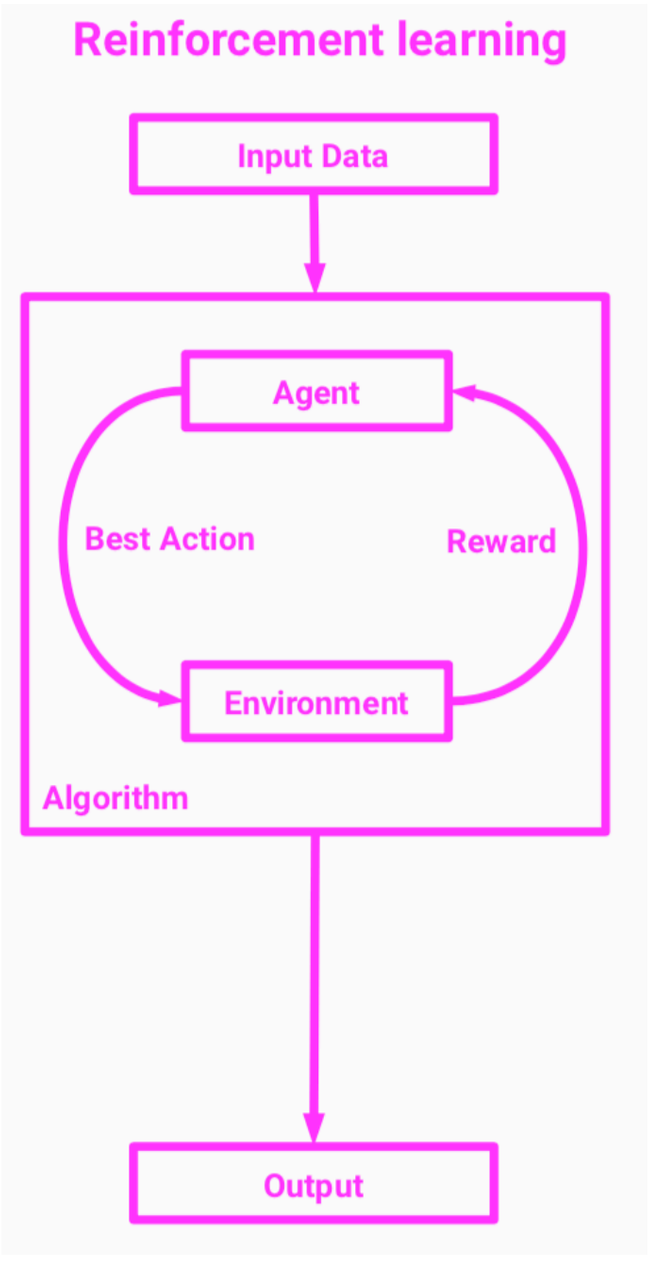
Supervised vs Unsupervised Learning



Lectures 1+2



Lecture 3



Lecture 3

Reinforcement Learning

So far we have considered **two main paradigms** in Machine Learning problems

Supervised Learning: starting from a training dataset with **labelled examples,** $\{x_i, y_i\}_{i=1,N}$, produce a **model f(x)** that predicts and generalises the info in the training sample.
The labels y_i can be continuous (underlying law is function) or discrete (classification)

Unsupervised Learning: starting from a training dataset with **unlabelled examples,** $\{x_i\}_{i=1,N}$, produce a **model** that takes a sample as input and as output produces the solution of a practical problem, such as **clustering**, **dimensional reduction**, or **outlier detection**

Reinforcement Learning

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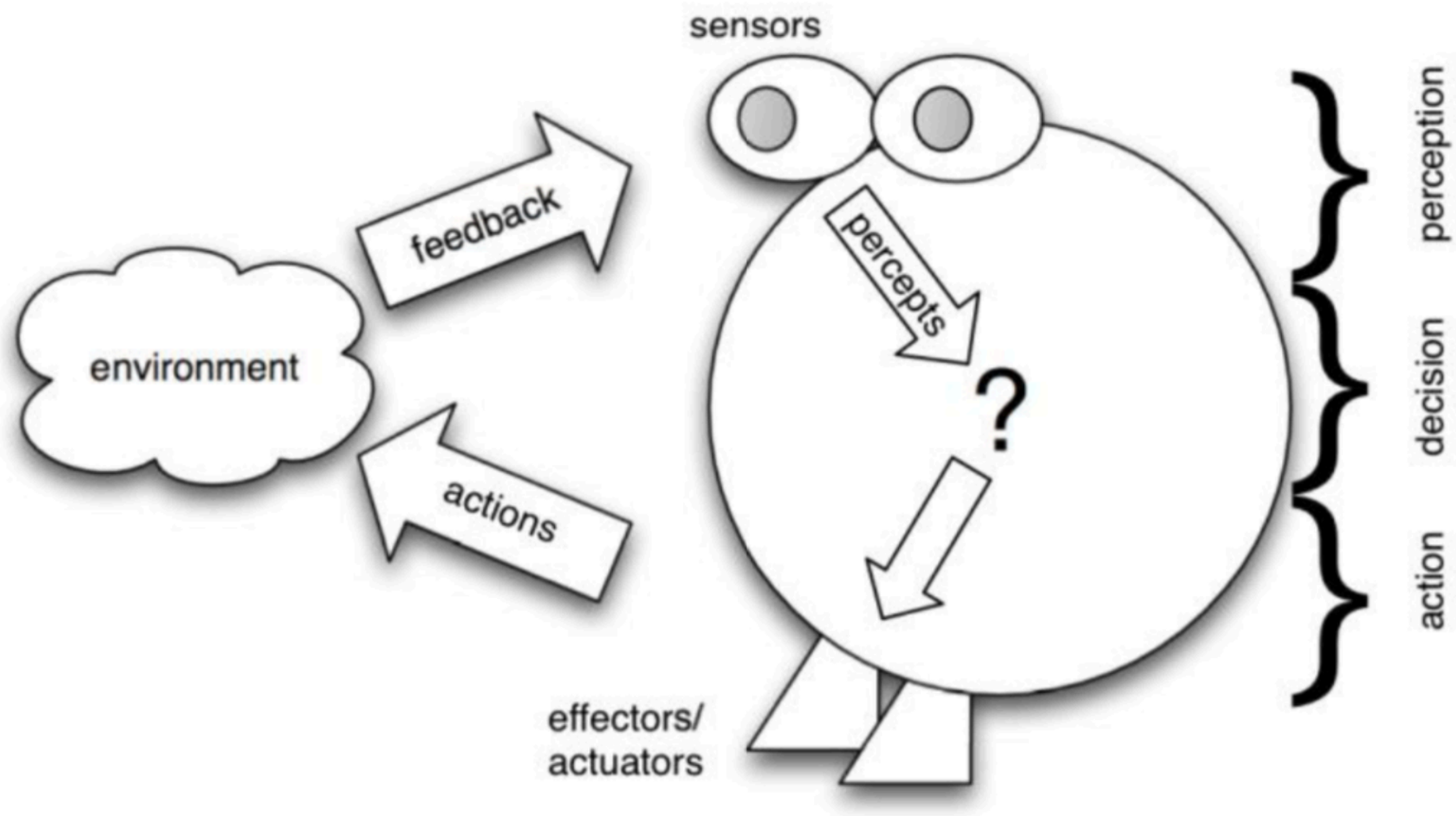
now we want to discuss a **third ML paradigm**

Reinforcement Learning: given a complex task in a complex environment (dynamic, non deterministic, only partly accessible) train an **agent** that carry out **autonomous action** in this environment and complete the requested task

Agents in Reinforcement Learning

In the context of **Reinforcement Learning,** an **agent** is a computer system capable **autonomous action** in some environment, in order to achieve its delegated goals



Agents in Reinforcement Learning

In the context of **Reinforcement Learning,** an **agent** is a computer system capable **autonomous action** in some environment, in order to achieve its delegated goals

Can you think of trivial ``agents''?

Agents in Reinforcement Learning

In the context of **Reinforcement Learning,** an **agent** is a computer system capable **autonomous action** in some environment, in order to achieve its delegated goals

trivial agents: thermostat, e-mail daemons, alarms, ….

Agents in Reinforcement Learning

In the context of **Reinforcement Learning,** an **agent** is a computer system capable **autonomous action** in some environment, in order to achieve its delegated goals

non-trivial agents should exhibit the following properties:

- ***Reactive*:** interact with environment and react its changes
- ***Proactive***: recognise opportunities and take initiative
- ***Social*:** cooperate with other agents (and humans!) via cooperation, negotiation, coordination
- ***Rational:*** the agent will always act to fulfil its goals
- ***Adaptability:*** the agent is able to improve its performance over time

Agents in Reinforcement Learning

Environments in RL can exhibit the following features:

- ***Accessible or Inaccessible*:** can the agent obtain updated and accurate information about the state of the environment?

- ***Deterministic or non-deterministic*** : has each action that the agent perform always associated the same effect?

- ***Static vs dynamics*:** is the environment stable expect for the action of the agent?

- ***Discrete vs continuous:*** are there a finite or infinite number of actions possible?

A Reinforcement Learning system

The ultimate goal of **Reinforcement Learning** is to

design an agent that **performs complex tasks** and **takes autonomous action** to fulfil its design goals, in an environment that is: partly inaccessible, non-deterministic, non-episodic, dynamic and continuous (*i.e.* the real world!).

☑ The agent receives the state of the environment as a **vector of features** (inputs)

☑ The agent can execute actions in every state, with different actions bringing **different** rewards

☑ Goal: **learn a policy**, i.e. a function that maps the features of an state vector to an optimal action to be taken in that stage

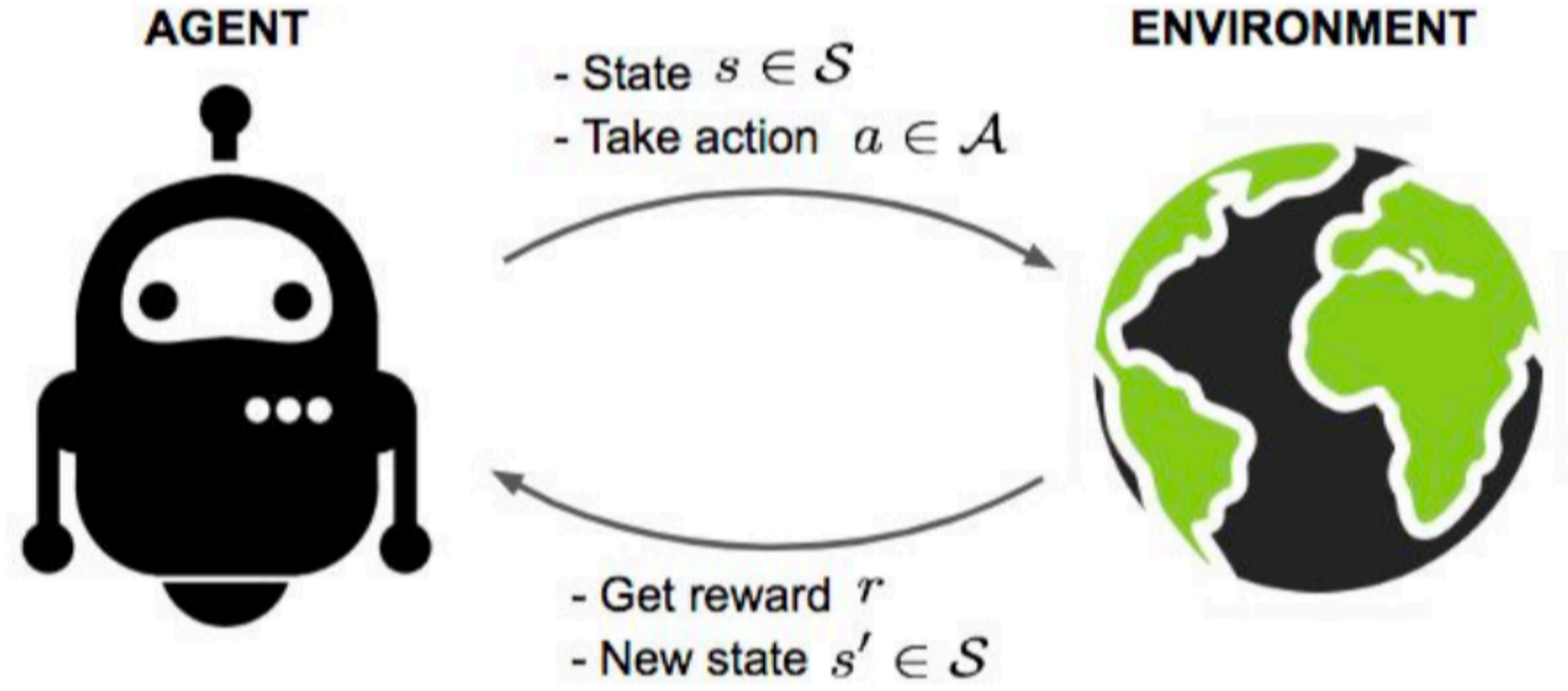
☑ An action is optimal if it **maximizes the expected average reward**

☑ In RL **decision making is sequential and the goal is long-term** (i.e. game playing, robotics, resource management, ...)

Agents in Reinforcement Learning

The ultimate goal of **Reinforcement Learning** is to

design an agent that **performs complex tasks** and **takes autonomous action** to fulfil its design goals, in an environment that is: partly inaccessible, non-deterministic, non-episodic, dynamic and continuous (*i.e.* the real world!).

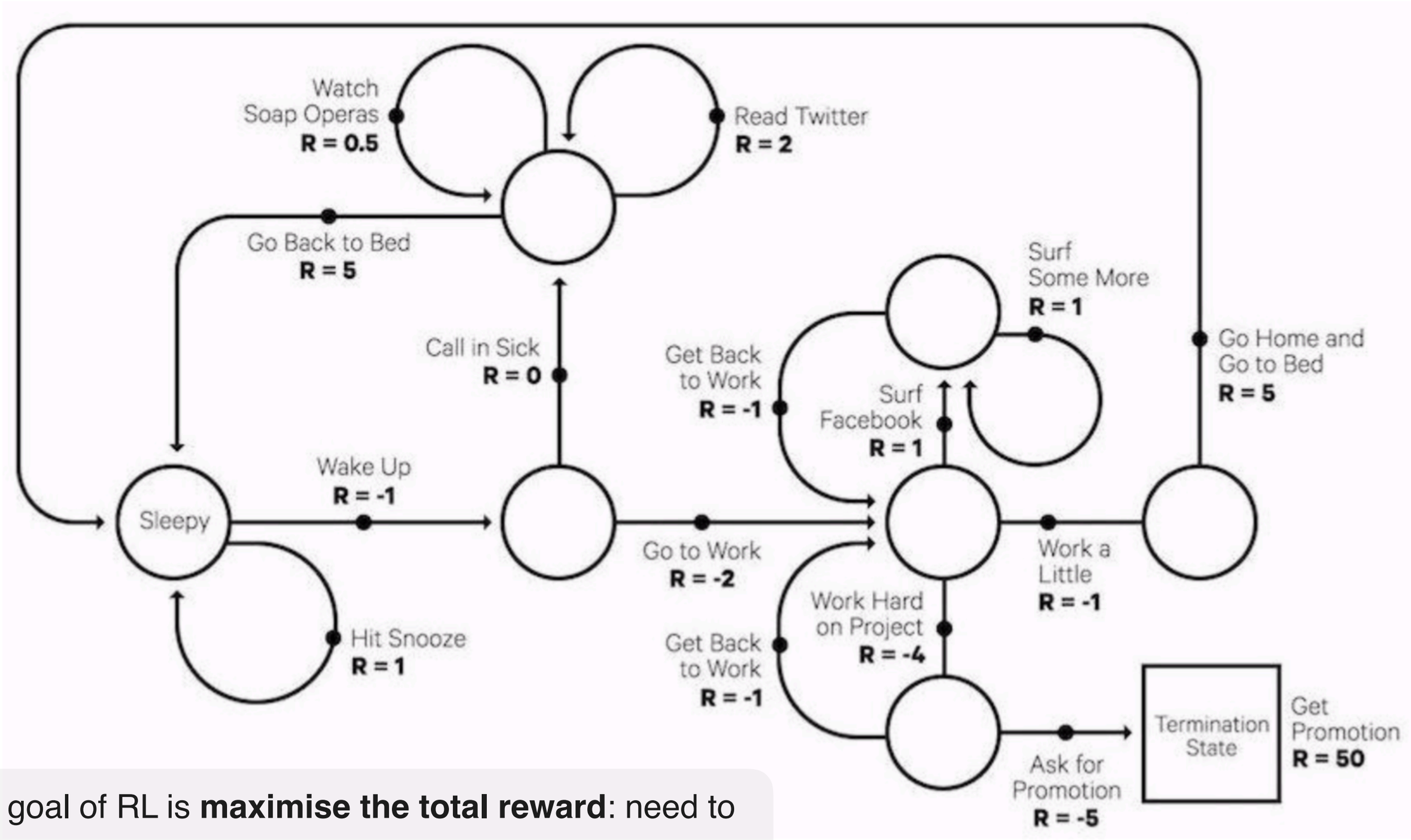


A Reinforcement Learning system

use **Reinforcement Learning** is to determine the actions that will get us a promotion at work!

the goal of RL is **maximise the total reward**: need to explore all possible options to determine the best policy for each action that it might need to carry

A Reinforcement Learning system



the goal of RL is **maximise the total reward**: need to explore all possible options to determine the best policy for each action that it might need to carry

Reinforcement Learning for Games

AlphaGo: using machine learning to master the ancient game of Go

BLOG POST
RESEARCH

04 DEC 2018

AlphaZero: Shedding new light on chess, shogi, and Go

In late 2017 we introduced AlphaZero, a single system that taught itself from scratch how to master the games of chess, shogi (Japanese chess), and Go, beating a world-champion program in each case. We were excited by the preliminary results and thrilled to see the response from members of the chess community, who saw in AlphaZero's games a ground-breaking, highly dynamic and "unconventional" style of play that differed from any chess playing engine that came before it.

BLOG POST
RESEARCH

24 JAN 2019

AlphaStar: Mastering the Real-Time Strategy Game StarCraft II

Reinforcement Learning for Games

DeepMind AlphaStar: AI breakthrough or pushing the limits of reinforcement learning?

By **Ben Dickson** - November 4, 2019

4 min read

DeepMind's AI program AlphaStar managed to defeat 99.8 percent of StarCraft II players.

Reinforcement Learning for Games

Q-learning

Q-learning is a **model-free reinforcement learning algorithm,** which aims to learn a **policy** about what actions should the agent carry out for different circumstances

no model of the environment need: the agent learns to maximise its future reward by repeatedly interacting with the environment

In Q-learning, the weight for a step into the future is calculated by the **discount factor**

$$0 \leq \gamma^{\Delta t} \leq 1$$

earlier rewards valued higher than later ones

analog of cost function in Supervised Learning is the **quality of state-action combination**

$$Q : S \times A \rightarrow \mathbb{R}$$

quality function *state* *action*

the goal of Q-learning is to determine the actions that the agent should take for each state in order to **maximise the total reward**

Q-learning

Schematically, at **each iteration of the Q-learning** algorithm the following steps take place:

- The agent selects an **action** a_t
- As a consequence of this action, the agent observes a **reward** r_t
- The agent then then enters into a **new state** s_t
- The quality function (cost function) Q is updated

$$Q^{\text{new}}(s_t, a_t) \leftarrow (1 - \alpha) \times Q^{\text{old}}(s_t, a_t) + \alpha \left(r_t + \gamma \times \max_a Q(s_{t+1}, a) \right)$$

reward

learning rate

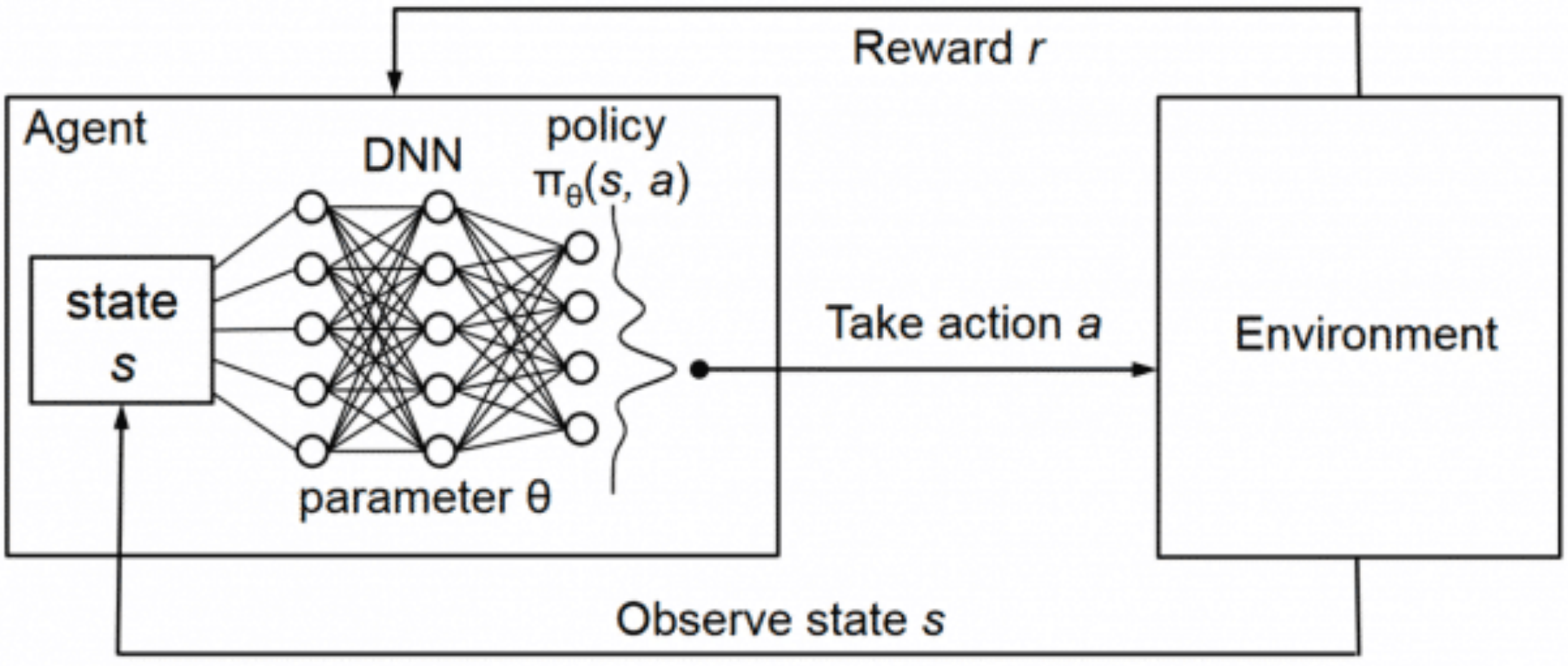
discount factor

(estimate of) future optimal value

After training, **the agent has a policy** Q which tells it how to act for each circumstance

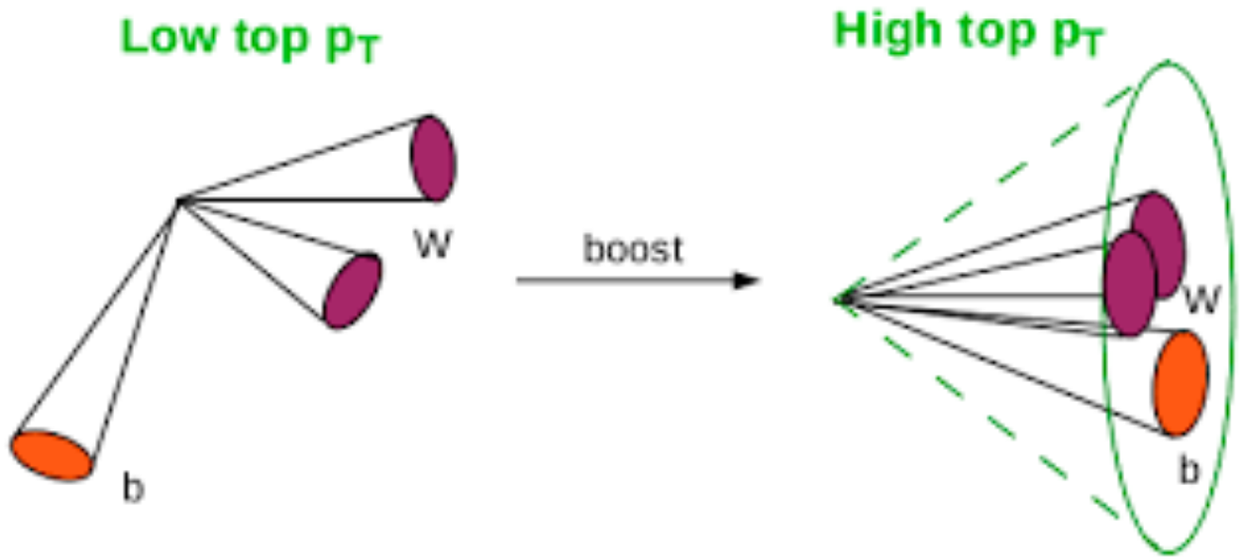
Deep Q-Networks

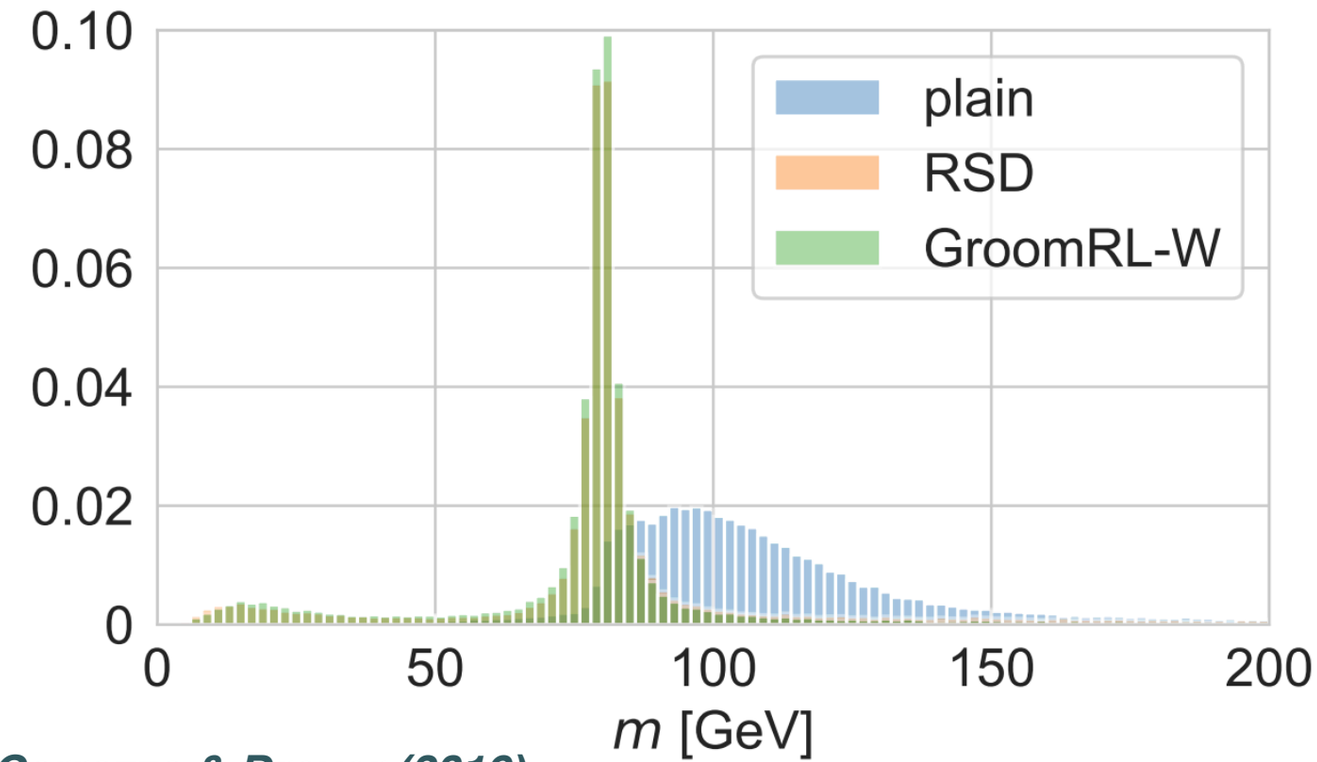
the model for the **policy function** (which action to take as function of the state) can be parametrised using Deep Neural Networks, in this case called Q-Networks



Reinforcement learning for jets

jet substructure allows separating interesting jets (collimated hadrons in high energy collisions) from background processes e.g. jets from top quark decay vs QCD jets





Carrazza & Dreyer (2019)

use RL to train an agent to ``groom'' jets removing background contamination: tune the **reward** to the **physics requirements**

bypasses need for algorithmic implementation of a grooming algorithm

Ensemble Methods

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

for fully correlated models →

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

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

$$\widehat{g}^{A}_{\mathcal{L}}(\boldsymbol{x}) = \frac{1}{M} \sum_{i=1}^{M} g^{A}_{\mathcal{L}_i}(\boldsymbol{x})$$

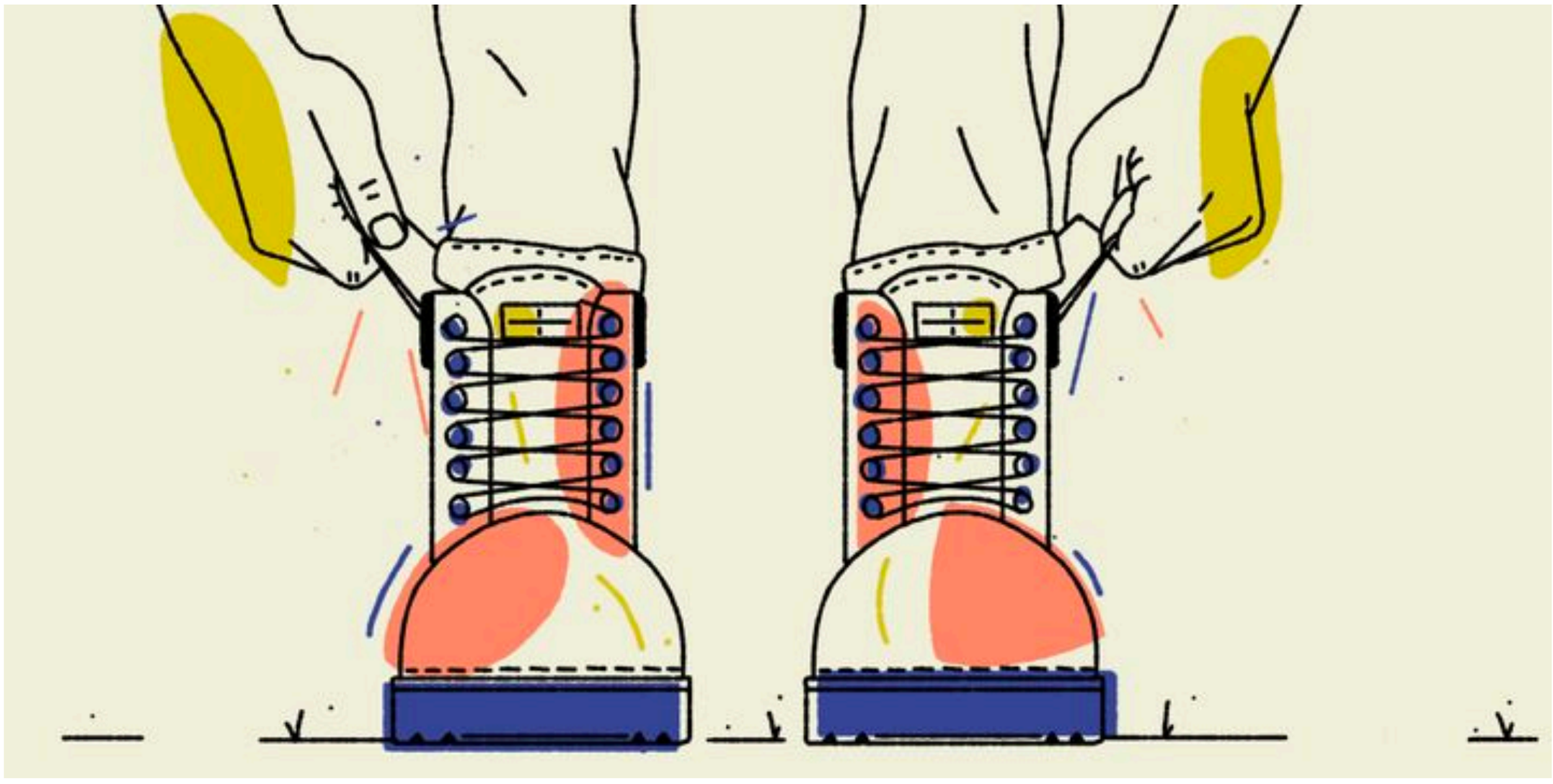
for continuous datasets, analogous expressions for discrete classifiers

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**

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

$$\vdots$$

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

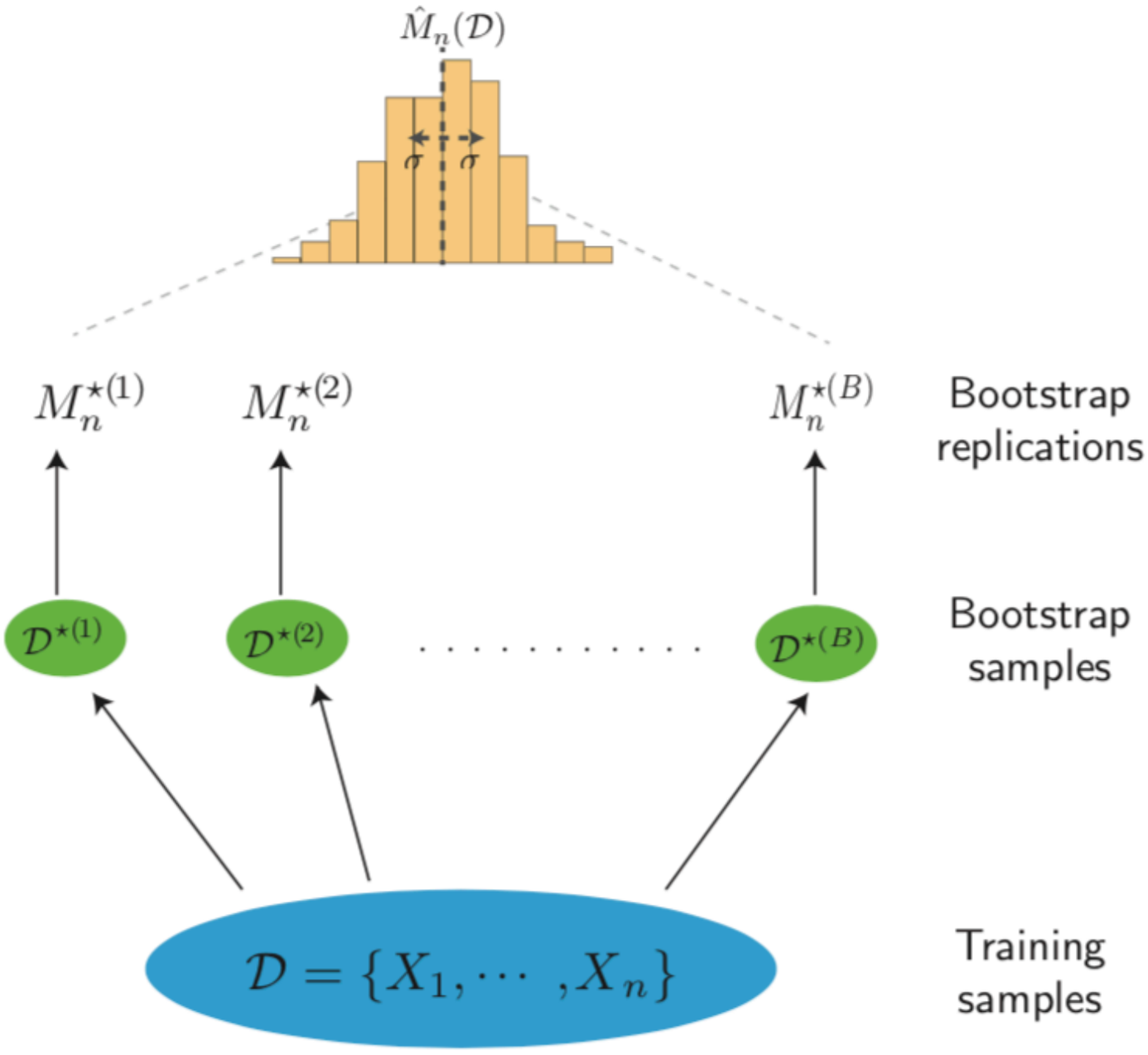
bootstrap samples (with repeated elements)

- 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

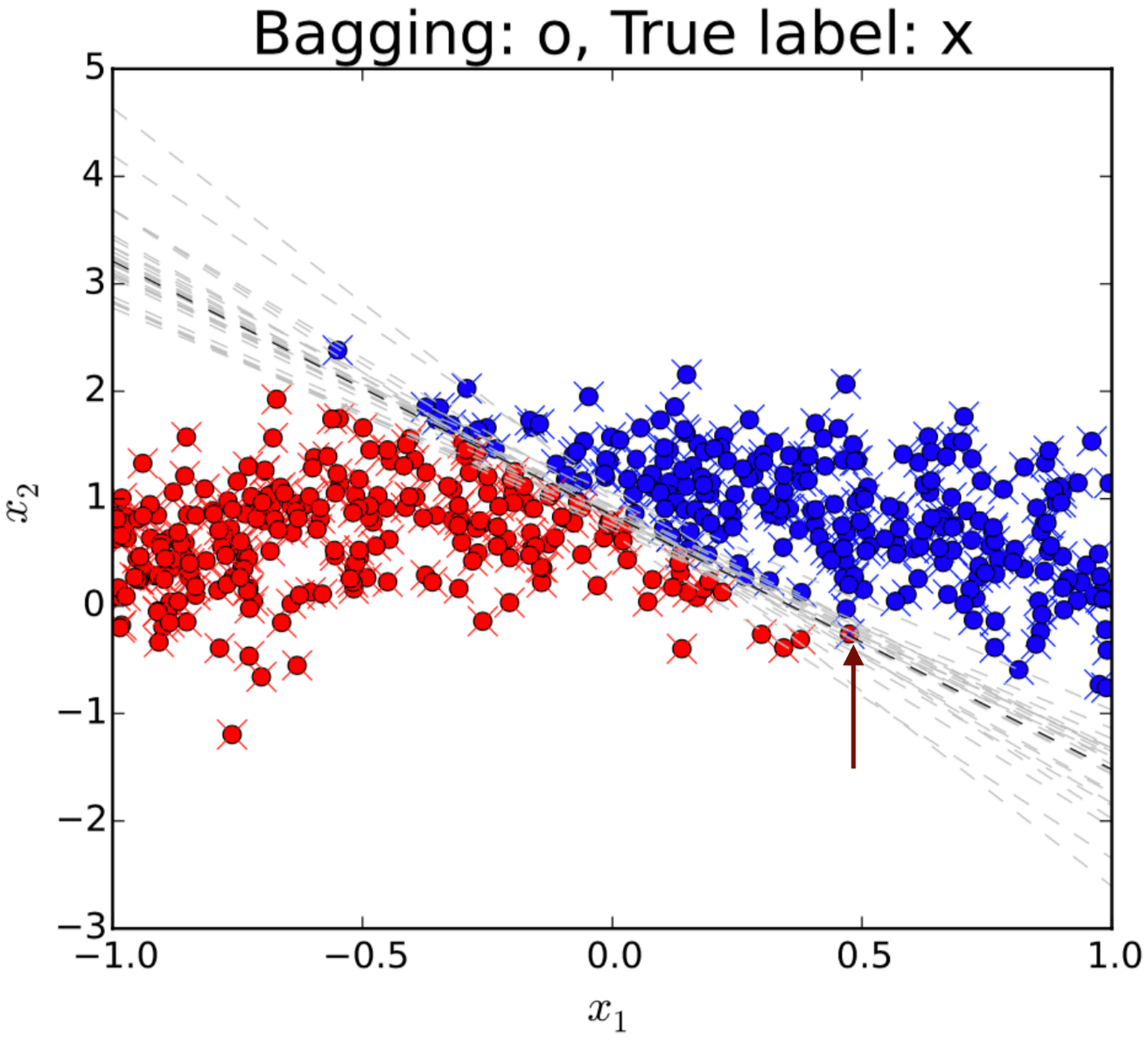
It can be shown that in the large *n* limit the **bootstrap distributions** approximate well the **sampling distributions** from which the training dataset was obtained

Bagging with bootstrap

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

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

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

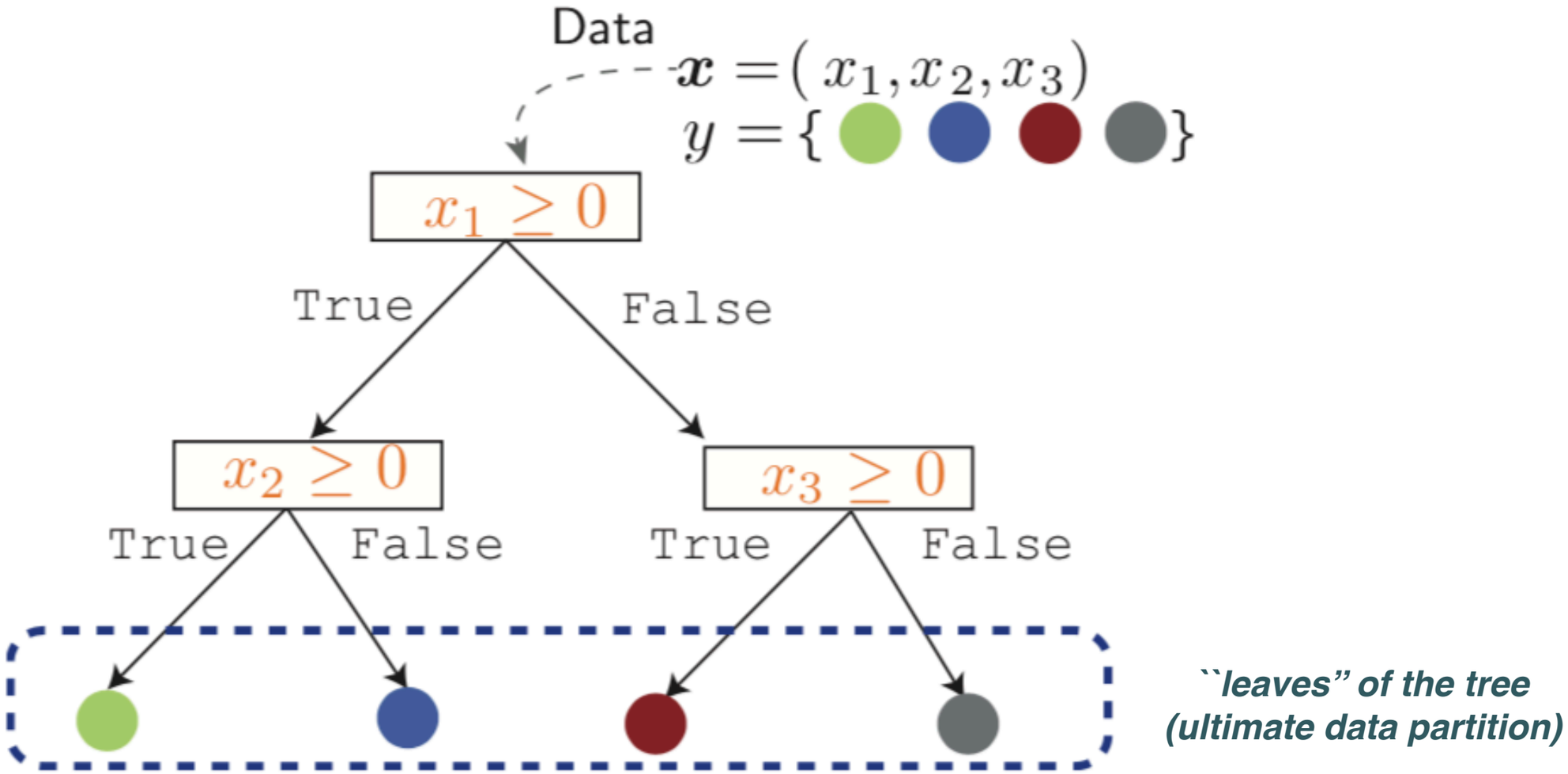
black dahed: bagging average

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

Random Forests

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



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

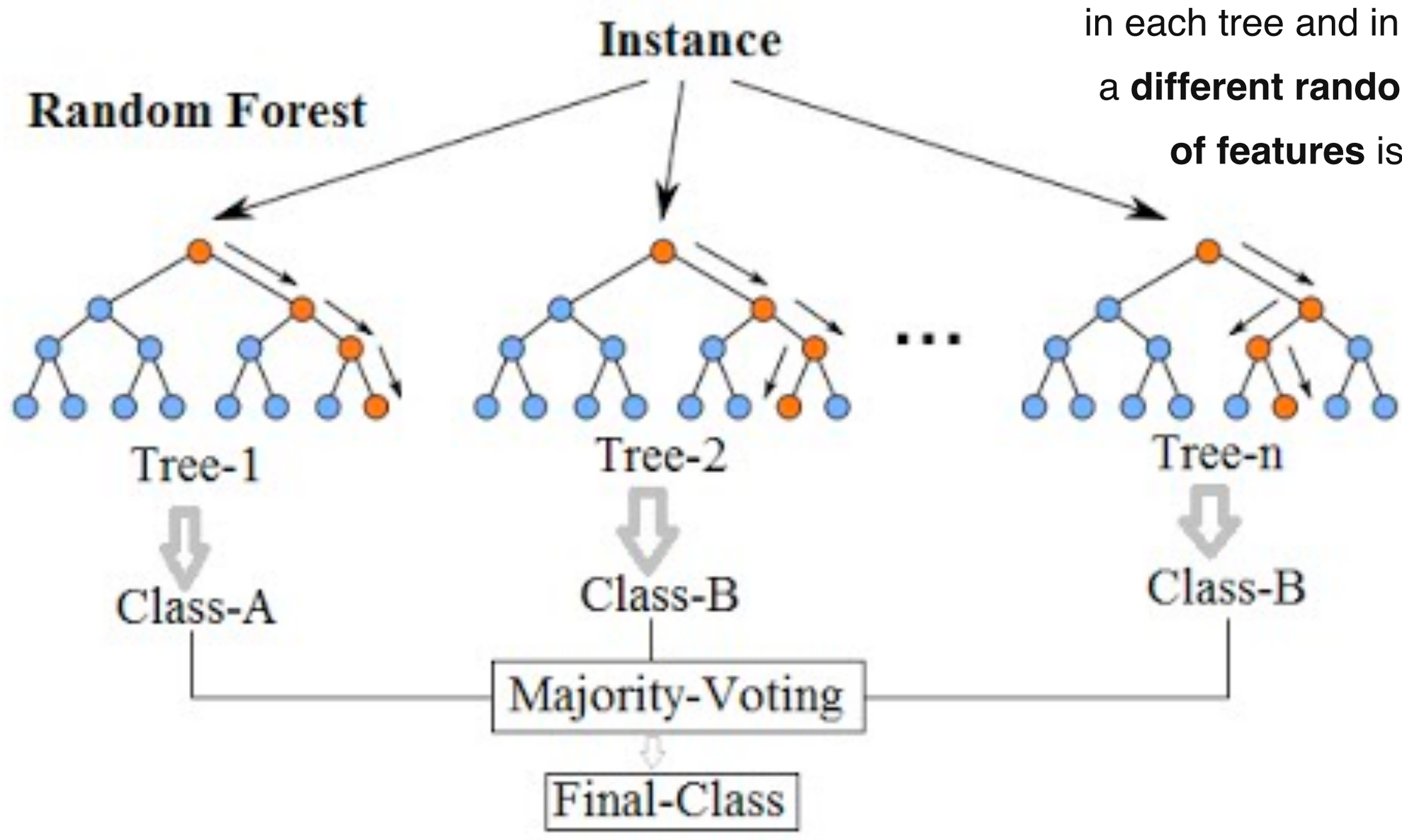
typically, a classification problem with p features, in RFs only $p^{1/2}$ features are used in each split

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**

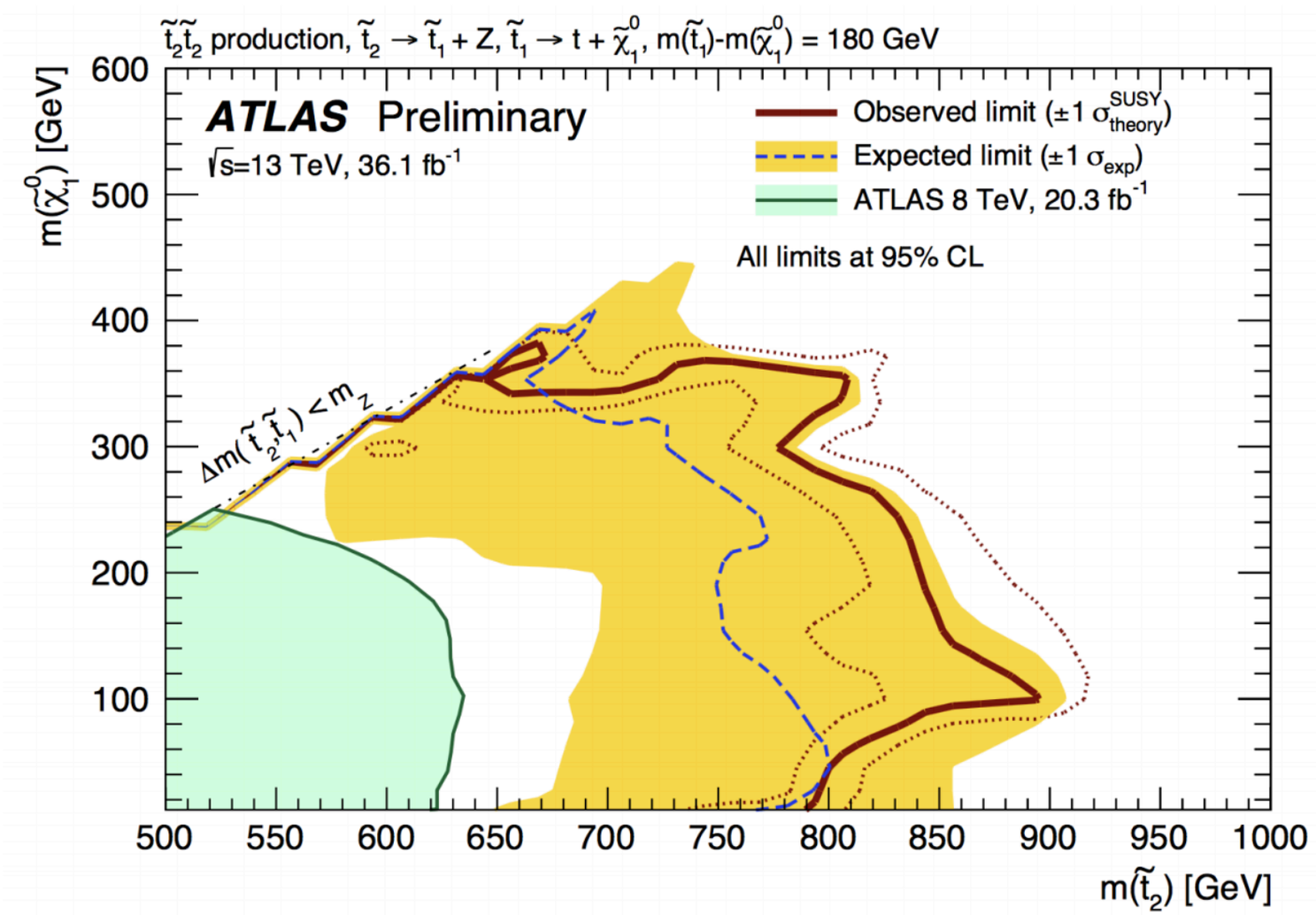
Case Study: limit setting in high-dimensional models with decision trees

S. Caron, J. S. Kim, K. Rolbiecki, R. Ruiz de Austri and B. Stienen,
`The BSM-AI project: SUSY-AI–generalizing LHC limits on supersymmetry with machine learning''
Eur. Phys. J. C 77, no. 4, 257 (2017), [arXiv:1605.02797 [hep-ph]].

Harvesting LHC data for BSM signals

- In the absence of new particles and/or interactions, LHC searches for BSM physics are used to **derive exclusion ranges for specific scenarios**

- Results presented as excluded ranges in **subset of the full parameter space**

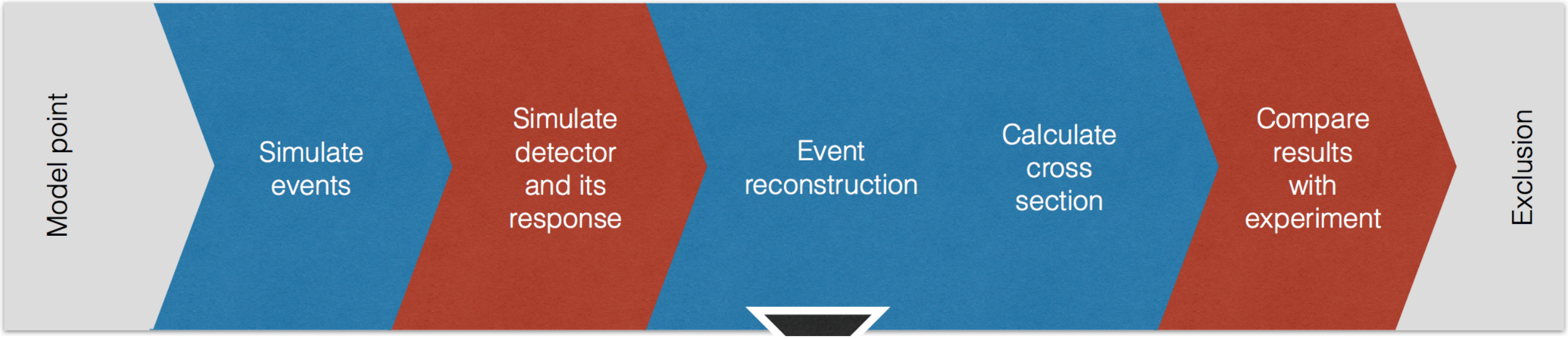


However this is only a **small part of the information contained by the LHC measurements**, ideally we would like the exclusion ranges in the full parameter space of the theory: *e.g.* **19 params in the pMSSM**

Harvesting LHC data for BSM signals

Exploring the full parameter space of a given BSM scenario is in general CPU time consuming

Time = O(hours)



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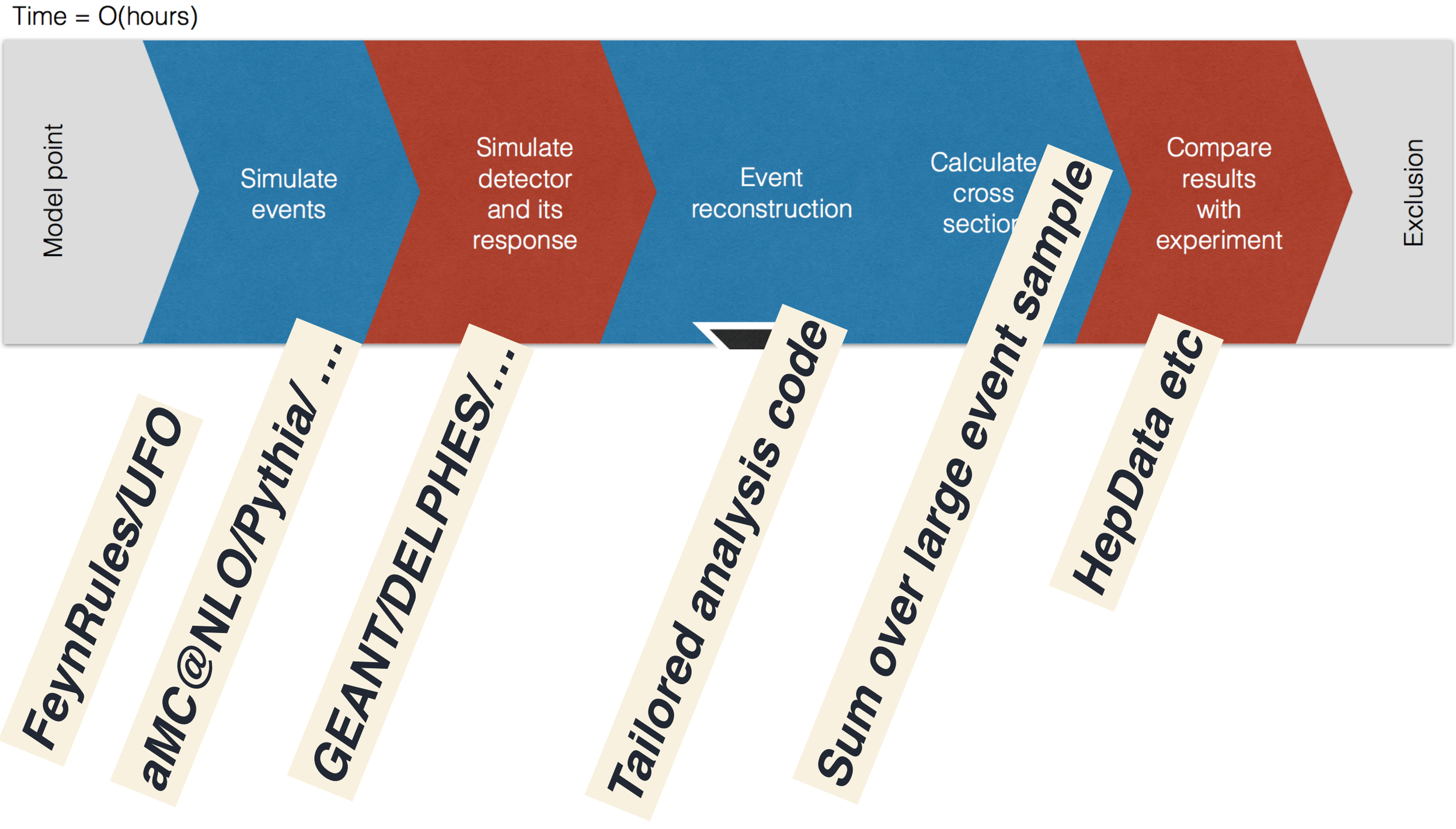

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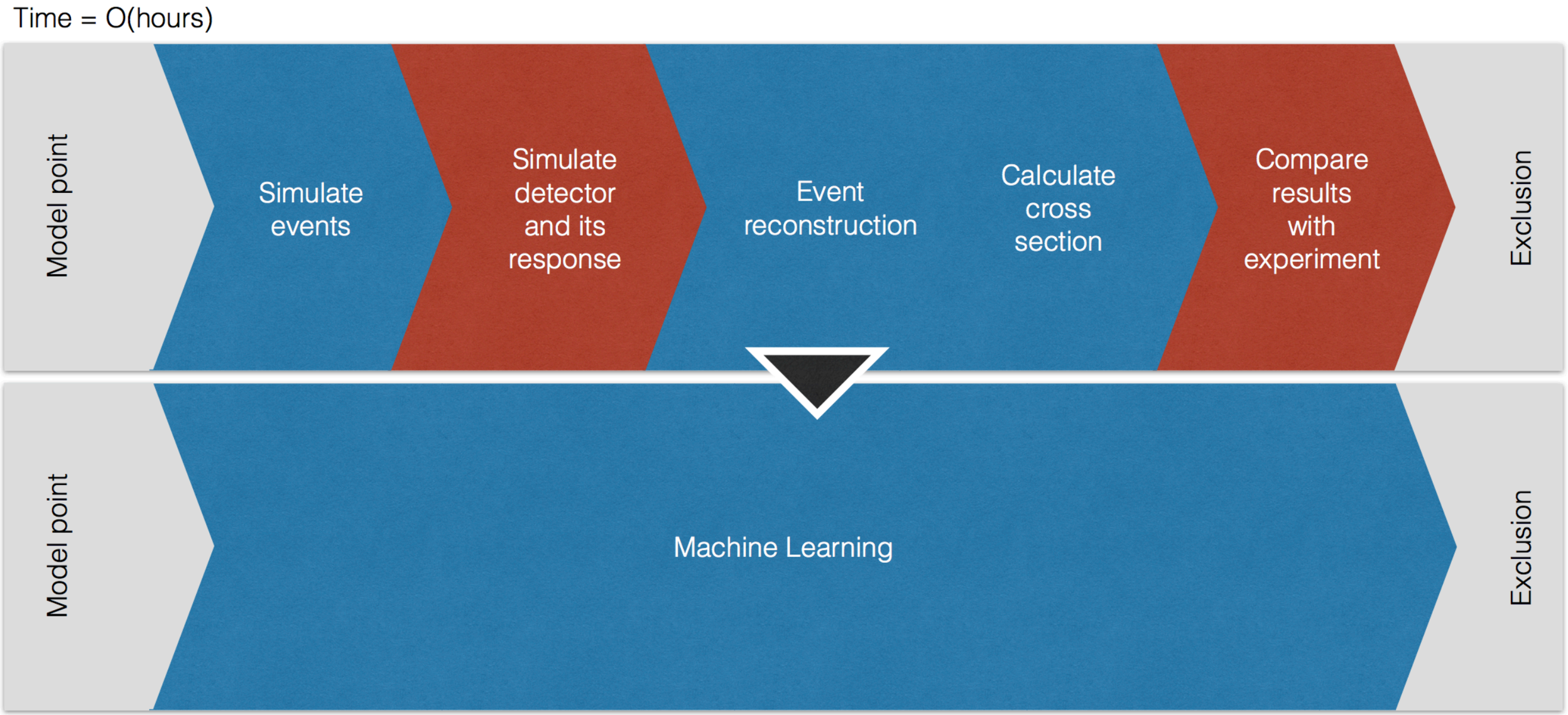

Use ML tools one can **speed-up the limit-setting procedure by orders of magnitude**, making possible an efficient exploration of the full parameter space

Harvesting LHC data for BSM signals

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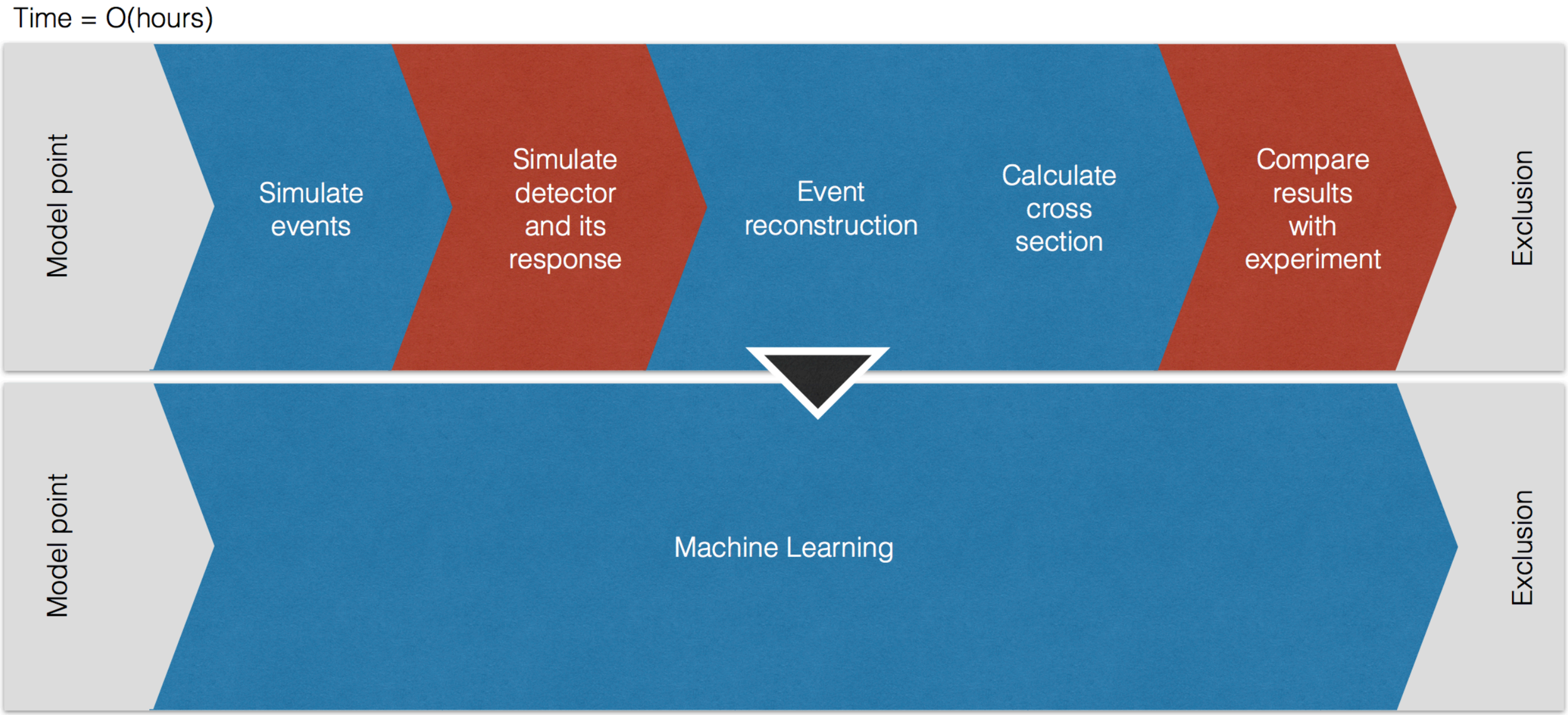

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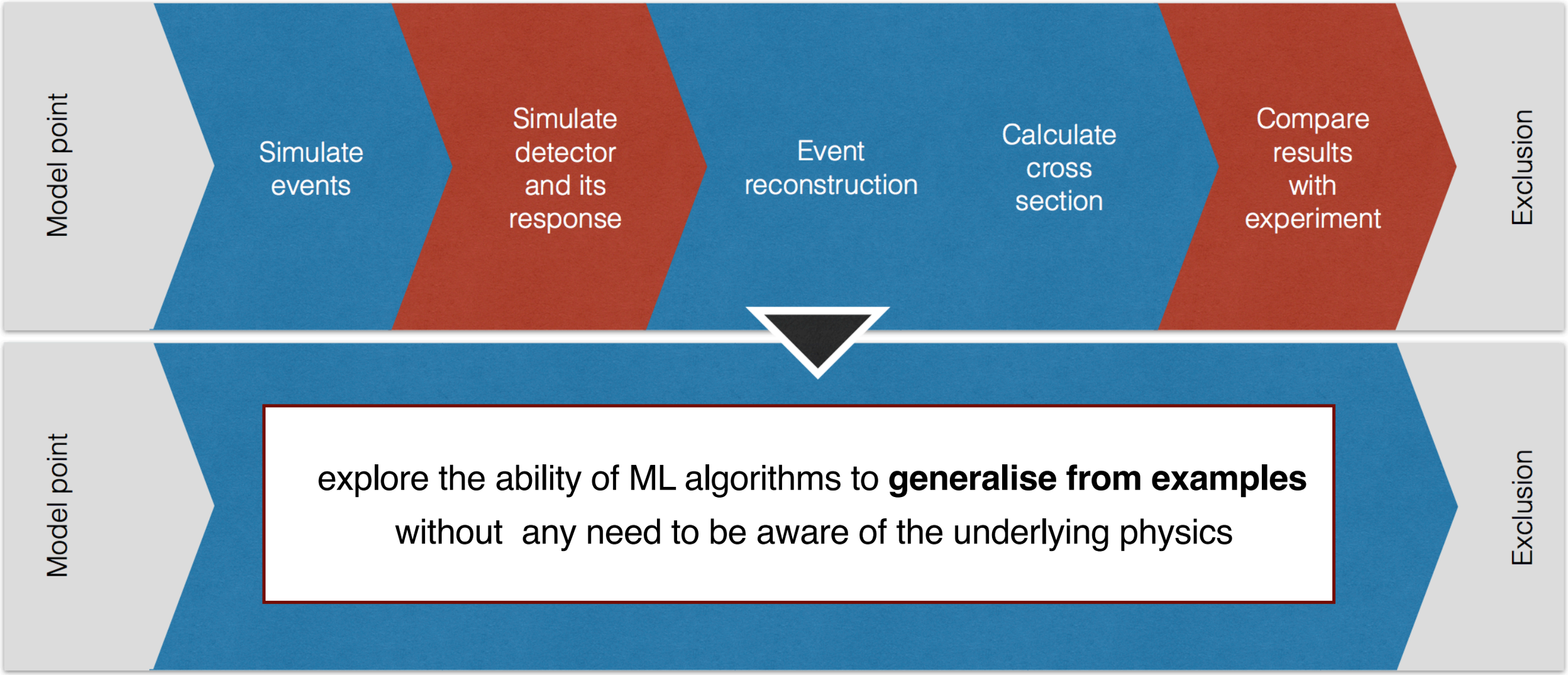


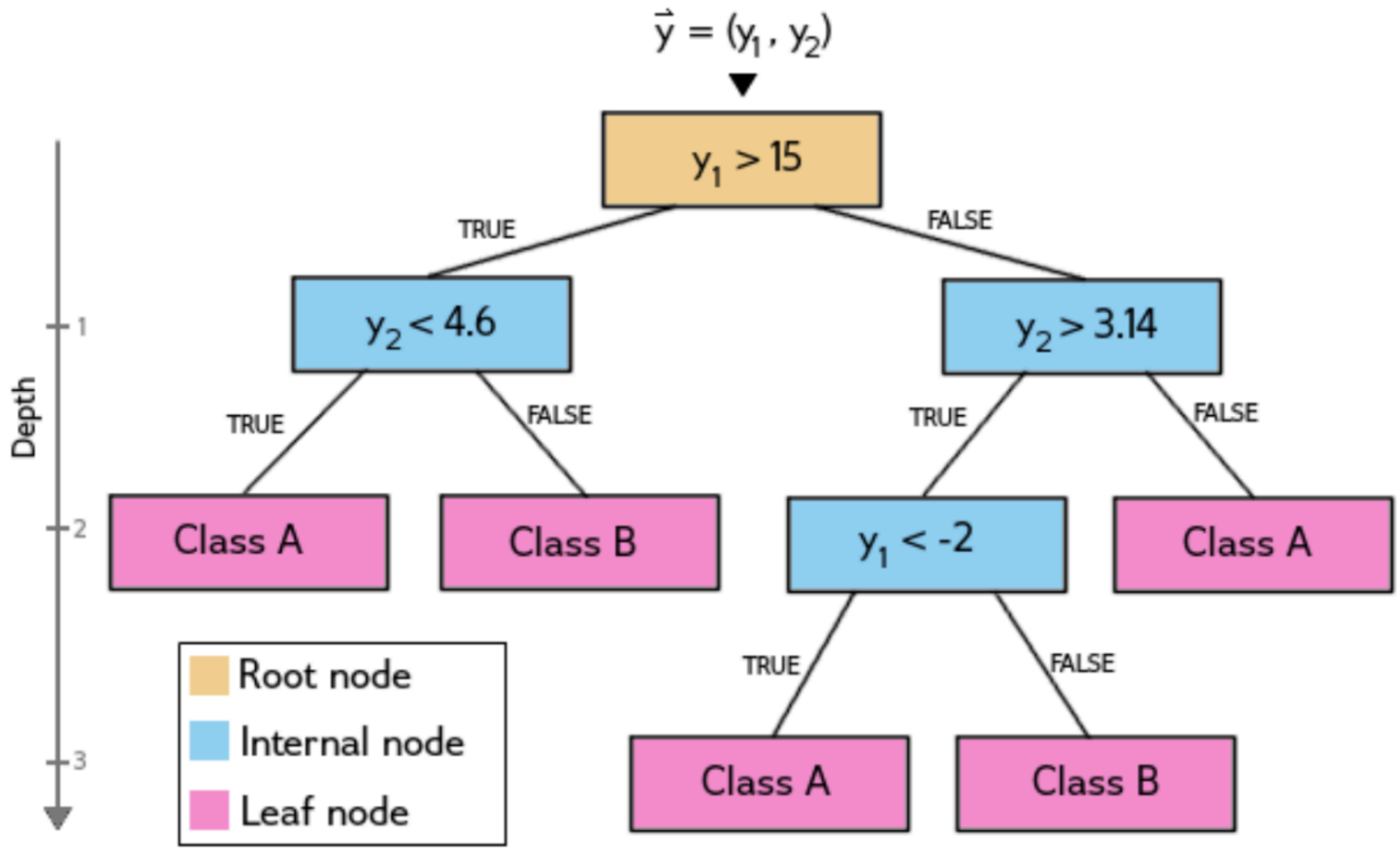
Time = O(ms)

Use ML tools one can **speed-up the limit-setting procedure by orders of magnitude**, making possible an efficient exploration of the full parameter space

Classification with Decision Trees

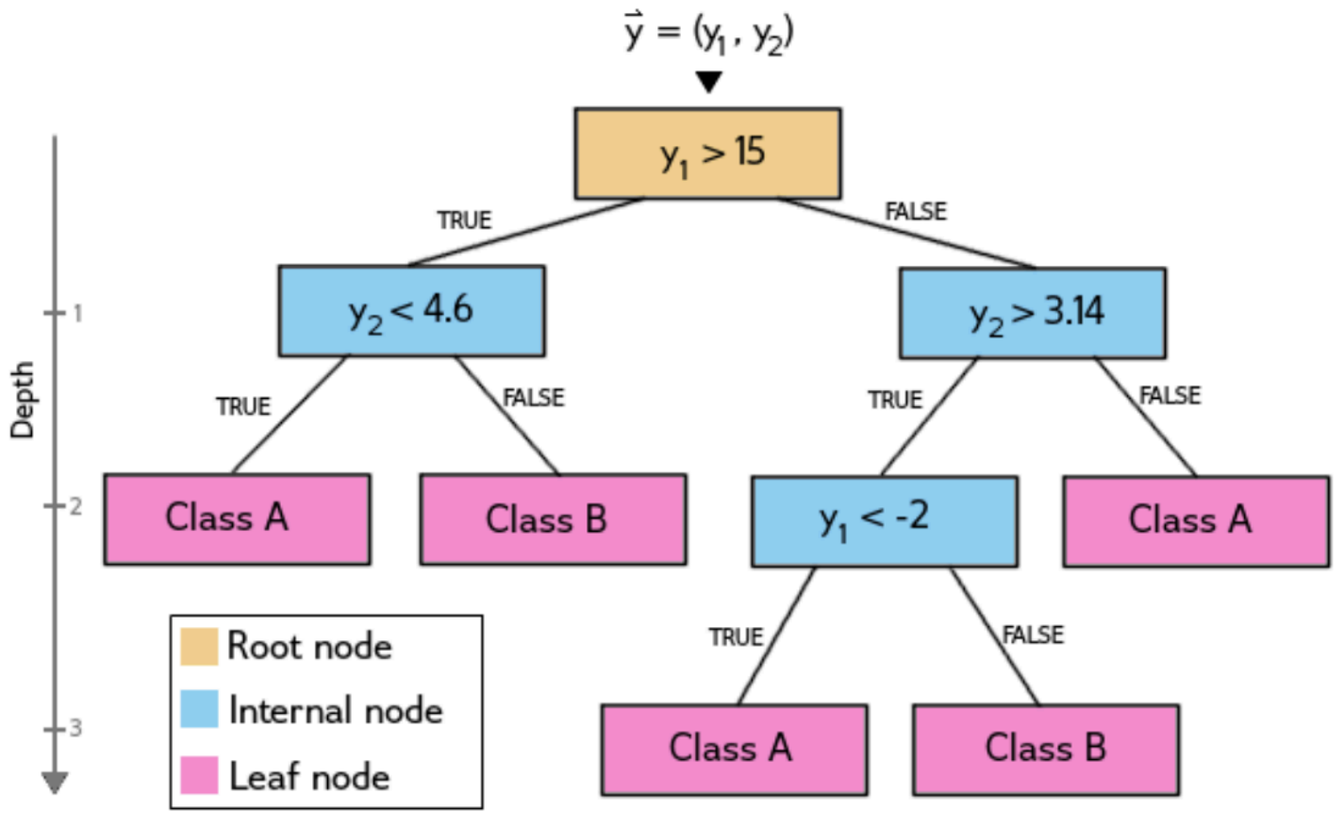
- This is an example of a discrete Classification problem: a given point in bSM parameter space can be either **allowed** or **excluded**, with no options in between

- **Decision Trees** classifiers, such as **Random Forest classifier**, exhibit good performance here



Procedure starts by presenting parameter sets and class labels, to **learn the patterns that the input data follow**

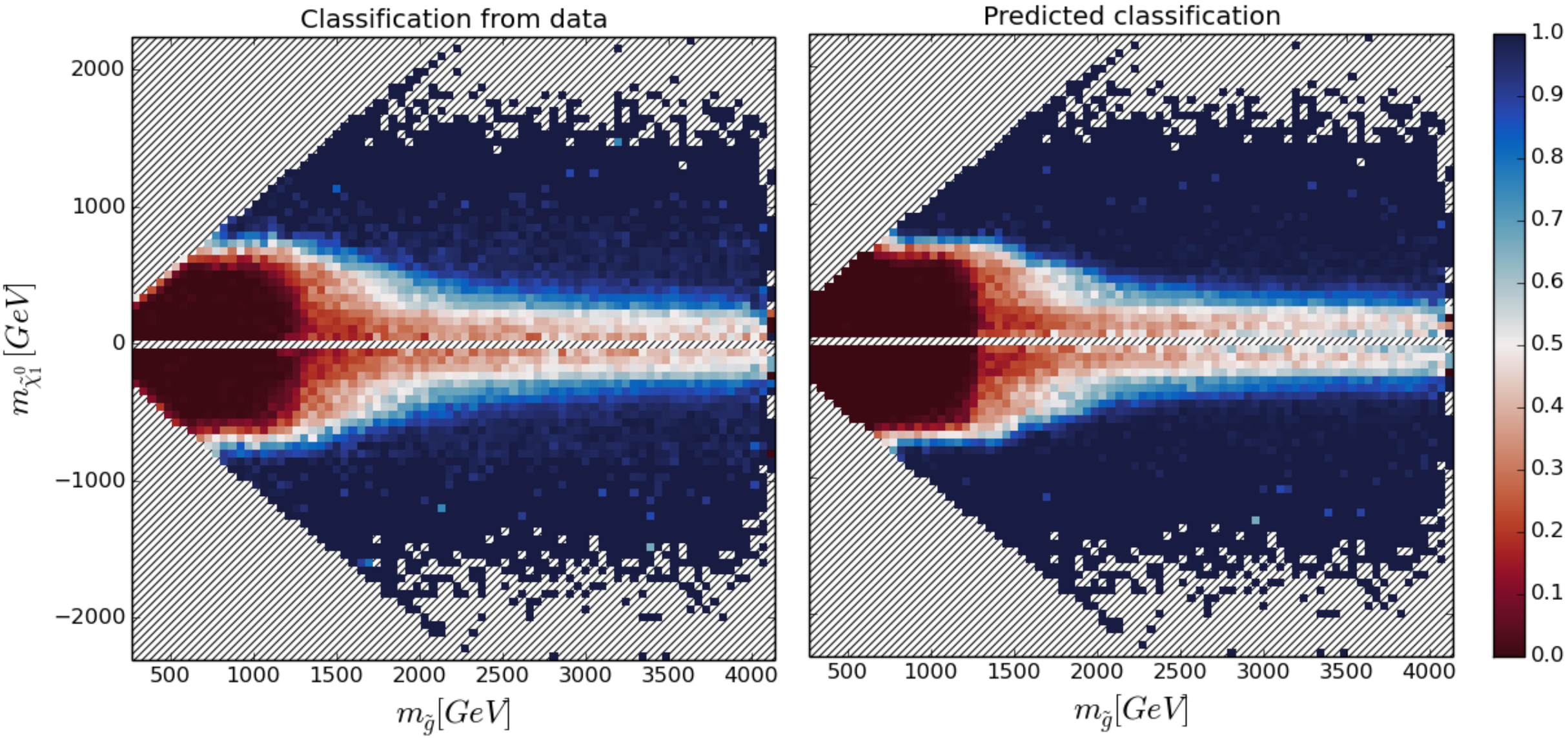
Classification with Decision Trees



- Each node in tree specifies a **test performed on the arriving attribute**
- The result of this test determines to which node the attribute set is sent next.
- Process is repeated until the f**inal leaf node is reached**,
- At final node a **class label is assigned to the set**, specifying its class
- Tree works on the **entire parameter space**: every test performed interpreted as a cut in this space.
- The **parameter space is split into disjunct regions**, each having borders defined by the cuts in the root and internal nodes, and a classification defined by a leaf node.

Harvesting LHC data for BSM signals

Compare classification (allowed vs excluded) in **real data** vs the **ML-trained classifier**



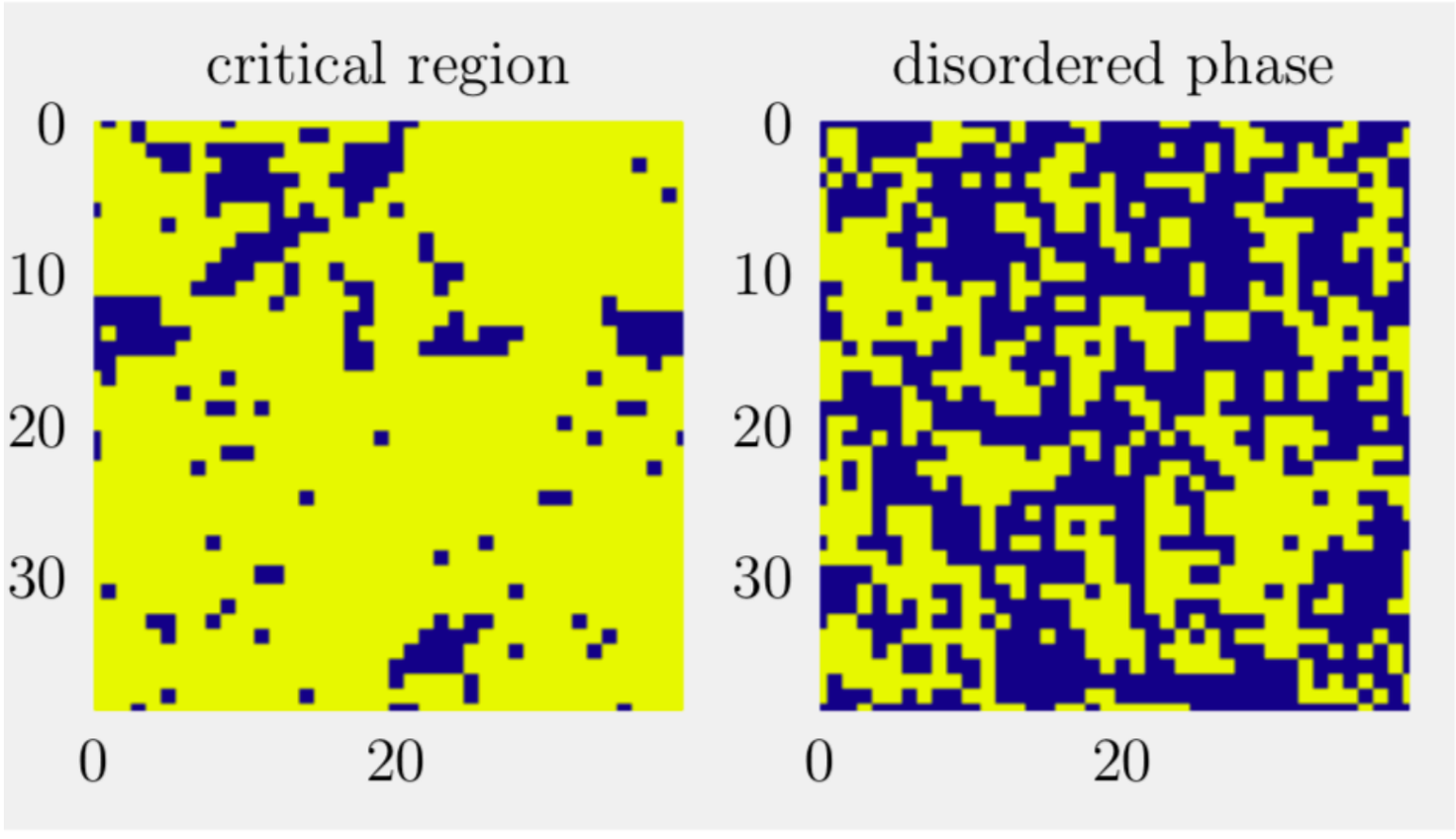
- Efficient exploration of the **full bSM parameter space**
- Can be **projected** in any of the dimensions of the 19-parameter space of the pMSSM
- Generalise to points outside training dataset in O(ms) as opposed to O(h)

Tutorial 3 Exercise 3b

starting point is the **Python script** that you will find in

https://github.com/juanrojochacon/ml-ditp-attp/blob/master/Tutorials/Tutorial3/

- Construct a **classifier based on Random Forests** and test it on the 2D Ising dataset



- What are advantages and disadvantages as compared to a classifier based on **logistic regression?**

- Investigate different methods to **visualise the results**, including with principal component analysis