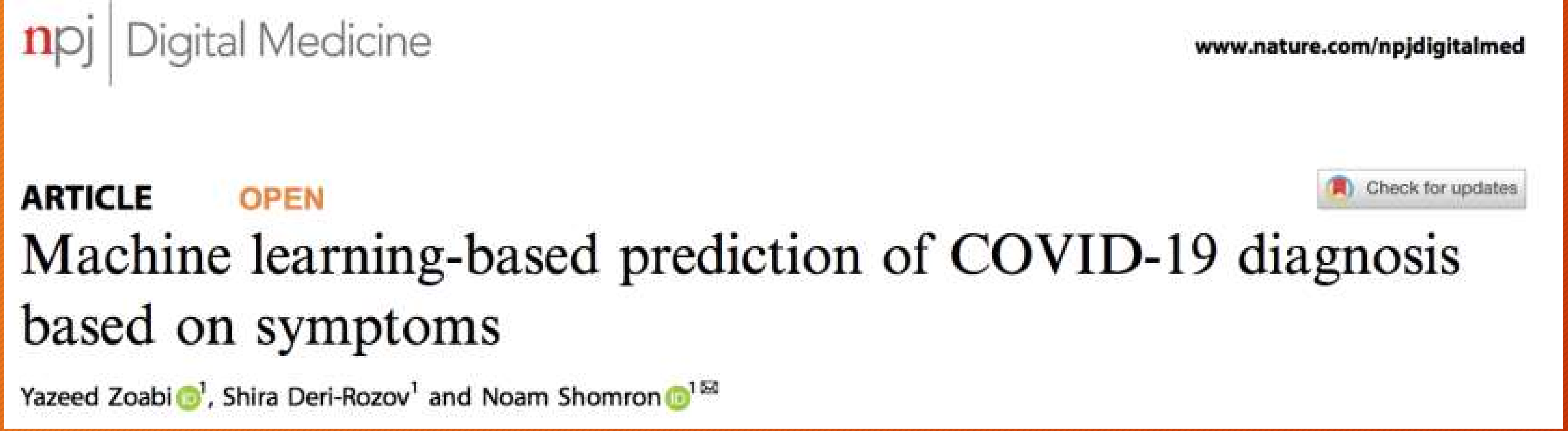

npj Digital Medicine www.nature.com/npjdigitalmed

ARTICLE OPEN

Check for updates

Machine learning-based prediction of COVID-19 diagnosis based on symptoms

Yazeed Zoabi[1], Shira Deri-Rozov[1] and Noam Shomron[1]

# Supervised and unsupervised learning

ADS2

Transit stations

-68%

compared to baseline

Mobility trends for places like public transp hubs such as subway, bus, and train statio

Workplaces

-35%

compared to baseline

Mobility trends for places of work.

Residential

+11%

compared to baseline

Mobility trends for places of residence.

+80%
+40%
Baseline
-40%
-80%
Sun Feb 16
Sun Mar 8
Sun Mar 29

Gedi Lukšys

April 15, 2024

Market Summary > Amazon.com, Inc.

2,295.45 USD

+1,334.10 (138.77%) ↑ past 5 years

Closed: 6 May, 19:56 GMT-4 • Disclaimer

After hours 2,290.50 −4.95 (0.22%)

1D
5D
1M
6M
YTD
1Y
5Y
Max
2,134.87 USD 14 Feb 2020
4,000
3,000
2,000
1,000
0
2018
2019
2020
2021
2022

## Learning objectives

Today’s plan:

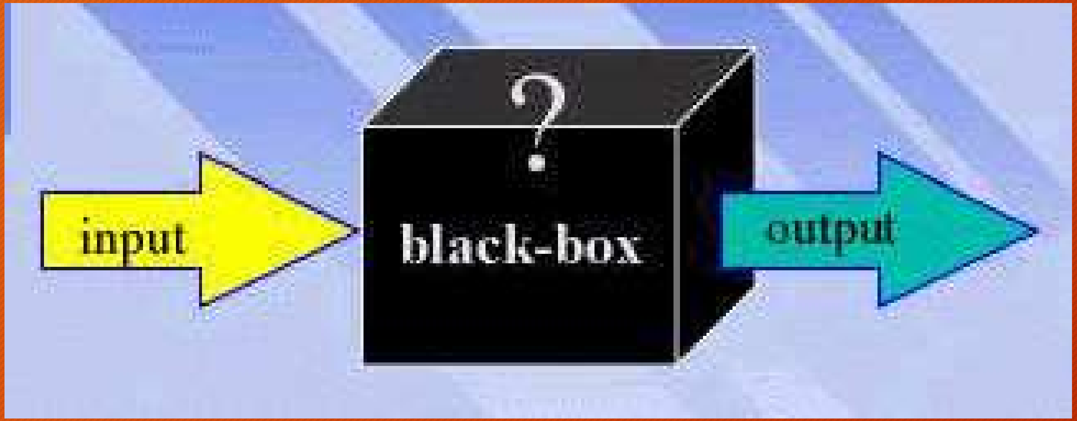
- main elements & techniques of supervised learning
- a simple example of supervised learning and gradient ascent approach
- an overview of different supervised and unsupervised learning techniques
- relevant considerations and applications of supervised and unsupervised learning

# Supervised learning: what is it for?

Learn to predict relations between 2 sets of data: „inputs“ ➔ „outputs“

Apt. size: 50, 75, 150, 67, 34, 80m$^2$

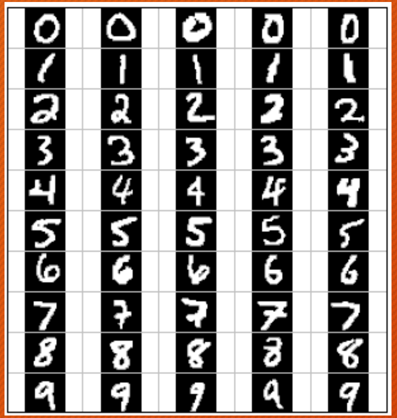
No of rooms: 2, 4, 5, 3, 2, 3



Rent: $700, 950, 1400, 1000, 550, 1200

0, 1, 2, ..., 9

Spam / no Spam



http://w3.impa.br/~lhf/sib2003/p023/img2.gif

„Abu Malik: CONFIDENTIAL TRUST REPLY URGENTLY“

„bahn.de: Vielen Dank für Ihren Fahrkartenkauf! (Auftrag ABCXYZ)“

**Input typically multidimensional**
(sometimes very much so...)

Output often unidimensional, **discrete** (classes) or **continuous**

# Formally speaking: classification vs. regression

- Supervised learning deals with learning a function $f(X, W) = Y$, based on a number of available data points $(x^{(1)},y^{(1)})$, $(x^{(2)},y^{(2)})$, … , $(x^{(N)},y^{(N)})$, also called **examples**
  - where $x^{(i)}$ is usually a vector $(x_1^{(i)}, x_2^{(i)}, \dots, x_M^{(i)})$
  - $y^{(i)}$ is either a number (=> **regression**)

  a class {0, 1} or a vector of classes (=> **classification**)

  W – model parameters (also a vector), M – dimensionality

- Most common example: linear regression / classifier

## Why is it called „supervised“?

- Suppose our model simulates a function y = f(x)
- We can apply it to inputs (x-s) from existing examples to calculate outputs, i.e. $f(x^{(1)}), f(x^{(2)}), \ldots$
- In the beginning the model has not learned to predict the function correctly yet, but as we have the corresponding example („teacher“) outputs, we can measure the mean squared error (MSE):

  MSE = $((y^{(1)} - f(x^{(1)}))^2 + \ldots + (y^{(n)} - f(x^{(n)}))^2)/n$

- Sometimes root mean square error (RMSE) is used instead.

This is called the **error** or **objective** function. The goal is to minimize it.

# A simple example – linear model

- Model: y = ax + b

Objective function: $$MSE = {}^{1}/_{N} \sum_{i=1}^{N} \left(y^{(i)} - ax^{(i)} - b\right)^{2}$$

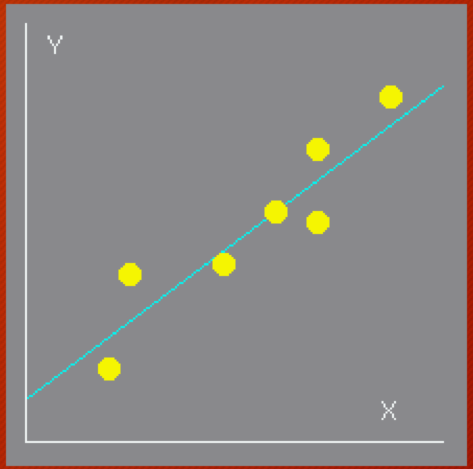
How can we make our model minimize the error?

We have 2 **parameters**: a & b

- We have to find their values that minimize the error!

How?

1. **Guess!** (need to start somewhere)



http://www.statslab.cam.ac.uk/~rrw1/stats/regress1.gif

**Parameter initialization**
Typically random

2. **Adjust guesses**, e.g. try neighboring values, go in the direction that decreases the error most => hill climbing

## A standard method: **gradient descent**

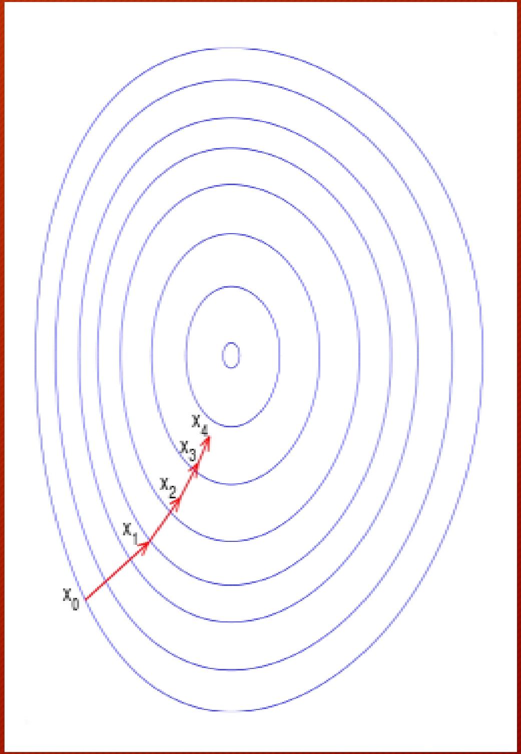
- Mean squared error (MSE) is a function of parameters (a and b)
- Derivatives $\delta MSE / \delta a$ and $\delta MSE / \delta b$ should be 0 at the minimum of MSE.
- How to get there fastest? (analytical solution aside ☺)

- Go along the steepest direction:

$$\Delta a = - \alpha \, \delta MSE / \delta a$$

$$\Delta b = - \alpha \, \delta MSE / \delta b$$

- Update of parameters is called a **learning rule**, and $\alpha$ is the learning rate.



http://en.wikipedia.org/wiki/File:Gradient_descent.svg

# Let‘s try!

$$MSE = \frac{1}{N} \mathop{\square}\limits_{i=1}^{N} \left(y^{(i)} - ax^{(i)} - b\right)^2$$

- Learning rules: $$\Delta a = -\frac{\alpha}{N} \sum_{i=1}^{N} 2\left(y^{(i)} - ax^{(i)} - b\right)\left(-x^{(i)}\right)$$ $$\Delta b = -\frac{\alpha}{N} \sum_{i=1}^{N} 2\left(y^{(i)} - ax^{(i)} - b\right)(-1)$$

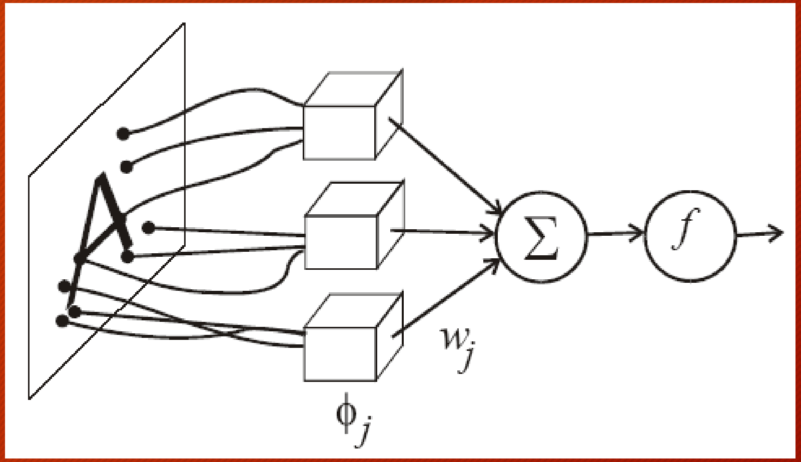
- Examples: (0,1), (1,3), (4,6), (2,4), (3,4)
- Try different learning rates

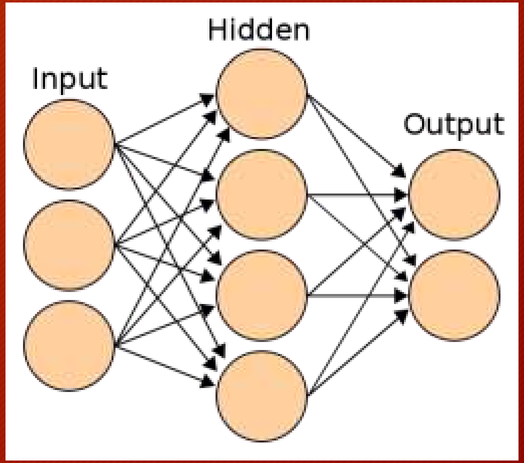
Too slow

| **α = 0.03** | **α = 0.08** | **α = 0.13** | **α = 0.16** ☹ |
|---|---|---|---|
| #1: a=0.56, b=0.22 | #1: a=1.5, b=0.58 | #1: a=2.44, b=0.94 | #1: a=3.01, b=1.15 |
| #2: a=0.9, b=0.35 | #2: a=1.38, b=0.58 | #2: a=0.59, b=0.36 | #2: a=-0.5, b=0.01 |
| #3: a=1.1, b=0.44 | #3: a=1.37, b=0.62 | #3: a=1.93, b=0.89 | #3: a=3.46, b=1.48 |
| #4: a=1.21, b=0.5 | #4: a=1.36, b=0.66 | #4: a=0.9, b=0.6 | #4: a=-1.12, b=-0.06 |
| #5: a=1.28, b=0.54 | #5: a=1.35, b=0.69 | #5: a=1.63, b=0.91 | #5: a=4.07, b=1.83 |
| #10: a=1.36, b=0.64 | #10: a=1.29, b=0.85 | #10: a=1.17, b=0.97 | #10: a=-4.25, b=-0.85 |
| #20: a=1.32, b=0.77 | #20: a=1.22, b=1.06 | #20: a=1.16, b=1.22 | #20: a=-19.92, b=-6.11 |
| #50: a=1.23, b=1.03 | #50: a=1.13, b=1.32 | #50: a=1.11, b=1.38 | #50: a=-1206.95, b=-422.37 |
| #100: a=1.15, b=1.25 | #100: a=1.1, b=1.39 | #100: a=1.1, b=1.4 | #100: a=-1030083.04, b=-361332.61 |
| #200: a=1.11, b=1.38 | #200: a=1.1, b=1.4 | #200: a=1.1, b=1.4 | #200: a=-748941284697.65, b=-262714417242.33 |

# Artificial neural networks (multi-layer perceptrons)

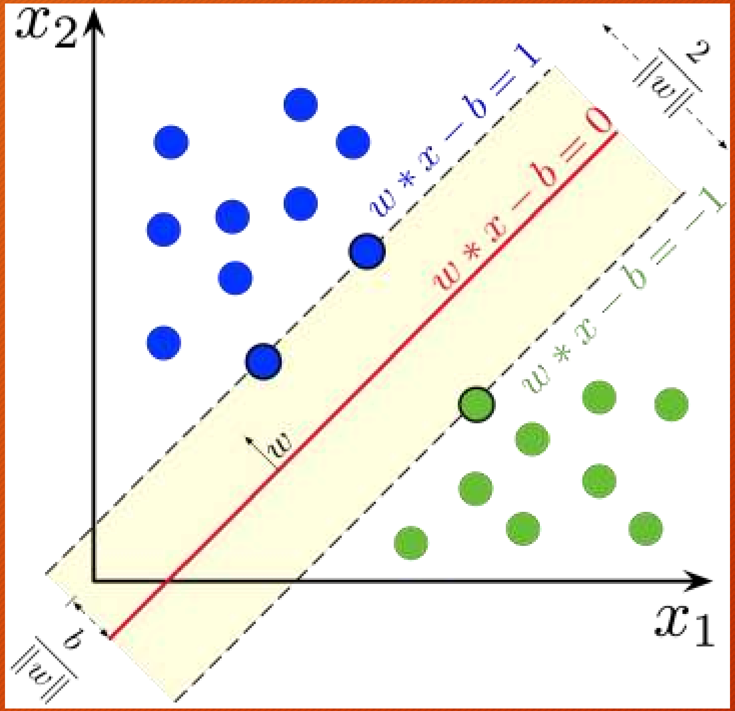
- Inspired by early ideas on neural networks in the brain, particularly the hierarchically organized visual system („the perceptron“)
- Trained using *backpropagation*
- Were shown to have *universal approximation property*
- Still very popular, although recently eclipsed by deep learning (which is a special case)

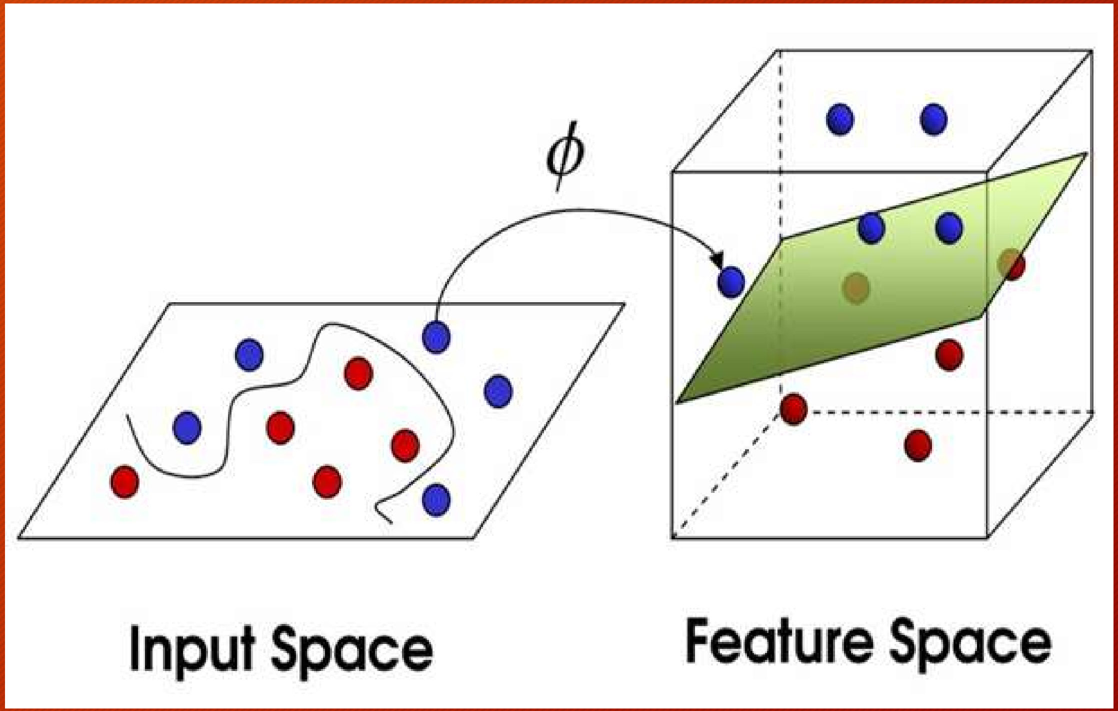




# Support vector machines (SVMs) and kernels

- Finding boundaries with largest margins between classes
- Kernels: projecting to higher dimensions





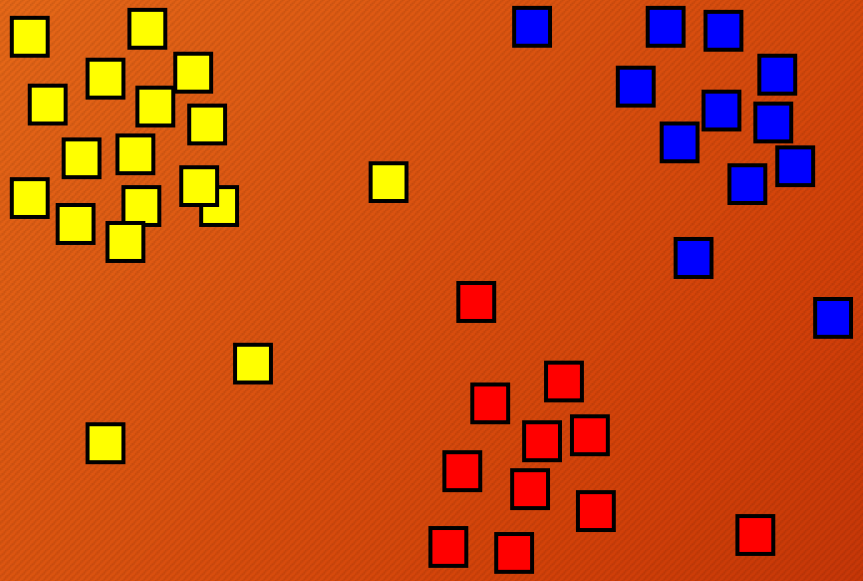
http://www.imtech.res.in/raghava/rbpred/svm.jpg

https://en.wikipedia.org/wiki/Support-vector_machine

Shooting fireworks into the sky or gene -> protein parallels ☺

## Unsupervised learning: a clustering example

- Can be solved with K-means



But…

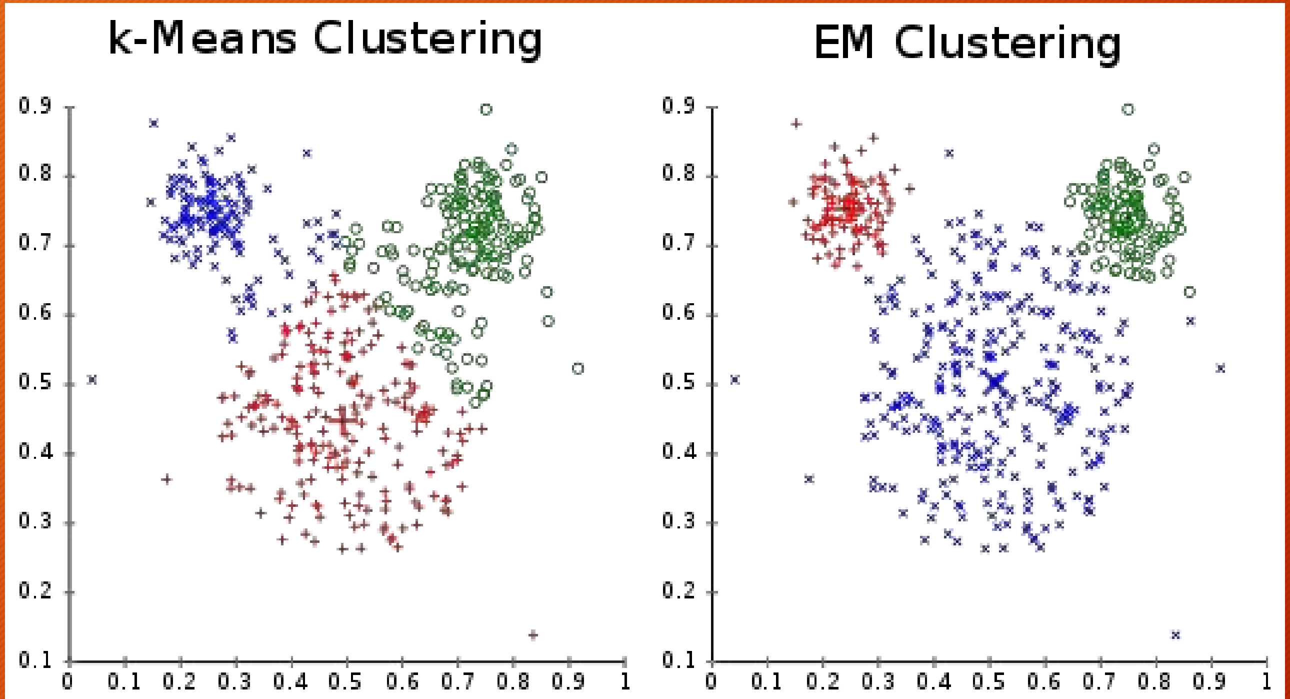
How many clusters?

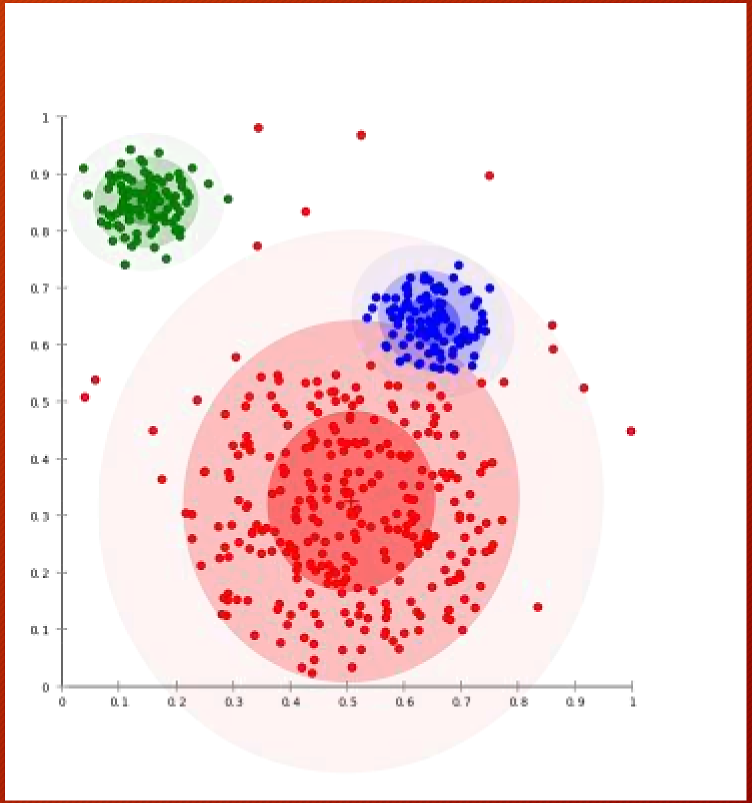
How to treat borderline points?

https://en.wikipedia.org/wiki/Cluster_analysis

# More on unsupervised learning: Gaussian mixtures

- Clusters vary in sizes & shapes, modeled by Gaussians
- Calculated using "expectation-maximization" algorithm



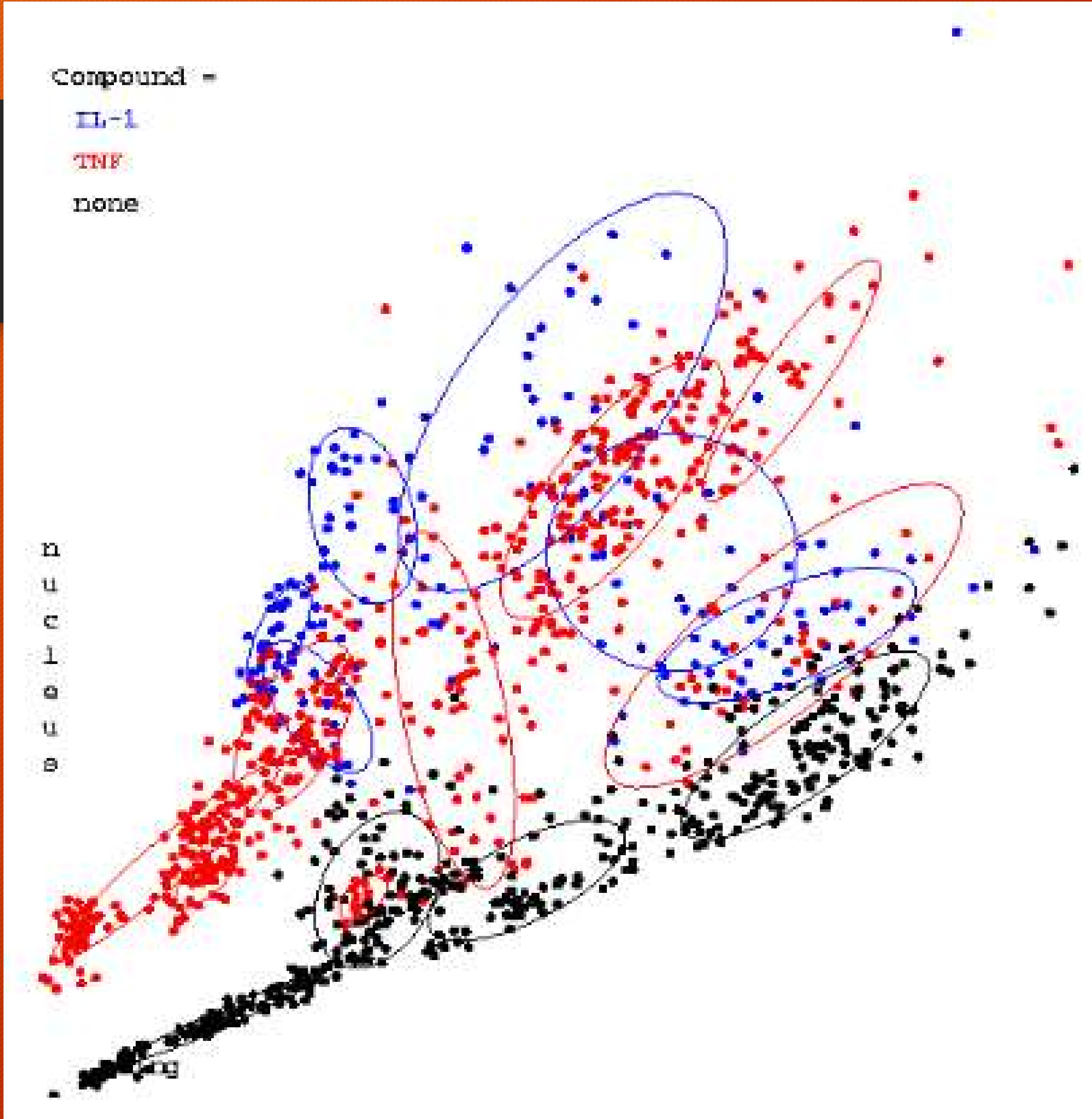


https://en.wikipedia.org/wiki/Cluster_analysis

## Gaussian mixtures for supervised learning

- Classes have complex distributions and may consist of multiple Gaussian clusters

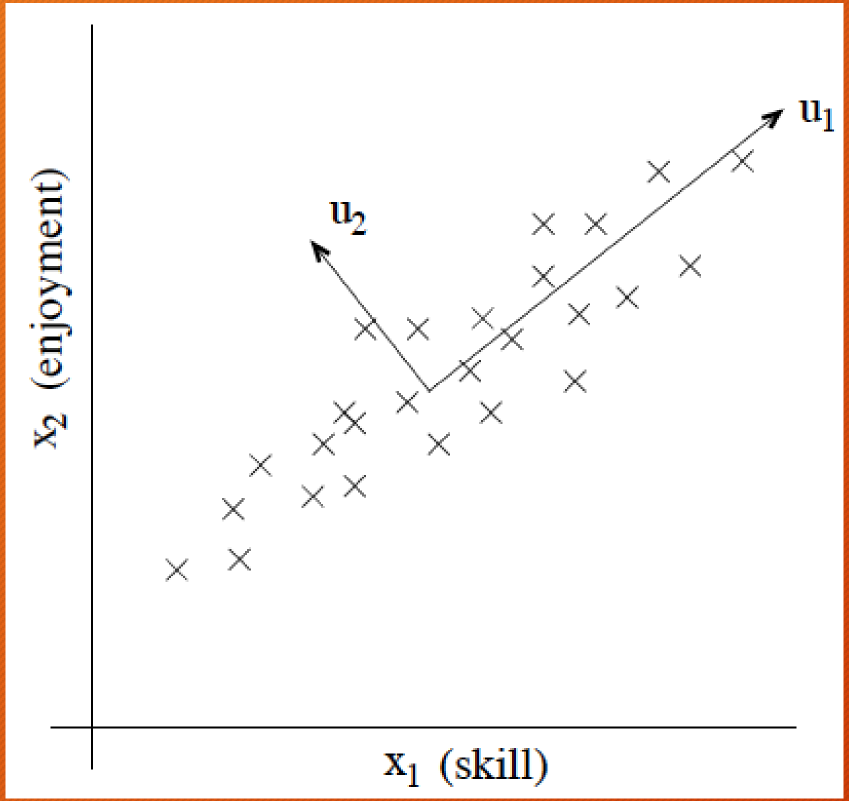
A.W.Moore's bioassay example



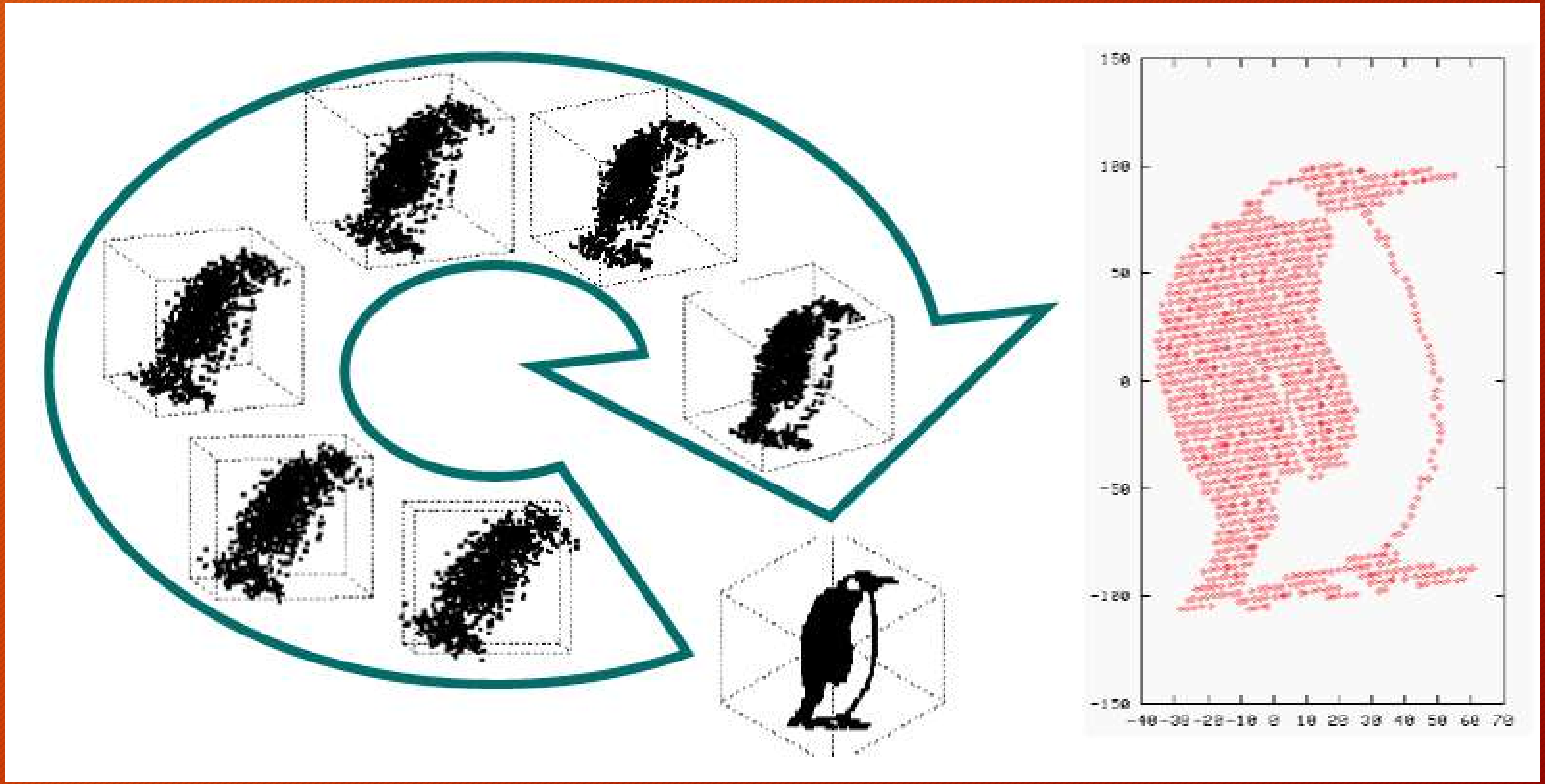
## Clustering vs. dimensionality reduction

- Clustering reduces the number of data points (into much fewer clusters)
  - *e.g. K-means, Gaussian mixtures*
- Dimensionality reduction reduces the number of dimensions per data point
  - *e.g. Principal/Independent Component Analyses*
- Use similar principles but in different direction / for different purpose (leading to either fewer data or fewer dimensions)
- In supervised learning dimensionality reduction often used before prediction – WHY?

# Principal component analysis – rotate data to maximize variance



Helicopter driving – Andrew Ng



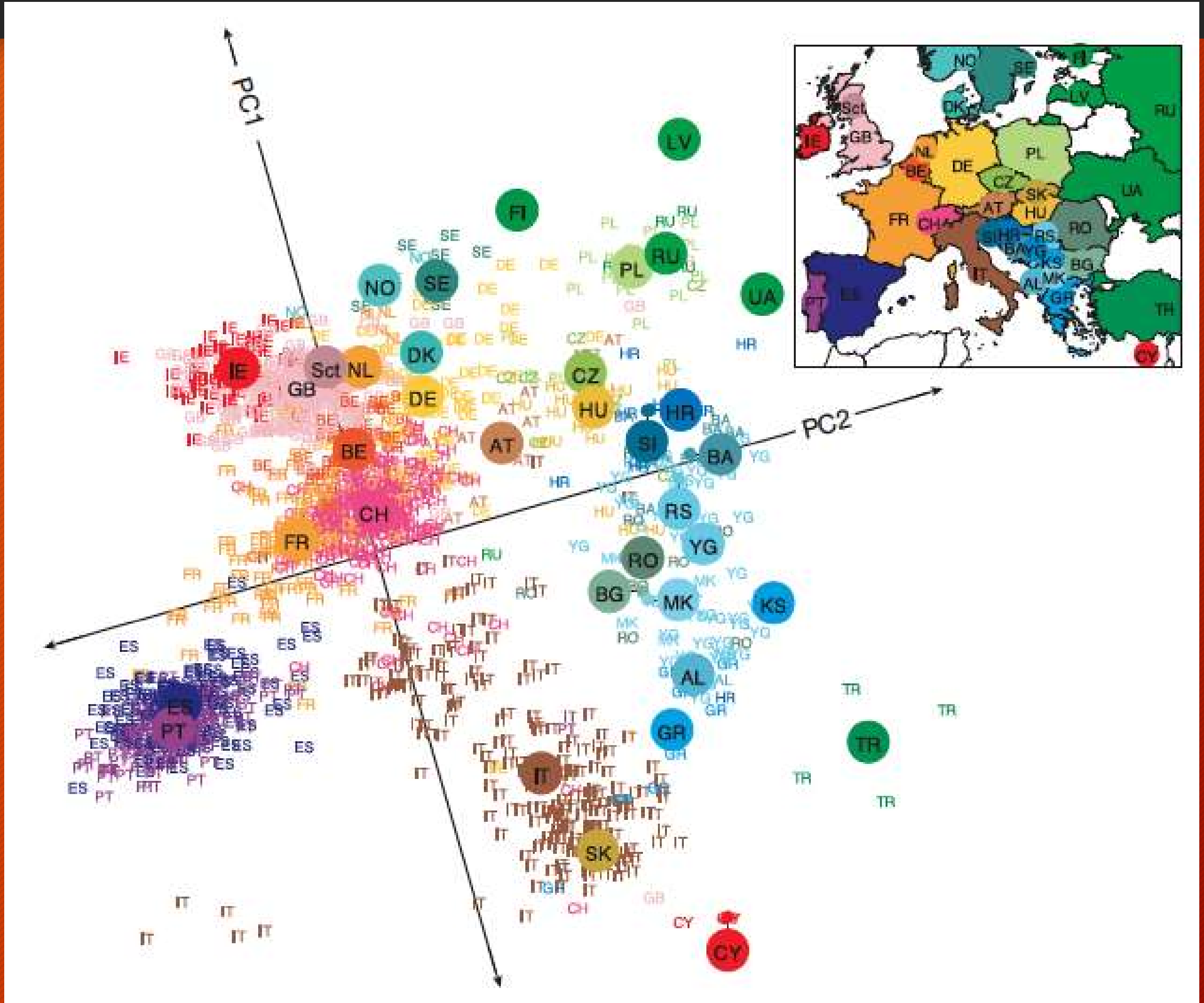
Example by R.Gutierrez-Osuna

# PCA can help finding good features

- Principal components are orthogonal / decorrelated, but not always easily interpretable

Where they are:

- Principal component analysis of genetic variation in Europe

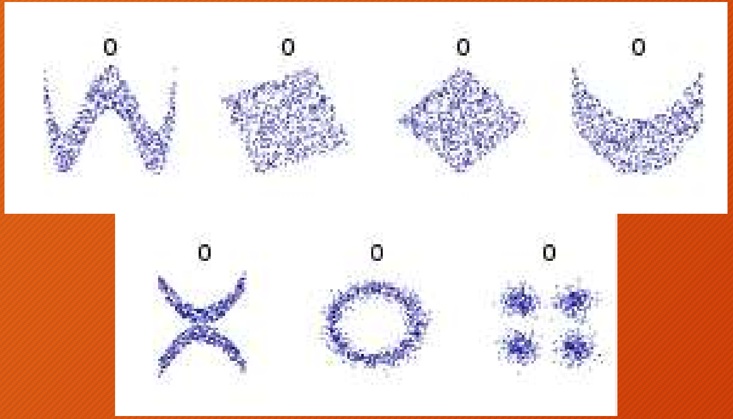


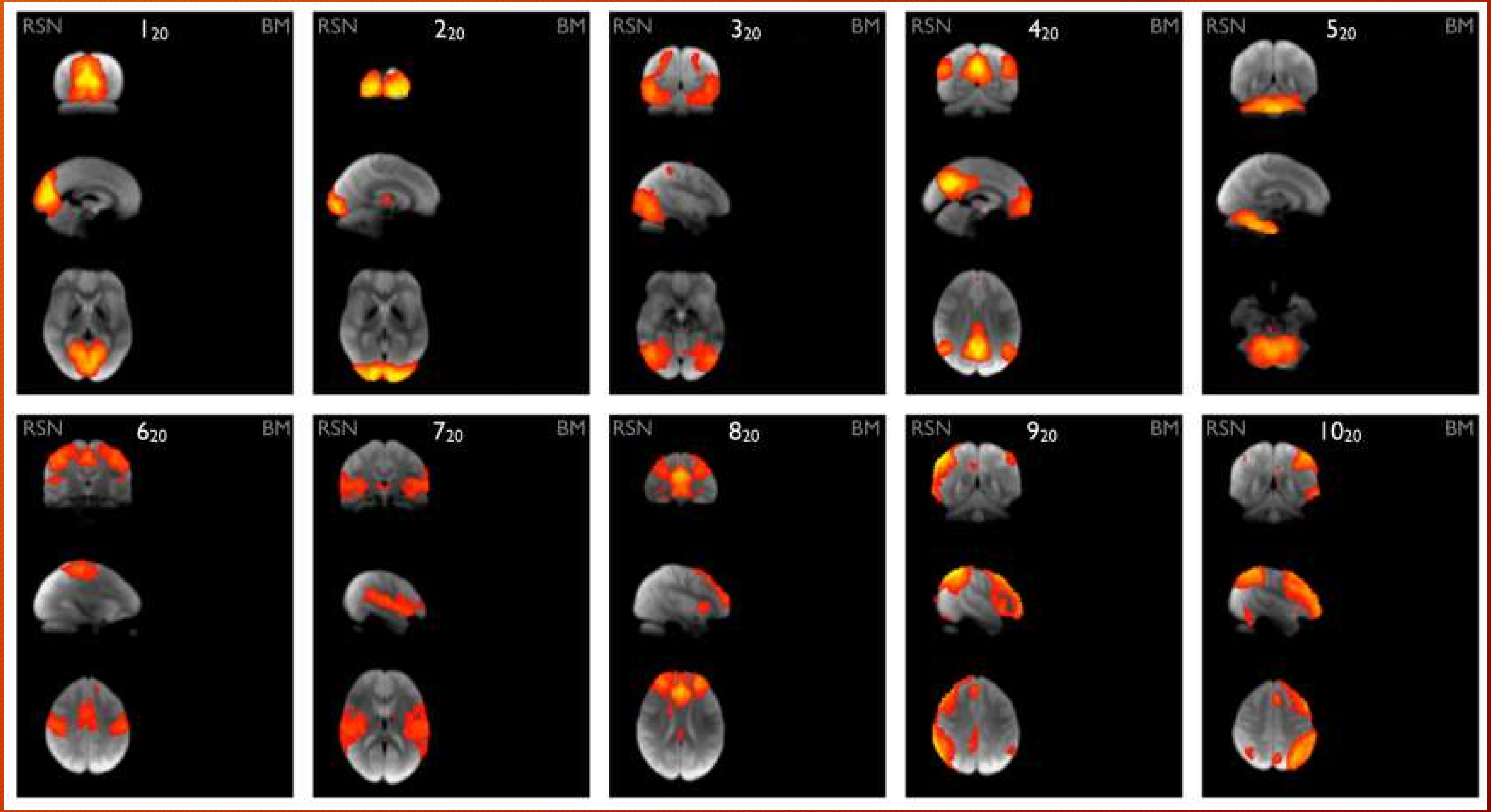
Novembre et al., Nature 2008

# Identification of brain's networks using fMRI + Independent Component Analysis during the resting state

Smith et al., PNAS 2009

**Independent Component analysis** – extract components that are not just uncorrelated but also independent!

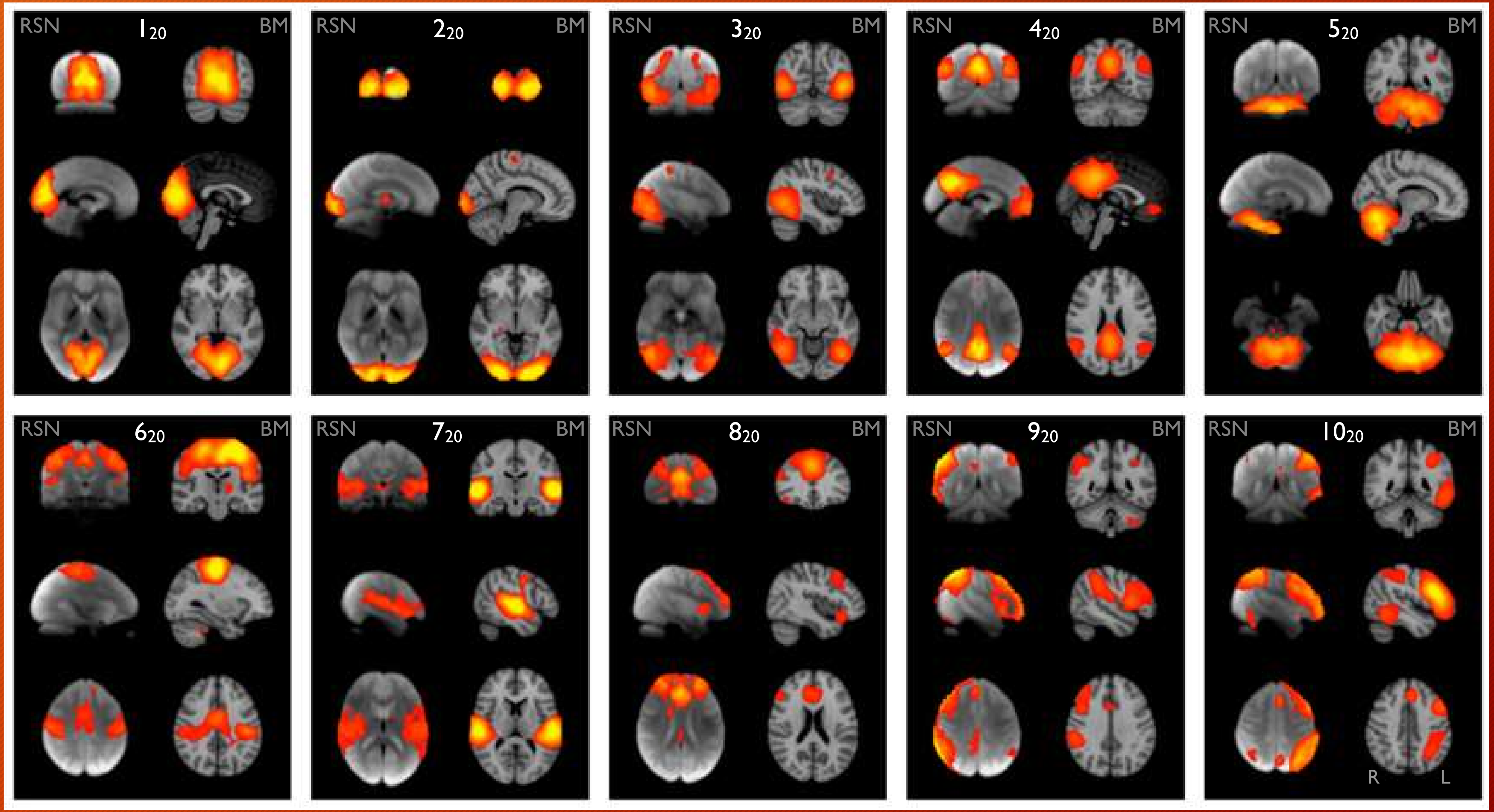




# Identification of brain's networks using fMRI + ICA during the resting state & task performance

Extracted components in the resting state and during a variety of task performances are similar!

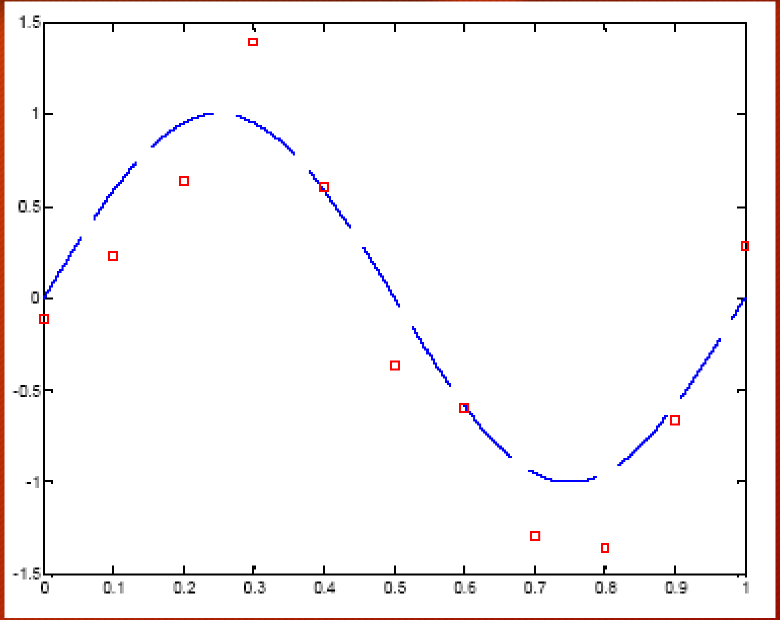
Smith et al., PNAS 2009

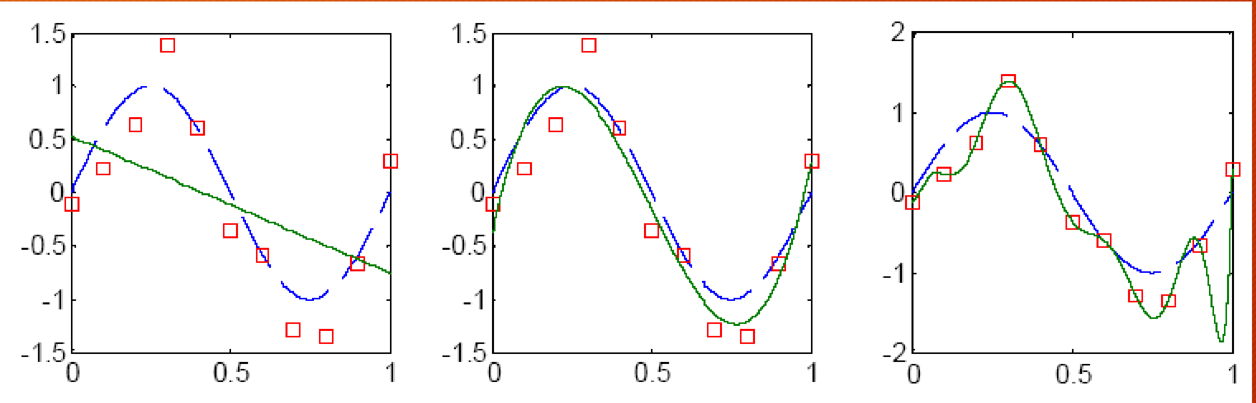


# Potential problem in supervised learning: **overfitting**

- Imagine a model: $p(x) = w_0 + w_1 x + \cdots + w_M x^M = \sum_{j=0}^{M} w_j x^j$ .
- No. of parameters = M+1
- Goal: minimize error

$$MSE_{train} = {}^{1}\!/\!_{N} \sum_{i=1}^{N} \left( p\left(x^{(i)}\right) - y^{(i)} \right)^2$$





Herbert Jaeger, *'Machine Learning'*, Bremen, 2003

M=1, MSE=0.4852
M=3, MSE=0.0703
M=10, MSE = 0!

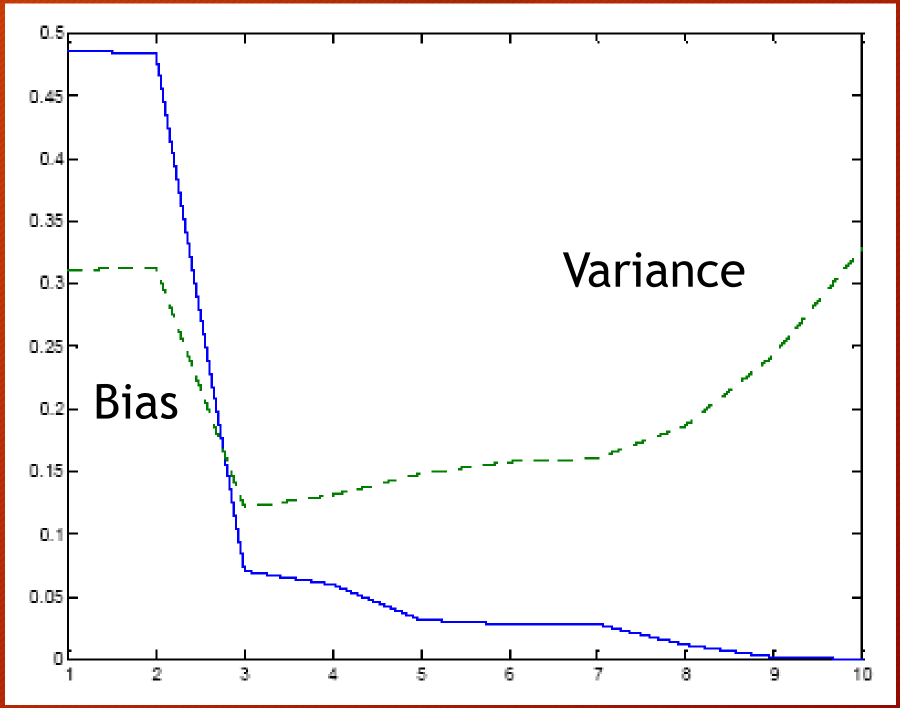
**Really?**

# Bias-variance dilemma

- Why does M=3 look better than M=10?
  - It better **generalizes** the function! But…
  - We typically don‘t know what the function is…
- Use the *testing error*!

$$MSE_{test} = \frac{1}{K}\sum_{j=1}^{K}\left(p\left(x^{(j)}\right) - y^{(j)}\right)^2$$

So M=3 is really the best ☺



H.Jaeger, ‘*Machine Learning*’, Bremen, 2003

Why „bias-variance“?

- Bias – fails to account for relevant data structure
- Variance – varies too much depending on training data

## Dealing with bias-variance dilemma

Finding a right balance (i.e. avoiding overfitting and underfitting) depends on two critical quantities:

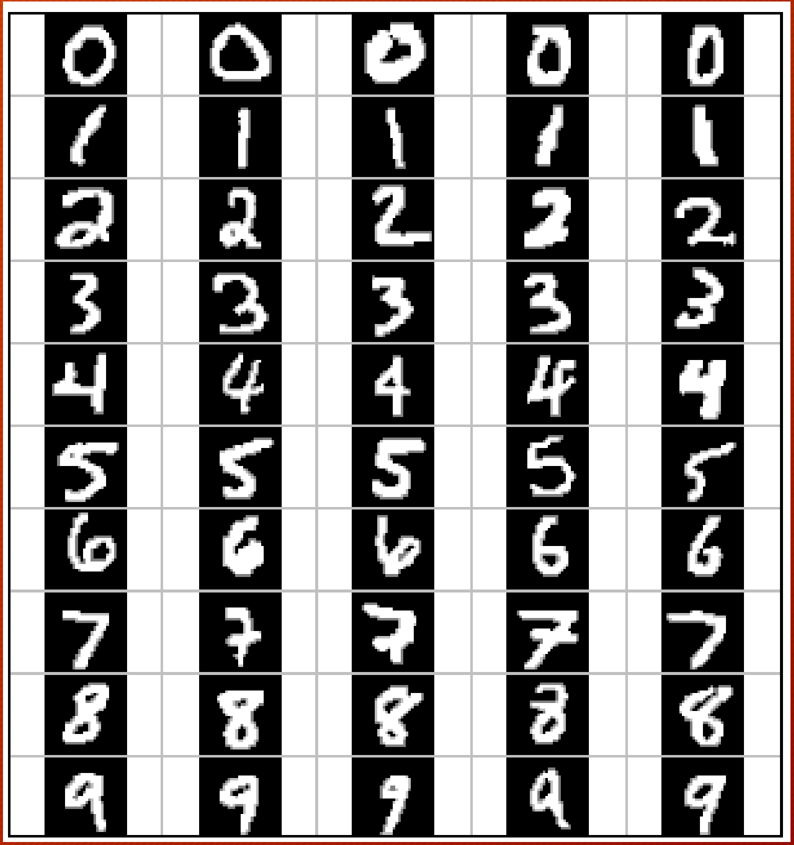
- **Model size** (the number of parameters M)
- The **number of samples** N

If M >= N, there will certainly be a substantial overfitting (system of linear equations analogy)

- Normally it's recommended that M would be **much smaller** than N, e.g. 50 or 100 parameters for 1000 samples

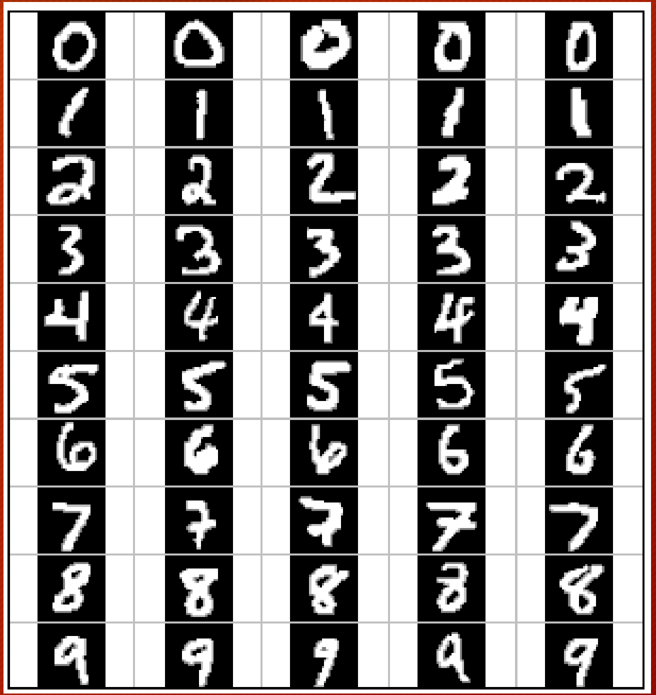
# How to evaluate over-/underfitting?

- Use **cross-validation**
  - Divide your data into **training** and **validation** sets
  - Use the training set for training the model, and the validation set for choosing the number of parameters
  - If have too little data, can use „leave-one-out“ cross validation

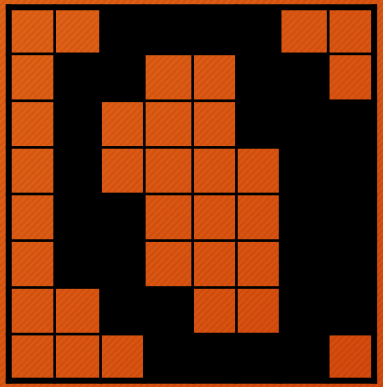

http://w3.impa.br/~lhf/sib2003/p023/img2.gif

# Dimensionality reduction: features

- So our model size is limited by the number of available samples. What‘s the problem with this?
- Model size is also constrained *(unfortunately from the opposite side)* by the dimensionality of data – usually for each input dimension there is at least 1 parameter



http://w3.impa.br/~lhf/sib2003/p023/img2.gif



**How to resolve this?**

- Use not the raw data, but **features**!
- Sometimes this can be done using task-dependent heuristics