Machine Learning: Unsupervised Learning

Konstantin Tretyakov
http://kt.era.ee

AACIMP 2012
August 2012

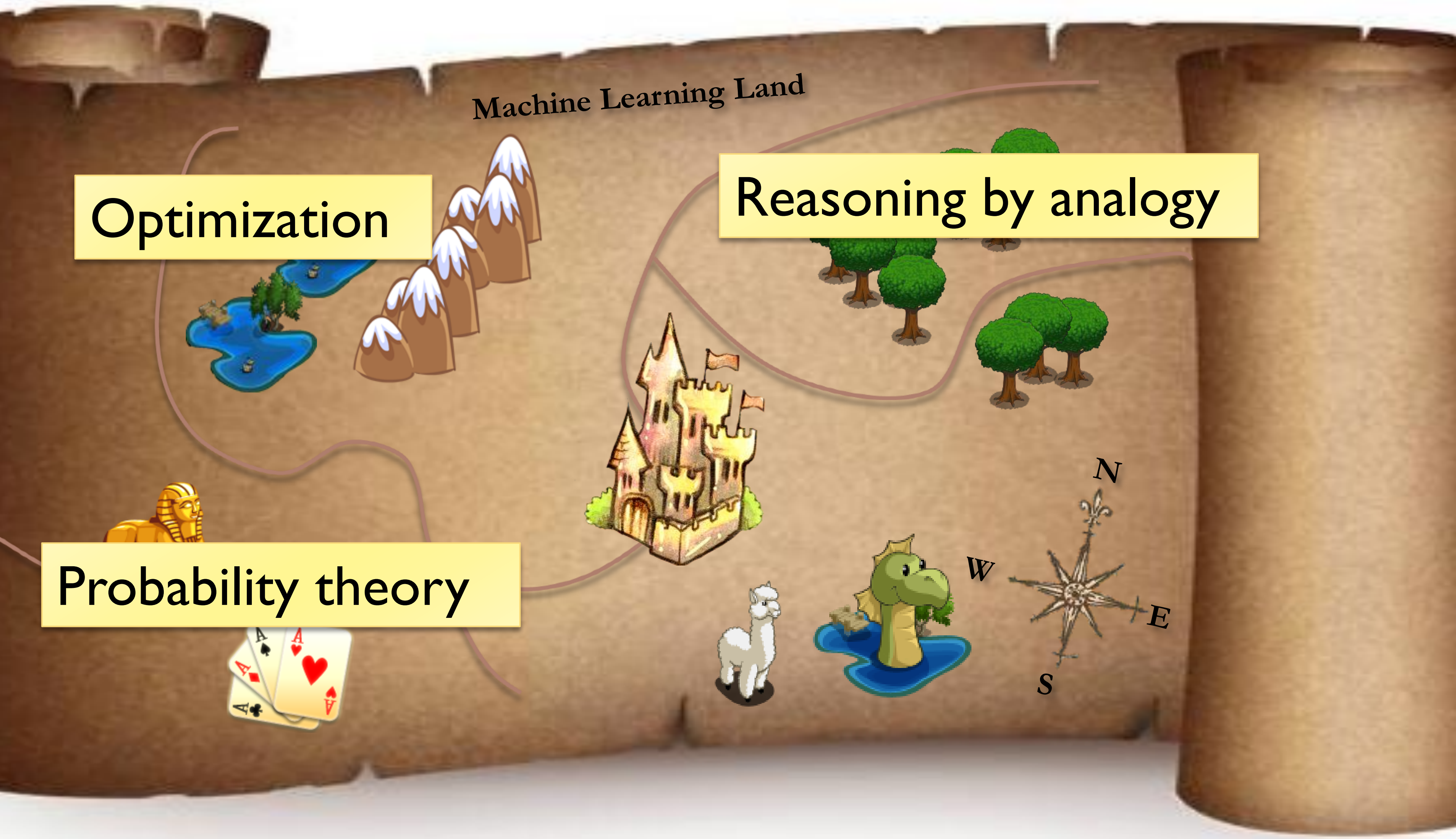
STACC Software Technology and Applications Competence Center

BIIT

TARTU ÜLIKOOL · UNIVERSITAS TARTUENSIS · 1632

So far…

So far…


Machine Learning Land
Optimization
Reasoning by analogy
Probability theory
N
W
E
S

So far…

Optimization

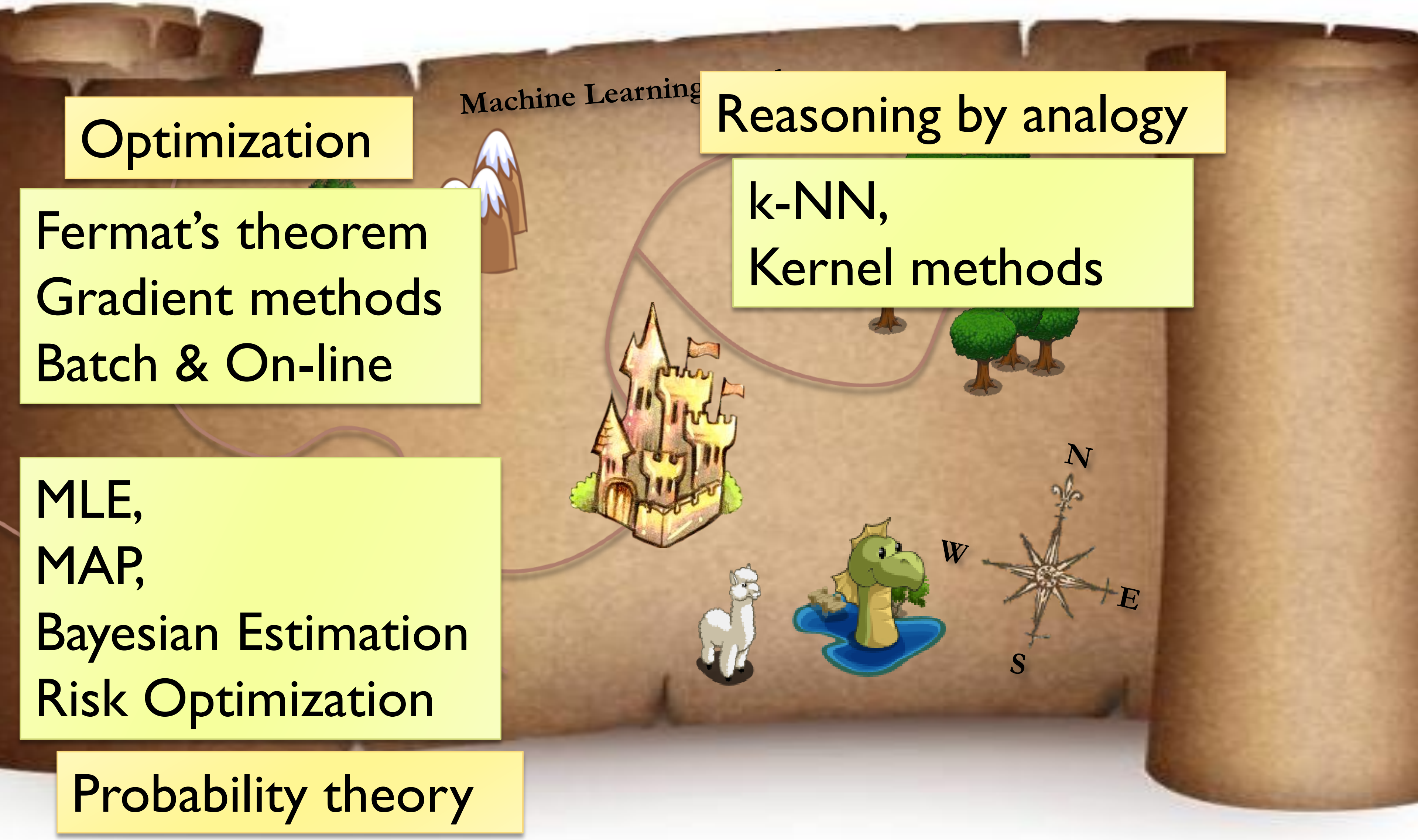
Fermat's theorem
Gradient methods
Batch & On-line

MLE,
MAP,
Bayesian Estimation
Risk Optimization

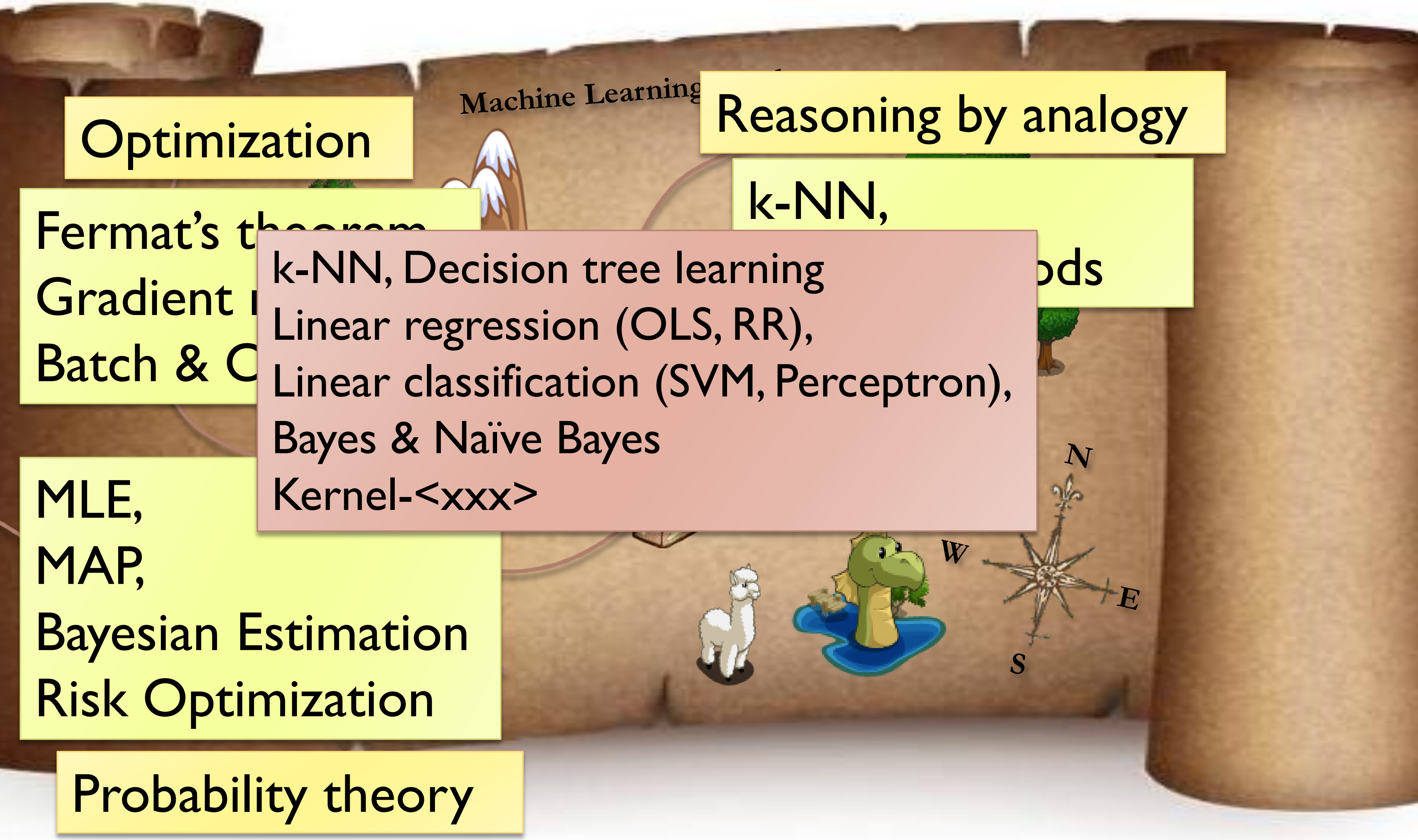
Probability theory

Reasoning by analogy

k-NN,
Kernel methods



So far…



Optimization

Fermat's th
Gradient
Batch & O

MLE,
MAP,
Bayesian Estimation
Risk Optimization

Probability theory

Reasoning by analogy

k-NN,
ods

k-NN, Decision tree learning
Linear regression (OLS, RR),
Linear classification (SVM, Perceptron),
Bayes & Naïve Bayes
Kernel-<xxx>

Today

Machine Learning

Optimization

Fermat's th
Gradient
Batch & O

Reasoning by analogy

k-NN,
ods

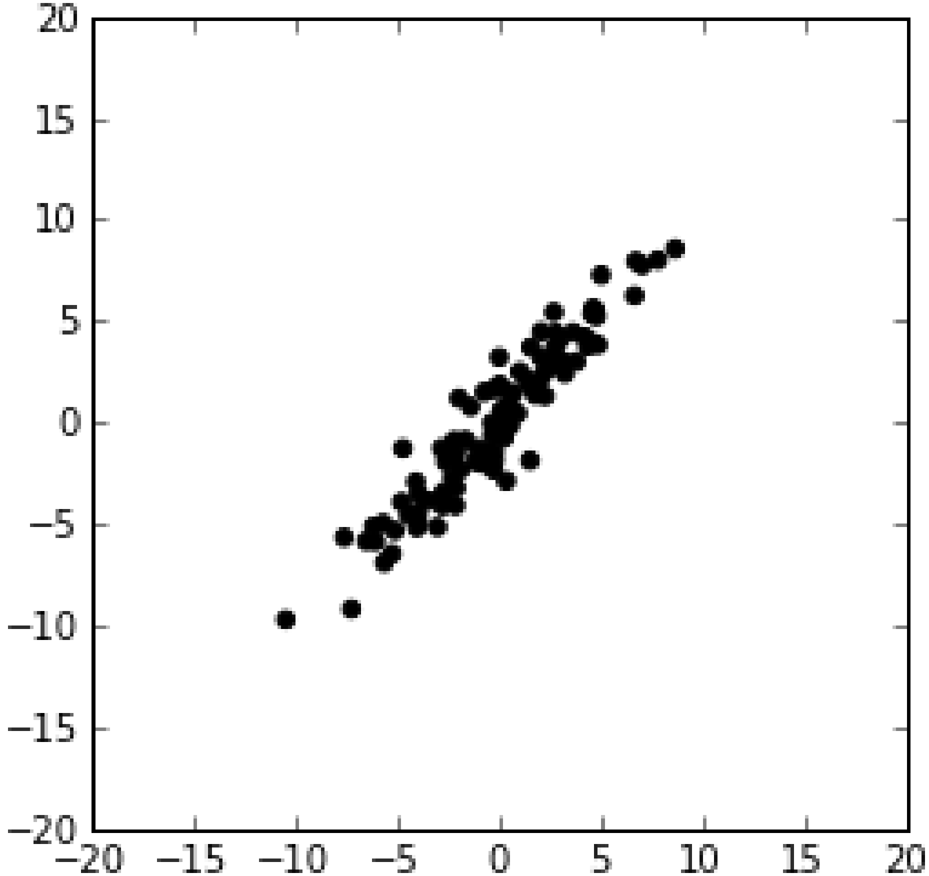
k-NN, Decision tree learning
Linear regression (OLS, RR),
Linear classification (SVM, Perceptron),
Bayes & Naïve Bayes
Kernel-<xxx>

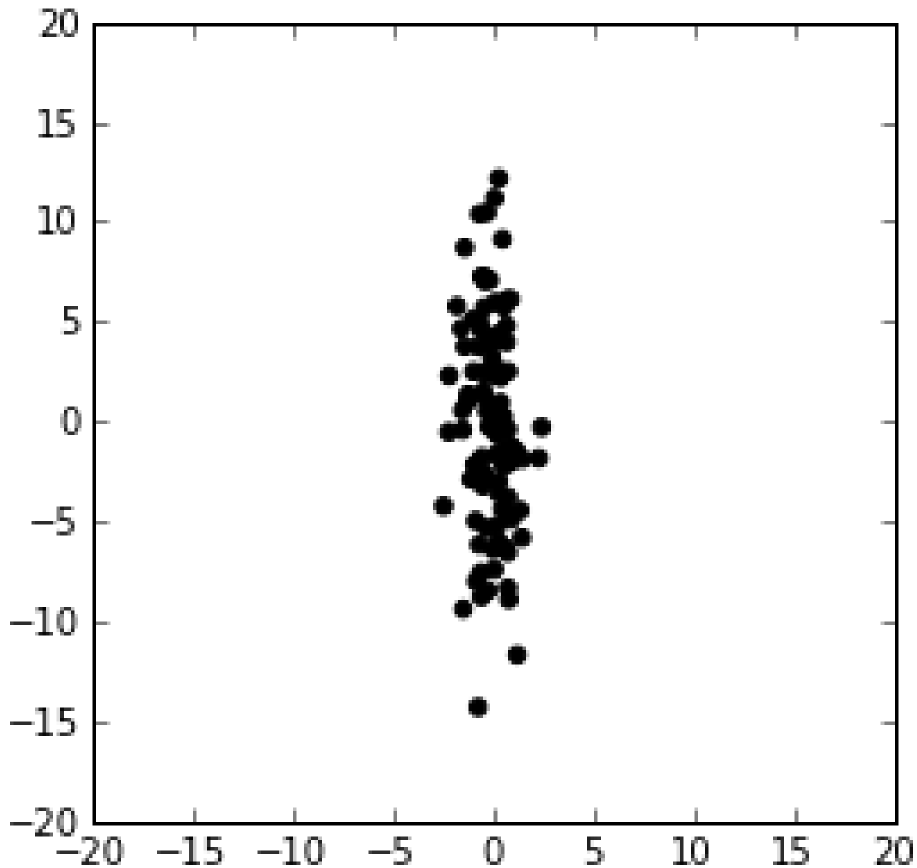
N

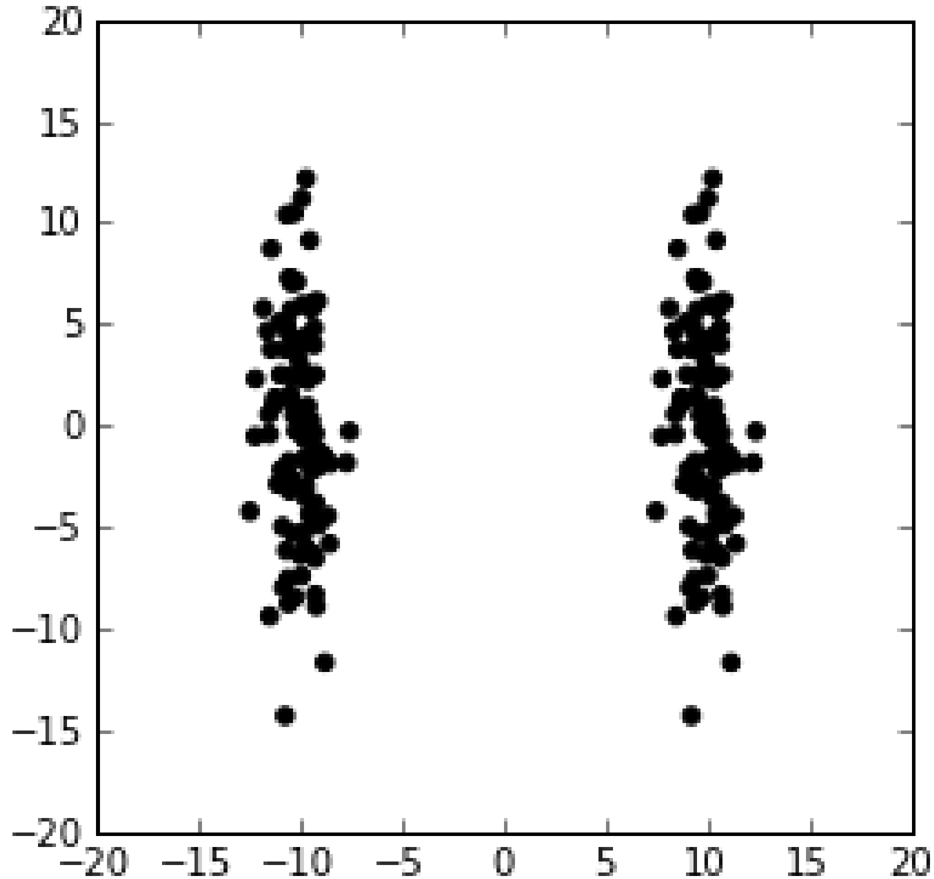
MLE,
MAP,
Bayesian Estimation
Risk Optimization

Unsupervised Learning

Probability theory


20
15
10
5
0
−5
−10
−15
−20
−20
−15
−10
−5
0
5
10
15
20


20
15
10
5
0
−5
−10
−15
−20
−20
−15
−10
−5
0
5
10
15
20



20
15
10
5
0
−5
−10
−15
−20
−20 −15 −10 −5 0 5 10 15 20

AATAACGGCCCGATGAGGAAACGAACGGTCGCACT

AAGATGAGACATGTCCCGAAAGGTGCATAAGTTAT

GGACGAAAAACTTTCTTCGCCCTTTGATGTGCCCC

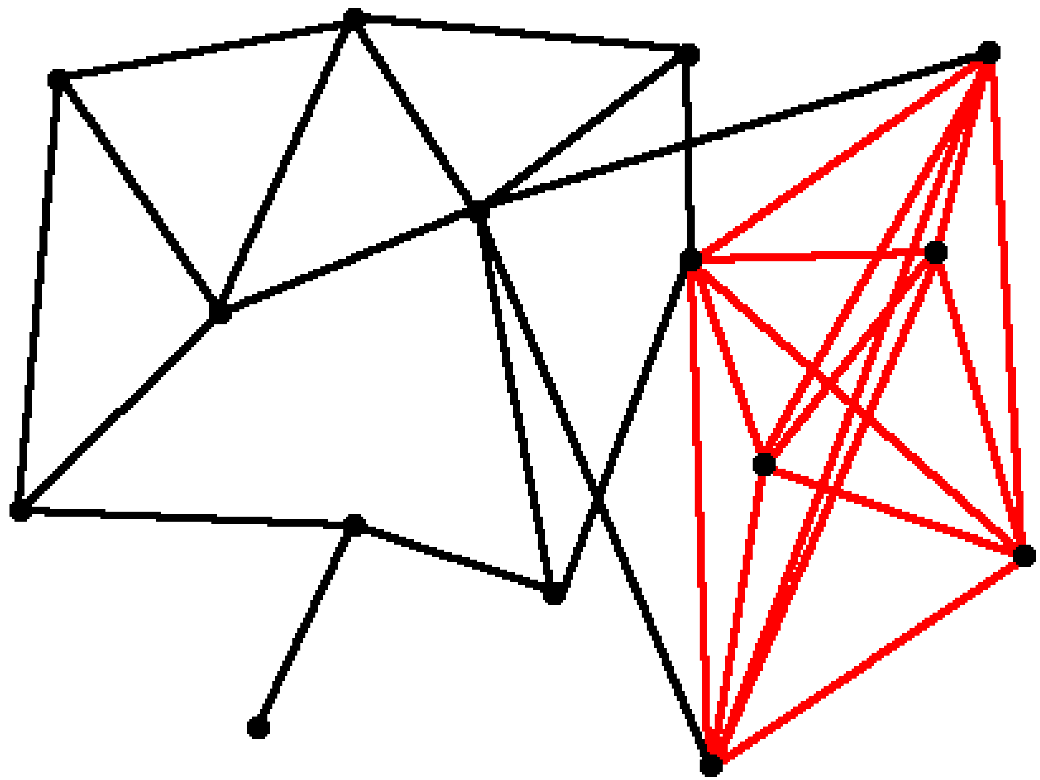
AGCGCGGGATGAGGATCAGCCCCCGCATTAGTTCA

ATATGCGAGCTTTCGCGCTCGGAAAGGGCAATAAA

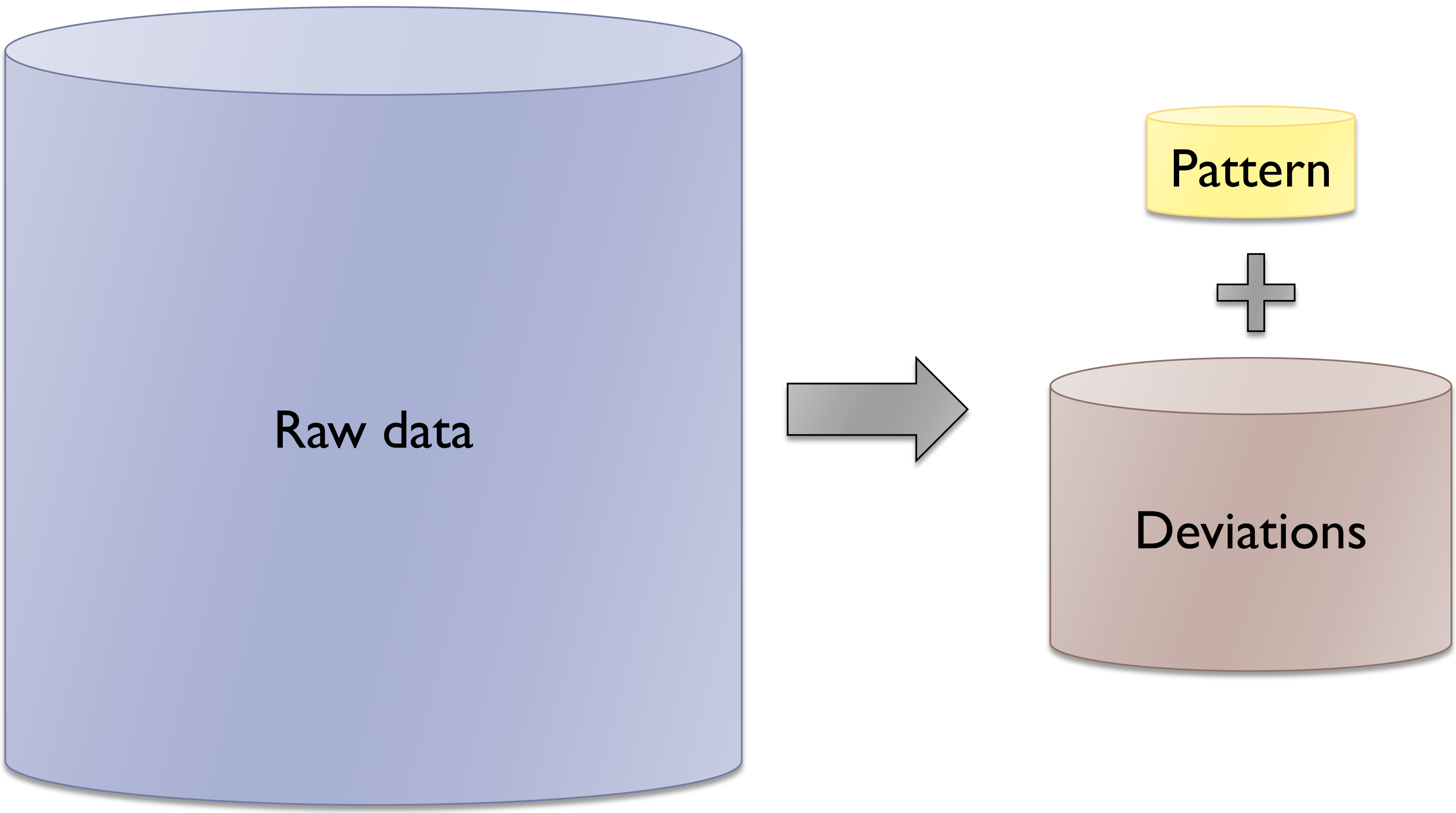
GCGACGGCCCCGATGAGGGGTGTTACTAGATTGGA

TGGGTGGTTCAGATCTCGGCTTACCCCCTTTATCA

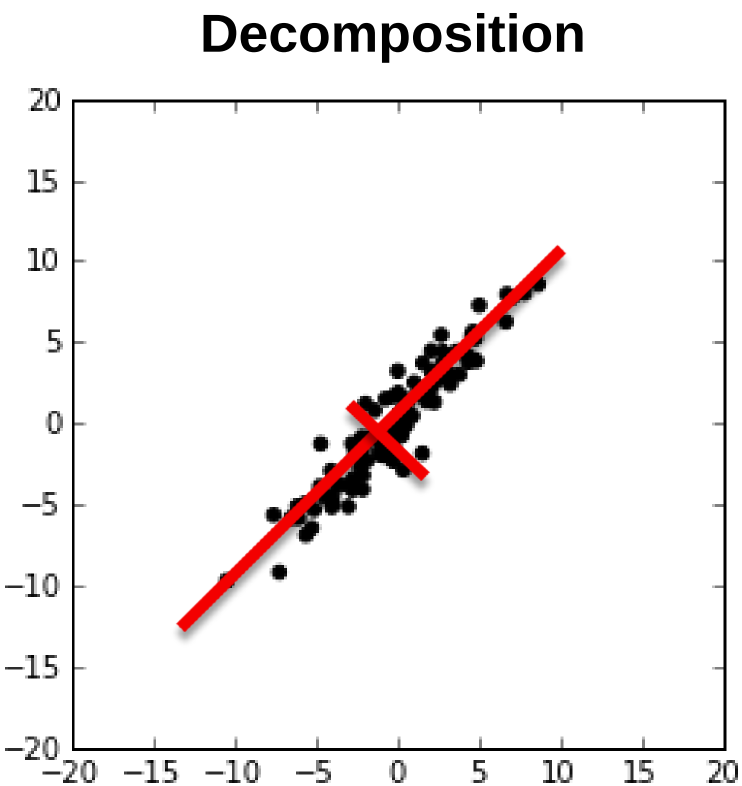
ACCCTGCTACAGACTCGTTGAGAATGCTACGGATC

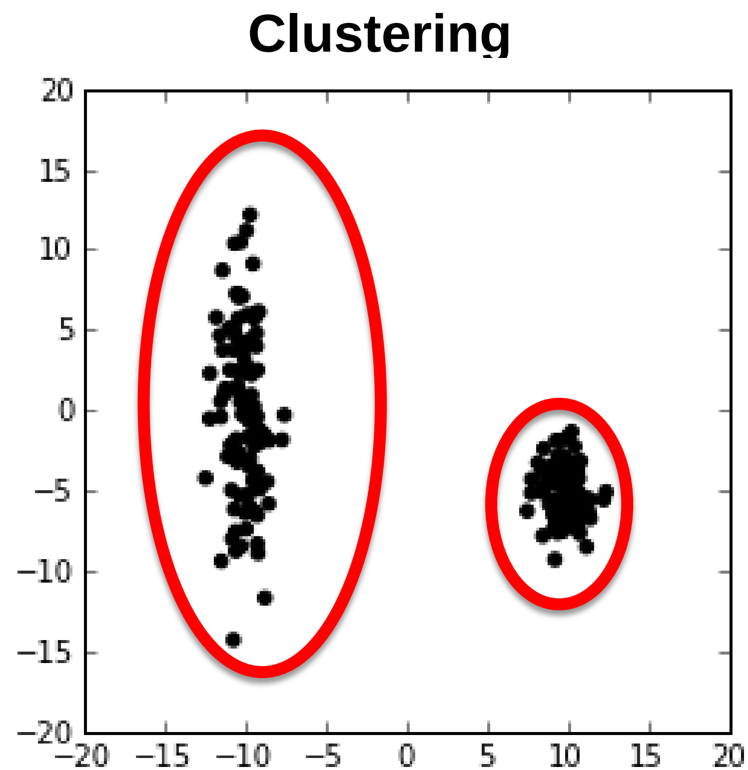


Data Mining



Today

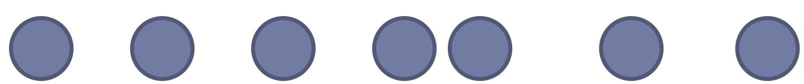

Decomposition
20
15
10
5
0
−5
−10
−15
−20
−20 −15 −10 −5 0 5 10 15 20


Clustering
20
15
10
5
0
−5
−10
−15
−20
−20 −15 −10 −5 0 5 10 15 20

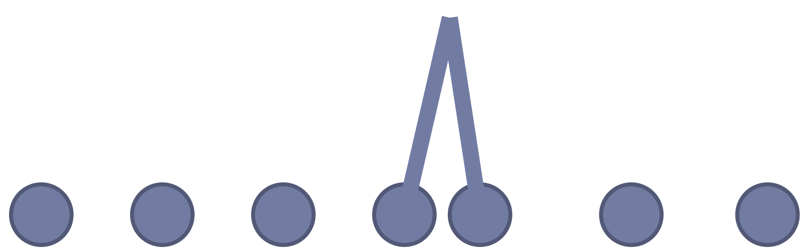
Quiz

- Why would one need clustering?

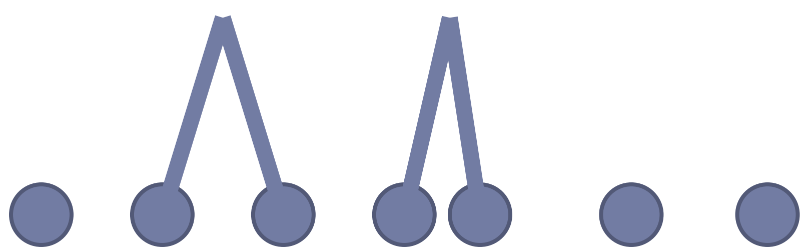
Hierarchical clustering



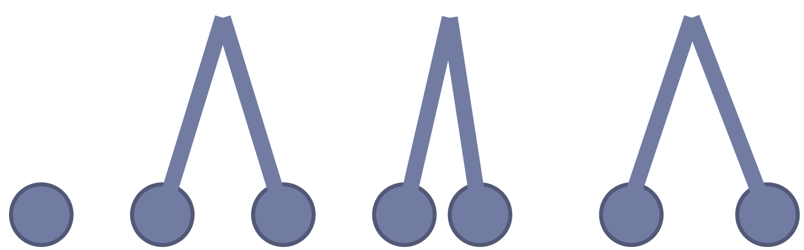
Hierarchical clustering



Hierarchical clustering

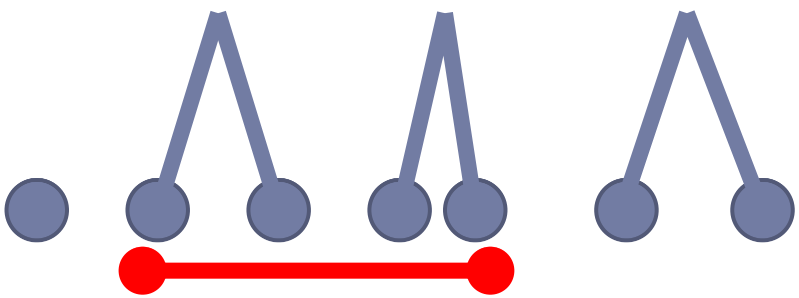


Hierarchical clustering



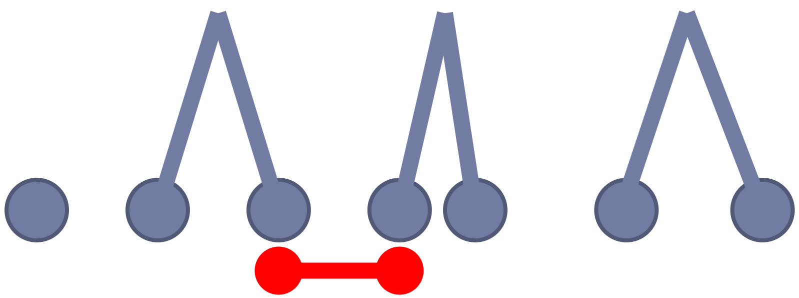
Hierarchical clustering

Complete linkage



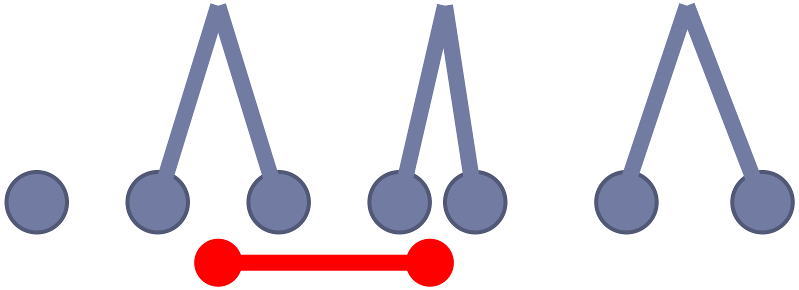
Hierarchical clustering

Single linkage



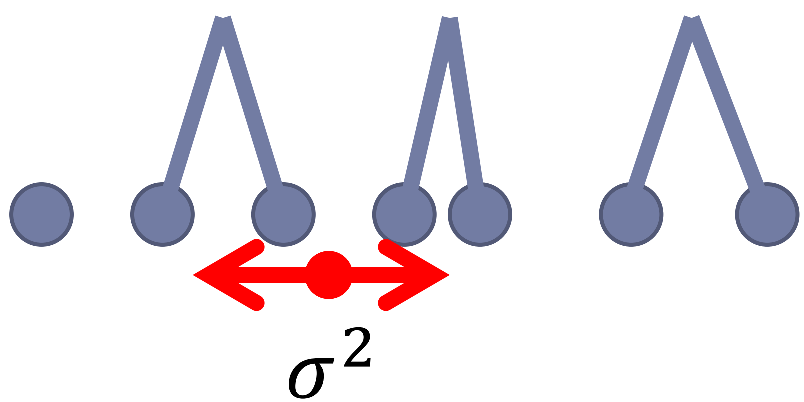
Hierarchical clustering

Average linkage

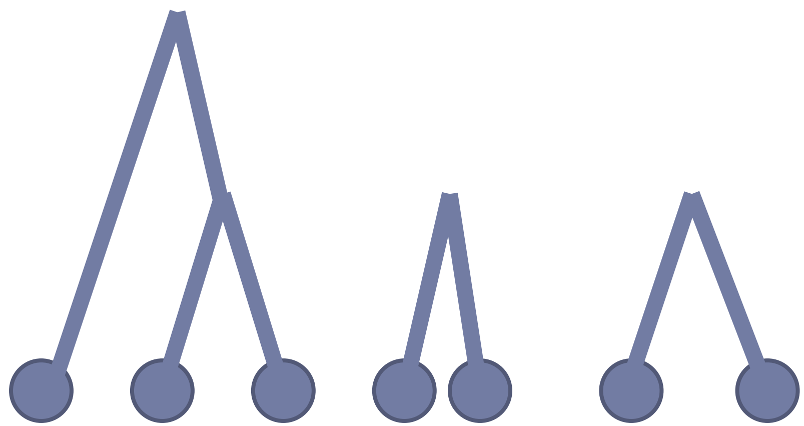


Hierarchical clustering

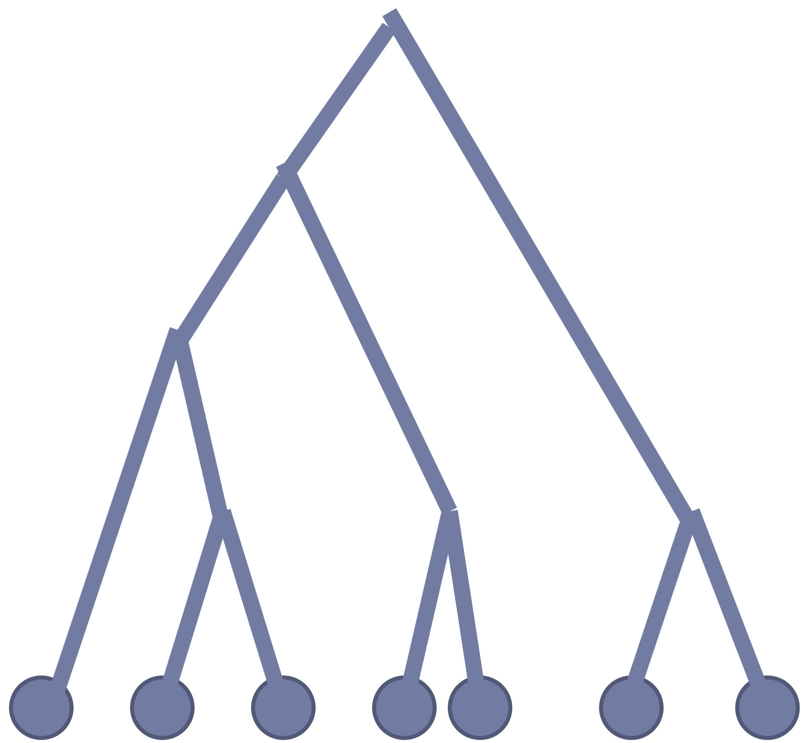
Ward linkage



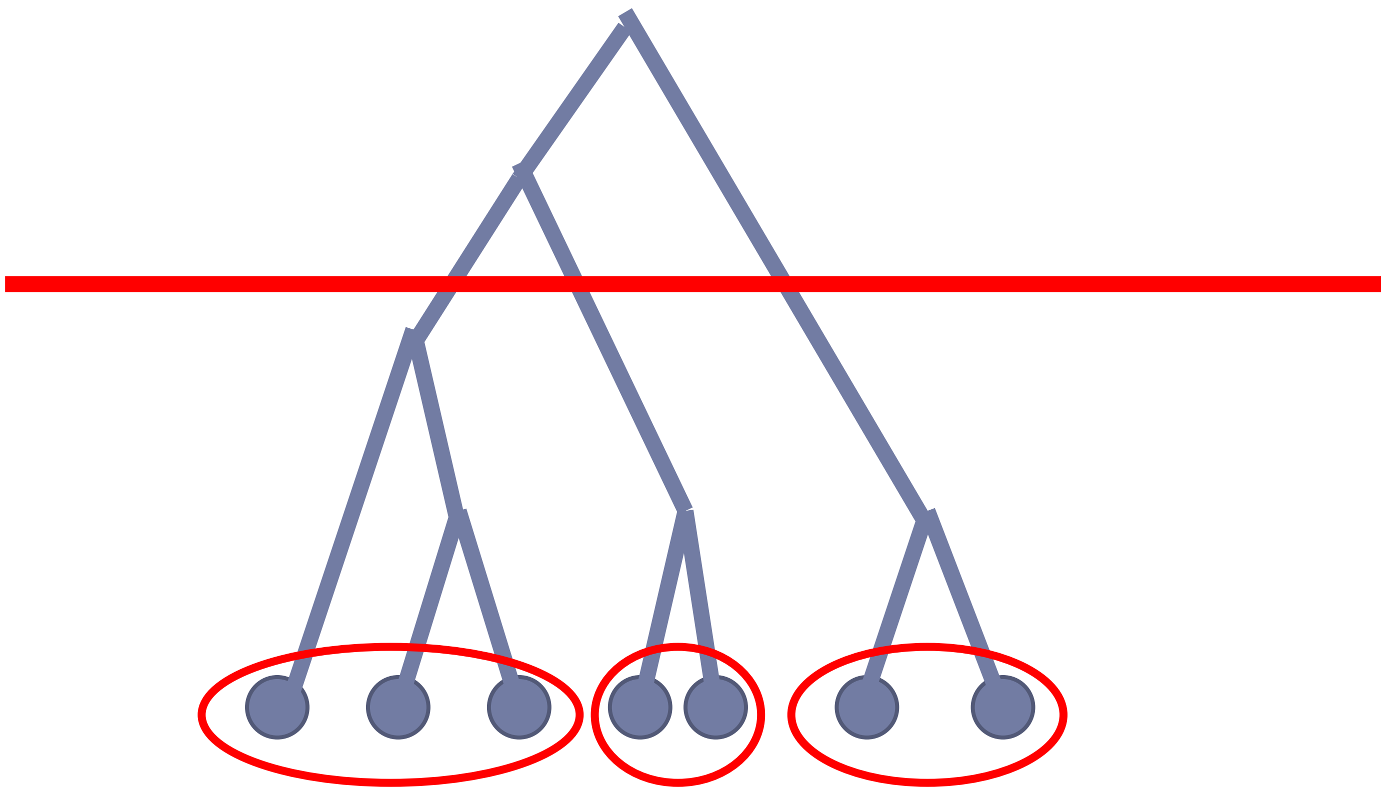
Hierarchical clustering



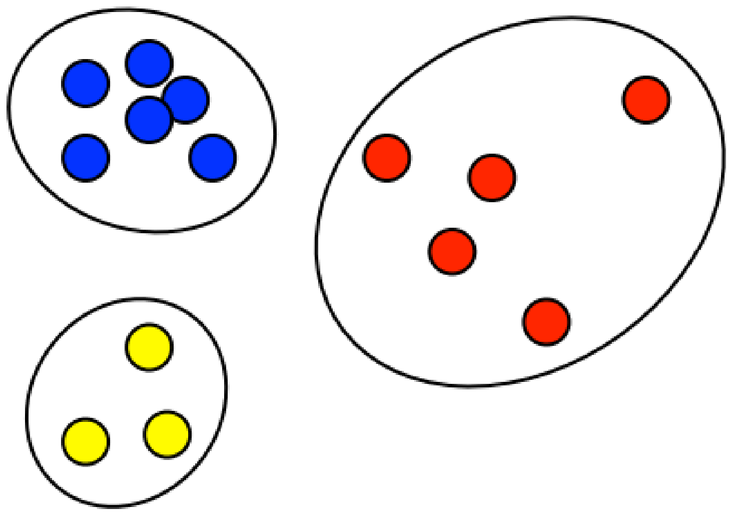
Hierarchical clustering



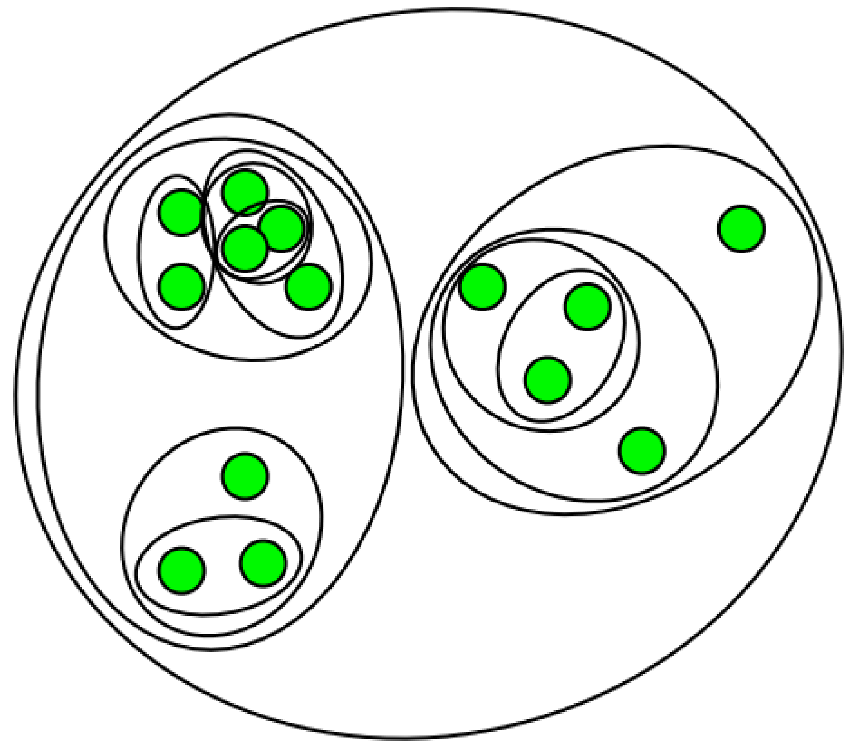
Hierarchical clustering



Partitional vs Hierarchical

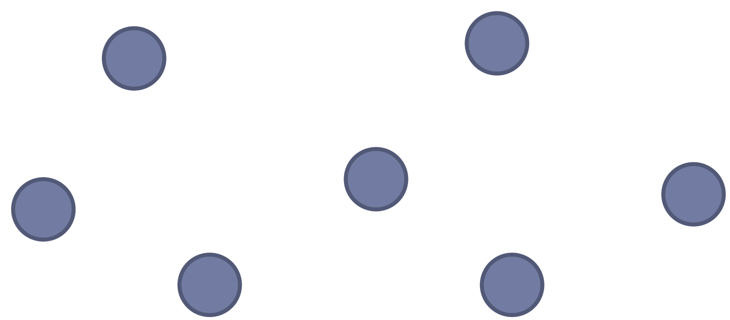


Partitional clustering finds a fixed number of clusters

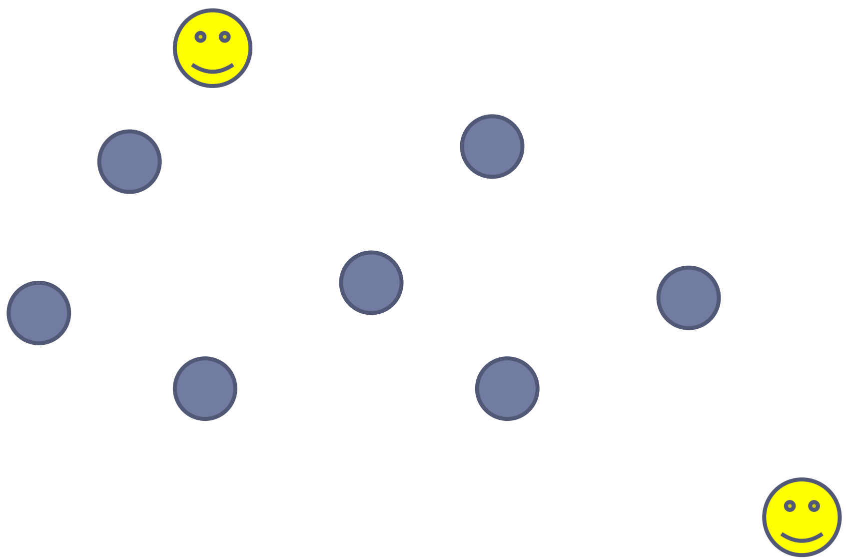


Hierarchical clustering creates a series of clusterings contained in each other

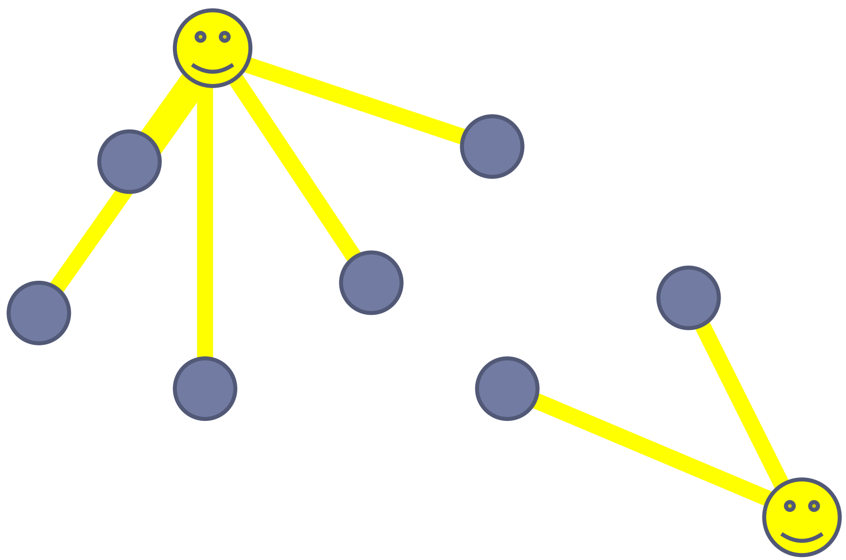
K-means



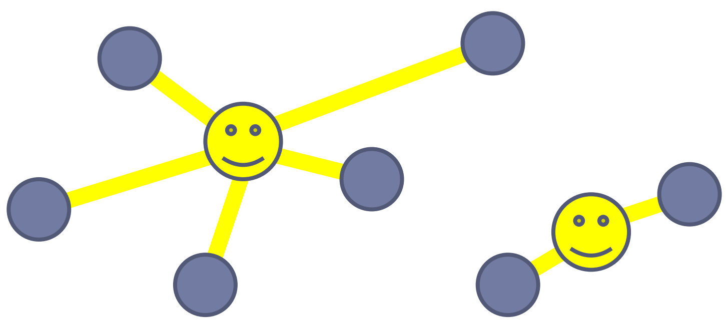
K-means



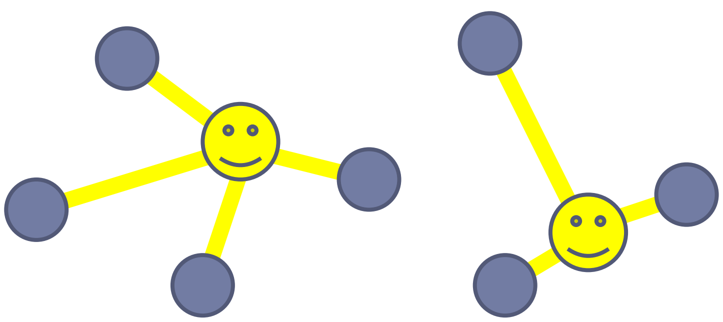
K-means



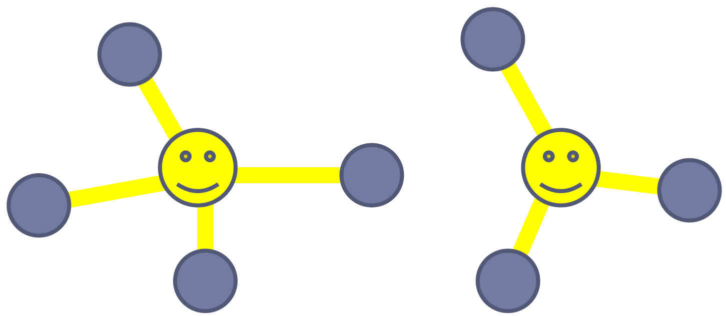
K-means



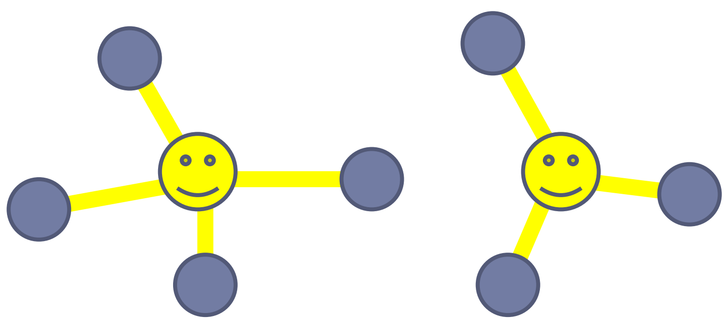
K-means



K-means



K-means



$$\text{argmin}_{c_1,\ldots,c_K} \sum_i \left\| x_i - c_{\text{closest\_to }(i)} \right\|^2$$

K-means

$$\operatorname{argmin}_{c_1,\ldots,c_K} \sum_i \left\| x_i - c_{\text{closest\_to}(i)} \right\|^2$$

- **Need to find cluster centers c_k.**

$$c_1 = ?, c_2 = ?, \ldots, c_K = ?$$

K-means

$$\mathrm{argmin}_{c_1,\ldots,c_K} \sum_i \left\| x_i - c_{\mathrm{closest\_to}(i)} \right\|^2$$

- **Need to find cluster centers c_k.**

$$c_1 = ?, c_2 = ?, \ldots, c_K = ?$$

- **Introduce *latent variables* (one for each x_i)**

$$a_i = \mathrm{closest\_cluster\_center}(i)$$

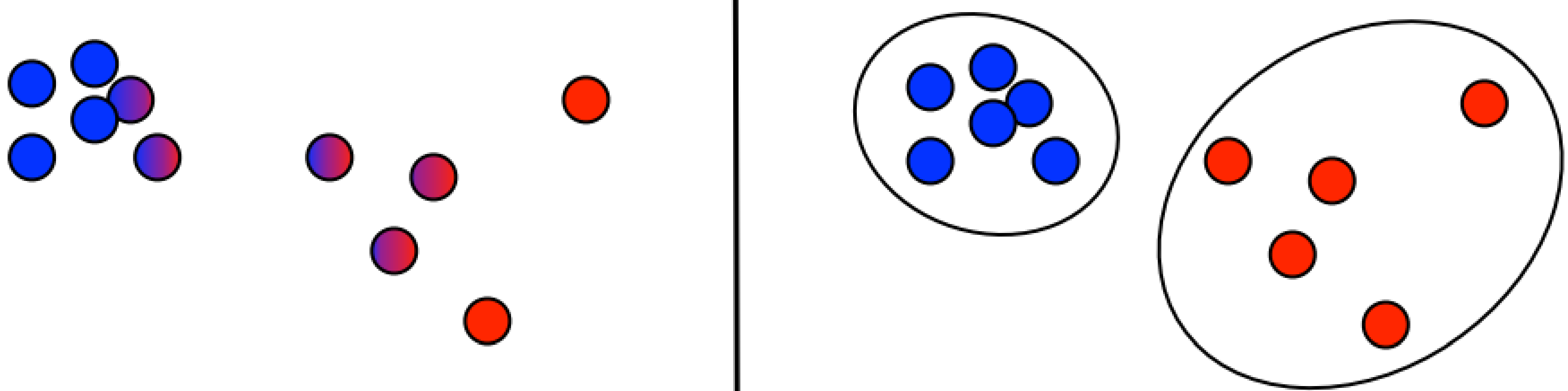
$$a_1 = ?, a_2 = ?, a_3 = ?, \ldots, a_n = ?$$

K-means

$$\operatorname{argmin}_{c_1,\ldots,c_K} \sum_i \left\| x_i - c_{\text{closest\_to}(i)} \right\|^2$$

- **For fixed c_k we can find optimal a_i**
- **For fixed a_i we can find optimal c_k.**
- **Iterate to convergence.**

Fuzzy vs Hard



Each object belongs to each cluster with some weight (the weight can be zero)

Each object belongs to exactly one cluster

Gaussian Mixture Modeling

$$\boldsymbol{X} \sim [N(\boldsymbol{\mu}_1, \sigma_1^2) \text{ or } N(\boldsymbol{\mu}_2, \sigma_2^2)]$$

Given X, estimate $\boldsymbol{\mu}_i, \boldsymbol{\sigma}_i^2$

Gaussian Mixture Modeling

$$\boldsymbol{X} \sim [N(\boldsymbol{\mu}_1, \sigma_1^2) \ \text{ or } \ N(\boldsymbol{\mu}_2, \sigma_2^2)]$$

Given X, estimate $\boldsymbol{\mu_i}, \boldsymbol{\sigma_i^2}$

→ **MLE**

Gaussian Mixture Modeling

$$\boldsymbol{X} \sim [N(\boldsymbol{\mu}_1, \sigma_1^2) \text{ or } N(\boldsymbol{\mu}_2, \sigma_2^2)]$$

Given X, estimate $\boldsymbol{\mu_i}, \boldsymbol{\sigma_i^2}$

- **MLE**
- **Expectation-Maximization (EM)**

SKLearn's Clustering

```
from sklearn.cluster
import
    Ward,
    KMeans,
    DBScan,
    MeanShift,
    SpectralClustering,
    AffinityPropagation
```

SKLearn's Clustering

```
from sklearn.cluster
import
    Ward,
    KMeans,
    DBScan,
    MeanShift,

    SpectralClustering,
    AffinityPropagation
```

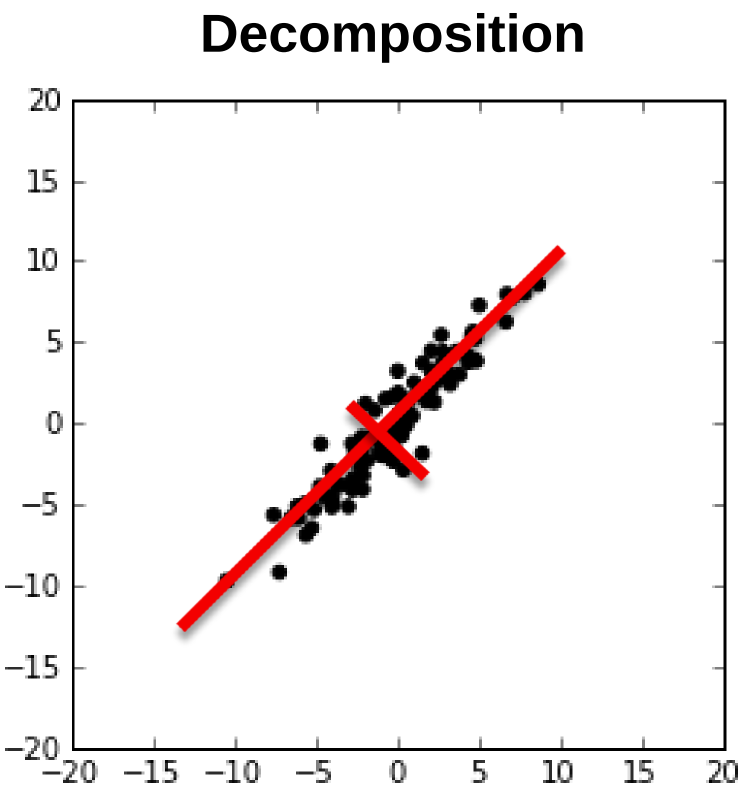
Use feature vectors

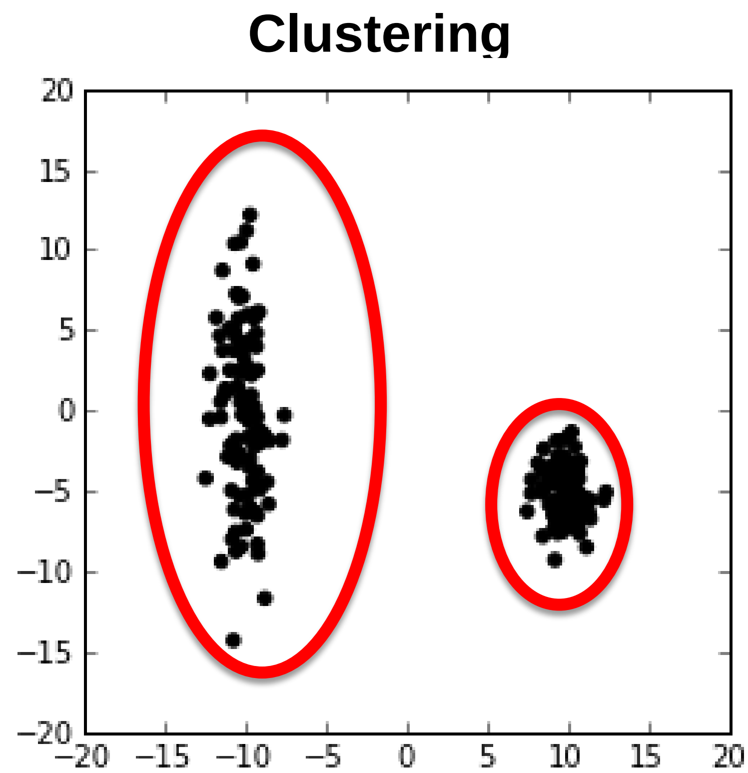
Use distance matrix

Quiz

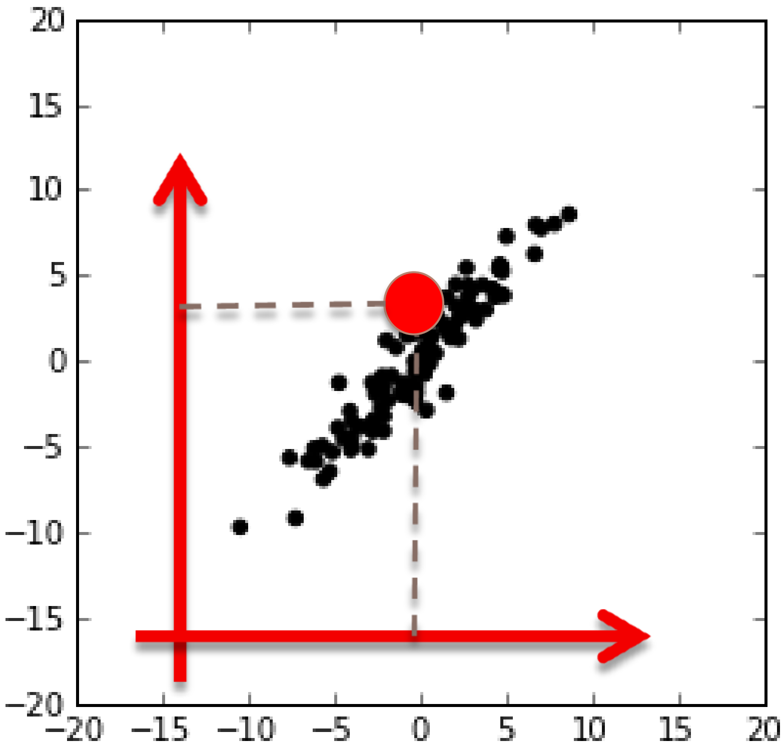
- Fuzzy clustering means that ________
- K-means finds a set of cluster centers, which have the smallest ______________
- K-means can get stuck in a local minimum (Y/N)?

Today


Decomposition
20
15
10
5
0
−5
−10
−15
−20
−20 −15 −10 −5 0 5 10 15 20

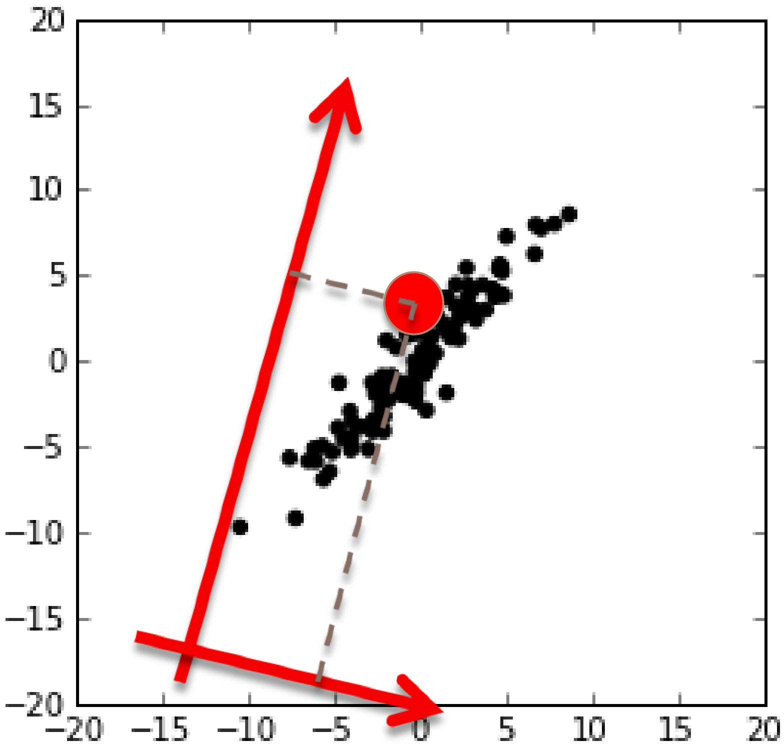

Clustering
20
15
10
5
0
−5
−10
−15
−20
−20 −15 −10 −5 0 5 10 15 20

Canonical basis



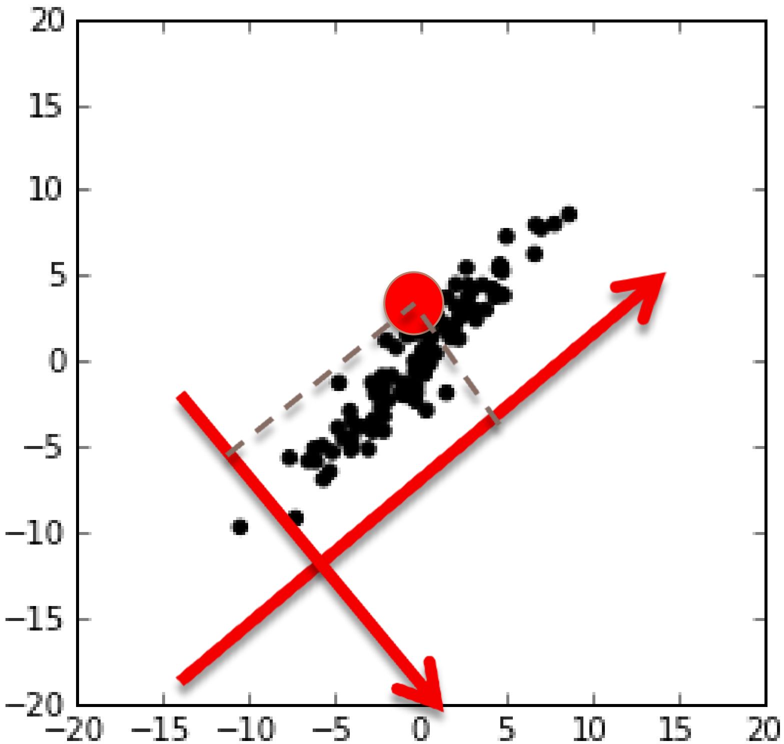
$$\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \alpha \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \beta \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Alternative basis



$$\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \alpha \begin{pmatrix} 0.9 \\ -0.1 \end{pmatrix} + \beta \begin{pmatrix} 0.1 \\ 0.9 \end{pmatrix}$$

Alternative basis



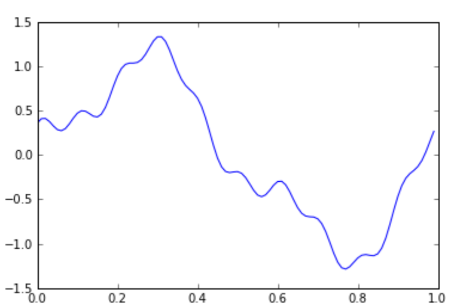
$$\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \alpha \begin{pmatrix} 0.4 \\ -0.6 \end{pmatrix} + \beta \begin{pmatrix} 0.6 \\ 0.4 \end{pmatrix}$$

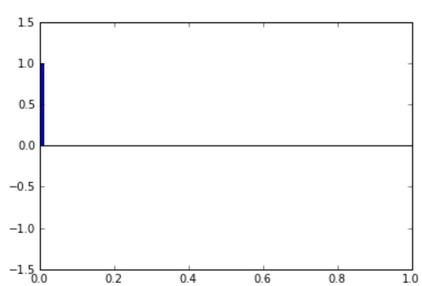
Linear Decomposition

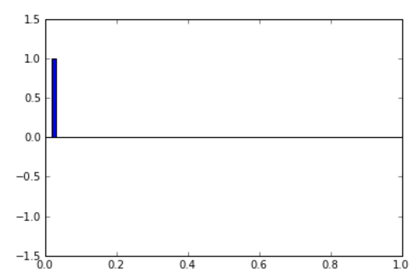
$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ \dots \\ x_{100000} \end{pmatrix} = \alpha_1 \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} + \alpha_2 \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} + \cdots + \alpha_m \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \vdots \\ 1 \end{pmatrix}$$

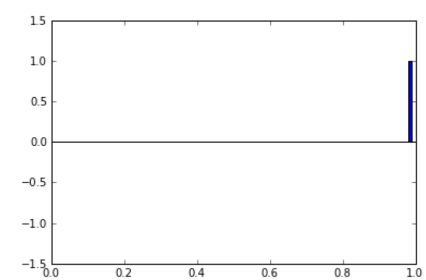
Linear Decomposition

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ \cdots \\ x_{100000} \end{pmatrix} = \alpha_1 \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} + \alpha_2 \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} + \cdots + \alpha_m \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \vdots \\ 1 \end{pmatrix}$$



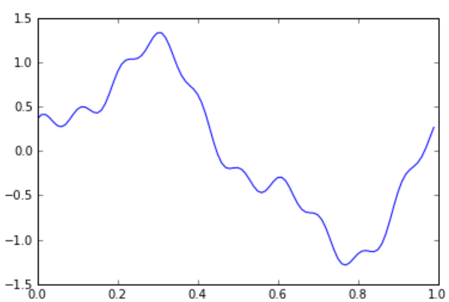


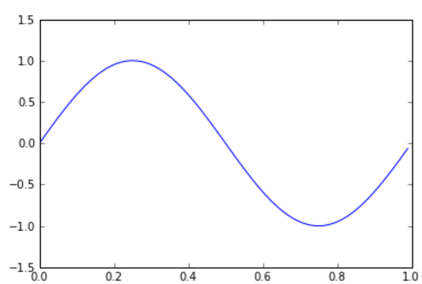


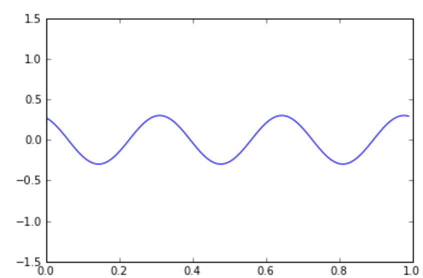


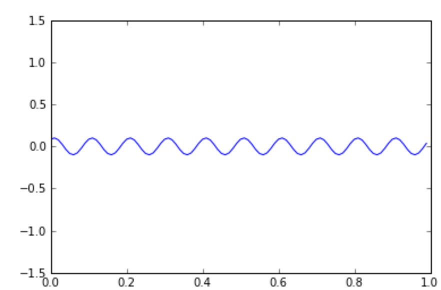
Linear Decomposition

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ \ldots \\ x_{100000} \end{pmatrix} = \alpha_1 \begin{pmatrix} 0.0 \\ 0.1 \\ 0.1 \\ 0.2 \\ \vdots \\ 0.0 \end{pmatrix} + \alpha_2 \begin{pmatrix} 0.3 \\ 0.2 \\ 0.2 \\ 0.1 \\ \vdots \\ 0.3 \end{pmatrix} + \alpha_m \begin{pmatrix} 0.1 \\ 0.1 \\ 0.1 \\ 0.0 \\ \vdots \\ 0.0 \end{pmatrix}$$



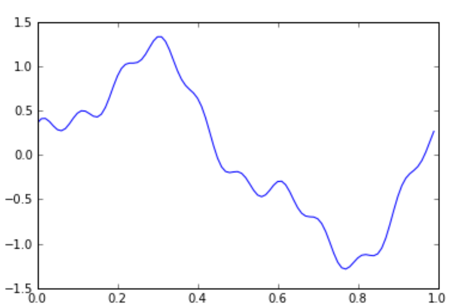






Linear Decomposition

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ \dots \\ x_{100000} \end{pmatrix} = \alpha_1 \begin{pmatrix} 0.0 \\ 0.1 \\ 0.1 \\ 0.2 \\ \vdots \\ 0.0 \end{pmatrix} + \alpha_2 \begin{pmatrix} 0.3 \\ 0.2 \\ 0.2 \\ 0.1 \\ \vdots \\ 0.3 \end{pmatrix} + \alpha_m \begin{pmatrix} 0.1 \\ 0.1 \\ 0.1 \\ 0.0 \\ \vdots \\ 0.0 \end{pmatrix}$$



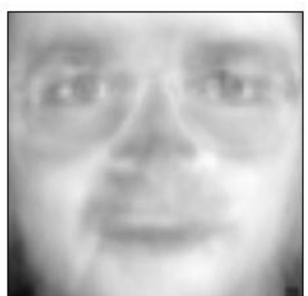
Linear Decomposition

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ \cdots \\ x_{100000} \end{pmatrix} = \alpha_1 \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} + \alpha_2 \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} + \cdots + \alpha_m \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \vdots \\ 1 \end{pmatrix}$$




Linear Decomposition

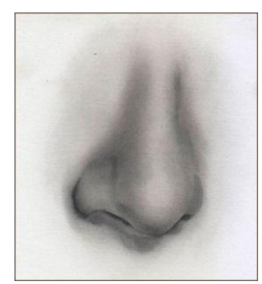
$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ \dots \\ x_{100000} \end{pmatrix} = \alpha_1 \begin{pmatrix} 0.0 \\ 0.1 \\ 0.1 \\ 0.2 \\ \vdots \\ 0.0 \end{pmatrix} + \alpha_2 \begin{pmatrix} 0.3 \\ 0.2 \\ 0.2 \\ 0.1 \\ \vdots \\ 0.3 \end{pmatrix} + \alpha_m \begin{pmatrix} 0.1 \\ 0.1 \\ 0.1 \\ 0.0 \\ \vdots \\ 0.0 \end{pmatrix}$$



Linear Decomposition

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ \dots \\ x_{100000} \end{pmatrix} = \alpha_1 \begin{pmatrix} 0.0 \\ 0.1 \\ 0.1 \\ 0.2 \\ \vdots \\ 0.0 \end{pmatrix} + \alpha_2 \begin{pmatrix} 0.3 \\ 0.2 \\ 0.2 \\ 0.1 \\ \vdots \\ 0.3 \end{pmatrix} + \alpha_m \begin{pmatrix} 0.1 \\ 0.1 \\ 0.1 \\ 0.0 \\ \vdots \\ 0.0 \end{pmatrix}$$






Linear Decomposition

$$\boldsymbol{x} = \alpha_1 \boldsymbol{v_1} + \alpha_2 \boldsymbol{v_2} + \cdots + \alpha_m \boldsymbol{v_m}$$

Linear Decomposition

$$\boldsymbol{x} = \alpha_1 \boldsymbol{v_1} + \alpha_2 \boldsymbol{v_2} + \cdots + \alpha_m \boldsymbol{v_m}$$

$$\boldsymbol{x} = \begin{pmatrix} \vdots & \vdots & \cdots & \vdots \\ \boldsymbol{v_1} & \boldsymbol{v_2} & & \boldsymbol{v_m} \\ \vdots & \vdots & \cdots & \vdots \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_m \end{pmatrix}$$

Linear Decomposition

$$\boldsymbol{x} = \alpha_1 \boldsymbol{v_1} + \alpha_2 \boldsymbol{v_2} + \cdots + \alpha_m \boldsymbol{v_m}$$

$$\boldsymbol{x} = \boldsymbol{V\alpha}$$

Linear Decomposition

$$\boldsymbol{x} = \alpha_1 \boldsymbol{v_1} + \alpha_2 \boldsymbol{v_2} + \cdots + \alpha_m \boldsymbol{v_m}$$

$$\boldsymbol{x} = \boldsymbol{V\alpha}$$

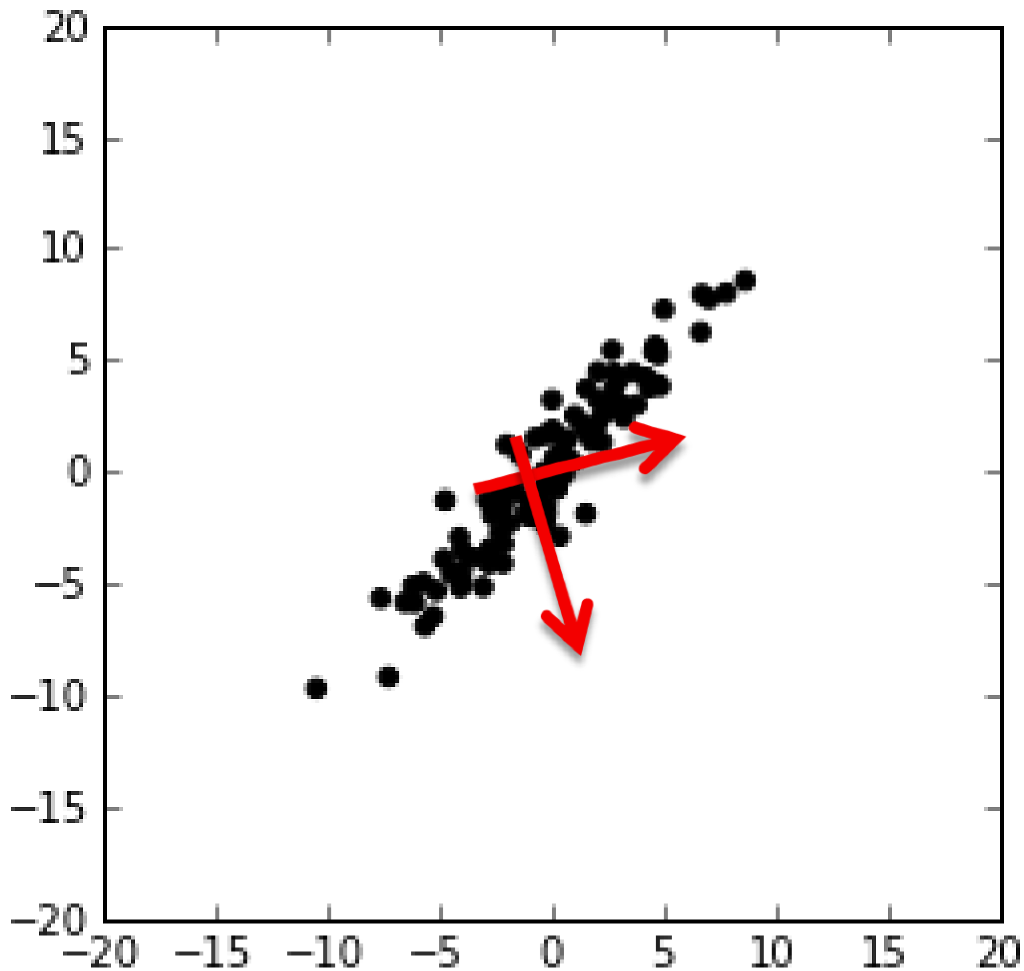
$$\boldsymbol{\alpha} = ?$$

Linear Decomposition

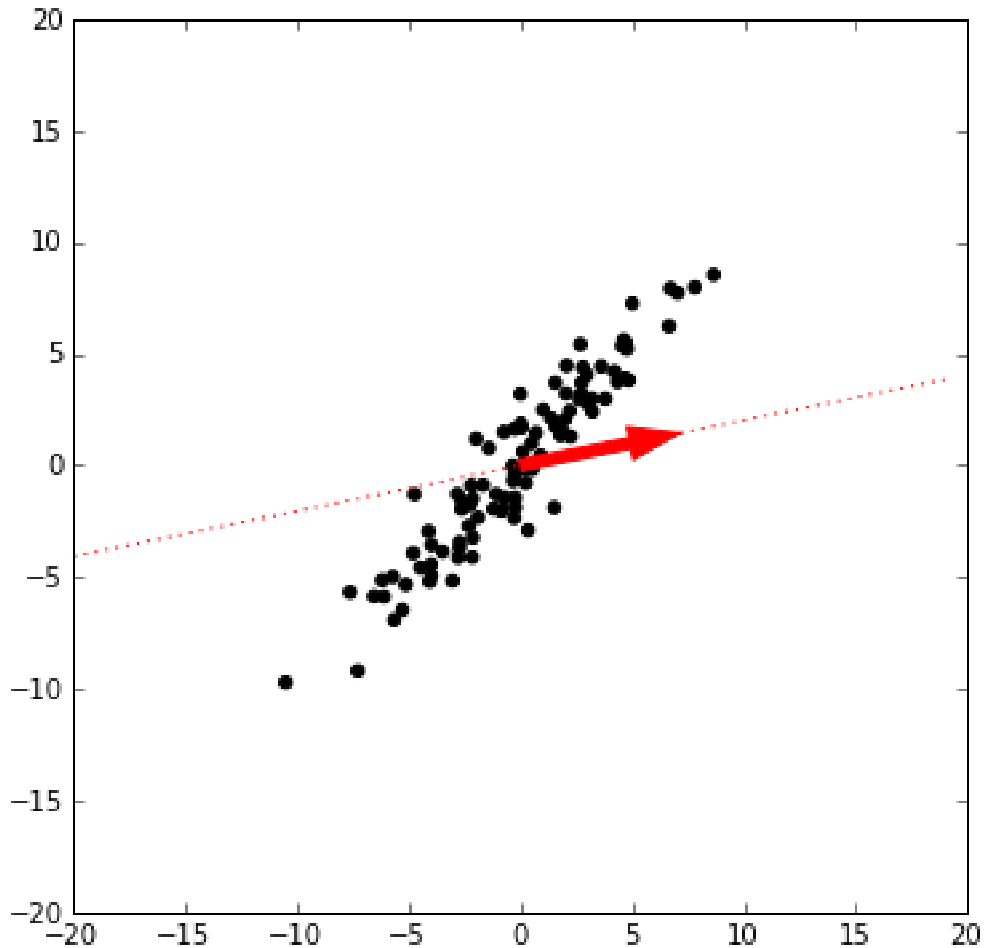
$$\boldsymbol{x} = \alpha_1 \boldsymbol{v}_1 + \alpha_2 \boldsymbol{v}_2 + \cdots + \alpha_m \boldsymbol{v}_m$$

$$\boldsymbol{x} = \boldsymbol{V}\boldsymbol{\alpha}$$
$$\boldsymbol{\alpha} = \boldsymbol{V}^{+}\boldsymbol{x}$$

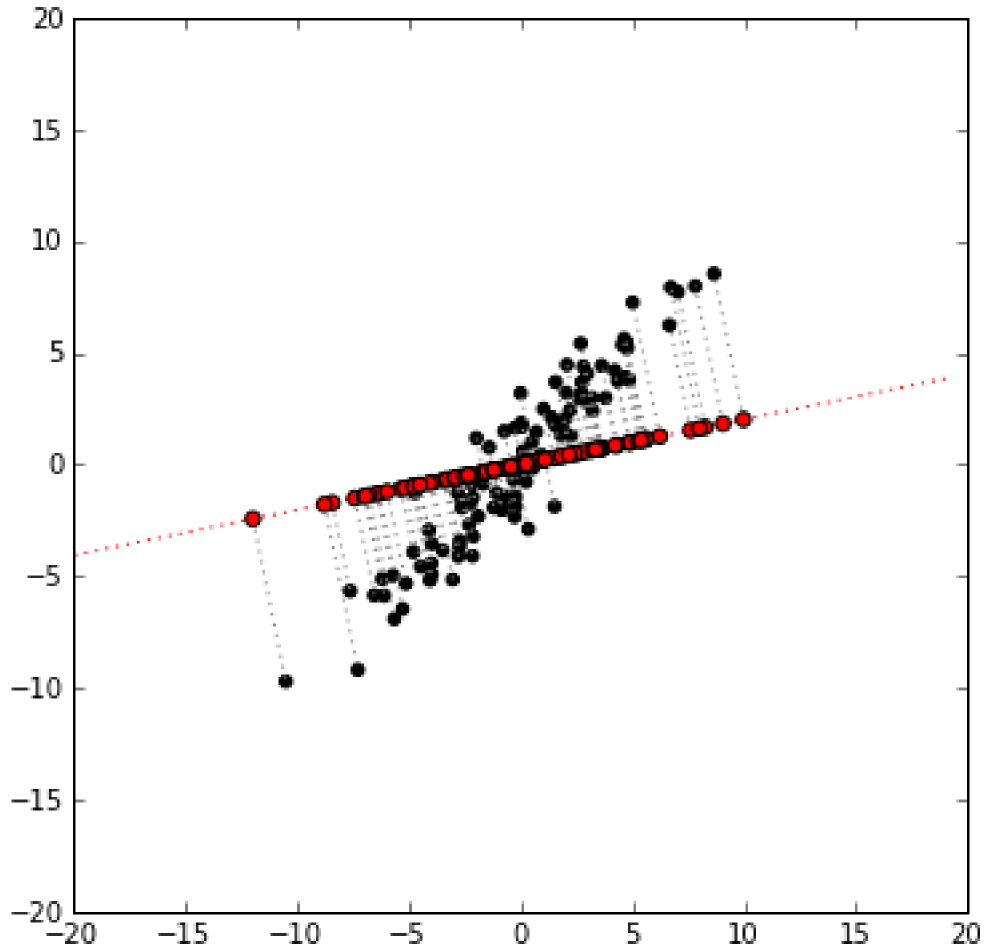
How do we find a good basis?



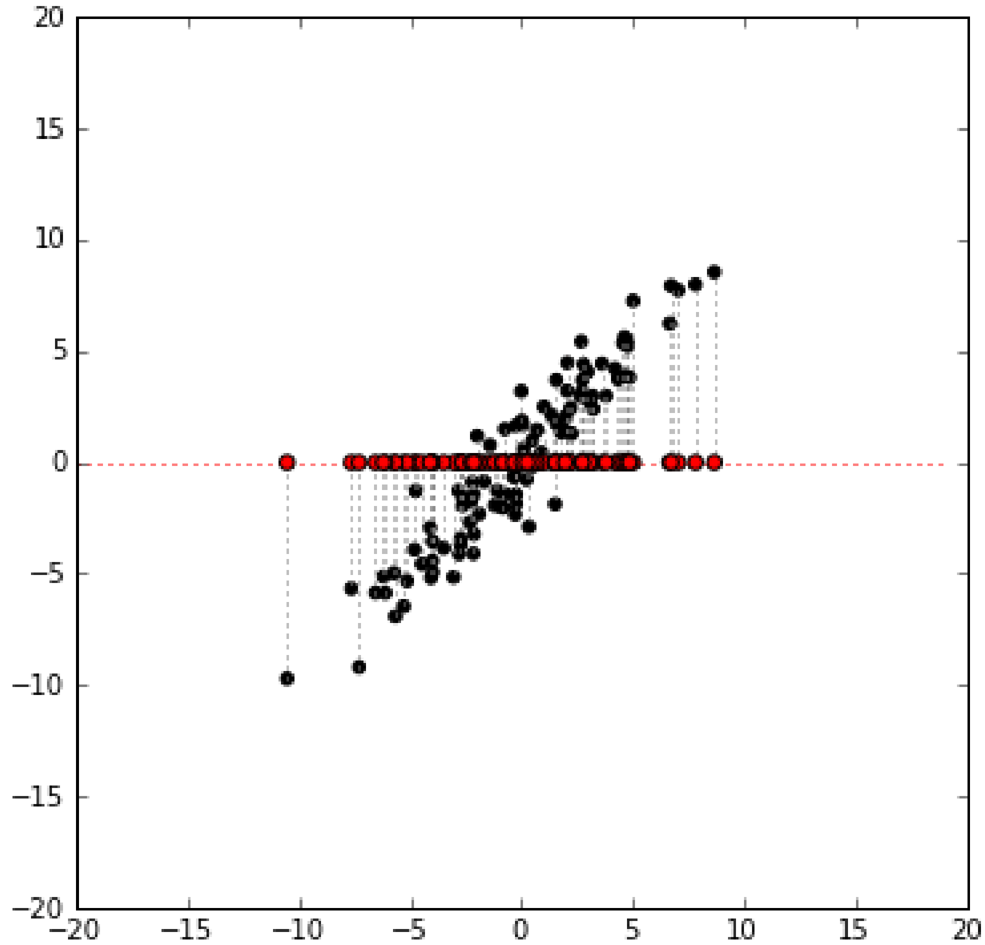
Linear projection



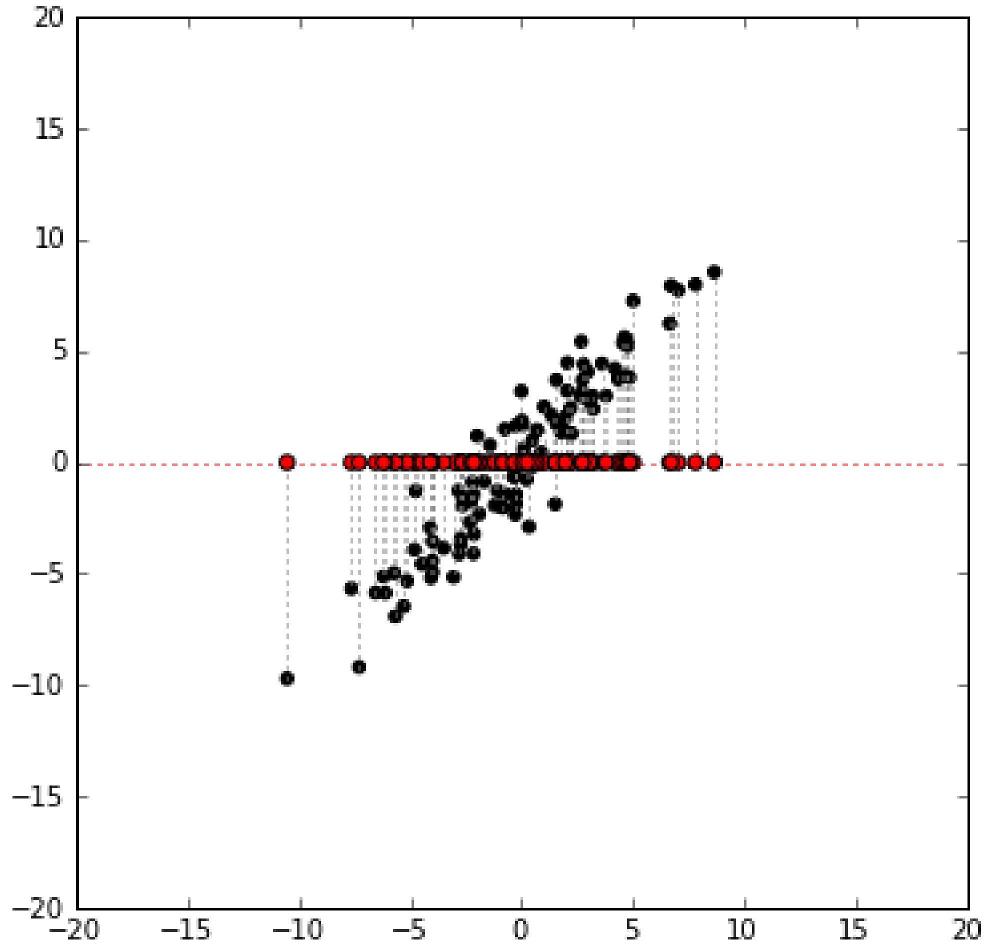
Linear projection



Linear projection



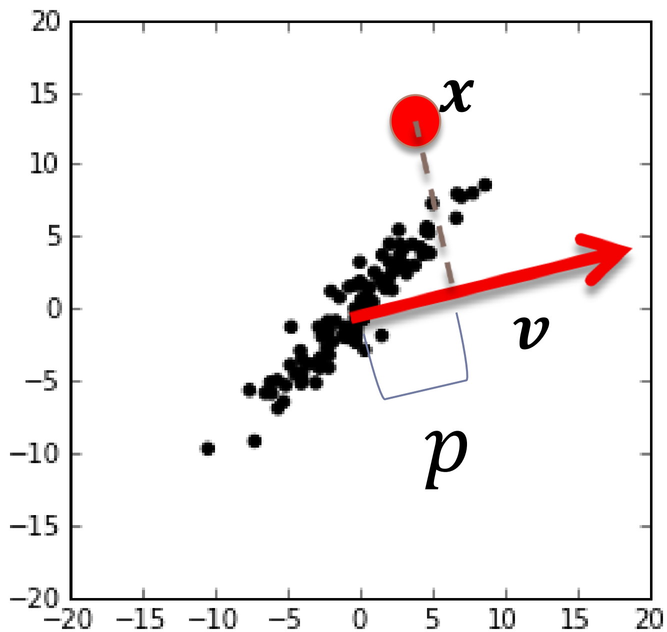
Linear projection



Idea: Maximize projection variance

- For a point $\boldsymbol{x}_i$ and a unit basis vector $\boldsymbol{v}$ the length of projection of $\boldsymbol{x}_i$ onto $\boldsymbol{v}$ is given by

$$p = \langle \boldsymbol{v}, \boldsymbol{x}_i \rangle = \boldsymbol{v}^T \boldsymbol{x}_i$$



Projection variance

$$p_i = \boldsymbol{v}^T \boldsymbol{x}_i$$

Projection variance

$$p_i = \boldsymbol{v}^T \boldsymbol{x}_i$$

$$\sigma_{\boldsymbol{v}}^2 = \frac{1}{n} \sum_i (p_i - \overline{p})^2$$

Projection variance

$$p_i = \boldsymbol{v}^T \boldsymbol{x}_i$$

$$\sigma_{\boldsymbol{v}}^2 = \frac{1}{n} \sum_i (p_i - \overline{p})^2$$

$$\boldsymbol{v} = \operatorname{argmax}_{\boldsymbol{v}} \sigma_{\boldsymbol{v}}^2$$

Projection variance

$$p_i = \boldsymbol{v}^T \boldsymbol{x}_i$$

$$\sigma_{\boldsymbol{v}}^2 = \frac{1}{n} \sum_i (p_i - \overline{p})^2$$

Pre-center data, so that $\overline{p} = \boldsymbol{v}^T \overline{\boldsymbol{x}} = 0$

Projection variance

$$p_i = \boldsymbol{v}^T \boldsymbol{x}_i$$

$$\sigma_{\boldsymbol{v}}^2 = \frac{1}{n} \sum_i (p_i)^2$$

Pre-center data, so that $\overline{p} = \boldsymbol{v}^T \overline{\boldsymbol{x}} = 0$

Projection variance

$$p_i = \boldsymbol{v}^T \boldsymbol{x}_i$$

$$\sigma_{\boldsymbol{v}}^2 = \frac{1}{n}\sum_i (p_i)^2 = \frac{1}{n}\|\boldsymbol{p}\|^2$$

Projection variance

$$p_i = \boldsymbol{v}^T \boldsymbol{x}_i$$

$$\sigma_{\boldsymbol{v}}^2 = \frac{1}{n}\sum_i (p_i)^2 = \frac{1}{n}\|\boldsymbol{p}\|^2$$

$$= \frac{1}{n}\|\boldsymbol{X}\boldsymbol{v}\|^2$$

Projection variance

$$p_i = \boldsymbol{v}^T \boldsymbol{x}_i$$

$$\sigma_{\boldsymbol{v}}^2 = \cdots$$

$$= \frac{1}{n} \|\boldsymbol{X}\boldsymbol{v}\|^2 = \frac{1}{n} (\boldsymbol{X}\boldsymbol{v})^T (\boldsymbol{X}\boldsymbol{v})$$

$$= \frac{1}{n} \boldsymbol{v}^T \boldsymbol{X}^T \boldsymbol{X} \boldsymbol{v} = \boldsymbol{v}^T \boldsymbol{\Sigma} \boldsymbol{v}$$

Projection variance

$$p_i = \boldsymbol{v}^T \boldsymbol{x}_i$$

$$\sigma_{\boldsymbol{v}}^2 = \boldsymbol{v}^T \boldsymbol{\Sigma} \boldsymbol{v}$$

Projection variance

$$p_i = \boldsymbol{v}^T \boldsymbol{x}_i$$

$$\sigma_{\boldsymbol{v}}^2 = \boldsymbol{v}^T \boldsymbol{\Sigma} \boldsymbol{v}$$

Data covariance matrix

$\boldsymbol{X}^T \boldsymbol{X}$

Objective function

$$\operatorname{argmax}_v \, \boldsymbol{v}^T \boldsymbol{\Sigma} \boldsymbol{v}$$

$$s.t. \, \|\boldsymbol{v}\|^2 = 1$$

Optimization

$$\text{argmax}_v \; \boldsymbol{v}^T \boldsymbol{\Sigma} \boldsymbol{v}$$

$$s.t. \|\boldsymbol{v}\|^2 = 1$$

Method of Lagrange multipliers…

$$\boldsymbol{\Sigma} \boldsymbol{v} = \lambda \boldsymbol{v}$$

Optimization

$$\text{argmax}_{\boldsymbol{v}}\ \boldsymbol{v}^T \boldsymbol{\Sigma} \boldsymbol{v}$$

$$s.t. ||\boldsymbol{v}||^2 = 1$$

Method of Lagrange multipliers…

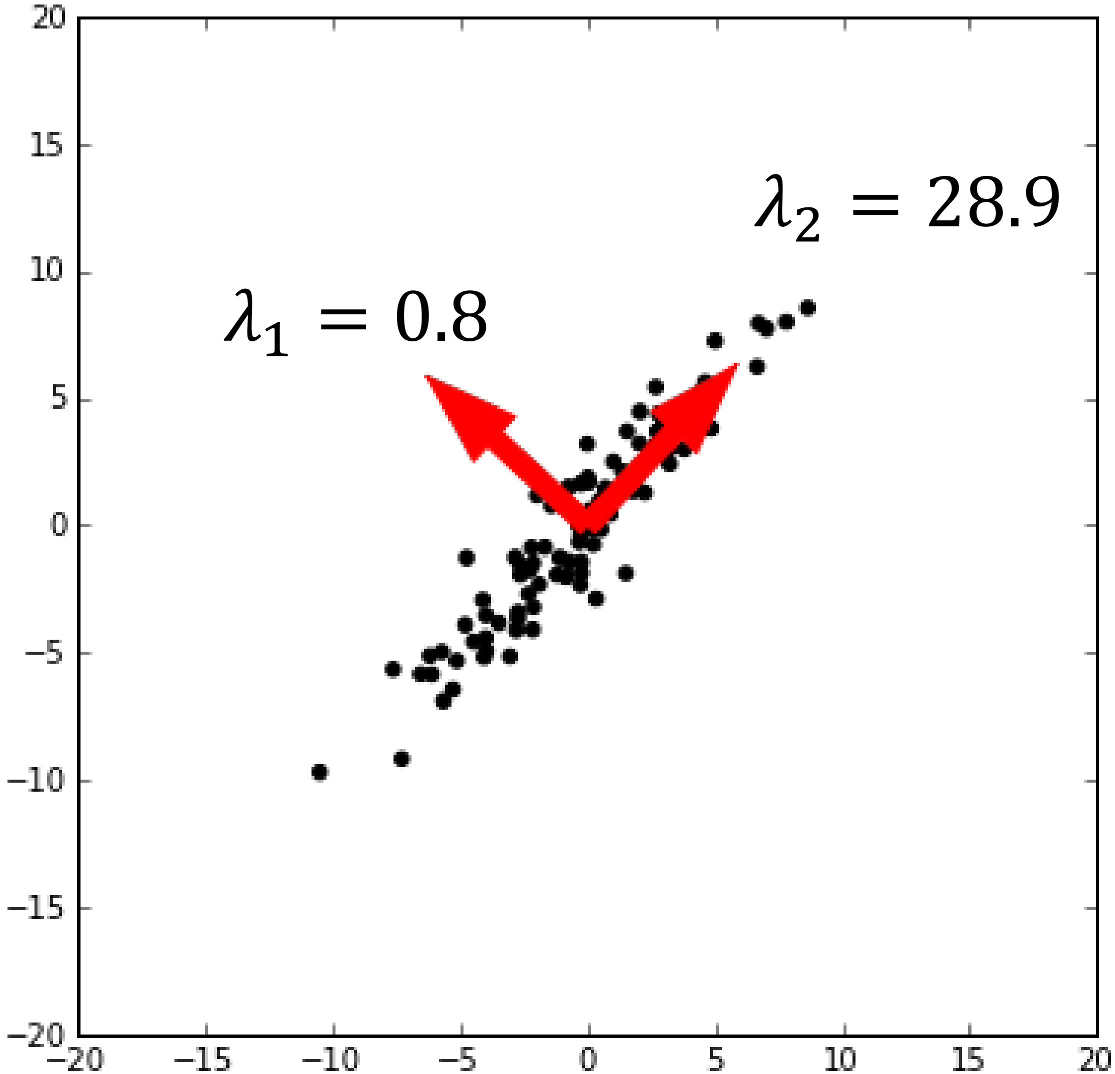
$$\boldsymbol{\Sigma}\boldsymbol{v} = \lambda \boldsymbol{v}$$

Eigenvector of Σ **Eigenvalue**

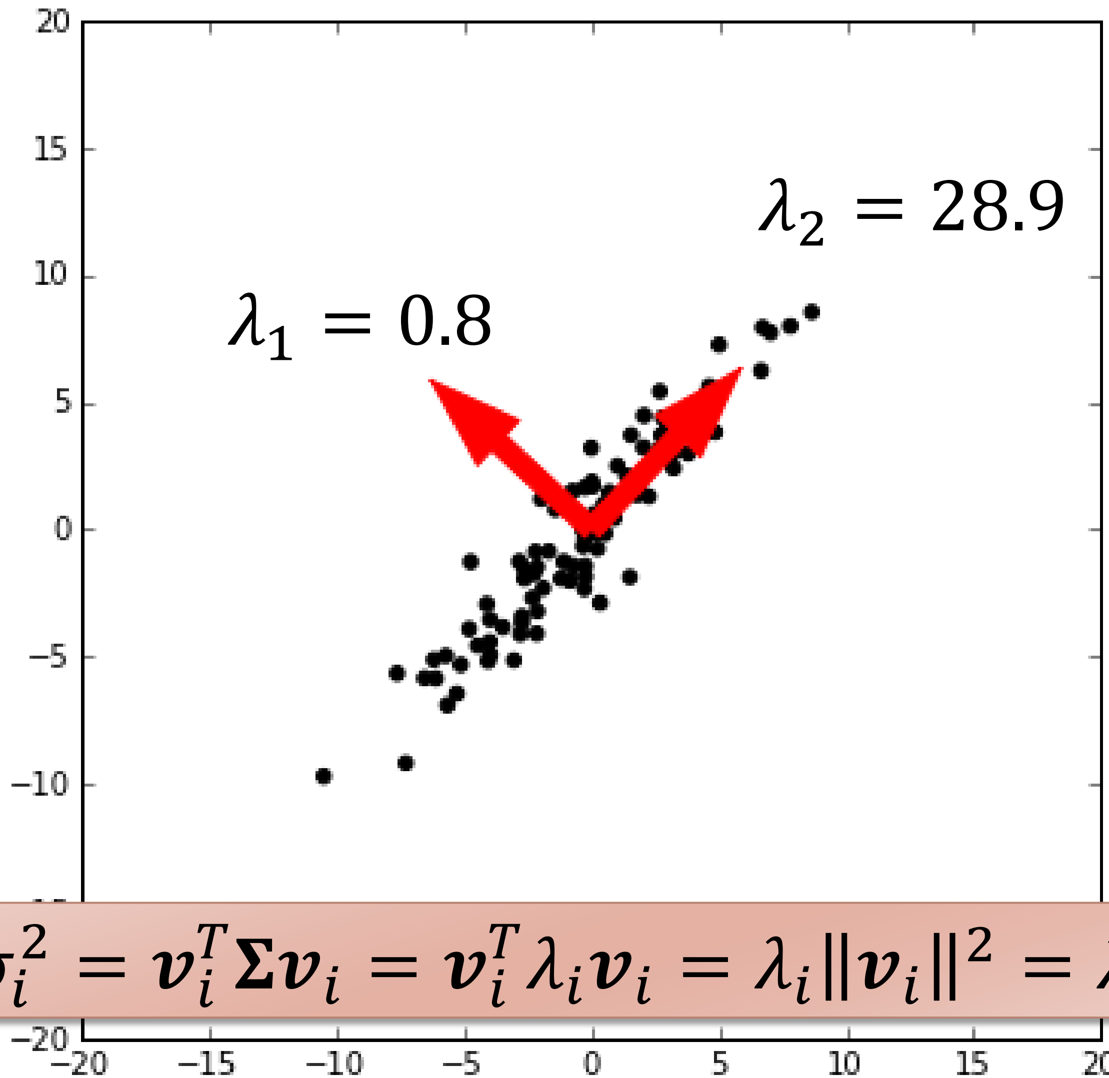
Example

```
Xc = X - mean(X, axis=0)

Sigma = Xc.T * Xc / n

            (= cov(Xc, rowvar=0))

lambdas, vs = eigh(Sigma)
```

Example

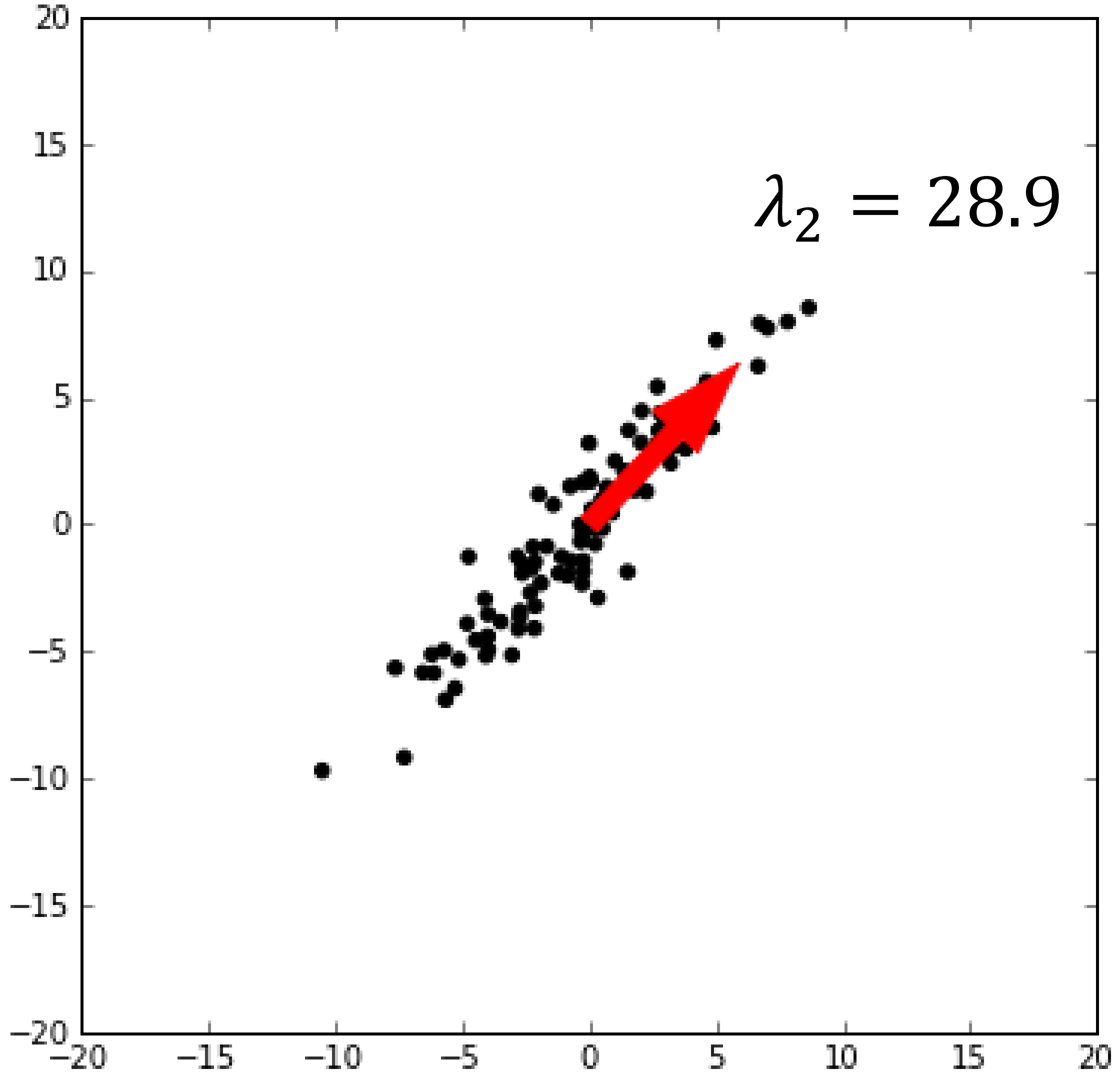


Example



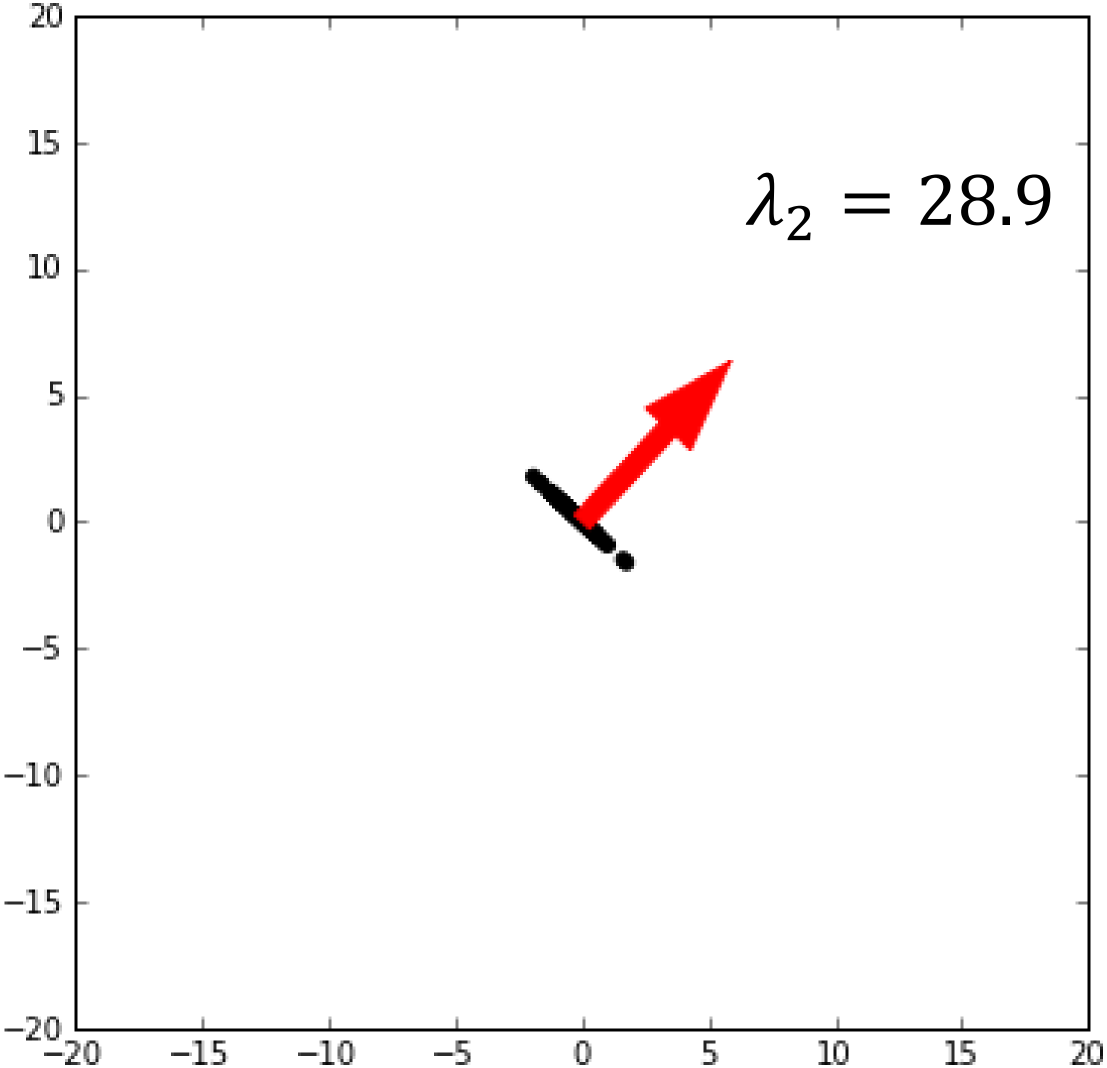
$$\sigma_i^2 = \boldsymbol{v}_i^T \boldsymbol{\Sigma} \boldsymbol{v}_i = \boldsymbol{v}_i^T \lambda_i \boldsymbol{v}_i = \lambda_i \|\boldsymbol{v}_i\|^2 = \lambda_i$$

Example



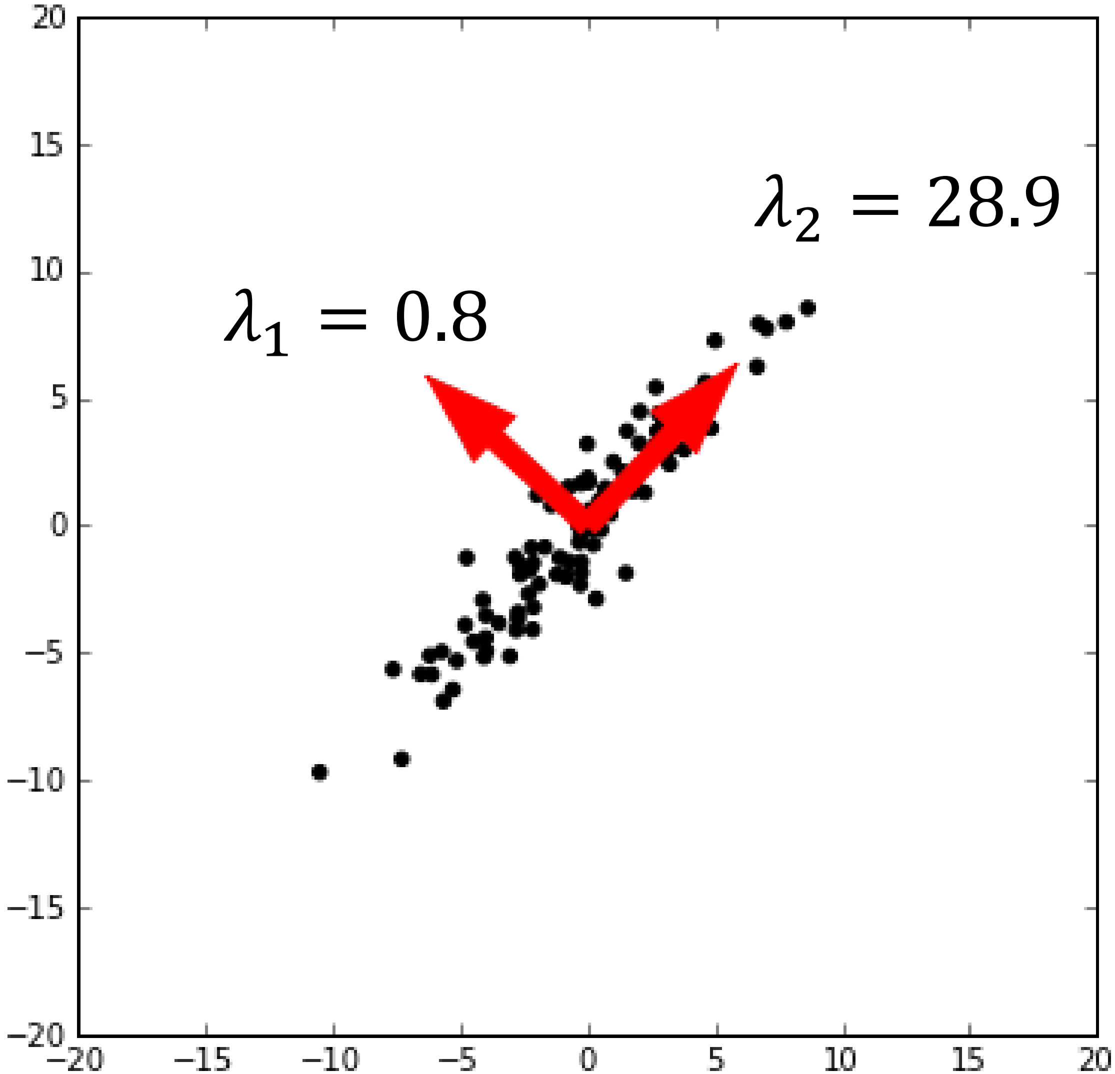
$\lambda_2 = 28.9$

Example



$\lambda_2 = 28.9$

Example



Principal Components Analysis

Principal components are the **eigenvectors** of the **covariance matrix**.

$$V, \lambda = \mathbf{eig}(\boldsymbol{\Sigma})$$

Principal Components Analysis

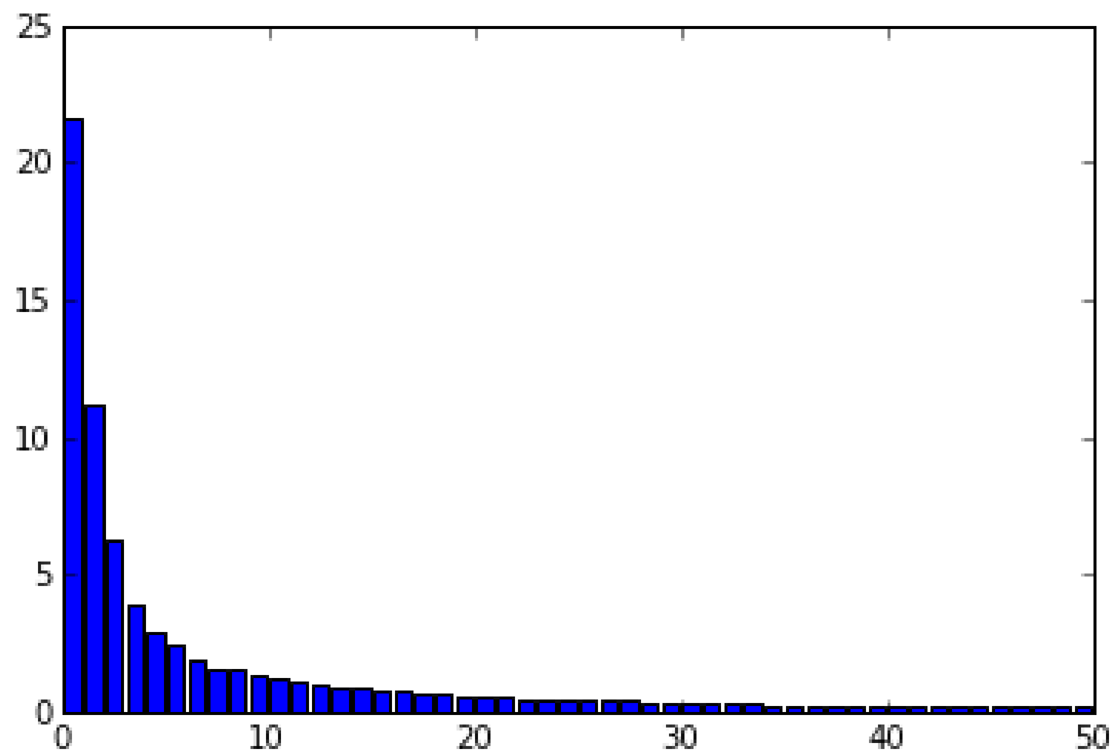
Principal components are the **eigenvectors** of the **covariance matrix**.

$$\boldsymbol{V}, \boldsymbol{\lambda} = \mathbf{eig}(\boldsymbol{\Sigma})$$

For each PC, the corresponding eigenvalue λ_i shows the **amount of variance explained** by the component.

Principal Components Analysis

Eigenvalue spectrum of Σ



Principal Components Analysis

Data projection onto PC i:

$$\boldsymbol{p} = \boldsymbol{X}\boldsymbol{v}_i$$

Data projection onto multiple PCs:

$$\boldsymbol{X}_{\text{proj}} = \boldsymbol{X}\boldsymbol{V}_*$$

Data reconstruction from PC coordinates:

$$\boldsymbol{X}_{\text{proj}}\boldsymbol{V}_*^T = \boldsymbol{X}$$

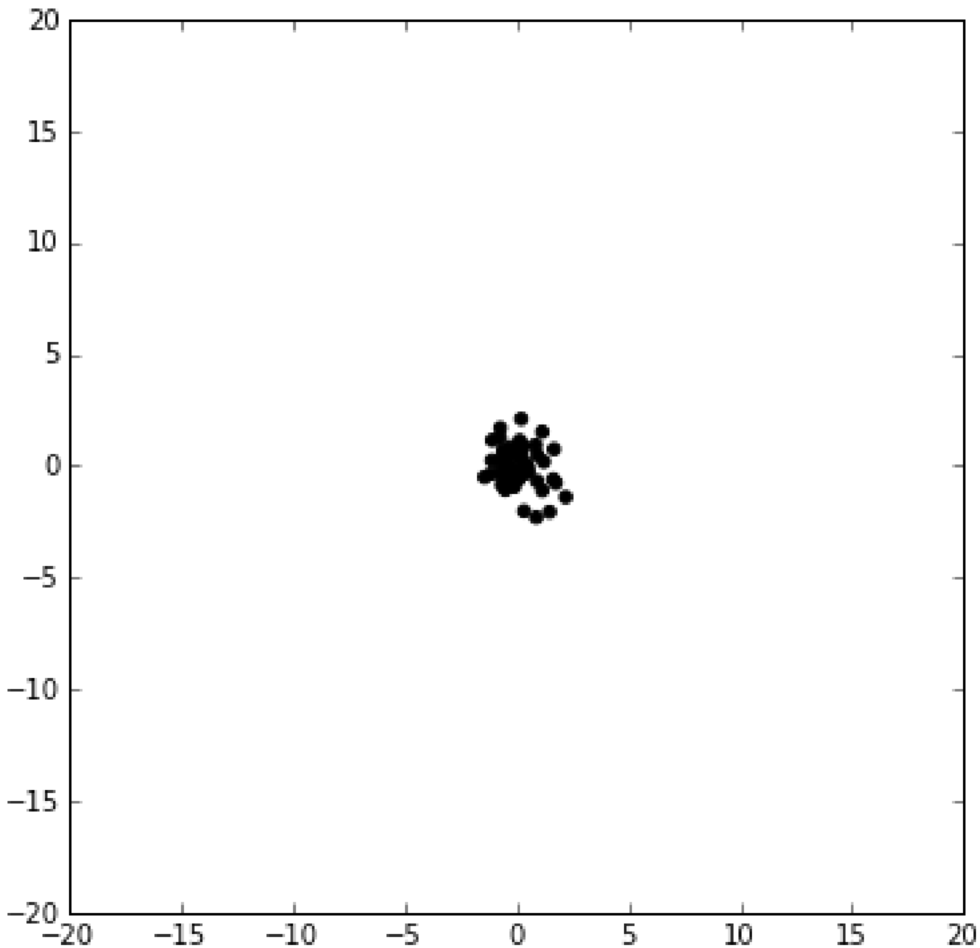
SKLearn's PCA

```
from sklearn.decomposition
                             import PCA

model = PCA(n_components=2)
model.fit(X)
X_t = model.transform(X)

model.components_[1,:]
```

SKLearn's PCA

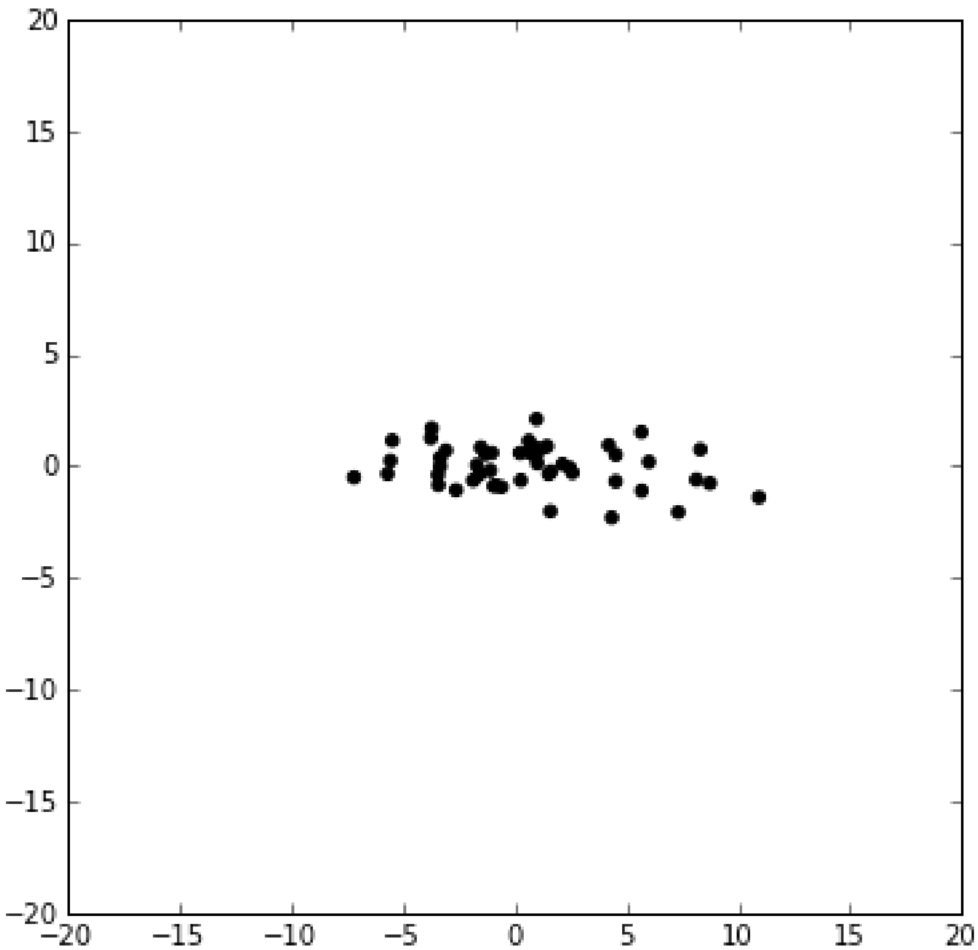
```
from sklearn.decomposition
import
    PCA,
    SparsePCA,
    ProbabilisticPCA,
    KernelPCA,
    FastICA,
    NMF,
    DictionaryLearning,
    ...
```

PCA: Geometric intuition



$$\boldsymbol{X} \sim N(0,1)$$

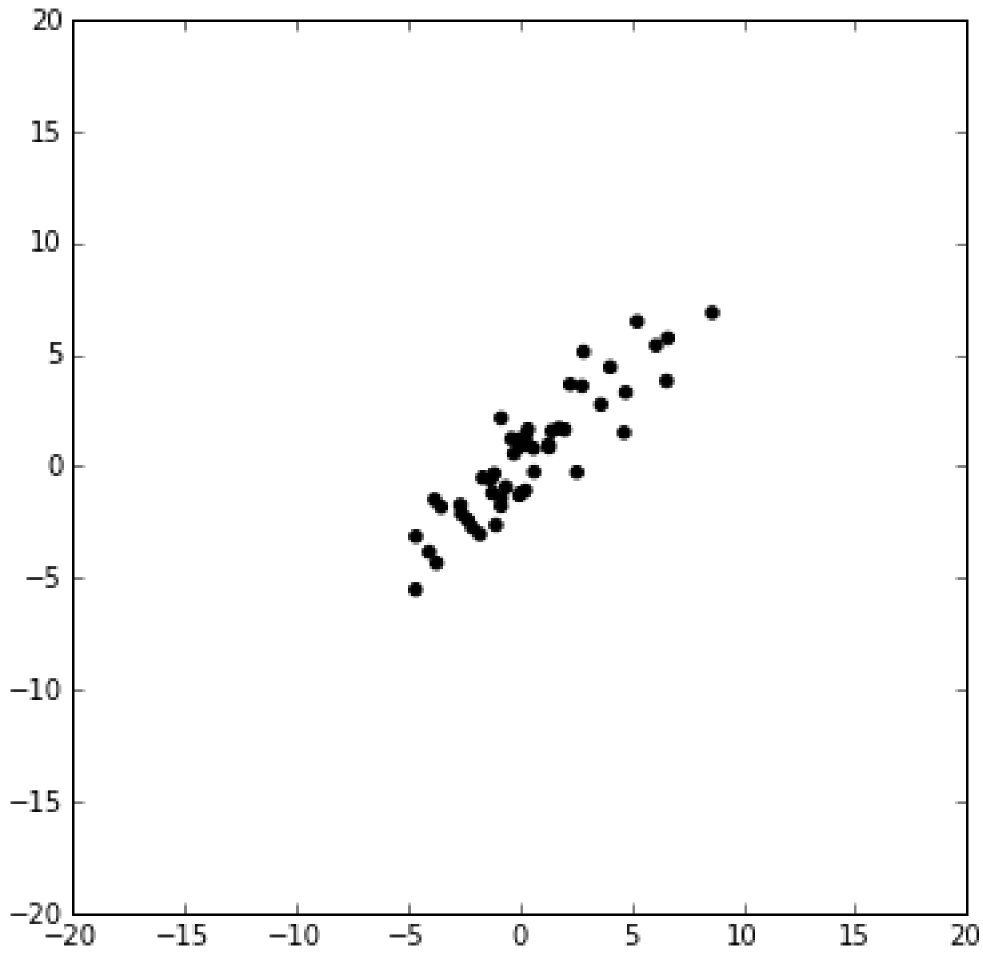
PCA: Geometric intuition



$$\boldsymbol{X} \sim N(0,1)$$

$$\boldsymbol{X}' = \boldsymbol{X}\begin{pmatrix} 5 & 0 \\ 0 & 0.9 \end{pmatrix}$$

PCA: Geometric intuition

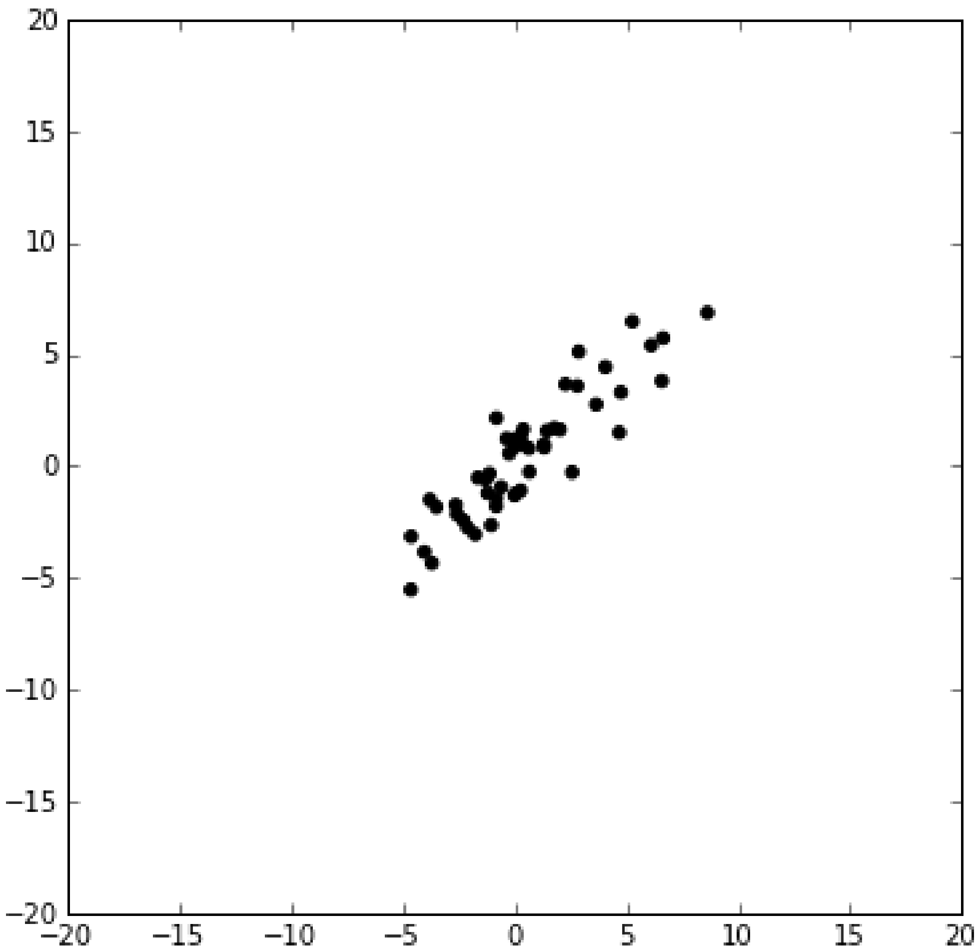


$$X \sim N(0,1)$$

$$X' = X\begin{pmatrix} 5 & 0 \\ 0 & 0.9 \end{pmatrix}$$

$$X'' = X'\begin{pmatrix} \cos 0.8 & -\sin 0.8 \\ \sin 0.8 & \cos 0.8 \end{pmatrix}$$

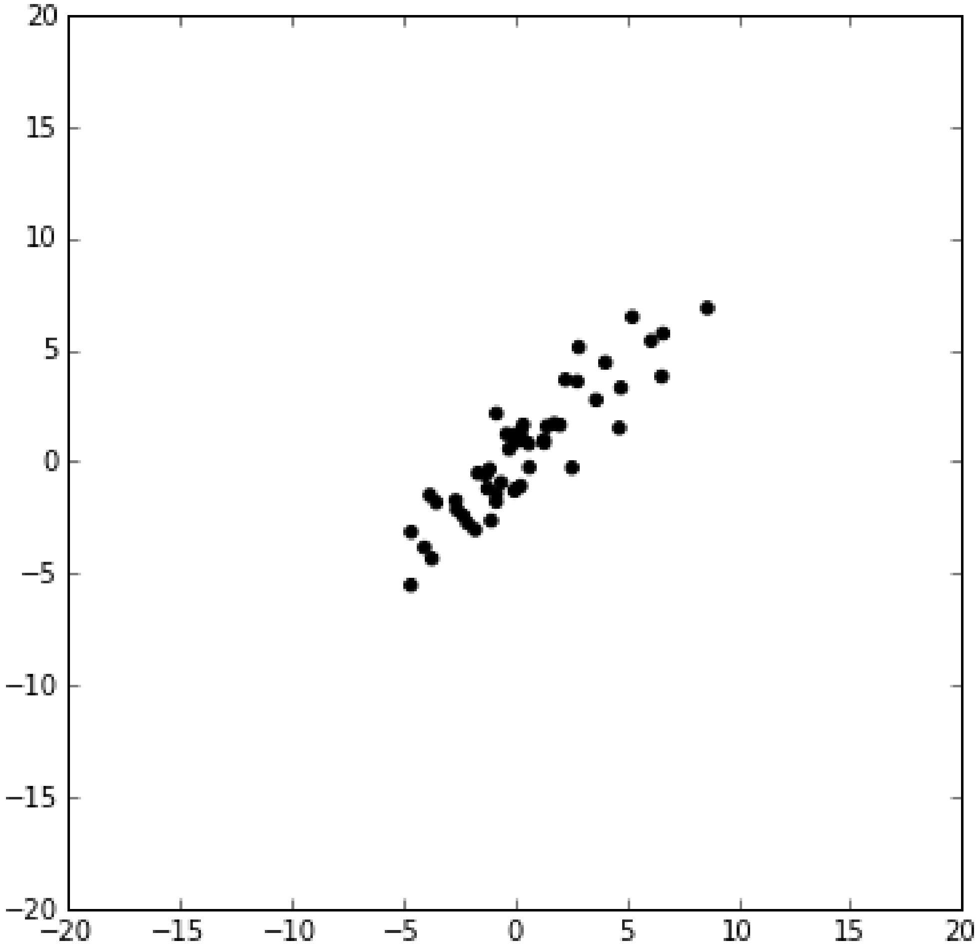
PCA: Geometric intuition



$$\boldsymbol{X} \sim N(0,1)$$

$$\boldsymbol{X}'' = \boldsymbol{X} \cdot \boldsymbol{D} \cdot \boldsymbol{R}$$

PCA: Geometric intuition

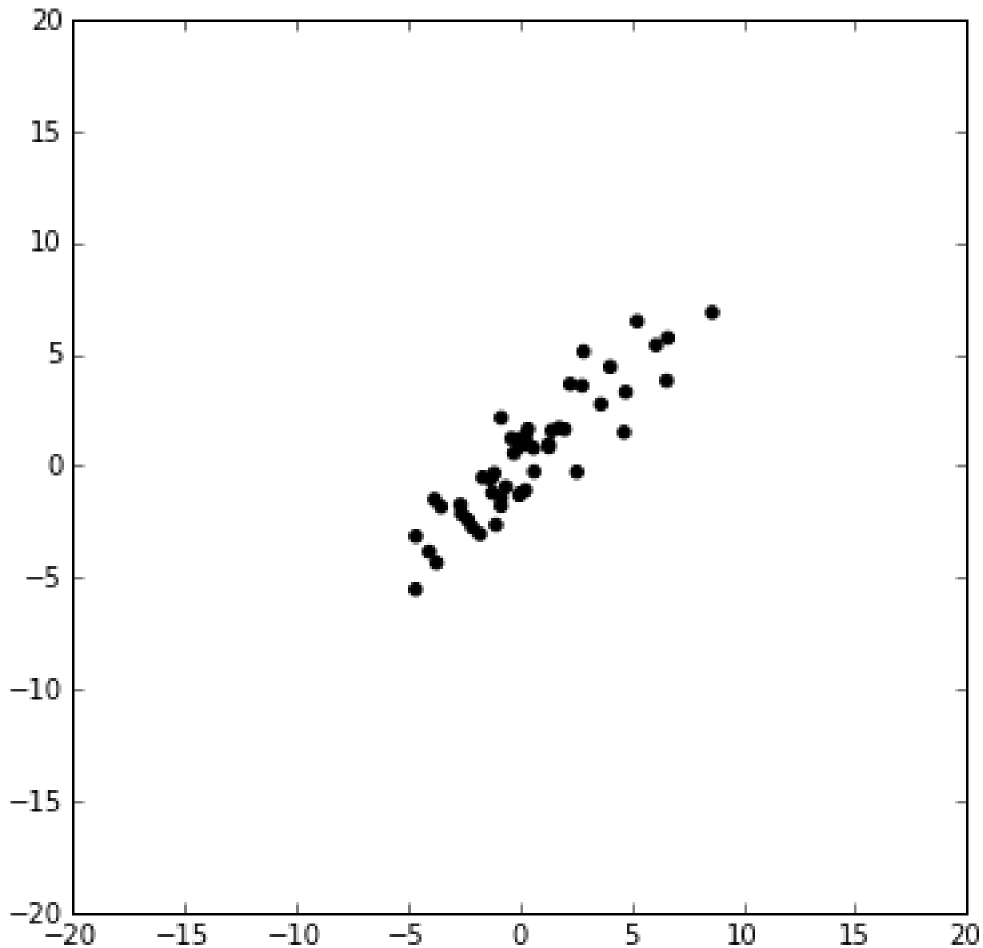


$$\boldsymbol{X} \sim N(0,1)$$

$$\boldsymbol{X}'' = \boldsymbol{X} \cdot \boldsymbol{D} \cdot \boldsymbol{R}$$

$$(\boldsymbol{X}'')^T(\boldsymbol{X}'') = (\boldsymbol{XDR})^T(\boldsymbol{XDR})$$

PCA: Geometric intuition

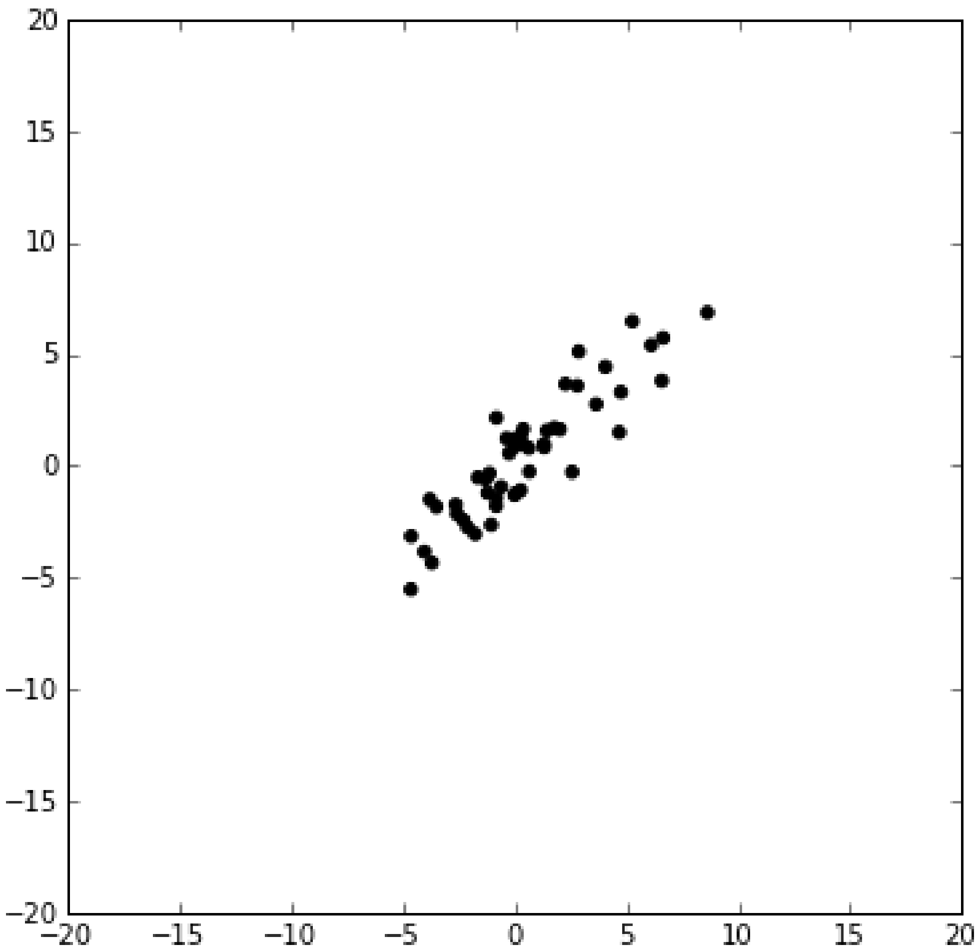


$$\boldsymbol{X} \sim N(0,1)$$

$$\boldsymbol{X''} = \boldsymbol{X} \cdot \boldsymbol{D} \cdot \boldsymbol{R}$$

$$(\boldsymbol{X''})^T(\boldsymbol{X''}) = (\boldsymbol{XDR})^T(\boldsymbol{XDR}) = \boldsymbol{R}^T\boldsymbol{D}^T\boldsymbol{X}^T\boldsymbol{XDR}$$

PCA: Geometric intuition

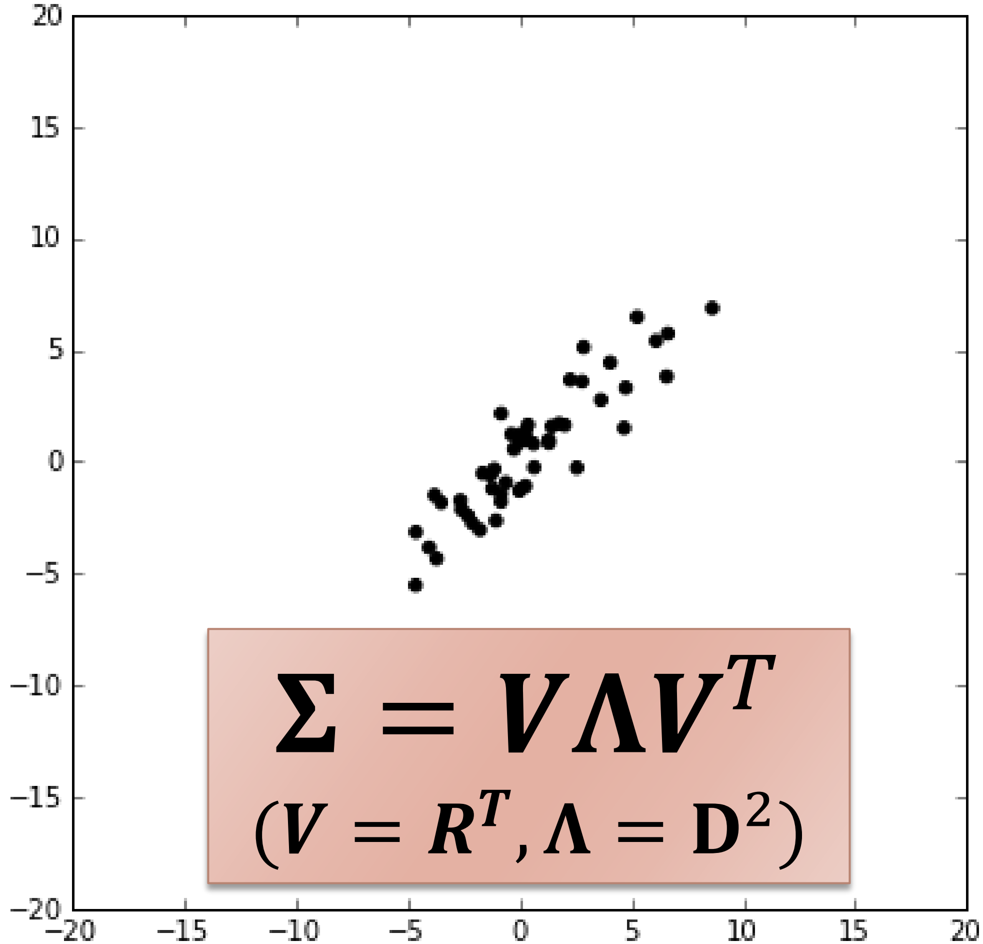


$$\boldsymbol{X} \sim N(0,1)$$

$$\boldsymbol{X''} = \boldsymbol{X} \cdot \boldsymbol{D} \cdot \boldsymbol{R}$$

$$(\boldsymbol{X''})^T(\boldsymbol{X''})$$
$$= (\boldsymbol{XDR})^T(\boldsymbol{XDR})$$
$$= \boldsymbol{R}^T\boldsymbol{D}^T\boldsymbol{X}^T\boldsymbol{XDR}$$
$$= \boldsymbol{R}^T\boldsymbol{D}^2\boldsymbol{R}$$

PCA: Geometric intuition



$$\Sigma = V\Lambda V^T$$

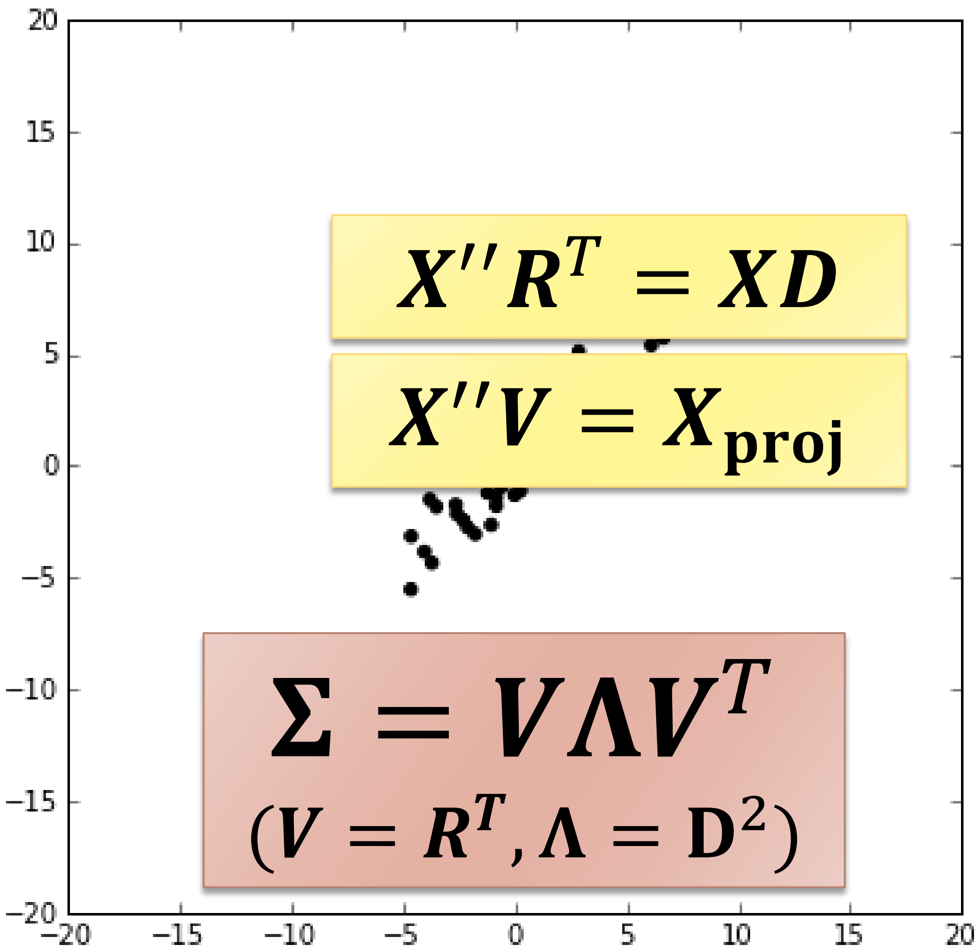
$$(V = R^T, \Lambda = \mathrm{D}^2)$$

$$X \sim N(0,1)$$

$$X'' = X \cdot D \cdot R$$

$$(X'')^T(X'') = (XDR)^T(XDR) = R^T D^T X^T X D R = R^T D^2 R$$

PCA: Geometric intuition



$$X''R^T = XD$$

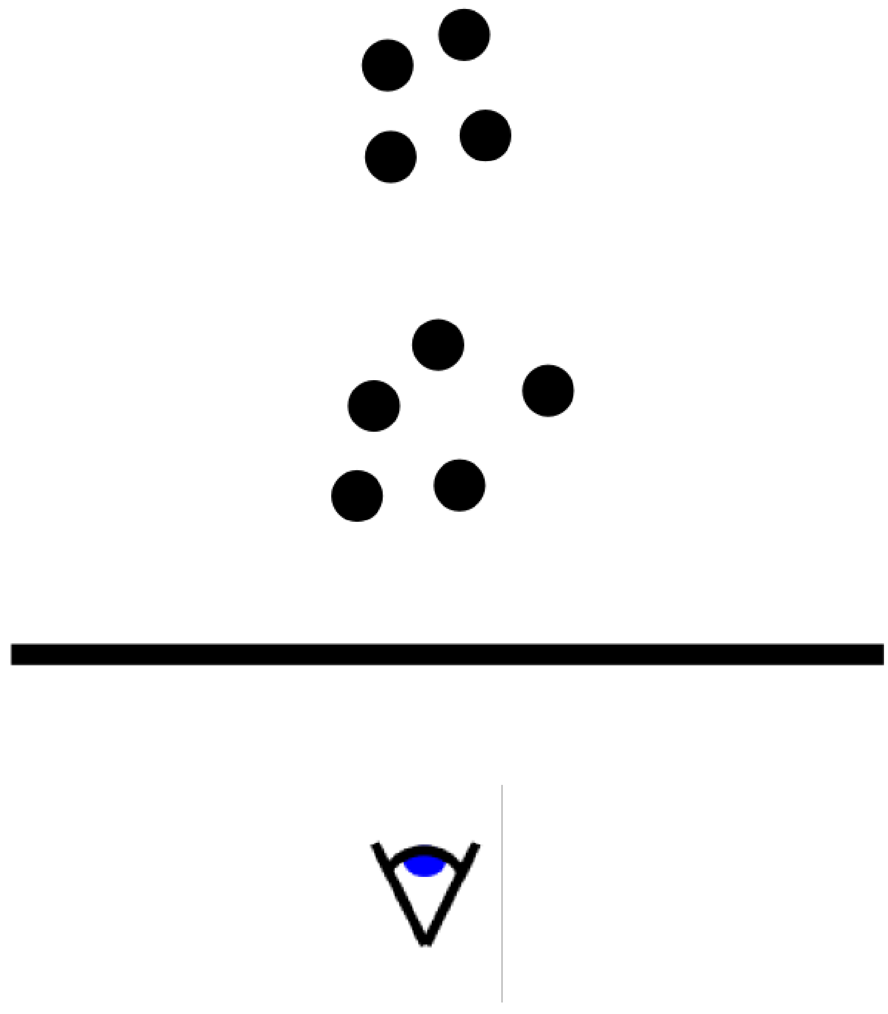
$$X''V = X_{\mathrm{proj}}$$

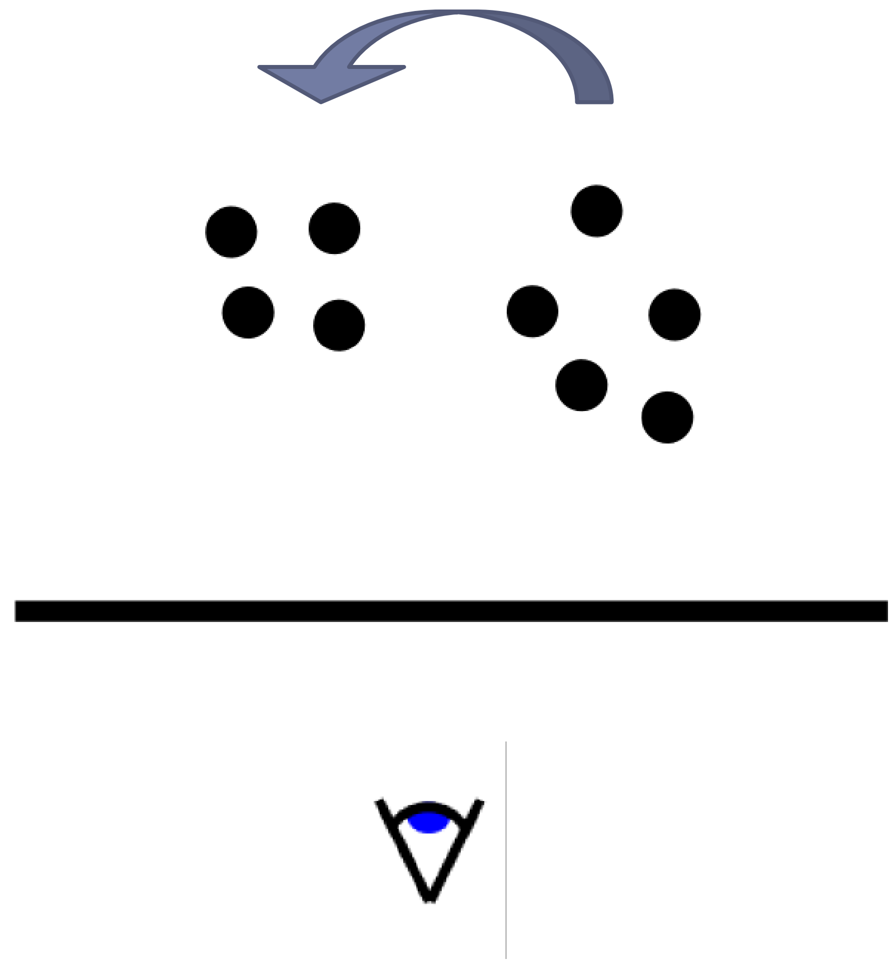
$$\Sigma = V\Lambda V^T$$
$$(V = R^T, \Lambda = \mathrm{D}^2)$$

$$X \sim N(0,1)$$

$$X'' = X \cdot D \cdot R$$

$$\begin{aligned}(X'')^T(X'') \\ &= (XDR)^T(XDR) \\ &= R^T D^T X^T X D R \\ &= R^T D^2 R\end{aligned}$$





Quiz

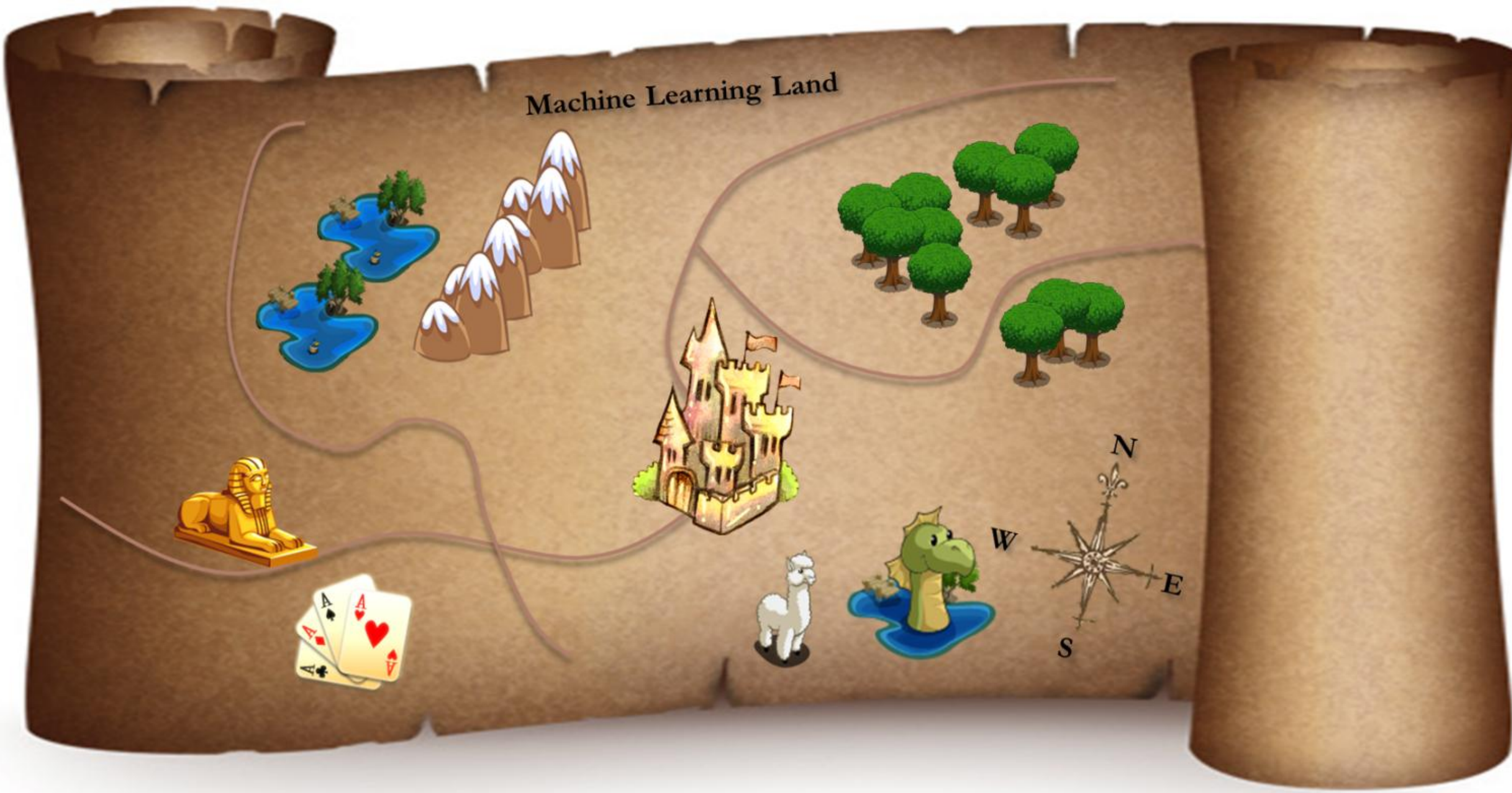
- Principal components are ______________ of the ______________ matrix.

- Eigenvalue spectrum shows how much ______________ is explained by each _______.

- If $\boldsymbol{\Sigma} = \boldsymbol{V}\boldsymbol{\Lambda}\boldsymbol{V}^T$, then

$$\boldsymbol{X}_{\mathbf{proj}} = \_\_\_\_\_\_$$

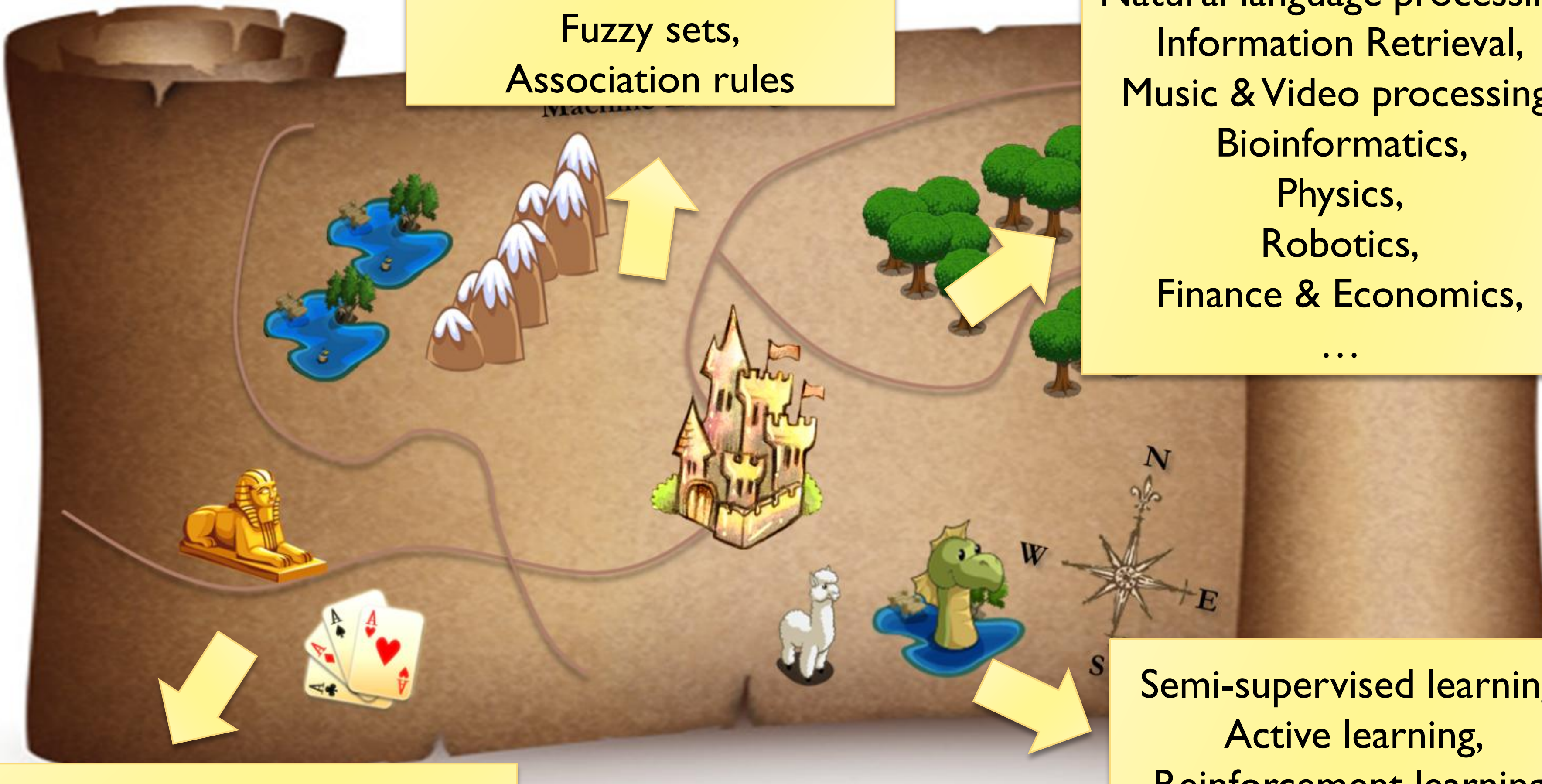
Conclusion



Conclusion

Graphical models,
Neural networks,
Fuzzy sets,
Association rules

Computer vision,
Natural language processing,
Information Retrieval,
Music & Video processing,
Bioinformatics,
Physics,
Robotics,
Finance & Economics,
…



Statistical Learning Theory,
PAC-theory

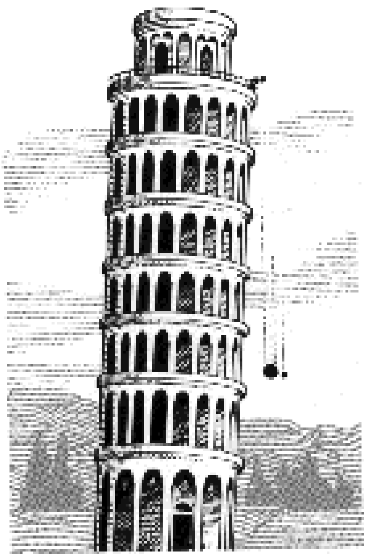
Semi-supervised learning,
Active learning,
Reinforcement learning,
Multi-instance learning,
Deep learning

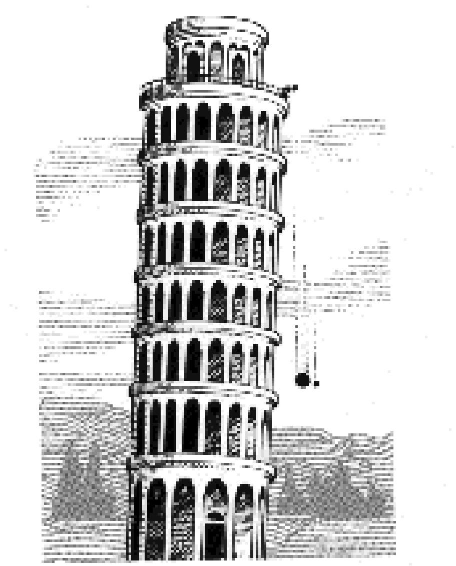
Where to go next

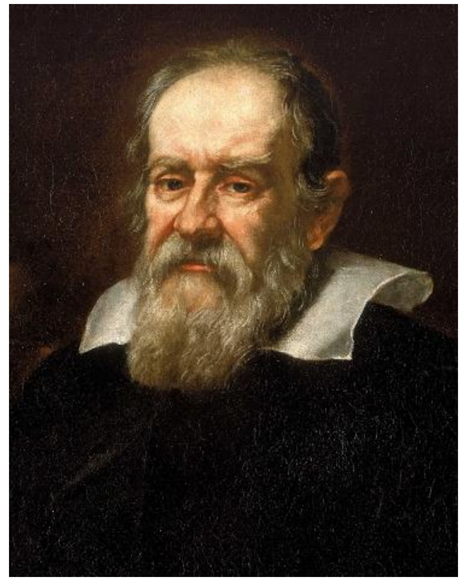
- Books:
  - "The Elements of Statistical Learning" (Hastie & Tibshirani)
  - "Pattern Recognition and Machine Learning" (Bishop)
  - "Kernel Methods for Pattern Analysis" (Shawe-Taylor & Cristianini)
- On-line materials:
  - http://videolectures.net
  - + Coursera, Udacity, edX
- Tools:
  - Python, R, RapidMiner, Weka, Matlab, Mathematica, …

Where to go next

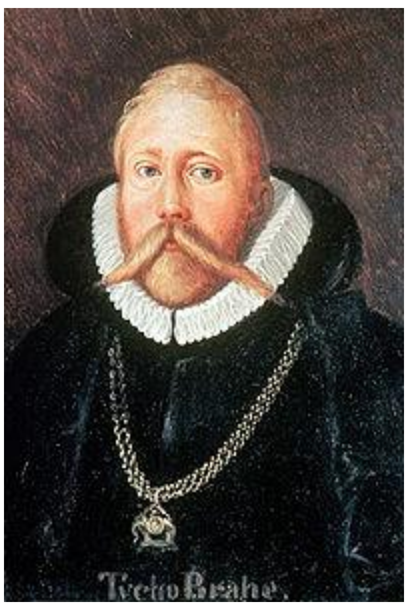
- http://kt.era.ee/aacimp

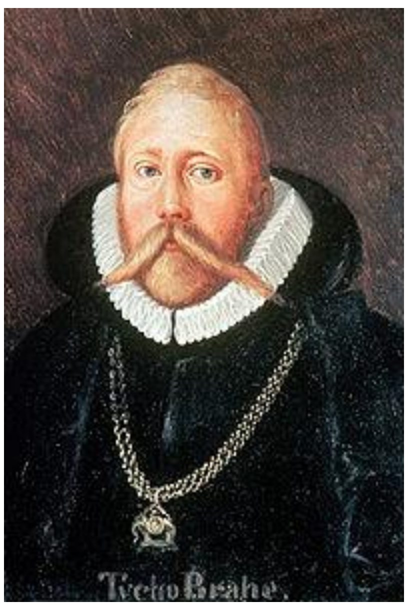


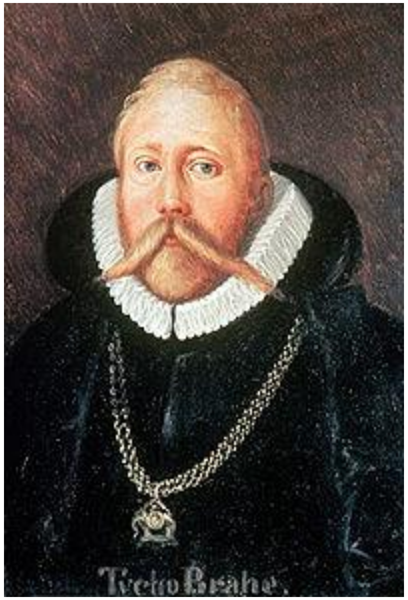


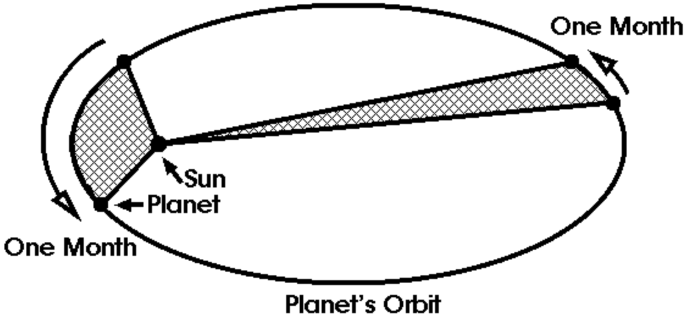


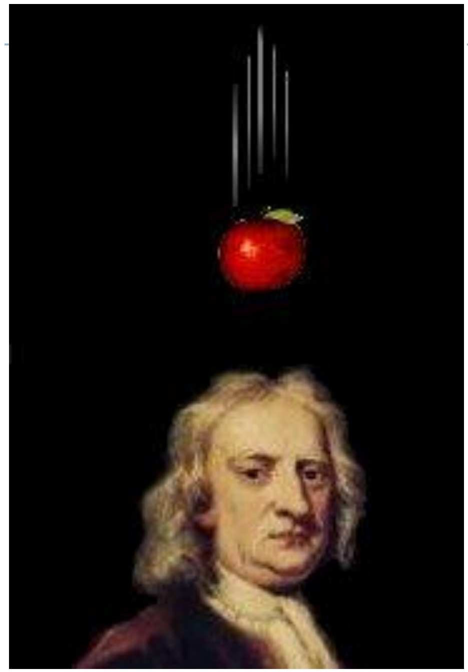
$$s = \frac{a}{2}t^2$$

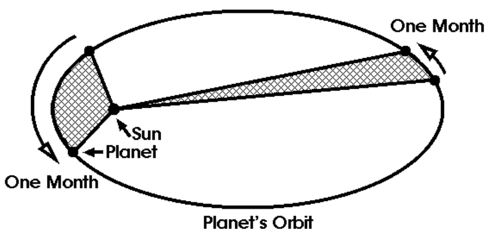

Tycho Brahe.

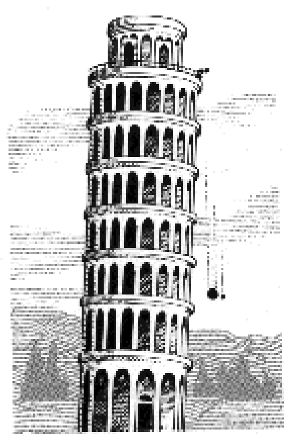

Tycho Brahe.

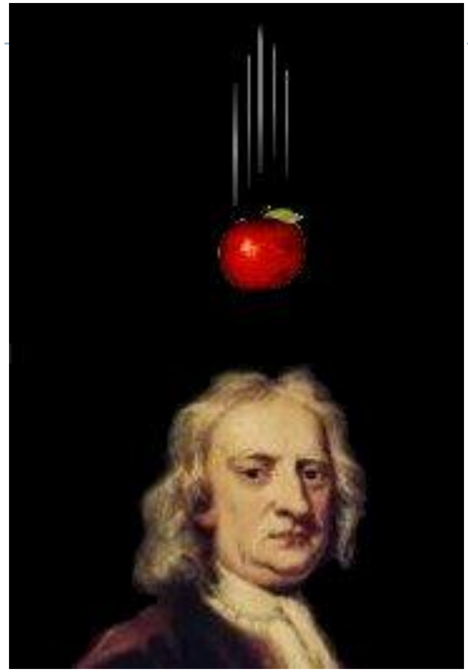

Tycho Brahe.

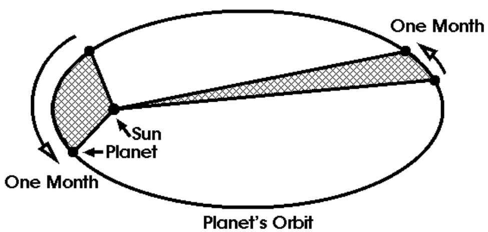

One Month
Sun
Planet
One Month
Planet's Orbit

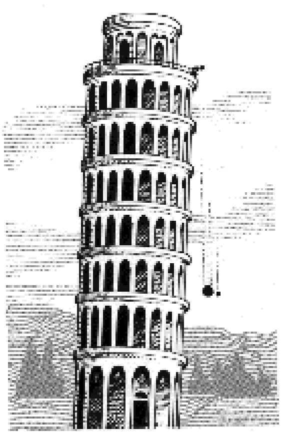



One Month
Sun
Planet
One Month
Planet's Orbit



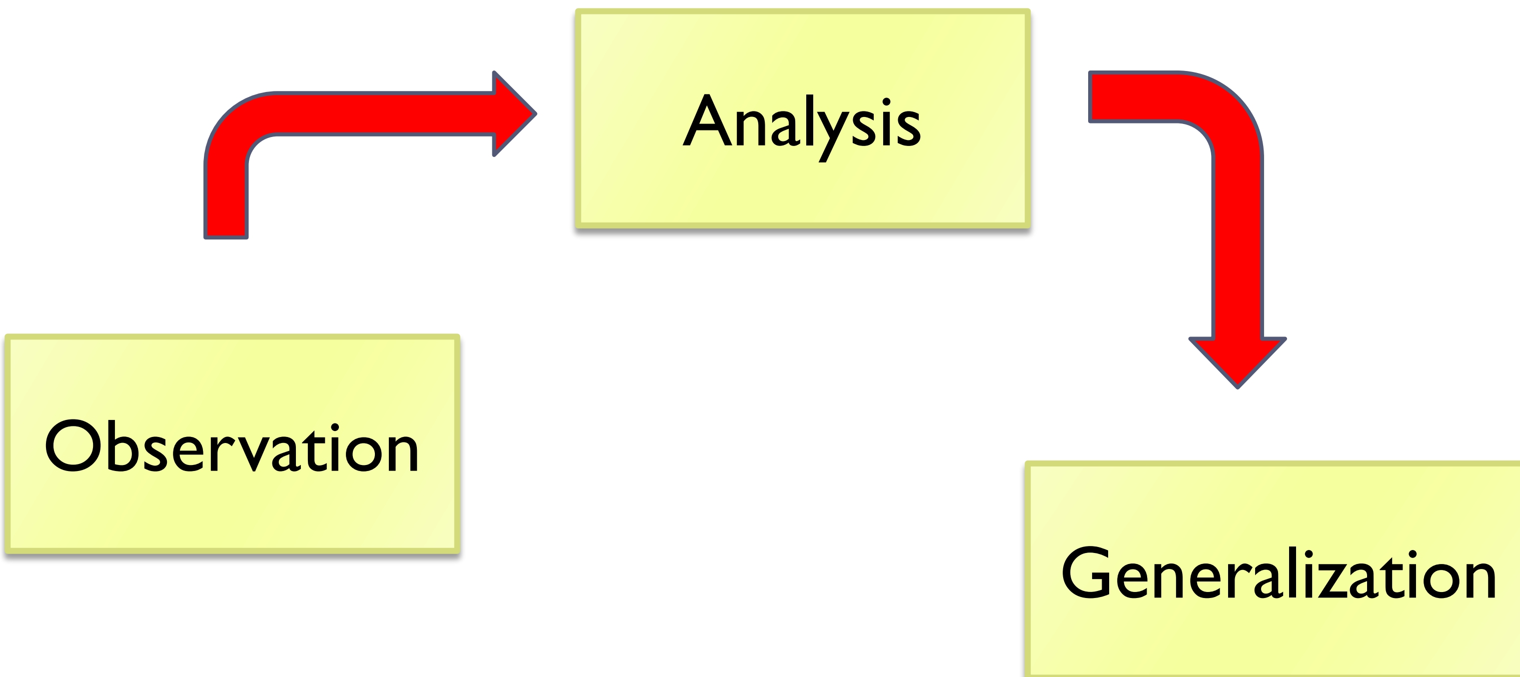


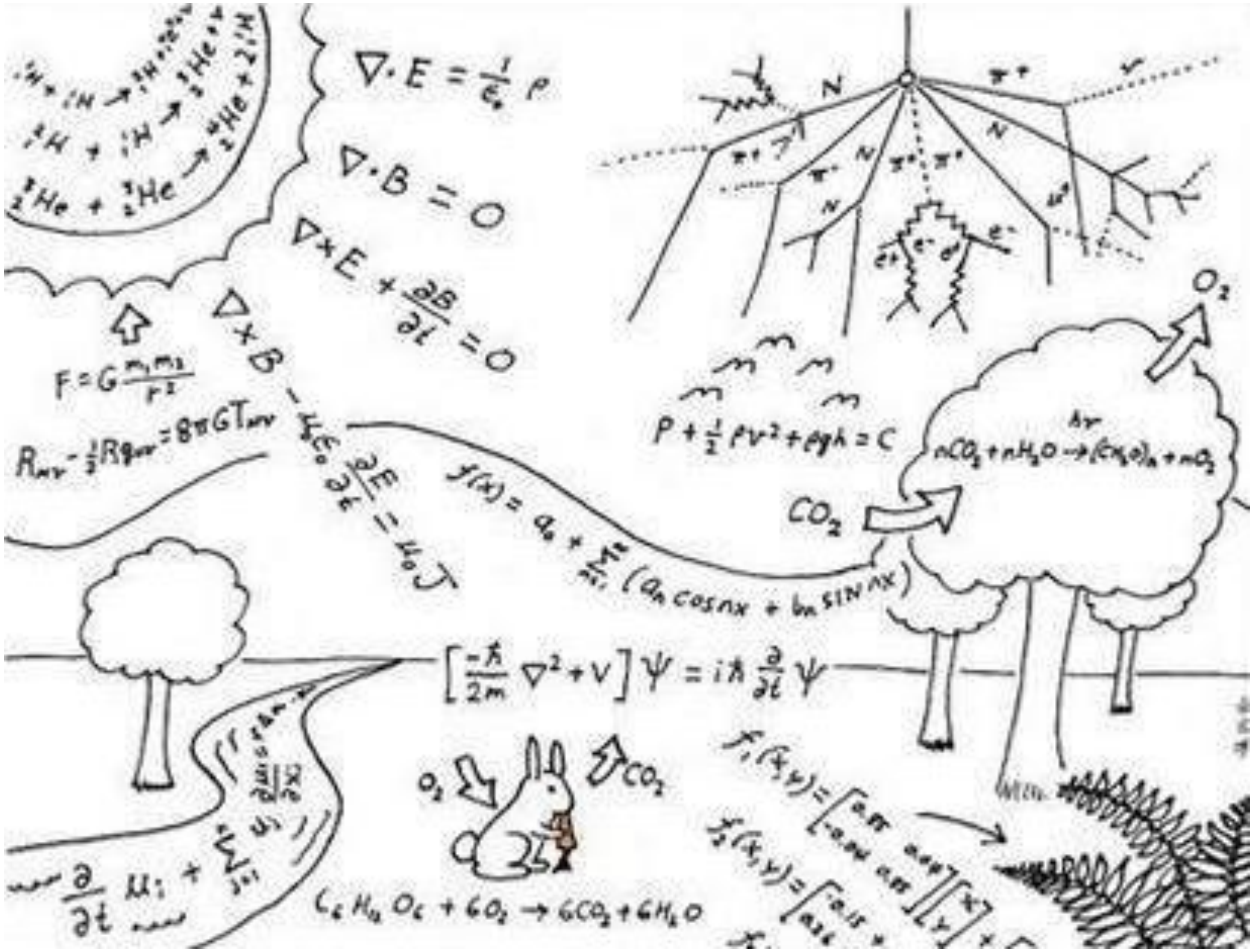




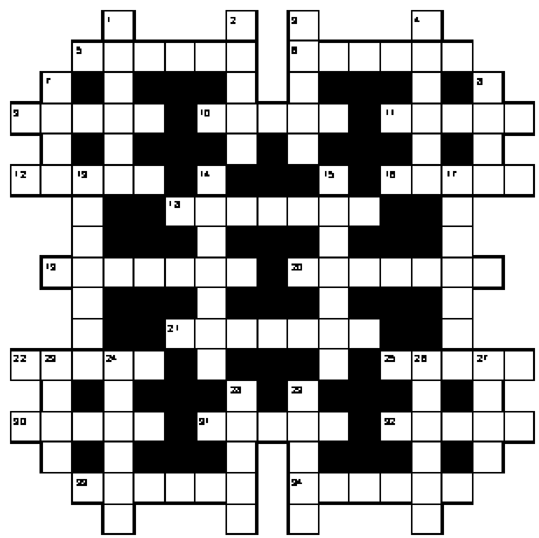
$$\vec{F} = m\vec{g}$$

Science



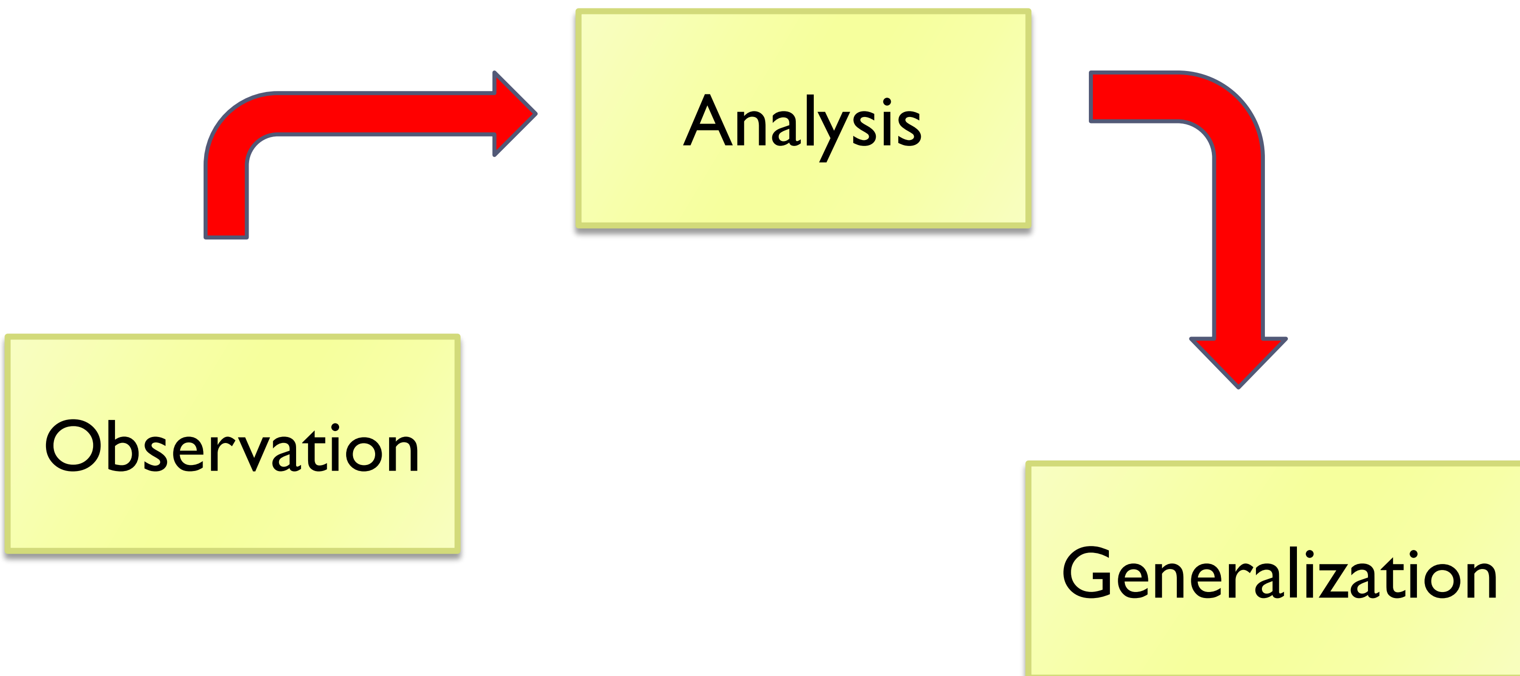

${}^3_2He + {}^3_2He \rightarrow {}^4_2He + 2{}^1_1H$
$\nabla\cdot E = \frac{1}{\epsilon_0}\rho$
$\nabla\cdot B = 0$
$\nabla\times E + \frac{\partial B}{\partial t} = 0$
$\nabla\times B - \mu_0\epsilon_0\frac{\partial E}{\partial t} = \mu_0 J$
$F = G\frac{m_1 m_2}{r^2}$
$R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu} = 8\pi G T_{\mu\nu}$
$P + \frac{1}{2}\rho v^2 + \rho g h = C$
$h\nu$
$nCO_2 + nH_2O \rightarrow (CH_2O)_n + nO_2$
O_2
CO_2
$f(x) = a_0 + \sum_{n=1}^{\infty}(a_n \cos nx + b_n \sin nx)$
$\left[\frac{-\hbar}{2m}\nabla^2 + V\right]\Psi = i\hbar\frac{\partial}{\partial t}\Psi$
O_2
CO_2
$C_6H_{12}O_6 + 6O_2 \rightarrow 6CO_2 + 6H_2O$

Why?



Why?

Contemporary Science



Contemporary Science

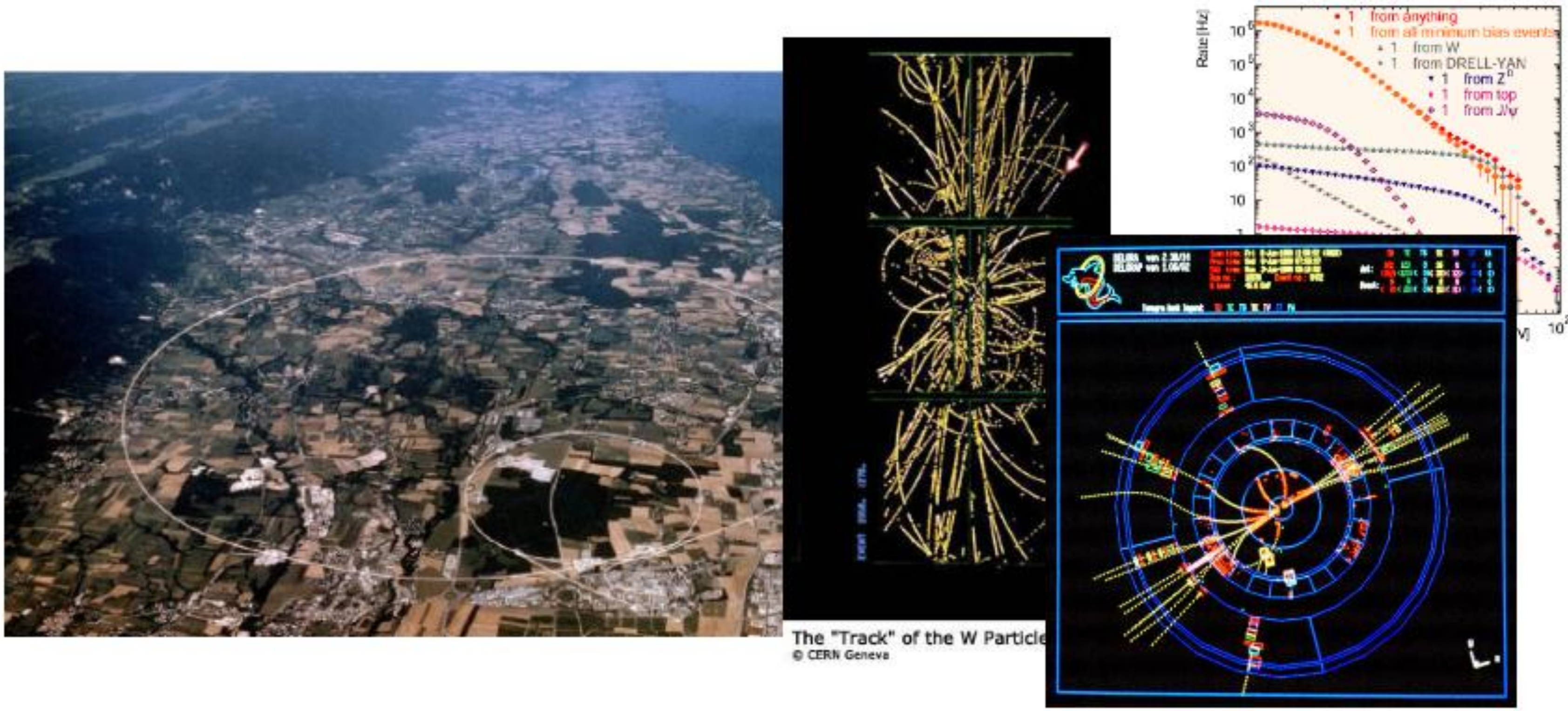
Analysis

Generalization

CS & EE

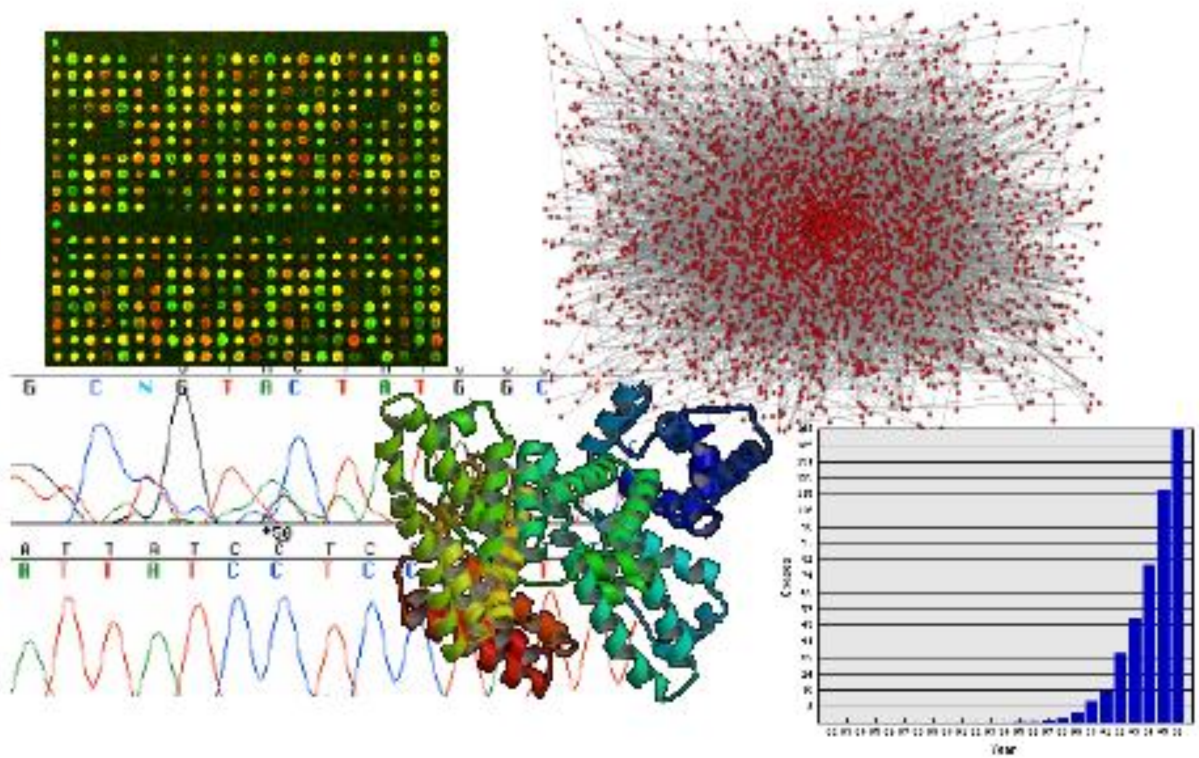
Contemporary Science

Contemporary Science



The "Track" of the W Particle
© CERN Geneva

Contemporary Science



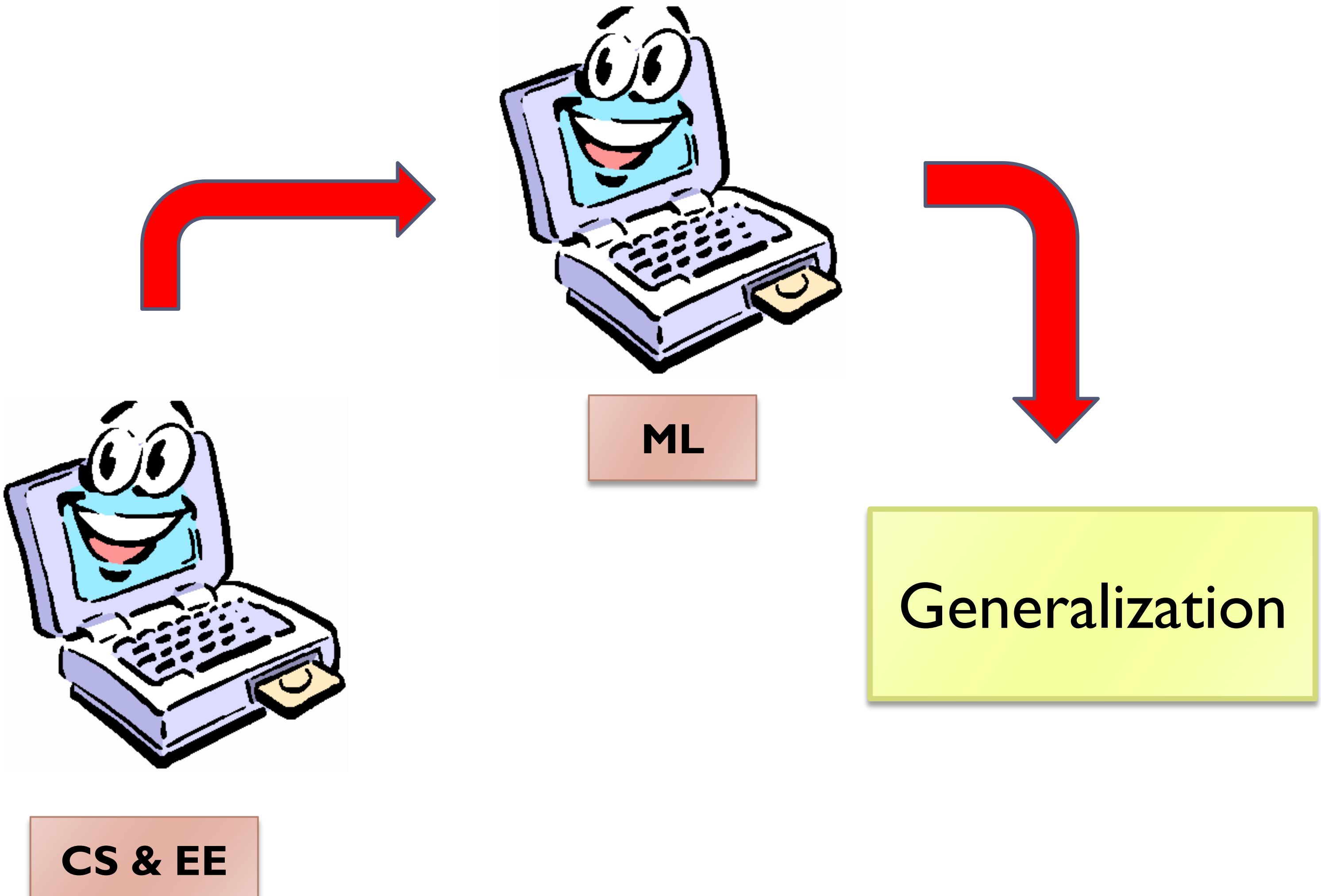
Contemporary Science

Analysis

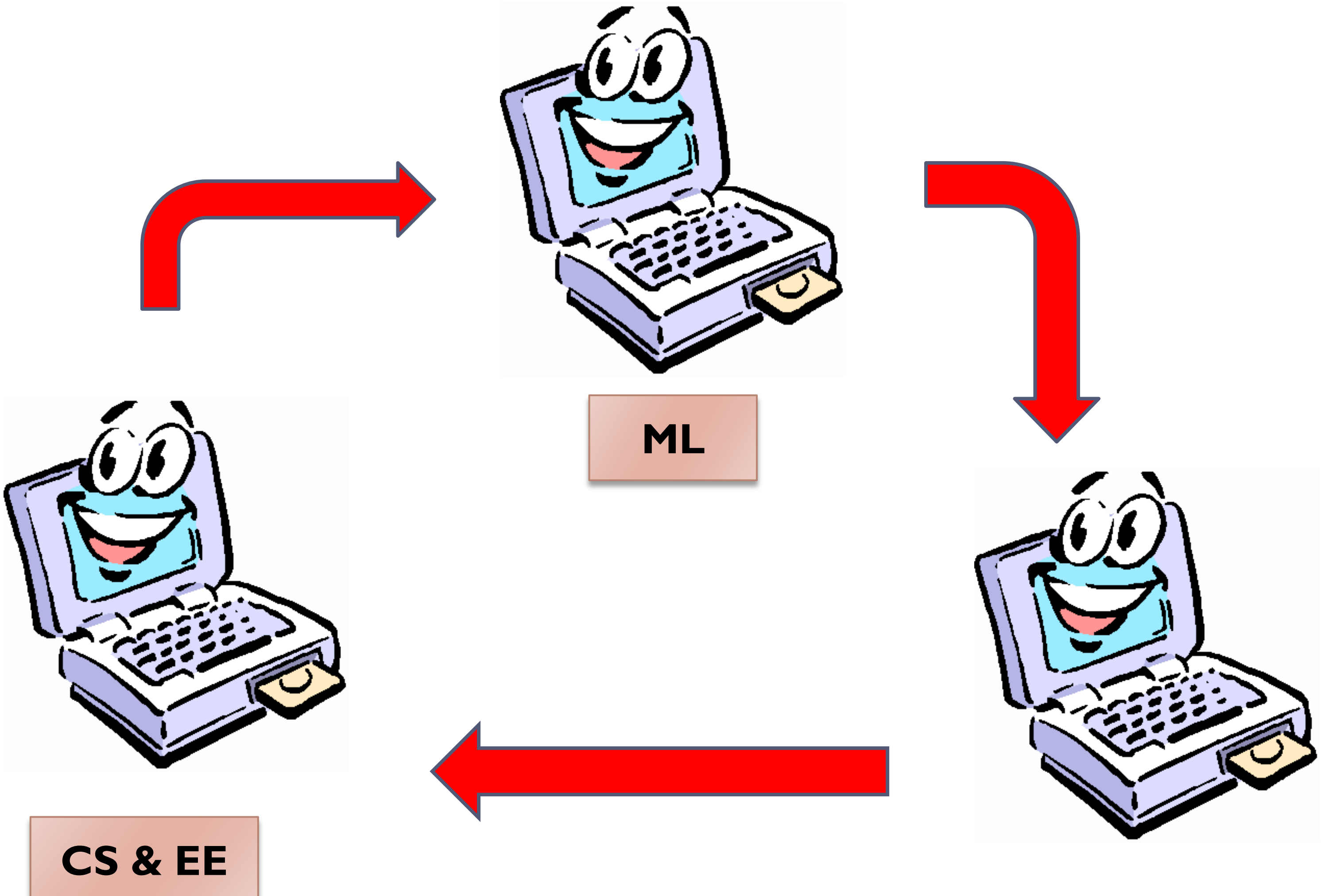
Generalization

CS & EE

Contemporary Science



Contemporary Science




Thank You!