Machine Learning

Clustering, Self-Organizing Maps

Clustering

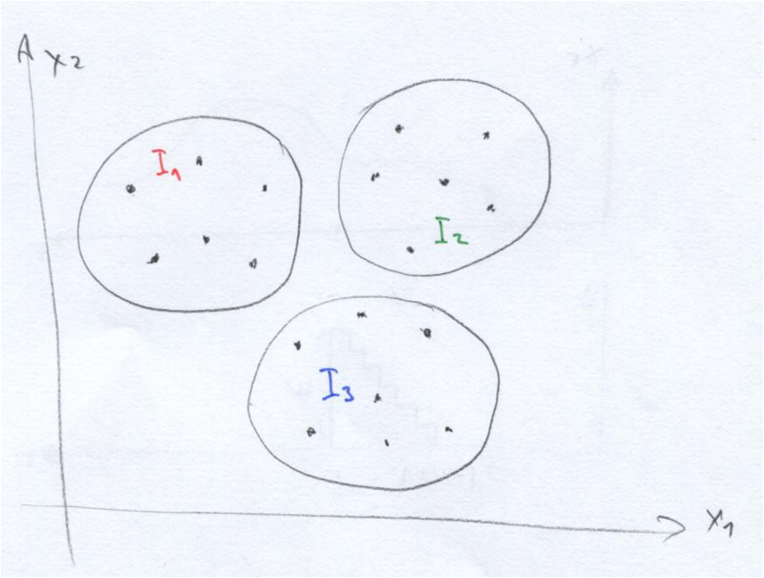
The task: partition a set of objects into "meaningful" subsets (clusters). The objects in a subset should be "similar".

Notations:

Set of Clusters K

Set of indices $I = \{1, 2, \dots, |I|\}$

Feature vectors $x^i,\ i \in I$



Partitioning

$$C = (I_1, I_2, \dots, I_{|K|}),\ I_k \cap I_{k'} = \emptyset \text{ for } k \neq k',\ \bigcup_k I_k = I$$

Clustering

Let $x^i \in \mathbb{R}^n$ and each cluster has a "representative" $y^k \in \mathbb{R}^n$

The task reads:

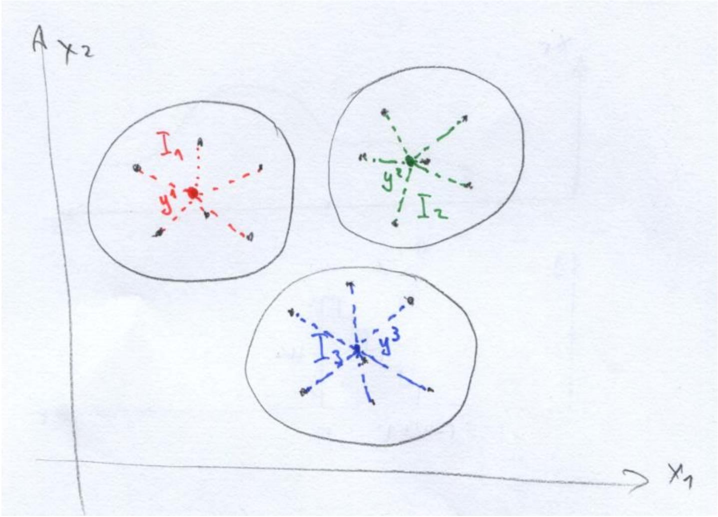
$$\sum_k \sum_{i \in I_k} ||x^i - y^k||^2 \to \min_{C,y}$$

Alternative variant is to consider the clustering C as a mapping $C : I \to K$ that assigns a cluster number to each $i \in I$

$$\sum_i ||x^i - y^{C(i)}||^2 \to \min_{y,C}$$

$$\sum_i \min_k ||x^i - y^k||^2 \to \min_y$$

K-Means Algorithm



Initialize centers randomly,

Repeat **until convergence**:

1. Classify:

$$C(i) = \arg\min_{k'} \|x^i - y^{k'}\|^2 \quad \Rightarrow \quad i \in I_k$$

2. Update centers:

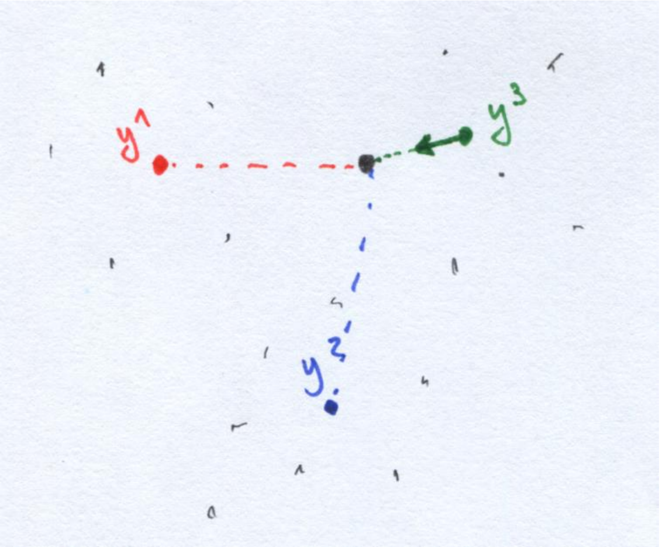
$$y^k = \arg\min_{y} \sum_{i \in I_k} \|x^i - y\|^2 = \frac{1}{|I_k|} \sum_{i \in I_k} x^i$$

- The task is NP
- converges to a local optimum (depends on the initialization)

Sequential K-Means

Repeat **infinitely**:

1. Chose randomly a feature vector x from the training data



2. Classify it:

$$k = \arg\min_{k'} \|x - y^{k'}\|$$

3. Update the k-th center:

$$y^k = y^k + \eta(t)(x - y^k)$$

with a decreasing step $\eta(t)$

- converges to the same, as the parallel version
- is a special case of Robbins-Monro Algorithm

Some variants

Other distances, e.g. $||x^i - y^k||$ instead of $||x^i - y^k||^2$

In the K-Means algorithm the classification step remains the same, the update step – the geometric median of $x^i,\ i \in I_k$

$$y_k = \arg\min_y \sum_{i \in I_k} ||x^i - y||$$

(a bit complicated as the average ☹).

Another problem: features may be not additive (y^k does not exist)

Solution: K-Medioid Algorithm (y^k is a feature vector from the training set)

A generalization

Observe (for the Euclidean distance):

$$\sum_i \|x^i - \bar{x}\|^2 \sim \sum_{ij} \|x^i - x^j\|^2$$

In what follows:

$$\sum_k \sum_{ij \in I_k} \|x^i - x^j\|^2 = \sum_k \sum_{ij \in I_k} d(i,j) \rightarrow \min_C$$

with a Distance Matrix d that can be defined in very different ways.

Example: Objects are nodes of a weighted graph, $d(i,j)$ is the length of the shortest path from i to j.

Distances for "other" objects (non-vectors):

- Edit (Levenshtein) distance between two symbolic sequences
- For graphs – distances based on graph isomorphism etc.

An application – color reduction

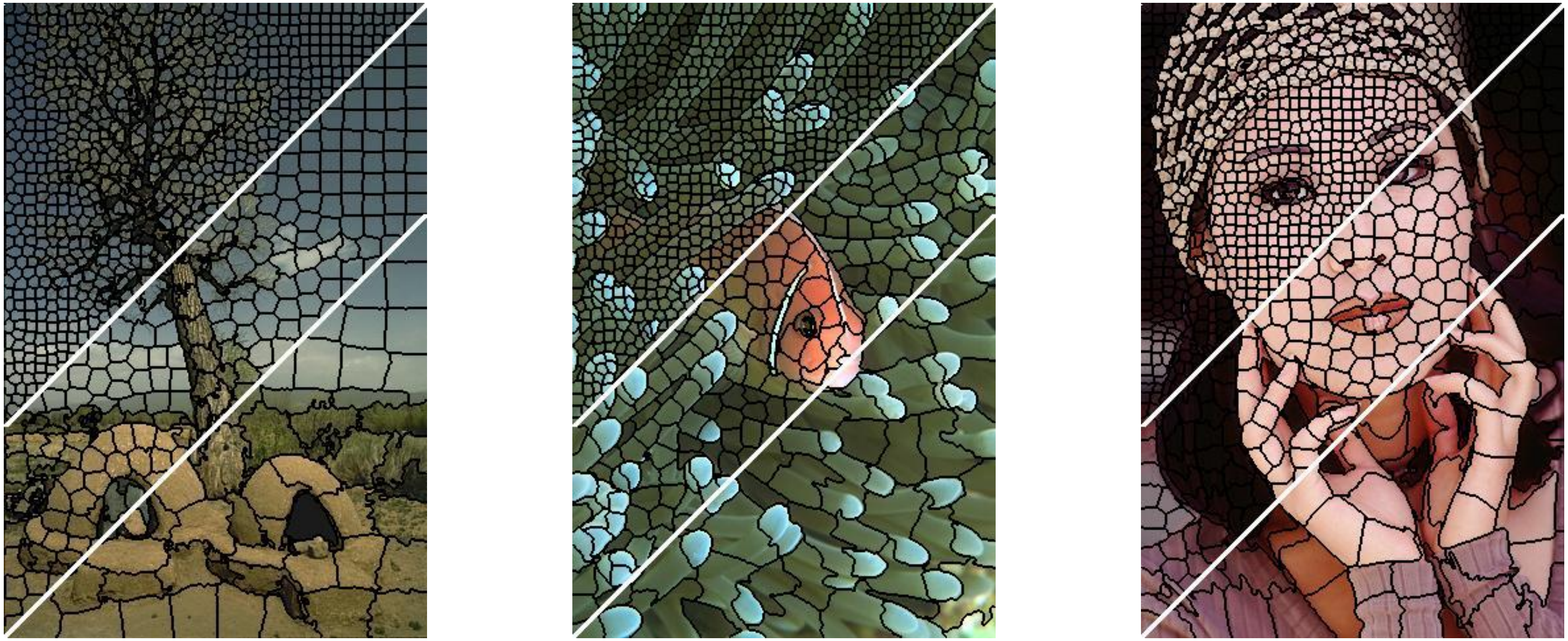
Objects are pixels, features are RGB-values.
Partition the RGB-space into “characteristic” colors.

(8 colors)

Another application – superpixel segmentation

Object are pixels. Features are RGBXY-values.

→ Those pixels belong to the same cluster that are close to each other both spatially and in in the RGB-space

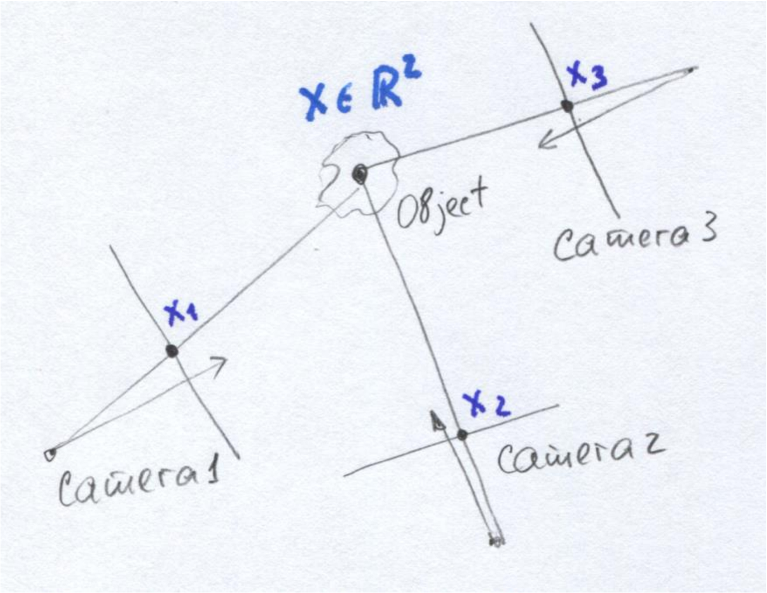


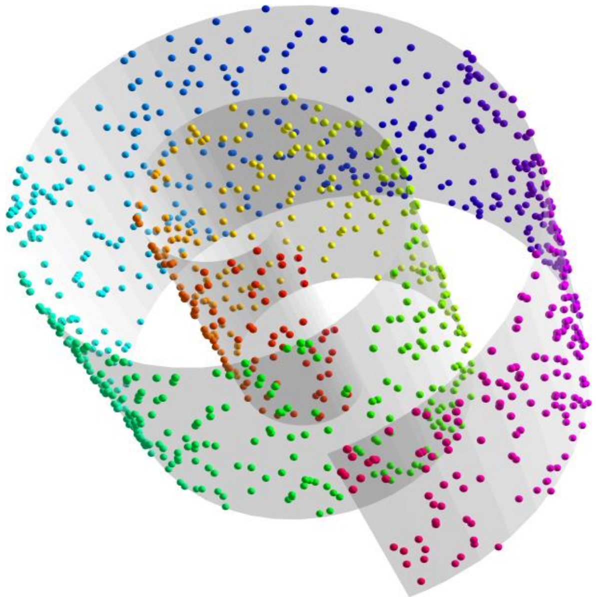
SLIC Superpixels: http://ivrg.epfl.ch/research/superpixels

Cohonen Networks, Self-Organizing Maps

The task is to “approximate” a dataset by a neural network of a certain **topology**.

An example – stereo in “flatland”.



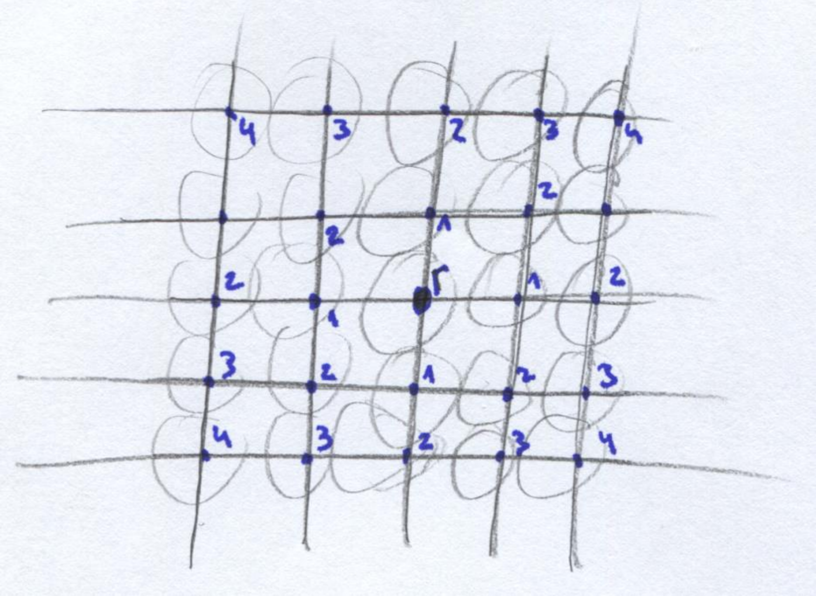


The input space is 3- (or more) dimensional, the set of points is however isomorphic to a 2D-space (up to noises).

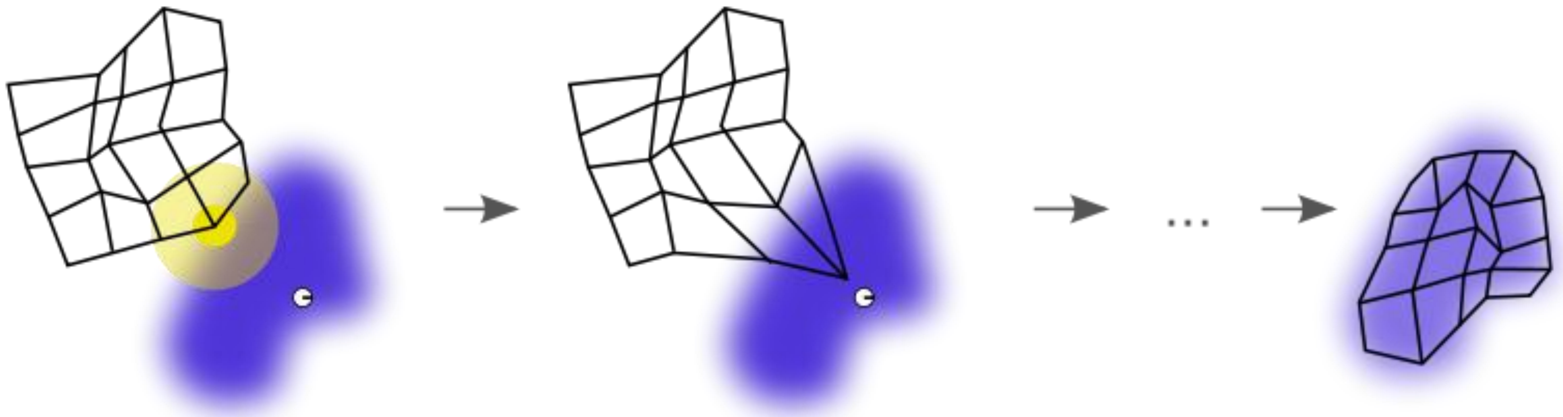
Self-Organizing Maps

SOM-s (usually) consist of RBF-neurons r, each one represents (covers) a "part" of the input space (specified by the centers μ^r).

The network topology is given by means of a distance $d(r, r')$. Example – neurons are nodes of a weighted graph, distances are shortest paths. For the "flatland" example the graph is a 2D-grid with unit weight for all edges.



Self-Organizing Maps, sequential algorithm



1. Chose randomly a feature vector x from the training data (white)
2. Compute the "winner"-neuron (dark-yellow)

$$r^* = \arg\min_r \|x - \mu^r\|$$

3. Compute the neighborhood of r^* **in the network** (yellow)

$$R = \{r | d(r^*, r) < \Theta\}$$

4. Update the weights of **all** neurons from R

$$\mu^r = \mu^r + (x - \mu^r) \cdot \eta\big(t, d(r^*, r)\big)$$

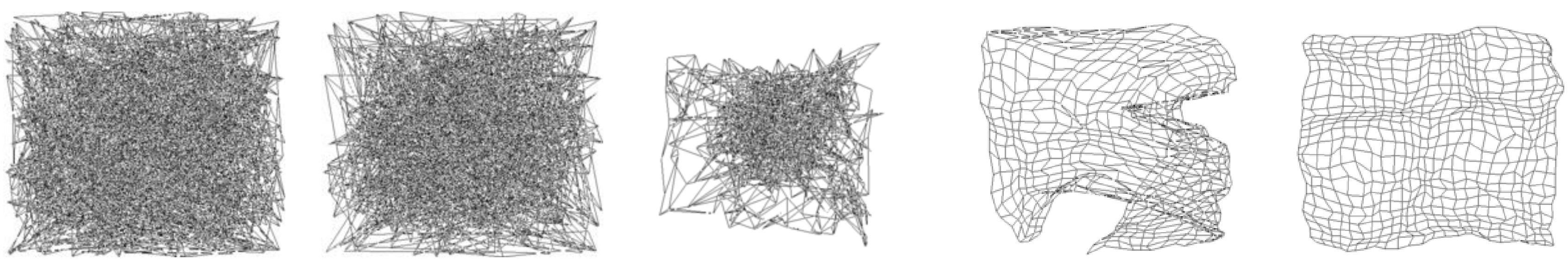
Self-Organizing Maps, algorithms

$\eta(t, d)$ is monotonously decreasing with respect to t (time) **and** d

Without 3) – the sequential K-Means.

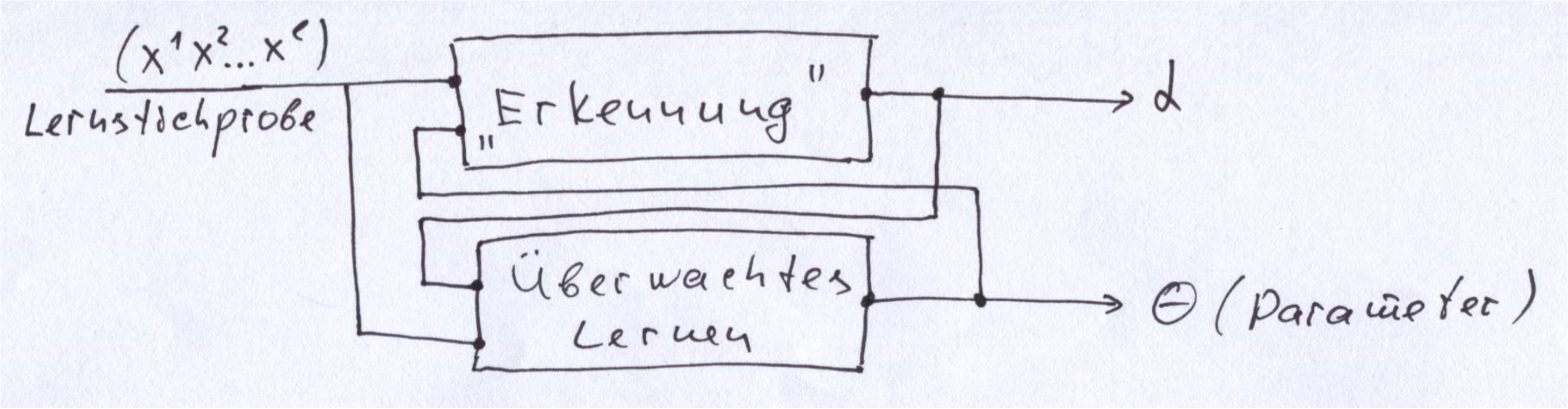
Parallel variants:
Go through all feature vectors, sum up the gradients, apply.

Example for $\mathbb{R}^2 \to \mathbb{R}^2$:

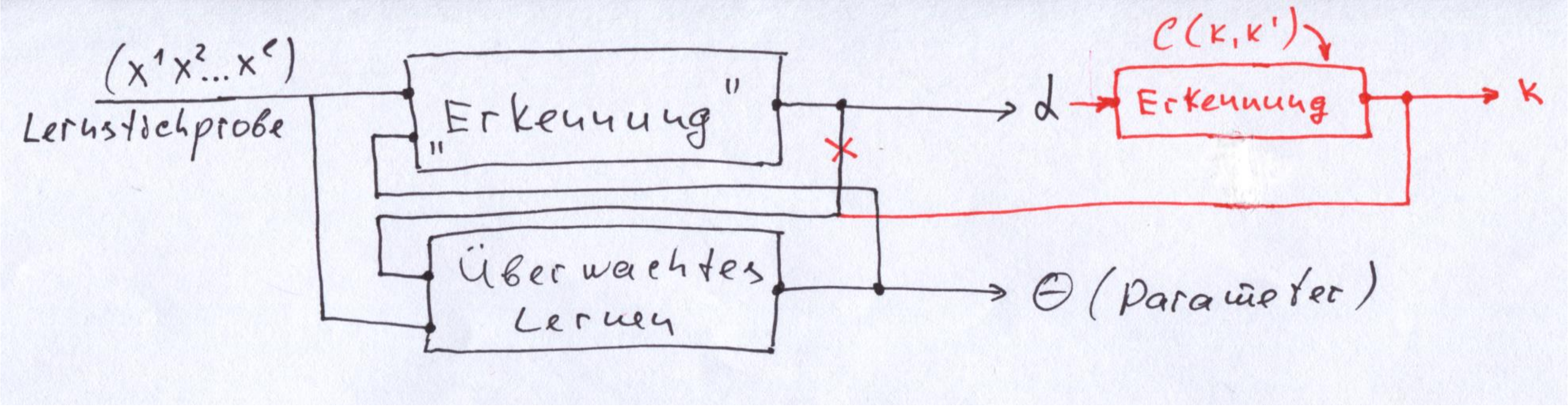


The network fits into the data distribution (unfolds).

EM – compute posteriors for the Expectation step



K-Means – classify object



Conclusion

Before:
1. Probability theory – models, inference, learning
2. → Discriminative learning → Classifiers

Neural networks:
1. Feed-Forward Networks – complex classifiers
2. Hopfield Networks – structured output
3. Cohonen Networks – clustering (unsupervised), model fitting

Next topics – further classifiers:
1. Support Vector Machines, Kernels
2. Empirical Risk minimization
3. Principal Component Analysis
4. Combining classifiers – Decision Trees, AdaBoost