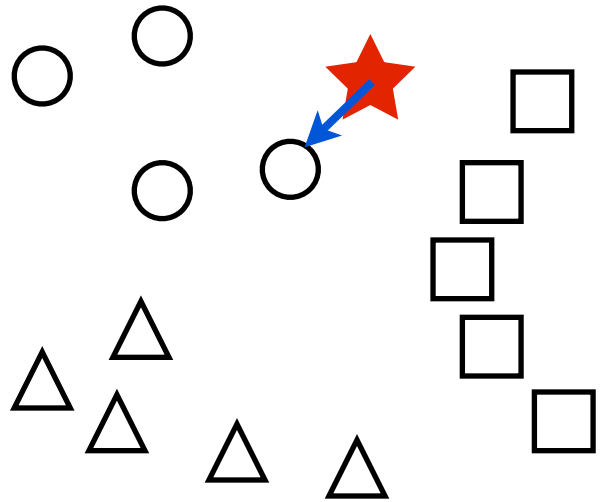
Lecture 5: Machine Learning III

Nearest Neighbors and Neural Networks

http://cs.nju.edu.cn/yuy/course_dm14ms.ashx

Nearest neighbor

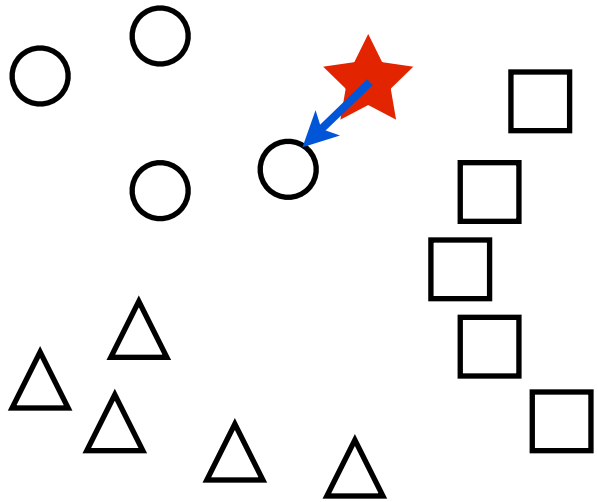
what looks similar are similar



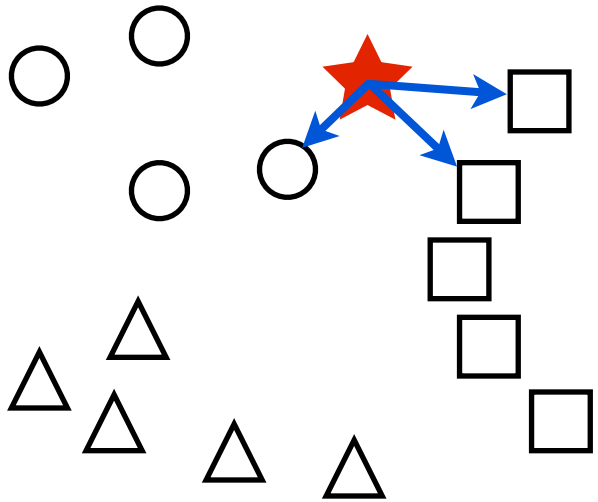
Nearest neighbor

for classification:

1-nearest neighbor:



k-nearest neighbor:

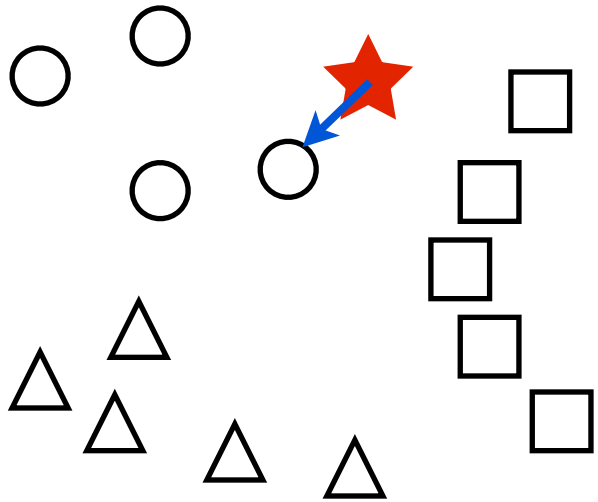


Predict the label as that of the NN
or the (weighted) majority of the k-NN

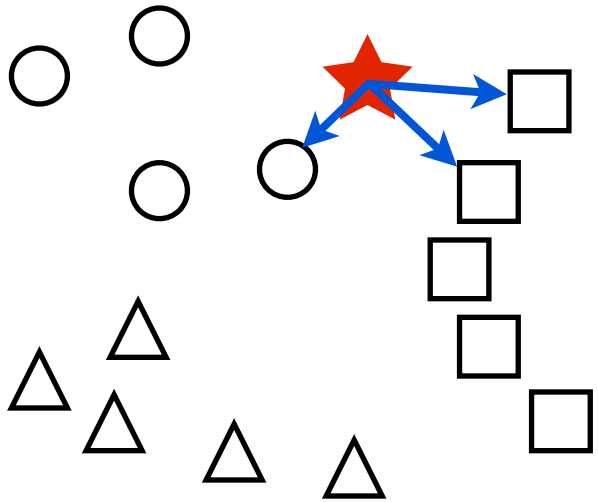
Nearest neighbor

for regression:

1-nearest neighbor:



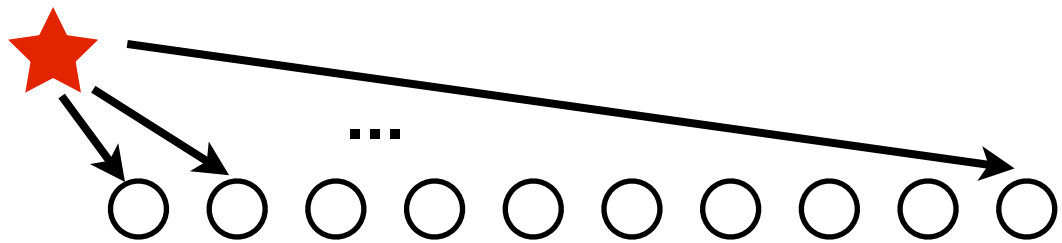
k-nearest neighbor:



Predict the label as that of the NN
or the (weighted) *average* of the k-NN

Search for the nearest neighbor

Linear search



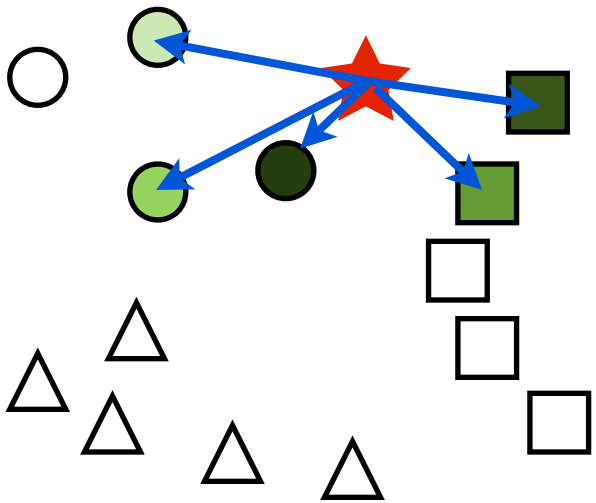
n times of distance calculations

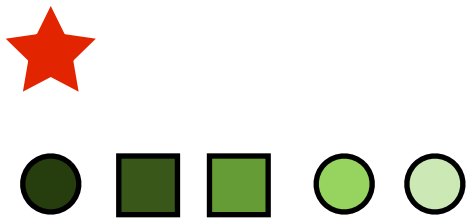
$O(dn \ln k)$

d is the dimension, *n* is the number of samples

Nearest neighbor

for retrieval:





Nearest neighbor classifier

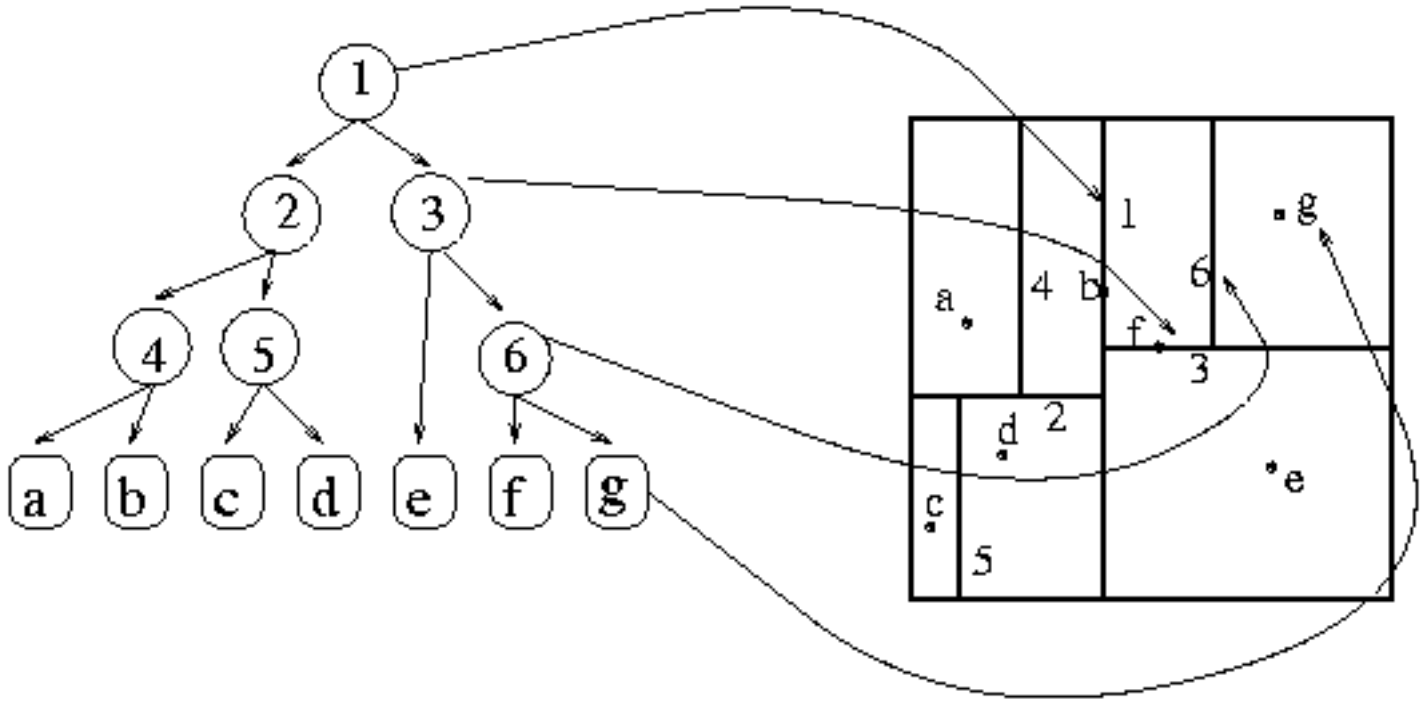
- as classifier, asymptotically less than 2 times of the optimal Bayes error
- naturally handle multi-class
- no training time
- nonlinear decision boundary

- slow testing speed for a large training data set
- have to store the training data
- sensitive to similarity function

nonparametric method

Accelerate NN search: branch-and-bound

k-d tree:



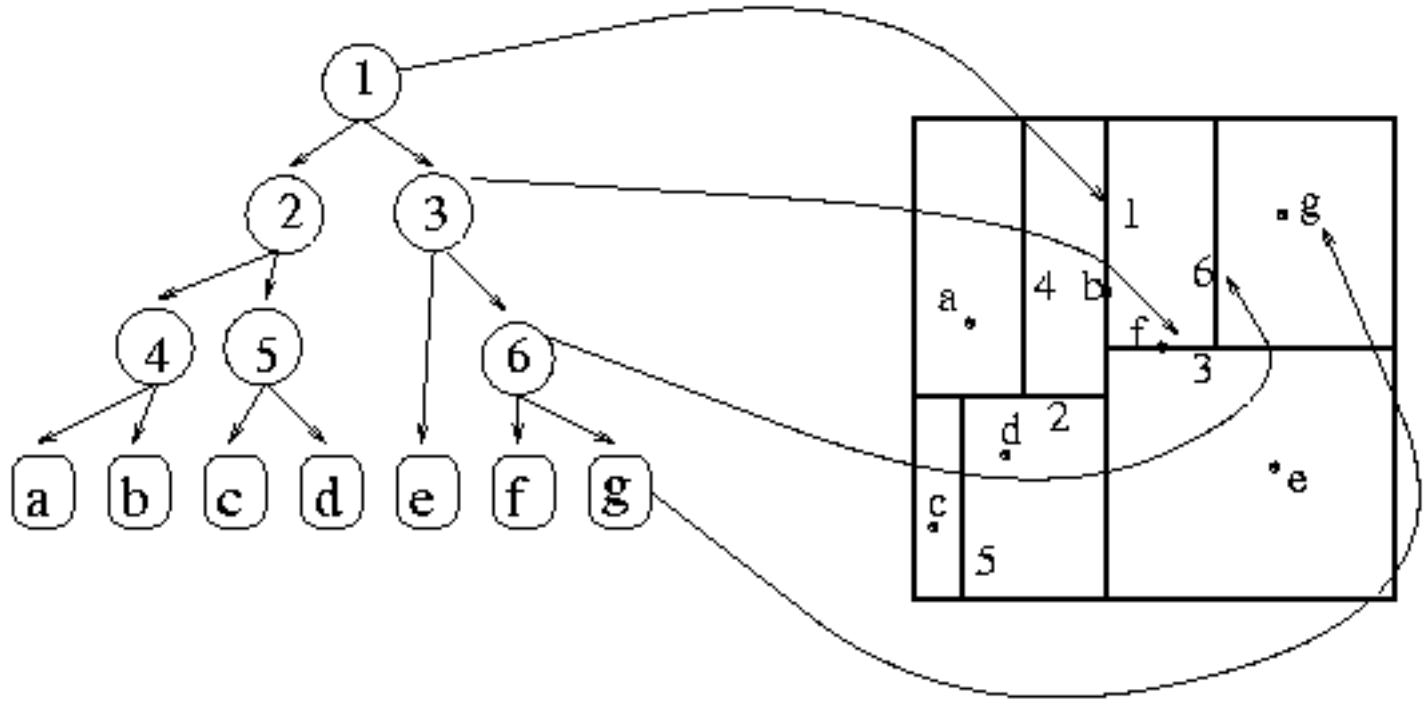
construction:

alternatively choose one dimension,
make a split by the median value.

[image from http://groups.csail.mit.edu/graphics/classes/6.838/S98/meetings/m13/kd.html]

Accelerate NN search: branch-and-bound

k-d tree:



linear search on *k*-d tree:

search(node,x):

1. if node is a leave, return the distance and the instance
2. compare *search*(left branch,x) and *search*(right branch,x)
3. return the instance with smaller distance

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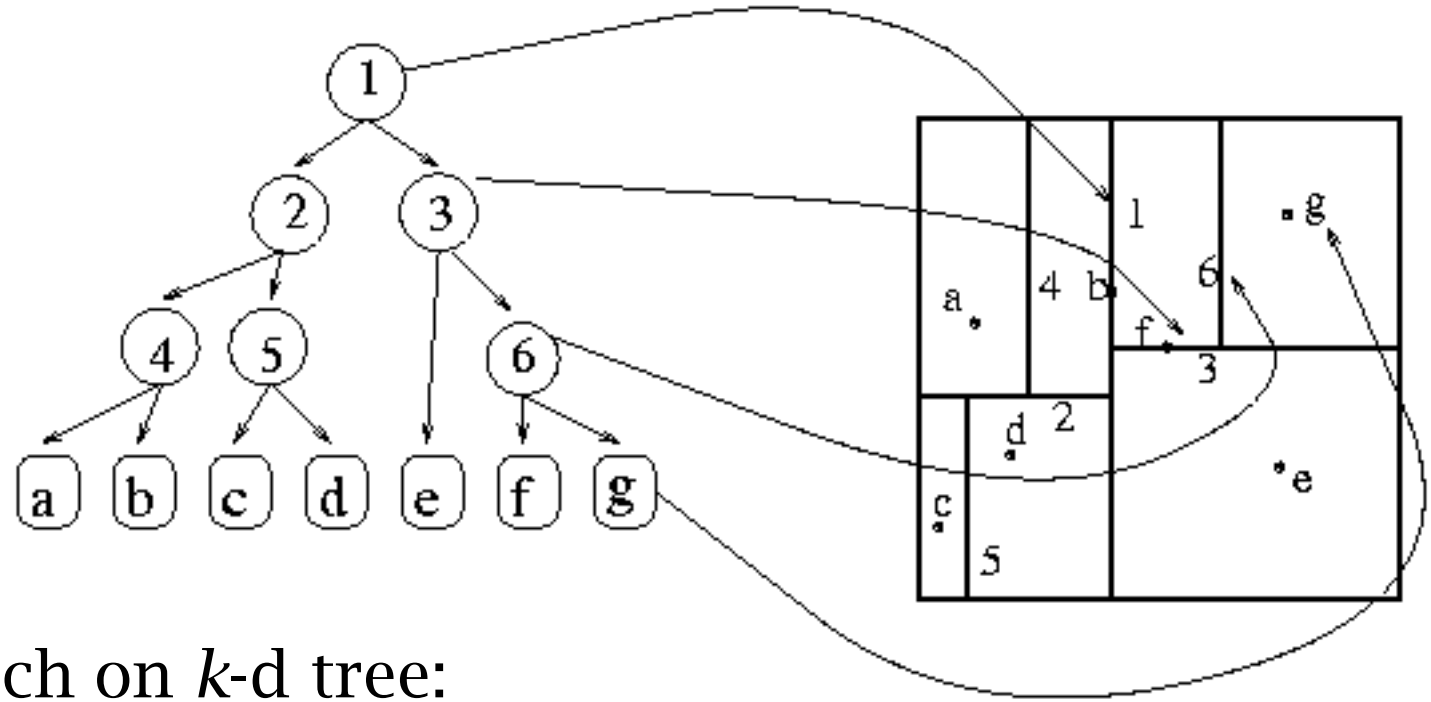
Accelerate NN search: branch-and-bound

k-d tree:



a smarter search on *k*-d tree:

search(node,x):

1. if node is a leave, return the distance and the instance
2. if ***out-of-best-range***, return infinity distance
2. compare *search*(left branch,x) and *search*(right branch,x)
3. return the instance with smaller distance

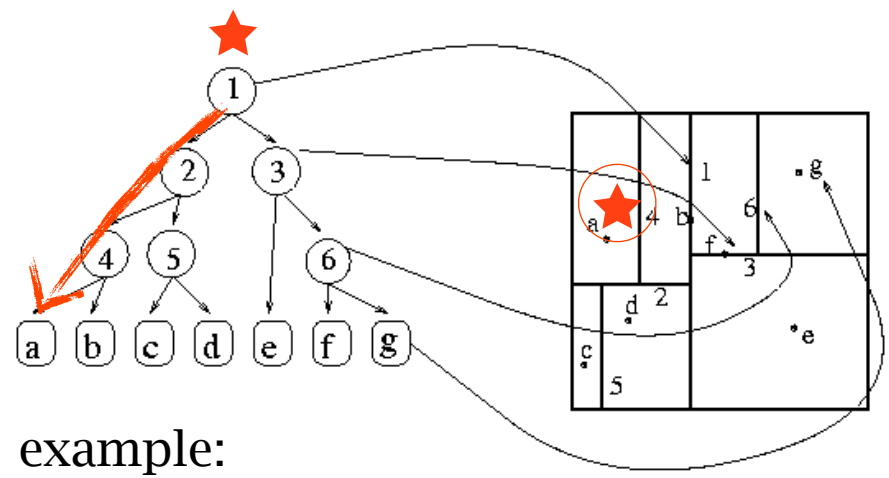
[image from http://groups.csail.mit.edu/graphics/classes/6.838/S98/meetings/m13/kd.html]

Accelerate NN search: branch-and-bound

k-d tree:

search for the nearest neighbor:
follow the depth-first search

1. find the leaf containing the test instance, and calculate the distance to training point *a*



example:
find ★ in the leaf of *a*, draw a cycle with diameter being the distance

[image from http://groups.csail.mit.edu/graphics/classes/6.838/S98/meetings/m13/kd.html]

Accelerate NN search: branch-and-bound

k-d tree:

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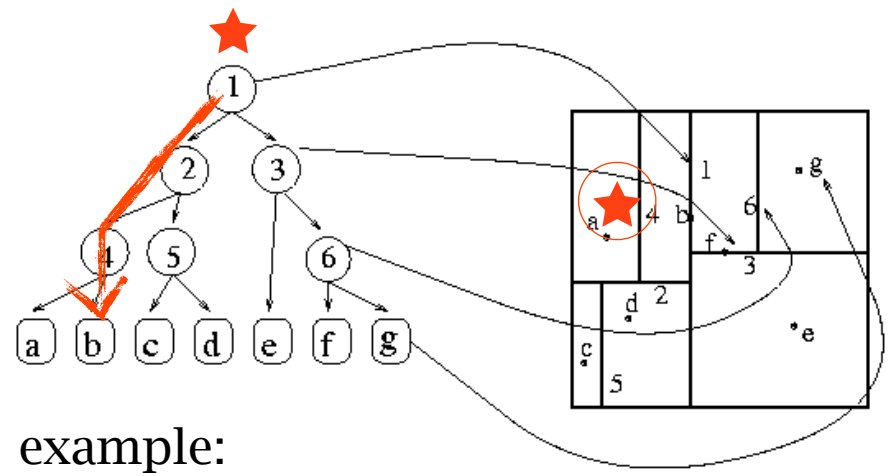
follow the depth-first search

1. find the leaf containing the test instance, and calculate the distance to training point *a*

2. back-tracing like the depth-first search. Skip nodes not overlapped with the current circle.



example:
find in the leaf of *a*, draw a cycle with diameter being the distance

the cycle overlaps with the box of *b*, so visit the leaf of *b*

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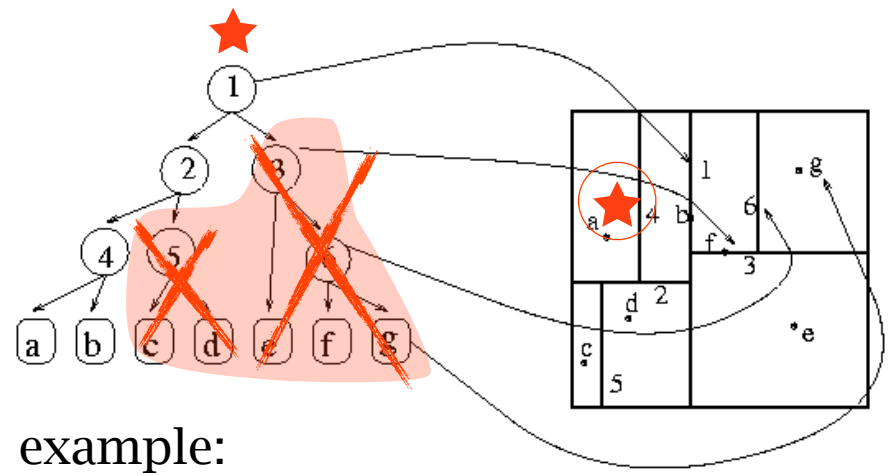


example:
find in the leaf of *a*, draw a cycle with diameter being the distance

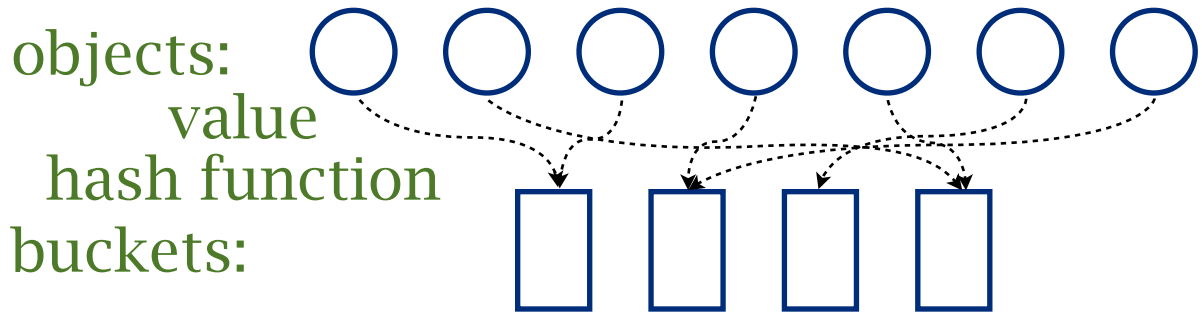
the cycle overlaps with the box of *b*, so visit the leaf of *b*

the cycle does not overlap with the box of node 5 and node 3, skip them

[image from http://groups.csail.mit.edu/graphics/classes/6.838/S98/meetings/m13/kd.html]

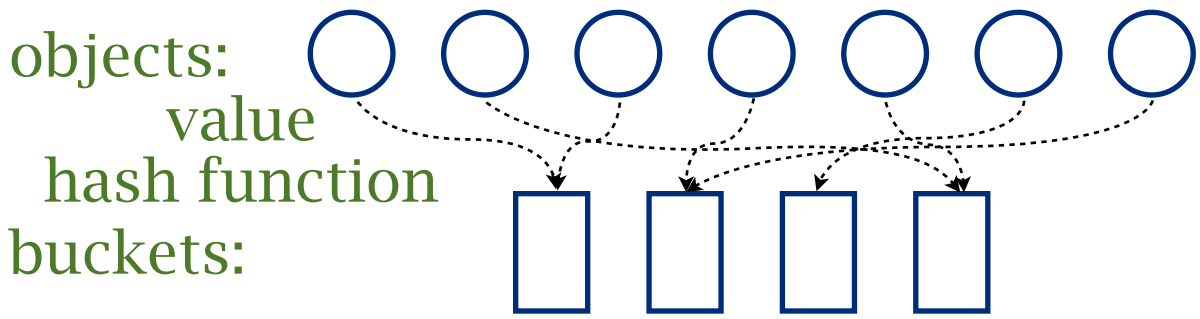
Accelerate NN search: hashing

hashing



Accelerate NN search: hashing

hashing

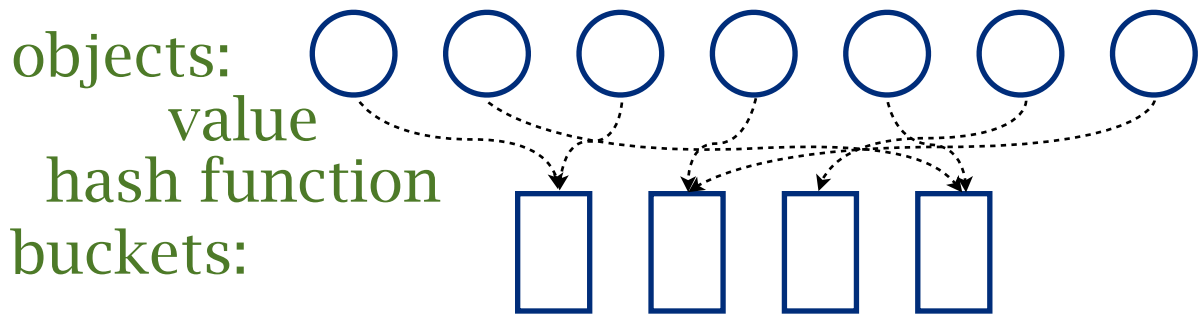


locality sensitive hashing:

similar objects in the same bucket

Accelerate NN search: hashing

hashing



locality sensitive hashing:

similar objects in the same bucket

A LSH function family $\mathcal{H}(c, r, P_1, P_2)$ has the following properties for any $\boldsymbol{x}_1, \boldsymbol{x}_2 \in S$

$$\text{if } \|\boldsymbol{x}_1 - \boldsymbol{x}_2\| \leq r, \text{then } P_{h\in\mathcal{H}}(h(\boldsymbol{x}_1) = h(\boldsymbol{x}_2)) \geq P_1$$

similar objects should be hashed in the same bucket with high probability

$$\text{if } \|\boldsymbol{x}_1 - \boldsymbol{x}_2\| \geq cr, \text{then } P_{h\in\mathcal{H}}(h(\boldsymbol{x}_1) = h(\boldsymbol{x}_2)) \leq P_2$$

dissimilar objects should be hashed in the same bucket with low probability

Accelerate NN search: hashing

Binary vectors in Hamming space

objects: (1100101101)

Hamming distance: count the number of positions with different elements

$$\|110101001, 110001100\|_H = 3$$

Accelerate NN search: hashing

Binary vectors in Hamming space

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$$\|110101001, 110001100\|_H = 3$$

LSH functions: $\mathcal{H} = \{h_1, \ldots, h_n\}$ where $h_i(\boldsymbol{x}) = x_i$

	h_2	h_5	h_9
110101001	1	0	1
110010100	1	1	0
000110110	0	1	0
111001001	1	0	1
000011101	0	1	1

Accelerate NN search: hashing

Binary vectors in Hamming space

objects: (1100101101)
Hamming distance: count the number of positions with different elements

$$\|110101001, 110001100\|_H = 3$$

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	h_2	h_5	h_9
110101001	1	0	1
110010100	1	1	0
000110110	0	1	0
111001001	1	0	1
000011101	0	1	1

$$P(h_i(\boldsymbol{x}_1) = h_i(\boldsymbol{x}_2)) = 1 - \frac{\|\boldsymbol{x}_1 - \boldsymbol{x}_2\|}{d}$$

↑

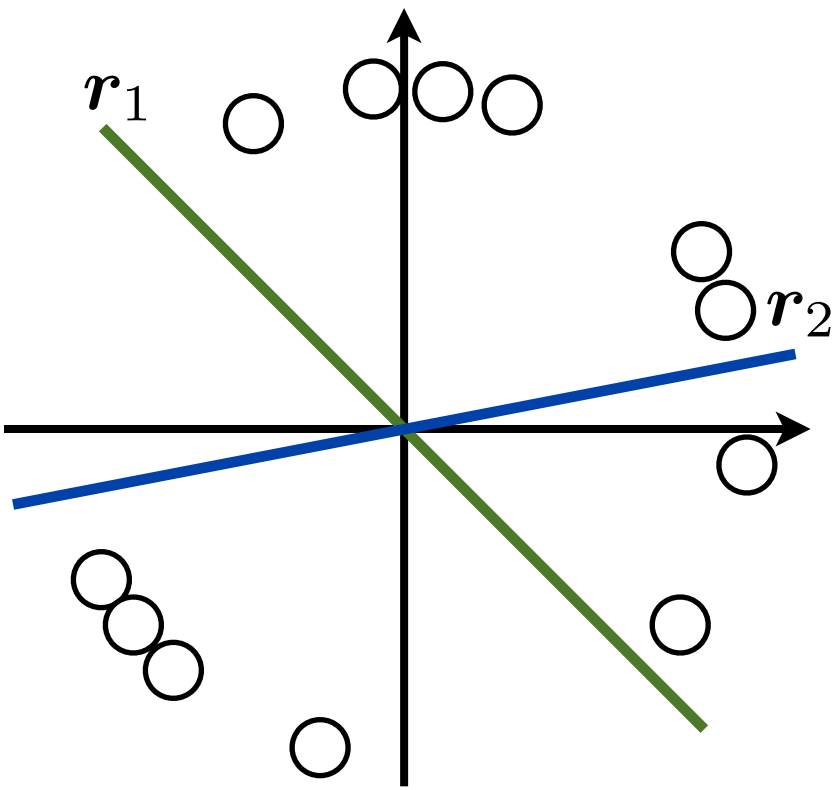
frequency in the same bucket for a sample of hashing functions

Accelerate NN search: hashing

Real vectors with angle similarity

$$\theta(\boldsymbol{x}_1, \boldsymbol{x}_2) = \arccos \frac{\boldsymbol{x}_1^\top \boldsymbol{x}_2}{\|\boldsymbol{x}_1\| \|\boldsymbol{x}_2\|}$$

LSH functions: $\mathcal{H} = \{h_{\boldsymbol{r}}\}(\boldsymbol{r} \in \mathbb{B}^n)$ where $h_r(\boldsymbol{x}) = \text{sign}(\boldsymbol{r}^\top \boldsymbol{x})$

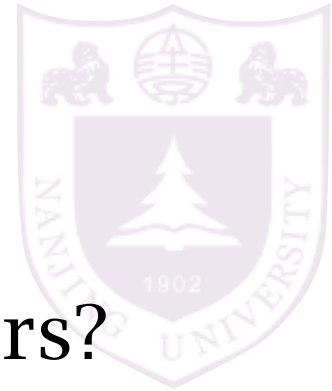


$$P(h_{\boldsymbol{r}}(\boldsymbol{x}_1) = h_{\boldsymbol{r}}(\boldsymbol{x}_2)) = 1 - \frac{\theta(\boldsymbol{x}_1, \boldsymbol{x}_2)}{\pi}$$

↑

frequency in the same bucket for a sample of hashing functions

Reduce the model complexity



What is the model complexity of NN classifiers?

How to make it simpler?

Reduce the model complexity

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How to make it simpler?

k-NN revisit:
1) build prototypes, which are exactly the training instances
2) find an class assignment of the prototypes to minimize the training error under *k*-NN

Reduce the model complexity

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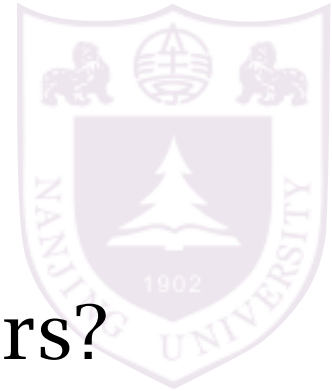
How to make it simpler?

k-NN revisit:
1) build prototypes, which are exactly the training instances
2) find an class assignment of the prototypes to minimize the training error under *k*-NN

model: data
hypothesis space: all class assignments

Reduce the model complexity



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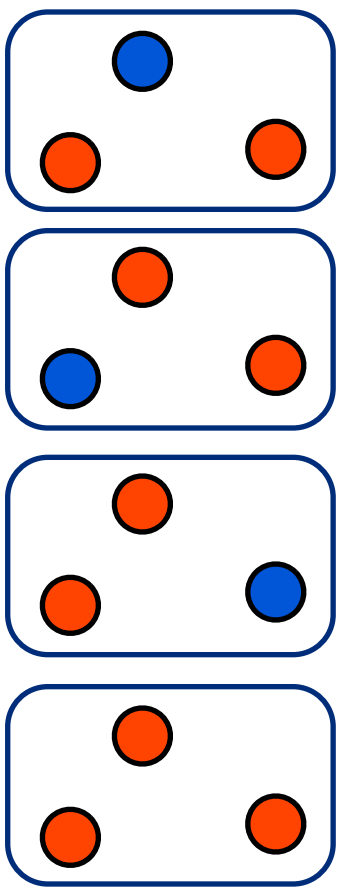

Reduce the model complexity

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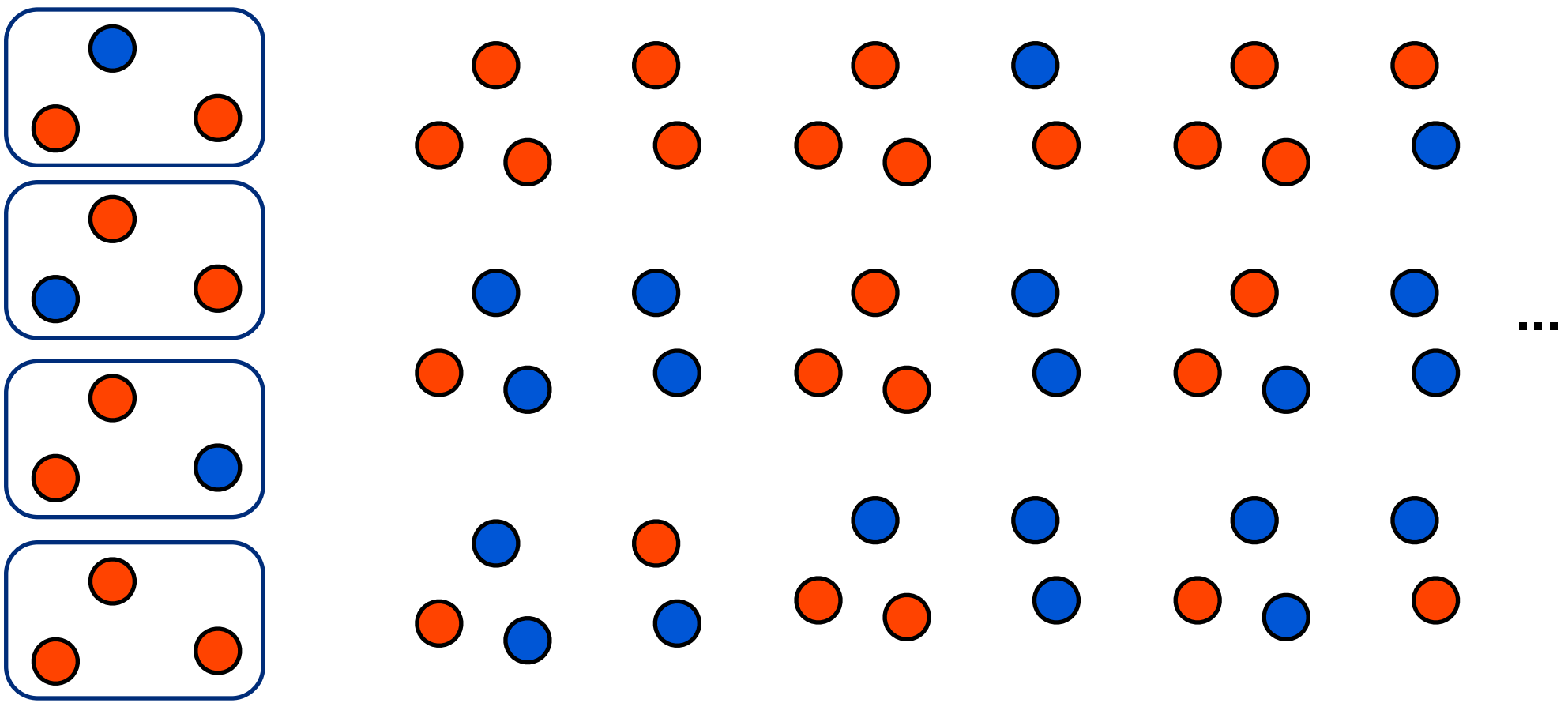

Data reduction

keep boundary examples only

Condensed kNN [Hart, TIT68]: iteratively record and remove a boundary example

Data reduction

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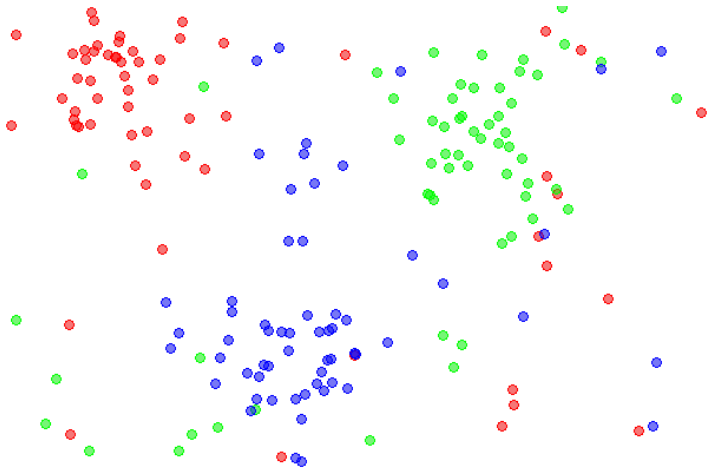

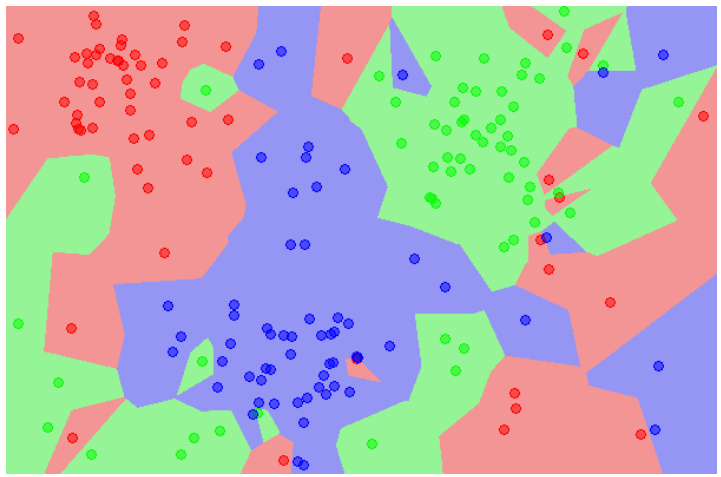

[images from http://en.wikipedia.org/wiki/K-nearest_neighbors_algorithm]

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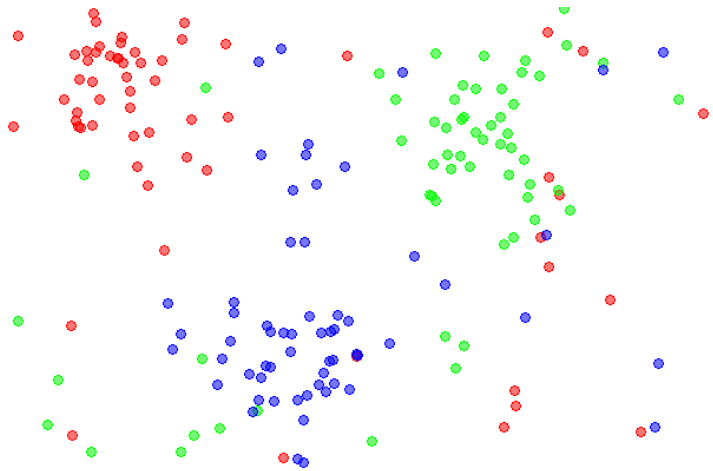

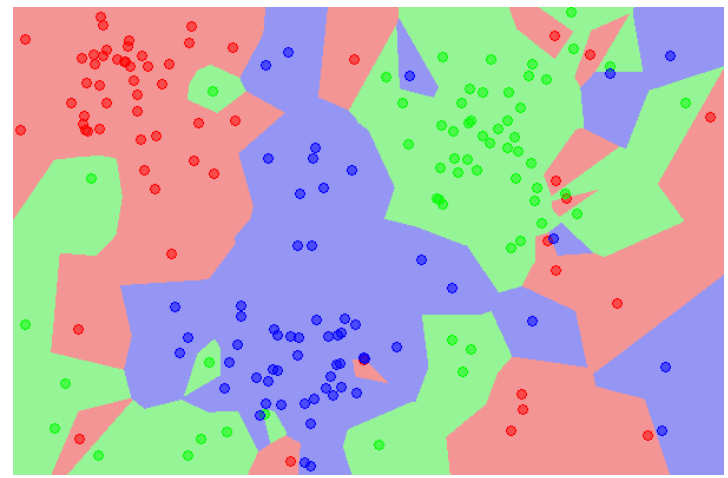

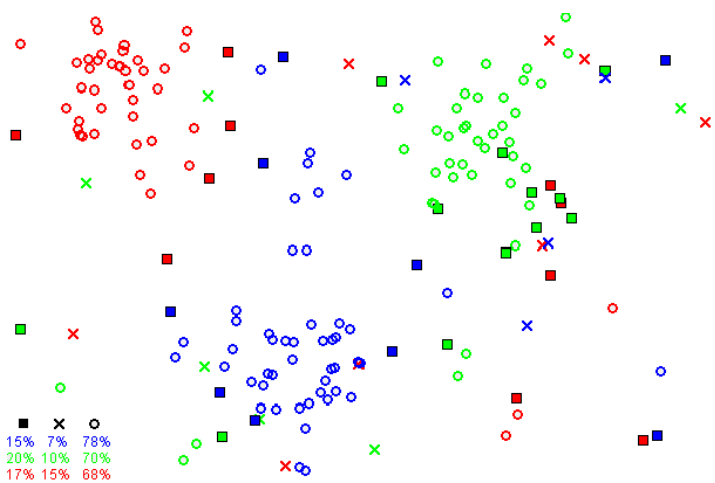

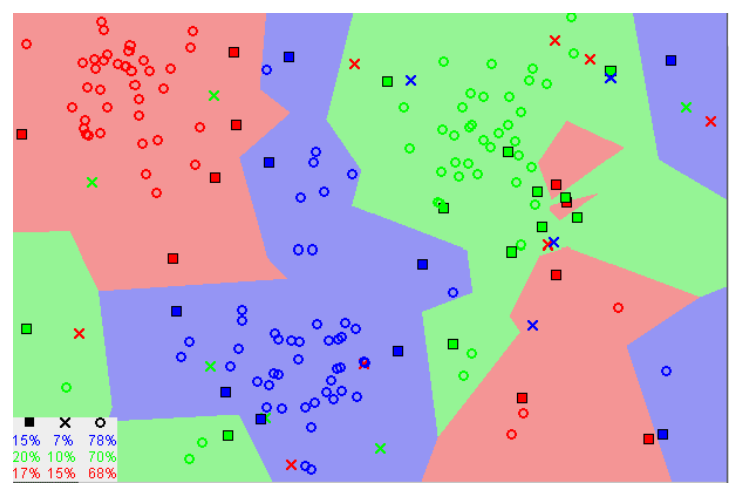

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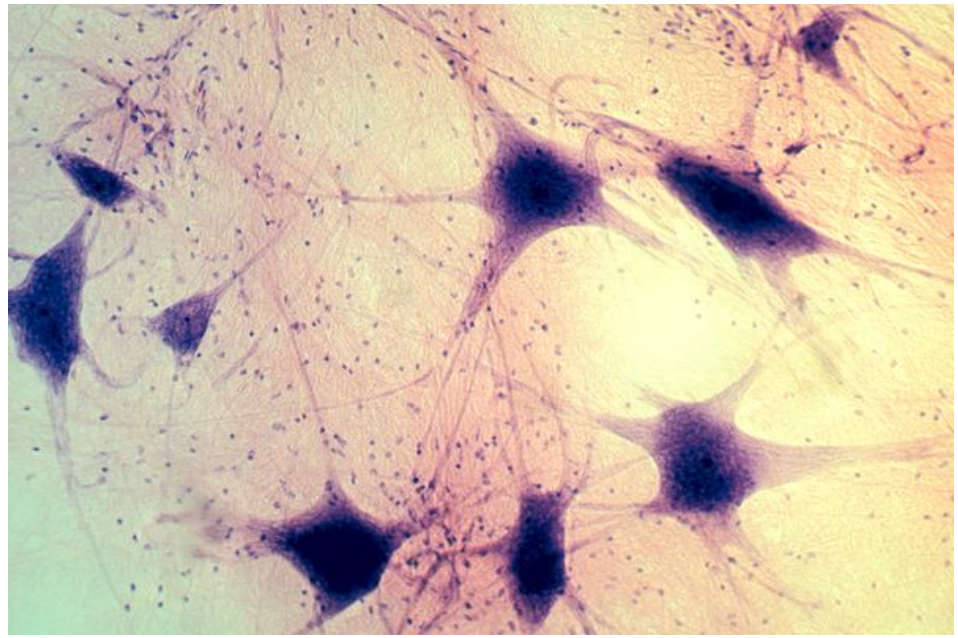
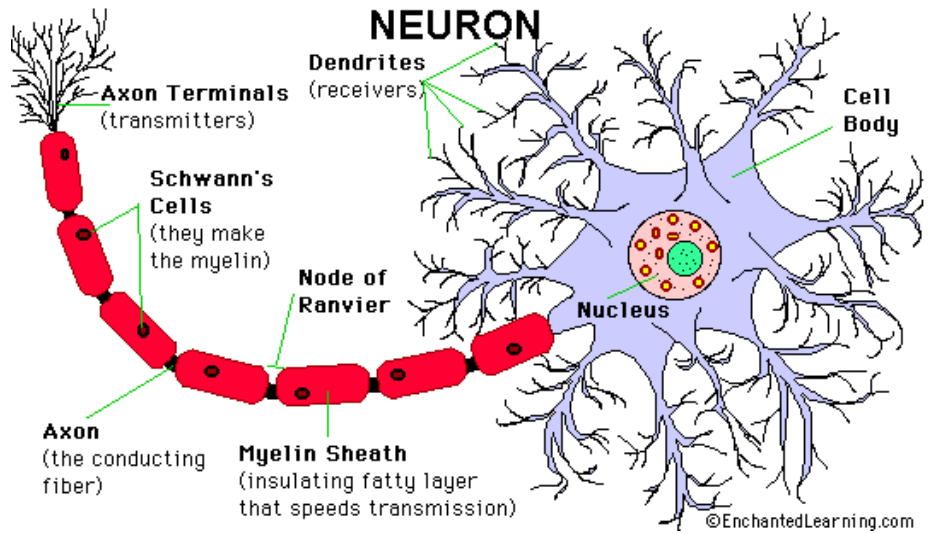
Neural networks





Neuron / perceptron

output a function of sum of input

linear function:

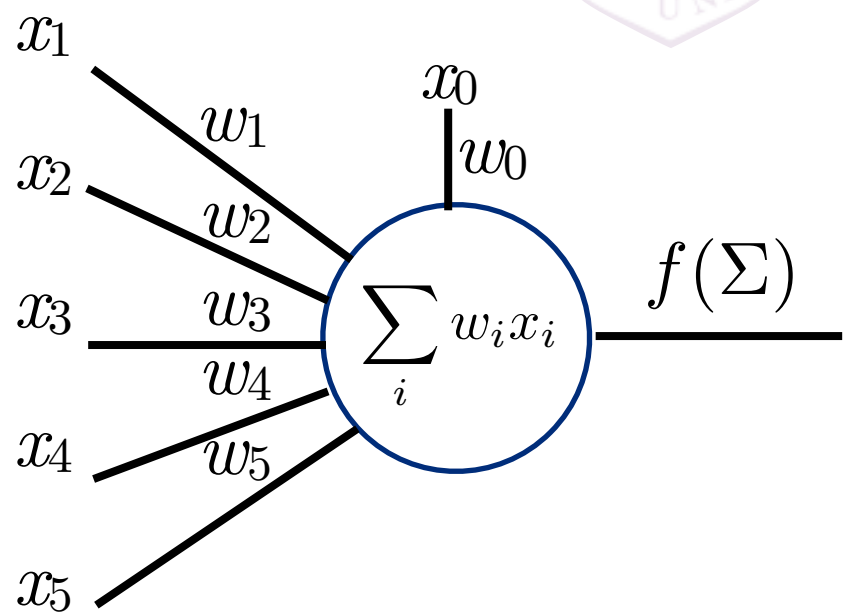
$$f(\sum_i w_i x_i) = \sum_i w_i x_i$$

threshold function:

$$f(\sum_i w_i x_i) = I(\sum_i w_i x_i > 0)$$

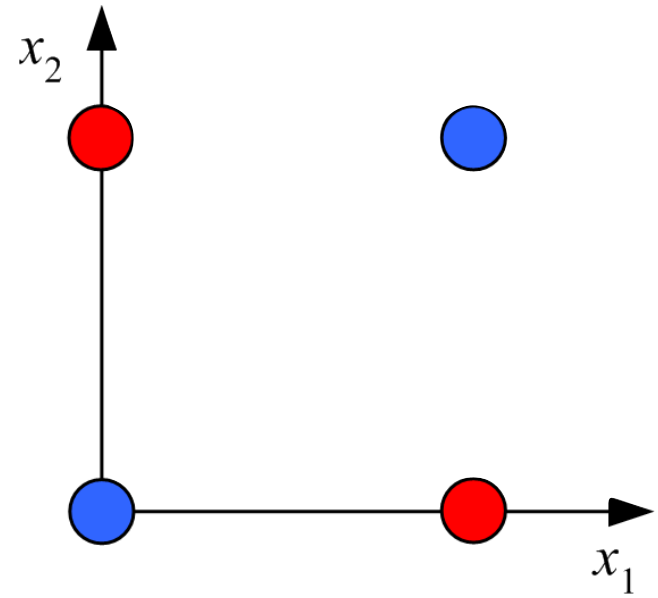
sigmoid function:

$$f(\sum_i w_i x_i) = \frac{1}{1 + e^{-\Sigma}}$$



Limitation of single neuron

x_1	x_2	r
0	0	0
0	1	1
1	0	1
1	1	0



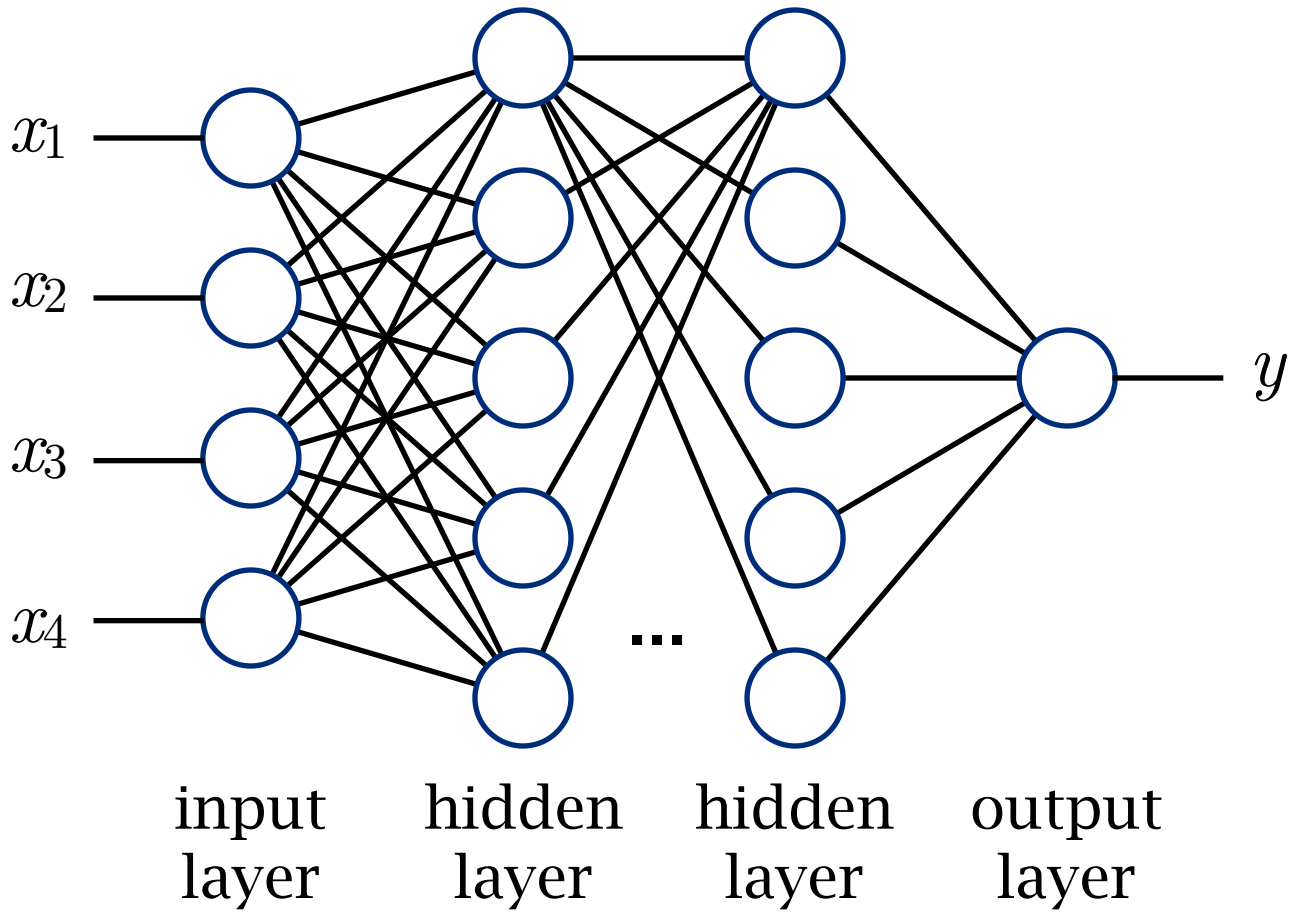
[Minsky and Papert, *Perceptrons,* 1969]

Marvin Minsky
Turing Award 1969

AI Winter

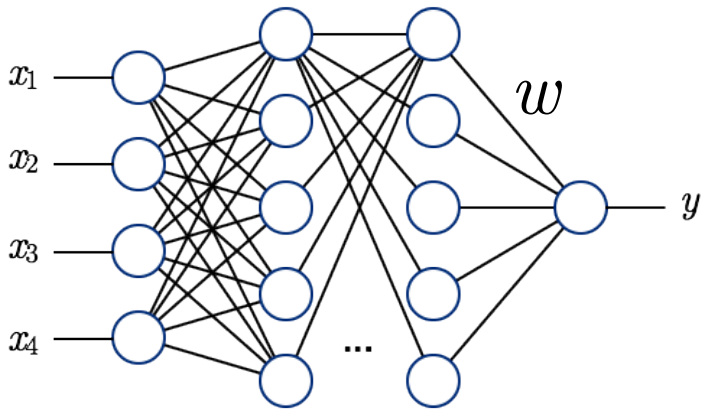
Multi-layer perceptrons

feed-forward network



sigmoid network with one hidden layer can approximate arbitrary function [Cybenko 1989]

Back-propagation algorithm



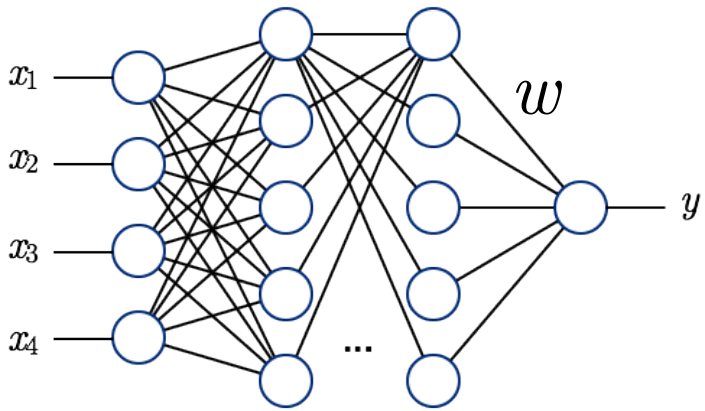
$$\hat{y} = F(\boldsymbol{x}) \quad f(\sum_i w_i x_i) = \frac{1}{1+e^{-\Sigma}}$$

gradient descent

error: $E(\boldsymbol{w}) = (F(\boldsymbol{x}) - y)^2$

[Rumelhart, Hinton, Williams. Nature 1986]

Back-propagation algorithm



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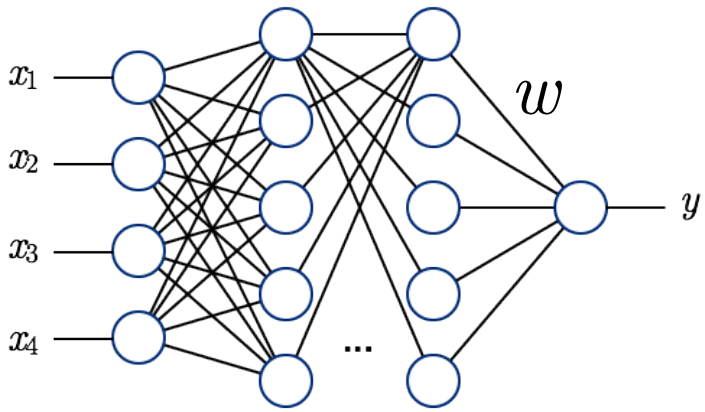
error: $E(\boldsymbol{w}) = (F(\boldsymbol{x}) - y)^2$

update one weight: $\Delta w_{i,j} = -\eta \frac{\partial E(\boldsymbol{w})}{\partial w_{i,j}}$

[Rumelhart, Hinton, Williams. Nature 1986]

Back-propagation algorithm



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update one weight: $\Delta w_{i,j} = -\eta \frac{\partial E(\boldsymbol{w})}{\partial w_{i,j}}$

weight of the laster layer

$$\frac{\partial E(\boldsymbol{w})}{\partial w_{i,j}} = \frac{\partial E(\boldsymbol{w})}{\partial F(\boldsymbol{x})} \frac{\partial F(\boldsymbol{x})}{\partial w_{i,j}}$$

[Rumelhart, Hinton, Williams. Nature 1986]

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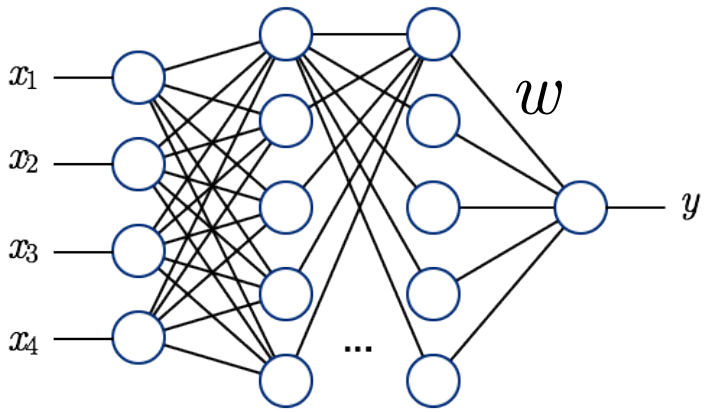

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weight of the laster layer

$$\frac{\partial E(\boldsymbol{w})}{\partial w_{i,j}} = \frac{\partial E(\boldsymbol{w})}{\partial F(\boldsymbol{x})} \frac{\partial F(\boldsymbol{x})}{\partial w_{i,j}}$$

weight of the first layer

$$\frac{\partial E(\boldsymbol{w})}{\partial w_{i,j}} = \frac{\partial E(\boldsymbol{w})}{\partial F(\boldsymbol{x})} \frac{\partial F(\boldsymbol{x})}{\partial \mathrm{HL2}} \frac{\partial \mathrm{HL2}}{\partial \mathrm{HL1}} \frac{\partial \mathrm{HL1}}{\partial w_{i,j}}$$

[Rumelhart, Hinton, Williams. Nature 1986]

Back-propagation algorithm

For each given training example (**x**, **y**), **do**

1. Input the instance **x** to the NN and compute the output value o_u of every output unit u of the network

2. **For each** network output unit k, calculate its error term δ_k

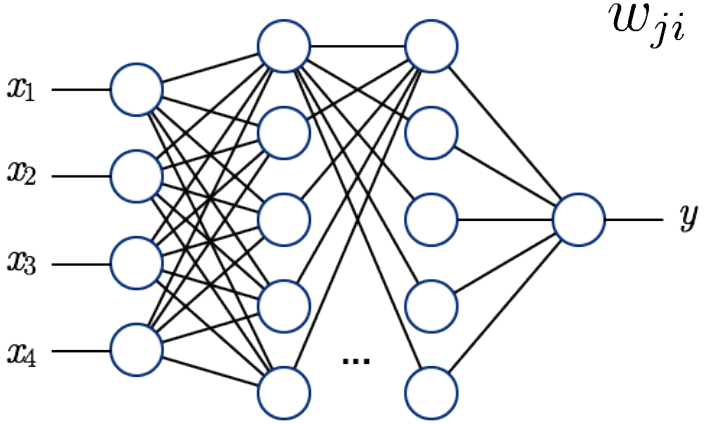
$$\delta_k \leftarrow o_k(1-o_k)(y_k-o_k)$$

3. **For each** hidden unit k, calculate its error term δ_h

$$\delta_h \leftarrow o_k(1-o_k)\sum_{k\in outputs} w_{kh}\delta_k$$

4. Update each network weight w_{ji} which is the weight associated with the i-th input value to the unit j

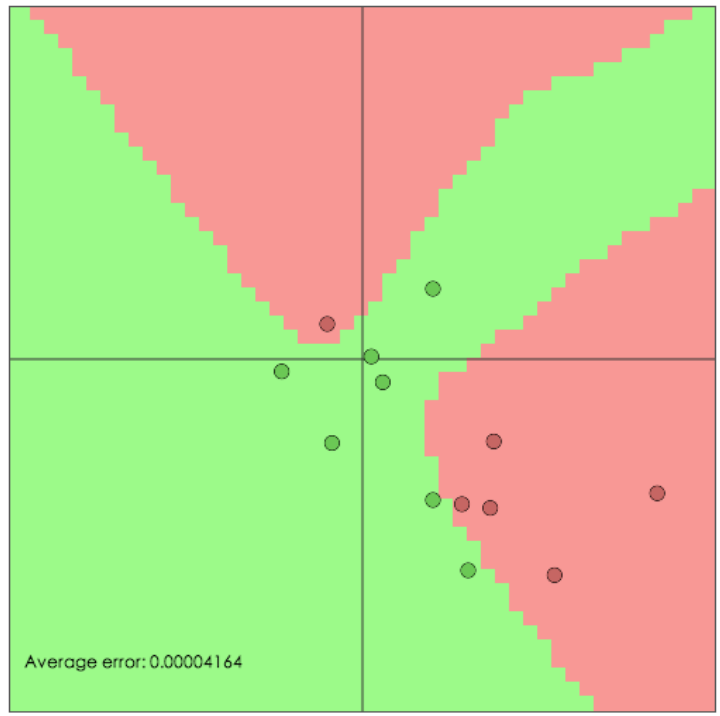
$$w_{ji} \leftarrow w_{ji} + \eta\delta_j x_{ji}$$



[Rumelhart, Hinton, Williams. Nature 1986]

Advantage and disadvantages

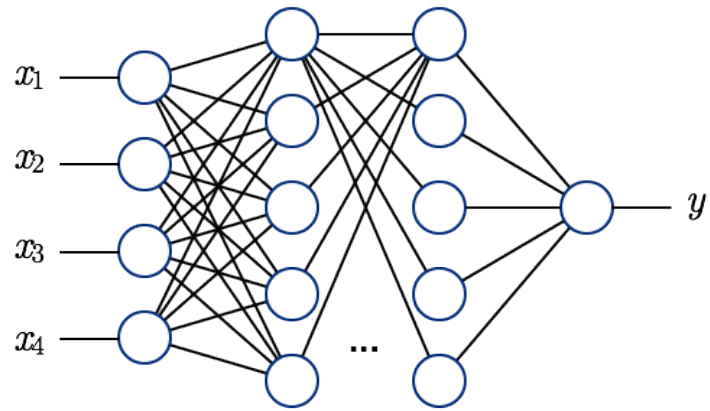
Smooth and nonlinear decision boundary



Slow convergence

Many local optima

Best network structure unknown



Hard to handle nominal features

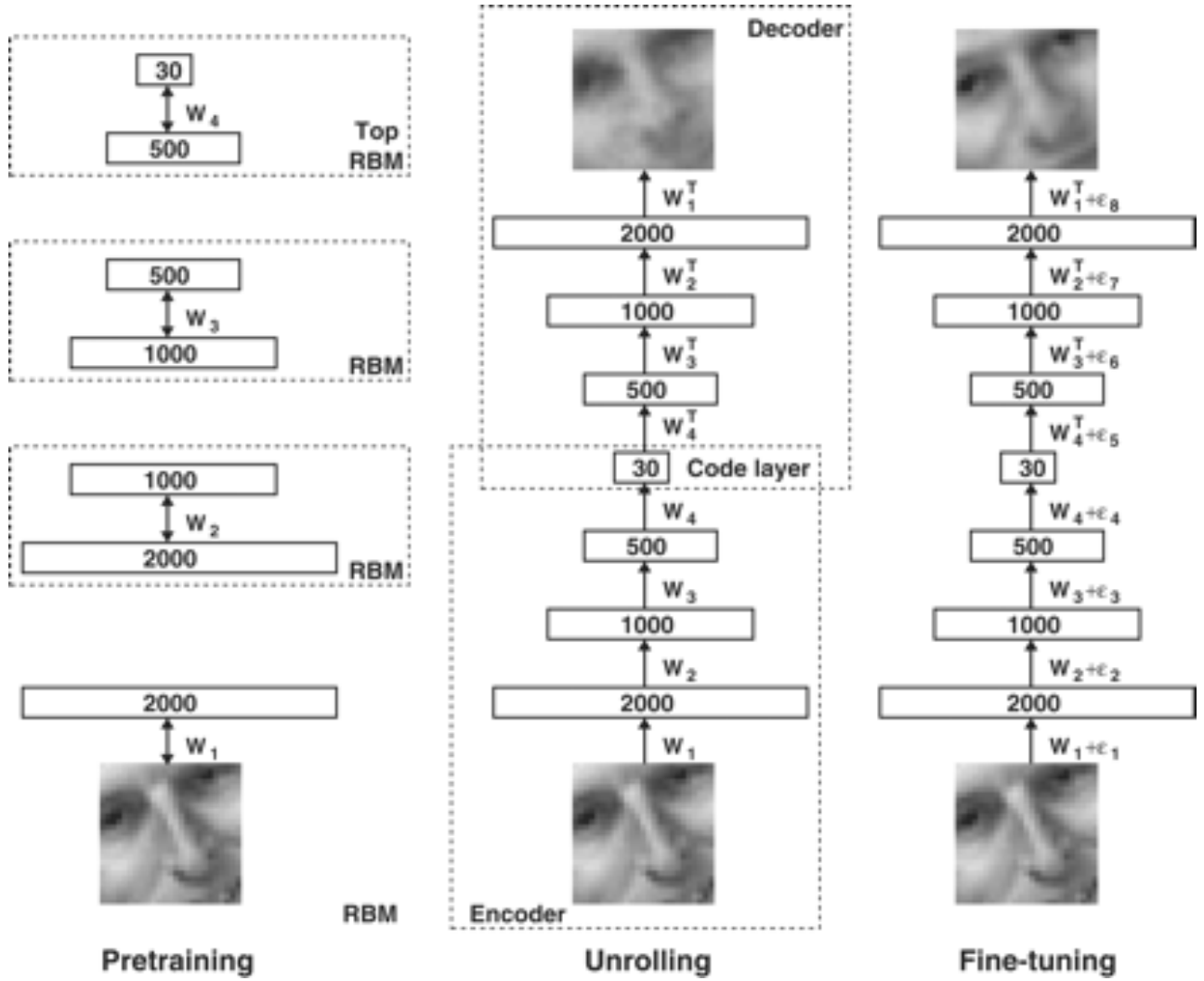
Complexity of networks

The number of free variables?

Leave to “linear models”

Deep network

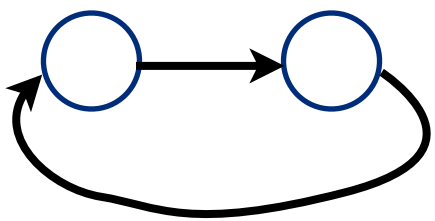
autoencoder:

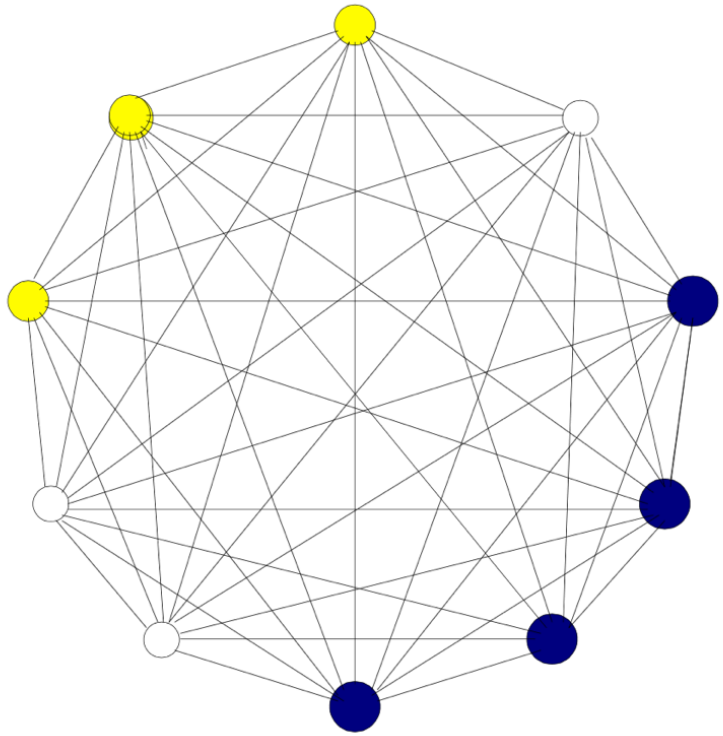


[Hinton and Salakhutdinov, Science 2006]

Hopfield networks

a fully connected recursive network





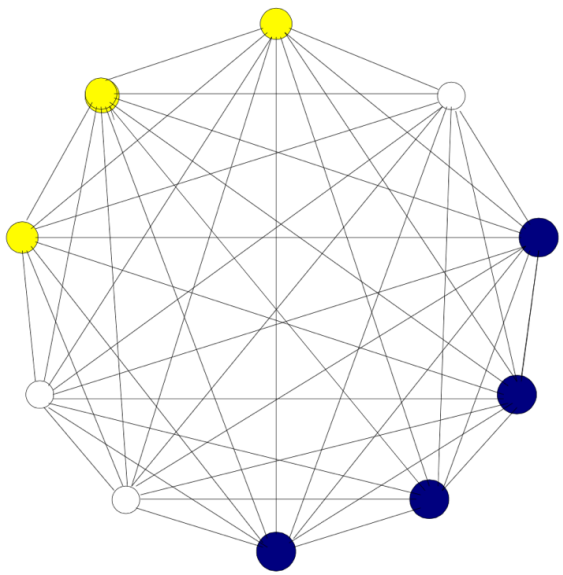
Hopfield networks

run:

1) set the input value of blue nodes

2) run the network

3) read the output from the yellow nodes



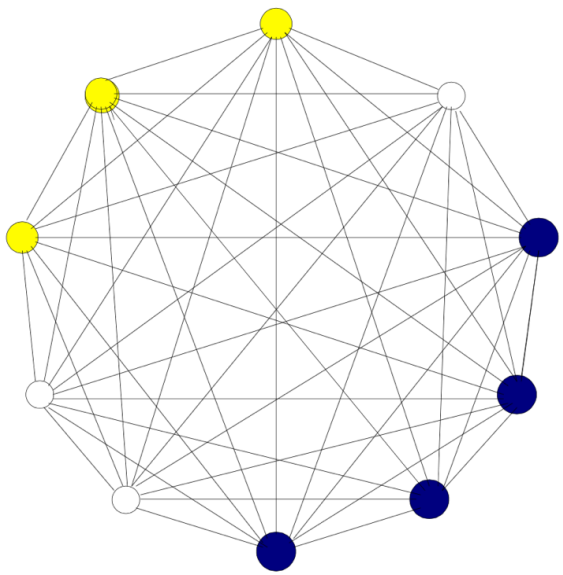
Hopfield networks

train:

set the input and the output the same pattern

associative rule:

$$w_{ij} = \frac{1}{N} x_i x_j$$



习题

多层神经网络为何能实现非线性分类?

BP算法能否收敛到全局最优解?

k近邻分类算法是否需要训练预测模型?