CS4442/9542b
Artificial Intelligence II
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Lecture 3

Machine Learning

K Nearest Neighbor Classifier

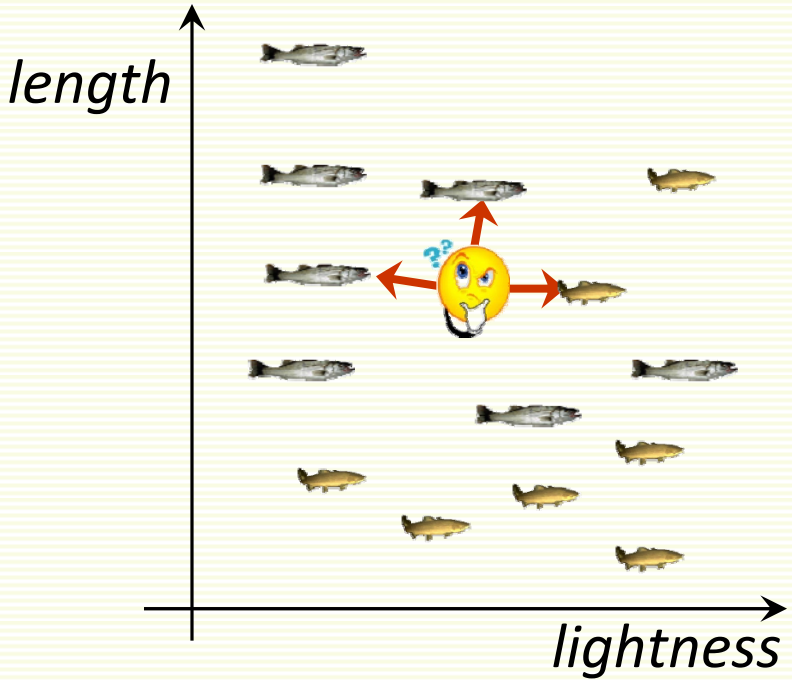
Today

- kNN classifier - the simplest classifier on earth
- matlab implementation of kNN

k-Nearest Neighbors

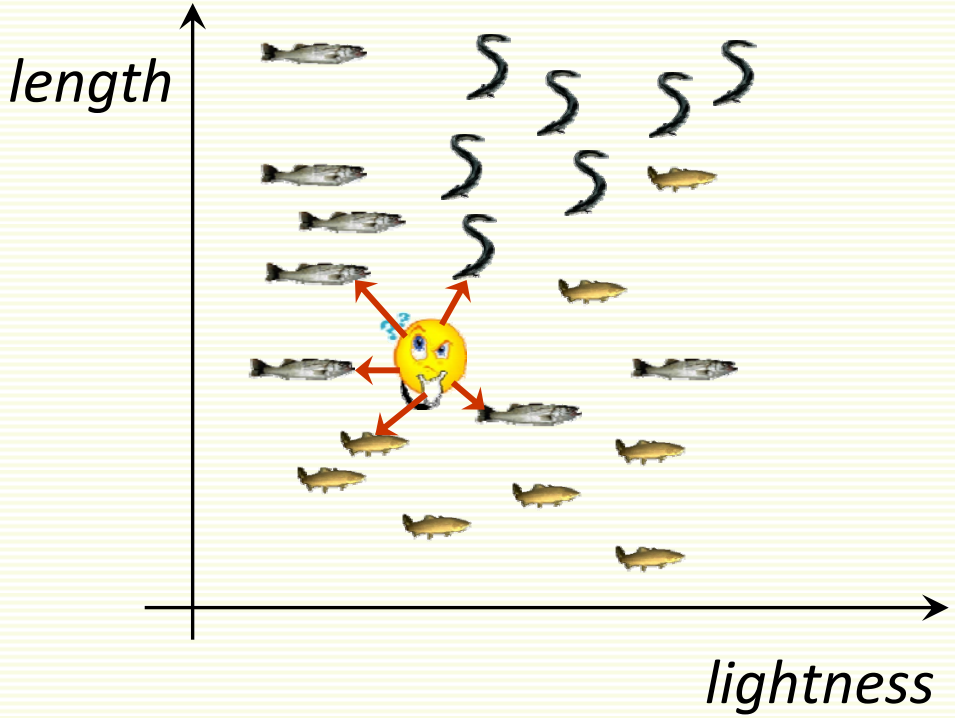
- classify an unknown example with the most common class among ***k*** closest examples
  - *"tell me who your neighbors are, and I'll tell you who you are"*

- Example:
  - ***k*** = 3
  - 2 sea bass, 1 salmon
  - Classify as sea bass



kNN: Multiple Classes

- Easy to implement for multiple classes
- Example for ***k*** = 5
  - 3 fish species: salmon, sea bass, eel
  - 3 sea bass, 1 eel, 1 salmon ⇒ classify as sea bass



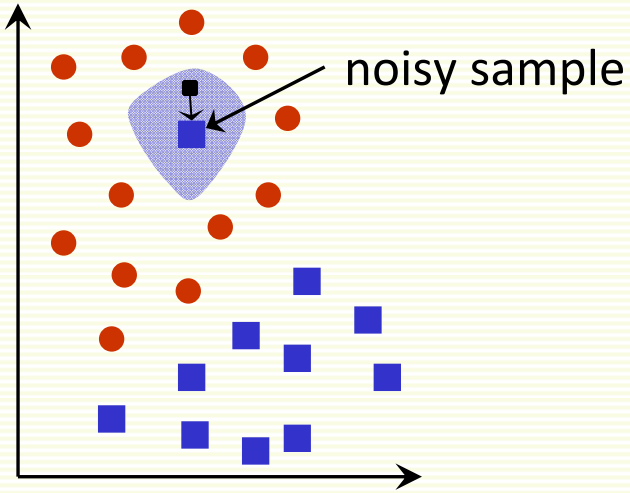
kNN: How to Choose k?

- In theory, if infinite number of samples available, the larger is ***k***, the better is classification
- But the caveat is that all ***k*** neighbors have to be close
  - Possible when infinite # samples available
  - Impossible in practice since # samples is finite

kNN: How to Choose k?

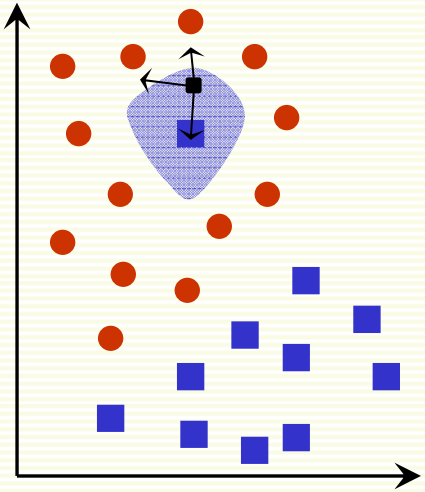
- Rule of thumb is ***k*** = sqrt(***n***), ***n*** is number of examples
  - interesting theoretical properties
- In practice, ***k*** = 1 is often used for efficiency, but can be sensitive to "noise"

1 NN



every example in the blue shaded area will be misclassified as the blue class

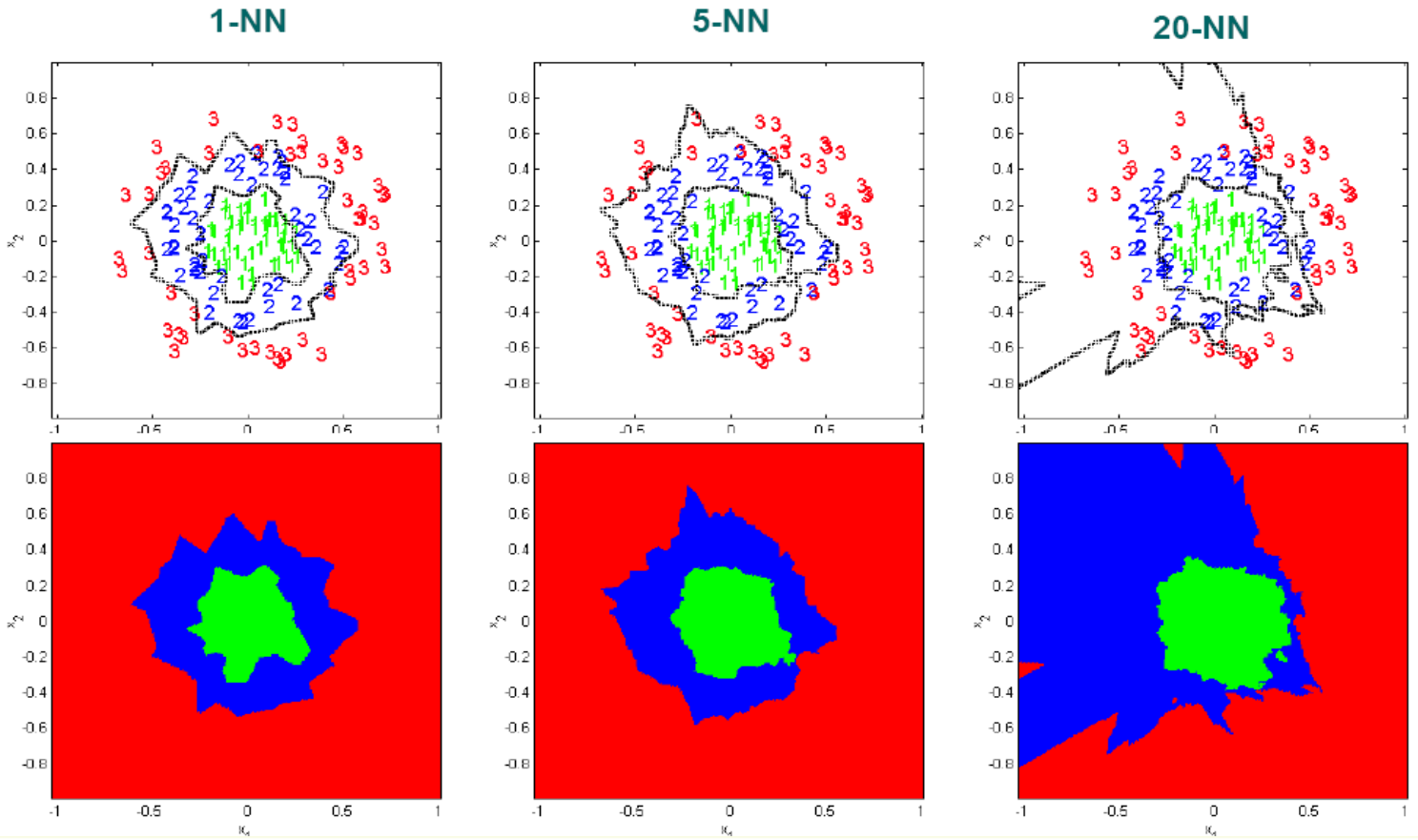
3 NN



every example in the blue shaded area will be classified correctly as the red class

kNN: How to Choose k?

- larger ***k*** may improve performance, but too large ***k*** destroys *locality*, i.e. end up looking at samples that are not neighbors
- cross-validation (study later) may be used to choose ***k***



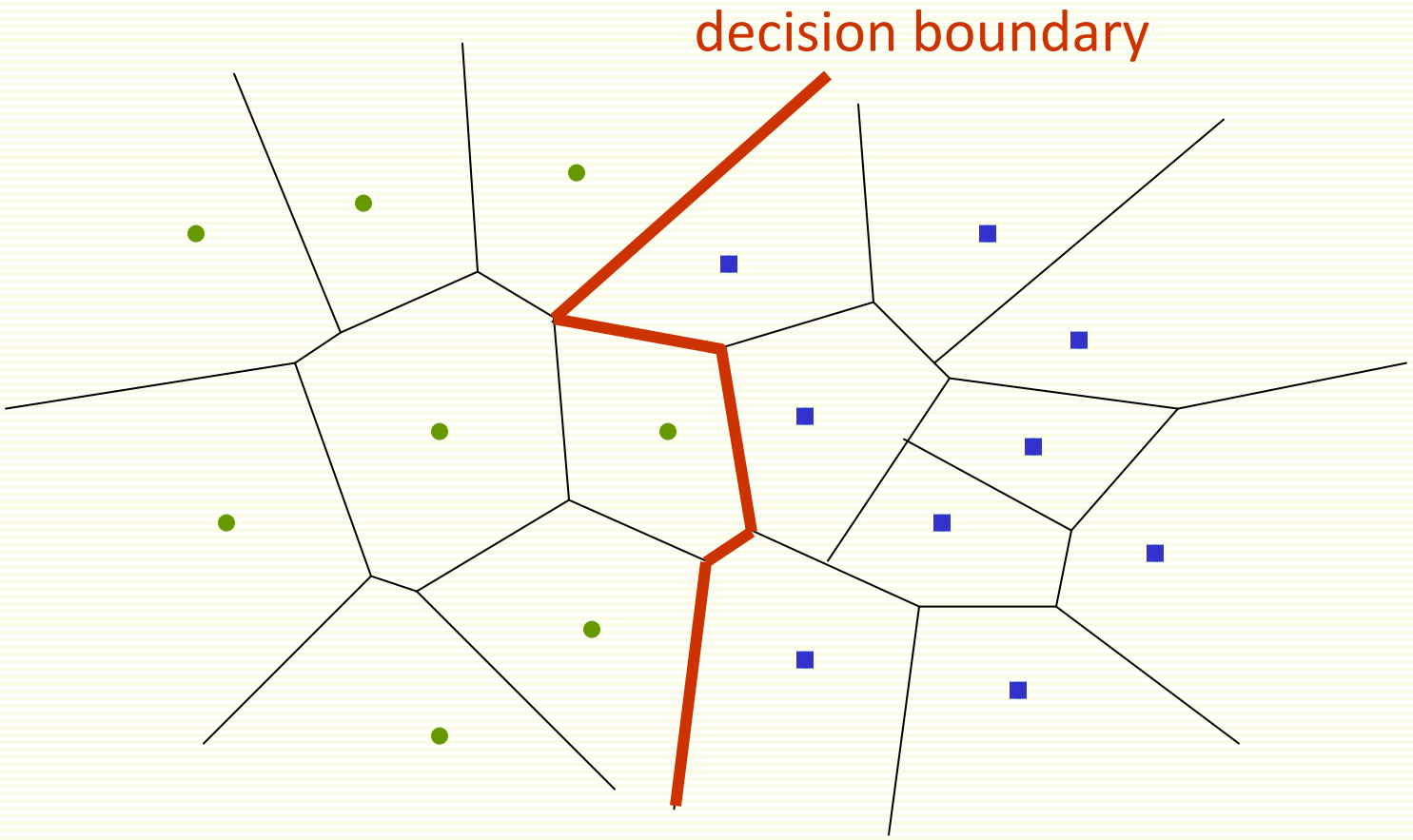
picture from R. Gutierrez-Osuna

kNN: How Well does it Work?

- kNN is simple and intuitive, but does it work?
- Theoretically, the best error rate is the Bayes rate ***E****
  - Bayes error rate is the best (smallest) error rate a classifier can have, for a given problem, but we do not study it in this course
- Assume we have an unlimited number of samples
- kNN leads to an error rate greater than ***E****
- But even for ***k*** =1, as $n \to \infty$, it can be shown that kNN error rate is smaller than ***2E****
- As we increase ***k***, the upper bound on the error gets better, that is the error rate (as $n \to \infty$) for the ***kNN*** rule is smaller than ***cE****,with smaller ***c*** for larger ***k***
- **If we have lots of samples, kNN works well**

1NN Visualization

- Voronoi tesselation is useful for visualization



kNN Selection of Distance

- So far we assumed we use Euclidian Distance to find the nearest neighbor:

$$D(a,b) = \sqrt{\sum_k \left(a_k - b_k\right)^2} = \sqrt{a \cdot b}$$

- Euclidean distance treats each feature as equally important
- However some features (dimensions) may be much more discriminative than other features

kNN Distance Selection: Extreme Example

- feature 1 gives the correct class: 1 or 2
- feature 2 gives irrelevant number from 100 to 200
- dataset: **[1 150]**

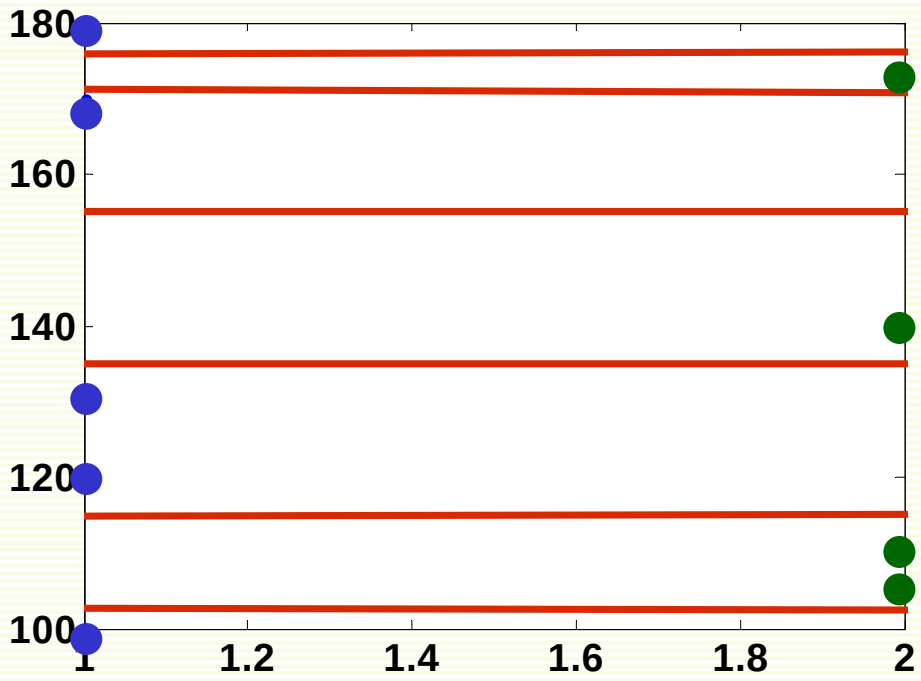
  [2 110]
- classify **[1 100]**

$$D\left(\begin{bmatrix}1\\100\end{bmatrix},\begin{bmatrix}1\\150\end{bmatrix}\right)=\sqrt{(1-1)^2+(100-150)^2}=50$$

$$D\left(\begin{bmatrix}1\\100\end{bmatrix},\begin{bmatrix}2\\110\end{bmatrix}\right)=\sqrt{(1-2)^2+(100-110)^2}=10.5$$

- **[1 100]** is misclassified!
- The denser the samples, the less of this problem
- But we rarely have samples dense enough

kNN Distance Selection: Extreme Example



- Decision boundary is in red, and is really wrong because
  - feature 1 is discriminative, but it's scale is small
  - feature 2 gives no class information but its scale is large, it dominates distance calculation

kNN: Feature Normalization

- Notice that 2 features are on different scales:
- First feature takes values between 1 or 2
- Second feature takes values between 100 to 200
- **Idea:** normalize features to be on the same scale
- Different normalization approaches
- Linearly scale the range of each feature to be, say, in range [0,1]

$$f_{new} = \frac{f_{old} - f_{old}^{\min}}{f_{old}^{\max} - f_{old}^{\min}}$$

kNN: Feature Normalization

- Linearly scale to **0** mean variance **1**:
- If Z is a random variable of mean m and variance σ^2, then $(Z - m)/\sigma$ has mean **0** and variance **1**
- For each feature f let the new rescaled feature be

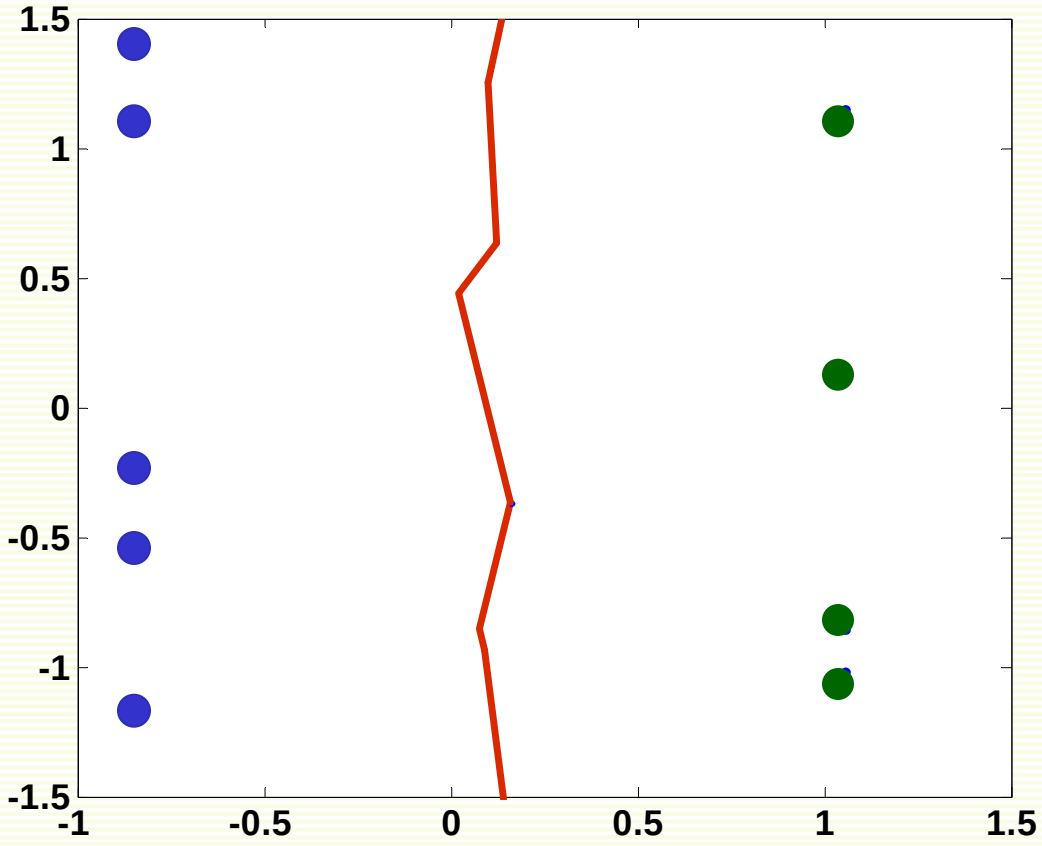
$$f_{new} = \frac{f_{old} - \mu}{\sigma}$$

- C is a matrix with all samples stored as rows, in Matlab can normalize all features simultaneously:

C_{new}=(C-repmat(mean(C),size(C,1),1))*diag(1./std(C))

- Let us apply this normalization to previous example

kNN: Feature Normalization



kNN: Selection of Distance

- Feature normalization does not help in high dimensional spaces if most features are irrelevant

$$D(a,b) = \sqrt{\sum_k (a_k - b_k)^2} = \sqrt{\underbrace{\sum_i (a_i - b_i)^2}_{\text{discriminative features}} + \underbrace{\sum_j (a_j - b_j)^2}_{\text{noisy features}}}$$

- If the number of useful features is smaller than the number of noisy features, Euclidean distance is dominated by noise

kNN: Feature Weighting

- Scale each feature by its importance for classification

$$D(a,b) = \sqrt{\sum_k w_k \left(a_k - b_k\right)^2}$$

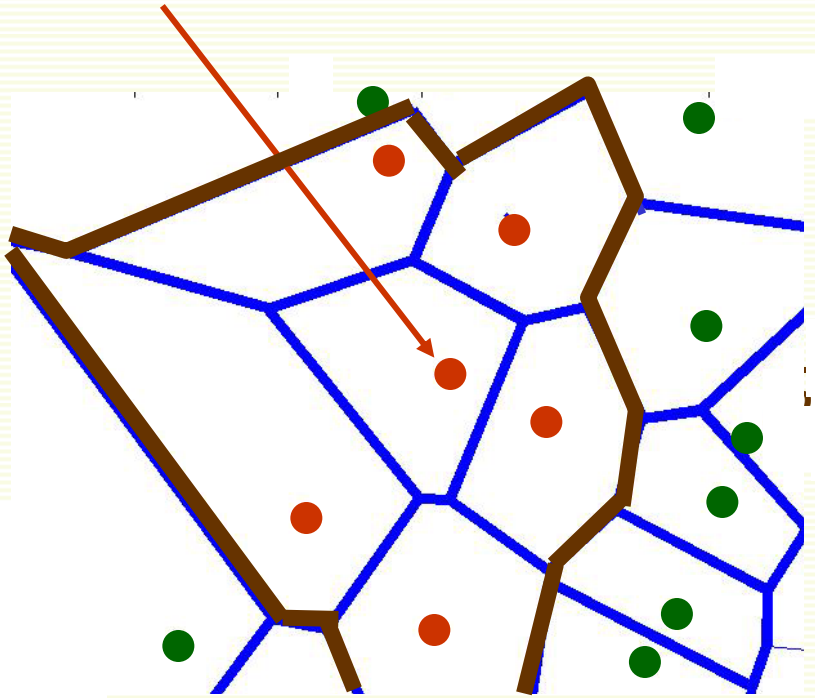
- Can use our prior knowledge about which features are more important
- Can learn the weights $\mathbf{w_k}$ using cross-validation (to be covered later)

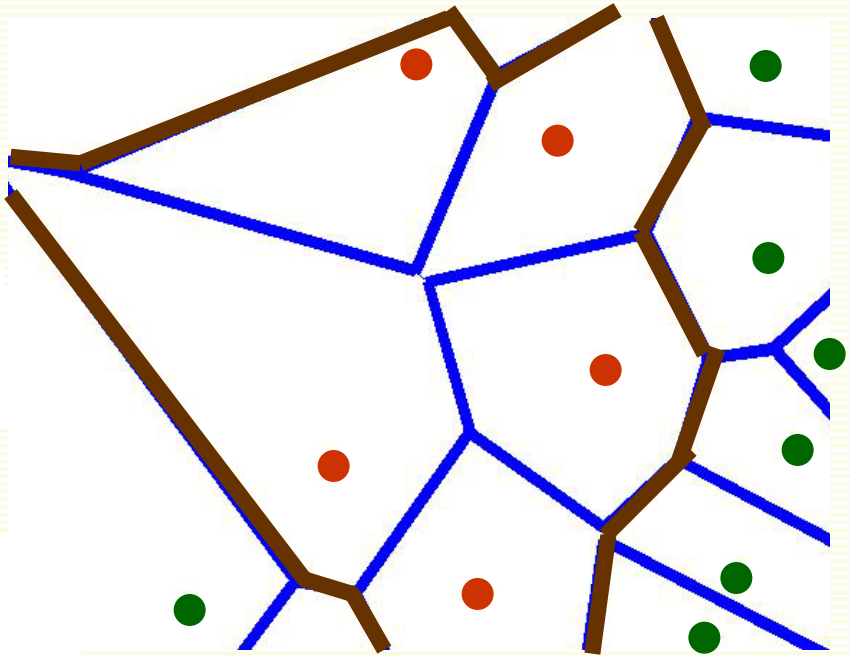
kNN: Computational Complexity

- Basic kNN algorithm stores all examples
- Suppose we have **n** examples each of dimension **d**
- **O(d)** to compute distance to one example
- **O(nd)** to find one nearest neighbor
- **O(knd)** to find **k** closest examples examples
- Thus total complexity is **O(knd)**
- Very expensive for a large number of samples
- But we need a large number of samples for kNN to work well!

Reducing Complexity: editing 1NN

- If all Voronoi neighbors have the same class, a sample is useless, remove it





- Number of samples decreases
- Decision boundary does not change

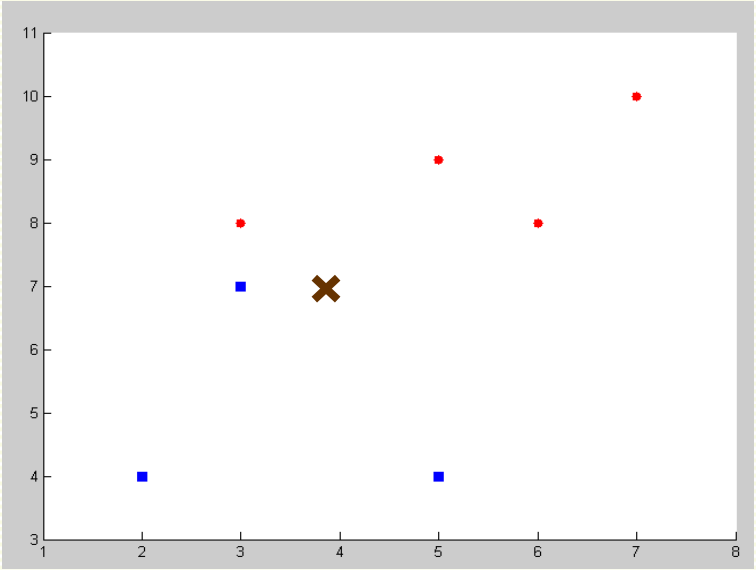
Reducing Complexity: Partial Distance

- Have current ***k*** closes samples
- Abort distance computation if partial distance is already greater than the full distance to the current ***k*** closest samples
- Advantages:
  - complexity decreases
  - we are guaranteed to find closes neighbor(s)
- Disadvantages:
  - how much complexity decreases depends on our luck and data layout

kNN in Matlab

$$\textbf{class1} = \begin{bmatrix} 2 & 4 \\ 3 & 7 \\ 5 & 4 \end{bmatrix}$$

$$\textbf{class2} = \begin{bmatrix} 3 & 8 \\ 5 & 9 \\ 7 & 10 \\ 6 & 8 \end{bmatrix}$$



- Want to classify $\mathbf{x} = \begin{bmatrix} 4 \\ 7 \end{bmatrix}$

kNN in Matlab without Loops

```
numClass1     = size(Class1,1);
numClass2     = size(Class2,1);
totalSamples  = numClass1+numClass2;

combinedSamples = [Class1;Class2];
trueClass = [zeros(numClass1,1)+1;zeros(numClass2,1)+2;];

testMatrix = repmat(newSample,totalSamples,1);
absDiff      = abs(combinedSamples-testMatrix);
absDiff      = absDiff.^2;
dist         = sum(absDiff,2);

[Y,I]              = sort(dist);
neighborsInd  = I(1:k);
neighbors       = trueClass(neighborsInd);

class1   = find(neighbors == 1);
class2   = find(neighbors == 2);
joint    = [size(class1,1);size(class2,1)];

[value class] = max(joint);
```

$$\mathbf{class1} = \begin{bmatrix} 2 & 4 \\ 3 & 7 \\ 5 & 4 \end{bmatrix}$$

$$\mathbf{class2} = \begin{bmatrix} 3 & 8 \\ 5 & 9 \\ 7 & 10 \\ 6 & 8 \end{bmatrix}$$

$$\mathbf{x} = \begin{bmatrix} 4 \\ 7 \end{bmatrix}$$

$$k = 3$$

kNN in Matlab

```
numClass1    = size(Class1,1);
numClass2    = size(Class2,1);
totalSamples = numClass1+numClass2;

combinedSamples = [Class1;Class2];
trueClass = [zeros(numClass1,1)+1;zeros(numClass2,1)+2;];
```

$$\mathbf{class1} = \begin{bmatrix} 2 & 4 \\ 3 & 7 \\ 5 & 4 \end{bmatrix}$$

$$\mathbf{class2} = \begin{bmatrix} 3 & 8 \\ 5 & 9 \\ 7 & 10 \\ 6 & 8 \end{bmatrix}$$

$$\mathbf{x} = \begin{bmatrix} 4 \\ 7 \end{bmatrix}$$

numClass1 = 3

numClass2 = 4

totalSamples = 7

$$combinedSamples = \begin{bmatrix} 2 & 4 \\ 3 & 7 \\ 5 & 4 \\ 3 & 8 \\ 5 & 9 \\ 7 & 10 \\ 6 & 8 \end{bmatrix} \qquad trueClass = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 2 \\ 2 \\ 2 \\ 2 \end{bmatrix}$$

kNN in Matlab

```
testMatrix = repmat(newSample,totalSamples,1);
absDiff    = abs(combinedSamples-testMatrix);
absDiff    = absDiff.^2;
dist       = sum(absDiff,2);
```

$$\mathbf{x} = \begin{bmatrix} 4 \\ 7 \end{bmatrix}$$

$$testMatrix = \begin{bmatrix} 4 & 7 \\ 4 & 7 \\ 4 & 7 \\ 4 & 7 \\ 4 & 7 \\ 4 & 7 \\ 4 & 7 \end{bmatrix} \qquad absDiff = \begin{bmatrix} 2 & 3 \\ 1 & 0 \\ 1 & 3 \\ 1 & 1 \\ 1 & 2 \\ 3 & 3 \\ 2 & 1 \end{bmatrix}$$

$$combinedSamples = \begin{bmatrix} 2 & 4 \\ 3 & 7 \\ 5 & 4 \\ 3 & 8 \\ 5 & 9 \\ 7 & 10 \\ 6 & 8 \end{bmatrix}$$

$$absDiff = \begin{bmatrix} 4 & 9 \\ 1 & 0 \\ 1 & 9 \\ 1 & 1 \\ 1 & 4 \\ 9 & 9 \\ 4 & 1 \end{bmatrix} \qquad dist = \begin{bmatrix} 13 \\ 1 \\ 10 \\ 2 \\ 5 \\ 18 \\ 5 \end{bmatrix}$$

$$trueClass = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 2 \\ 2 \\ 2 \\ 2 \end{bmatrix}$$

kNN in Matlab

```
[Y,I]          = sort(dist);
neighborsInd   = I(1:k);
neighbors      = trueClass(neighborsInd);
```

$$dist = \begin{bmatrix} 13 \\ 1 \\ 10 \\ 2 \\ 5 \\ 18 \\ 5 \end{bmatrix}$$

$$Y = \begin{bmatrix} 1 \\ 2 \\ 5 \\ 5 \\ 10 \\ 13 \\ 18 \end{bmatrix} \qquad I = \begin{bmatrix} 2 \\ 4 \\ 5 \\ 7 \\ 3 \\ 1 \\ 6 \end{bmatrix}$$

$$trueClass = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 2 \\ 2 \\ 2 \\ 2 \end{bmatrix}$$

$$neighborsInd = \begin{bmatrix} 2 \\ 4 \\ 5 \end{bmatrix} \qquad neighbors = \begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix}$$

$$k = 3$$

kNN in Matlab

```
class1  = find(neighbors == 1);
class2  = find(neighbors == 2);
joint   = [size(class1,1);size(class2,1)];

[value class] = max(joint);
```

$$neighbors = \begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix}$$

$$class1 = \begin{bmatrix} 1 \end{bmatrix}$$

$$class2 = \begin{bmatrix} 2 \\ 3 \end{bmatrix}$$

$$joint = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$$

$$class = 2$$

kNN in Matlab

Video

- http://videolectures.net/aaai07_bosch_knnc/

kNN Summary

- Advantages
  - Can be applied to the data from any distribution
    - for example, data does not have to be separable with a linear boundary
  - Very simple and intuitive
  - Good classification if the number of samples is large enough
- Disadvantages
  - Choosing ***k*** may be tricky
  - Test stage is computationally expensive
    - No training stage, all the work is done during the test stage
    - This is actually the opposite of what we want. Usually we can afford training step to take a long time, but we want fast test step
  - Need large number of samples for accuracy