CS4442/9542b
Artificial Intelligence II
prof. Olga Veksler

Lecture 3

Machine Learning

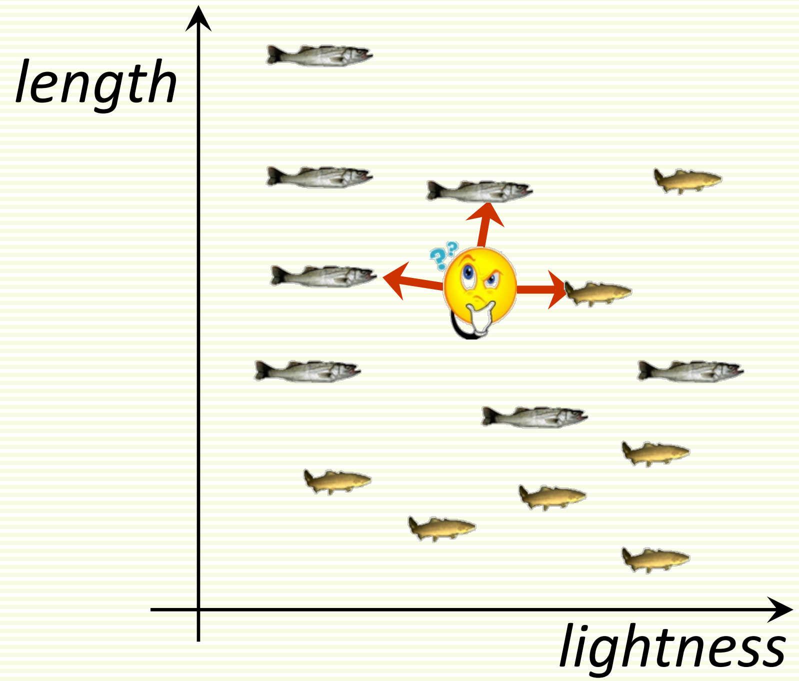
K Nearest Neighbor Classifier

Today

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

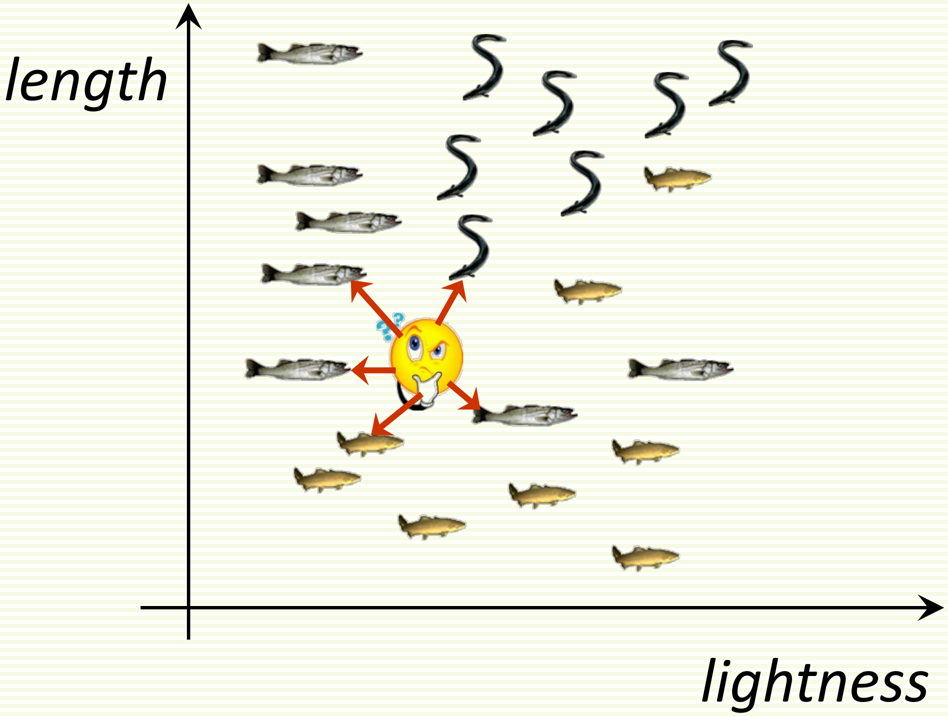
k-Nearest Neighbors

- 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



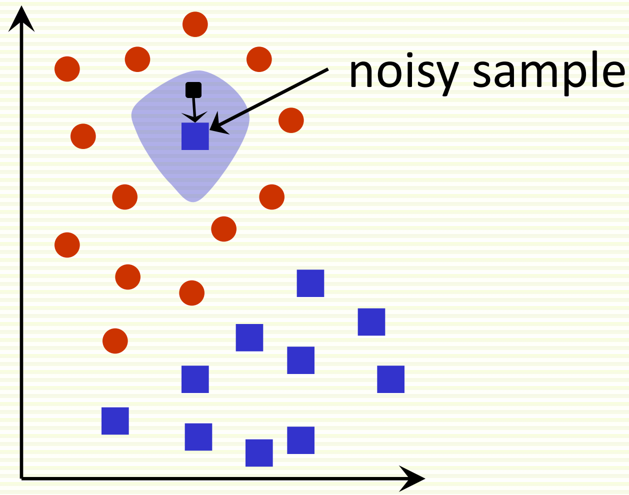
kNN: How to Choose k?

- 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?

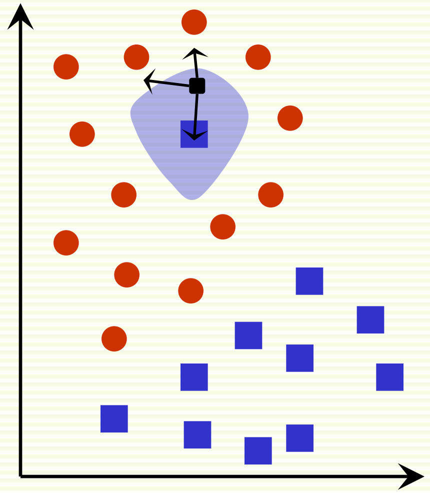
- Rule of thumb is ***k*** = sqrt(***n***), ***n*** is number of examples
  - interesting theoretical properties
- In practice, ***k*** = 1 is often used for efficiency, but can be sensitive to “noise”

1 NN



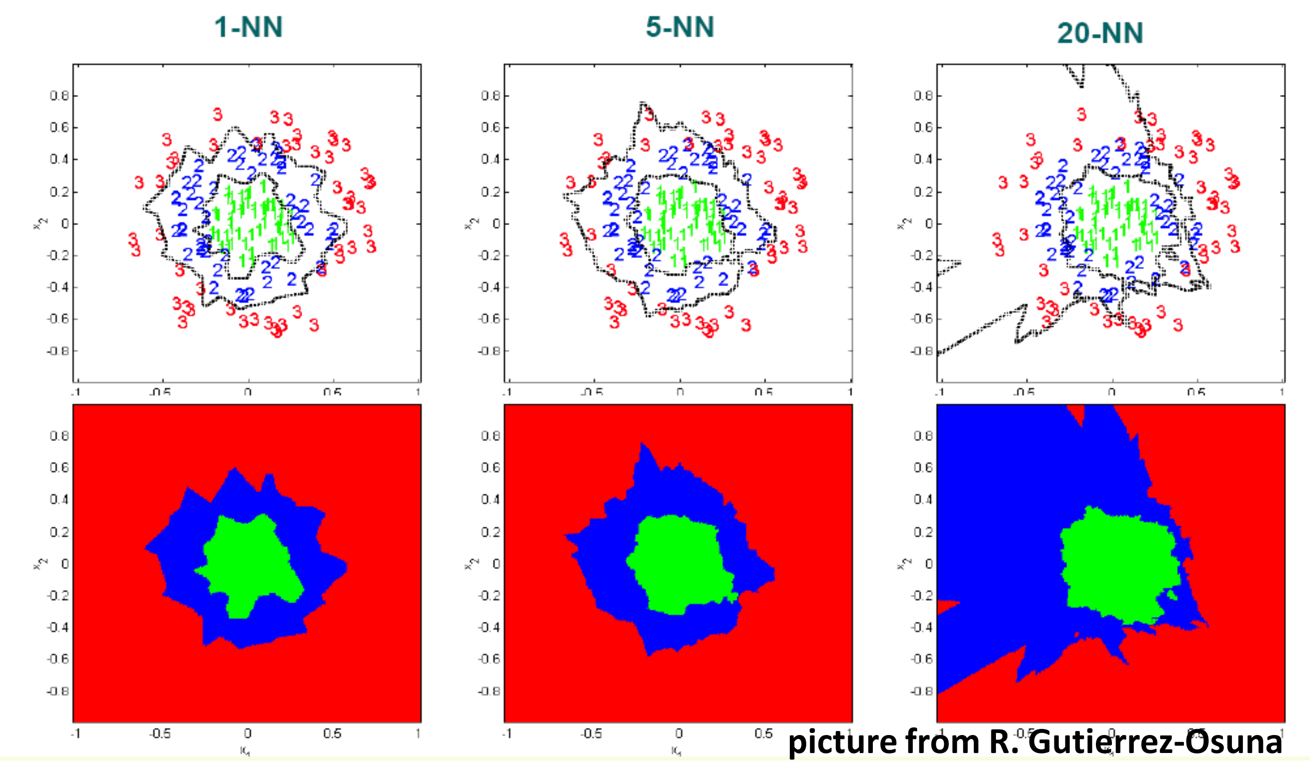
every example in the blue shaded area will be misclassified as the blue class

3 NN



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

kNN: How to Choose k?



picture from R. Gutierrez-Osuna

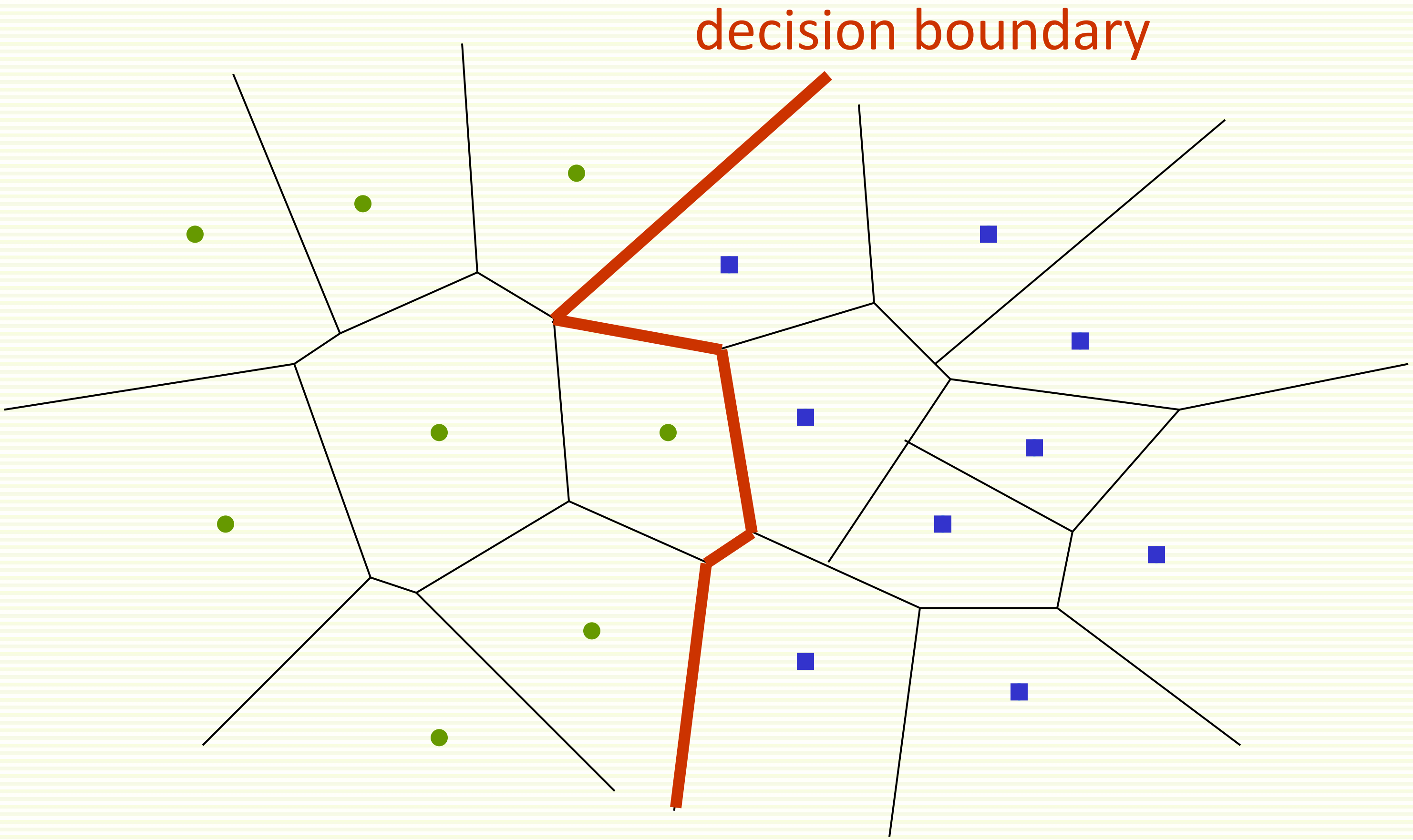
- Larger ***k*** gives smoother boundaries, better for generalization
  - But only if *locality* is preserved. Locality is not preserved if end up looking at samples too far away, not from the same class.
- Interesting theoretical properties if ***k*** < sqrt(***n***), ***n*** is # of examples
- Can choose ***k*** through cross-validation (study soon)

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 $n \rightarrow \infty$, 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 $n \rightarrow \infty$) 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:

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

- 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]**

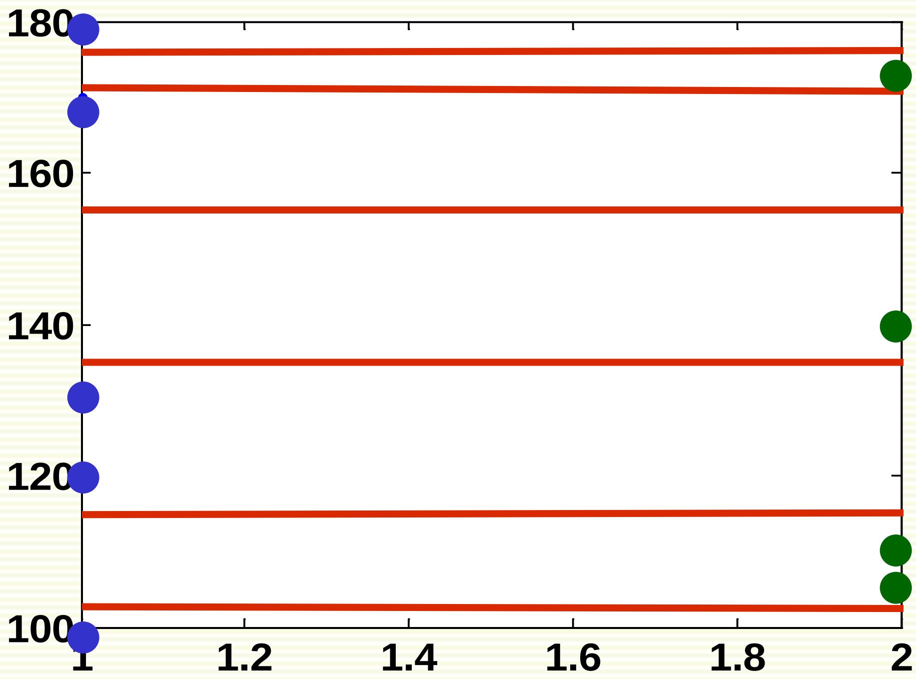
  [2 110]
- classify **[1 100]**

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

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

- **[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 $\boldsymbol{\mu}$ and variance $\boldsymbol{\sigma}^2$, then $(\boldsymbol{Z} - \boldsymbol{\mu})/\boldsymbol{\sigma}$ 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

$\boldsymbol{C}_{\boldsymbol{new}}$=(***C***-repmat(mean(***C***), size(***C***,1), 1))*diag(1./std(***C***))

kNN: Feature Normalization

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

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

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

$$C = \begin{bmatrix} 1 & 180 \\ 1 & 100 \\ 1 & 160 \\ 2 & 120 \\ 2 & 150 \\ 2 & 170 \end{bmatrix}$$

size(***C***,1) = 6

kNN: Feature Normalization

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

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

C

C_{new}=(***C***-repmat(mean(***C***), 6, 1))*diag(1./std(***C***))

[1.5 146.7]

$$C = \begin{bmatrix} 1 & 180 \\ 1 & 100 \\ 1 & 160 \\ 2 & 120 \\ 2 & 150 \\ 2 & 170 \end{bmatrix}$$

repmat Function

$$repmat\left(\begin{bmatrix}1 & 2\\ 3 & 4\end{bmatrix}, 2, 3\right) = \begin{bmatrix}\begin{bmatrix}1 & 2\\ 3 & 4\end{bmatrix} & \begin{bmatrix}1 & 2\\ 3 & 4\end{bmatrix} & \begin{bmatrix}1 & 2\\ 3 & 4\end{bmatrix}\\ \begin{bmatrix}1 & 2\\ 3 & 4\end{bmatrix} & \begin{bmatrix}1 & 2\\ 3 & 4\end{bmatrix} & \begin{bmatrix}1 & 2\\ 3 & 4\end{bmatrix}\end{bmatrix}$$

kNN: Feature Normalization

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

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

C

$\boldsymbol{C}_{\boldsymbol{new}}$=(***C***-repmat(mean(***C***), 6, 1))*diag(1./std(***C***))

$$\begin{bmatrix} 1.5 & 146.7 \\ 1.5 & 146.7 \\ 1.5 & 146.7 \\ 1.5 & 146.7 \\ 1.5 & 146.7 \\ 1.5 & 146.7 \end{bmatrix}$$

mean(***C***) = [1.5 146.7]

kNN: Feature Normalization

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

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

C*$_{new}$**= (C*** - repmat(mean(***C***),6,1))*diag(1./std(***C***))

$$\begin{bmatrix} 1 & 180 \\ 1 & 100 \\ 1 & 160 \\ 2 & 120 \\ 2 & 150 \\ 2 & 170 \end{bmatrix} - \begin{bmatrix} 1.5 & 146.7 \\ 1.5 & 146.7 \\ 1.5 & 146.7 \\ 1.5 & 146.7 \\ 1.5 & 146.7 \\ 1.5 & 146.7 \end{bmatrix} = \begin{bmatrix} -0.5 & 33.3 \\ -0.5 & -46.7 \\ -0.5 & 13.3 \\ 0.5 & -26.7 \\ 0.5 & 3.3 \\ 0.5 & 23.3 \end{bmatrix}$$

kNN: Feature Normalization

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

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

$\boldsymbol{C_{new}}$= (***C***-repmat(mean(***C***), 6, 1))*diag(1./std(***C***))

std(***C***) = [0.55   30.8]

$$C = \begin{bmatrix} 1 & 180 \\ 1 & 100 \\ 1 & 160 \\ 2 & 120 \\ 2 & 150 \\ 2 & 170 \end{bmatrix}$$

kNN: Feature Normalization

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

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

C_{new}= (***C***-repmat(mean(***C***), 6, 1))*diag(1./std(***C***))

1./std(***C***) = [1.83   0.03]

std(***C***) = [0.55   30.8]

kNN: Feature Normalization

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

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

C

C_{new}= (***C***-repmat(mean(***C***), 6, 1))*diag(1./std(***C***))

$$\begin{pmatrix} 1.83 & 0 \\ 0 & 0.03 \end{pmatrix}$$

1./std(***C***) = [1.83   0.03]

kNN: Feature Normalization

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

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

C_new = (***C***-repmat(mean(***C***), 6, 1))*diag(1./std(***C***))

$$\begin{bmatrix} -0.5 & 33.3 \\ -0.5 & -46.7 \\ -0.5 & 13.3 \\ 0.5 & -26.7 \\ 0.5 & 3.3 \\ 0.5 & 23.3 \end{bmatrix} \begin{bmatrix} 1.83 & 0 \\ 0 & 0.03 \end{bmatrix} = \begin{bmatrix} -0.9 & 1.08 \\ -0.9 & -1.51 \\ -0.9 & 0.43 \\ 0.9 & -0.87 \\ 0.9 & 0.11 \\ 0.9 & 0.76 \end{bmatrix}$$

kNN: Feature Normalization

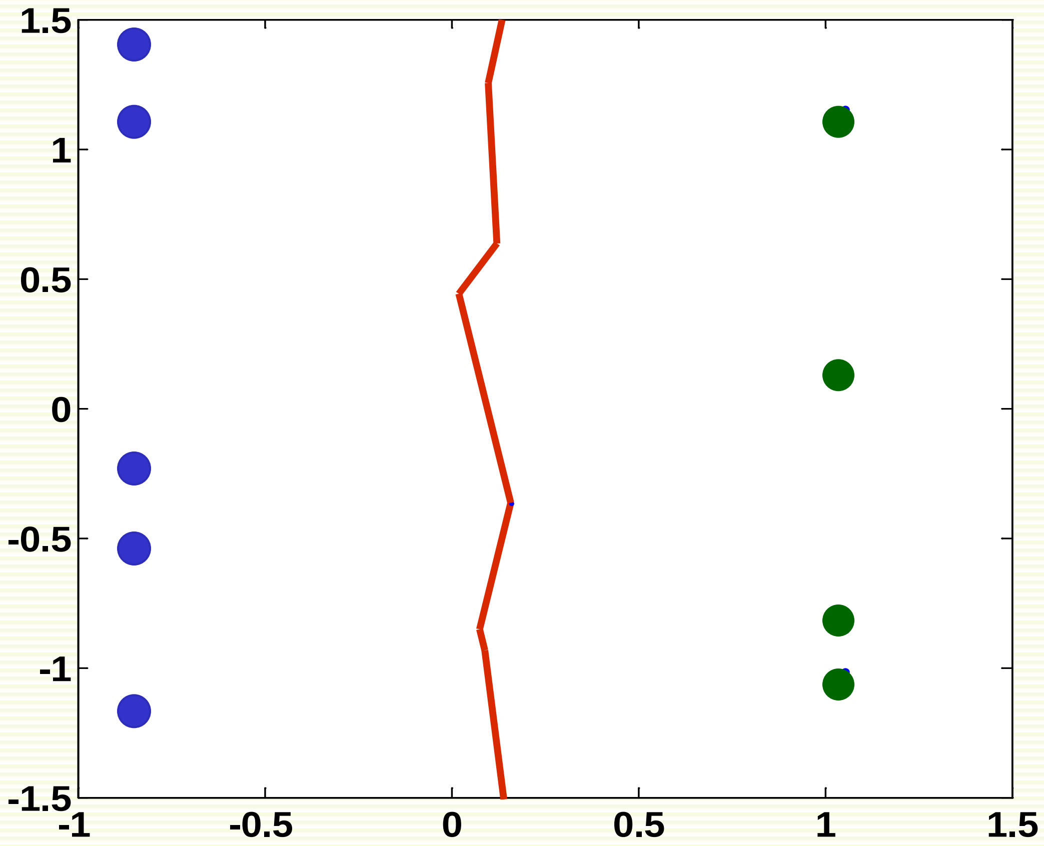
- ***C*** is a matrix with all samples stored as rows, in Matlab can normalize all features simultaneously

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

C_{new} = (***C***-repmat(mean(***C***), 6, 1))*diag(1./std(***C***))

$$\begin{bmatrix} -0.5 & 33.3 \\ -0.5 & -46.7 \\ -0.5 & 13.3 \\ 0.5 & -26.7 \\ 0.5 & 3.3 \\ 1.5 & 23.3 \end{bmatrix} \begin{bmatrix} 1.83 & 0 \\ 0 & 0.03 \end{bmatrix} = \begin{bmatrix} -0.9 & 1.08 \\ -0.9 & -1.21 \\ -0.9 & 0.43 \\ 0.9 & -0.87 \\ 0.9 & 0.11 \\ 0.9 & 0.76 \end{bmatrix}$$

kNN: Feature Normalization



kNN: Selection of Distance

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

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

discriminative features — **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

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

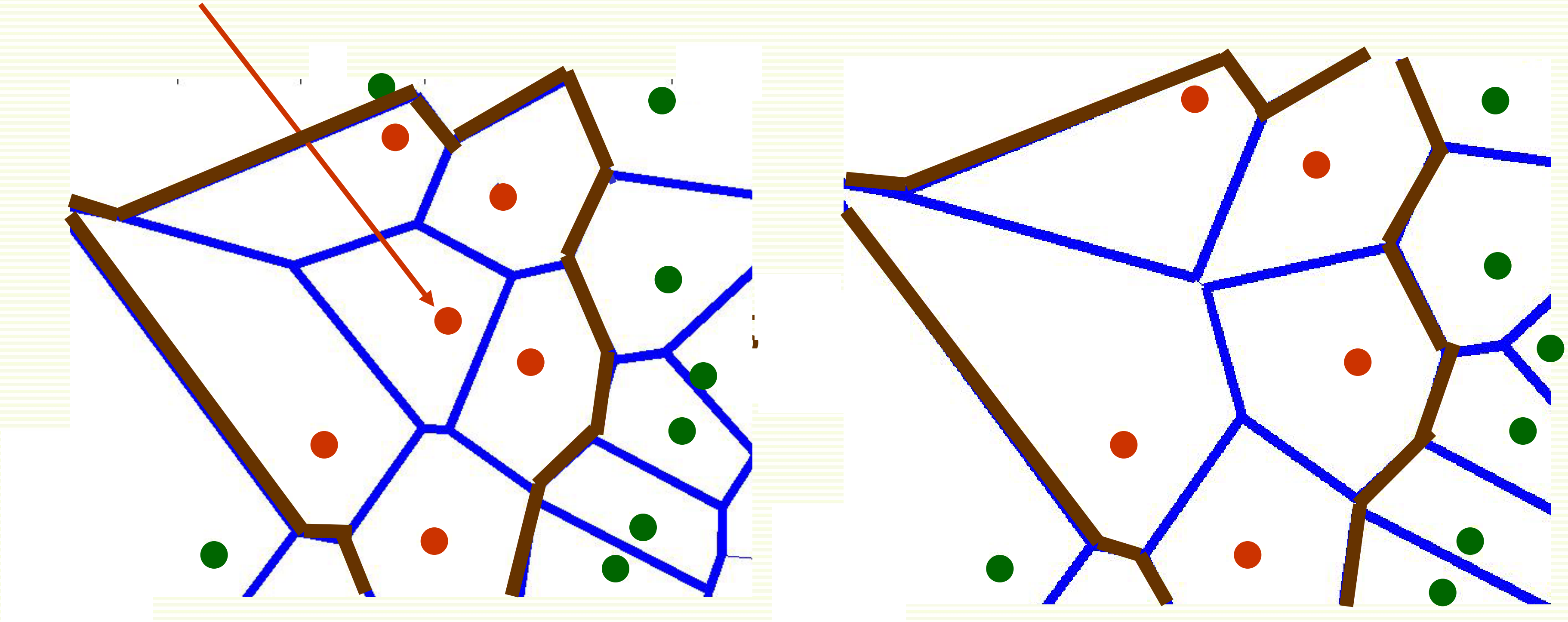
- Can use our prior knowledge about which features are more important
- Can learn the weights $\mathbf{w_k}$

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 distances to all examples
- **O(knd)** to find **k** closest examples examples
  - **O(nd)** + **O(kn)** if careful
- 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

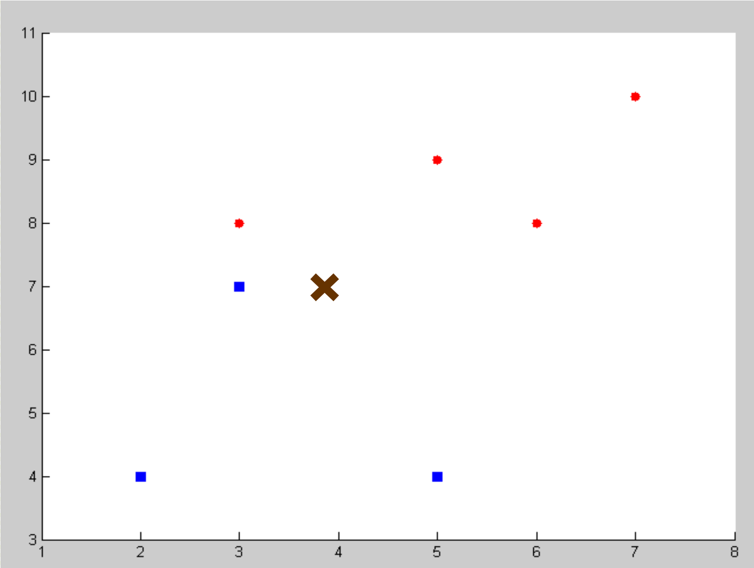
- Have current ***k*** closes samples
- Abort distance computation if partial distance is already greater than the full distance to the current ***k*** closest samples

- 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 for 2 classes

$$class1 = \begin{bmatrix} 3 & 8 \\ 5 & 9 \\ 7 & 10 \\ 6 & 8 \end{bmatrix}$$

$$class2 = \begin{bmatrix} 2 & 4 \\ 3 & 7 \\ 5 & 4 \end{bmatrix}$$



- Want to classify **newSample = [4   7]**

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);
```

$$class1 = \begin{bmatrix} 3 & 8 \\ 5 & 9 \\ 7 & 10 \\ 6 & 8 \end{bmatrix}$$

$$class2 = \begin{bmatrix} 2 & 4 \\ 3 & 7 \\ 5 & 4 \end{bmatrix}$$

$$\mathbf{newSample} = \begin{bmatrix} 4 & 7 \end{bmatrix}$$

$$k = 3$$

kNN in Matlab

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

$$class1 = \begin{bmatrix} 3 & 8 \\ 5 & 9 \\ 7 & 10 \\ 6 & 8 \end{bmatrix}$$

$$class2 = \begin{bmatrix} 2 & 4 \\ 3 & 7 \\ 5 & 4 \end{bmatrix}$$

$$\mathbf{newSample} = \begin{bmatrix} 4 & 7 \end{bmatrix}$$

numClass1 = 4

numClass2 = 3

totalSamples = 7

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

kNN in Matlab

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

$$newSample = \begin{bmatrix} 4 & 7 \end{bmatrix}$$

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

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

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

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

kNN in Matlab

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

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

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

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

$$neighborsInd = \begin{bmatrix} 6 \\ 1 \\ 2 \end{bmatrix} \qquad neighbors = \begin{bmatrix} 2 \\ 1 \\ 1 \end{bmatrix}$$

$$k = 3$$

kNN in Matlab

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

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

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

$$class1 = \begin{bmatrix} 2 \\ 3 \end{bmatrix}$$

$$class2 = \begin{bmatrix} 1 \end{bmatrix}$$

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

$$class = 1$$

kNN in Matlab

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

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

Also can use **class = mode(neighbors)** instead

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

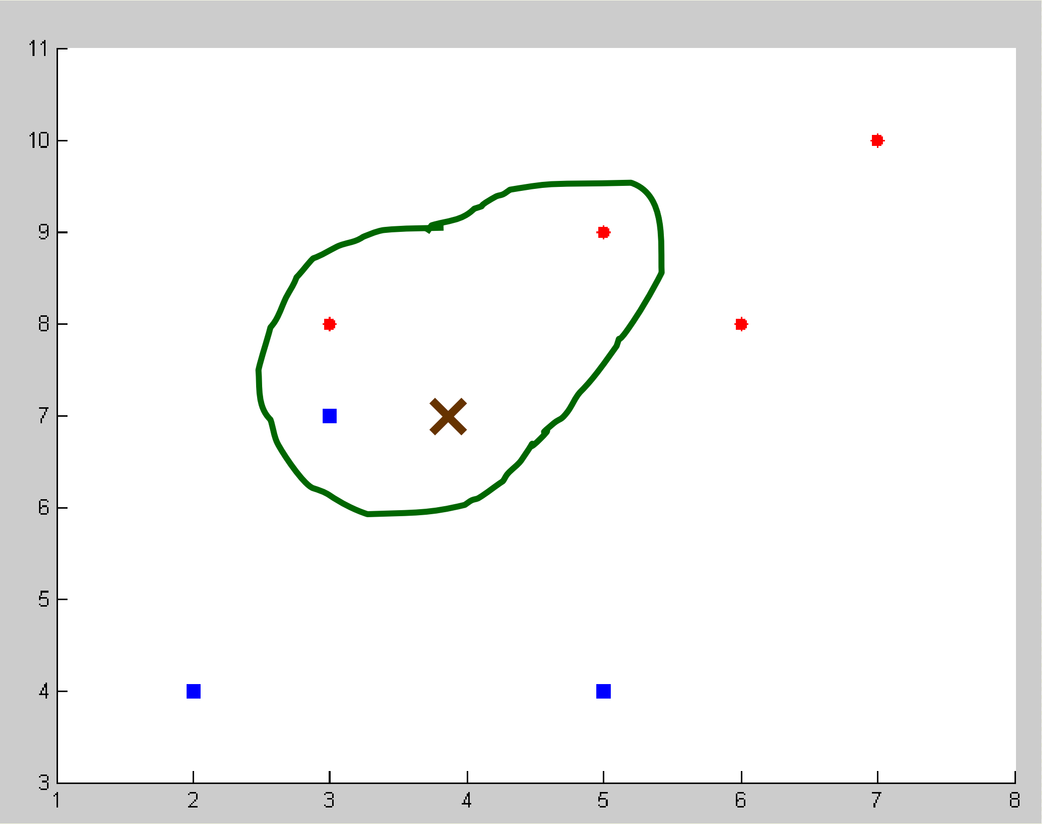
$$class1 = \begin{bmatrix} 2 \\ 3 \end{bmatrix}$$

$$class2 = \begin{bmatrix} 1 \end{bmatrix}$$

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

$$class = 1$$

kNN in Matlab



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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);

class   = mode(neighbors);
```

- Simpler code if use matlab **mode** function

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