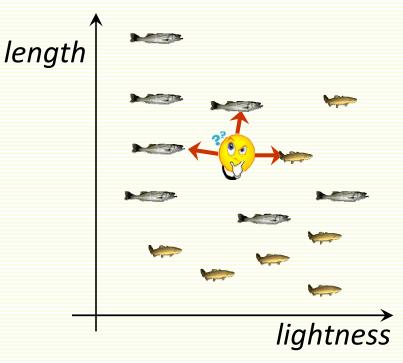
CS840a Machine Learning in Computer Vision Olga Veksler

Lecture 2 k Nearest Neighbors

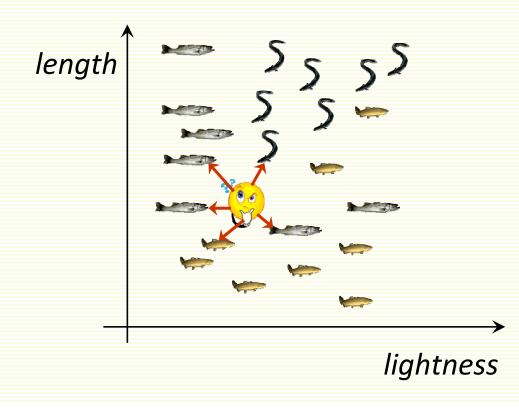
k-Nearest Neighbors

- 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 \Rightarrow classify as sea bass

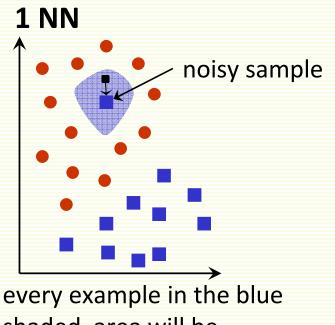


kNN: How to Choose k?

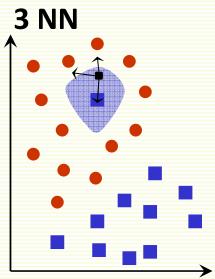
- In theory, if infinite number of samples available, the larger is *k*, the better is classification
- The caveat is that all k neighbors have to be close
 - Possible when infinite # samples available
 - Impossible in practice since # samples is finite

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"



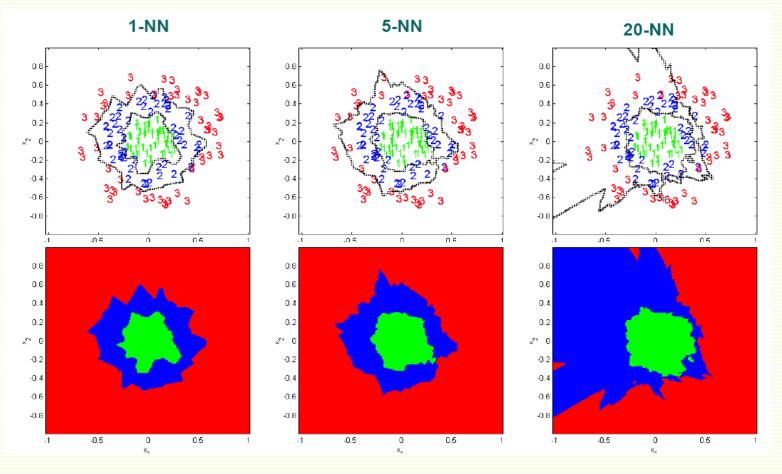
shaded area will be misclassified as the blue class



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



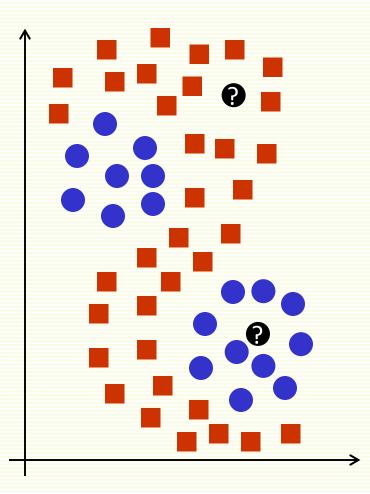
picture from R. Gutierrez-Osuna

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 → ∞, 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 → ∞) for the kNN rule is smaller than cE*, with smaller c for larger k
- If we have lots of samples, kNN works well

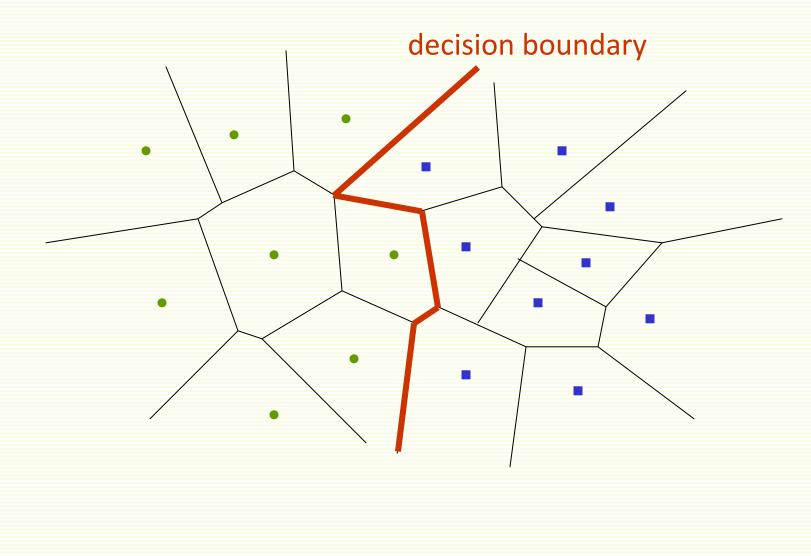
kNN: Multi-Modal Distributions

- Most parametric distributions would not work for this 2 class classification problem:
- Nearest neighbors will do reasonably well, provided we have a lot of samples



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:

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

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

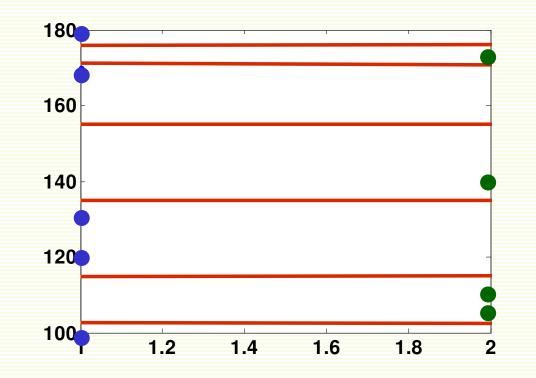
kNN Distance Selection: Extreme Example

- 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]

$$D(\begin{bmatrix} 1\\100 \end{bmatrix}, \begin{bmatrix} 1\\150 \end{bmatrix}) = \sqrt{(1-1)^2 + (100-150)^2} = 50$$
$$D(\begin{bmatrix} 1\\100 \end{bmatrix}, \begin{bmatrix} 2\\110 \end{bmatrix}) = \sqrt{(1-2)^2 + (100-110)^2} = 10.5$$

- [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]

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

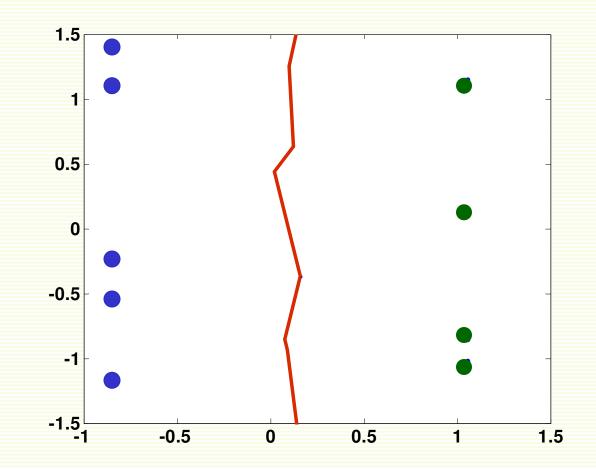
kNN: Feature Normalization

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

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

• 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

$$D(a,b) = \sqrt{\sum_{k} (a_{k} - b_{k})^{2}} = \sqrt{\sum_{i} (a_{i} - b_{i})^{2} + \sum_{j} (a_{j} - b_{j})^{2}}$$

discriminative noisy
features 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

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

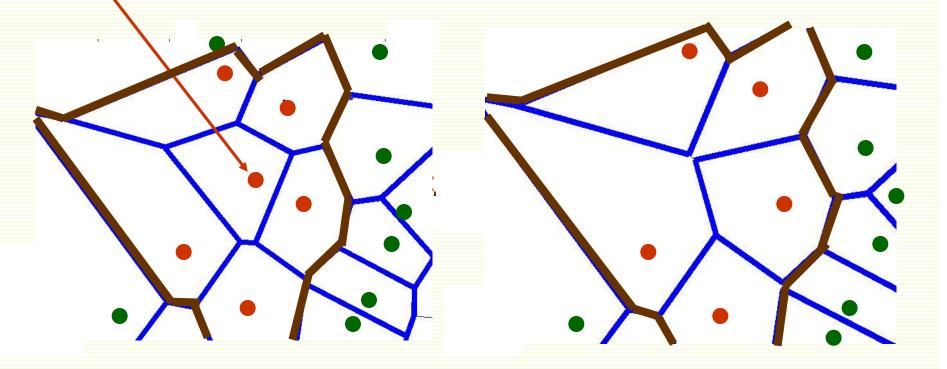
- Can use our prior knowledge about which features are more important
- Can learn the weights w_k using cross-validation (to be covered later)

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

Reducing Complexity

- Other methods for reducing complexity
 - reduce dimensionality of the data
 - find projection to a lower dimensional space so that the distances between samples are approximately the same
 - PCA
 - Projection to a Random subspace
 - use smart data structures, like kd trees

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