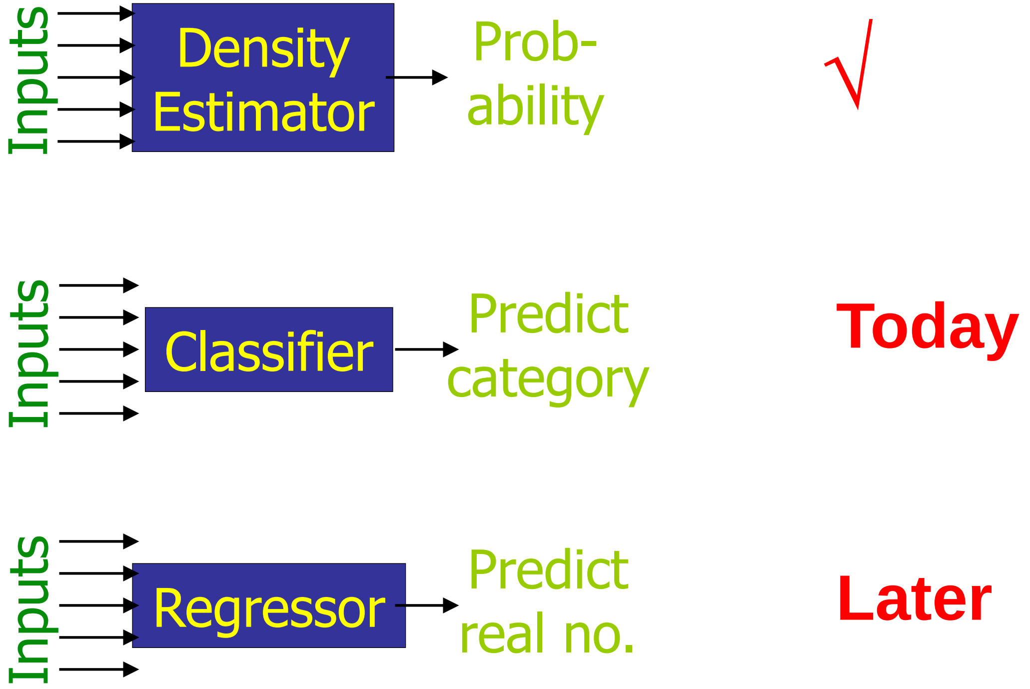
10-701
Machine Learning

Classification

Related reading: Mitchell 8.1,8.2; Bishop 1.5

Where we are


Inputs
Density Estimator
Prob-ability
√
Inputs
Classifier
Predict category
Today
Inputs
Regressor
Predict real no.
Later

Classification

- Assume we want to teach a computer to distinguish between cats and dogs …








Bayes decision rule

x – input feature set
y - label

- If we know the conditional probability p(x | y) and class priors p(y) we can determine the appropriate class by using Bayes rule:

$$P(y=i\mid x)=\frac{P(x\mid y=i)P(y=i)}{P(x)}\stackrel{def}{=}q_i(x)$$

Minimizes our probability of making a mistake

Note that p(x) does not affect our decision

- We can use $q_i(x)$ to select the appropriate class.
- We chose class 0 if $q_0(x) \geq q_1(x)$ and class 1 otherwise
- This is termed the 'Bayes decision rule' and leads to optimal classification.
- However, it is often very hard to compute …

Bayes decision rule

$$P(y=i \mid x) = \frac{P(x \mid y=i)P(y=i)}{P(x)} \stackrel{def}{=} q_i(x)$$

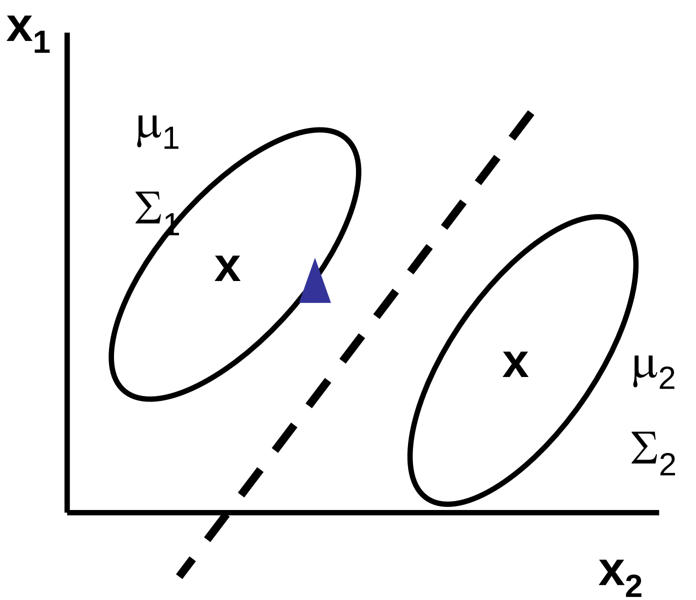
- We can also use the resulting probabilities to determine our **confidence** in the class assignment by looking at the likelihood ratio:

$$L(x) = \frac{q_0(x)}{q_1(x)}$$

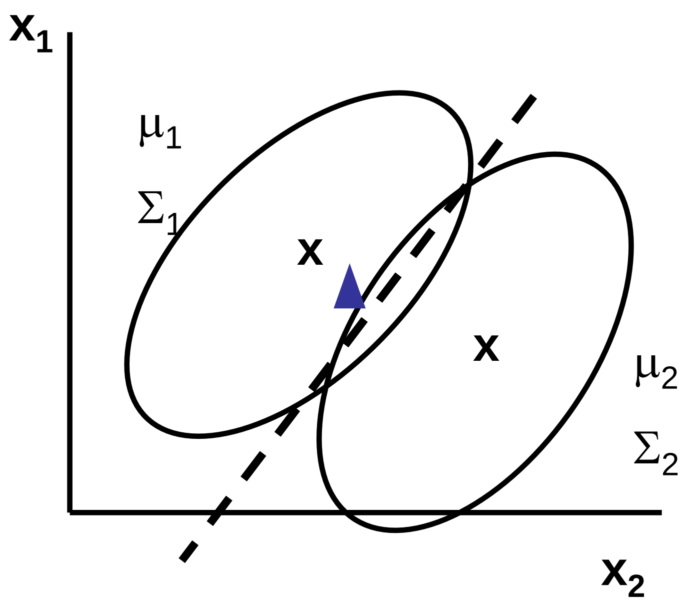
Also known as likelihood ratio, we will talk more about this later

Confidence: Example

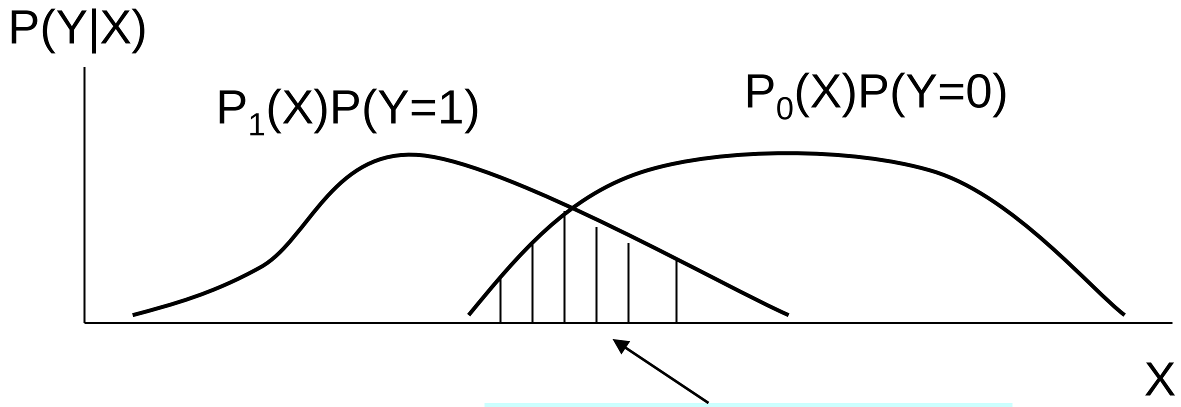
Normal Gaussians



Normal Gaussians



Bayes error and risk



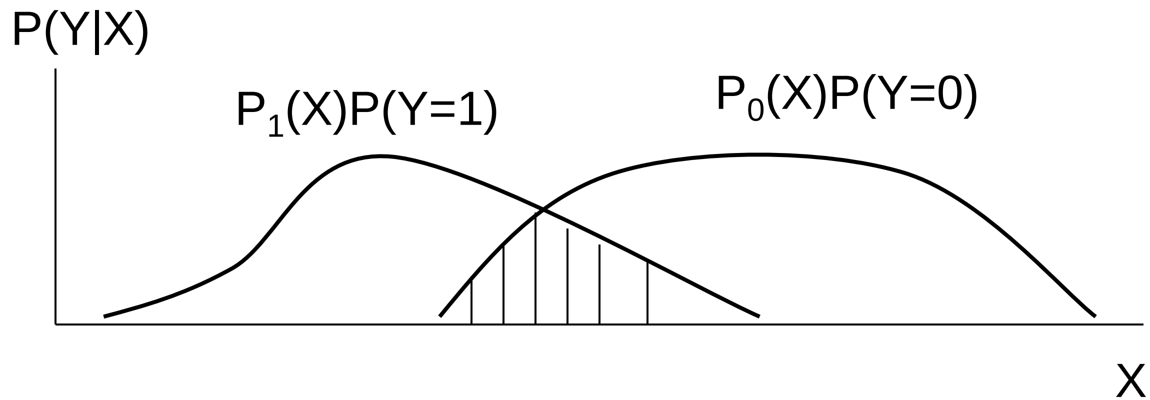
x values for which we will have errors

• Risk for sample x is defined as:

$$R(x) = \min\{P_1(x)P(y=1),\ P_0(x)P(y=0)\} \ / \ P(x)$$

Risk can be used to determine a ‘reject’ region

Bayes risk



- The probability that we assign a sample to the wrong class, is known as the **risk**

- The risk for sample x is:

$R(x) = \min\{P_1(x)P(y=1), P_0(x)P(y=0)\} / P(x)$

- We can also compute the expected risk (the risk for the entire range of values of x):

$$
\begin{aligned}
E[r(x)] &= \int_x r(x)p(x)dx \\
&= \int_x \min\{p_1(x)p(y=1), p_0(x)p(y=0)\}dx \\
&= p(y=0)\int_{L_1} p_0(x)dx + p(y=1)\int_{L_0} p_1(x)dx
\end{aligned}
$$

L_1 is the region where we assign instances to class 1

Loss function

- The risk value we computed assumes that both errors (assigning instances of class 1 to class 0 and vice versa) are equally harmful.
- However, this is not always the case.
- Why?
- In general our goal is to minimize loss, often defined by a loss function: $L_{0,1}(x)$ which is the penalty we pay when assigning instances of class 0 to class 1

$$E[L] = L_{0,1}\, p(y=0)\int_{L_1} p_0(x)dx + L_{1,0}\, p(y=1)\int_{L_0} p_1(x)dx$$

Types of classifiers

- We can divide the large variety of classification approaches into roughly two main types

1. Instance based classifiers
   - Use observation directly (no models)
   - e.g. K nearest neighbors

2. Generative:
   - build a generative statistical model
   - e.g., Naïve Bayes

3. Discriminative
   - directly estimate a decision rule/boundary
   - e.g., decision tree

Classification

- Assume we want to teach a computer to distinguish between cats and dogs …




Several steps:
1. feature transformation
2. Model / classifier specification
3. Model / classifier estimation (with regularization)
4. feature selection

Classification

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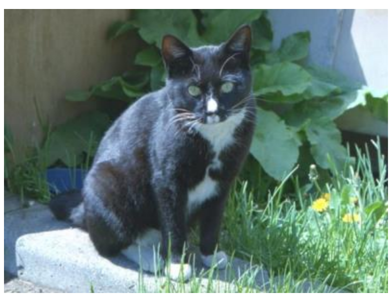


Several steps:

1. feature transformation
2. Model / classifier specification
3. Model / classifier estimation (with regularization)
4. feature selection

How do we encode the picture? A collection of pixels? Do we use the entire image or a subset? …

Classification

- Assume we want to teach a computer to distinguish between cats and dogs …




Several steps:

1. feature transformation
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3. Model / classifier estimation (with regularization)
4. feature selection

What type of classifier should we use?

Classification

- Assume we want to teach a computer to distinguish between cats and dogs …




Several steps:

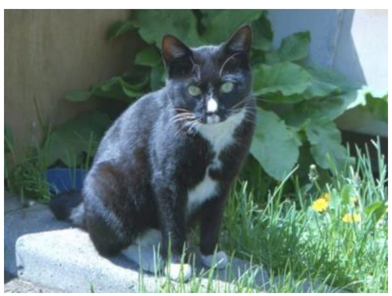
1. feature transformation
2. Model / classifier specification
3. Model / classifier estimation (with regularization)
4. feature selection

How do we learn the parameters of our classifier? Do we have enough examples to learn a good model?

Classification

- Assume we want to teach a computer to distinguish between cats and dogs …





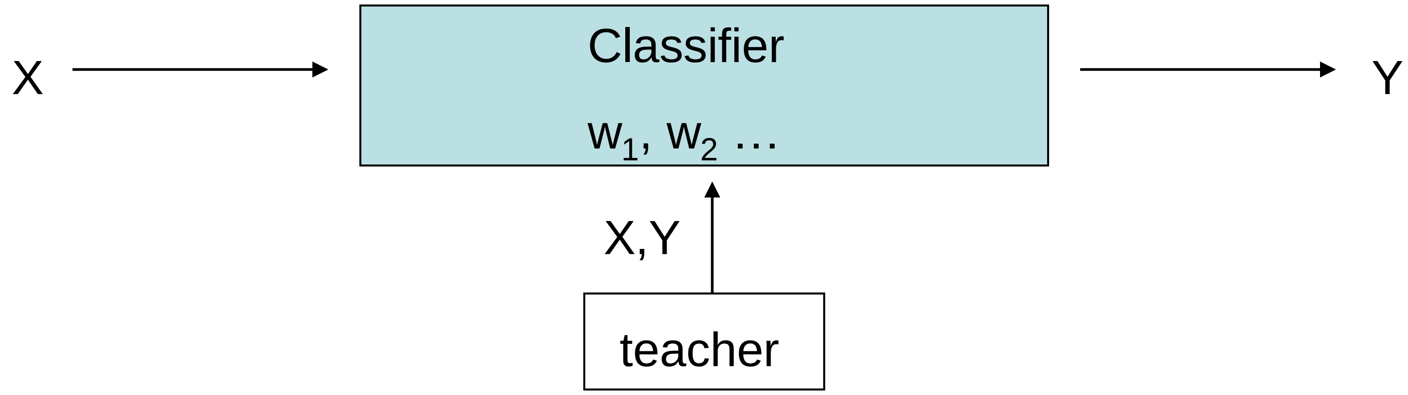

Several steps:

1. feature transformation
2. Model / classifier specification
3. Model / classifier estimation (with regularization)
4. feature selection

Do we really need all the features? Can we use a smaller number and still achieve the same (or better) results?

Supervised learning

- Classification is one of the key components of ‘supervised learning’
- Unlike other learning paradigms, in supervised learning the teacher (us) provides the algorithm with the solutions to some of the instances and the goal is to generalize so that a model / method can be used to determine the labels of the unobserved samples



Types of classifiers

- We can divide the large variety of classification approaches into roughly two main types

1. Instance based classifiers
   - Use observation directly (no models)
   - e.g. K nearest neighbors

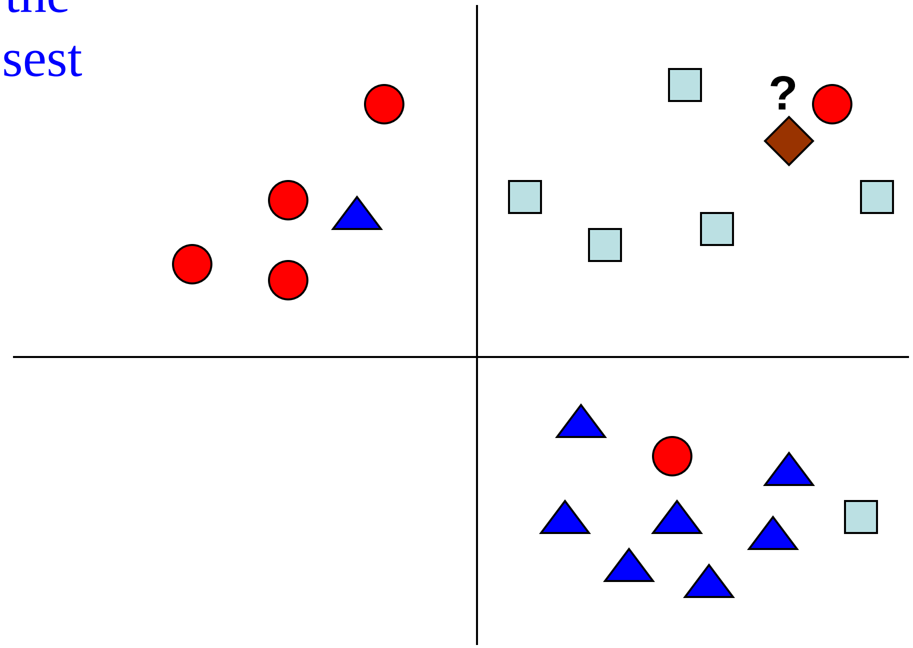
2. Generative:
   - build a generative statistical model
   - e.g., Bayesian networks

3. Discriminative
   - directly estimate a decision rule/boundary
   - e.g., decision tree

K nearest neighbors

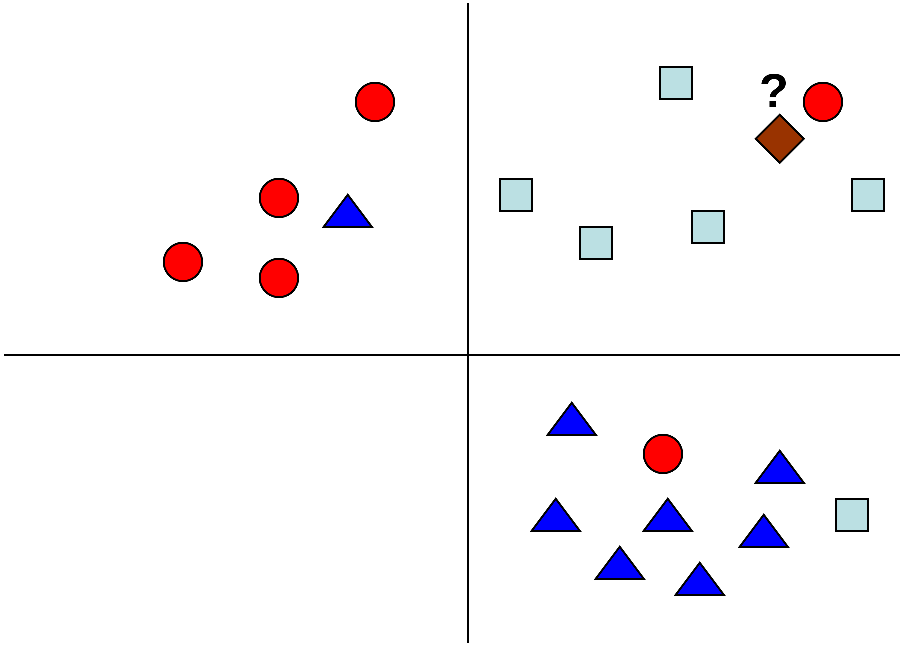
K nearest neighbors (KNN)

- A simple, yet surprisingly efficient algorithm
- Requires the definition of a distance function or similarity measures between samples
- Select the class based on the majority vote in the k closest points



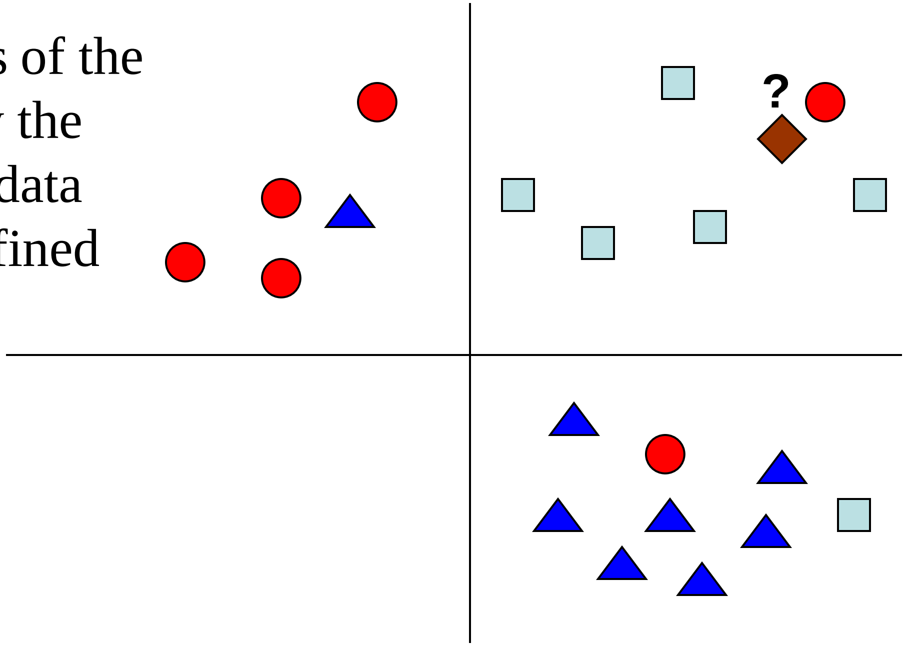
K nearest neighbors (KNN)

- Need to determine an appropriates value for k
- What happens if we chose k=1?
- What if k=3?

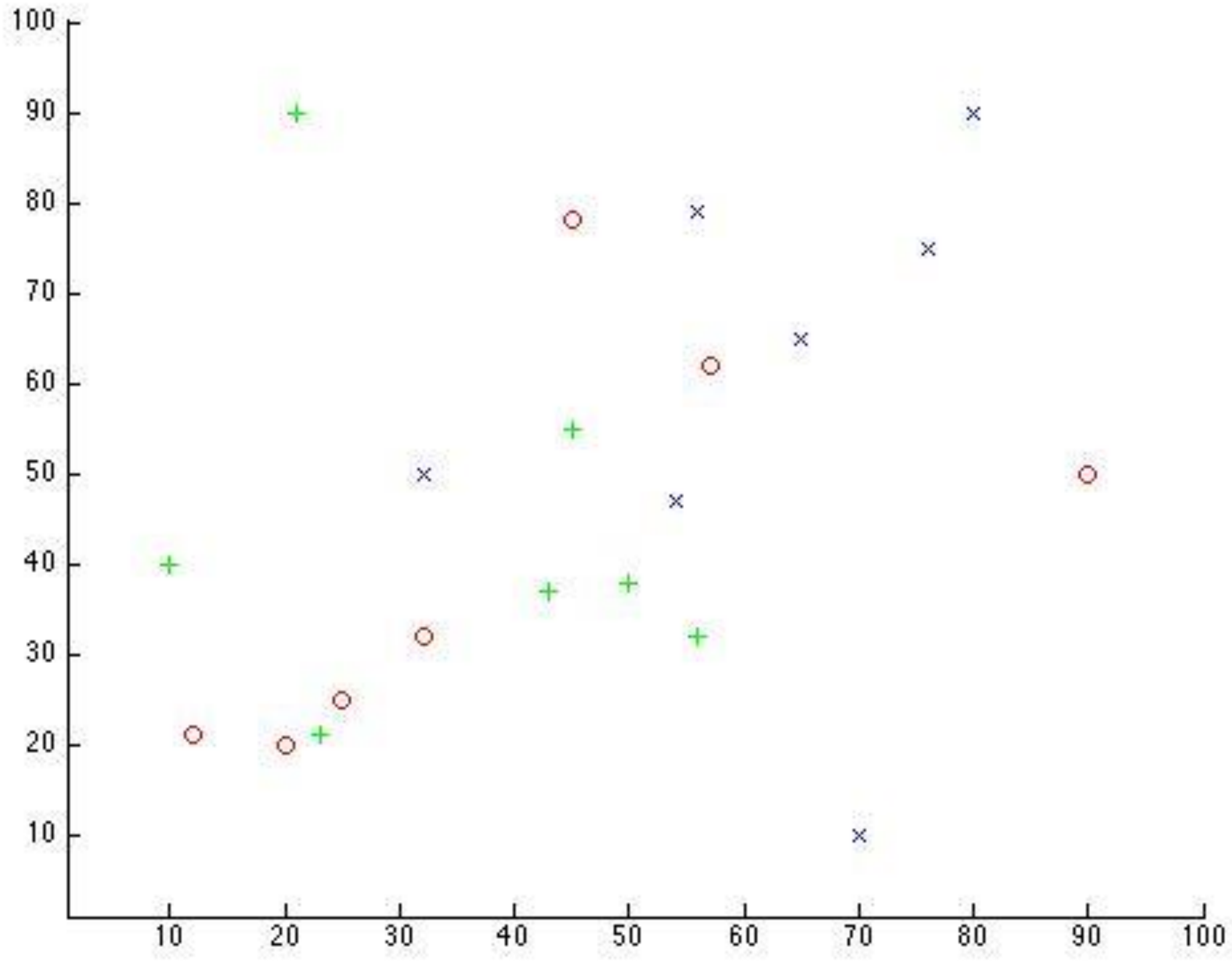


K nearest neighbors (KNN)

- Choice of k influences the 'smoothness' of the resulting classifier
- In that sense it is similar to a kernel methods (discussed later in the course)
- However, the smoothness of the function is determined by the actual distribution of the data (p(x)) and not by a predefined parameter.



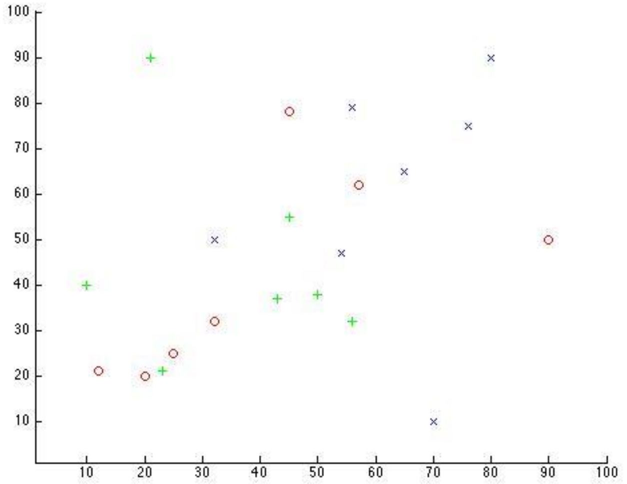
The effect of increasing k



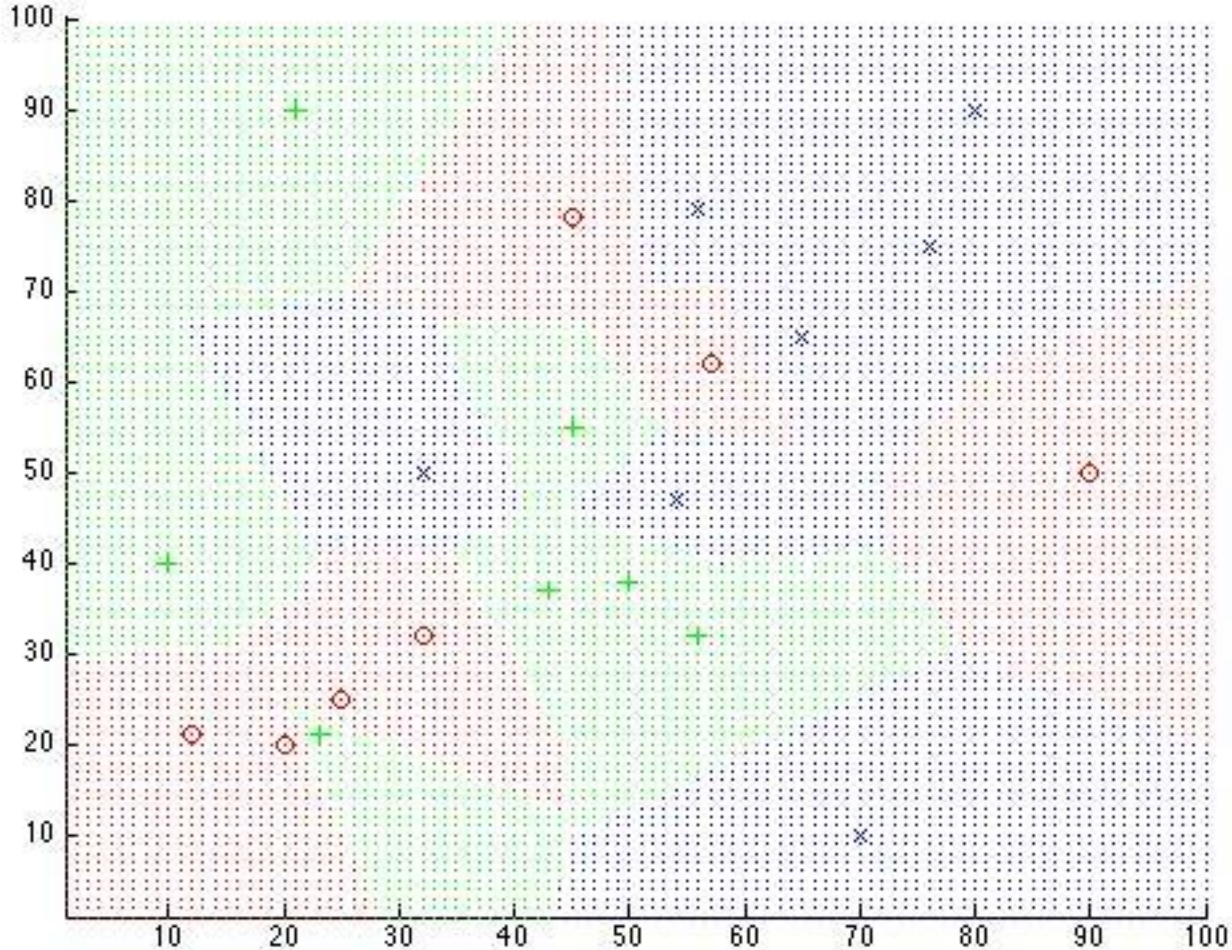
The effect of increasing k

We will be using Euclidian distance to determine what are the k nearest neighbors:

$$d(x,x') = \sqrt{\sum_i (x_i - x_i')^2}$$



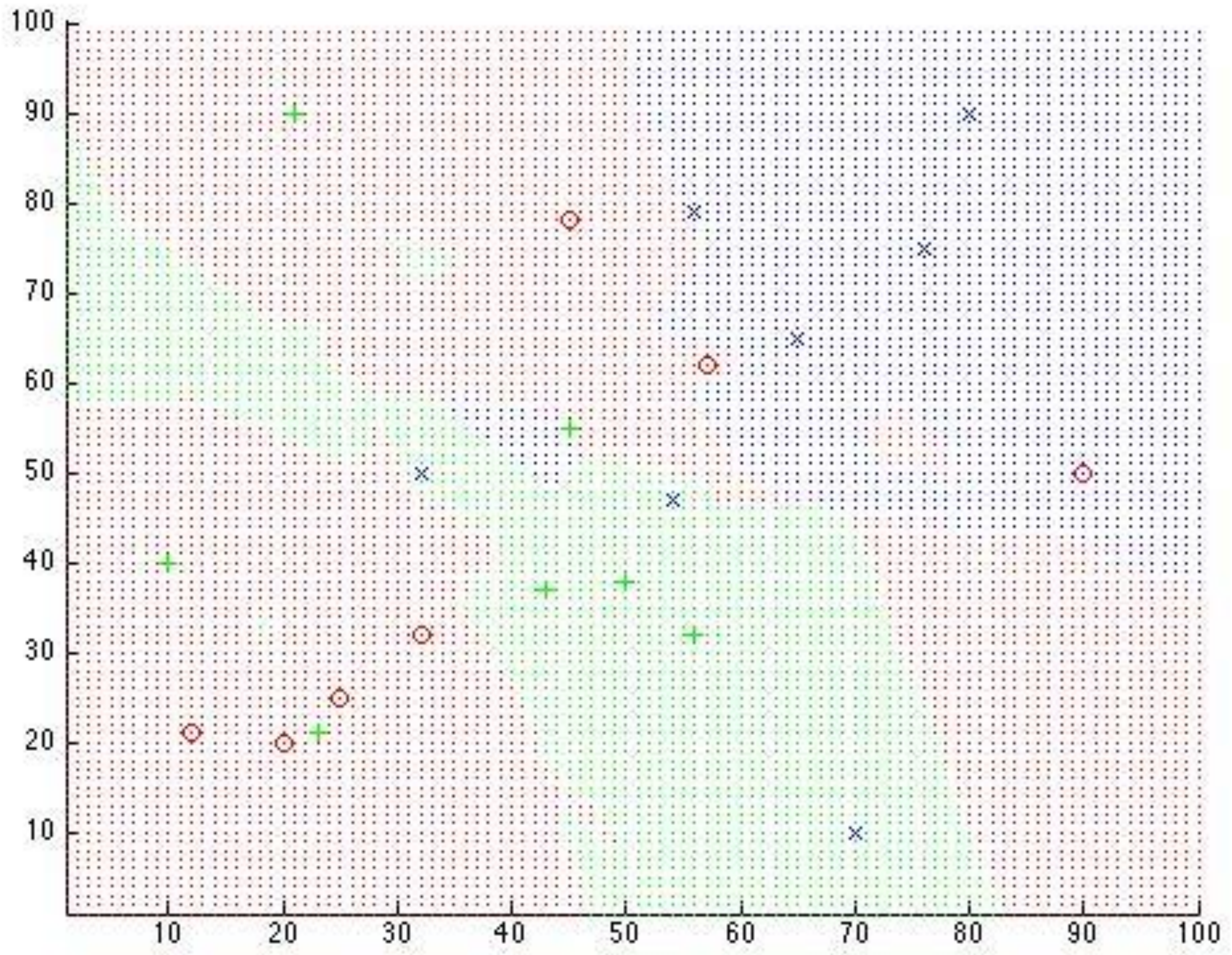
KNN with k=1



KNN with k=3

Ties are broken using the order:

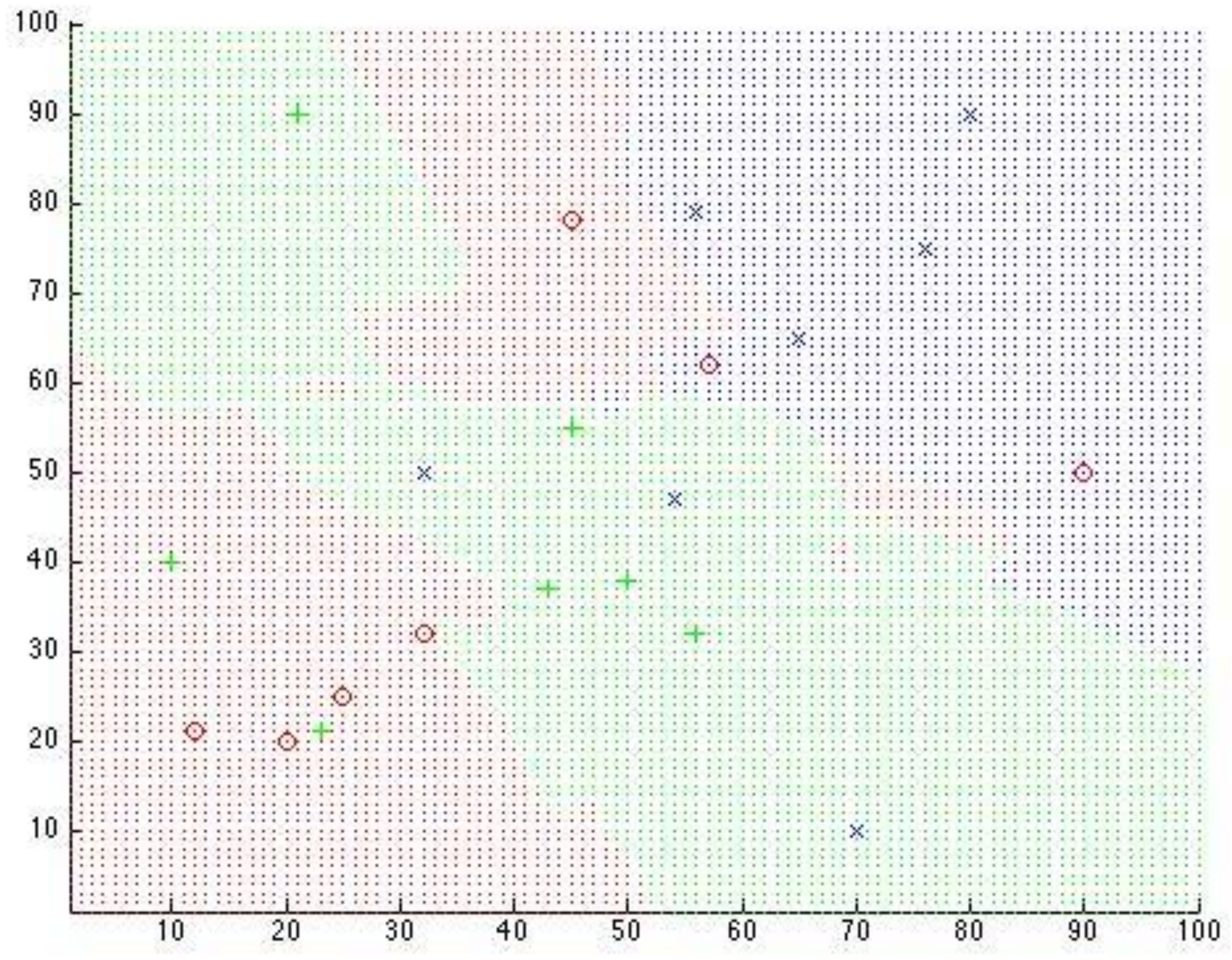
Red , Green, Blue



KNN with k=5

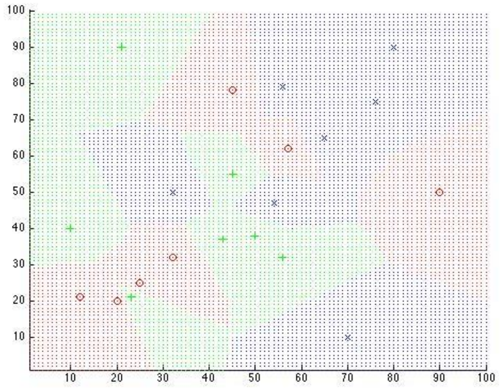
Ties are broken using the order:

Red , Green, Blue

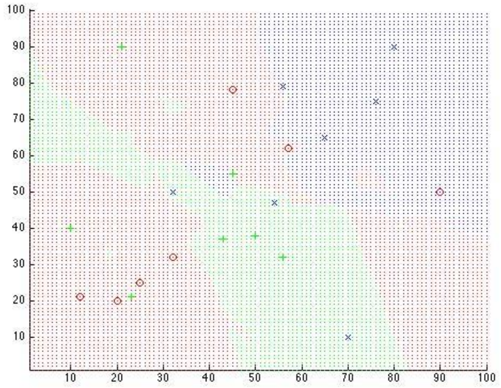


Comparisons of different k's

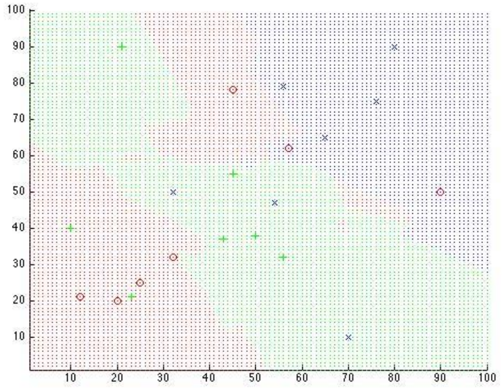
K = 1



K = 3



K = 5



A probabilistic interpretation of KNN

- The decision rule of KNN can be viewed using a probabilistic interpretation
- What KNN is trying to do is approximate the Bayes decision rule on a subset of the data
- To do that we need to compute certain properties including the conditional probability of the data given the class ($p(x|y)$), the prior probability of each class ($p(y)$) and the marginal probability of the data ($p(x)$)
- These properties would be computed for some small region around our sample and the size of that region will be *dependent on the distribution of the test samples**

* Remember this idea. We will return to it when discussing kernel functions

Computing probabilities for KNN

- Let *V* be the volume of the *m* dimensional ball around *z* containing the *k* nearest neighbors for *z* (where *m* is the number of features).
- Then we can write

$$p(x)V = P = \frac{K}{N} \qquad p(x) = \frac{K}{NV} \qquad p(x \mid y=1) = \frac{K_1}{N_1 V} \qquad p(y=1) = \frac{N_1}{N}$$

- Using Bayes rule we get:

$$p(y=1 \mid z) = \frac{p(z \mid y=1)\, p(y=1)}{p(z)} = \frac{K_1}{K}$$

z – new data point to classify

V - selected ball

P – probability that a random point is in V

N - total number of samples

K - number of nearest neighbors

N_1 - total number of samples from class 1

K_1 - number of samples from class 1 in K

Computing probabilities for KNN

N - total number of samples

V - Volume of selected ball

K - number of nearest neighbors

N_1 - total number of samples from class 1

K_1 - number of samples from class 1 in K

- Using Bayes rule we get:

$$p(y=1 \mid z) = \frac{p(z \mid y=1)\, p(y=1)}{p(z)} = \frac{K_1}{K}$$

Using Bayes decision rule we will chose the class with the highest probability, which in this case is the class with the highest number of samples in K

Important points

- Optimal decision using Bayes rule
- Types of classifiers
- Effect of values of k on knn classifiers
- Probabilistic interpretation of knn
- Possible reading: Mitchell, Chapters 1,2 and 8.