

10-601

Machine Learning

Classification

Where we are



Today



Later

Classification

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



Bayes decision rule

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

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

Minimizes our probability of making a mistake

- 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 ...

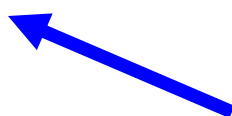
Note that $p(x)$ does not affect our decision

Bayes decision rule

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

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

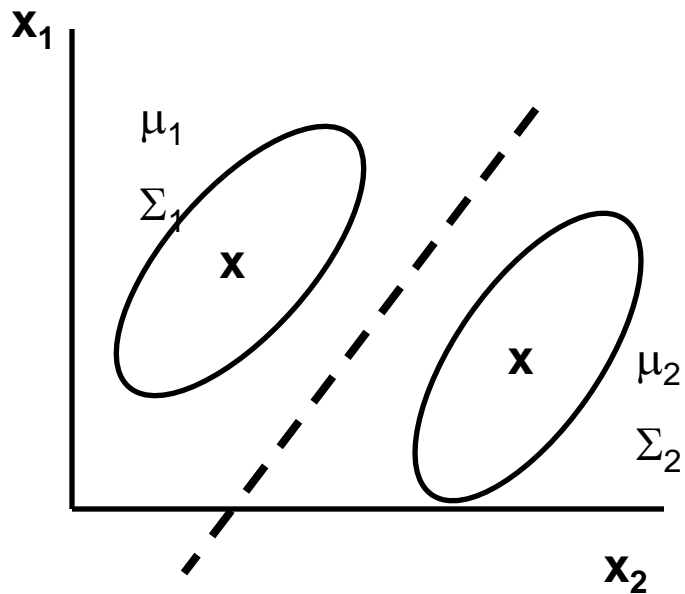
$$L(x) = \frac{q_0(x)}{q_1(x)}$$



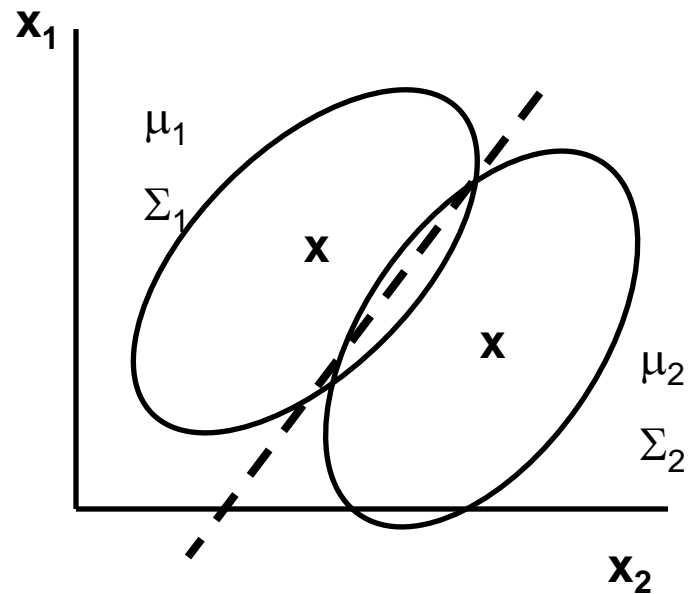
Also known as likelihood ratio test, we will talk more about this later

Bayes decision rule: Example

Normal Gaussians

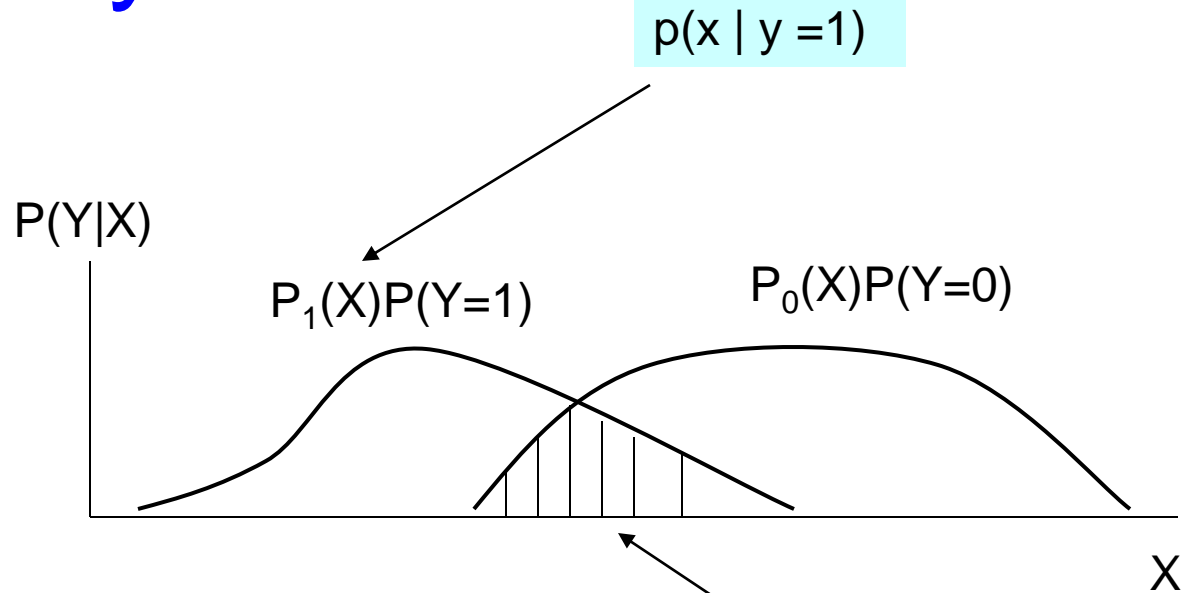


Normal Gaussians



Bayes error

- For the Bayes decision rule we can calculate the probability of an error
- This is the probability that we assign a sample to the wrong class, also known as the **risk**



- The risk for sample x is:

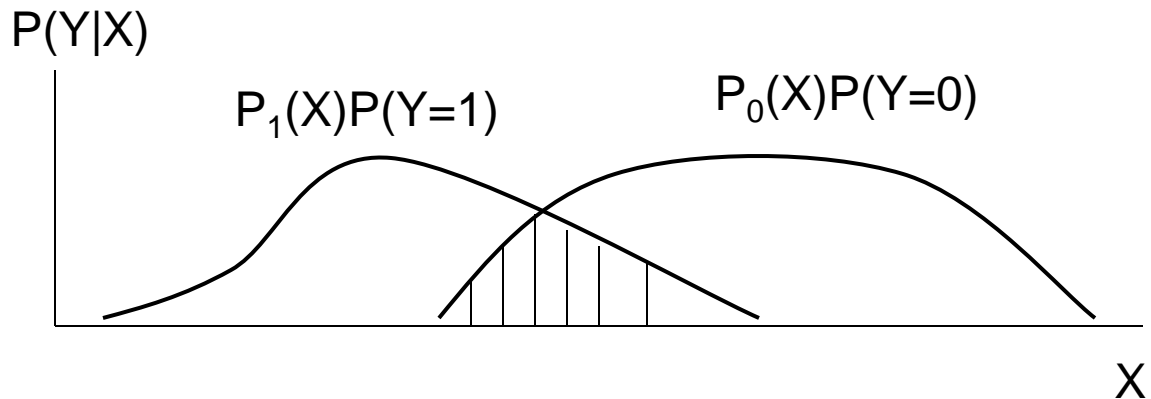
$$R(x) = \min\{P_1(x)P(y=1), P_0(x)P(y=0)\}$$

x values for which we will have errors

Risk can be used to determine a 'reject' region

Bayes error

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



- The risk for sample x is:

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

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

Assuming all values equally likely

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

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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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
2. Model / classifier specification
3. Model / classifier estimation (with regularization)
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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
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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 ...



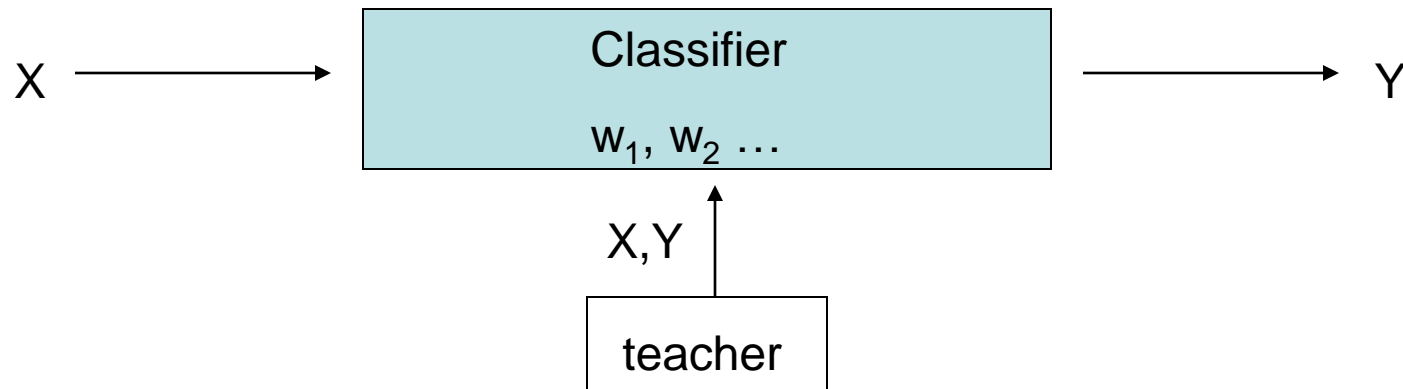
Several steps:

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



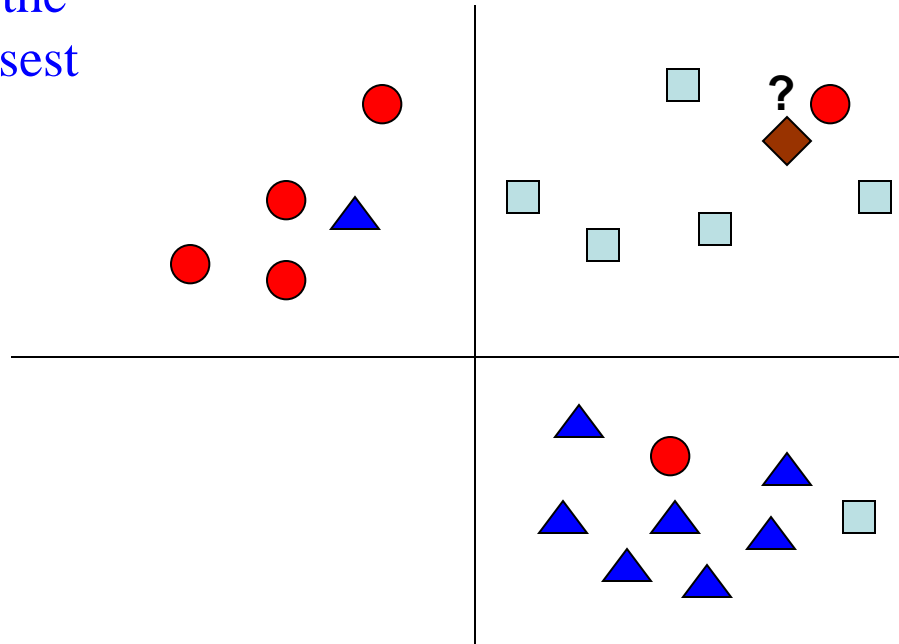
Types of classifiers

- 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

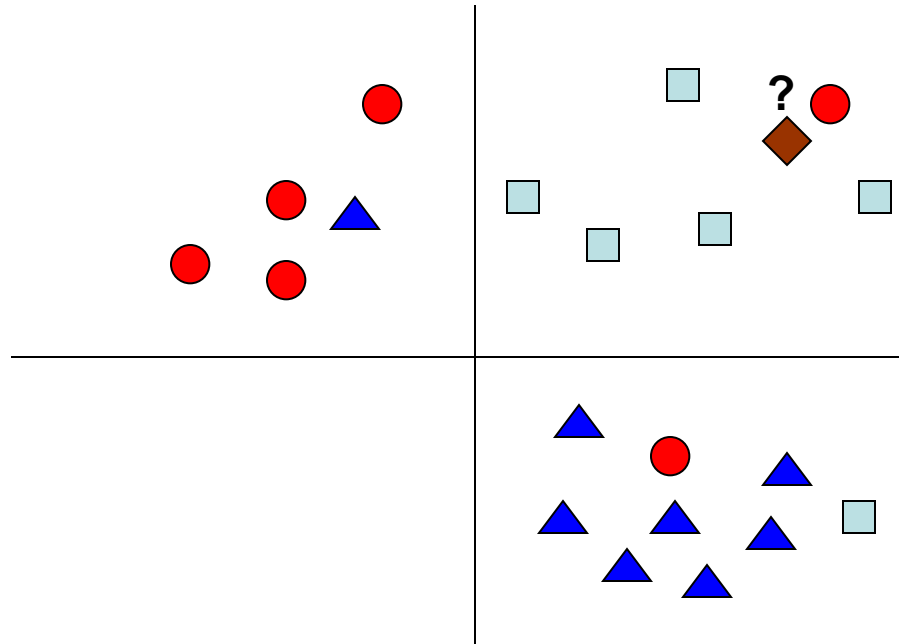
K nearest neighbors (KNN)

- 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



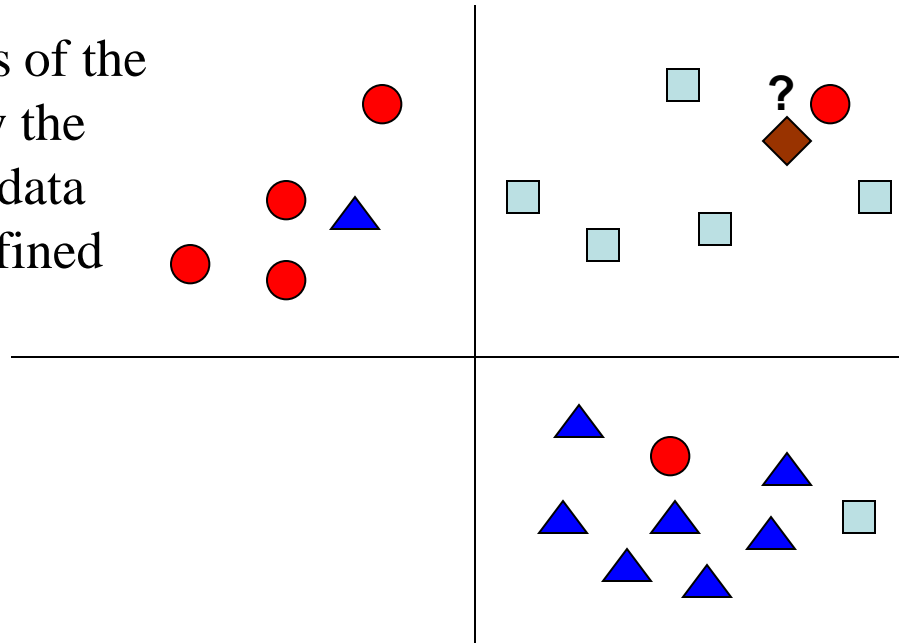
K nearest neighbors (KNN)

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

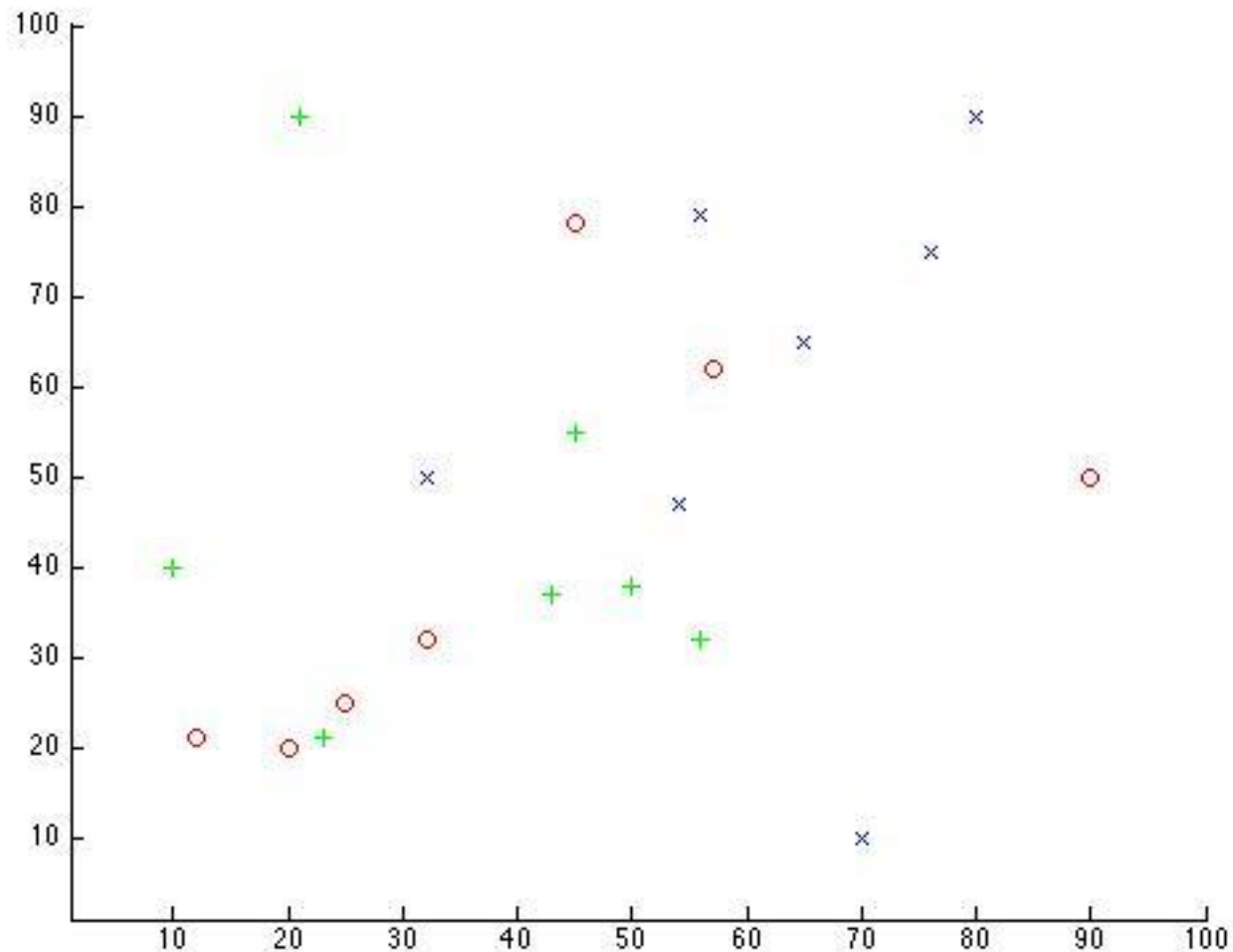


K nearest neighbors (KNN)

- 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.



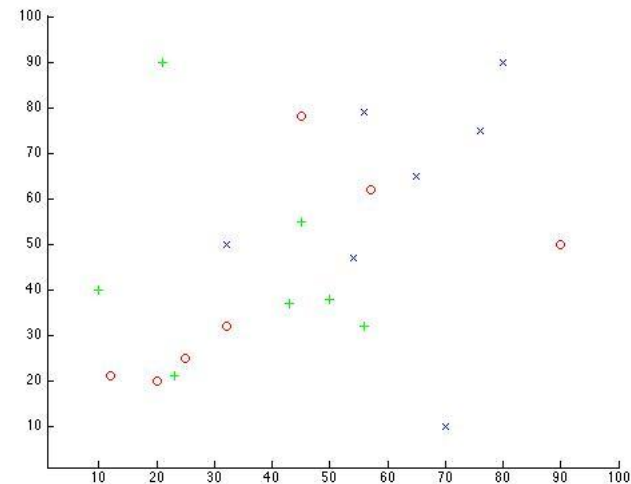
The effect of increasing k



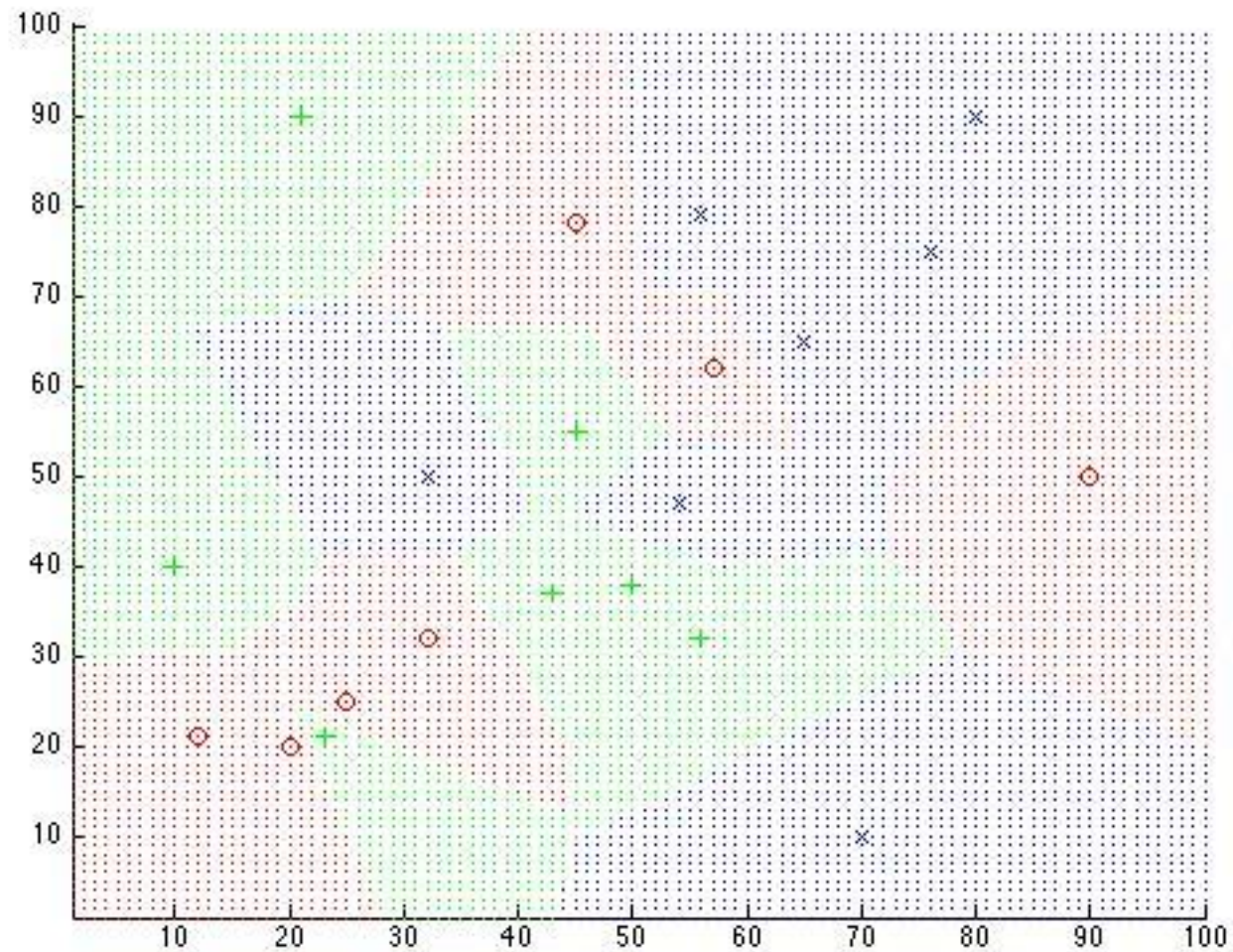
The effect of increasing k

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

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



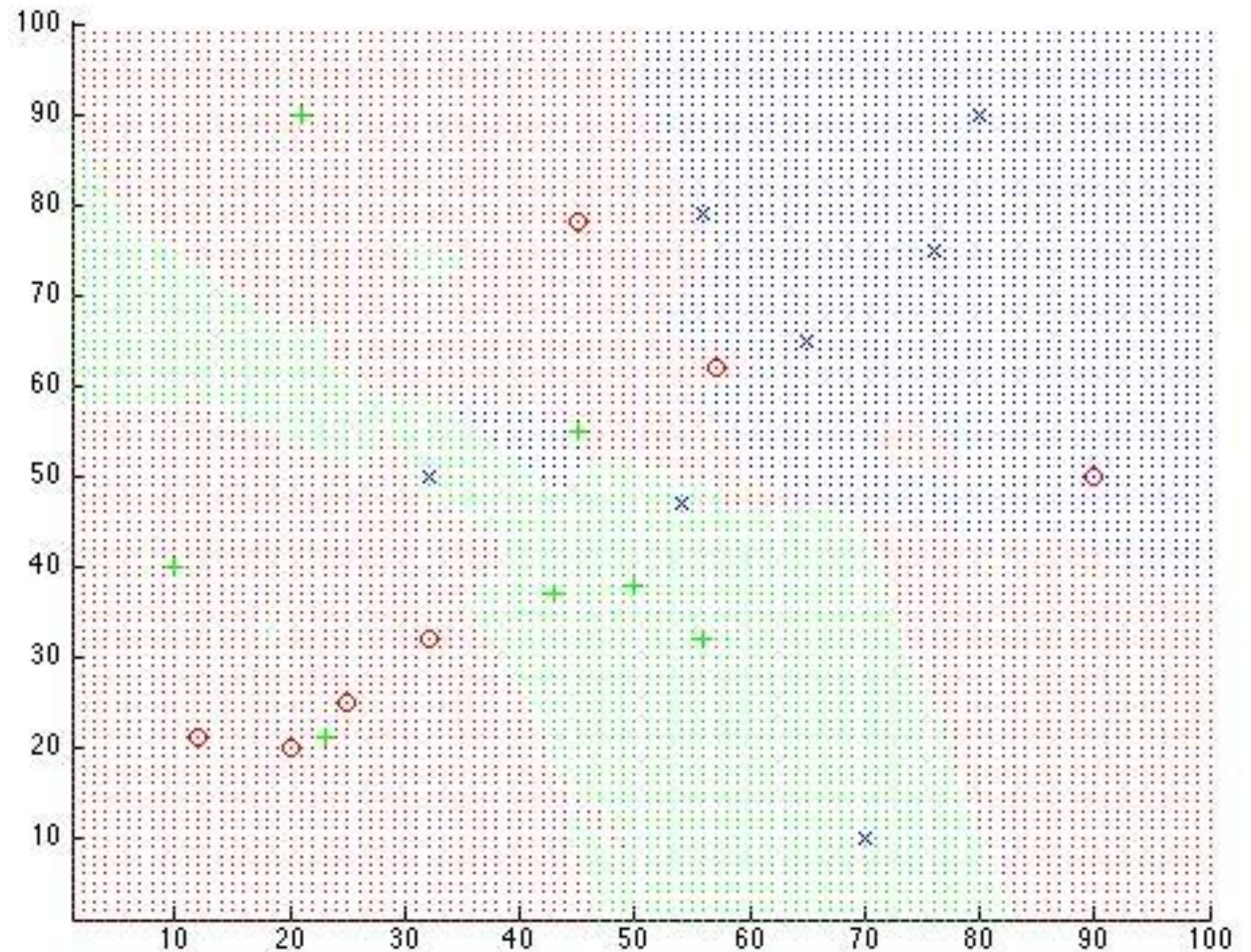
KNN with $k=1$



KNN with $k=3$

Ties are broken
using the order:

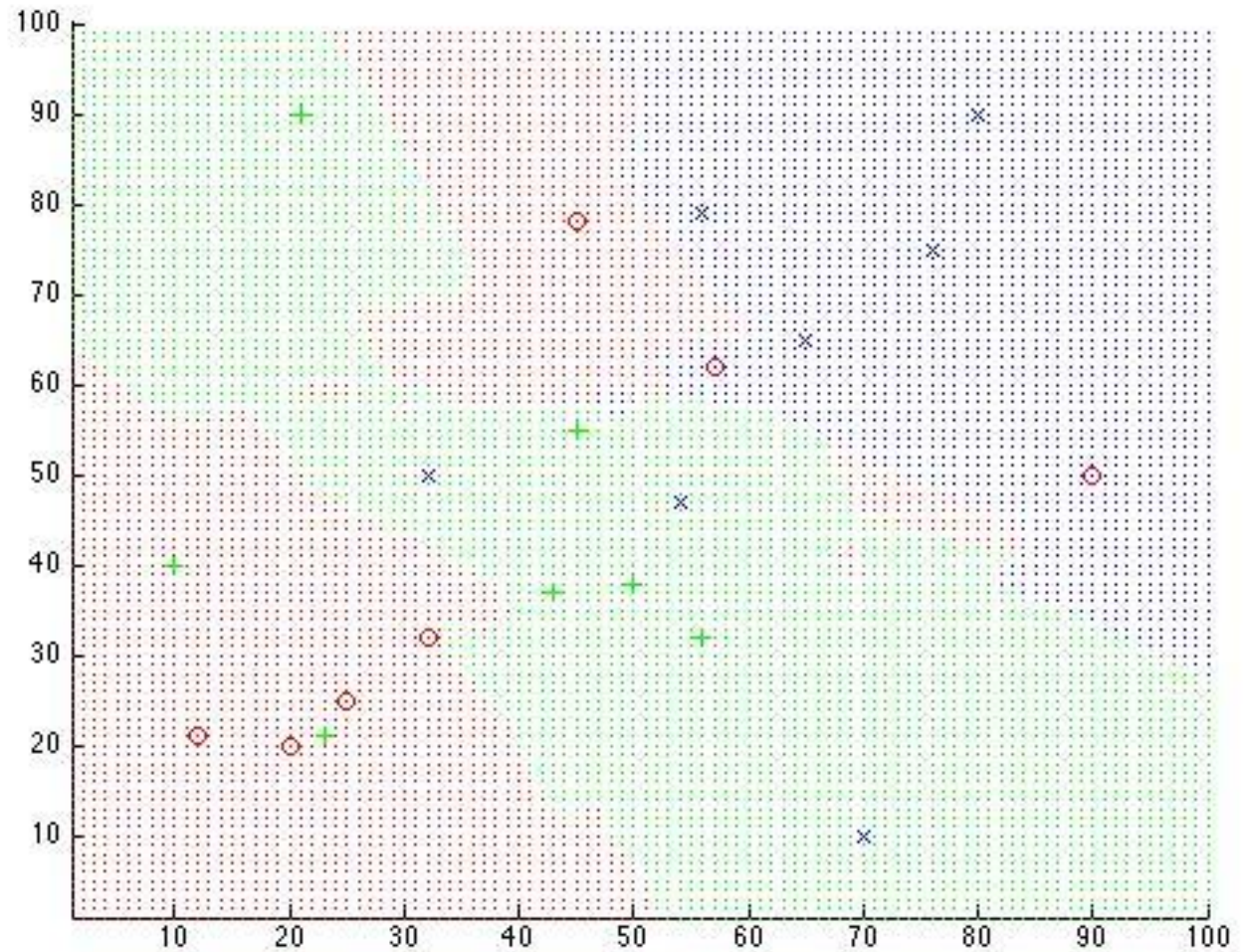
Red , Green, Blue



KNN with $k=5$

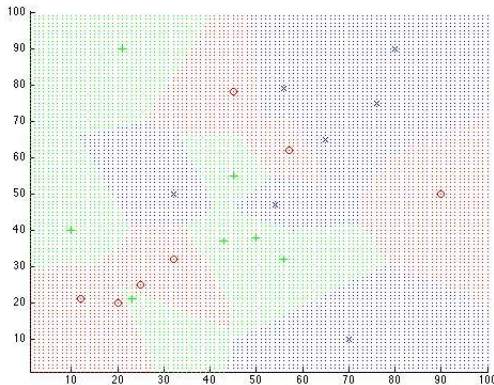
Ties are broken
using the order:

Red , Green, Blue

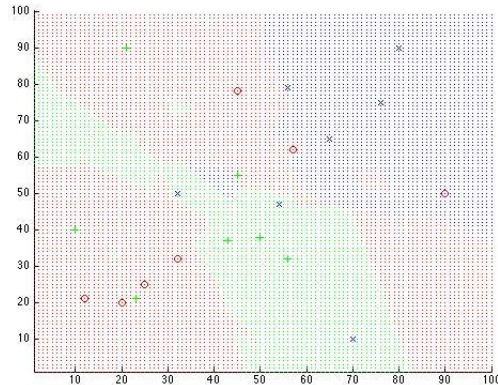


Comparisons of different k's

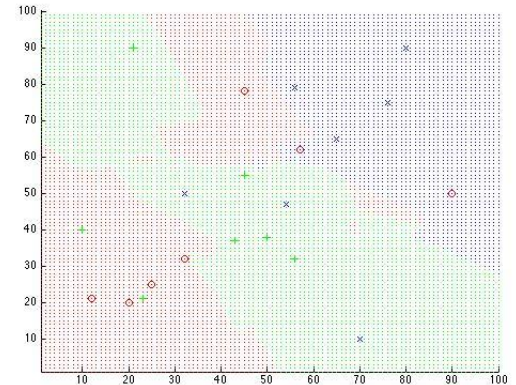
$K = 1$



$K = 3$



$K = 5$



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*

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 in z).
- Then we can write

$$p(x)V = P = \frac{K}{N} \quad p(x) = \frac{K}{NV} \quad p(x | y = 1) = \frac{K_1}{N_1V} \quad p(y = 1) = \frac{N_1}{N}$$

- Using Bayes rule we get:

$$p(y = 1 | x) = \frac{p(x | y = 1)p(y = 1)}{p(x)} = \frac{K_1}{K}$$

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:

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

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