K Nearest Neighbors and Kernel Regression

STAT5241 Section 2

Statistical Machine Learning

Xiaofei Shi

Tasks

Input → Regressor → Predict real number

Input → Classifier → Predict category

Input → Density Estimator → Probability

COLUMBIA UNIVERSITY

Types of classifiers

- Discriminative classifiers:
  - Directly estimate a decision rule/boundary
  - e.g. decision tree, SVM
- Instance based classifiers:
  - Use observation directly
  - e.g. K nearest neighborhood
- Generative classifiers:
  - Build a generative statistical model
  - e.g. Bayesian Network

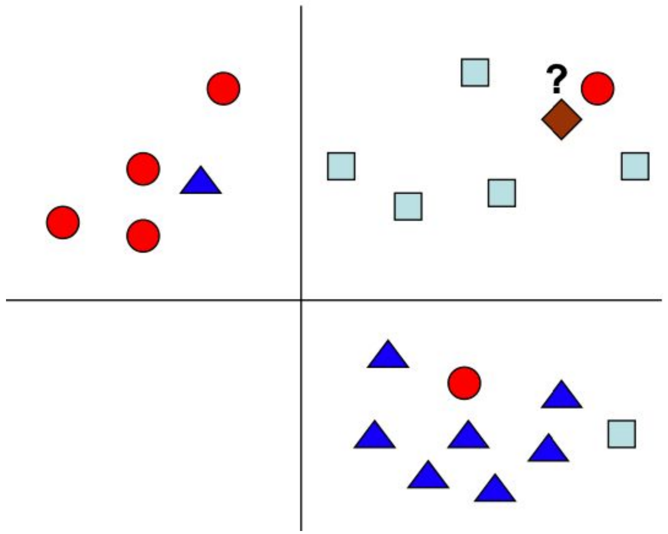
Loss function

Recall the loss function in previous classifiers:

- Logistic Regression: MLE of conditional (log)likelihood
- Decision Tree: maximum information gain
- What else?

K nearest neighbors (KNN)

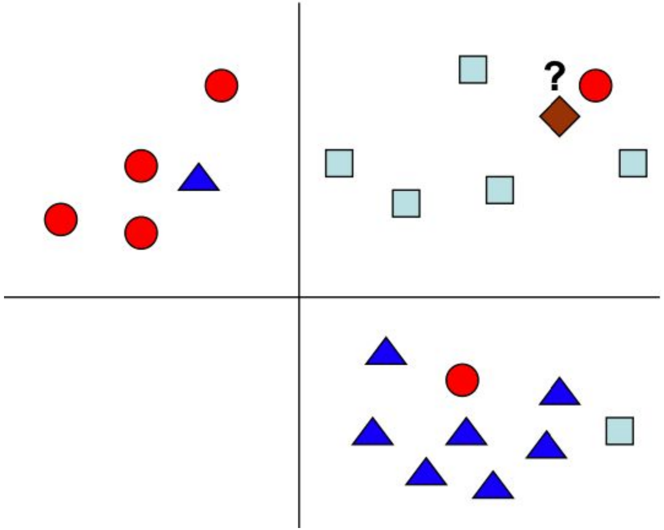
- A simple yet surprisingly efficient algorithm
- Requires the definition of a similarity measure or a distance function between sample points
- Select the class based on the majority vote among the K nearest sample points



K nearest neighbors (KNN)

- A simple yet surprisingly efficient algorithm
- Requires the definition of a similarity measure or a distance function between sample points
- Select the class based on the majority vote among the K nearest sample points

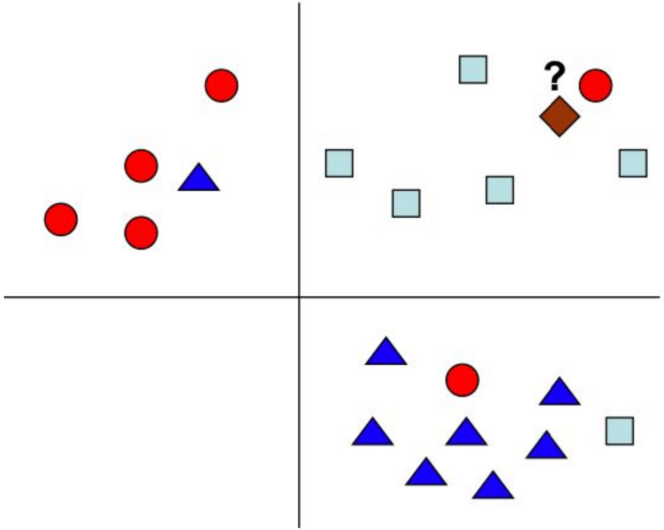
What is the best value of K?



COLUMBIA UNIVERSITY

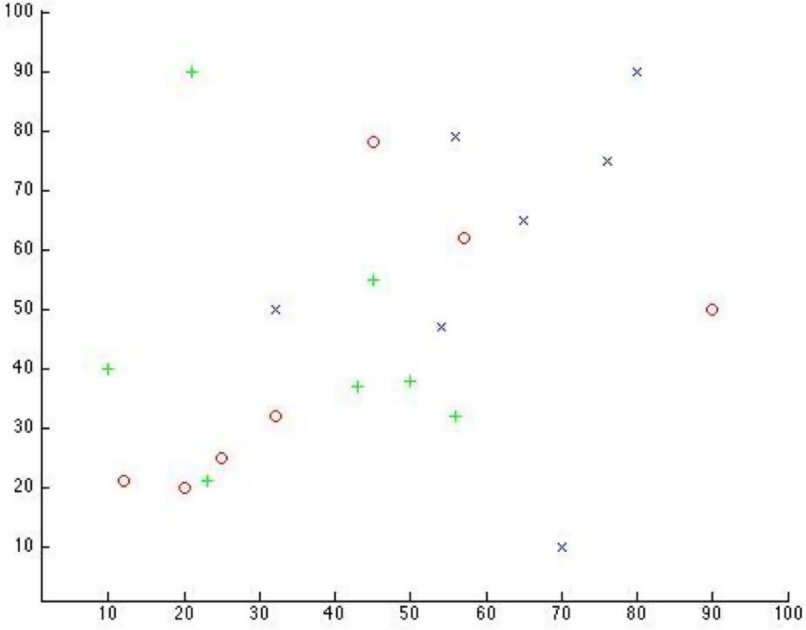
K nearest neighbors (KNN)

- Choice of K influences the “smoothness” of the resulting classifier
- In this sense, the KNN classifier is similar to a kernel methods
- However, the smoothness of the classifier should be determined by the actual distribution of the data, i.e. the density function p(x) of the data, not any predefined parameter.



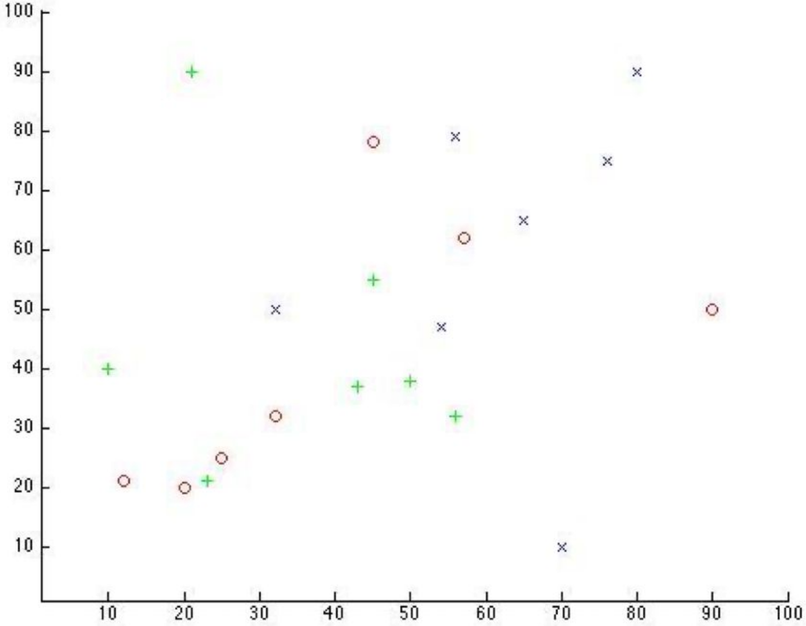
COLUMBIA UNIVERSITY

The effect of increasing K



COLUMBIA UNIVERSITY

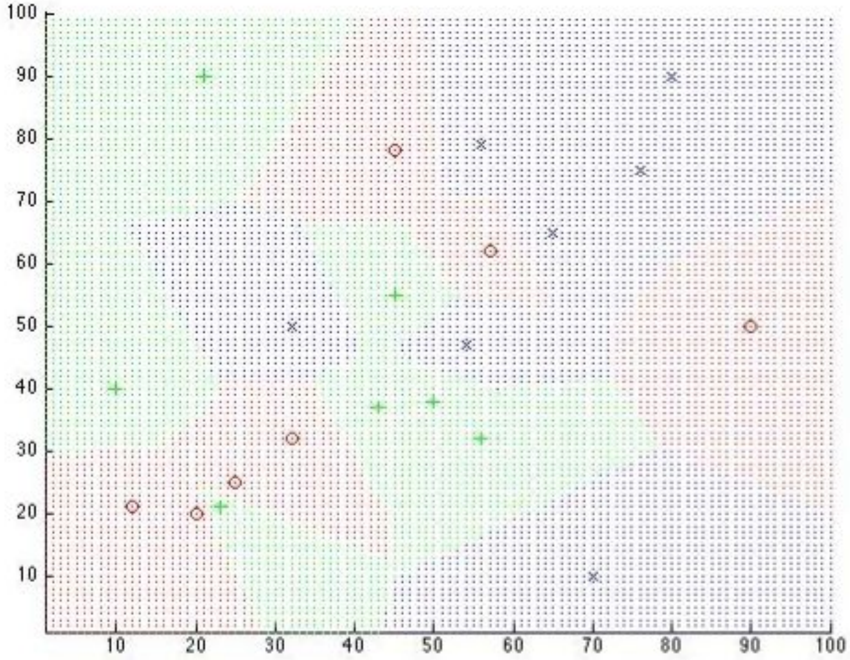
The effect of increasing K



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

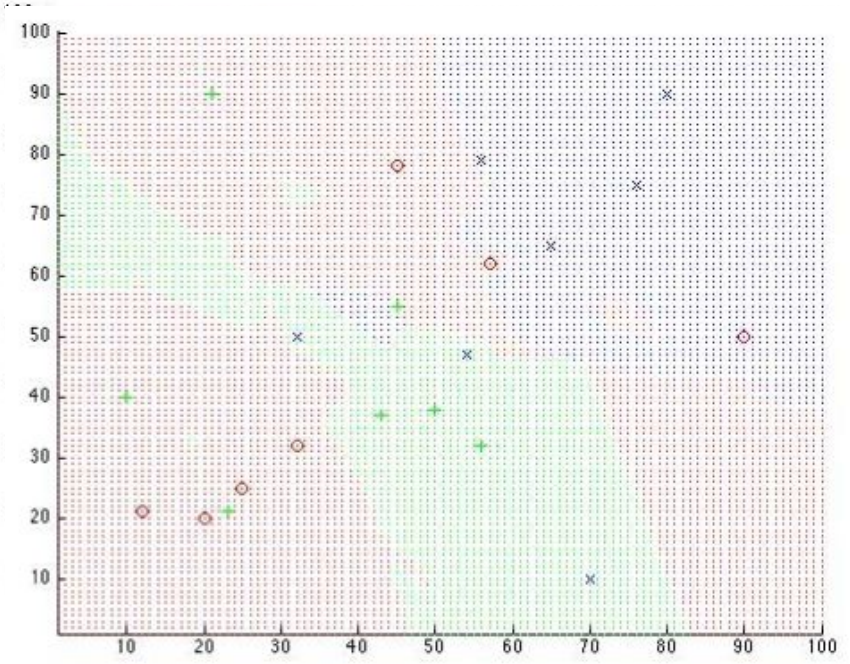
$$d(x,x') = \sqrt{\sum_i (x_i - x_i')^2}$$

The effect of increasing K



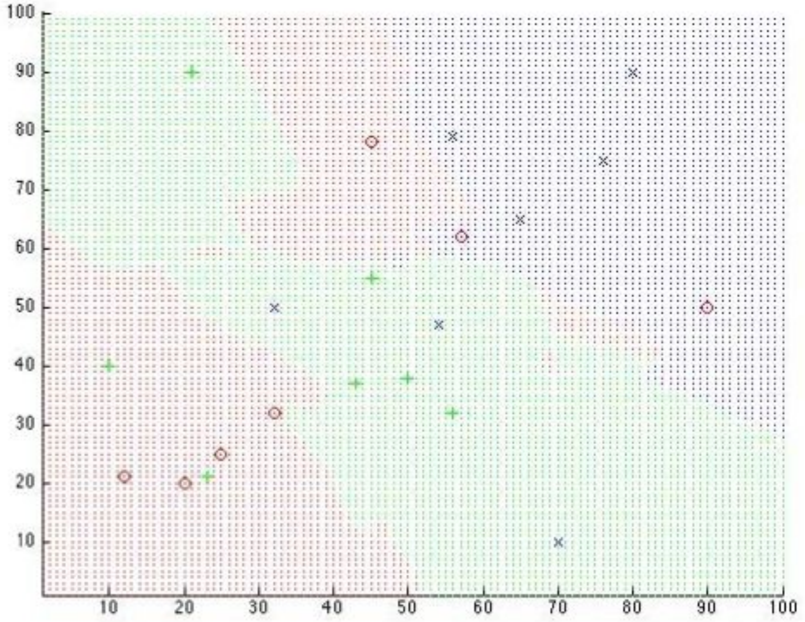
K =1

The effect of increasing K



K =3

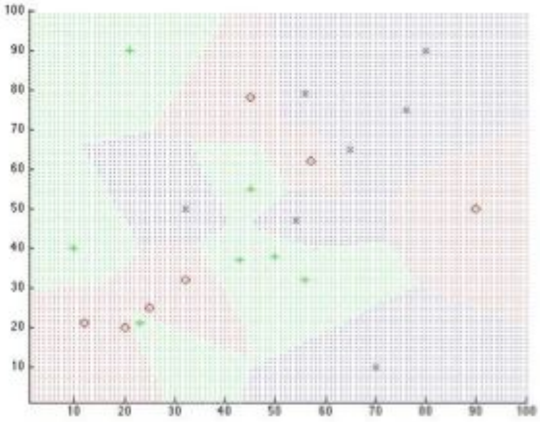
The effect of increasing K



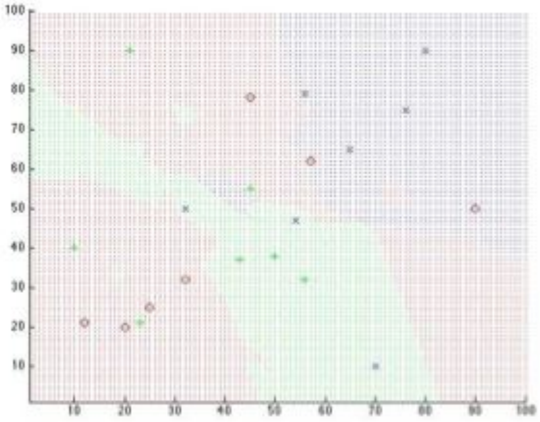
K =5

Comparison of different values of K

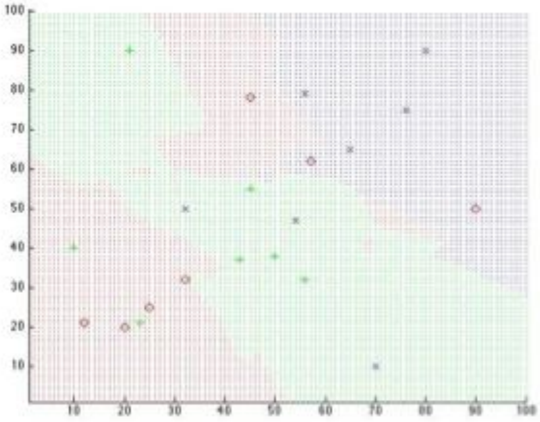
K = 1



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*

COLUMBIA UNIVERSITY

- 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:

Choose the class with the highest probability

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

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

Bayes decision rule

Bayes Rule: $$P(Y|X) = \frac{P(X|Y)P(Y)}{P(X)}$$

$$P(Y = y|X = x) = \frac{P(X = x|Y = y)P(Y = y)}{P(X = x)}$$

COLUMBIA UNIVERSITY

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 …

Columbia University

Bayes decision rule

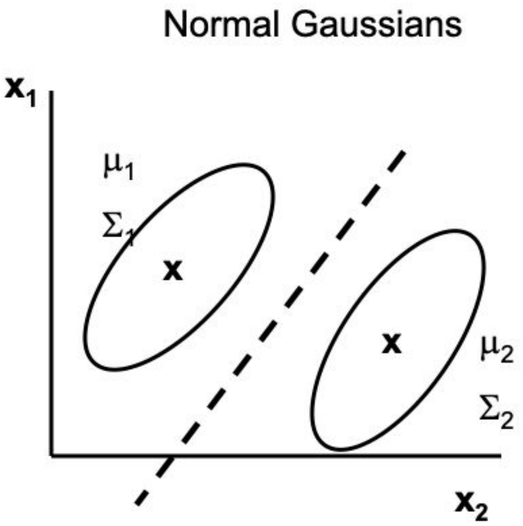
$$P(y=i \mid x) = \frac{P(x \mid y=i)P(y=i)}{P(x)} \stackrel{def}{=} q_i(x)$$

- 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

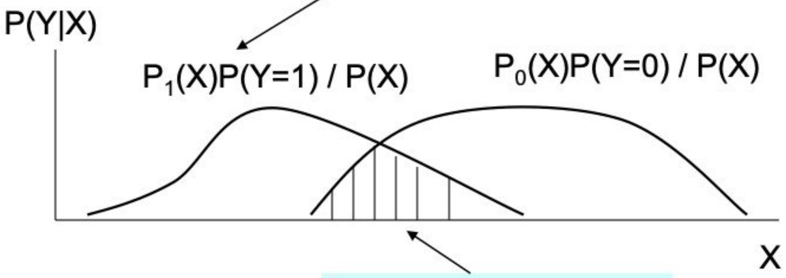
Binary case: separable v.s. non-separable



Classification 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**

p(x | y =1)



x values for which we will have errors

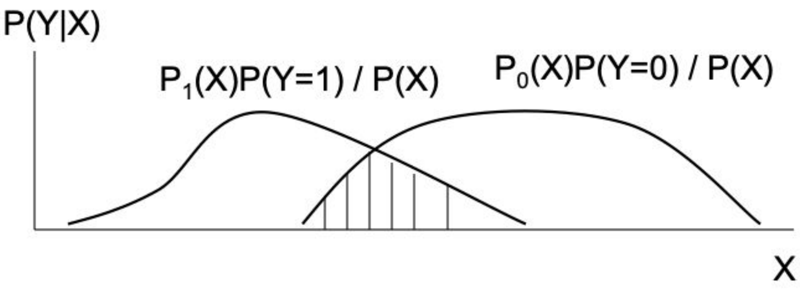
- The risk for sample x is:

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

Risk can be used to determine a 'reject' region

COLUMBIA UNIVERSITY

Bayes error



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

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

- 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

COLUMBIA UNIVERSITY

Takeaways

- Optimal decision using Bayes rule
- Type of classifiers
- Effect of values of K on KNN classifiers
- Probabilistic interpretation of KNN

References

- Tom Mitchell: Machine Learning, Chapter 8
- Kevin Murphy: Machine Learning: A probabilistic perspective, Chapter 14
- Trevor Hastie, Robert Tibshirani, Jerome Friedman: The Elements of Statistical Learning: Data Mining, Inference and Prediction, Chapter 6, 13
- Ziv Bar-Joseph, Tom Mitchell, Pradeep Ravikumar and Aarti Singh: CMU 10-701

Columbia University