Machine Learning

KNN Classifier and r-fold Cross Validation

Indian Institute of Information Technology
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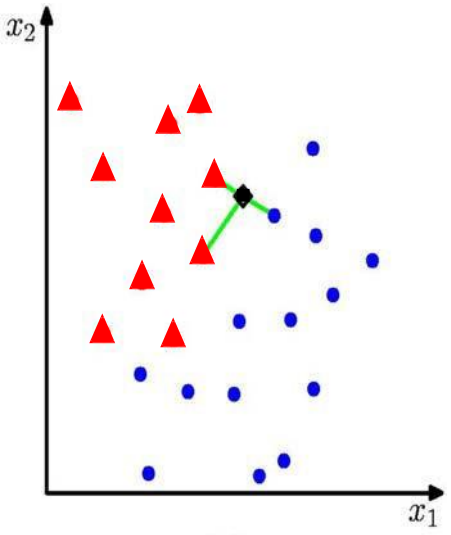
Today's Agenda

- K-Nearest Neighbor Classifier
- r-fold Cross validation

K-Nearest Neighbor Classifier

- Algorithm
  - For each test point, x, to be classified, find the K nearest samples in the training data
  - Classify the point, x, according to the majority vote of their class labels

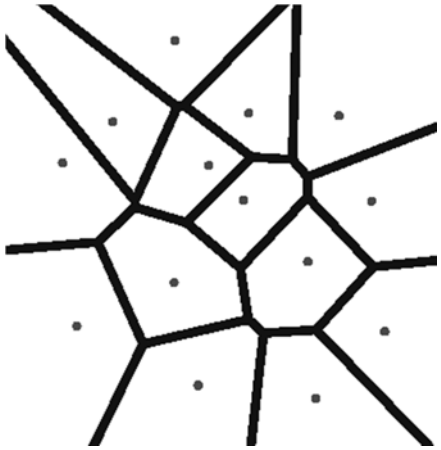
- e.g. K = 3



- applicable to multi-class case

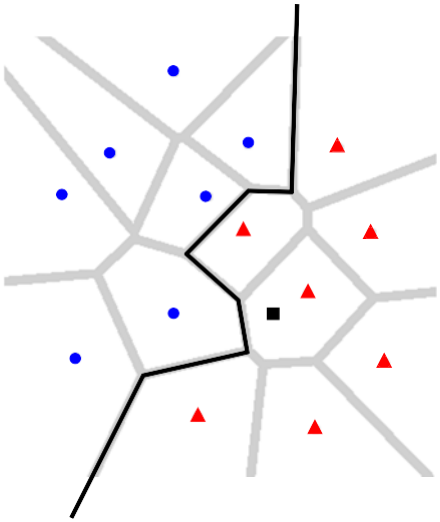
K-Nearest Neighbor Classifier

K = 1



Voronoi diagram:

- partitions the space into regions
- boundaries are equal distance from training points



Classification boundary:

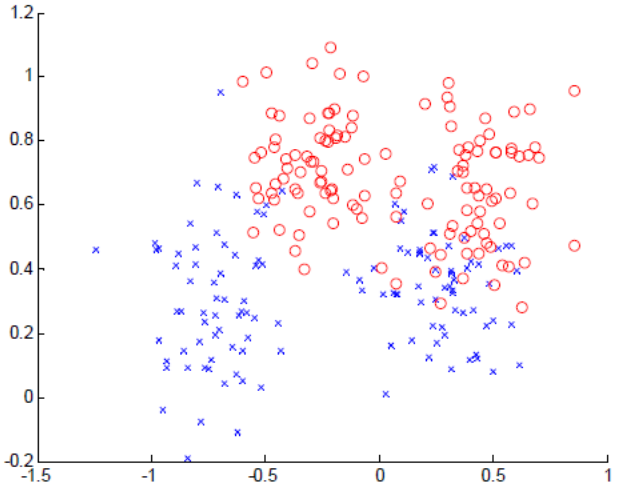
- non-linear

K-Nearest Neighbor Classifier

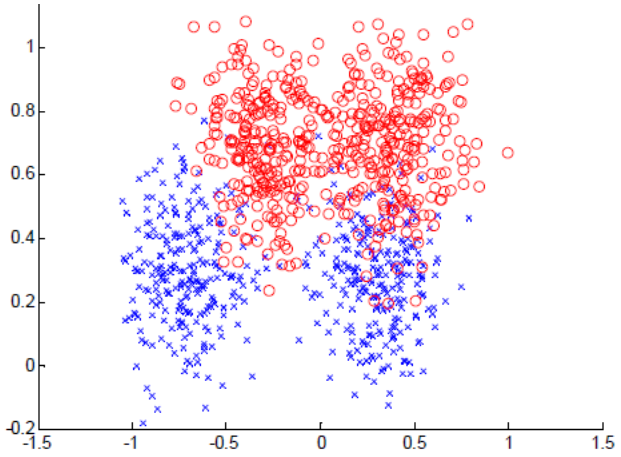
• Assume that the training examples are drawn independently from the set of all possible examples.

• This makes it very unlikely that a strong regularity in the training data will be absent in the test data.

• Measure classification error as = $\frac{1}{N}\sum_{i=1}^{N}\underbrace{[\mathbf{y}_i \neq f(\mathbf{x}_i)]}_{\text{loss function}}$ The "risk"



Training data

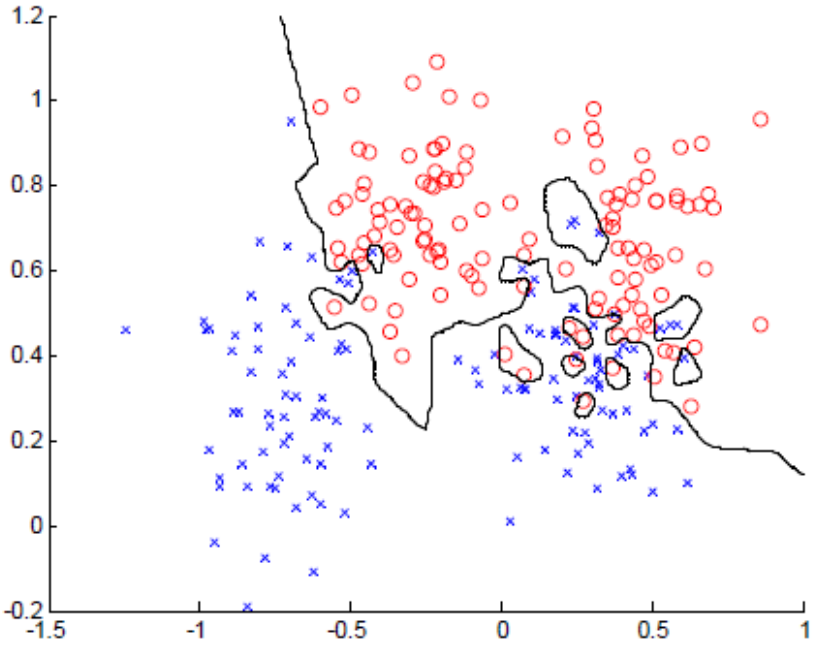


Testing data

K-Nearest Neighbor Classifier

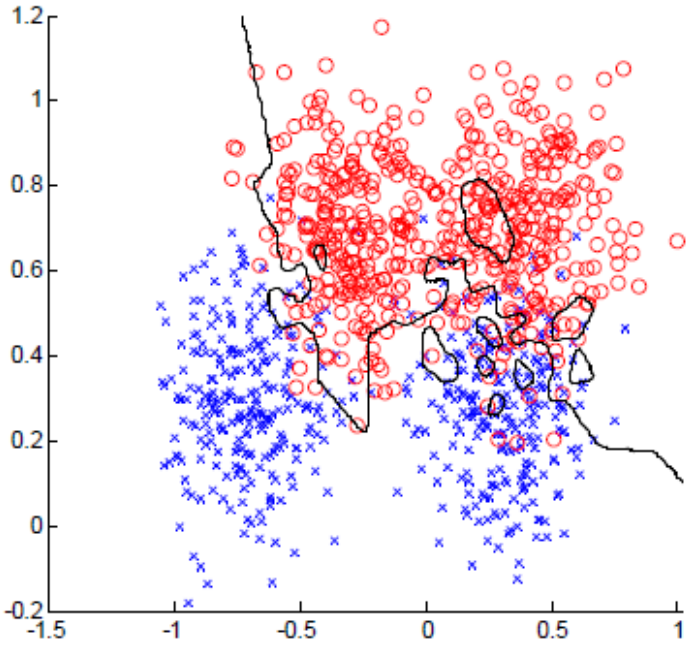
K=1

Training data



error = 0.0

Testing data



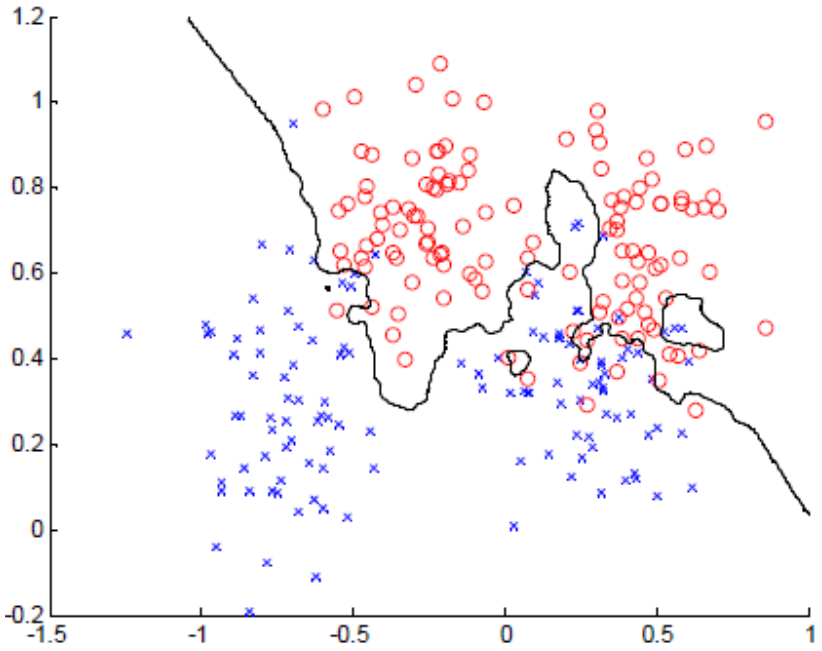
error = 0.15

Slide adapted from Andrew Zisserman

K-Nearest Neighbor Classifier

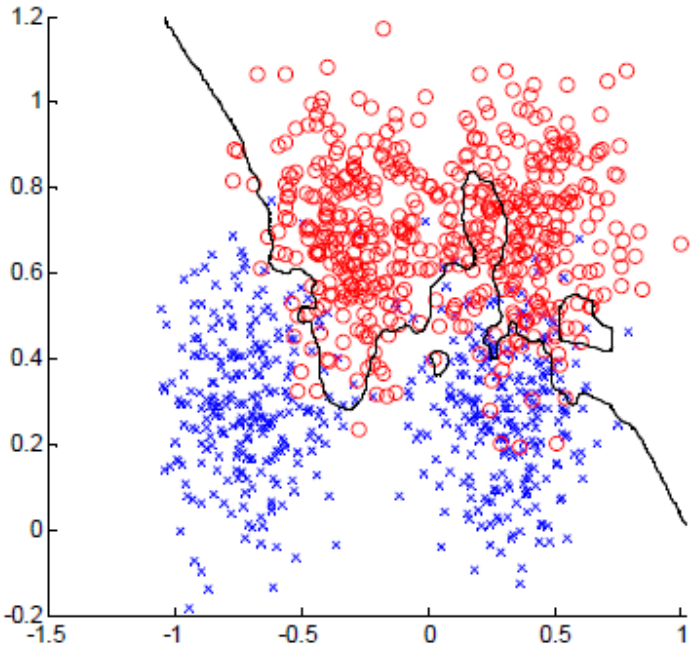
K=3

Training data



error = 0.0760

Testing data



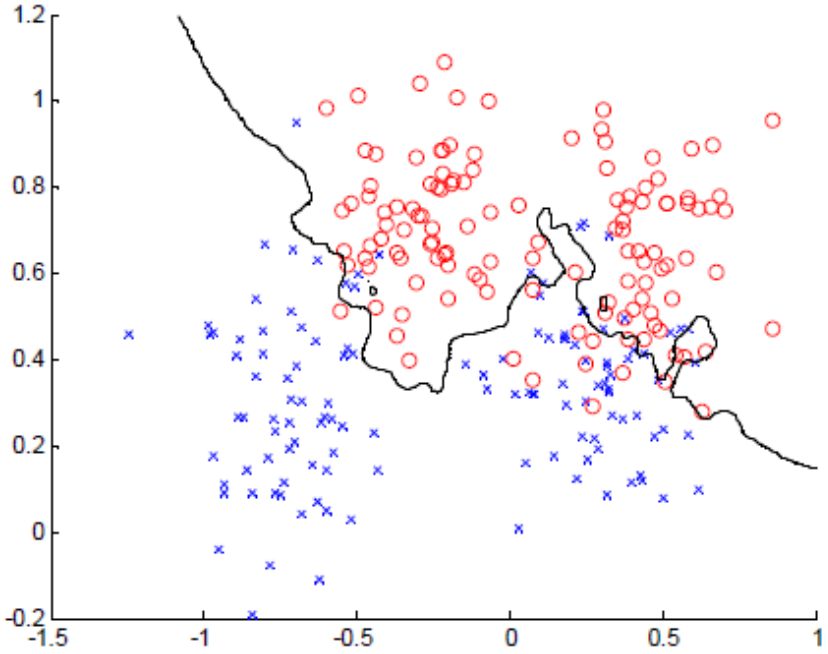
error = 0.1340

Slide adapted from Andrew Zisserman

K-Nearest Neighbor Classifier

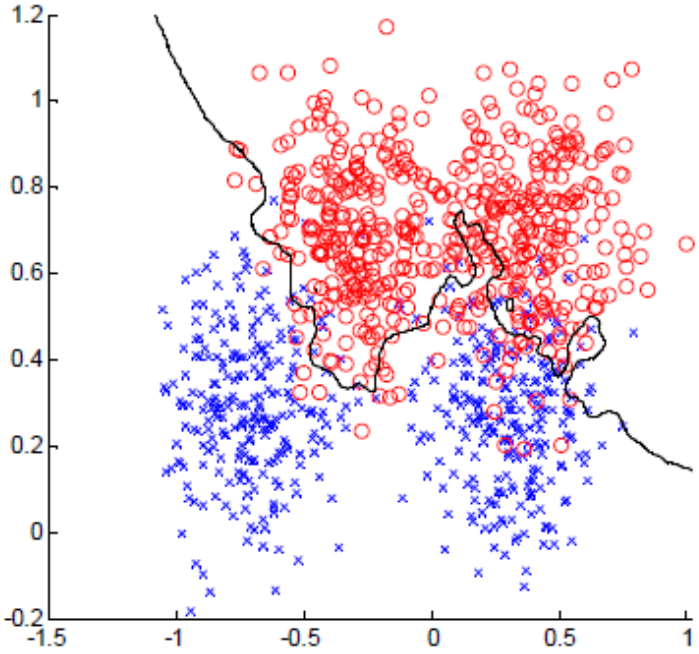
K=7

Training data



error = 0.1320

Testing data



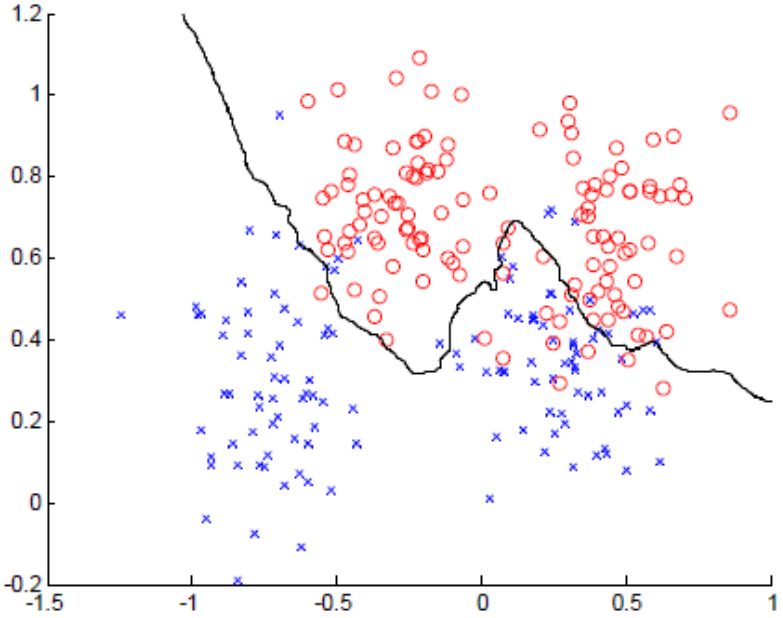
error = 0.1110

Slide adapted from Andrew Zisserman

K-Nearest Neighbor Classifier

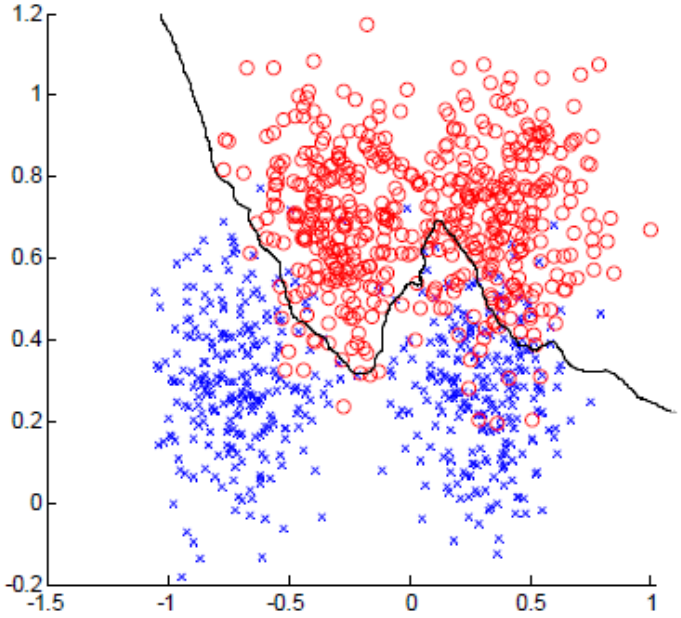
K=21

Training data



error = 0.1120

Testing data



error = 0.0920

Slide adapted from Andrew Zisserman

K-Nearest Neighbor Classifier

- The real aim of supervised learning is to do well on test data that is not known during learning
- Choosing the values for the parameters that minimize the loss function on the training data is not necessarily the best policy
- We want the learning machine to model the true regularities in the data and to ignore the noise in the data.

K-Nearest Neighbor Classifier

As K increases:

- Classification boundary becomes smoother
- Training error can increase

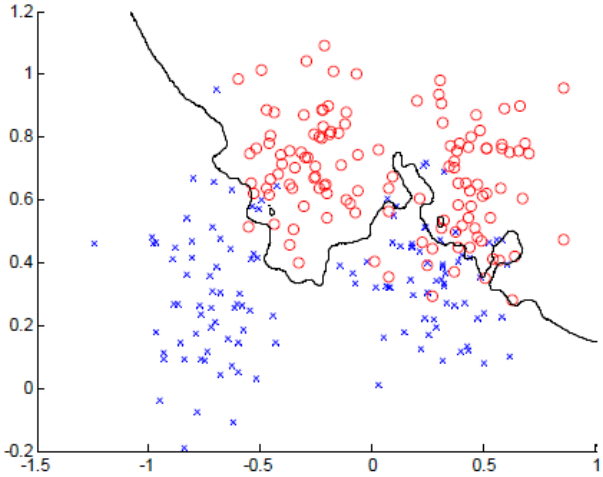
Choose (learn) K by cross-validation

- Split training data into training and validation
- Hold out validation data and measure error on this

K-Nearest Neighbor Classifier

Advantages:

- K-NN is a simple but effective classification procedure
- Applies to multi-class classification
- Decision surfaces are non-linear
- Quality of predictions automatically improves with more training data
- Only a single parameter, K; easily tuned by cross-validation

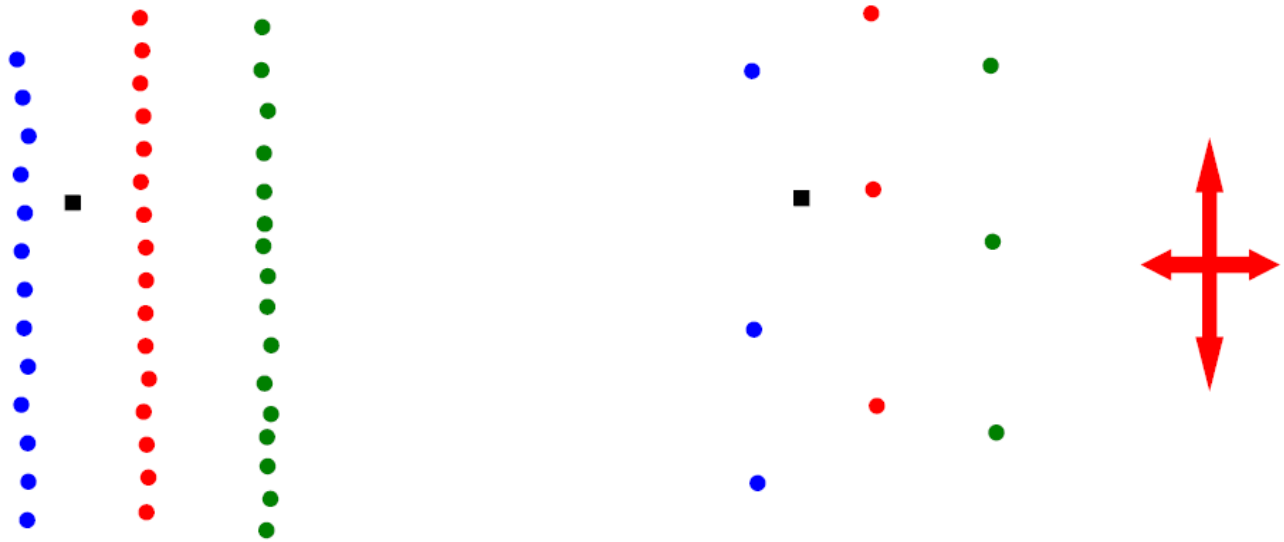


Slide adapted from Andrew Zisserman

K-Nearest Neighbor Classifier

Disadvantages:

- What does nearest mean? Need to specify a distance metric.
- Computational cost: must store and search through the entire training set at test time. Can alleviate this problem by thinning, and use of efficient data structures like KD trees.



Slide adapted from Andrew Zisserman

Cross Validation

- How to find appropriate k value for k-NNC.
- Some improvements to k-NNC

Cross Validation

r-fold cross validation:

1. Partition the training set into r blocks. Let these are $D_1, D_2, \ldots, D_r$.
2. For i = 1 to r do
   I. Consider $D - D_i$ as the training set and D_i as the validation set.
   II. For a range of k values (say from 1 to m) find the error rates on the validation set.
   III. Let these error rates are $e_{i1}, e_{i2}, \ldots, e_{im}$
3. Take e_i = mean of $\{e_{1i}, e_{2i}, \ldots., e_{ri}\}$, for i = 1 to m.
4. k value = $\underset{j}{\text{argmin}} \{e_1, e_2, \ldots.,e_j, \ldots, e_m\}$

Slide adapted from Dr. P. Viswanath

Cross Validation

- One should not use *the test set* to decide the value of K.
- Test set should be used only after fixing K, to get the final *error-rate* for the classifier.
- Cross validation is only to fix the value of parameters like K . So the error rates on validation sets should be called *validation error rates*.

Slide adapted from P. Viswanath

Thank You: Question?