CS6510

Applied Machine Learning

Classifiers: kNN, Decision Trees

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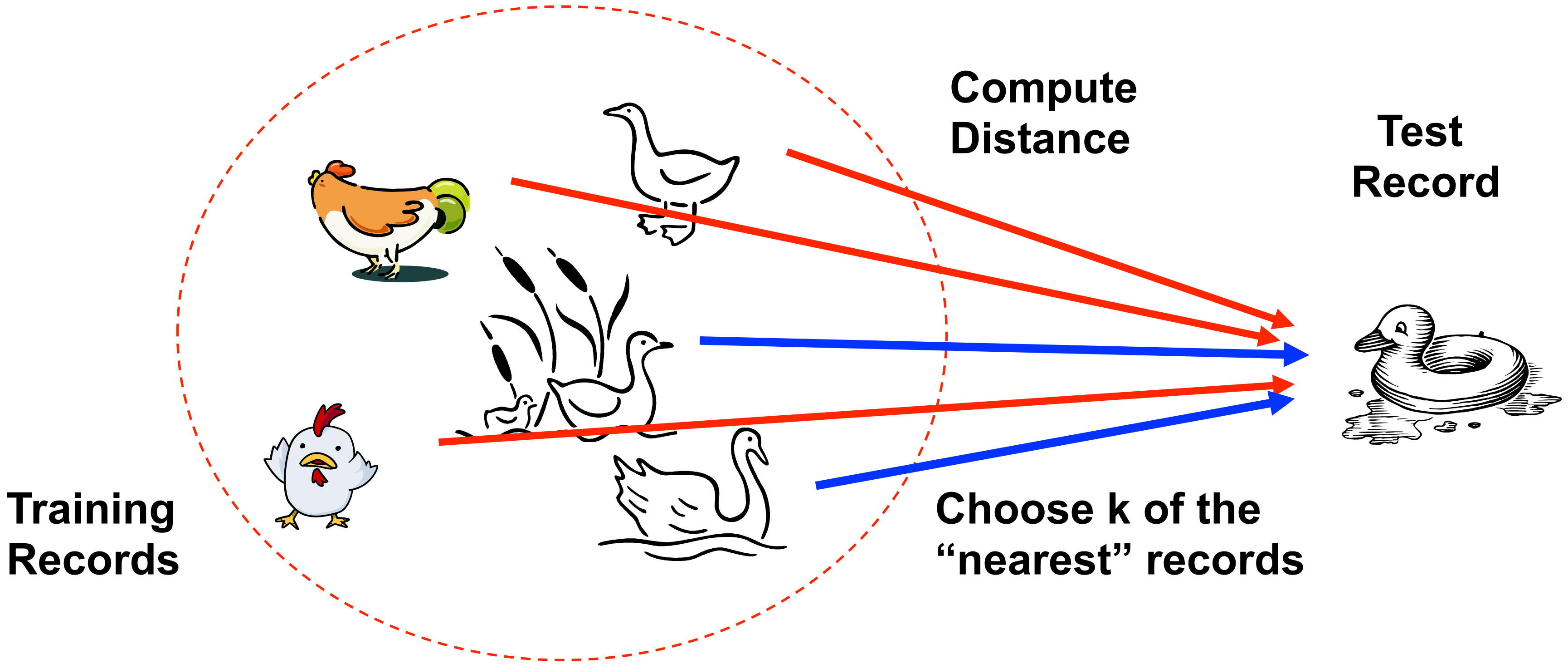
Classification Methods

- k-Nearest Neighbors
- Decision Trees
- Naïve Bayes
- Support Vector Machines
- Logistic Regression
- Neural Networks
- Ensemble Methods (Boosting, Random Forests)

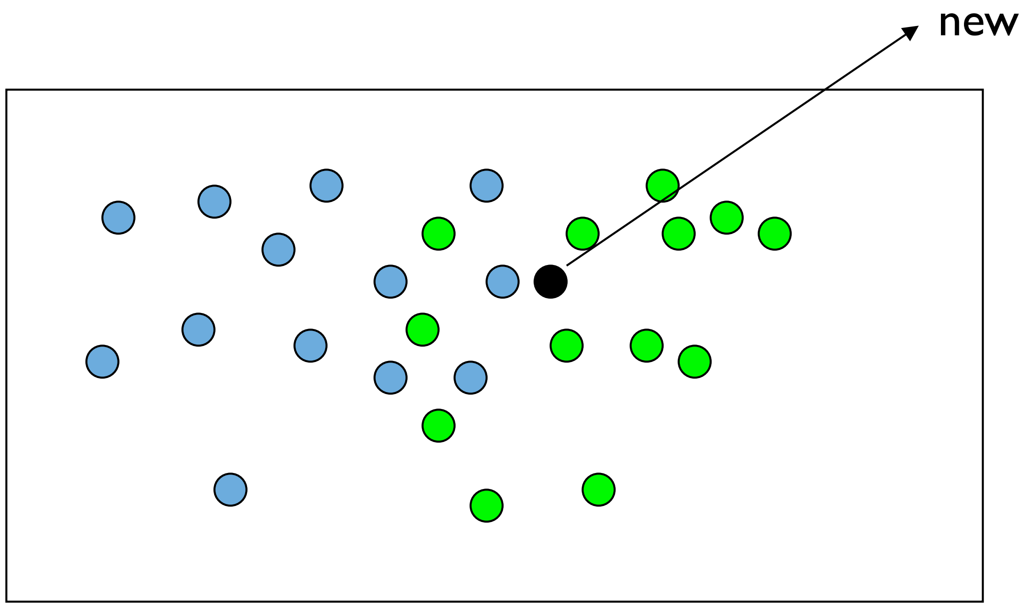
k-Nearest Neighbors

- Basic idea:
  - If it walks like a duck, quacks like a duck, then it's probably a duck



k-Nearest Neighbors

- Majority vote within the k nearest neighbors



K= 1: blue

K= 3: green

k-Nearest Neighbors

- An arbitrary instance is represented by $\mathbf{(a_1(x), a_2(x), a_3(x),.., a_n(x))}$
  - $\mathbf{a_i(x)}$ denotes features
- Euclidean distance between two instances
  - **$d(x_i, x_j)$=sqrt (sum for r=1 to n $(a_r(x_i) - a_r(x_j))^2$)**
- L_p distance
  - p=2: Euclidean distance
  - p=1: Manhattan distance
  - p =∞: Max distance
  - p= 0: Count non-zero distance
- In case of continuous-valued target function
  - Mean value of k nearest training examples

Other Distance Metrics

- Cosine Distance Metric

$$\rho(\vec{x}_1, \vec{x}_2) = \cos(\angle(\vec{x}_1, \vec{x}_2)) = \frac{\vec{x}_1 \cdot \vec{x}_2}{\|\vec{x}_1\|_2 \ \|\vec{x}_2\|_2}$$

- Edit Distance

x_1 = AAATCCCGTAA

x_2 = AATCGCGTAA

Minimum number of insertions, deletions and mutations needed

$$\rho(x_1, x_2) = 2$$

- Kendell-Tau Distance

x_1 = [o1 o2 o3 o4 o5]

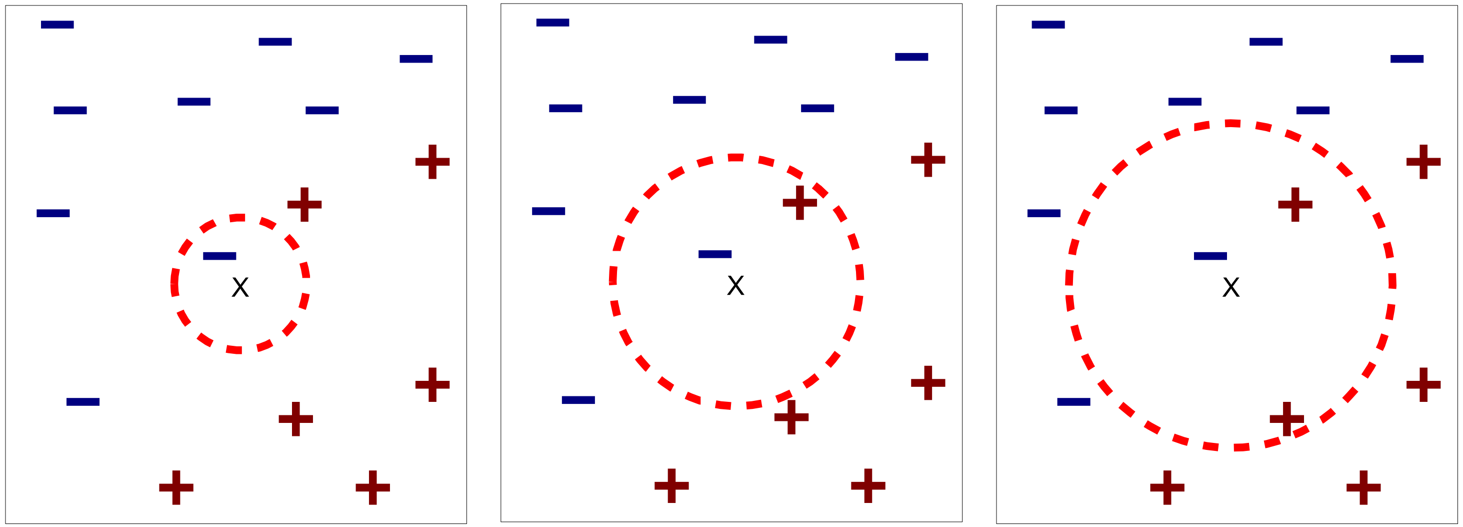
x_2 = [o2 o1 o3 o4 o5]

Bubble sort distance to make one ranking order same as the other

$$\rho(x_1, x_2) = 1$$

k-Nearest Neighbors

- Choosing k is important
  - If k is too small, sensitive to noise points
  - If k is too large, neighborhood may include points from other classes



(a) 1-nearest neighbor (b) 2-nearest neighbor (c) 3-nearest neighbor

How to determine k

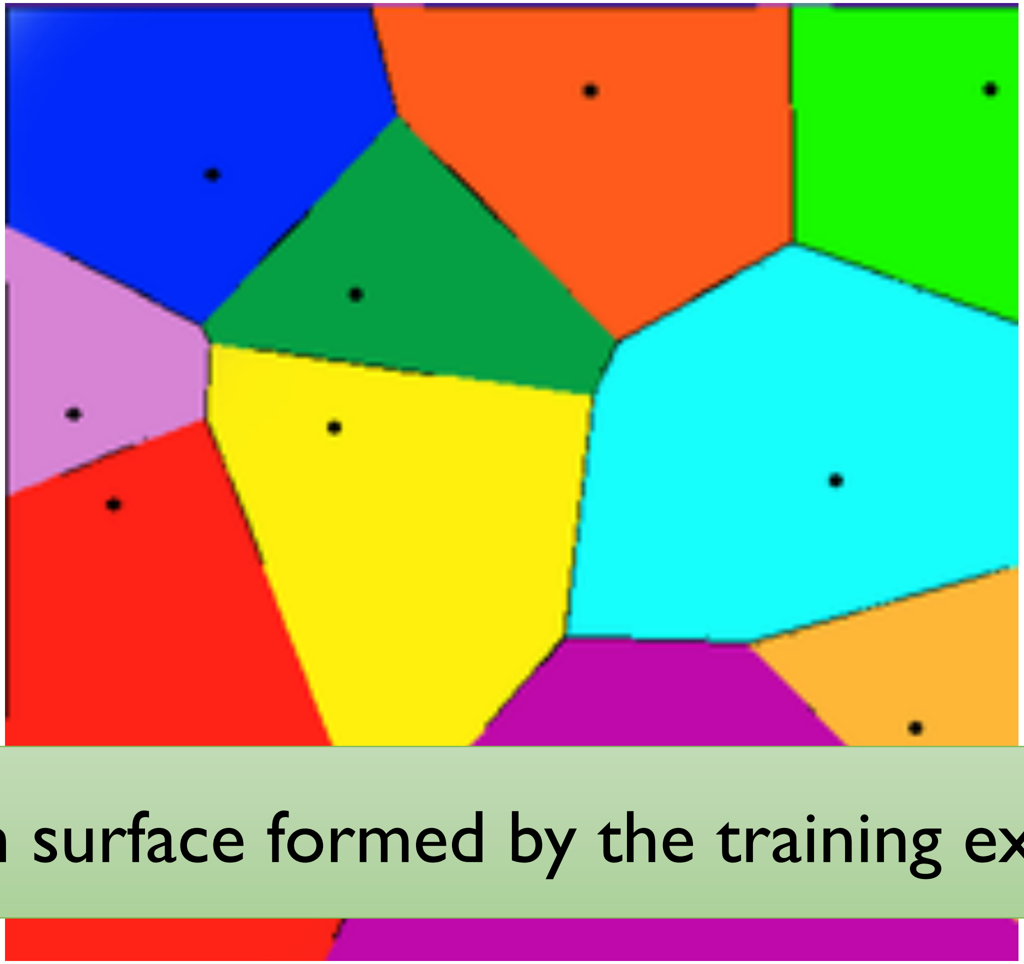
- Determined experimentally (think cross-validation!)
  - Start with k=1 and use a test set to validate the error rate of the classifier
  - Repeat with k=k+2
  - Choose the value of k for which the error rate is minimum
  - Note: k typically an odd number to avoid ties in binary classification

k-Nearest Neighbors

- Eager Learning (Induction)
  - Explicit description of target function on the whole training set
- Instance-based Learning (Transduction)
  - Learning=storing all training instances
  - Classification=assigning target function to a new instance
  - Referred to as "Lazy" learning

Similar Keywords: K-Nearest Neighbors, Memory-Based Reasoning, Example-Based Reasoning, Instance-Based Learning, Case-Based Reasoning, Lazy Learning

Voronoi Diagram



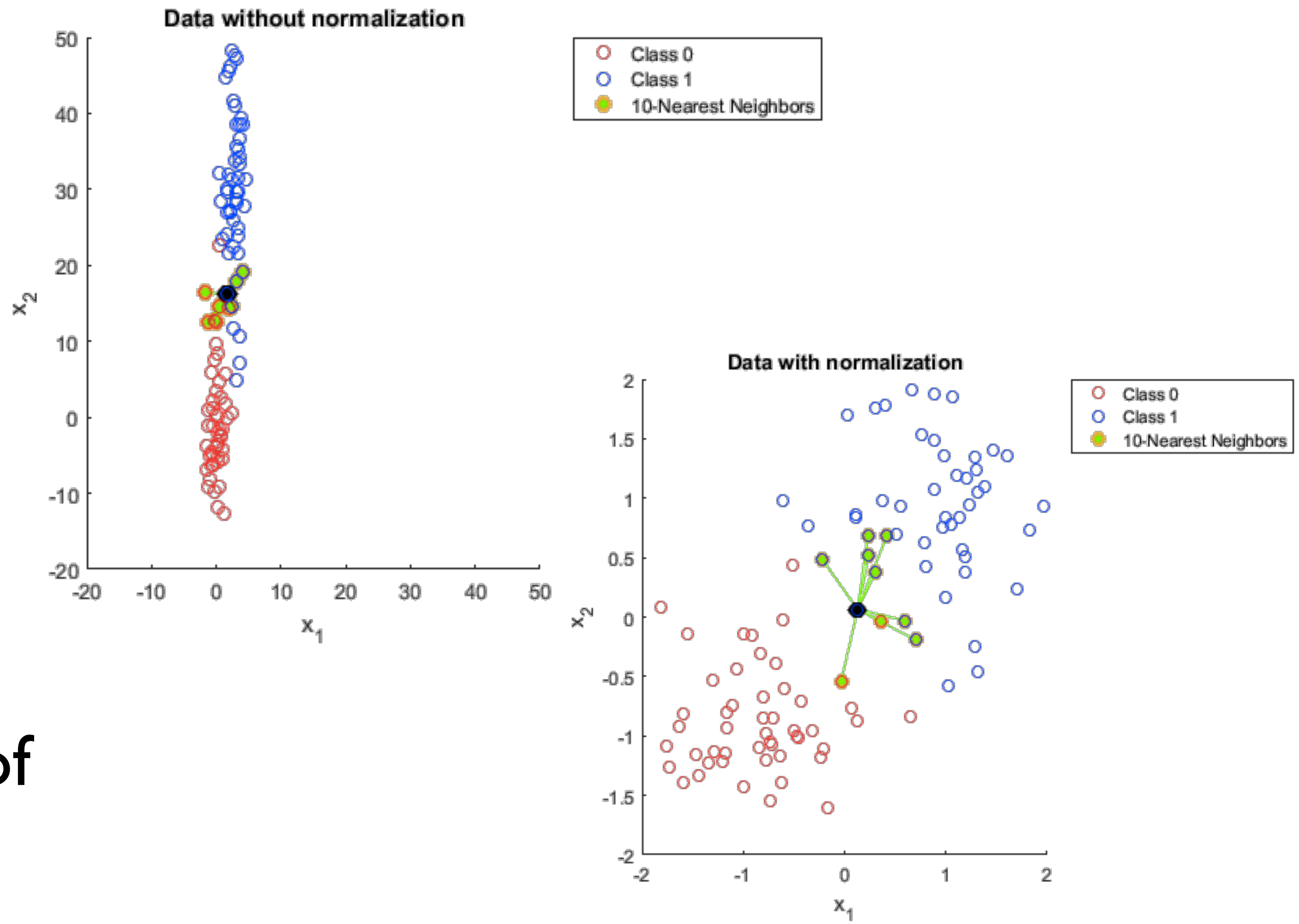
Decision surface formed by the training examples!

Pros and Cons

- Pros
  - Highly effective inductive inference method for noisy training data and complex target functions
  - Target function for a whole space may be described as a combination of less complex local approximations
  - Trains very fast ("Lazy" learner)
- Cons
  - Curse of dimensionality
    - In higher dimensions, all data points lie on the surface of the unit hypersphere!
  - Closeness in raw measurement space may not be good for the task
  - Storage: all training examples are saved in memory
    - A decision tree or linear classifier is much smaller
  - Slow at query time
    - Can be overcome and presorting and indexing training samples

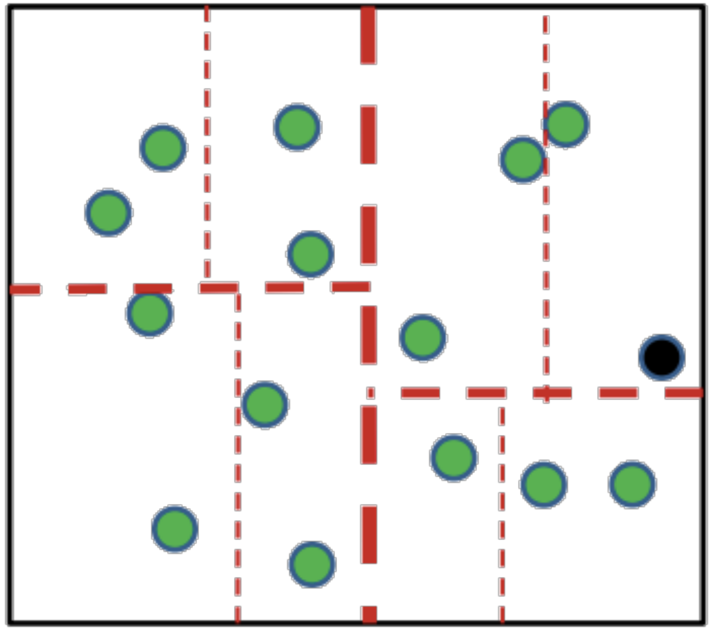
Improvements

- Measure “closeness” differently
- Distance-Weighted Nearest Neighbors
  - Assign weights to the neighbors based on their ‘distance’ from the query point (E.g., weight ‘may’ be inverse square of the distances)
  - Can also learn this -> “**Metric Learning**”
- Scaling (**normalization**) attributes for fair computation of distances



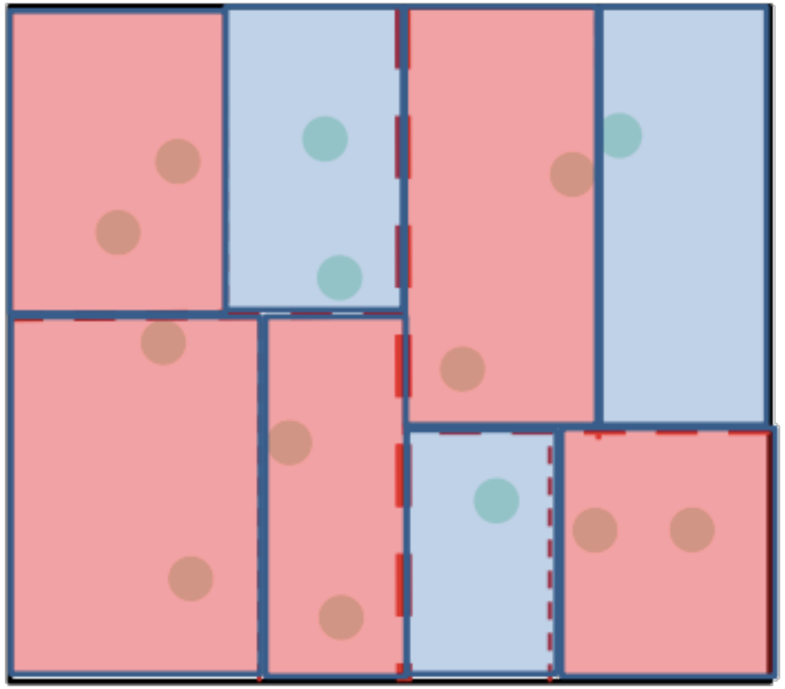
Improvements

- Finding "close" examples in a large training set quickly
  - E.g. Efficient memory indexing using kd-trees
    - In 1-dimension, can reduce complexity from O(n) to O(log n) – assuming data is sorted
  - Other methods
    - Cover trees, Ball trees, spill trees
    - Locality-Sensitive Hashing, Vector Quantization, Clustering-based methods



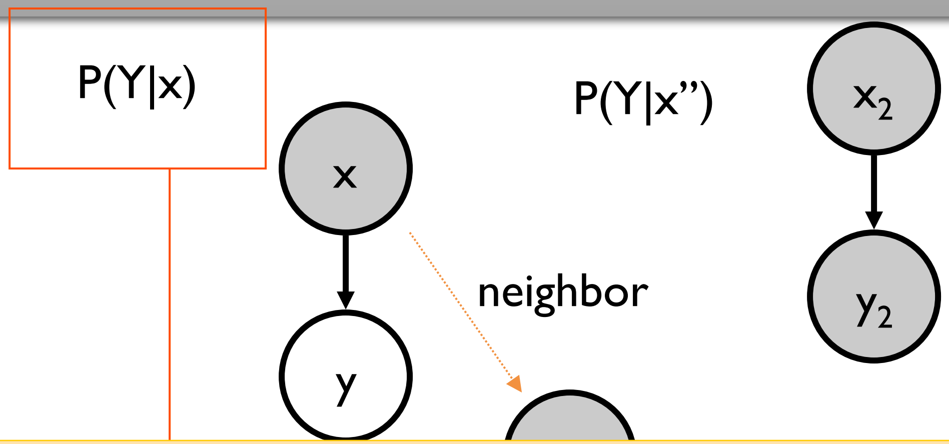
Improvements

- Not storing all examples
  - We can label each cell instead and discard the training data
  - What's the space requirement then?
  - # cells (of width r) = min{n,~$(1/r)^d$}



Convergence of 1-NN

$$P(\text{knnError})$$
$$= 1 - \Pr(y = y_1)$$
$$= 1 - \sum_{y'} \Pr(Y = y' | x)^2$$



Possible to show that: as the size of training data set approaches infinity, the one nearest neighbor classifier guarantees an error rate of no worse than twice the Bayes error rate (the minimum achievable error rate given the distribution of the data). We will see this later.

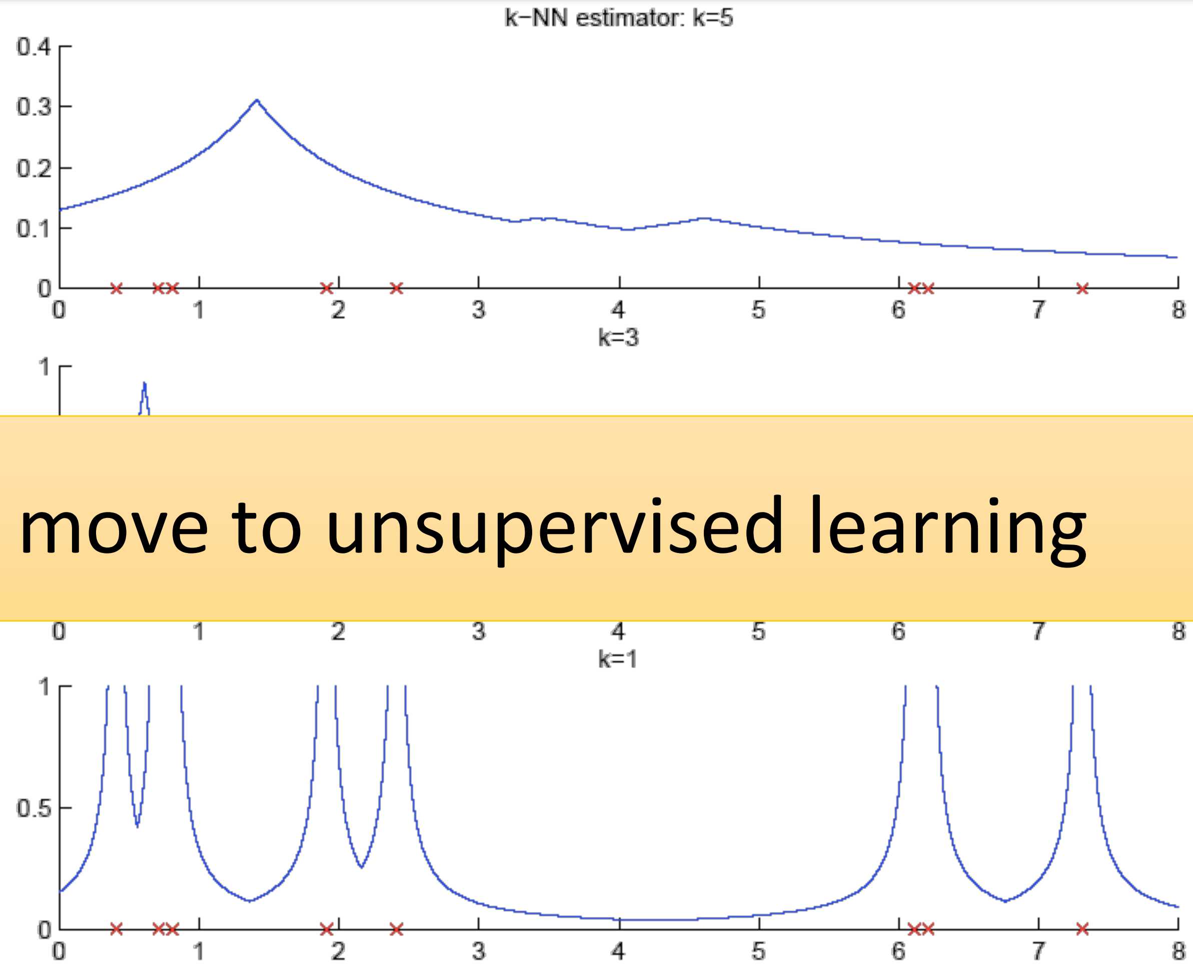
Non-parametric Density Estimation using kNNs

- **K-Nearest Neighbor estimator**
- Instead of fixing bin width h and counting the number of instances, fix

More later when we move to unsupervised learning

$$\hat{p}(x) = \frac{k}{2Nd_k(x)}$$

$d_k(x)$, distance to kth closest instance to x



Source: Ethem Alpaydin, Introduction to Machine Learning, 3rd Edition (Slides)

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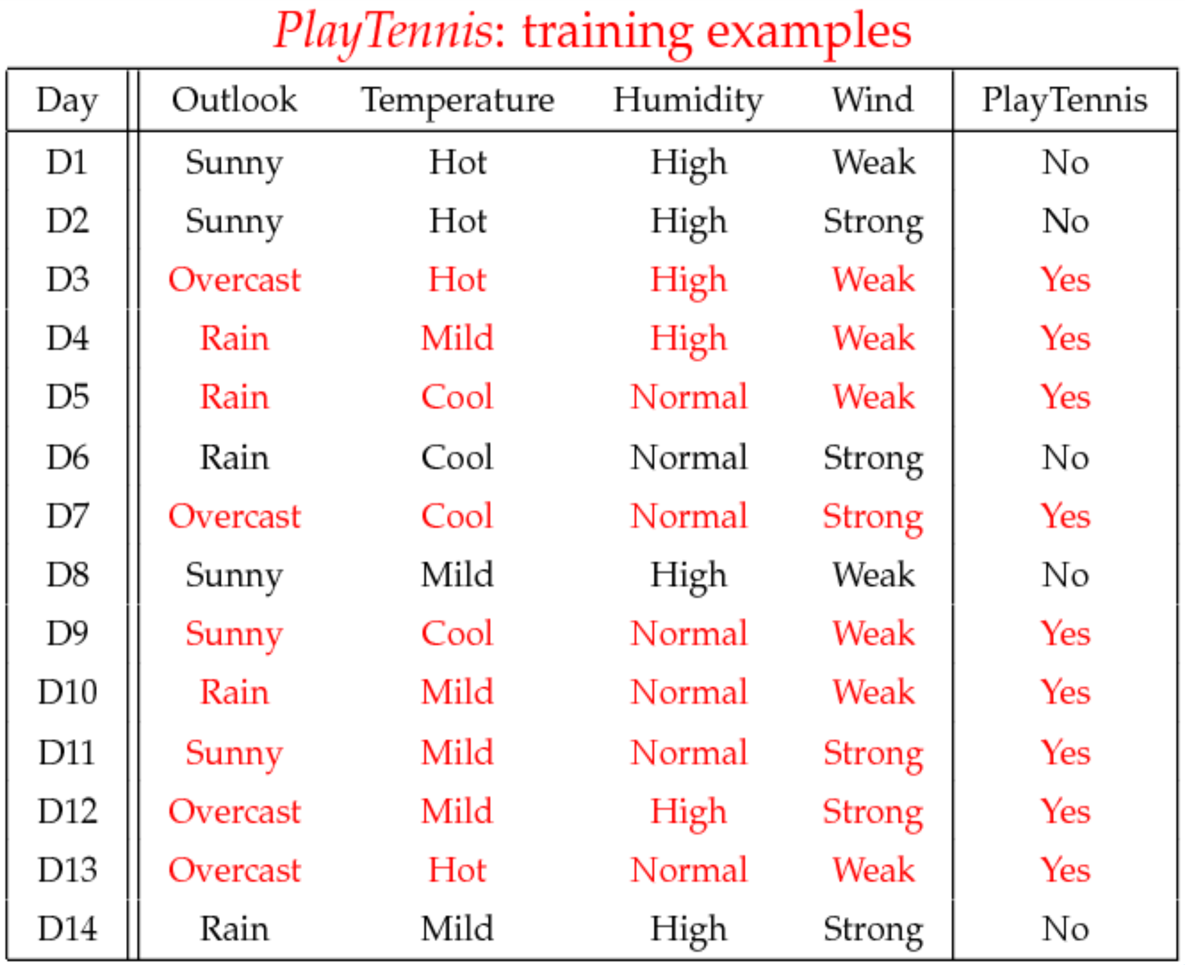
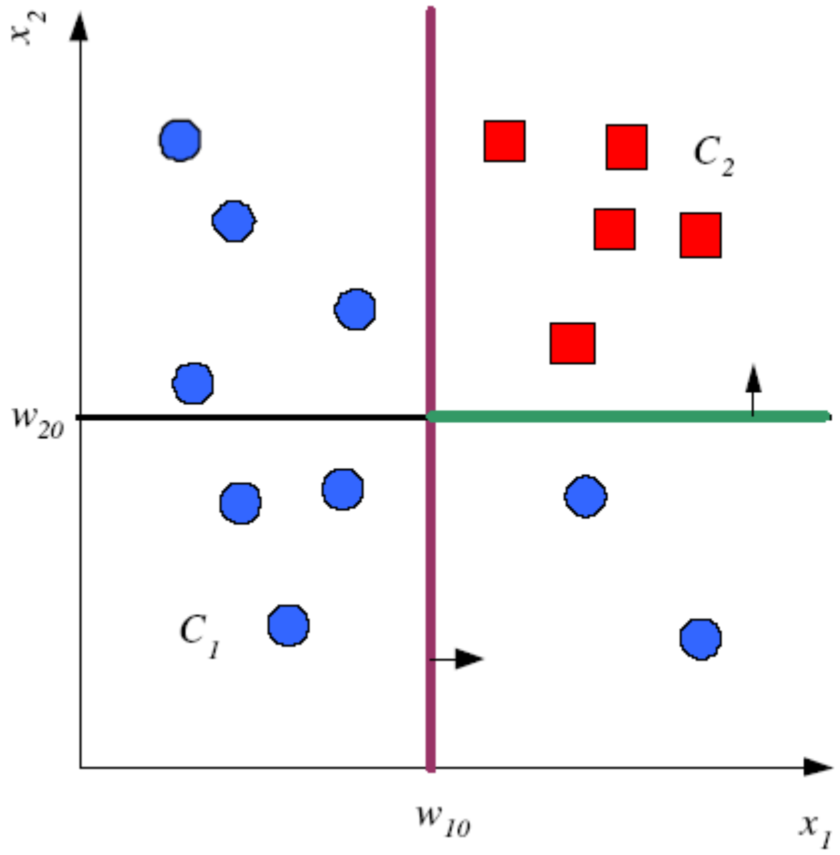
Example

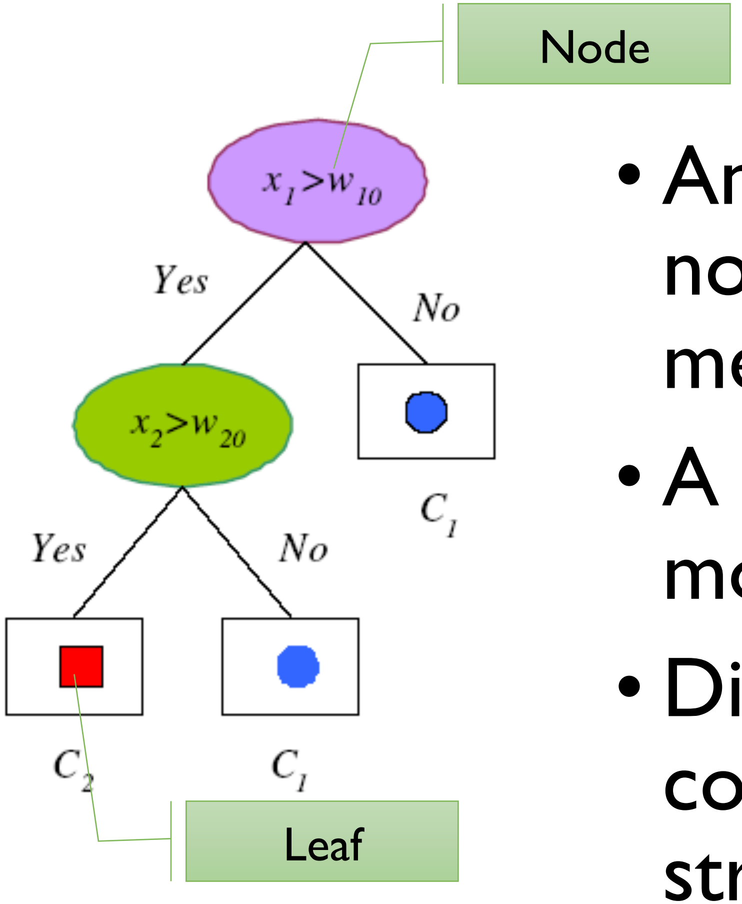


PlayTennis: training examples

Day	Outlook	Temperature	Humidity	Wind	PlayTennis
D1	Sunny	Hot	High	Weak	No
D2	Sunny	Hot	High	Strong	No
D3	Overcast	Hot	High	Weak	Yes
D4	Rain	Mild	High	Weak	Yes
D5	Rain	Cool	Normal	Weak	Yes
D6	Rain	Cool	Normal	Strong	No
D7	Overcast	Cool	Normal	Strong	Yes
D8	Sunny	Mild	High	Weak	No
D9	Sunny	Cool	Normal	Weak	Yes
D10	Rain	Mild	Normal	Weak	Yes
D11	Sunny	Mild	Normal	Strong	Yes
D12	Overcast	Mild	High	Strong	Yes
D13	Overcast	Hot	Normal	Weak	Yes
D14	Rain	Mild	High	Strong	No

Decision Trees





- An efficient nonparametric method
- A hierarchical model
- Divide-and–conquer strategy

Source: Ethem Alpaydin, Introduction to Machine Learning, 3rd Edition (Slides)

Divide and Conquer

- Internal decision nodes
  - Univariate: Uses a single attribute, x_i
    - Numeric x_i :
      - Binary split : $x_i > w_m$
    - Discrete x_i :
      - *n*-way split for *n* possible values
  - Multivariate: Uses more than one attributes, $\boldsymbol{x}$
- Leaves
  - Classification: Class labels, or proportions
  - Regression: Numeric; *r* average, or local fit
- Learning is greedy; find the best split recursively

Source: Ethem Alpaydin, Introduction to Machine Learning, 3rd Edition (Slides)

Classification Trees (C4.5, J48)

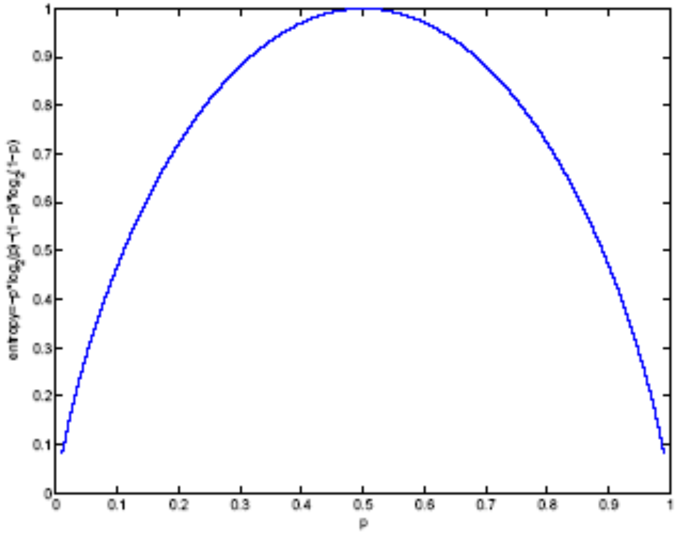
- For node *m*, N_m instances reach *m*, N^i_m belong to C_i

$$\hat{P}(C_i \mid \mathbf{x}, m) \equiv p^i_m = \frac{N^i_m}{N_m}$$

- Node *m* is **pure** if p^i_m is 0 or 1
- Measure of **impurity** is **entropy**

$$\mathcal{I}_m = -\sum_{i=1}^{K} p^i_m \log_2 p^i_m$$

2-class problem



Entropy in information theory specifies the average (expected) amount of information derived from observing an event

Source: Ethem Alpaydin, Introduction to Machine Learning, 3rd Edition (Slides)

Classification Trees

- If node *m* is pure, generate a leaf and stop, otherwise split and continue recursively
- **Impurity after split:** N_{mj} of N_m take branch *j*. N^i_{mj} belong to C_i

$$\hat{P}(C_i \mid \mathbf{x}, m, j) \equiv p^i_{mj} = \frac{N^i_{mj}}{N_{mj}}$$

$$\mathcal{I}'_m = -\sum_{j=1}^{n} \frac{N_{mj}}{N_m} \sum_{i=1}^{K} p^i_{mj} \log_2 p^i_{mj}$$

- **Information Gain:** Expected reduction in impurity measure after split
- Choose the *best* attribute(s) (**with maximum information gain**) to split the remaining instances and make that attribute a decision node
  - You can use same logic to find best splitting value too

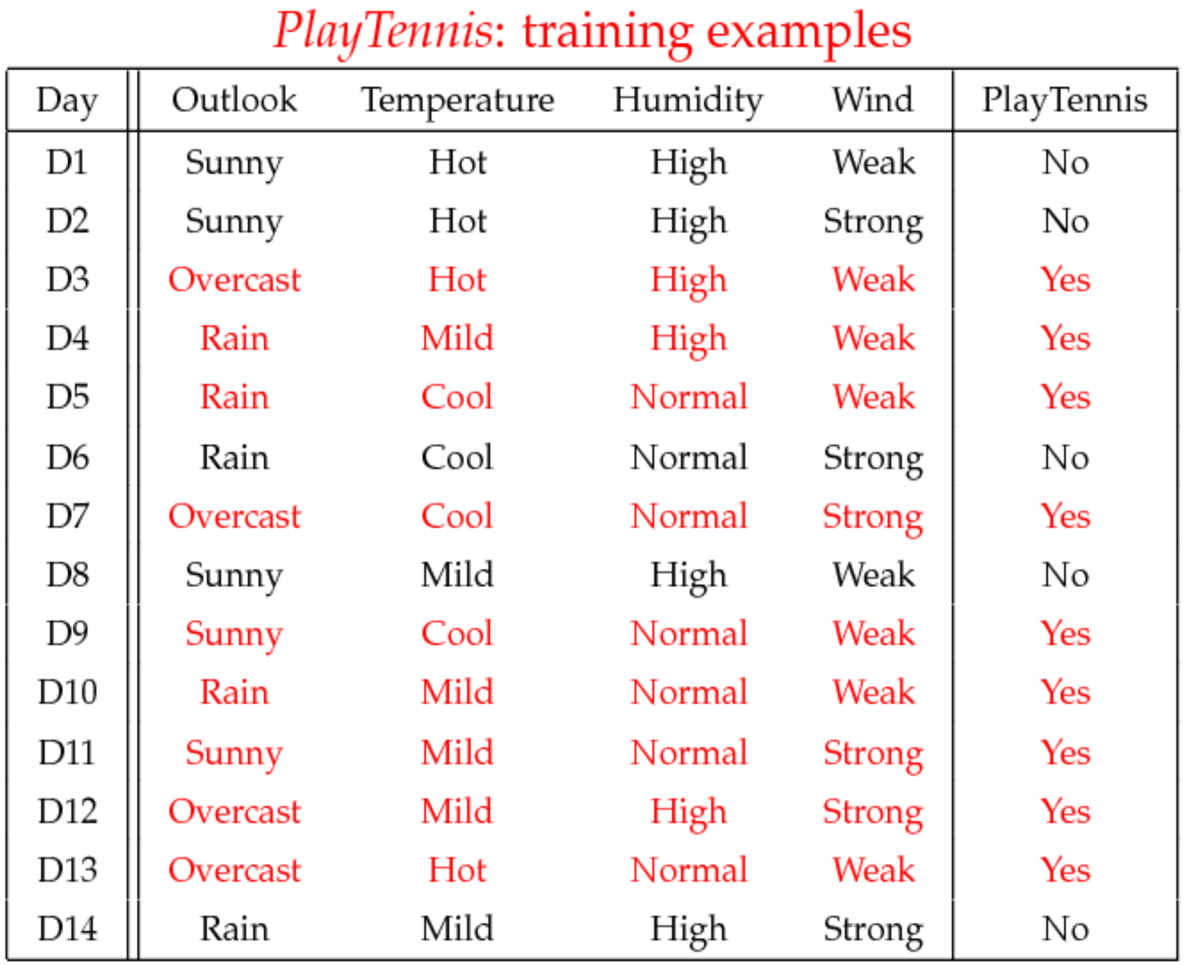
Source: Ethem Alpaydin, Introduction to Machine Learning, 3rd Edition (Slides)

Other Measures of Impurity

- The properties of functions measuring the **impurity** of a split:
  - $\phi(1/2,1/2) \geq \phi(p,1-p)$, for any $p \in [0,1]$
  - $\phi(0,1) = \phi(1,0) = 0$
  - $\phi(p,1-p)$ is increasing in p on $[0,\frac{1}{2}]$

    and decreasing in p on $[\frac{1}{2},1]$
- Examples (other than entropy)
  - **Gini impurity/index:** $1 - \sum_{j=1}^{c} p_j^2$

Decision Trees: Example



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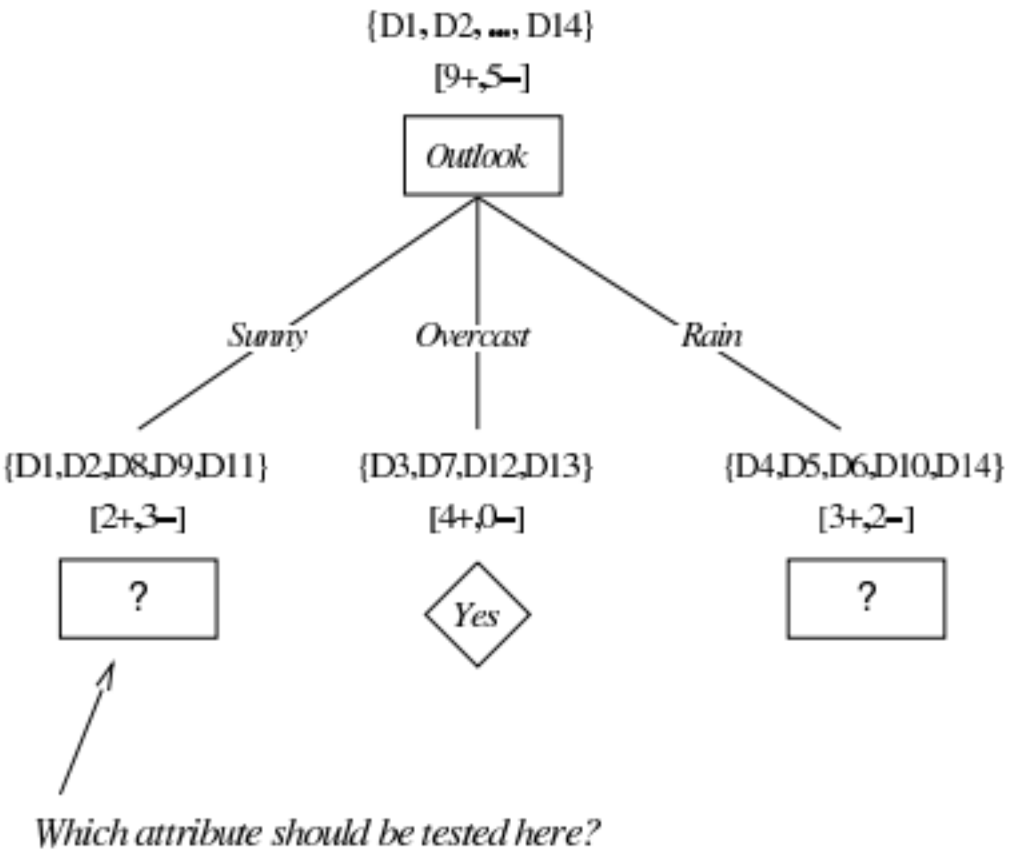
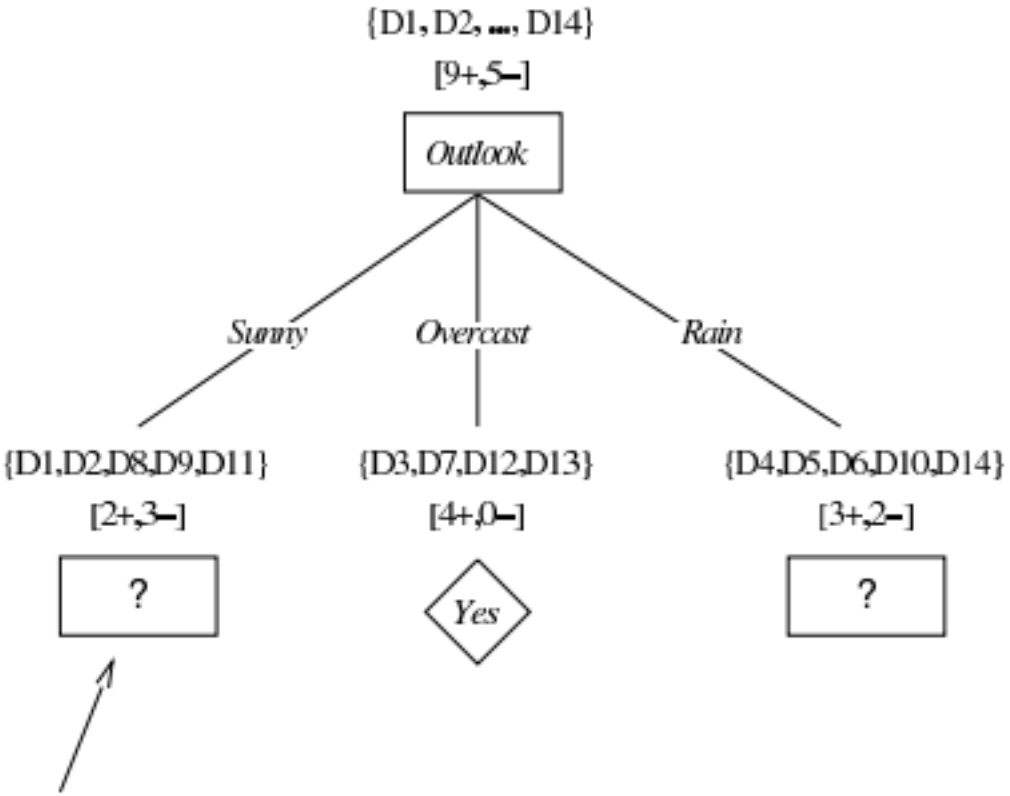


Decision Trees: Example



Which attribute should be tested here?

$S_{sunny} = \{D1,D2,D8,D9,D11\}$

$Gain\ (S_{sunny}, Humidity) = .970 - (3/5)\ 0.0 - (2/5)\ 0.0 = .970$

$Gain\ (S_{sunny}, Temperature) = .970 - (2/5)\ 0.0 - (2/5)\ 1.0 - (1/5)\ 0.0 = .570$

$Gain\ (S_{sunny}, Wind) = .970 - (2/5)\ 1.0 - (3/5)\ .918 = .019$

Overfitting and Generalization

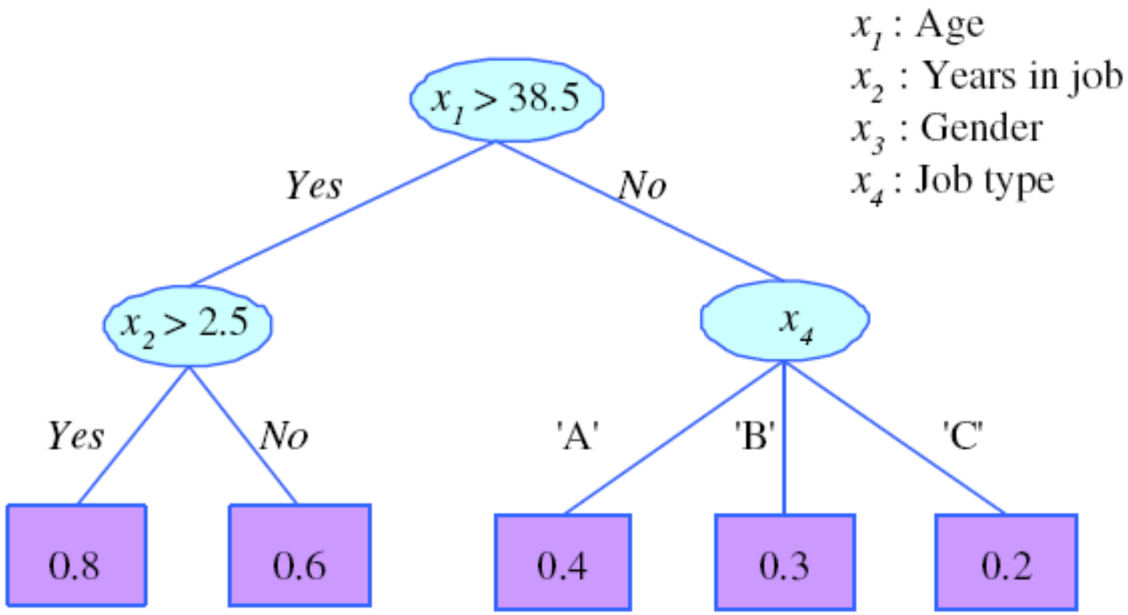
- Overfitting can occur with noisy training examples, also when small numbers of examples are associated with leaf nodes. How to handle?
- **Pruning:** Remove subtrees for better generalization (decrease variance)
  - Prepruning: Early stopping
  - Postpruning: Grow the whole tree then prune subtrees which overfit on the pruning set
  - Prepruning is faster, postpruning is more accurate

Overfitting and Generalization

- **Occam's Razor principle:** when multiple hypotheses can solve a problem, choose the simplest one
  - a short hypothesis that fits data unlikely to be coincidence
  - a long hypothesis that fits data might be coincidence

- How to select "best" tree:
  - Measure performance over training data
  - Measure performance over separate validation data set
  - **Minimum Description Length:** Minimize `size(tree) + size(misclassifications(tree))`

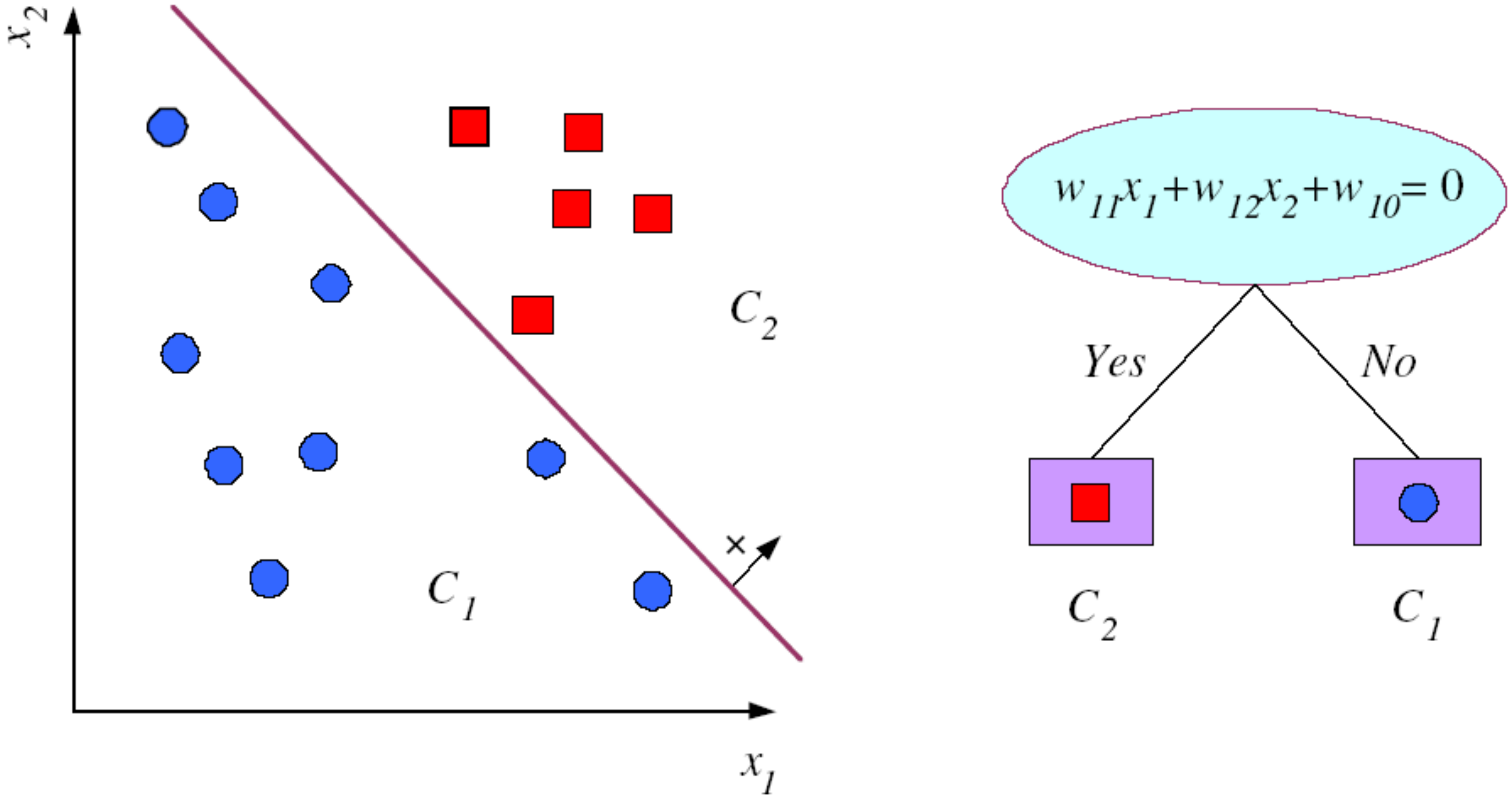
Rule Extraction from Trees



R1: IF (age>38.5) AND (years-in-job>2.5) THEN y =0.8
R2: IF (age>38.5) AND (years-in-job≤2.5) THEN y =0.6
R3: IF (age≤38.5) AND (job-type='A') THEN y =0.4
R4: IF (age≤38.5) AND (job-type='B') THEN y =0.3
R5: IF (age≤38.5) AND (job-type='C') THEN y =0.2

- Convert tree to equivalent set of rules
- Prune each rule independently of others, by removing any preconditions that result in improving its estimated accuracy
- Sort final rules into desired sequence for use

Multivariate Trees



Readings

- Chapters 8, 9, EA Introduction to ML 2nd Edn
- Chapter 14 (Sec 14. 4) + Chapter 2 (Sec 2. 5), Bishop, PRML