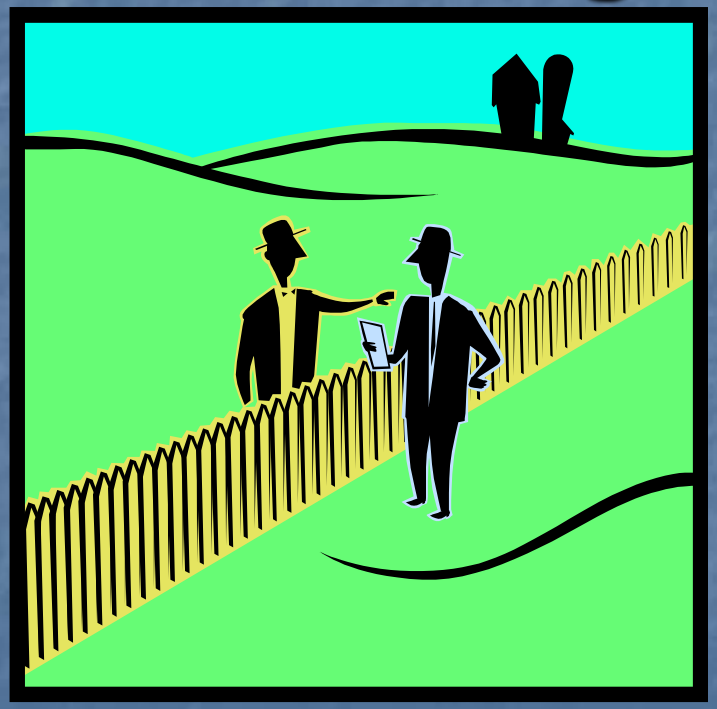
Classification Model

K-Nearest Neighbor



Classifier

Lazy vs. Eager Learning

- Lazy vs. eager learning
  - Lazy learning (e.g., instance-based learning): Simply stores training data (or only minor processing) and waits until it is given a test tuple
  - Eager learning : Given a set of training set, constructs a classification model before receiving new (e.g., test) data to classify
- Lazy: less time in training but more time in predicting
- Accuracy
  - Lazy method effectively uses a richer hypothesis space since it uses many local linear functions to form its implicit global approximation to the target function
  - Eager: must commit to a single hypothesis that covers the entire instance space

Lazy Learner: Instance-Based Methods

- Instance-based learning:
  - Store training examples and delay the processing ("lazy evaluation") until a new instance must be classified
- Typical approaches
  - *k*-nearest neighbor approach
    - Instances represented as points in a Euclidean space.
  - Locally weighted regression
    - Constructs local approximation
  - Case-based reasoning
    - Uses symbolic representations and knowledge-based inference

K-Nearest Neighbor Classifiers

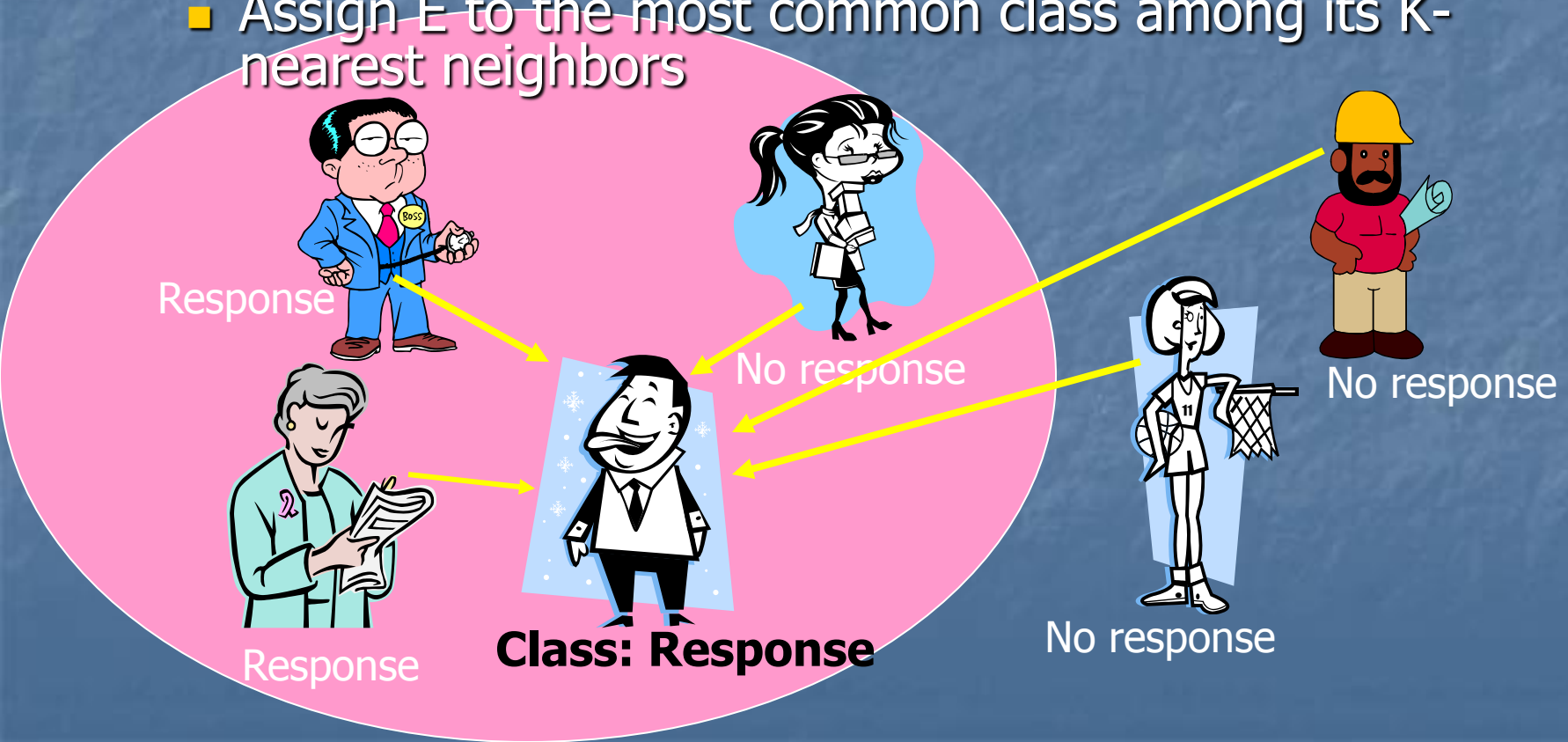
Learning by analogy:

Tell me who your friends are and I'll tell you who you are

A new example is assigned to the most common class among the (K) examples that are most similar to it.

K-Nearest Neighbor Algorithm

- To determine the class of a new example E:
  - Calculate the distance between E and all examples in the training set
  - Select K-nearest examples to E in the training set
  - Assign E to the most common class among its K-nearest neighbors



Distance Between Neighbors

- Each example is represented with a set of numerical attributes

John:
Age=35
Income=95K
No. of credit cards=3

Rachel:
Age=41
Income=215K
No. of credit cards=2

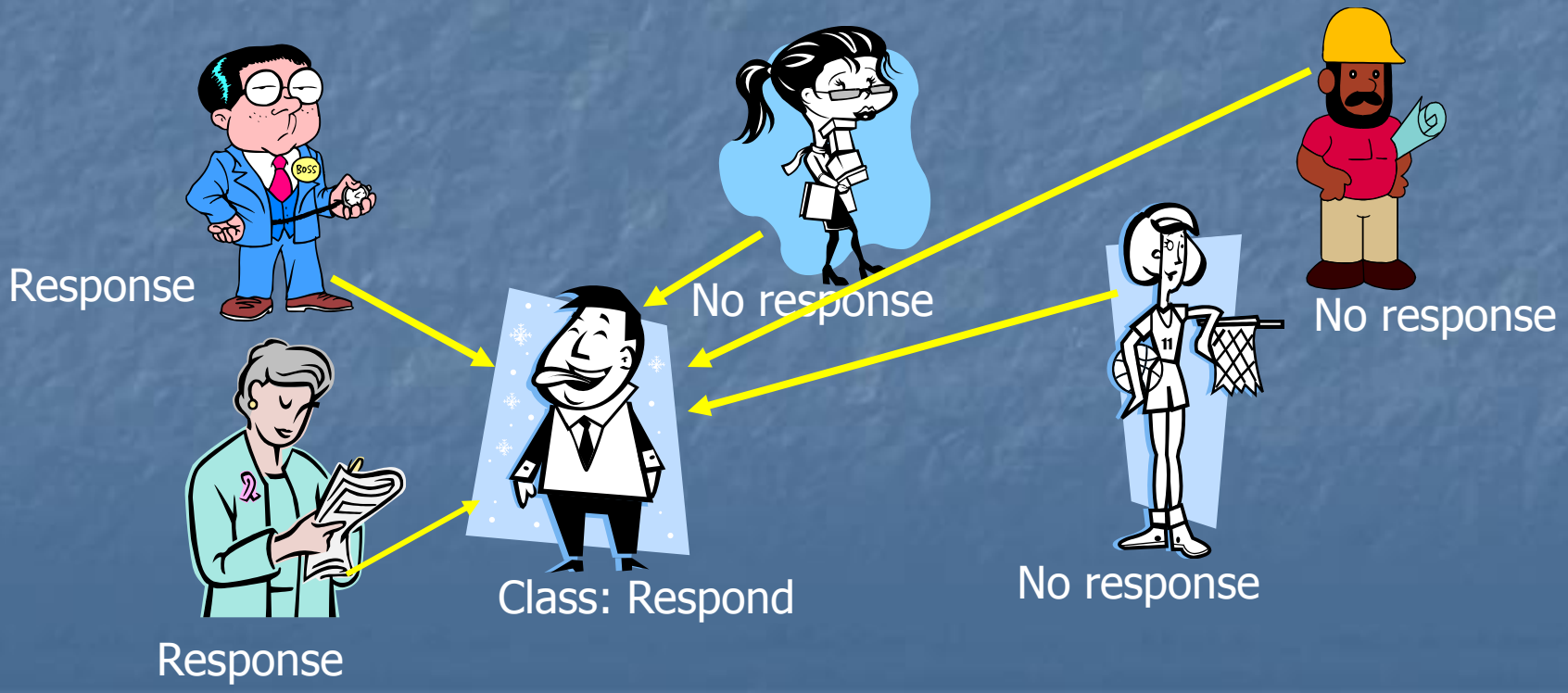
- "Closeness" is defined in terms of the *Euclidean* distance between two examples.
  - The Euclidean distance between $X=(x_1, x_2, x_3,\ldots x_n)$ and $Y=(y_1,y_2, y_3,\ldots y_n)$ is defined as:

$$D(X,Y)=\sqrt{\sum_{i=1}^{n}(x_i-y_i)^2}$$

  - Distance (John, Rachel)=sqrt $[(35-41)^2+(95K-215K)^2+(3-2)^2]$

K-Nearest Neighbor: Instance Based Learning

- No model is built: Store all training examples
- Any processing is delayed until a new instance must be classified.



Example : 3-Nearest Neighbors

Customer	Age	Income	No. credit cards	Response
John 	35	35K	3	No
Rachel 	22	50K	2	Yes
Hannah 	63	200K	1	No
Tom 	59	170K	1	No
Nellie 	25	40K	4	Yes
David 	37	50K	2	?

Example

Customer	Age	Income (K)	No. cards	Response	Distance from David
John 	35	35	3	No	sqrt $[(35-37)^2+(35-50)^2+(3-2)^2]=\mathbf{15.16}$
Rachel 	22	50	2	Yes	sqrt $[(22-37)^2+(50-50)^2+(2-2)^2]=\mathbf{15}$
Hannah 	63	200	1	No	sqrt $[(63-37)^2+(200-50)^2+(1-2)^2]=\mathbf{152.23}$
Tom 	59	170	1	No	sqrt $[(59-37)^2+(170-50)^2+(1-2)^2]=\mathbf{122}$
Nellie 	25	40	4	Yes	sqrt $[(25-37)^2+(40-50)^2+(4-2)^2]=\mathbf{15.74}$
David 	37	50	2	**Yes**	

Strengths and Weaknesses

Strengths:

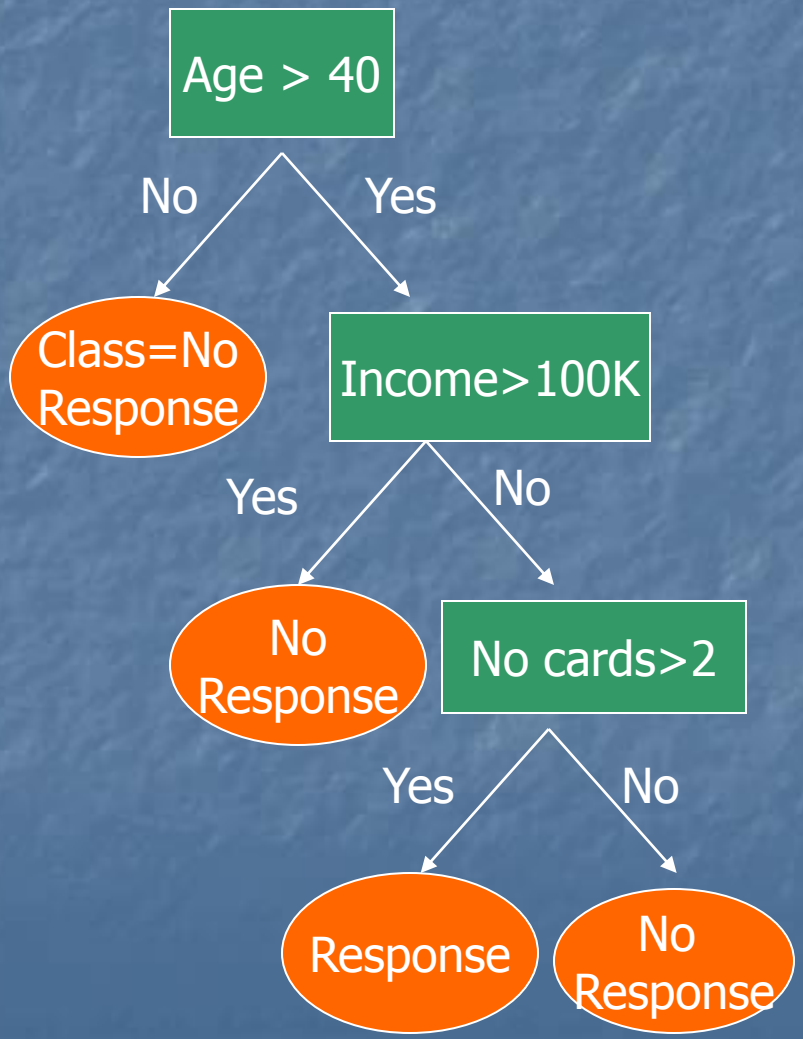
- Simple to implement and use
- Powerful
- Nonparametric architecture
- Comprehensible – easy to explain prediction
- Robust to noisy data by averaging k-nearest neighbors.
- Requires no training time

Weaknesses:

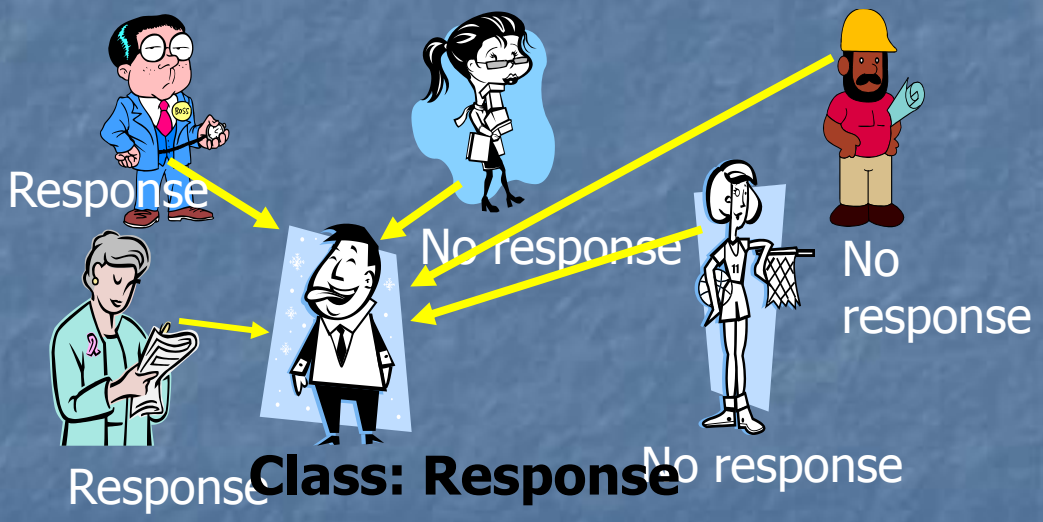
- Need a lot of space to store all examples.
- Takes more time to classify a new example than with a model (need to calculate and compare distance from new example to all other examples).

K-Nearest Neighbor Classifier

Classification Tree Modes



K-Nearest Neighbors



Strengths and Weaknesses K-Nearest Neighbor Classifier

John:
Age=35
Income=95K
No. of credit cards=3

Rachel:
Age=41
Income=215K
No. of credit cards=2

Distance (John, Rachel)=sqrt $[(35-45)^2+(95{,}000-215{,}000)^2+(3-2)^2]$

- Distance between neighbors could be dominated by some attributes with relatively large numbers (e.g., income in our example). Important to normalize some features (e.g., map numbers to numbers between 0-1)

  Exmaple: Income

  Highest income = 500K

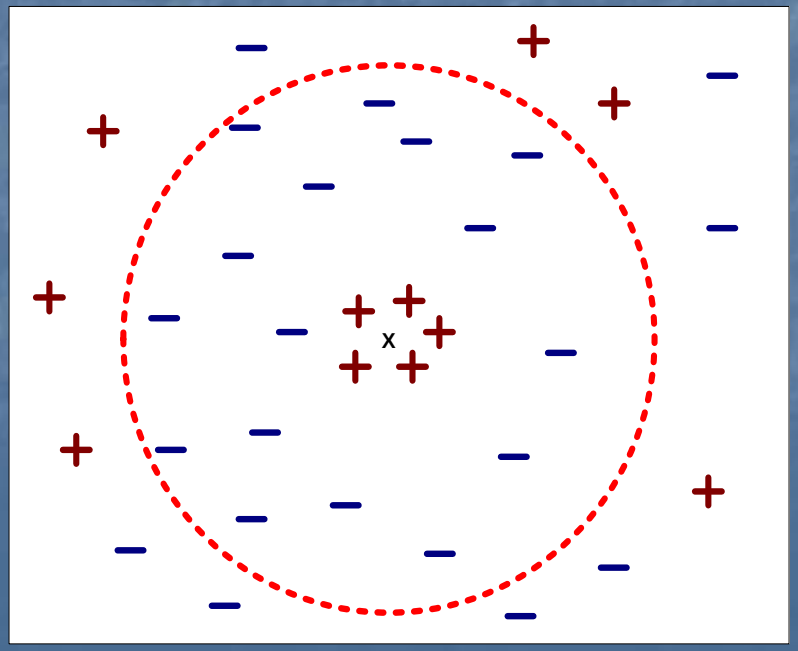
  Davis's income is normalized to 95/500, Rachel income is normalized to 215/500, etc.)

Normalization of Variables

Customer	Age	Income (K)	No. cards	Response
John 	55/63= 0.55	35/200= 0.175	¾= 0.75	No
Rachel 	22/63= 0.34	50/200= 0.25	2/4= 0.5	Yes
Hannah 	63/63= 1	200/200 =1	¼= 0.25	No
Tom 	59/63= 0.93	170/200 =0.85	¼= 0.25	No
Nellie 	25/63= 0.39	40/200= 0.2	4/4= 1	Yes
David 	37/63= 0.58	50/200= 0.25	2/4= 0.5	**Yes**

Nearest Neighbor Classification…

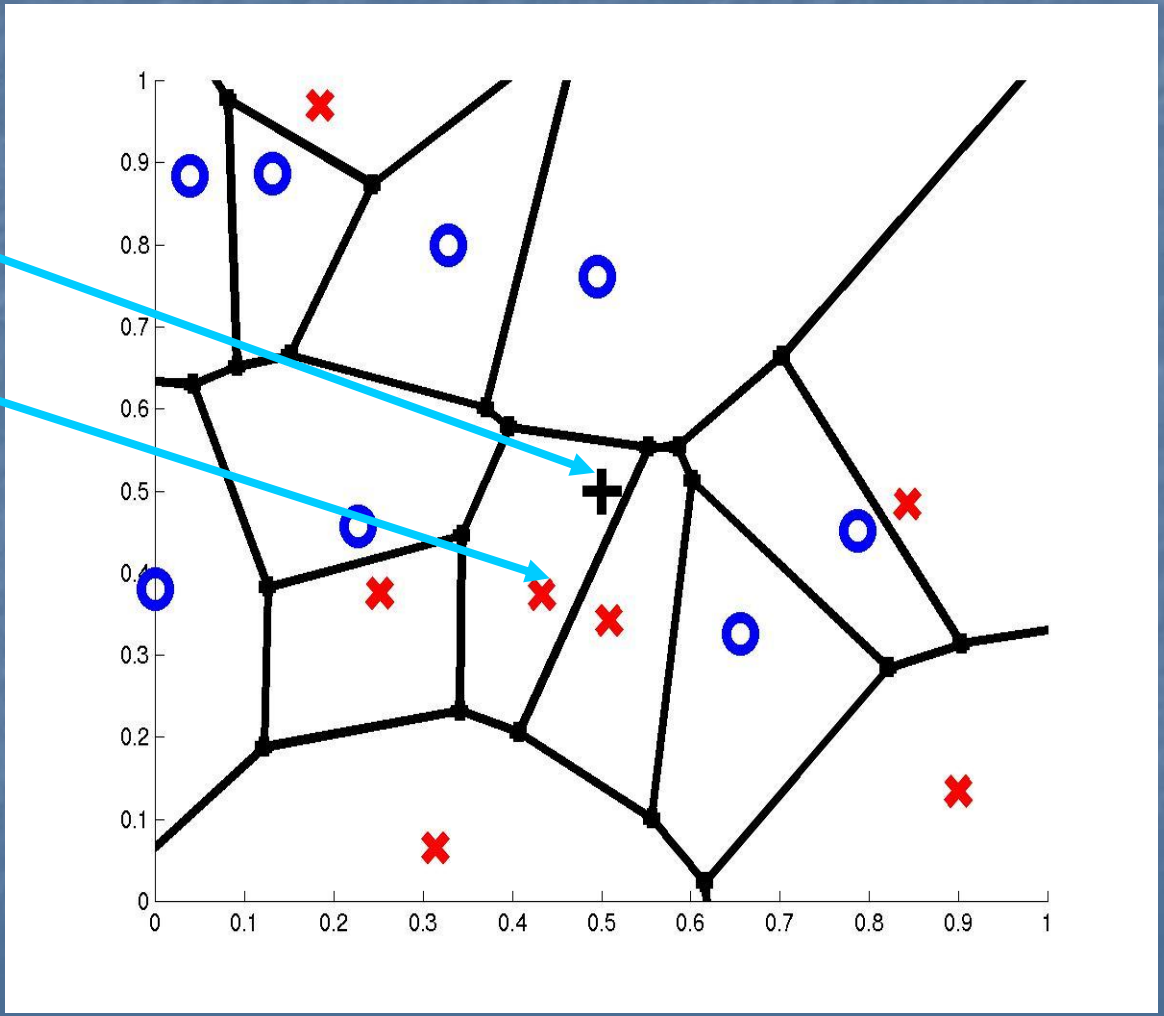
- Choosing the value of k:
  - If k is too small, sensitive to noise points
  - If k is too large, neighborhood may include points from other classes



1-Nearest Neighbor

query point q_f

nearest neighbor q_i

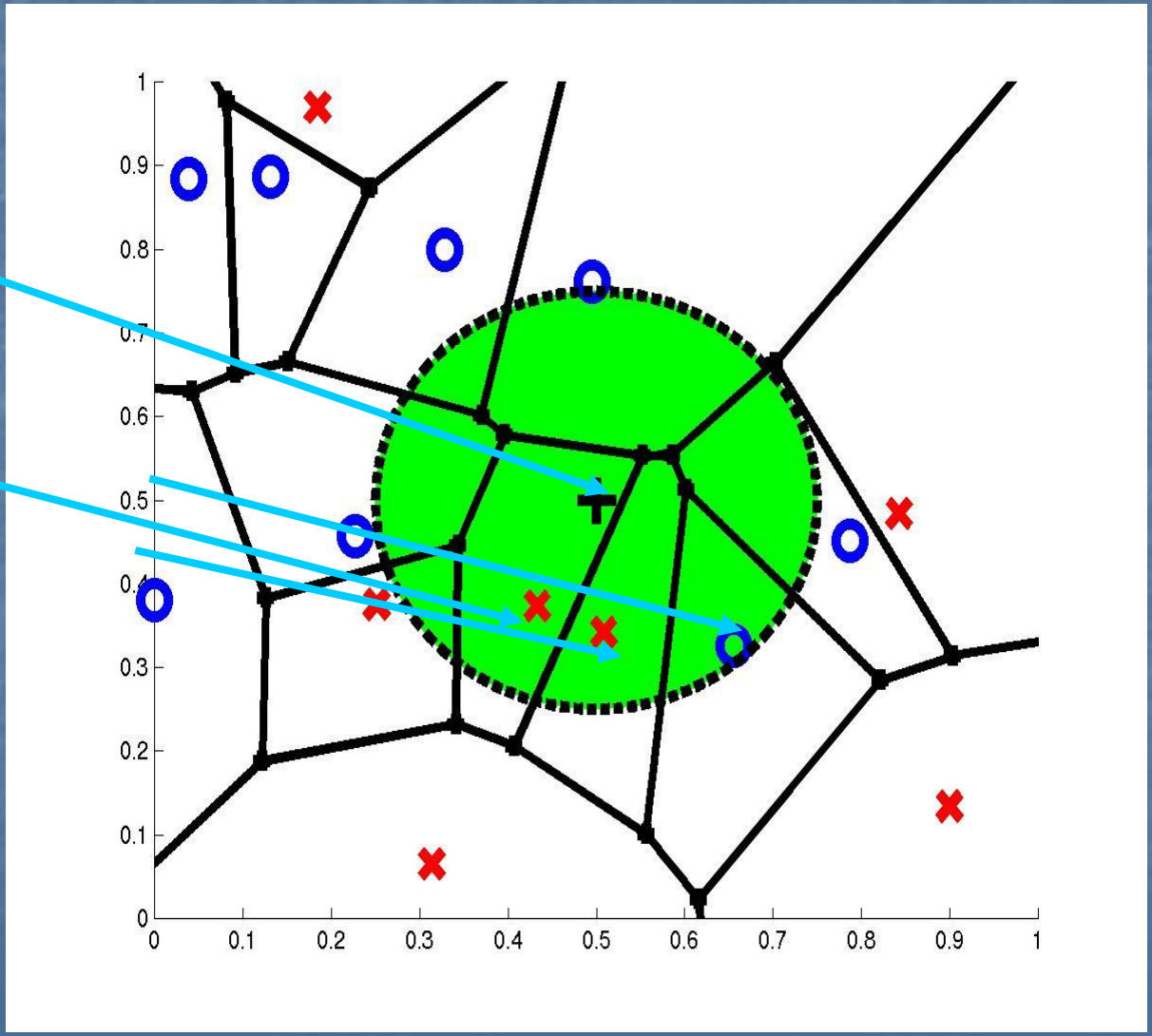


3-Nearest Neighbors

query point q_f

3 nearest neighbors

2x,1o

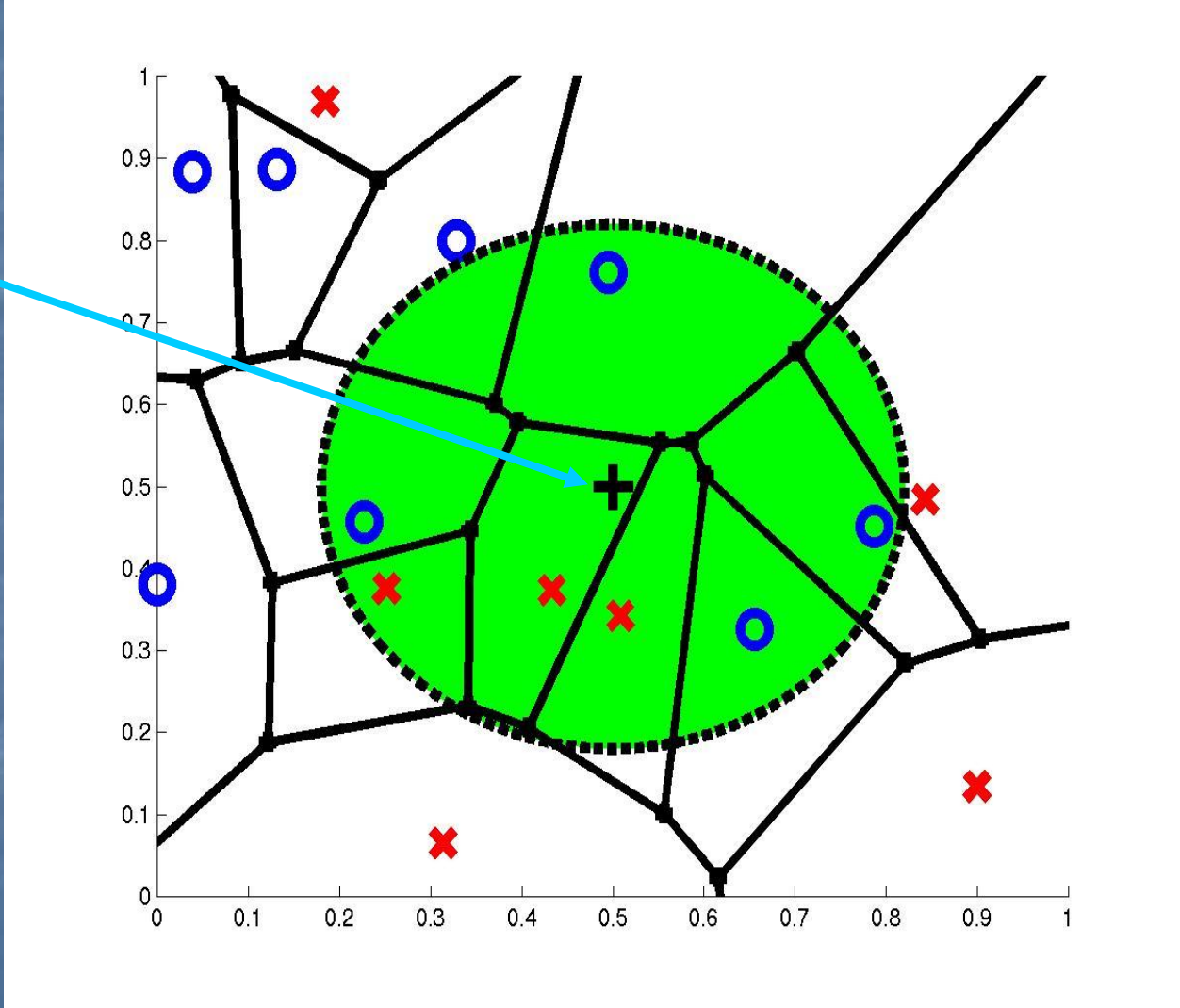


7-Nearest Neighbors

query point q_f

7 nearest neighbors

3x,4o



How to determine the good value for k?

- Determined experimentally
- 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 should be odd number to avoid ties

Strengths and Weaknesses K-Nearest Neighbor Classifier

- Distance works naturally with numerical attributes

D(Rachel&Johm)= sqrt $[(35-37)^2+(35-50)^2+(3-2)^2]$=**15.16**

What if we have nominal attributes?

Example: married

Customer	Married	Income (K)	No. cards	Response
John	Yes	35	3	No
Rachel	No	50	2	Yes
Hannah	No	200	1	No
Tom	Yes	170	1	No
Nellie	No	40	4	Yes
David	Yes	50	2	

What Is Prediction?

- (Numerical) prediction is similar to classification
  - construct a model
  - use model to predict continuous or ordered value for a given input
- Prediction is different from classification
  - Classification refers to predict categorical class label
  - Prediction models continuous-valued functions
- Major method for prediction: regression
  - model the relationship between one or more *independent* or **predictor** variables and a *dependent* or **response** variable
- Regression analysis
  - Linear and multiple regression
  - Non-linear regression
  - Other regression methods: generalized linear model, Poisson regression, log-linear models, regression trees

Linear Regression

- Linear regression: involves a response variable y and a single predictor variable x

  $y = w_0 + w_1 x$

  where w_0 (y-intercept) and w_1 (slope) are regression coefficients
- Method of least squares: estimates the best-fitting straight line

$$w_1 = \frac{\sum_{i=1}^{|D|}(x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{|D|}(x_i - \bar{x})^2} \qquad w_0 = \bar{y} - w_1 \bar{x}$$

- Multiple linear regression: involves more than one predictor variable
  - Training data is of the form $(\mathbf{X_1}, y_1)$, $(\mathbf{X_2}, y_2)$,…, $(\mathbf{X_{|D|}}, y_{|D|})$
  - Ex. For 2-D data, we may have: $y = w_0 + w_1 x_1 + w_2 x_2$
  - Solvable by extension of least square method or using SAS, S-Plus
  - Many nonlinear functions can be transformed into the above

Nonlinear Regression

- Some nonlinear models can be modeled by a polynomial function
- A polynomial regression model can be transformed into linear regression model. For example,

  $y = w_0 + w_1 x + w_2 x^2 + w_3 x^3$

  convertible to linear with new variables: $x_2 = x^2$, $x_3 = x^3$

  $y = w_0 + w_1 x + w_2 x_2 + w_3 x_3$
- Other functions, such as power function, can also be transformed to linear model
- Some models are intractable nonlinear (e.g., sum of exponential terms)
  - possible to obtain least square estimates through extensive calculation on more complex formulae

Other Regression-Based Models

- Generalized linear model:
  - Foundation on which linear regression can be applied to modeling categorical response variables
  - Variance of y is a function of the mean value of y, not a constant
  - Logistic regression: models the prob. of some event occurring as a linear function of a set of predictor variables
  - Poisson regression: models the data that exhibit a Poisson distribution
- Log-linear models: (for categorical data)
  - Approximate discrete multidimensional prob. distributions
  - Also useful for data compression and smoothing
- Regression trees and model trees
  - Trees to predict continuous values rather than class labels

Regression Trees and Model Trees

- Regression tree: proposed in CART system (Breiman et al. 1984)
  - CART: Classification And Regression Trees
  - Each leaf stores a *continuous-valued prediction*
  - It is the *average value of the predicted attribute* for the training tuples that reach the leaf
- Model tree: proposed by Quinlan (1992)
  - Each leaf holds a regression model—a multivariate linear equation for the predicted attribute
  - A more general case than regression tree
- Regression and model trees tend to be more accurate than linear regression when the data are not represented well by a simple linear model

Estimating Error Rates I

- Training Error:
  - The proportion of training records that are misclassified
  - Overly optimistic. Classifiers that overfit the datasets can have poor accuracy on unseen data

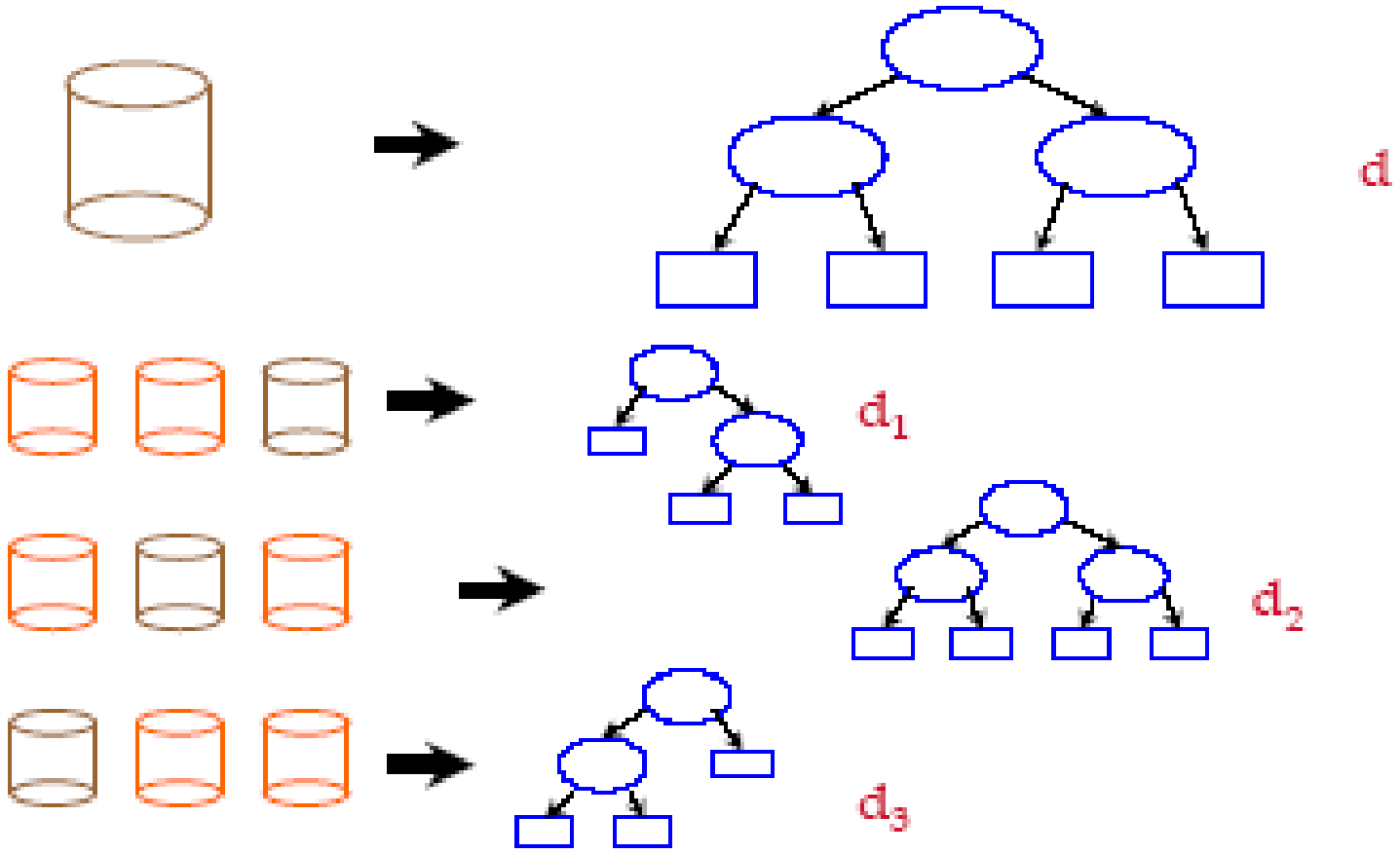
Estimating Error Rates II

- Holdout method
  - Partition: Training-and-testing
    - Given data is randomly partitioned into two independent sets
    - Training set (e.g., 2/3) for model construction
    - Test set (e.g., 1/3) for accuracy estimation
    - Unbiased, efficient. But require a large number of samples
    - used for data set with large number of samples
  - Random sampling: a variation of holdout
    - Repeat holdout k times, accuracy = avg. of the accuracies obtained

Estimating Error Rates III

- Cross-validation (*k*-fold, where k = 10 is most popular)
  - Randomly partition the data into *k mutually exclusive* subsets, each approximately equal size
  - At *i*-th iteration, use D_i as test set and others as training set
  - Leave-one-out: k folds where k = # of tuples, for small sized data
  - Stratified cross-validation: folds are stratified so that class dist. in each fold is approx. the same as that in the initial data

Cross-Validation: Example



Cross-Validation

- Misclassification estimate obtained through cross-validation is usually nearly unbiased
- Costly computation (we need to compute d, and d_1, ..., d_V); computation of d_i is nearly as expensive as computation of d
- Preferred method to estimate quality of learning algorithms in the machine learning literature

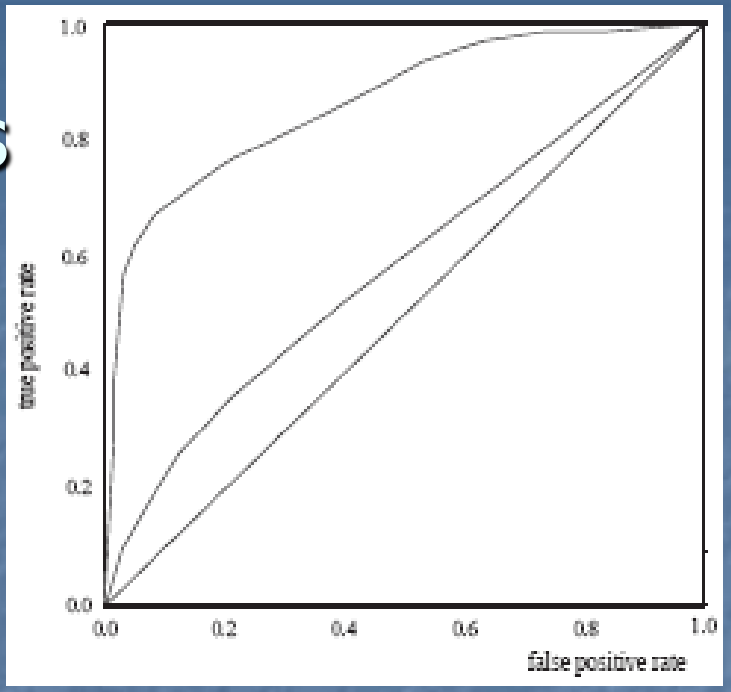
Estimating Error Rates IV

- Bootstrap
  - Works well with small data sets
  - Samples the given training tuples uniformly *with replacement*
    - i.e., each time a tuple is selected, it is equally likely to be selected again and re-added to the training set
- Several boostrap methods, and a common one is **.632 boostrap**
  - Suppose we are given a data set of d tuples. The data set is sampled d times, with replacement, resulting in a training set of d samples. The data tuples that did not make it into the training set end up forming the test set. About 63.2% of the original data will end up in the bootstrap, and the remaining 36.8% will form the test set (since $(1 - 1/d)^d \approx e^{-1} = 0.368$)
  - Repeat the sampling procedue k times, overall accuracy of the model:

$$acc(M) = \sum_{i=1}^{k} (0.632 \times acc(M_i)_{test\_set} + 0.368 \times acc(M_i)_{train\_set})$$

Model Selection: ROC Curves

- ROC (Receiver Operating Characteristics) curves: for visual comparison of classification models
- Originated from signal detection theory
- Shows the trade-off between the true positive rate and the false positive rate
- The area under the ROC curve is a measure of the accuracy of the model
- Rank the test tuples in decreasing order: the one that is most likely to belong to the positive class appears at the top of the list
- The closer to the diagonal line (i.e., the closer the area is to 0.5), the less accurate is the model



- Vertical axis represents the true positive rate
- Horizontal axis rep. the false positive rate
- The plot also shows a diagonal line
- A model with perfect accuracy will have an area of 1.0

Metrics for Performance Evaluation

- Focus on the predictive capability of a model
  - Rather than how fast it takes to classify or build models, scalability, etc.
- Confusion Matrix:

		PREDICTED CLASS	
		Class=Yes	Class=No
ACTUAL CLASS	Class=Yes	a	b
	Class=No	c	d

a: TP (true positive)

b: FN (false negative)

c: FP (false positive)

d: TN (true negative)

Metrics for Performance

		PREDICTED CLASS	
		Class=Yes	Class=No
ACTUAL CLASS	Class=Yes	a (TP)	b (FN)
	Class=No	c (FP)	d (TN)

$$\text{Accuracy} = \frac{a+d}{a+b+c+d} = \frac{TP+TN}{TP+TN+FP+FN}$$

- Most widely-used metric:

Limitation of Accuracy

- Consider a 2-class problem
  - Number of Class 0 examples = 9990
  - Number of Class 1 examples = 10

- If model predicts everything to be class 0, accuracy is 9990/10000 = 99.9 %
  - Accuracy is misleading because model does not detect any class 1 example

Cost Matrix

		PREDICTED CLASS	
ACTUAL CLASS	C(i|j)	**Class=Yes**	**Class=No**
	Class=Yes	C(Yes|Yes)	C(No|Yes)
	Class=No	C(Yes|No)	C(No|No)

C(i|j): Cost of misclassifying class j example as class i

Computing Cost of Classification

Cost Matrix	PREDICTED CLASS		
	C(i|j)	+	-
ACTUAL CLASS	+	-1	100
	-	1	0

Model M_1	PREDICTED CLASS		
		+	-
ACTUAL CLASS	+	150	40
	-	60	250

Model M_2	PREDICTED CLASS		
		+	-
ACTUAL CLASS	+	250	45
	-	5	200

Accuracy = 80%

Cost = 3910

Accuracy = 90%

Cost = 4255

Cost vs Accuracy

Count		PREDICTED CLASS	
		Class=Yes	Class=No
ACTUAL CLASS	Class=Yes	a	b
	Class=No	c	d

Cost		PREDICTED CLASS	
		Class=Yes	Class=No
ACTUAL CLASS	Class=Yes	p	q
	Class=No	q	p

Accuracy is proportional to cost if
1. C(Yes|No)=C(No|Yes) = q
2. C(Yes|Yes)=C(No|No) = p

$N = a + b + c + d$

$Accuracy = (a + d)/N$

$$\begin{aligned} Cost &= p\,(a + d) + q\,(b + c) \\ &= p\,(a + d) + q\,(N - a - d) \\ &= q\,N - (q - p)(a + d) \\ &= N\,[q - (q-p) \times Accuracy] \end{aligned}$$

Cost-Sensitive Measures

$$\text{Precision (p)} = \frac{a}{a+c}$$

$$\text{Recall (r)} = \frac{a}{a+b}$$

$$\text{F - measure (F)} = \frac{2rp}{r+p} = \frac{2a}{2a+b+c}$$

- Precision is biased towards C(Yes|Yes) & C(Yes|No)
- Recall is biased towards C(Yes|Yes) & C(No|Yes)
- F-measure is biased towards all except C(No|No)

$$\text{Weighted Accuracy} = \frac{w_1 a + w_4 d}{w_1 a + w_2 b + w_3 c + w_4 d}$$

More measures

- True Positive Rate (TPR) (Sensitivity)
  - a/a+b
- True Negative Rate (TNR) (Specificity)
  - d/c+d
- False Positive Rate (FPR)
  - c/c+d
- False Negative Rate (FNR)
  - b/a+b

Predictor Error Measures

- Measure predictor accuracy: measure how far off the predicted value is from the actual known value
- **Loss function**: measures the error betw. y_i and the predicted value y_i'
  - Absolute error: $| y_i - y_i' |$
  - Squared error: $(y_i - y_i')^2$
- Test error (generalization error): the average loss over the test set
  - Mean absolute error: $\frac{\sum_{i=1}^{d} | y_i - y_i' |}{d}$ Mean squared error: $\frac{\sum_{i=1}^{d} (y_i - y_i')^2}{d}$
  - Relative absolute error: $\frac{\sum_{i=1}^{d} | y_i - y_i' |}{\sum_{i=1}^{d} | y_i - \bar{y} |}$ Relative squared error: $\frac{\sum_{i=1}^{d} (y_i - y_i')^2}{\sum_{i=1}^{d} (y_i - \bar{y})^2}$

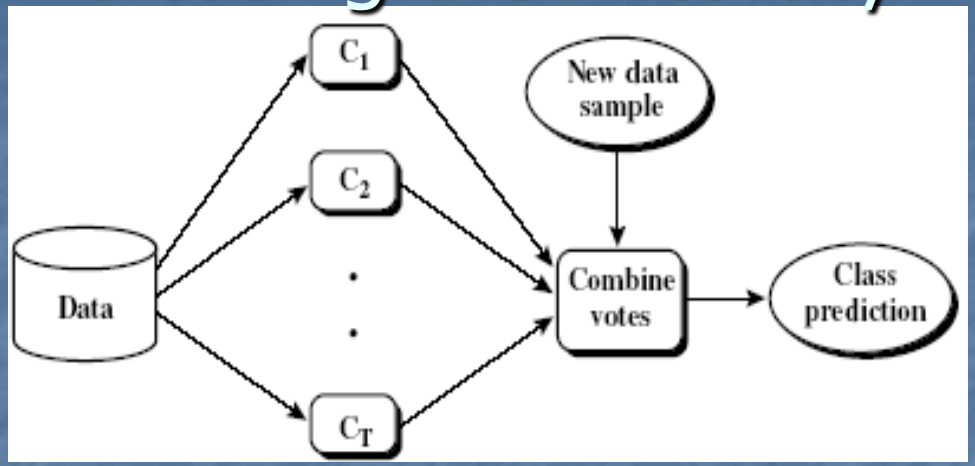
The mean squared-error exaggerates the presence of outliers

Popularly use (square) root mean-square error, similarly, root relative squared error

Ensemble Methods

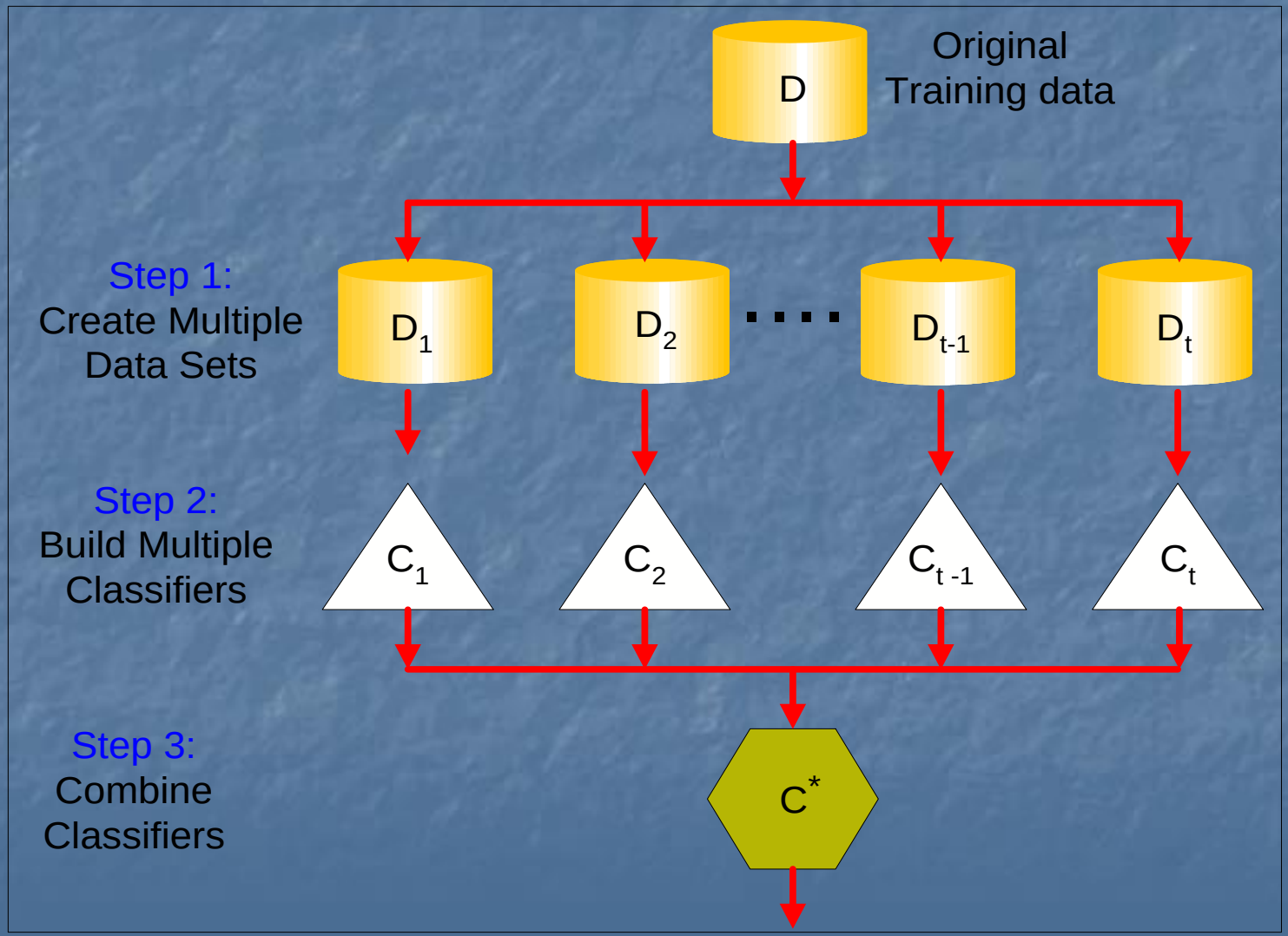
- Construct a set of classifiers from the training data
- Predict class label of previously unseen records by aggregating predictions made by multiple classifiers

Ensemble Methods: Increasing the Accuracy



- Ensemble methods
  - Use a combination of models to increase accuracy
  - Combine a series of k learned models, M_1, M_2, …, M_k, with the aim of creating an improved model M*
- Popular ensemble methods
  - Bagging: averaging the prediction over a collection of classifiers
  - Boosting: weighted vote with a collection of classifiers
  - Ensemble: combining a set of heterogeneous classifiers

General Idea



Why does it work?

- Suppose there are 25 base classifiers
  - Each classifier has error rate, $\varepsilon = 0.35$
  - Assume classifiers are independent
  - Probability that the ensemble classifier makes a wrong prediction:

$$\sum_{i=13}^{25} \binom{25}{i} \varepsilon^i (1-\varepsilon)^{25-i} = 0.06$$

Examples of Ensemble Methods

- How to generate an ensemble of classifiers?
  - Bagging
  - Boosting

Bagging: Boostrap Aggregation

- Analogy: Diagnosis based on multiple doctors' majority vote
- Training
  - Given a set D of *d* tuples, at each iteration *i*, a training set D_i of *d* tuples is sampled with replacement from D (i.e., boostrap)
  - A classifier model M_i is learned for each training set D_i
- Classification: classify an unknown sample **X**
  - Each classifier M_i returns its class prediction
  - The bagged classifier M* counts the votes and assigns the class with the most votes to **X**
- Prediction: can be applied to the prediction of continuous values by taking the average value of each prediction for a given test tuple
- Accuracy
  - Often significant better than a single classifier derived from D
  - For noise data: not considerably worse, more robust
  - Proved improved accuracy in prediction

Bagging

- Sampling with replacement

Original Data	1	2	3	4	5	6	7	8	9	10
Bagging (Round 1)	7	8	10	8	2	5	10	10	5	9
Bagging (Round 2)	1	4	9	1	2	3	2	7	3	2
Bagging (Round 3)	1	8	5	10	5	5	9	6	3	7

- Build classifier on each bootstrap sample

- Each sample has probability $(1 - 1/n)^n$ of being selected

Boosting

- An iterative procedure to adaptively change distribution of training data by focusing more on previously misclassified records
  - Initially, all N records are assigned equal weights
  - Unlike bagging, weights may change at the end of boosting round

Boosting

- Analogy: Consult several doctors, based on a combination of weighted diagnoses—weight assigned based on the previous diagnosis accuracy
- How boosting works?
  - Weights are assigned to each training tuple
  - A series of k classifiers is iteratively learned
  - After a classifier M_i is learned, the weights are updated to allow the subsequent classifier, M_{i+1}, to pay more attention to the training tuples that were misclassified by M_i
  - The final M* combines the votes of each individual classifier, where the weight of each classifier's vote is a function of its accuracy
- The boosting algorithm can be extended for the prediction of continuous values
- Comparing with bagging: boosting tends to achieve greater accuracy, but it also risks overfitting the model to misclassified data

Boosting

- Records that are wrongly classified will have their weights increased
- Records that are classified correctly will have their weights decreased

Original Data	1	2	3	4	5	6	7	8	9	10
Boosting (Round 1)	7	3	2	8	7	9	4	10	6	3
Boosting (Round 2)	5	4	9	4	2	5	1	7	4	2
Boosting (Round 3)	4	4	8	10	4	5	4	6	3	4

- Example 4 is hard to classify
- Its weight is increased, therefore it is more likely to be chosen again in subsequent rounds

Adaboost (Freund and Schapire, 1997)

- Given a set of *d* class-labeled tuples, ($\mathbf{X_1}$, y_1), …, ($\mathbf{X_d}$, y_d)
- Initially, all the weights of tuples are set the same (1/d)
- Generate k classifiers in k rounds. At round i,
  - Tuples from D are sampled (with replacement) to form a training set D_i of the same size
  - Each tuple's chance of being selected is based on its weight
  - A classification model M_i is derived from D_i
  - Its error rate is calculated using D_i as a test set
  - If a tuple is misclssified, its weight is increased, o.w. it is decreased
- Error rate: err($\mathbf{X_j}$) is the misclassification error of tuple $\mathbf{X_j}$. Classifier M_i error rate is the sum of the weights of the misclassified tuples:

$$error(M_i) = \sum_j^d w_j \times err(\mathbf{X_j})$$

- The weight of classifier M_i's vote is $\log \frac{1-error(M_i)}{error(M_i)}$

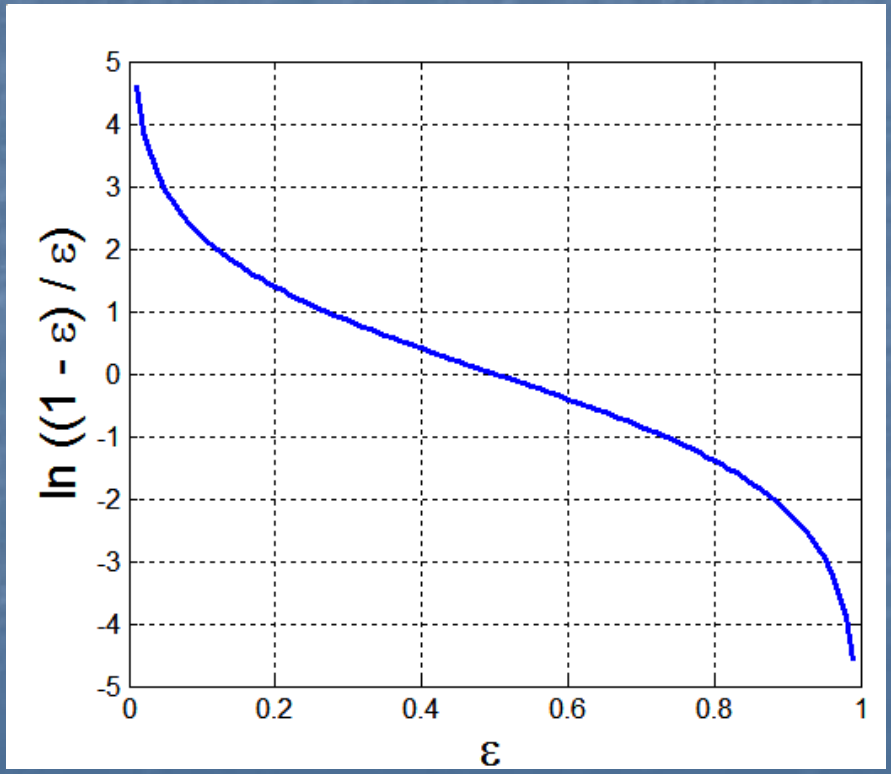
Example: AdaBoost

- Base classifiers: C_1, C_2, …, C_T
- Error rate:

$$\varepsilon_i = \frac{1}{N}\sum_{j=1}^{N} w_j \delta\left(C_i(x_j) \neq y_j\right)$$

- Importance of a classifier:

$$\alpha_i = \frac{1}{2}\ln\left(\frac{1-\varepsilon_i}{\varepsilon_i}\right)$$



Example: AdaBoost

- Weight update:

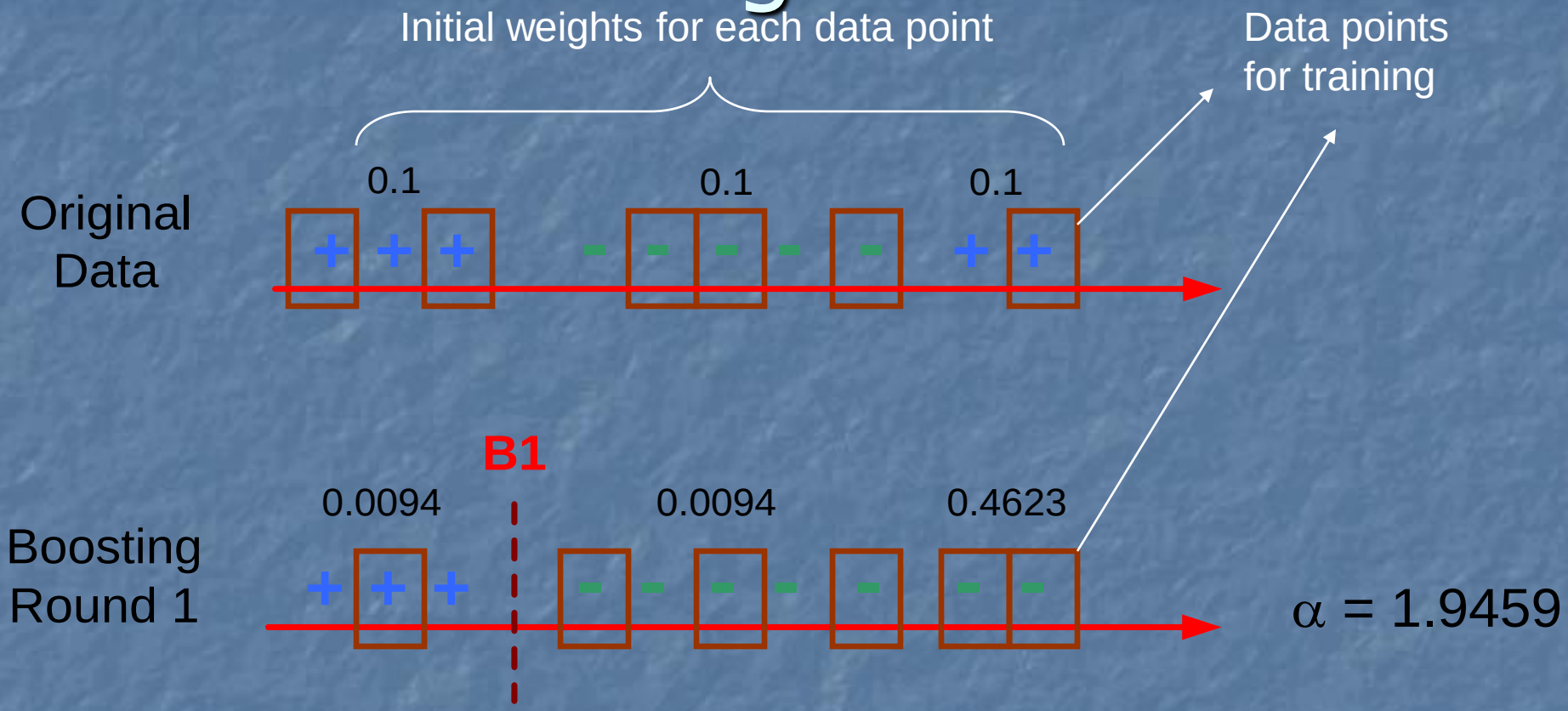
$$w_i^{(j+1)} = \frac{w_i^{(j)}}{Z_j} \begin{cases} \exp^{-\alpha_j} & \text{if } C_j(x_i) = y_i \\ \exp^{\alpha_j} & \text{if } C_j(x_i) \neq y_i \end{cases}$$

$$\text{where } Z_j \text{ is the normalization factor}$$

- If any intermediate rounds produce error rate higher than 50%, the weights are reverted back to 1/n and the resampling procedure is repeated
- Classification:

$$C^*(x) = \arg\max_y \sum_{j=1}^{T} \alpha_j \delta\left(C_j(x) = y\right)$$

Illustrating AdaBoost



Illustrating AdaBoost