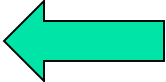


# Lecture No. 4 – Decision Tree Learning I

- Classification and Prediction 
- Overview of Decision Tree Learning
- Avoiding Overfitting

# Classification vs. Prediction

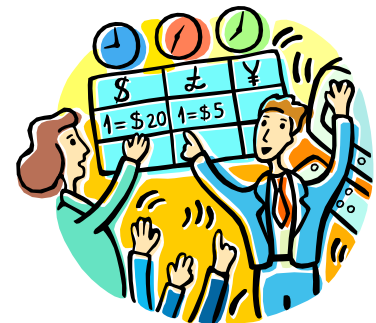
## ■ Classification

- predicts categorical class labels (discrete or nominal)
- Default predicted class: *majority voting*
- Optional: class probability estimation



## ■ Prediction / Regression

- models continuous-valued functions, i.e., predicts unknown or missing values
- Default prediction: *expected value*
- Optional: confidence interval

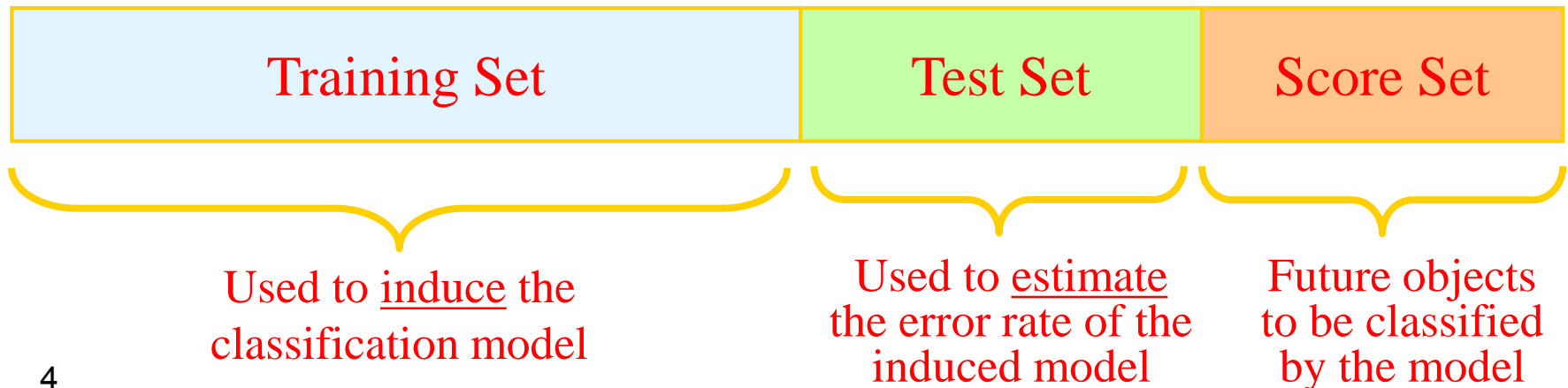


# Examples of typical classification / prediction tasks

- Typical classification tasks
  - Credit approval: approve / deny
  - Target marketing: will buy / will not buy
  - Medical diagnosis: Hepatitis B / Hepatitis C
  - Fraud detection: lawful transaction / fraudulent transaction
- Typical prediction / regression tasks
  - Weather forecast: predict tomorrow's temperature
  - Stock trading: predict stock's price tomorrow

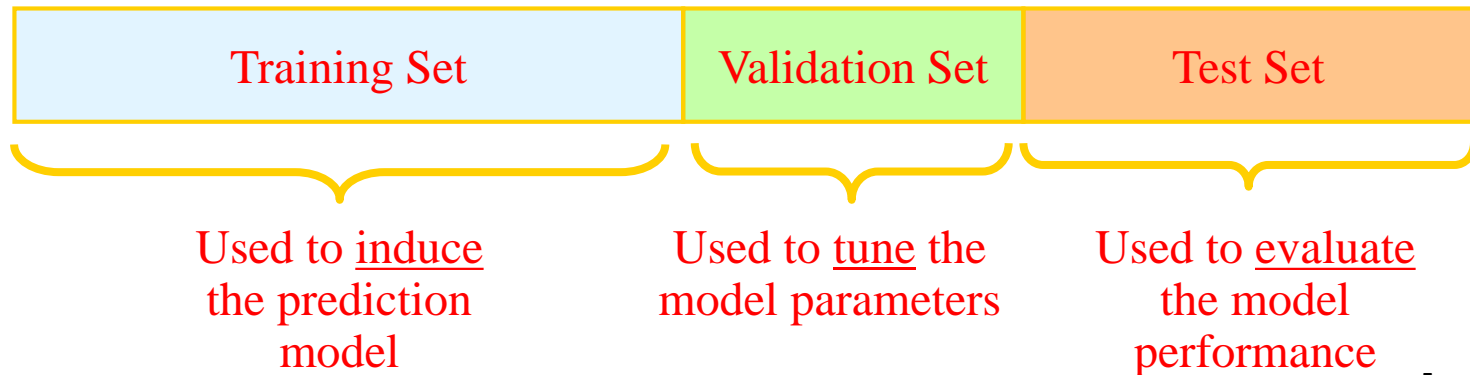
# Classification—A Two-Step Process

- Model construction / induction
  - Record labeling
  - Building a *training set*
  - Inducing the model(s)
- Model usage
  - Comparing to the *default (majority) rule*
  - Measuring the accuracy rate over time



# Model Evaluation and Selection

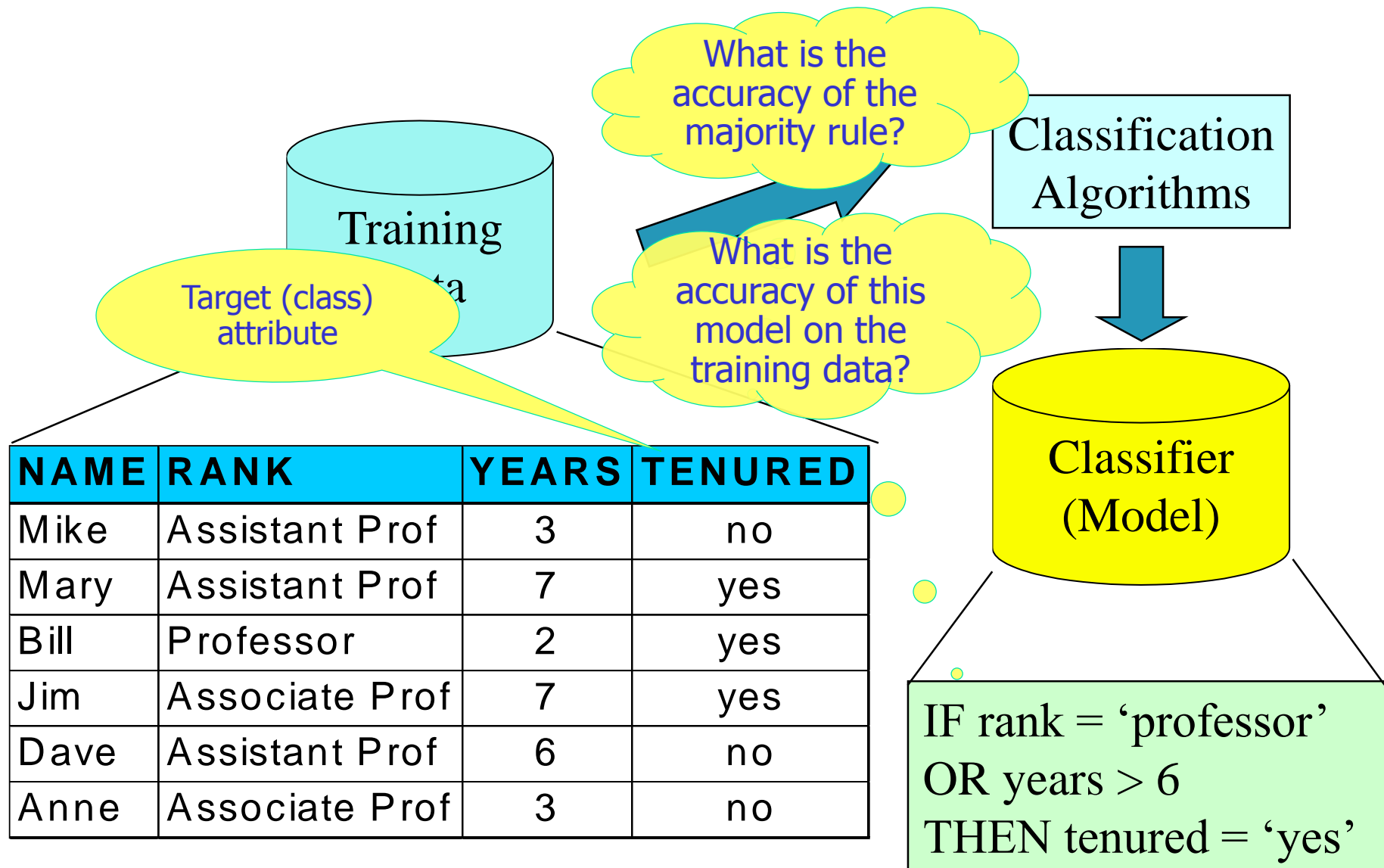
- Evaluation metrics: How can we measure accuracy? Other metrics to consider?
- Use **test set** of class-labeled tuples instead of training set when assessing accuracy
  - The model should generalize beyond the training instances
- Use **validation set** to tune model parameters
  - Common splits: 50:20:30 or 40:20:40



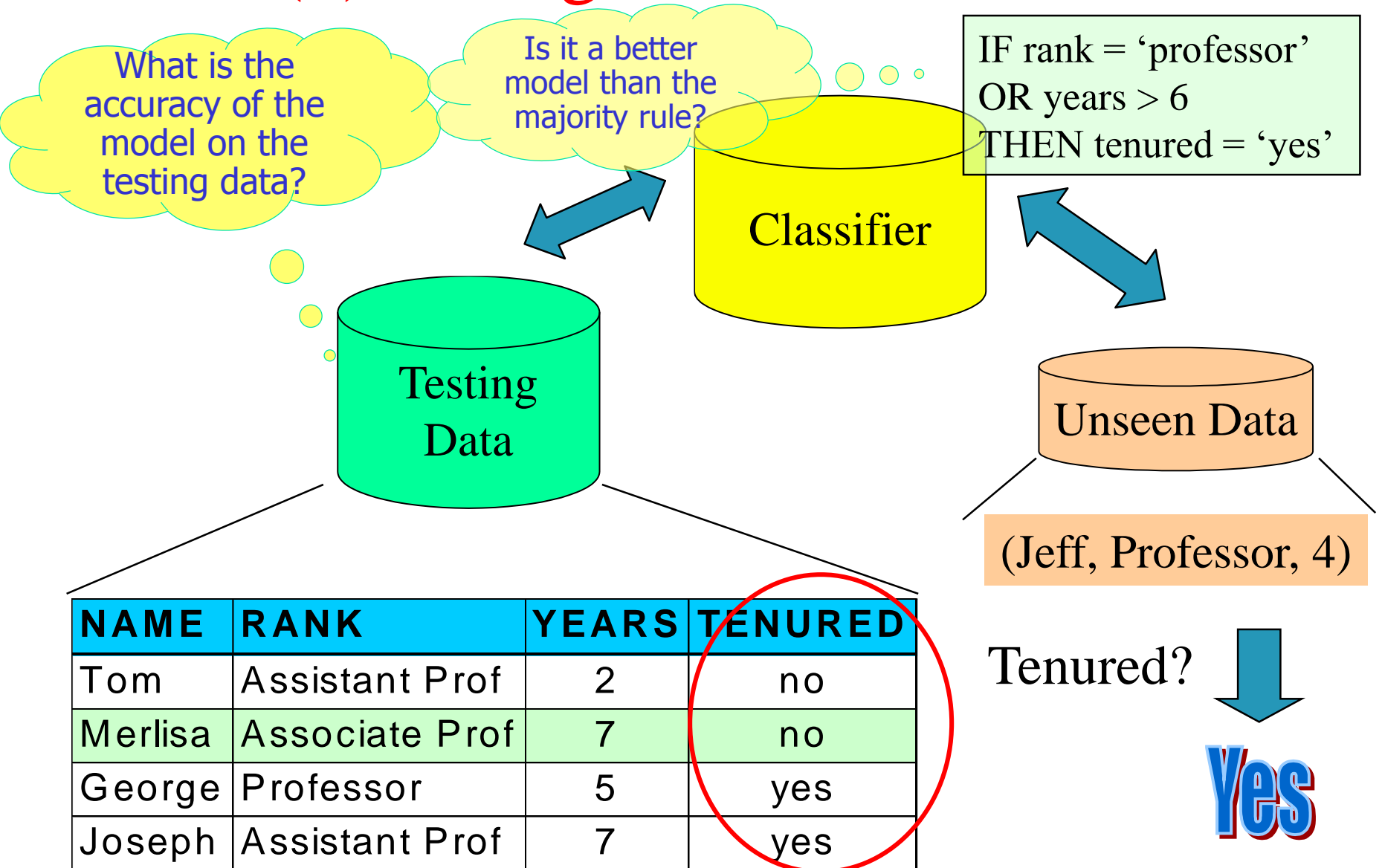
5

- **k-Fold Cross Validation**

# Process (1): Model Construction



# Process (2): Using the Model in Prediction



# Classification—Accuracy Estimation

- Estimate accuracy of the model
  - The known label is compared to the predicted label
  - Training Accuracy Rate =  $1 - Err_{Tr}$ 
    - The percentage of *training set* samples that are correctly classified by the model
  - Testing Accuracy Rate =  $1 - Err_{Test}$ 
    - The percentage of *test set* samples that are correctly classified by the model
    - Test set is independent of training set, otherwise over-fitting will occur
- If the accuracy is acceptable, use the model to **classify data** tuples whose class labels are not known



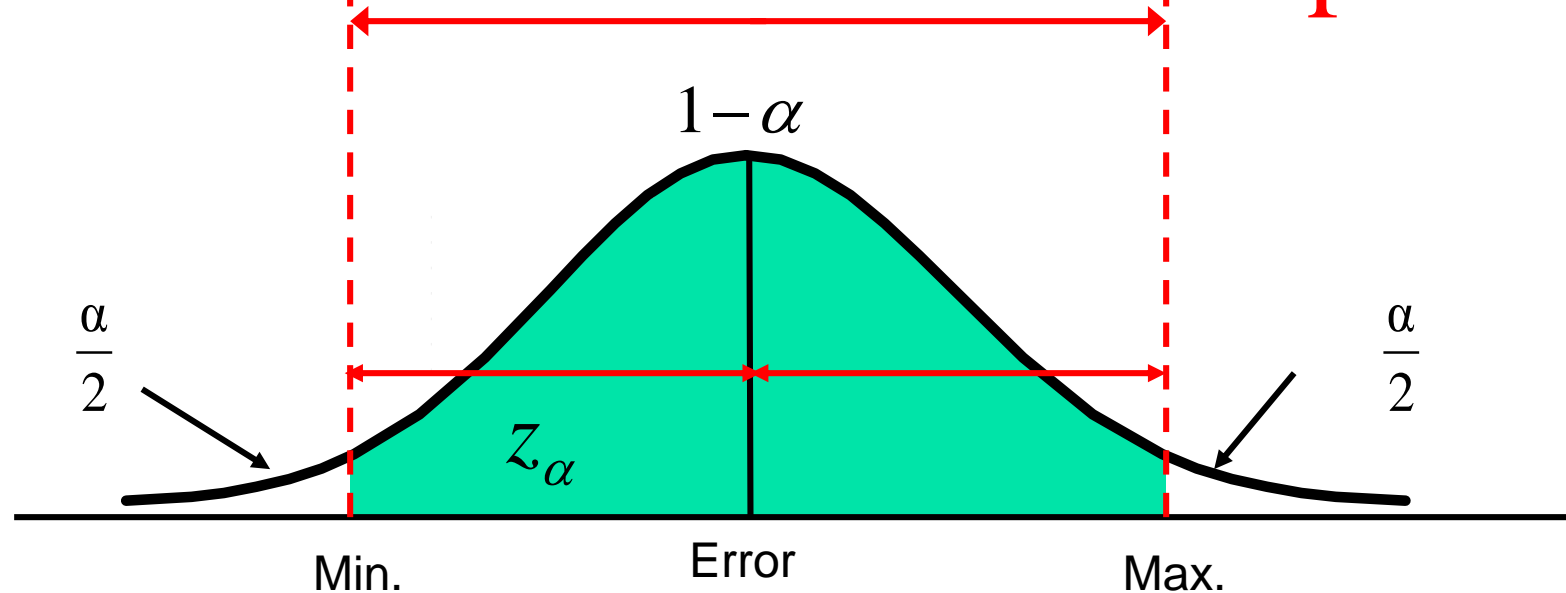
# Confidence Interval for an Error Rate

- Test error  $Err_{Test}$  is an *estimate* of the true error rate  $Err_{True}$  on the entire population
- $Err_{Test}$  is governed by Binomial distribution approximated by Normal when  $n \geq 30$ 
  - Assumption:  $n$  test samples are drawn randomly and independently from the entire population
- With the probability  $1 - \alpha$ , the true error rate  $Err_{True}$  lies in the *confidence interval*

How to estimate the true accuracy rate?

$$\left[ Err_{Test} - z_{\alpha} \sqrt{\frac{Err_{Test}(1 - Err_{Test})}{n}}; Err_{Test} + z_{\alpha} \sqrt{\frac{Err_{Test}(1 - Err_{Test})}{n}} \right]$$

# Confidence Interval - Example



alpha	0.2	0.1	0.05	0.01	0.001
Z_alpha	1.282	1.645	1.960	2.576	3.291

Error	n	alpha	z_alpha	min.	max.
0.200	30	0.010	2.576	0.0119	0.3881
0.200	30	0.050	1.960	0.0569	0.3431
0.200	30	0.100	1.645	0.0799	0.3201

# Difference between Classifiers

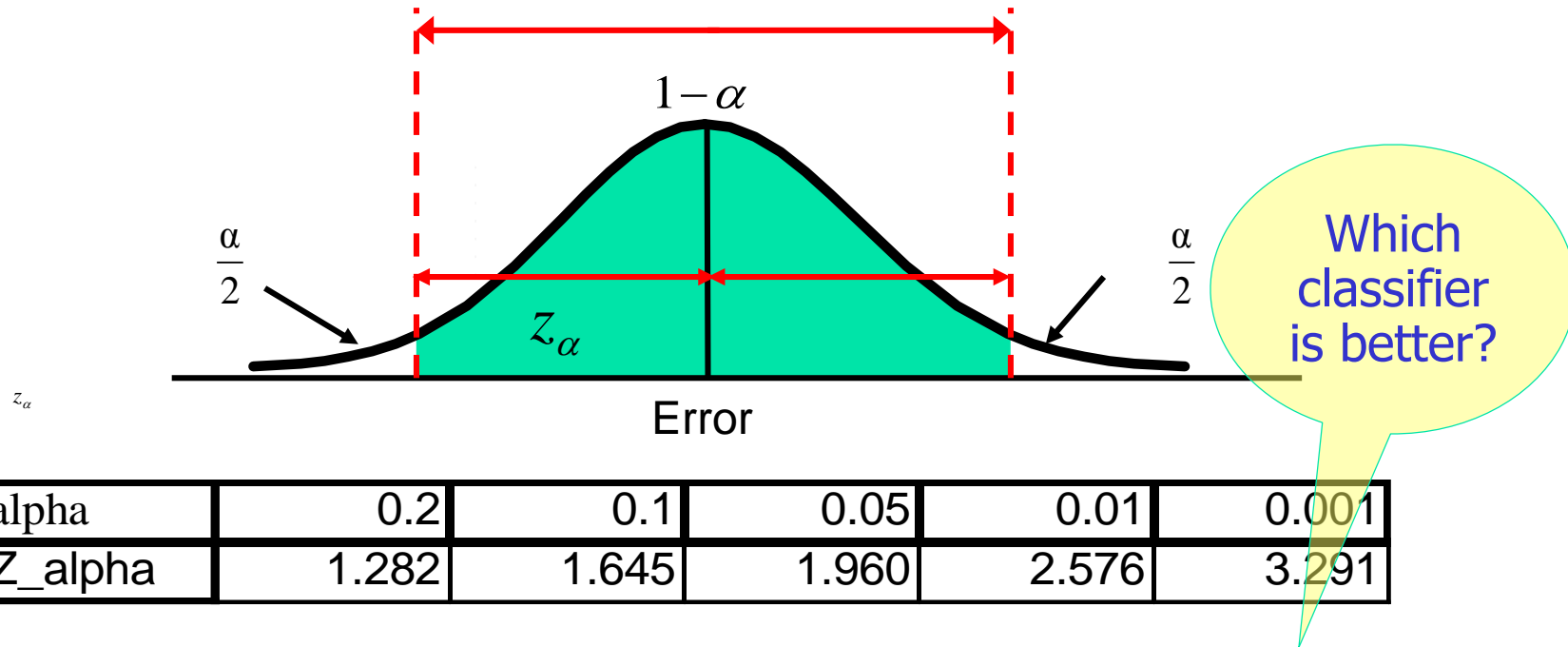
- Estimated difference between error rates

$$\hat{d} = Err_{Test1} - Err_{Test2}$$

- $\hat{d}$  is governed by Binomial distribution approximated by Normal when  $n_1, n_2 \geq 30$
- With the probability  $1 - \alpha$ , the true difference  $d$  lies in the *confidence interval*

$$\hat{d} \pm z_{\alpha} \sqrt{\frac{Err_{Test1}(1 - Err_{Test1})}{n_1} + \frac{Err_{Test2}(1 - Err_{Test2})}{n_2}}$$

# Difference between Classifiers – Example (Error1 vs. Error 2)

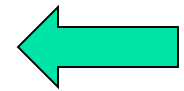


alpha	0.2	0.1	0.05	0.01	0.001
Z_alpha	1.282	1.645	1.960	2.576	3.291

Error1	n1	Error2	n2	d	alpha	z_alpha	min.	max.
0.200	30	0.400	40	0.20	0.010	2.326	-0.048	0.448
0.200	30	0.400	40	0.20	0.050	1.645	0.025	0.375
0.200	30	0.400	40	0.20	0.100	1.282	0.064	0.336

# Lecture No. 5 – Decision Tree Learning

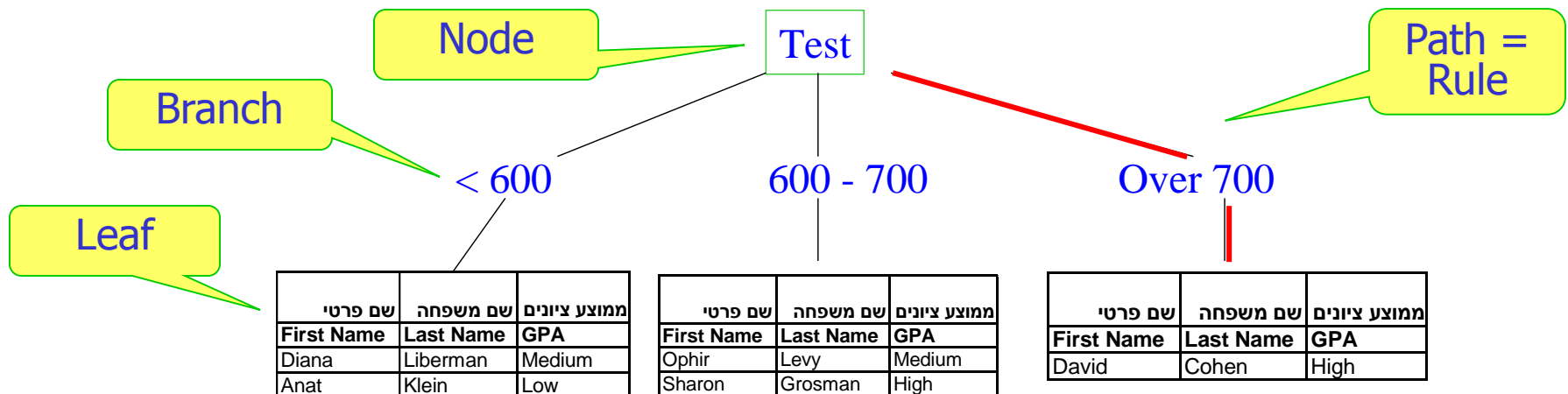
- Classification and Prediction
- Overview of Decision Tree Learning
- Avoiding Overfitting



# Decision Tree Structure

## Main Components

- *Nodes* - tests of some attribute
- *Branch* - one of possible values for the attribute
- *Leaves* (*terminal nodes*) - classifications
- *Path* (from the tree root to a leaf) - conjunction of attribute tests



# Decision Tree Learning

## Appropriate Problems + Student Example

- Instances are described by a *fixed* set of attributes
  - Example: *Gender, Place of Birth, and Test Grade*
- Each predicting attribute takes a *small* number of disjoint possible values
  - Example: Place of Birth (Israel vs. Abroad)
- The target function has *discrete* output values (each value = class / concept)
  - Example: GPA (Low, Medium, High)
- *Disjunctive* rules are required
  - Example:
    - If (Test < 600) Then GPA = Low
    - If (Test ≥ 600) Then GPA = Medium or High
- The training data may contain *errors* (noise)
- The training data may contain *missing attribute values*

# Algorithm for Decision Tree Induction

- Basic algorithm (a greedy algorithm – e.g., ID3)
  - Tree is constructed in a top-down recursive divide-and-conquer manner
  - At start, all the training examples are at the root
  - Attributes are categorical (if continuous-valued, they are discretized in advance)
  - Examples are partitioned recursively based on selected attributes
  - Test attributes are selected on the basis of a heuristic or statistical measure (e.g., information gain)
- Conditions for stopping partitioning
  - All samples for a given node belong to the same class
  - There are no remaining attributes for further partitioning – majority voting is employed for classifying the leaf
  - There are no samples left



# Detailed Example: Student Admission

All data in this  
example is  
fictional!

## Historical (Training) Data:

ת"ז	שם פרטי	שם משפחה	מגדר	תאריך לידה	מקום לידה	שנת קבלה	ציון פסיכומטרי	שנת סיום	ממוצע ציונים
ID	First Name	Last Name	Gender	Date of Birth	Place of Birth	Admission Year	Test Grade	Graduation Year	GPA
543406619	David	Cohen	M	18/12/1979	USA	2002	730	2006	93.5
951984264	Ophir	Levy	M	11/07/1980	Israel	2002	680	2006	87.5
683168092	Sharon	Grosman	F	19/05/1981	Israel	2002	640	2006	94.3
100900927	Diana	Liberman	F	11/02/1980	Russia	2002	585	2006	85.8
516120403	Anat	Klein	F	03/02/1982	Israel	2002	570	2006	78.7

## New (Scoring) Data:

ת"ז	שם פרטי	שם משפחה	מגדר	תאריך לידה	מקום לידה	שנת הגשת מועמדות	ציון פסיכומטרי	שנת סיום מתוכננת	ממוצע ציונים צפוי
ID	First Name	Last Name	Gender	Date of Birth	Place of Birth	Application Year	Test Grade	Expected Graduation Year	Expected GPA
537793401	Boaz	Bazak	M	22/09/1985	Israel	2007	580	2011	?
808943728	Ophir	Levy	M	10/02/1985	Israel	2007	650	2011	?
537362102	Maria	Neuman	F	03/12/1987	Ukraine	2007	720	2011	?

# Pre-processing: Removing Irrelevant Features

ת"ז	שם פרטי	שם משפחה	מגדר	תאריך לידה	מקום לידה	שנת קבלה	ציון פסיכומטרי	שנת סיום	ממוצע ציונים
ID	First Name	Last Name	Gender	Date of Birth	Place of Birth	Admission Year	Test Grade	Graduation Year	GPA
543406619	David	Cohen	M	18/12/1979	USA	2002	730	2006	93.5
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683168092	Sharon	Grosman	F	19/05/1981	Israel	2002	640	2006	94.3
100900927	Diana	Liberman	F	11/02/1980	Russia	2002	585	2006	85.8
516120403	Anat	Klein	F	03/02/1982	Israel	2002	570	2006	78.7

Remained features (attributes)

- Gender
- Place of Birth
- Test Grade

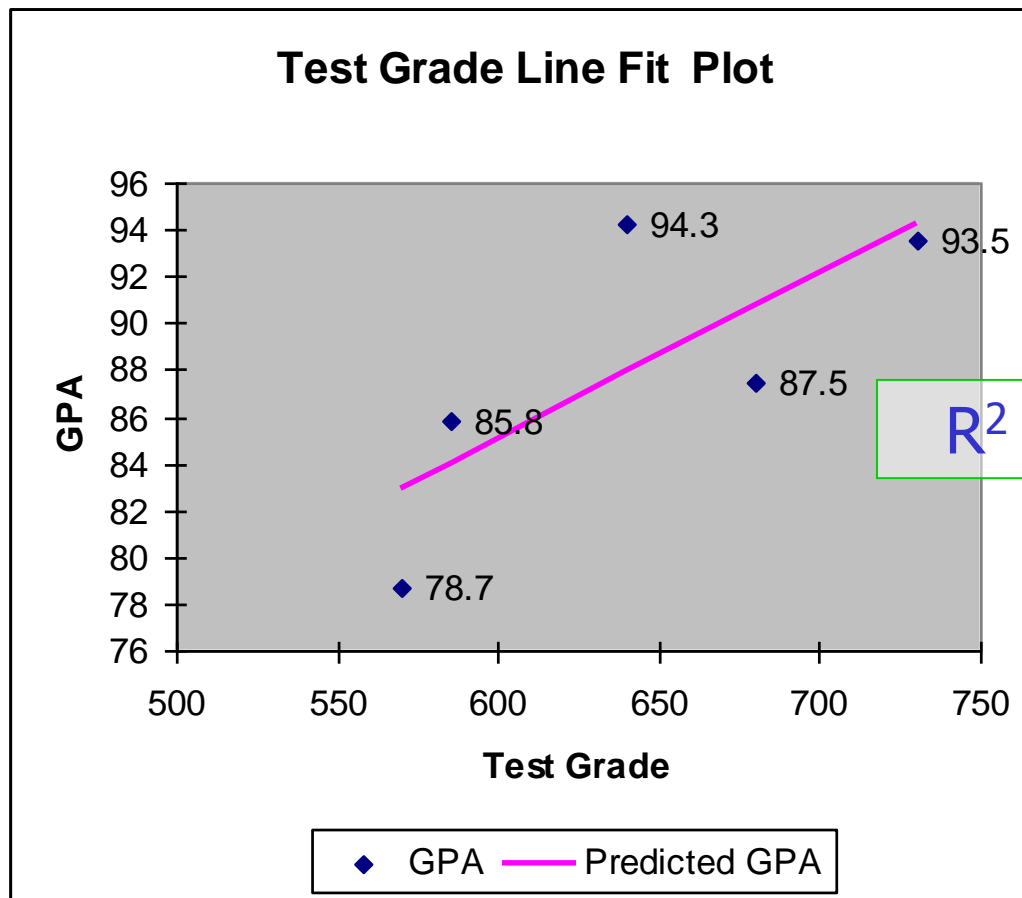
Predicted attribute: GPA

**The problem:** find the best (most accurate) model predicting GPA

# Try 1:

## Predict GPA Using a Linear Fit

Predictive attribute: Test Grade



# More Pre-processing

Goal: reduce the number of values

Generalize to two values  
(Israel vs. Diaspora)

Discretize to  
three intervals

Discretize to  
three intervals

Low	0-79
Medium	80-89
High	90-100

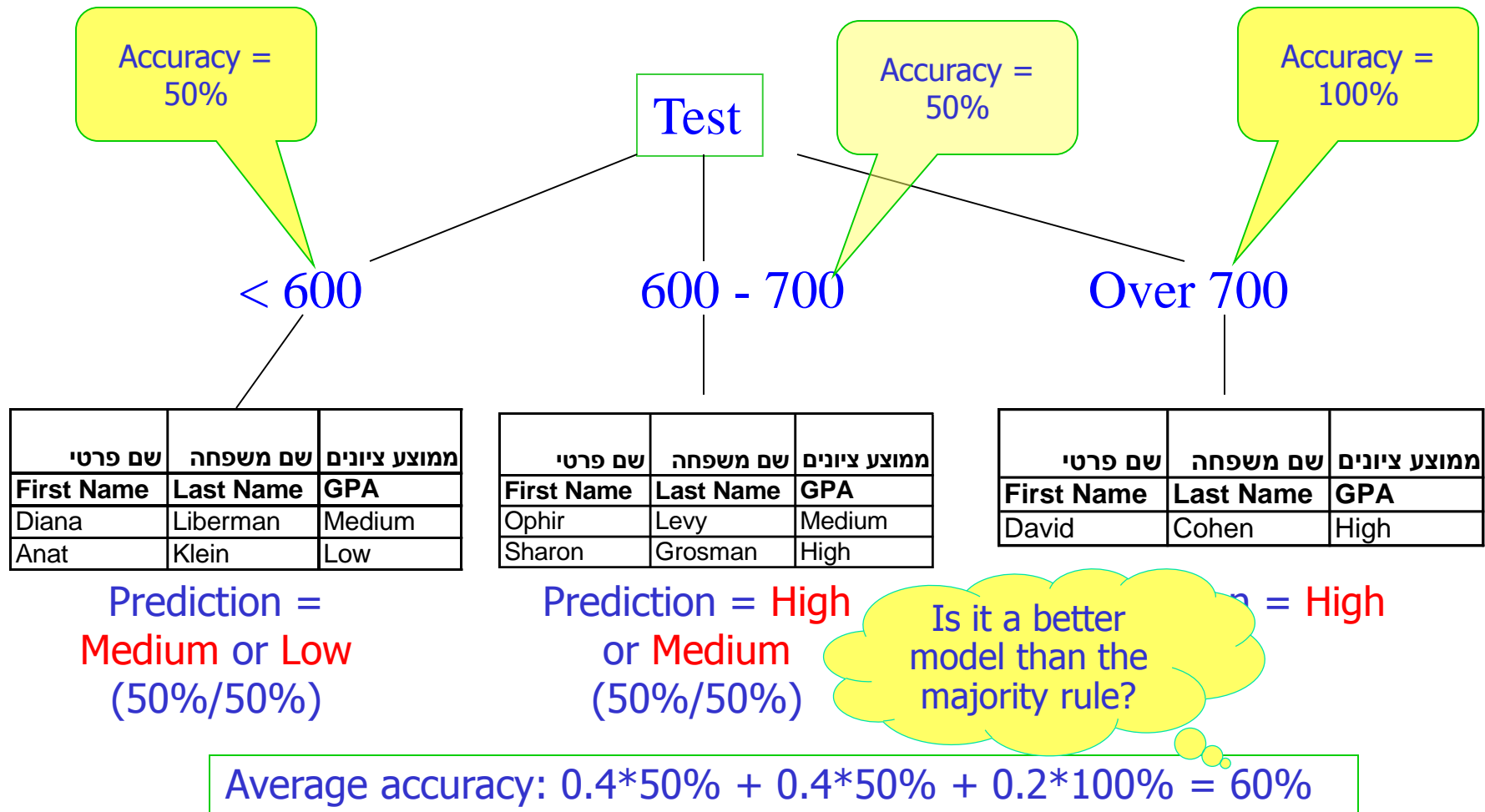
שם פרטי	שם משפחה	מגדר	מקום לידה	ציון פסיכומטרי	ממוצע ציונים
First Name	Last Name	Gender	Place of Birth	Test Grade	GPA
David	Cohen	M	Diaspora	Over 700	High
Ophir	Levy	M	Israel	600-700	Medium
Sharon	Grosman	F	Israel	600-700	High
Diana	Liberman	F	Diaspora	0-600	Medium
Anat	Klein	F	Israel	0-600	Low
	Use:			Output	Target

What is the  
accuracy of the  
majority rule?



# Try 2: Predict GPA Using a *Tree*

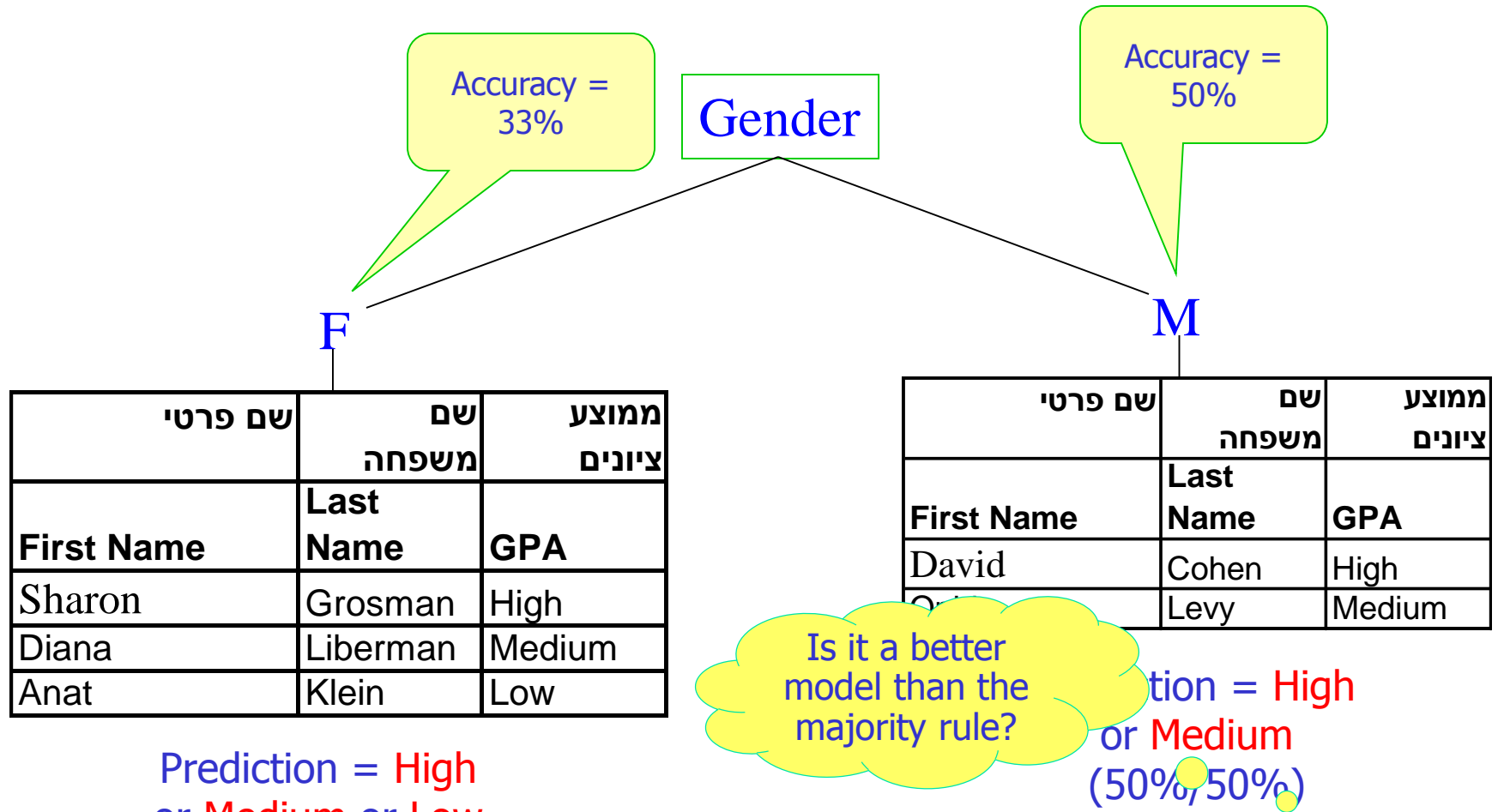
## Predictive attribute: Test Grade





# Try 2: Predict GPA Using a *Tree*

## Predictive attribute: Gender

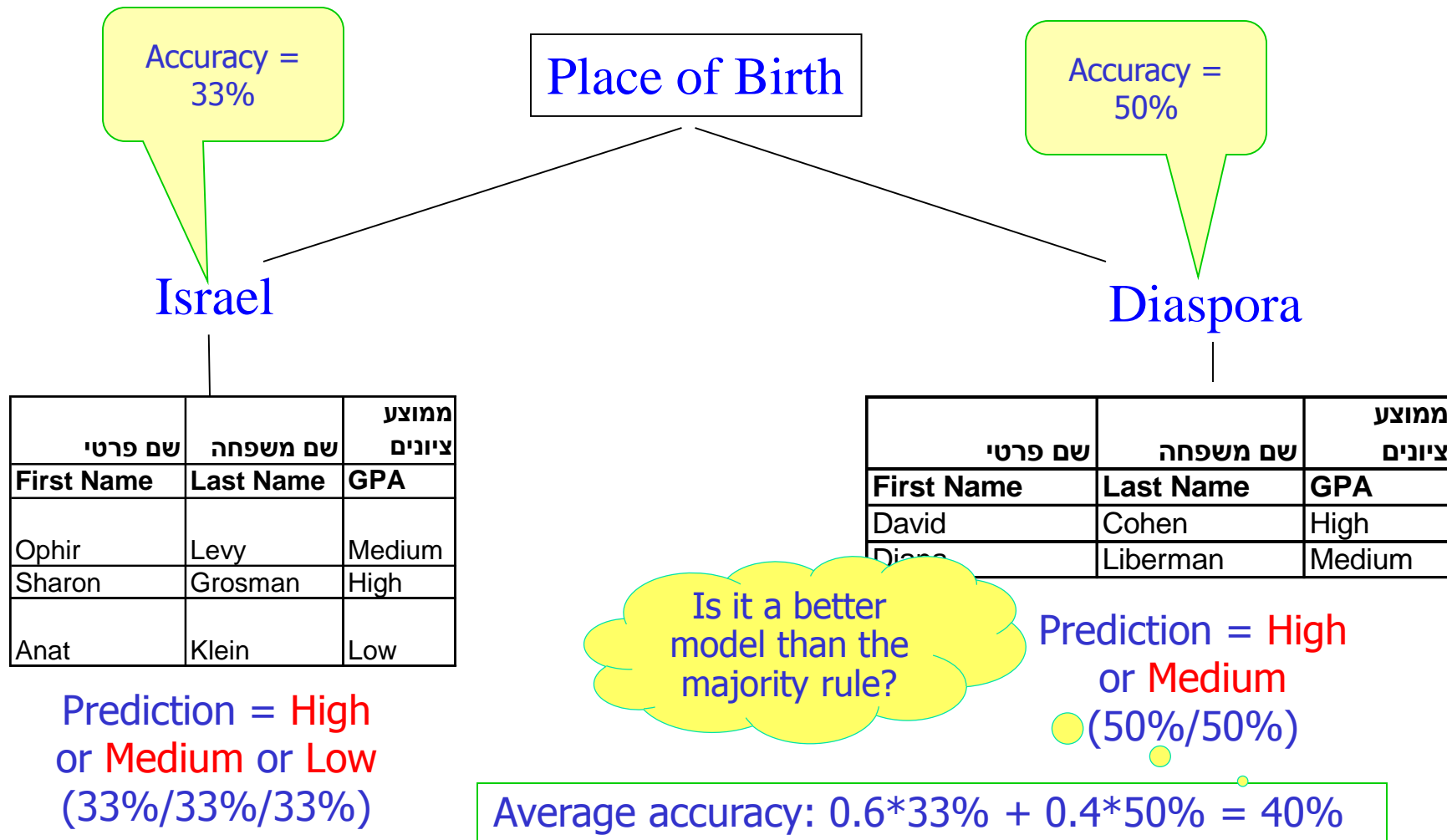


$$\text{Average accuracy: } 0.4 \cdot 50\% + 0.6 \cdot 33\% = 40\%$$



# Try 2: Predict GPA Using a *Tree*

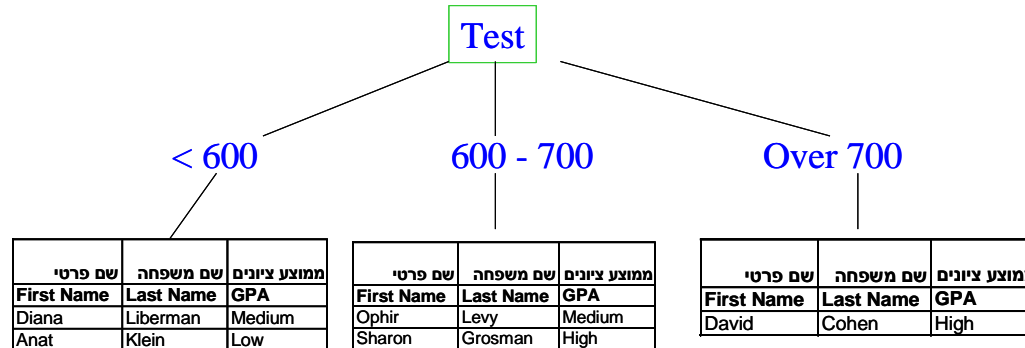
## Predictive attribute: Place of Birth



# How to choose the best tree?

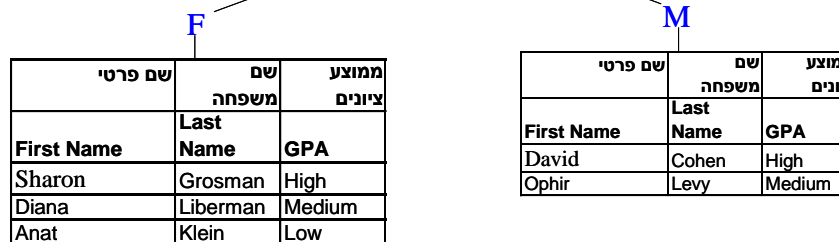
Training accuracy:

$$0.4 \cdot 50\% + 0.4 \cdot 50\% + 0.2 \cdot 100\% = 60\%$$



Test,  
Gender  
or Place  
of  
Birth?

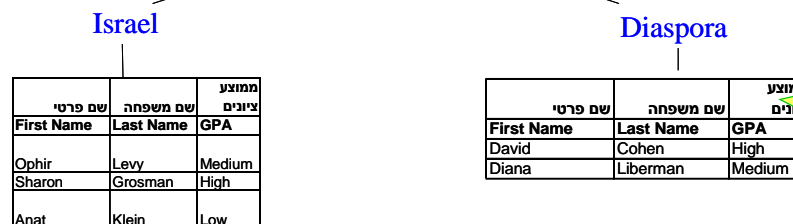
Gender



Training accuracy:

$$0.4 \cdot 50\% + 0.6 \cdot 33\% = 40\%$$

Place of Birth



Training accuracy:

$$0.6 \cdot 33\% + 0.4 \cdot 50\% = 40\%$$

ID3: Use  
Information  
Gain





# Attribute Selection Measure in ID3:

## Information Gain

- Select the attribute with the highest information gain
- Let  $p_i$  be the probability that an arbitrary tuple in  $D$  belongs to class  $C_i$ , estimated by  $|C_i \cap D|/|D|$
- **Expected information** (entropy) needed to classify a tuple in  $D$ :

$$Info(D) = - \sum_{i=1}^m p_i \log_2(p_i)$$

- **Information** (conditional entropy) needed (after using  $A$  to split  $D$  into  $v$  partitions) to classify  $D$ :

$$Info_A(D) = \sum_{j=1}^v \frac{|D_j|}{|D|} \times I(D_j)$$

- **Information gained** (mutual information) by branching on attribute  $A$

$$Gain(A) = Info(D) - Info_A(D)$$

# Student Admission Example

Expected information  
(entropy) needed to  
classify a tuple in  $D$ :

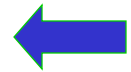
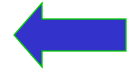
$$Info(D) = -\sum_{i=1}^m p_i \log_2(p_i)$$

Number of classes ( $m$ ): 3

The classes:

- **Low** (one example)
- **Medium** (two examples)
- **High** (two examples)

Low	1
p	0.200
-logp	2.322
Medium	2
p	0.400
-logp	1.322
High	2
p	0.400
-logp	1.322
Total	5
p	1.00
<b>Entropy</b>	<b>1.522</b>



$$0.2 * 2.322 + 0.4 * 1.322 + 0.4 * 1.322 = 1.522$$

# Student Admission Example (cont.)

Attribute:

Test Grade

Values:

- 0-600
- 600-700
- Over 700

$$Info(D) = -\sum_{i=1}^m p_i \log_2(p_i)$$

$$Info_A(D) = \sum_{j=1}^v \frac{|D_j|}{|D|} \times Info(D_j)$$

$$Gain(A) = Info(D) - Info_A(D)$$

$$Info(D) = 1.522$$

	Test Grade			Total
	0-600	600-700	Over 700	
Low	1	0	0	1
p	0.500	0.000	0.000	
-logp	1.000	0.000	0.000	
Medium	1	1	0	2
p	0.500	0.500	0.000	
-logp	1.000	1.000	0.000	
High	0	1	1	2
p	0.000	0.500	1.000	
-logp	0.000	1.000	0.000	
Total	2	2	1	5
p	0.40	0.40	0.20	1.00
Entropy	1.000	1.000	0.000	0.800
Gain				0.722

$$0.5 \times 1.0 + 0.5 \times 1.0 = 1.0 \quad 0.4 \times 1.0 + 0.4 \times 1.0 + 0.2 \times 0.0 = 0.8$$

# Student Admission Example (cont.)

Attribute:

Gender

$$Info(D) = -\sum_{i=1}^m p_i \log_2(p_i)$$

$$Info_A(D) = \sum_{j=1}^v \frac{|D_j|}{|D|} \times I(D_j)$$

$$Gain(A) = Info(D) - Info_A(D)$$

$$Info(D) = 1.522$$

	Gender		Total
	M	F	
Low	0	1	1
p	0.000	0.333	
-logp	0.000	1.585	
Medium	1	1	2
p	0.500	0.333	
-logp	1.000	1.585	
High	1	1	2
p	0.500	0.333	
-logp	1.000	1.585	
Total	2	3	5
p	0.40	0.60	1.00
Entropy	1.000	1.585	1.351
Gain			0.171

# Student Admission Example (cont.)

Attribute:

Place of Birth

$$Info(D) = -\sum_{i=1}^m p_i \log_2(p_i)$$

$$Info_A(D) = \sum_{j=1}^v \frac{|D_j|}{|D|} \times I(D_j)$$

$$Gain(A) = Info(D) - Info_A(D)$$

$$Info(D) = 1.522$$

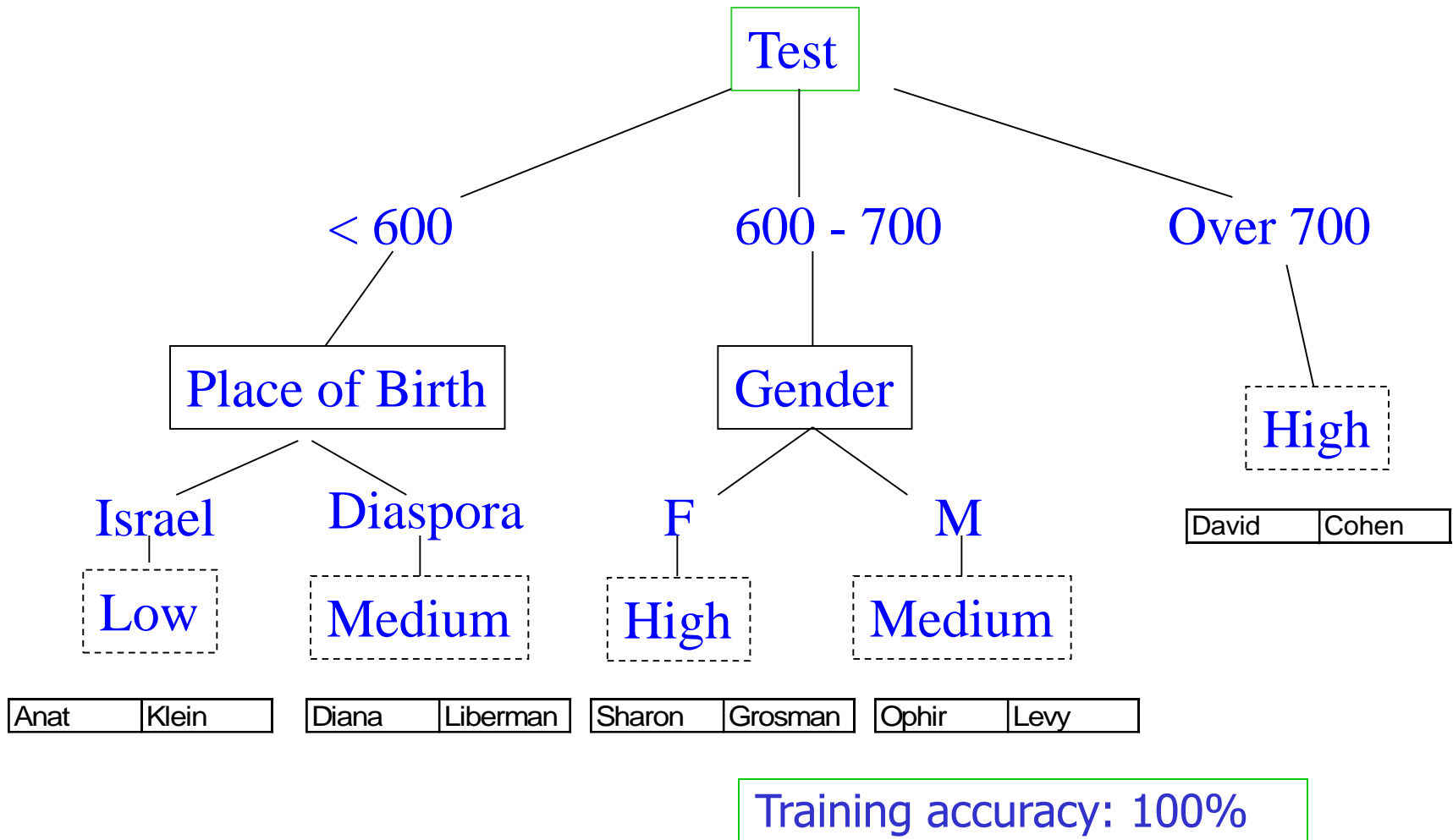
	Place of Birth		Total
	Israel	Abroad	
Low	1	0	1
p	0.333	0.000	
-logp	1.585	0.000	
Medium	1	1	2
p	0.333	0.500	
-logp	1.585	1.000	
High	1	1	2
p	0.333	0.500	
-logp	1.585	1.000	
Total	3	2	5
p	0.60	0.40	1.00
Entropy	1.585	1.000	1.351
Gain			0.171

# Student Admission Example (cont.)

- Gain (*Test Grade*) = 0.722
- Gain (*Gender*) = 0.171
- Gain (*Place of Birth*) = 0.171
- Selected attribute: **Test Grade**

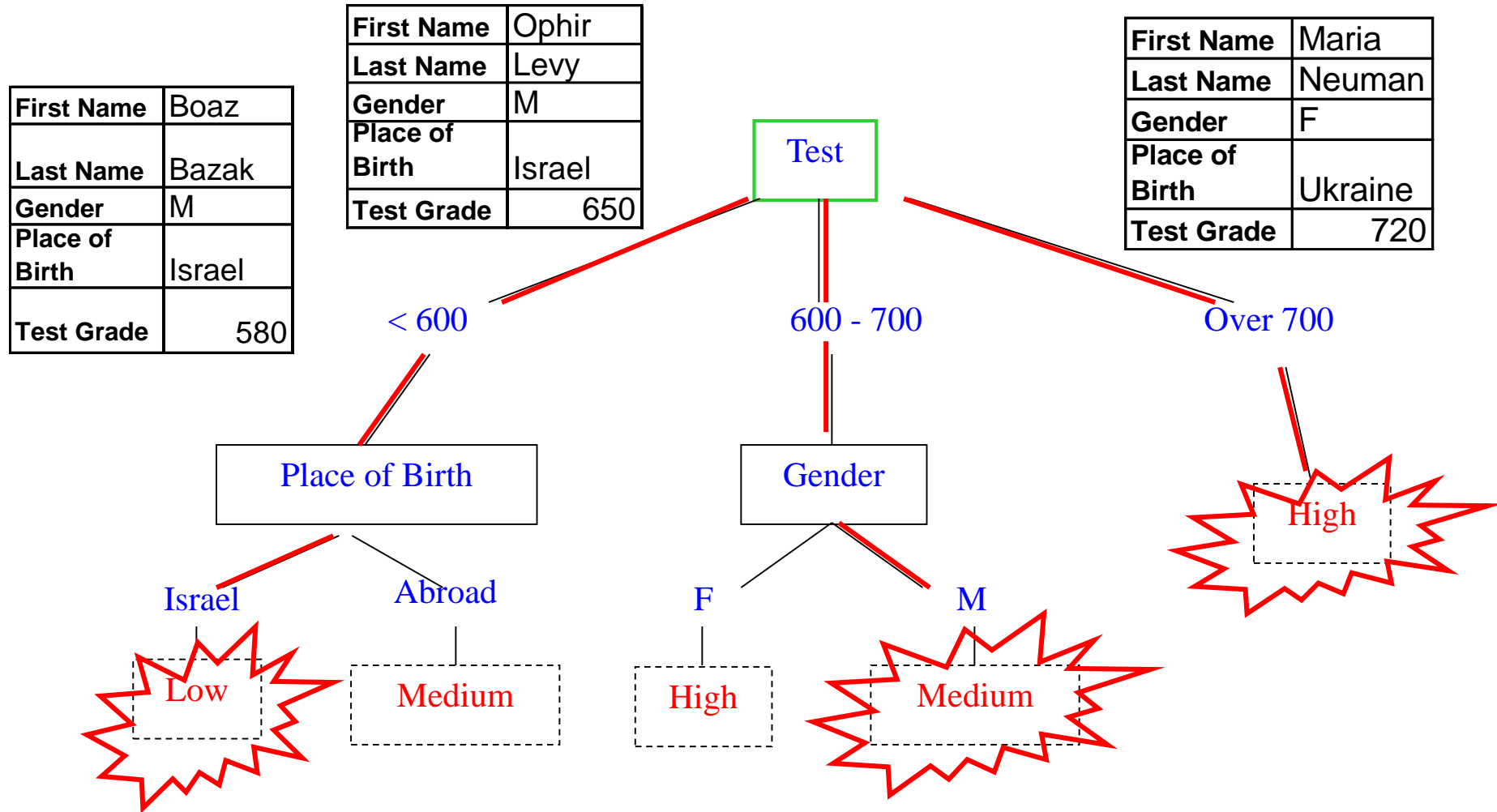
# Student Admission Example

## Complete Decision Tree



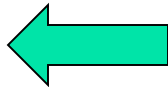
# Student Admission Example

## Classification with Decision Tree





# Lecture No. 5 – Decision Tree Learning

- Classification and Prediction
- Overview of Decision Tree Learning
- Avoiding Overfitting 

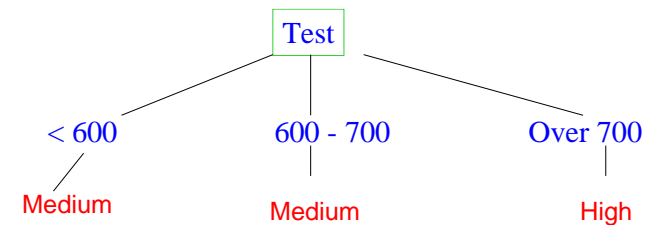
# Overfitting

- Overfitting: An induced tree may overfit the training data
  - Too many branches, some may reflect anomalies due to noise or outliers
  - Poor accuracy for unseen samples
- Definition of overfitting
  - $h$  – hypothesis (e.g., decision tree) in a *hypothesis space*  $H$
  - Training data:  $error_{train}(h)$
  - Entire population  $D$ :  $error_D(h)$
  - Hypothesis  $h \in H$  **overfits** training data if there is an alternative hypothesis  $h' \in H$  such that
    - $error_{train}(h) < error_{train}(h')$  and
    - $error_D(h) > error_D(h')$

# Overfitting – Student Example

Tree1 ( $h'$ ):

ID	First Name	Last Name	Expected GPA	Actual GPA	Error
537793401	Boaz	Bazak	Medium	Medium	No
808943728	Ophir	Levy	Medium	Medium	No
537362102	Maria	Neuman	High	High	No



$$error_D(h') = 0\%$$

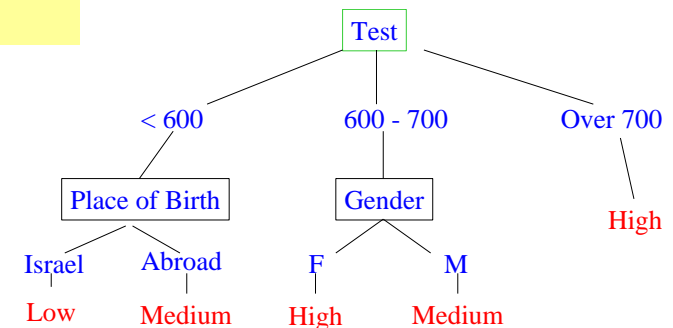
$$error_{train}(h') = 40\%$$

$$error_{train}(h) < error_{train}(h')$$

$$error_D(h) > error_D(h')$$

Tree2 ( $h$ ):

ID	First Name	Last Name	Expected GPA	Actual GPA	Error
537793401	Boaz	Bazak	Low	Medium	Yes
808943728	Ophir	Levy	Medium	Medium	No
537362102	Maria	Neuman	High	High	No



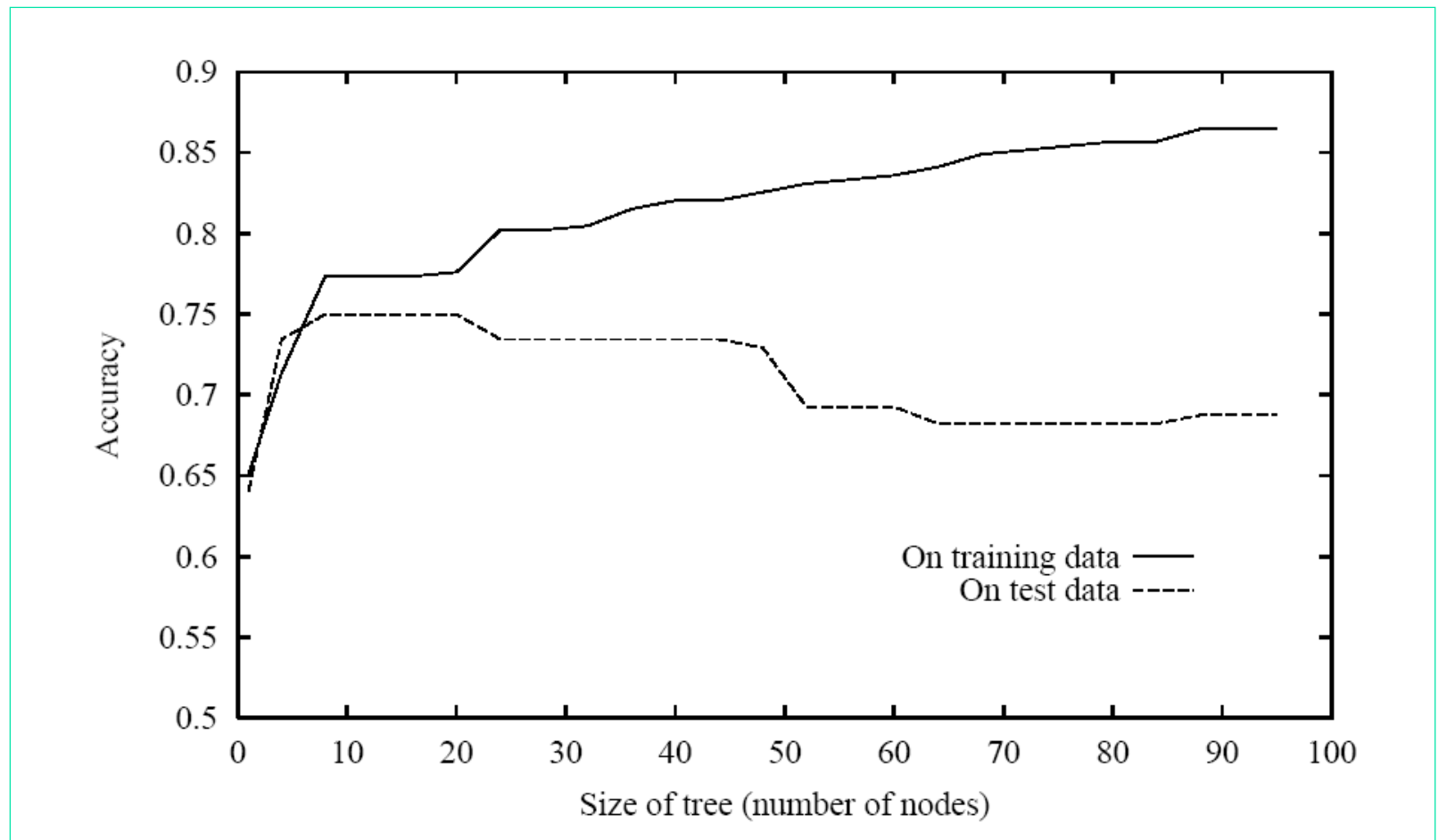
$$error_D(h) = 33\%$$

$$error_{train}(h) = 0\%$$

Which tree is better?

# Overfitting in Decision Tree Learning

(Source: Mitchell, 1997)



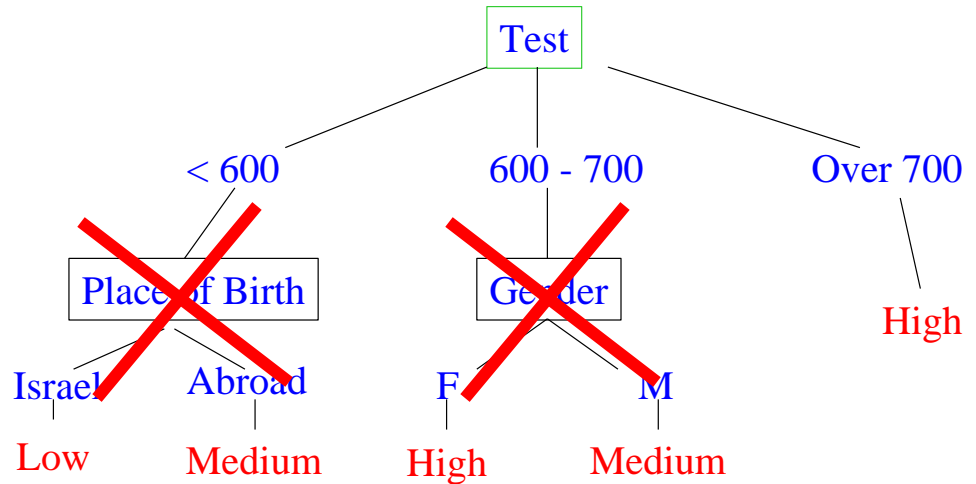
# Avoiding Overfitting

- Two approaches to avoid overfitting
  - Prepruning: Halt tree construction early —do not split a node if this would result in the goodness measure falling below a threshold
    - Difficult to choose an appropriate threshold
  - Postpruning: Remove branches from a “fully grown” tree—get a sequence of progressively pruned trees
    - Use a set of data different from the training data to decide which is the “best pruned tree”

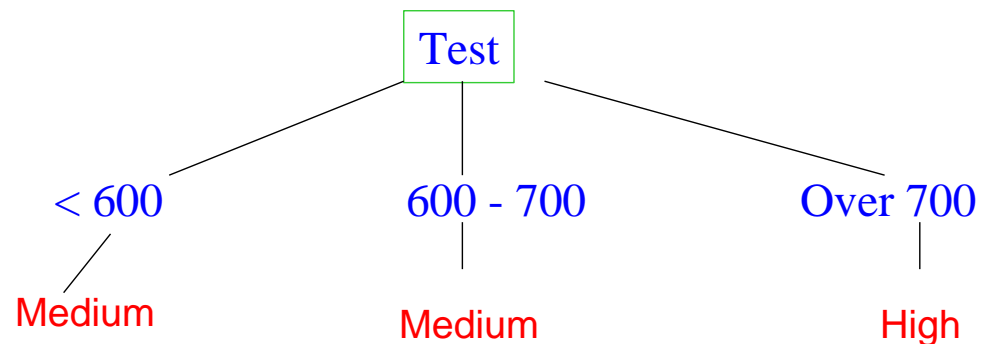
# Avoiding Overfitting - Student Example

“Fully grown” tree:

Prune two nodes:



Pruned tree:



# Approaches to Avoid Overfitting and Determine the Final Tree Size

- Separate training (2/3) and testing (1/3) sets
- Use cross validation, e.g., 10-fold cross validation
- Use all the data for training
  - but apply a statistical test (e.g., chi-square) to estimate whether expanding or pruning a node may improve the entire distribution
- Use minimum description length (MDL) principle
  - halting growth of the tree when the encoding is minimized

# Chi-Square Test

(based on Quinlan, Induction of Decision Trees, 1986)

## ■ Notation

- $A$  - splitting (branching) attribute (e.g., Test)
- $v$  - domain size of attribute  $A$  (3: 0-600, 600-700, 700+)
- $C_i$  - subset of records containing value  $i$  of attribute  $A$  (Test < 600: 2)
- $c$  - number of classes (3: low, medium, high)
- $e_j$  - number of records belonging to class  $j$  in the entire data set  $C$  ( $Low = 1$ ,  $Medium = 2$ ,  $High = 2$ )
- $o_{ij}$  - number of records belonging to class  $j$  in subset  $C_i$  (Test < 600, GPA = Low : 1)
- $\alpha$  - significance level



# Chi-Square Test (cont.)

- **Null Hypothesis:** attribute  $A$  is irrelevant to classifying the records in data set  $C$
- **Alternative Hypothesis:** attribute  $A$  affects the class distribution in data set  $C$
- Expected number of class  $j$  records in subset  $C_i$ :
- $e_j$  – actual number of records in class  $j$
- $o_{ij}$  - actual number of class  $j$  records in subset  $C_i$

$$e'_{ij} = \frac{e_j}{\sum_{j=1}^c e_j} \sum_{j=1}^c o_{ij}$$

## Statistic:

$v$  - domain size of  $A$

$c$  – number of classes

$$\sum_{j=1}^c \sum_{i=1}^v \frac{(o_{ij} - e'_{ij})^2}{e'_{ij}} \sim \chi^2_{((v-1)(c-1))}$$

# Chi-Square Test – Student Example

$$e'_{ij} = \frac{e_j}{\sum_{j=1}^c e_j} \sum_{j=1}^c o_{ij}$$

- Entire data set (before splitting):  $e_{Low} = 1, e_{Medium} = 2, e_{High} = 2$
- Splitting by *Test*
  - **Test < 600:**  $Low = 1, Medium = 1$   $\sum_{j=1}^c o_{ij} = 2$ 
    - $e'_{low} = (1/5)*2 = 0.4, e'_{medium} = (2/5)*2 = 0.8. e'_{high} = (2/5)*2 = 0.8.$
  - **Test = 600-700:**  $Medium = 1, High = 1$   $\sum_{j=1}^c o_{ij} = 2$ 
    - $e'_{low} = (1/5)*2 = 0.4, e'_{medium} = (2/5)*2 = 0.8. e'_{high} = (2/5)*2 = 0.8.$
  - **Test > 700:**  $High = 1$   $\sum_{j=1}^c o_{ij} = 1$ 
    - $e'_{low} = (1/5)*1 = 0.2, e'_{medium} = (2/5)*1 = 0.4. e'_{high} = (2/5)*1 = 0.4.$

# Chi-Square Test – Student Example (cont.)

		Test Grade (i)			Total	p <sub>j</sub>
GPA (j)		0-600	600-700	Over 700		
Low	Actual	1	0	0	1	0.2
	<b>Expected</b>	<b>0.4</b>	<b>0.4</b>	<b>0.2</b>	1	
	<b>Statistic</b>	<b>0.9</b>	<b>0.4</b>	<b>0.2</b>	<b>1.5</b>	
Medium	Actual	1	1	0	2	0.4
	<b>Expected</b>	<b>0.8</b>	<b>0.8</b>	<b>0.4</b>	2	
	<b>Statistic</b>	<b>0.05</b>	<b>0.05</b>	<b>0.4</b>	<b>0.5</b>	
High	Actual	0	1	1	2	0.4
	<b>Expected</b>	<b>0.8</b>	<b>0.8</b>	<b>0.4</b>	2	
	<b>Statistic</b>	<b>0.8</b>	<b>0.05</b>	<b>0.9</b>	<b>1.75</b>	
Total		2	2	1	<b>3.75</b>	5

Statistic:

$$\sum_{j=1}^c \sum_{i=1}^v \frac{(o_{ij} - e'_{ij})^2}{e'_{ij}} = 3.75$$

$$\chi^2_{0.05}(4) = 9.49$$

Conclusion: do not split the node on *Test Grade*

# Pessimistic Error Pruning (PEP)

- Uses training set to estimate error on new data
- Error estimate (relative frequency with continuity correction)
  - probability of error (apparent error rate)

$$q = \frac{N - n_C + 0.5}{N}$$

- where
  - $N$  = #examples
  - $n_C$  = #examples in majority class

# Pessimistic Error Pruning (cont.)

- Error of a node  $v$  (if pruned)

$$q(v) = \frac{N_v - n_{C,v} + 0.5}{N_v}$$

- where

- $N_v$  = #examples at node  $v$
- $n_{C,v}$  = #examples in majority class at node  $v$

- Error of a subtree  $T$

- Where

- $l$  = leaf node of sub-tree  $T$

$$q(T) = \frac{\sum_{l \in \text{leaves}(T)} (N_l - n_{C,l} + 0.5)}{\sum_{l \in \text{leaves}(T)} N_l}$$

- Prune if  $q(v) \leq q(T)$
- Prunes in bottom-up fashion
  - fast
  - considered a weakness (on accuracy)

# Example of Post-Pruning

Class = Yes	20
Class = No	10
Error = 10/30	

Training Error (Before splitting) = 10/30

Pessimistic error =  $q(v) = (10 + 0.5)/30 = 10.5/30$

Training Error (After splitting) = 9/30

Pessimistic error (After splitting)  $q(T) = (9 + 4 \times 0.5)/30 = 11/30$

