UNIVERSITÄT MANNHEIM

Data Mining I
Classification, Part 2

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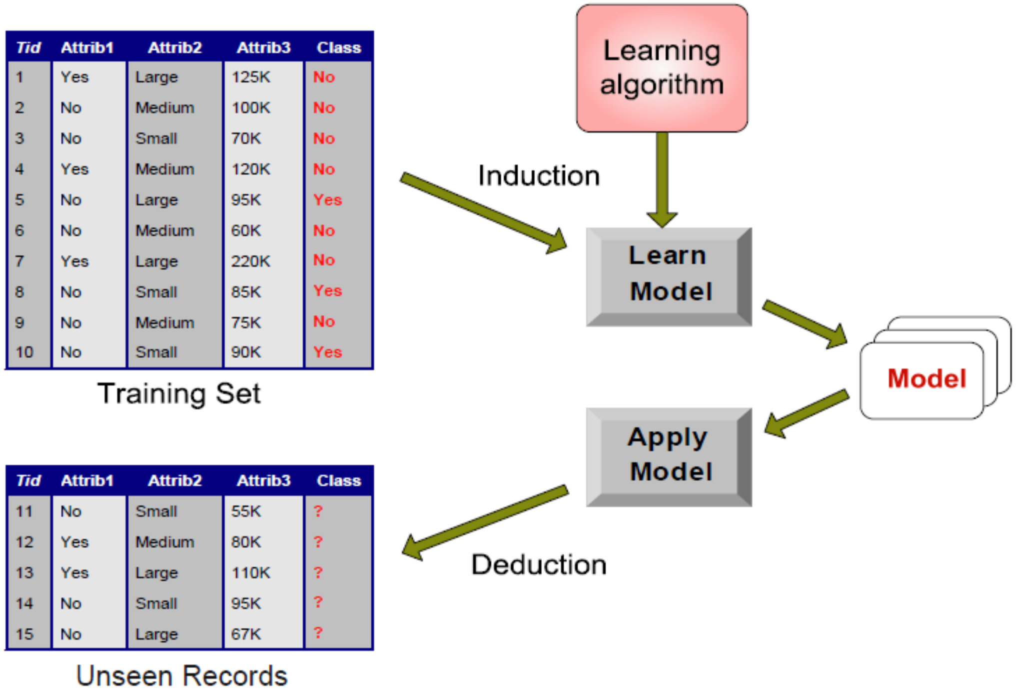
Outline

Lazy vs. Eager Learning

- Both k-NN and Naïve Bayes are “lazy” methods
- They do not build an explicit model!
  - “learning” is only performed on demand for unseen records



Tid	Attrib1	Attrib2	Attrib3	Class
1	Yes	Large	125K	No
2	No	Medium	100K	No
3	No	Small	70K	No
4	Yes	Medium	120K	No
5	No	Large	95K	Yes
6	No	Medium	60K	No
7	Yes	Large	220K	No
8	No	Small	85K	Yes
9	No	Medium	75K	No
10	No	Small	90K	Yes

Tid	Attrib1	Attrib2	Attrib3	Class
11	No	Small	55K	?
12	Yes	Medium	80K	?
13	Yes	Large	110K	?
14	No	Small	95K	?
15	No	Large	67K	?

Today: Eager Learning

- Actually, we have two goals
  - classify unseen instances
  - learn a model

Explainable AI

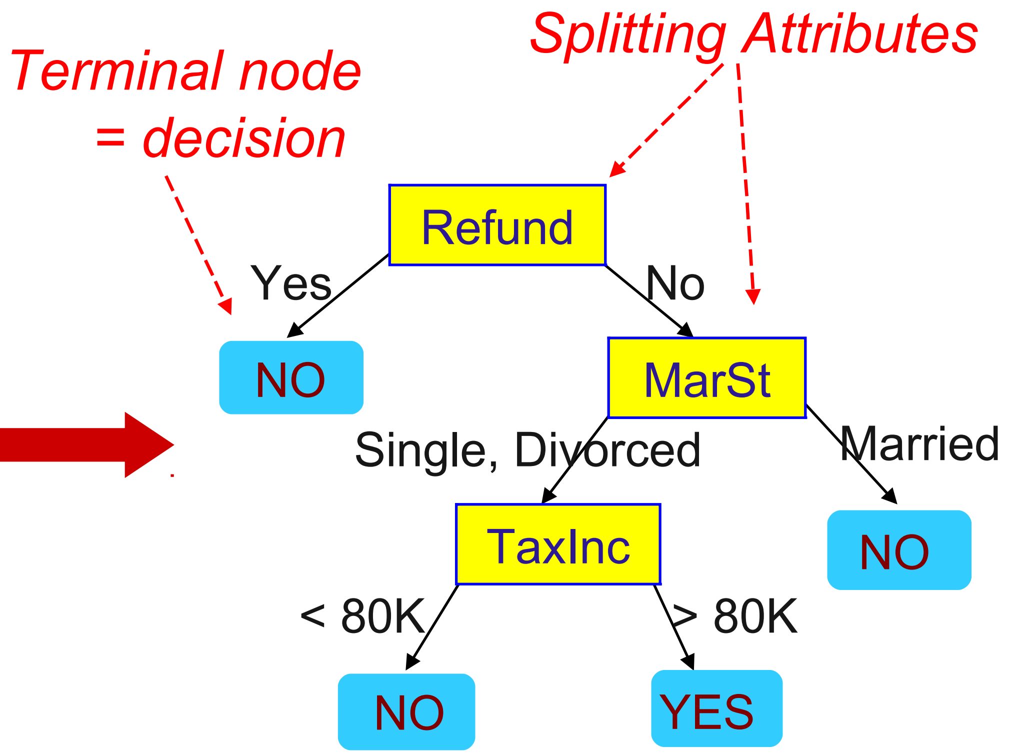
- Model
  - explains how to classify unseen instances
  - sometimes: interpretable by humans

Decision Tree Classifiers

Tid	Refund	Marital Status	Taxable Income	Cheat
1	Yes	Single	125K	**No**
2	No	Married	100K	**No**
3	No	Single	70K	**No**
4	Yes	Married	120K	**No**
5	No	Divorced	95K	**Yes**
6	No	Married	60K	**No**
7	Yes	Divorced	220K	**No**
8	No	Single	85K	**Yes**
9	No	Married	75K	**No**
10	No	Single	90K	**Yes**

categorical, categorical, continuous, class

Training Data



Model: Decision Tree

Another Example of a Possible Decision Tree

categorical categorical continuous class

Tid	Refund	Marital Status	Taxable Income	Cheat
1	Yes	Single	125K	No
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3	No	Single	70K	No
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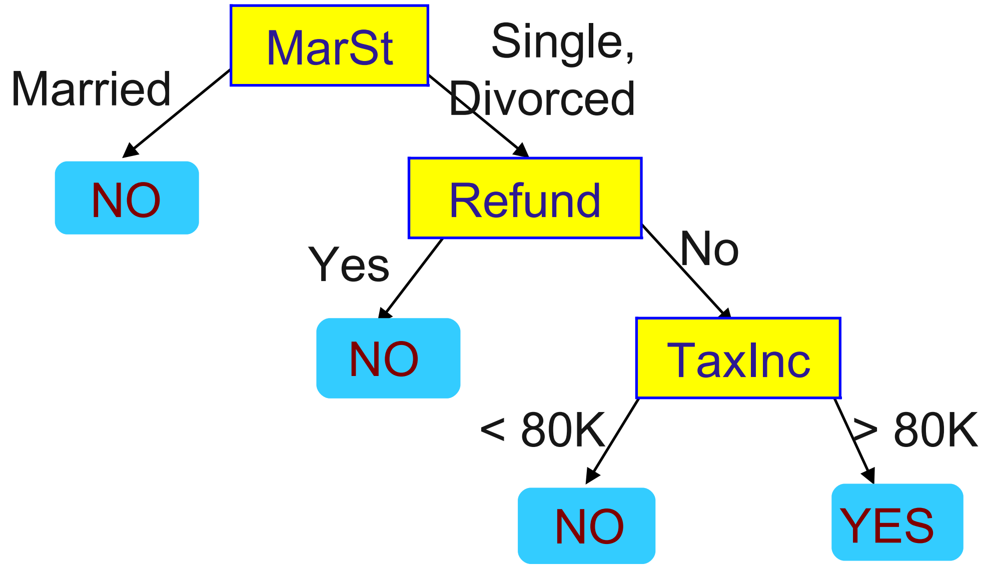
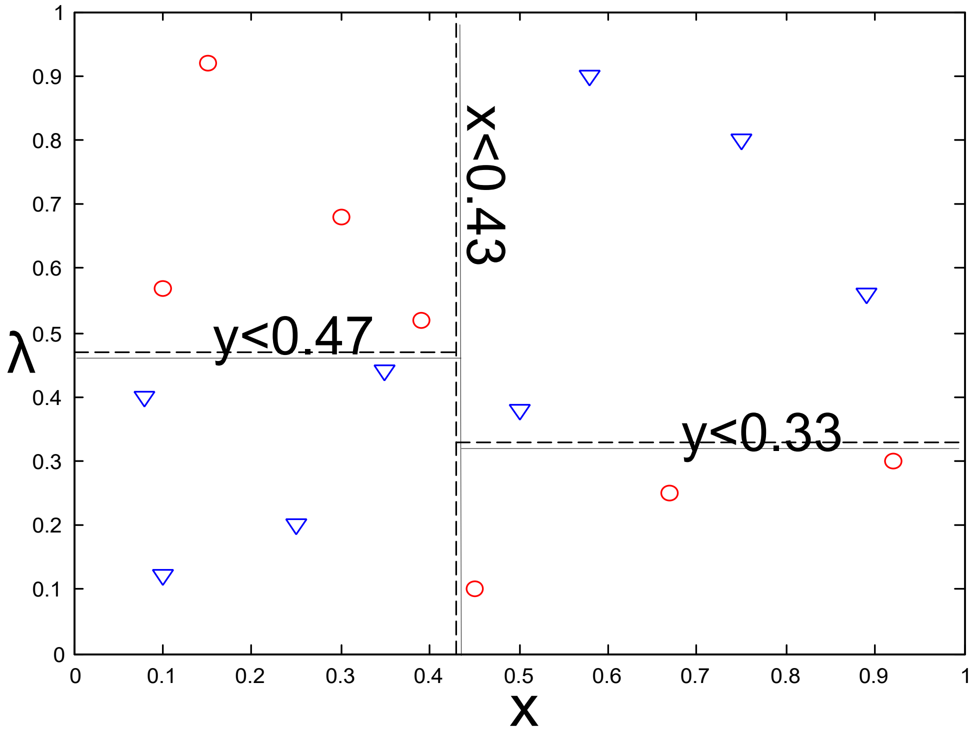
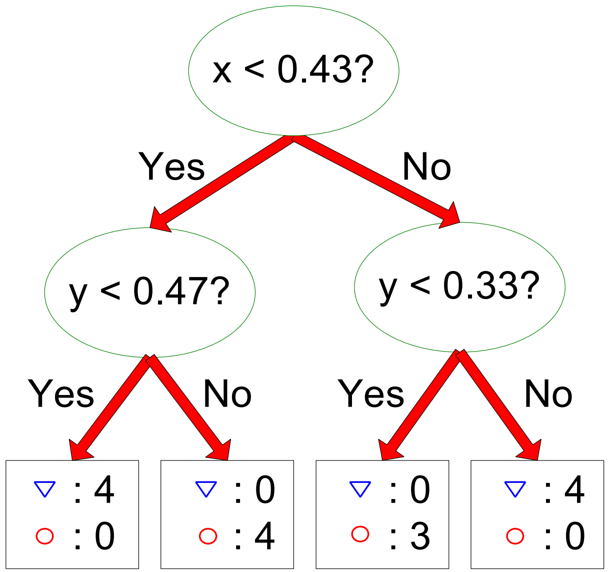


There can be more than one tree that fits the same data!

Decision Boundary





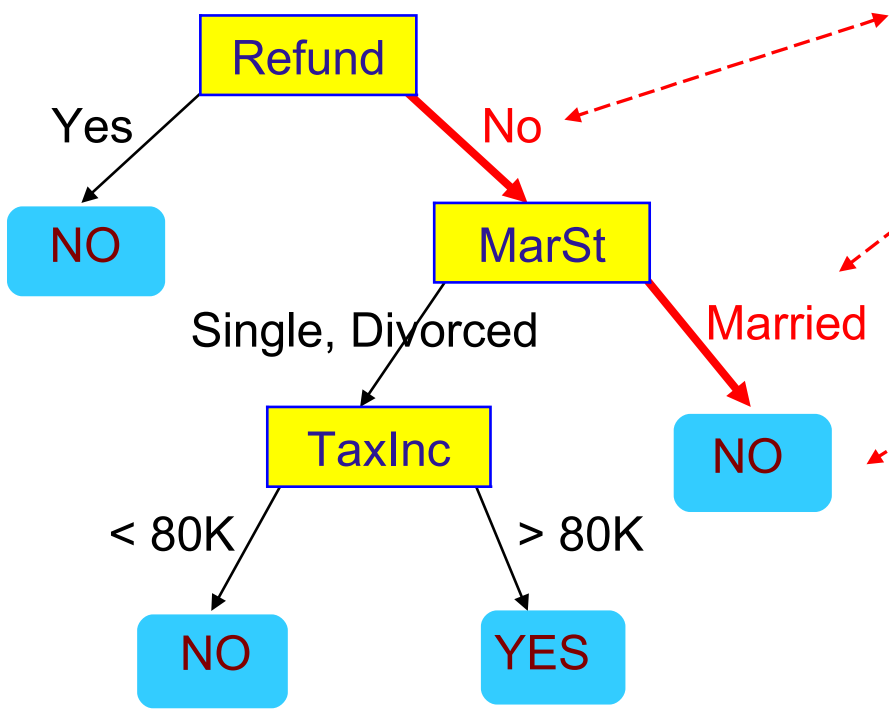
- Border line between two neighboring regions of different classes is known as decision boundary
- Decision boundary is parallel to axes because test condition involves a single attribute at-a-time

Applying a Decision Tree to Test Data

Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?

Start from the root of tree.



Assign Cheat to “No”

Decision Tree Induction

- How to learn a decision Tree from test data?
- Finding an optimal decision tree is NP-hard
- Tree building algorithms use a greedy, top-down, recursive partitioning strategy to induce a reasonable solution
  - also known as: divide and conquer
- Many different algorithms have been proposed:
  - Hunt’s Algorithm
  - ID3
  - CHAID
  - C4.5

General Structure of Hunt's Algorithm

- Let D_t be the set of training records that reach a node t
- General Procedure:
  - If D_t contains only records that belong to the same class y_t, then t is a leaf node labeled as y_t
  - If D_t contains records that belong to more than one class, use an attribute test to split the data into smaller subsets
  - Recursively apply the procedure to each subset

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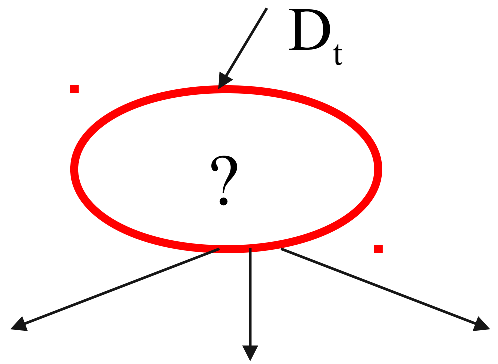
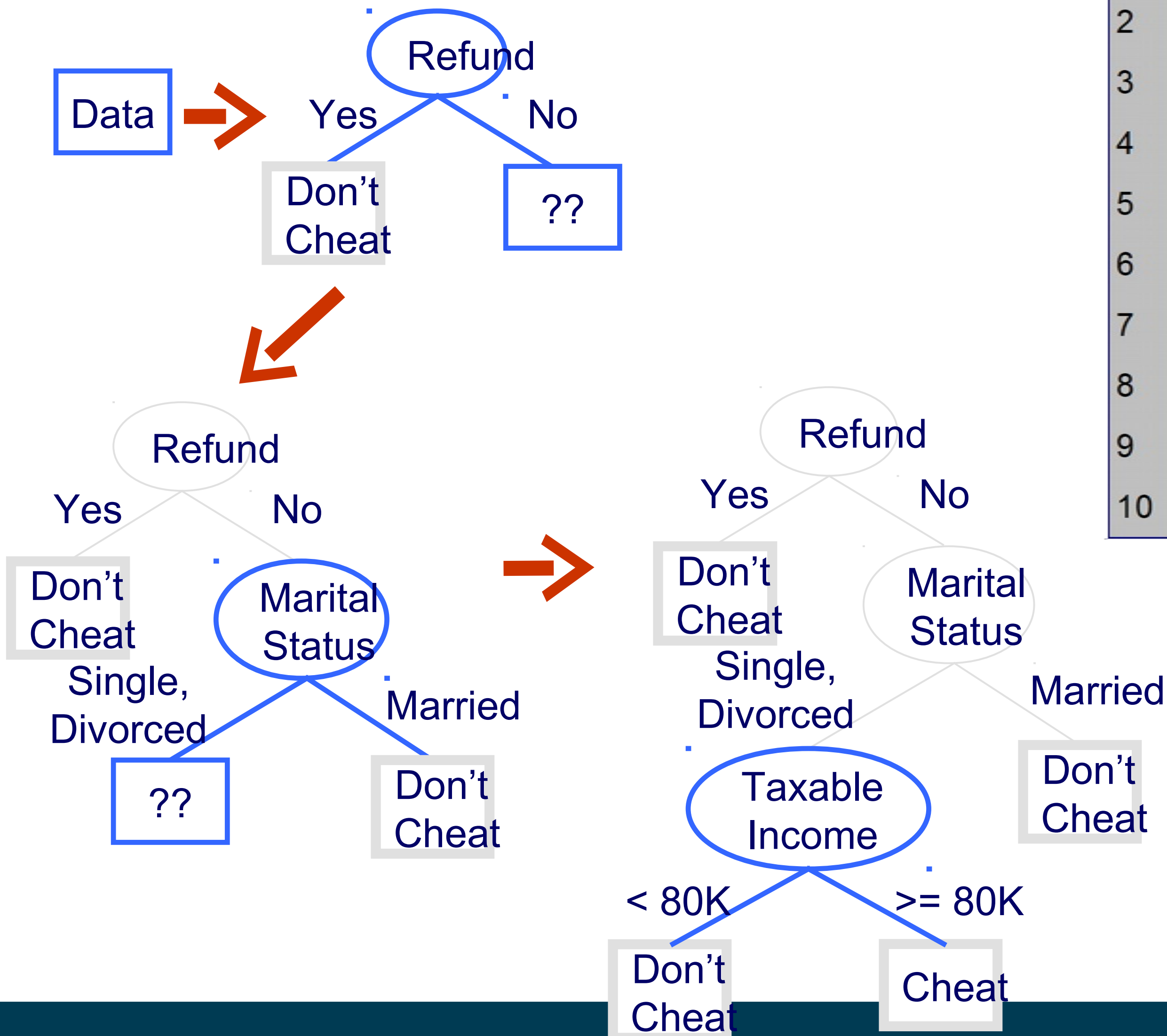


Hunt’s Algorithm



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10	No	Single	90K	Yes

Tree Induction Issues

- Determine how to split the records
  - How to specify the attribute test condition?
  - How to determine the best split?
- Determine when to stop splitting

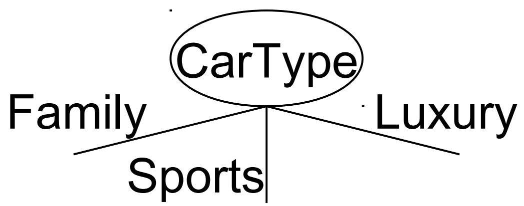
How to Specify the Attribute Test Condition?

- Depends on attribute types
  - Nominal
  - Ordinal
  - Continuous

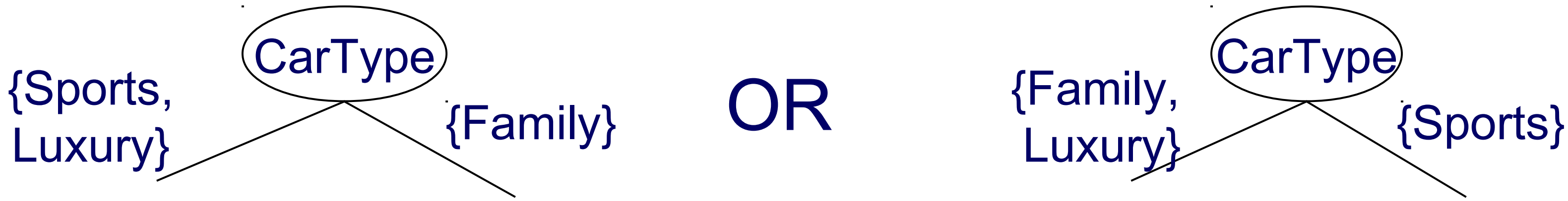
- Depends on number of ways to split
  - 2-way split
  - Multi-way split

Splitting Based on Nominal Attributes

- Multi-way split: Use as many partitions as distinct values

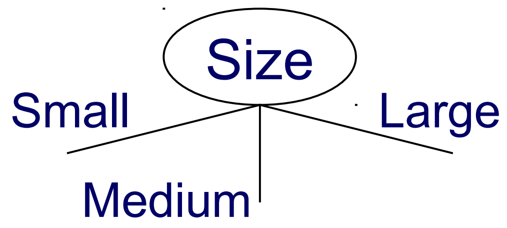


- Binary split: Divides values into two subsets.
  Need to find optimal partitioning

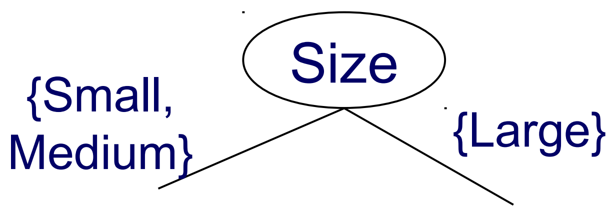


Splitting Based on Ordinal Attributes

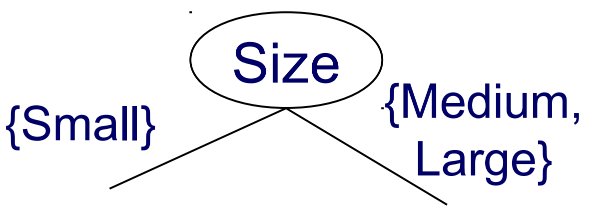
- Multi-way split: Use as many partitions as distinct values.



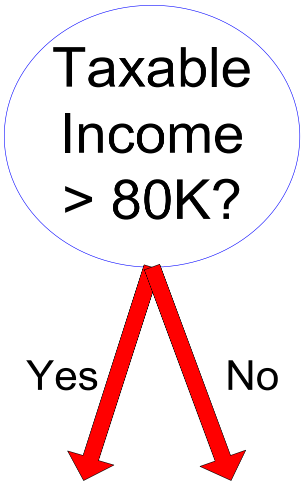
- Binary split: Divides values into two subsets, while keeping the order. Need to find optimal partitioning.



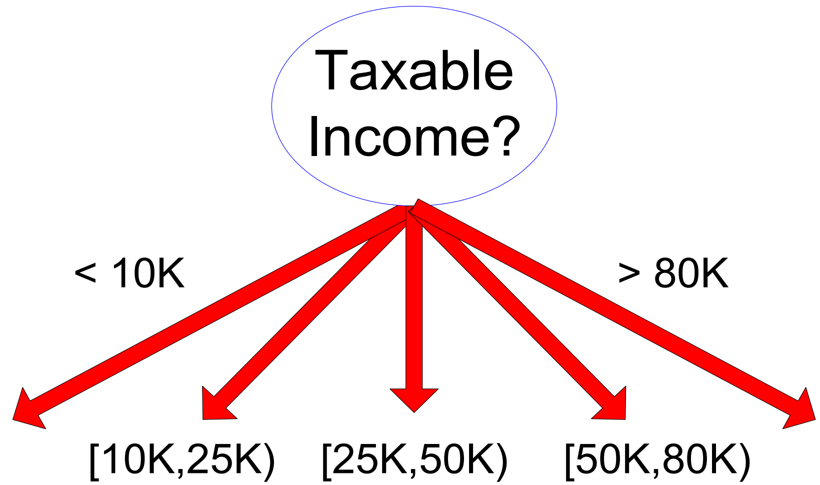
OR



Splitting Based on Continuous Attributes



(i) Binary split



(ii) Multi-way split

Splitting Based on Continuous Attributes

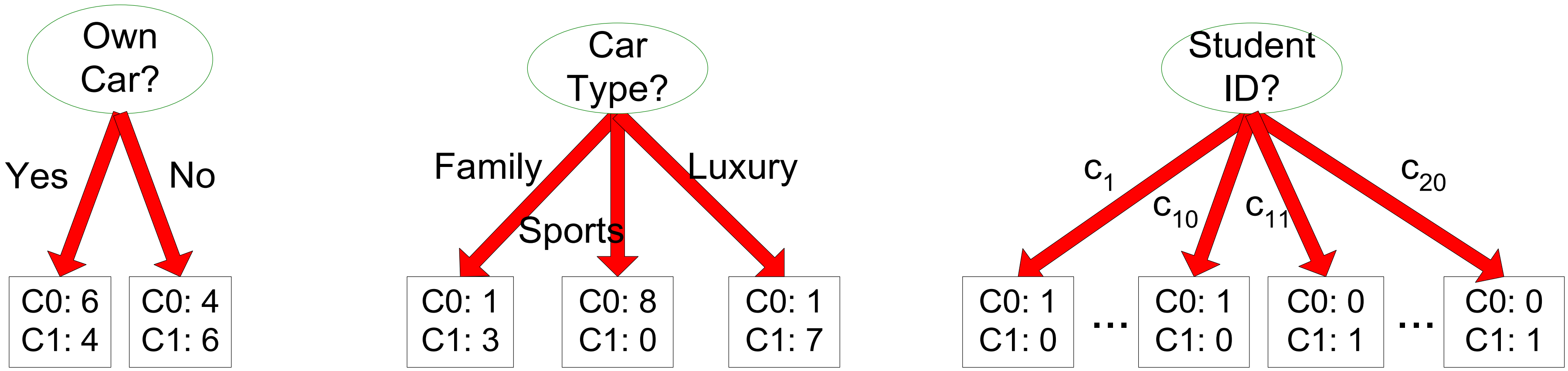
- Different ways of handling
  - Discretization to form an ordinal categorical attribute
    - equal-interval binning
    - equal-frequency binning
    - binning based on user-provided boundaries
  - Binary Decision: $(A < v)$ or $(A \geq v)$
    - usually sufficient in practice
    - consider all possible splits
    - find the best cut (i.e., the best v) based on a purity measure (see later)
    - can be computationally expensive

Discretization Example

- Attribute values (for one attribute e.g., age):
  – 0, 4, 12, 16, 16, 18, 24, 26, 28
- Equal-width binning – for bin width of e.g., 10:
  – Bin 1: 0, 4 [-∞,10) bin
  – Bin 2: 12, 16, 16, 18 [10,20) bin
  – Bin 3: 24, 26, 28 [20,+∞) bin
    - ∞ denotes negative infinity, +∞ positive infinity
- Equal-frequency binning – for bin density of e.g., 3:
  – Bin 1: 0, 4, 12 [-∞, 14) bin
  – Bin 2: 16, 16, 18 [14, 21) bin
  – Bin 3: 24, 26, 28 [21,+∞] bin

How to determine the Best Split?

**Before Splitting: 10 records of class 0,
10 records of class 1**



Which test condition is the best?

How to determine the Best Split?

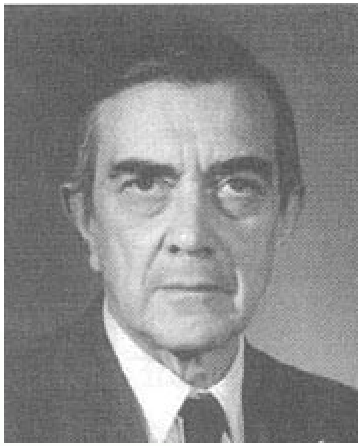
- Nodes with homogeneous class distribution are preferred
- Need a measure of node impurity:

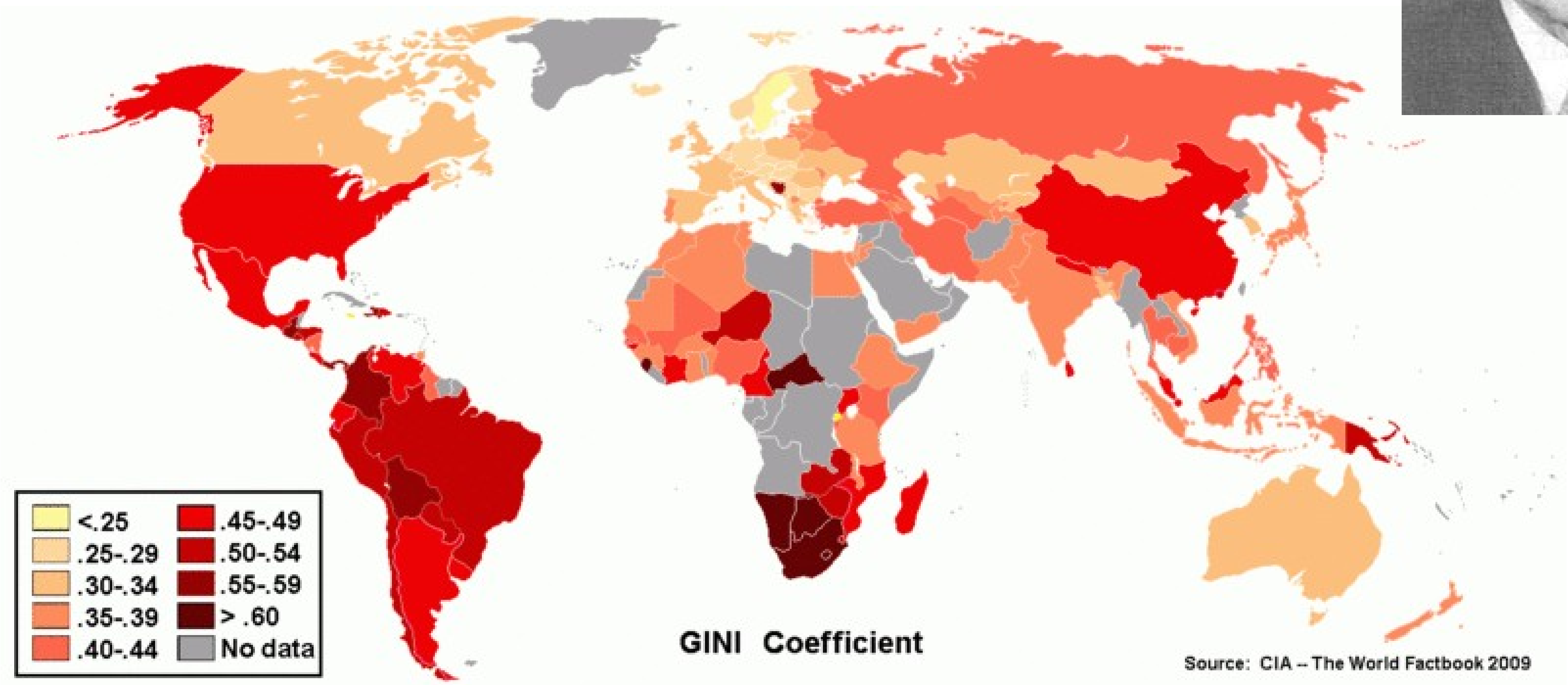
C0: 5 C1: 5	C0: 9 C1: 1
Non-homogeneous, High degree of impurity	Homogeneous, Low degree of impurity

- Common measures of node impurity:
  - Gini Index
  - Entropy
  - Misclassification error

Gini Index

- Named after Corrado Gini (1885-1965)
- Used to measure the distribution of income
  - 1: somebody gets everything
  - 0: everybody gets an equal share





Measure of Impurity: GINI

- Gini-based purity measure for a given node t :

$$GINI(t) = 1 - \sum_j [p(j \mid t)]^2$$

(NOTE: $p(j \mid t)$ is the relative frequency of class j at node t).

– Maximum $(1 - 1/n_c)$ when records are equally distributed among all classes, implying least interesting information

– Minimum (0.0) when all records belong to one class, implying most interesting information

C1	**0**
C2	**6**
Gini=0.000	

C1	**1**
C2	**5**
Gini=0.278	

C1	**2**
C2	**4**
Gini=0.444	

C1	**3**
C2	**3**
Gini=0.500	

Splitting Based on GINI

- When a node p is split into k partitions (children), the quality of split is computed as

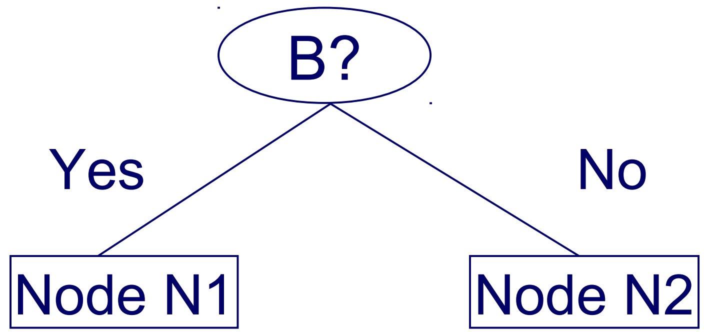
$$GINI_{split} = \sum_{i=1}^{k} \frac{n_i}{n} GINI(i)$$

  - where n_i = number of records at child i,
  - n = number of records at node p.

- Intuition:
  - The GINI index of each partition is weighted
  - according to the partition's size

Binary Attributes: Computing GINI Index

- Splits into two partitions



	Parent
C1	**6**
C2	**6**
Gini = 0.500	

Gini(N1)
$= 1 – (5/7)^2 – (2/7)^2$
$= 0.408$

Gini(N2)
$= 1 – (1/5)^2 – (4/5)^2$
$= 0.320$

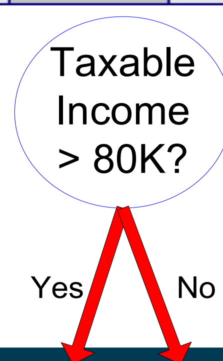
	N1	N2
C1	**5**	**1**
C2	**2**	**4**
Gini=0.371		

Gini(Children)
$= 7/12 * 0.408 +$
$5/12 * 0.320$
$= 0.371$

Continuous Attributes: Computing Gini Index

- Use Binary Decisions based on one value
- Several Choices for the splitting value
  - Number of possible splitting values = Number of distinct values
- Each splitting value has a count matrix associated with it
  - Class counts in each of the partitions, A < v and A ≥ v
- Simple method to choose best v
  - For each v, scan the database to gather count matrix and compute its Gini index
  - Computationally Inefficient! Repetition of work

Tid	**Refund**	**Marital Status**	**Taxable Income**	**Cheat**
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes



Continuous Attributes: Computing Gini Index

- For efficient computation: for each attribute,
  - Sort the attribute on values
  - Linearly scan these values, each time updating the count matrix and computing gini index
  - Choose the split position that has the least gini index

Sorted Values →

Cheat	No	No	No	Yes	Yes	Yes	No	No	No	No
	Taxable Income									
	60	70	75	85	90	95	100	120	125	220

Split Positions →

	55		65		72		80		87		92		97		110		122		172		230	
	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>
Yes	0	3	0	3	0	3	0	3	1	2	2	1	3	0	3	0	3	0	3	0	3	0
No	0	7	1	6	2	5	3	4	3	4	3	4	3	4	4	3	5	2	6	1	7	0
Gini	0.420		0.400		0.375		0.343		0.417		0.400		<u>*0.300*</u>		0.343		0.375		0.400		0.420	

Continuous Attributes: Computing Gini Index

- Note: it is enough to compute the GINI for those positions where the label changes!

Cheat	No	No	No	Yes	Yes	Yes	No	No	No	No
	Taxable Income									
Sorted Values →	60	70	75	85	90	95	100	120	125	220

Split Positions →	55		65		72		80		87		92		97		110		122		172		230	
	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>
Yes	0	3	0	3	0	3	0	3	1	2	2	1	3	0	3	0	3	0	3	0	3	0
No	0	7	1	6	2	5	3	4	3	4	3	4	3	4	4	3	5	2	6	1	7	0
Gini	0.420		0.400		0.375		0.343		0.417		0.400		***0.300***		0.343		0.375		0.400		0.420	

Alternative Splitting Criteria: Information Gain

- Entropy at a given node t:

$$Entropy(t) = -\sum_j p(j\,|\,t)\log_2 p(j\,|\,t)$$

(NOTE: p(j | t) is the relative frequency of class j at node t).

  – Measures homogeneity of a node
    - Maximum (log nc) when records are equally distributed among all classes implying least information
    - Minimum (0.0) when all records belong to one class, implying most information
  – Entropy based computations are similar to the GINI index computations

Splitting Based on Information Gain

- Information Gain:

$$GAIN_{split} = Entropy(p) - \left(\sum_{i=1}^{k} \frac{n_i}{n} Entropy(i) \right)$$

  - Parent Node, p is split into k partitions;
  - n_i is number of records in partition i

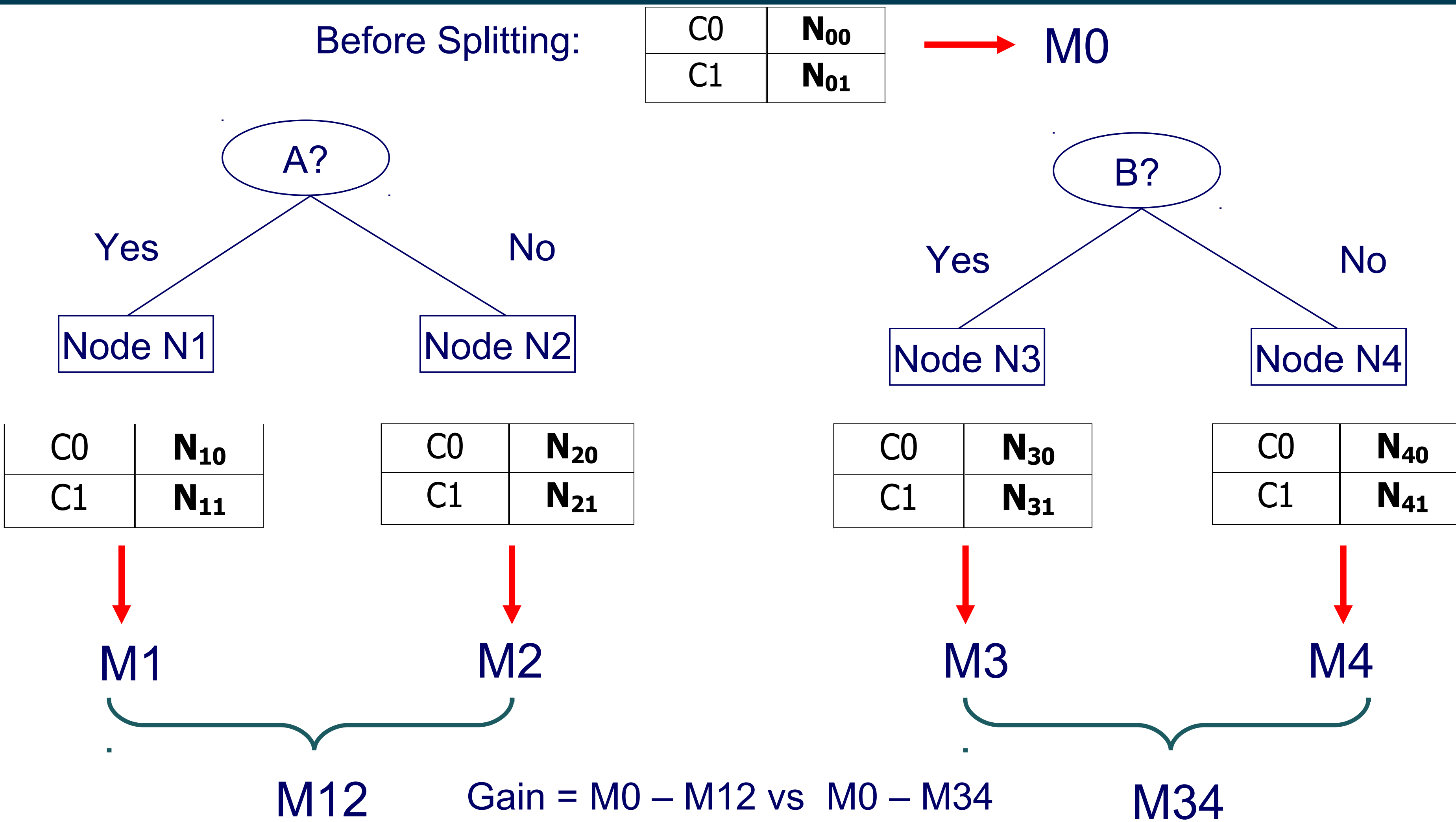
– Measures reduction in entropy achieved because of the split

  - Choose the split that achieves most reduction (maximizes GAIN)

– Disadvantage: Tends to prefer splits that result in large number of partitions, each being small but pure

  - e.g,. split by ID attribute

How to Find the Best Split



Discussion of Decision Trees

- Advantages:
  - Inexpensive to construct
  - Fast at classifying unknown records
  - Easy to interpret by humans for small-sized trees
  - Accuracy is comparable to other classification techniques for many simple data sets
- Disadvantages:
  - Decisions are based only one a single attribute at a time
  - Can only represent decision boundaries that are parallel to the axes

Comparing Decision Trees and k-NN

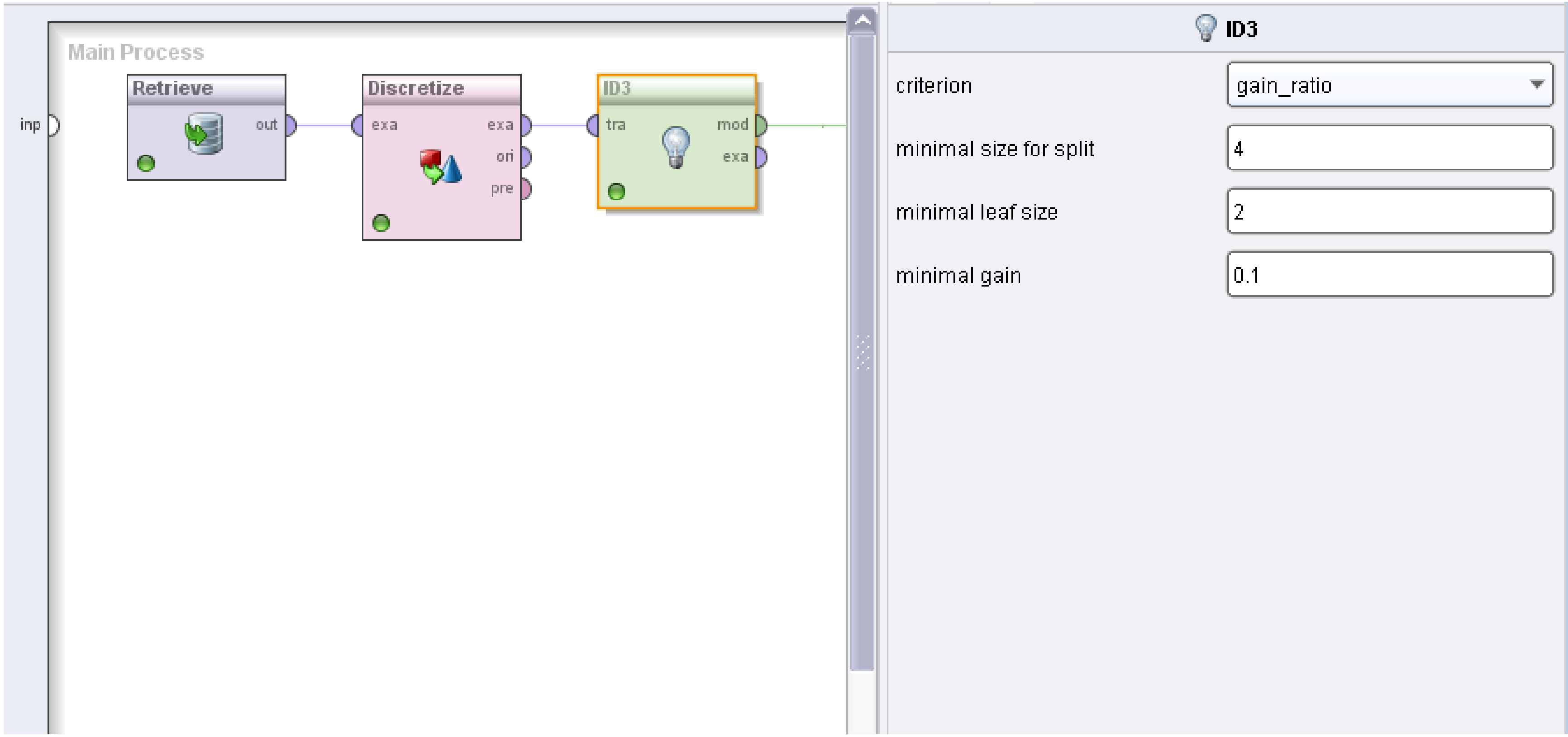
- Decision boundaries
  - k-NN: arbitrary
  - Decision trees: rectangular

- Sensitivity to scales
  - k-NN: needs normalization
  - Decision tree: does not require normalization (recap: Gini splitting)

- Runtime & memory
  - k-NN is cheap to train, but expensive for classification
  - decision tree is expensive to train, but cheap for classification

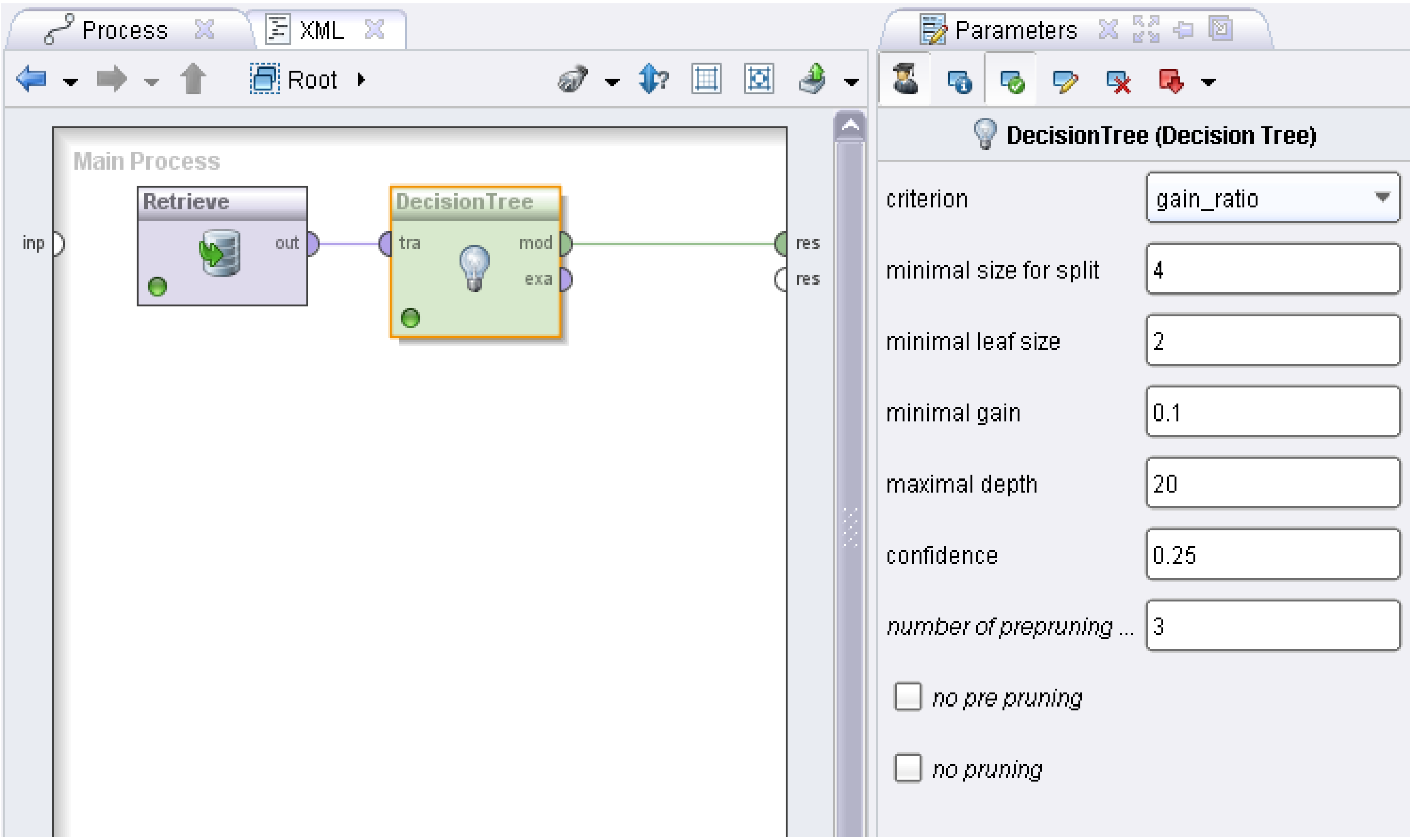
Decision Trees in RapidMiner (ID3)

Learns an un-pruned decision tree from nominal attributes only.



Decision Trees in RapidMiner

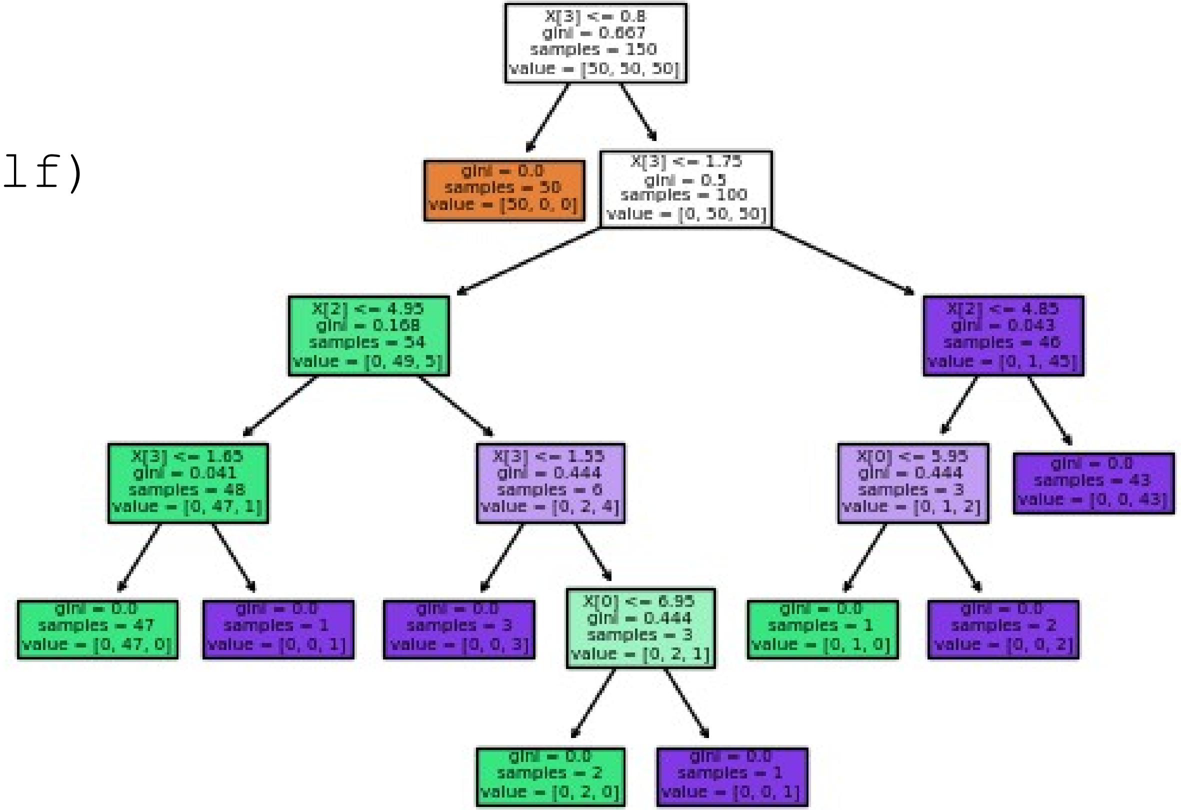
More flexible algorithm that includes pruning and discretization



Tree Induction in Python

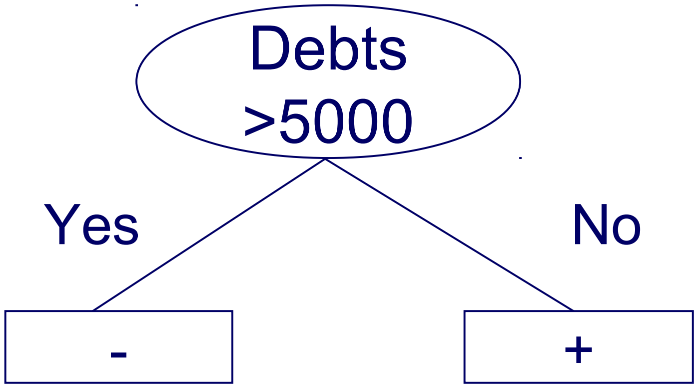
```
clf = DecisionTreeClassifier()
clf = clf.fit(X,X_labels)

# Visualization
tree.plot_tree(clf)
```



Practical Issue: Overfitting

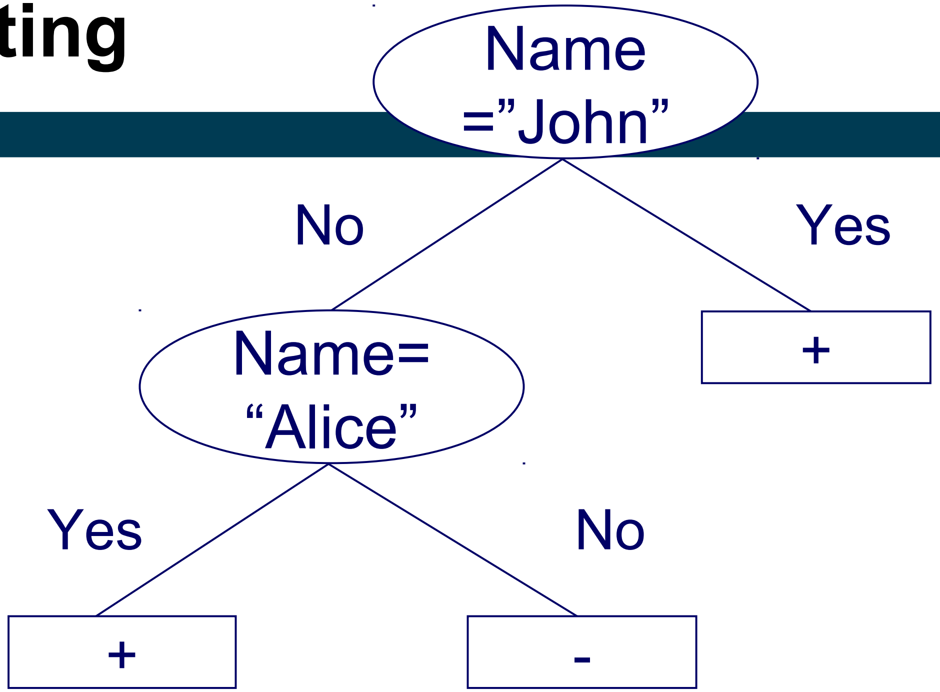
- Example: predict credit rating
  - possible decision tree:



Name	Net Income	Job status	Debts	Rating
John	40000	employed	0	+
Mary	38000	employed	10000	-
Stephen	21000	self-employed	20000	-
Eric	2000	student	10000	-
Alice	35000	employed	4000	+

Practical Issue: Overfitting

- Example: predict credit rating
  - alternative decision tree:



Name	Net Income	Job status	Debts	Rating
John	40000	employed	0	+
Mary	38000	employed	10000	-
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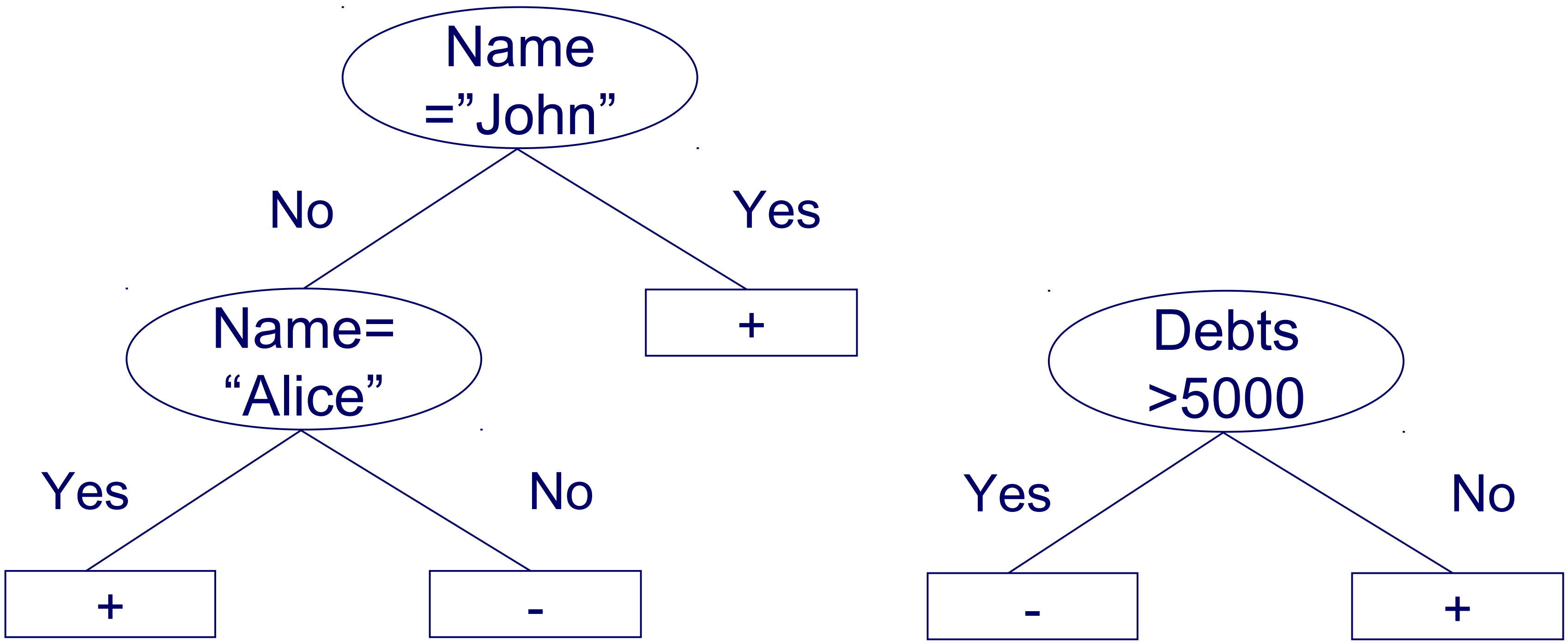
Eric	2000	student	10000	-
Alice	35000	employed	4000	+

Practical Issue: Overfitting

- Both trees seem equally good
  - Classify all instances in the training set correctly
  - Which one do you prefer?

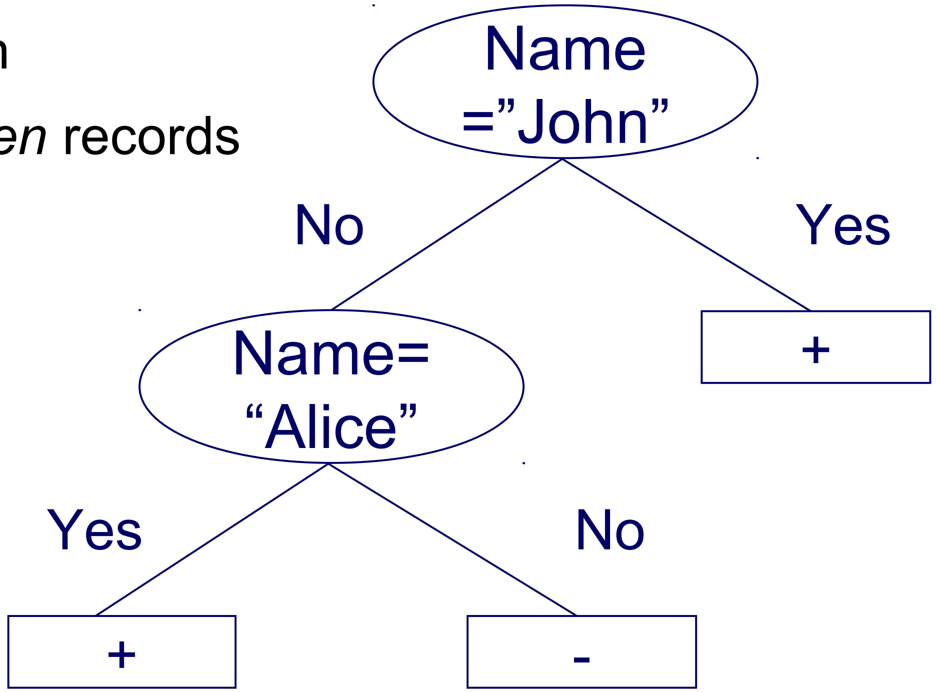


Occam's Razor

- Named after William of Ockham (1287-1347)
- A fundamental principle of science
  - if you have two theories
  - that explain a phenomenon equally well
  - choose the simpler one
- Example:
  - phenomenon: the street is wet
  - theory 1: *it has rained*
  - theory 2: *a beer truck has had an accident, and beer has spilled. The truck has been towed, and magpies picked the glass pieces, so only the beer remains*

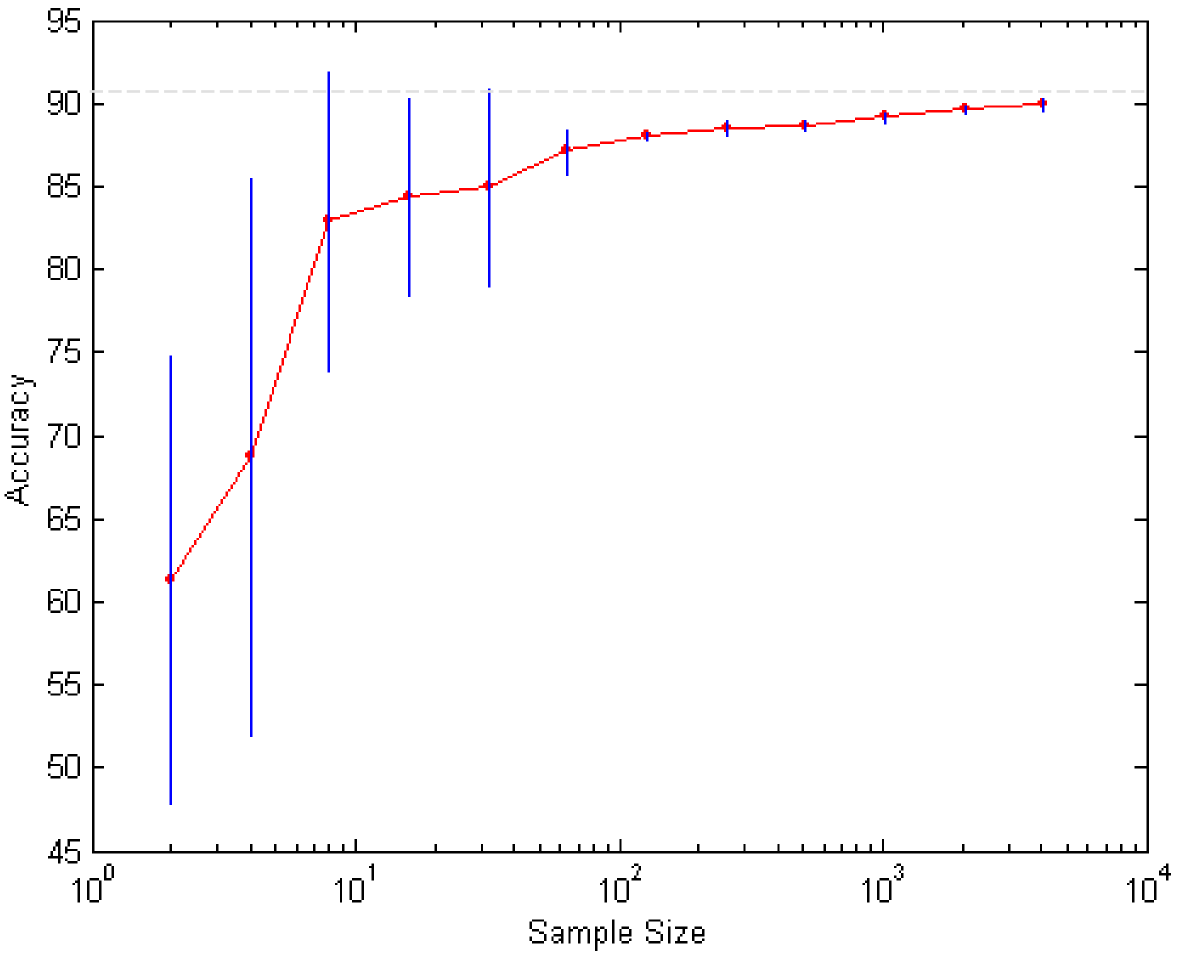
Training and Testing Data

- Consider the decision tree again
- Our ultimate goal: classify *unseen* records



- Assume you measure the performance using the training data
- Conclusion:
  - We need separate data for testing

Learning Curve



- Learning curve shows how accuracy changes with varying sample size
- Conclusion: Use as much data as possible for training
- At the same time: variation drops with larger evaluation sets
- Conclusion: use as much data as possible for evaluation

Holdout Method

- The *holdout* method reserves a certain amount for testing and uses the remainder for training
- Typical: one third for testing, the rest for training
- applied when lots of sample data is available
- For unbalanced datasets, samples might not be representative
  - Few or none instances of some classes
- *Stratified sample: balances the data*
  - Make sure that each class is represented with approximately equal proportions in both subsets

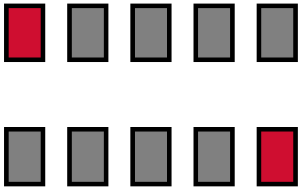
Leave One Out

- Iterate over all examples
  - train a model on all examples but the current one
  - evaluate on the current one

- Yields a very accurate estimate
- Uses as much data for training as possible
  - but is computationally infeasible in most cases

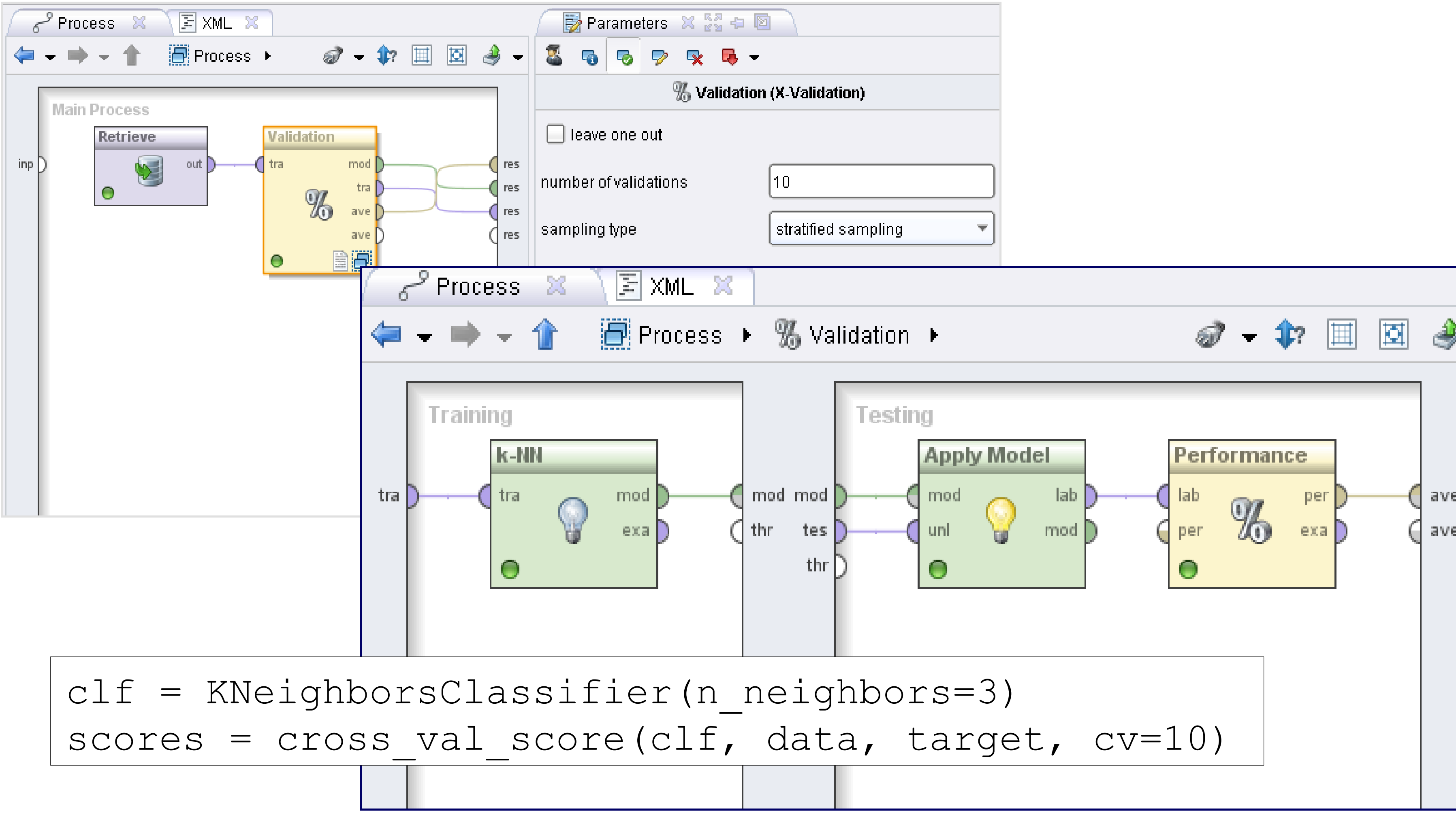
- Imagine: a dataset with a million instances
  - one minute to train a single model
  - Leave one out would take almost two years

Cross-Validation



- Compromise of Leave One Out and decent runtime
- *Cross-validation* avoids overlapping test sets
  - First step: data is split into *k* subsets of equal size
  - Second step: each subset in turn is used for testing and the remainder for training
- This is called *k-fold cross-validation*
- The error estimates are averaged to yield an overall error estimate
- Frequently used value for k : 10
  - Why ten? Extensive experiments have shown that this is the good choice to get an accurate estimate
- Often the subsets are stratified before the cross-validation is performed

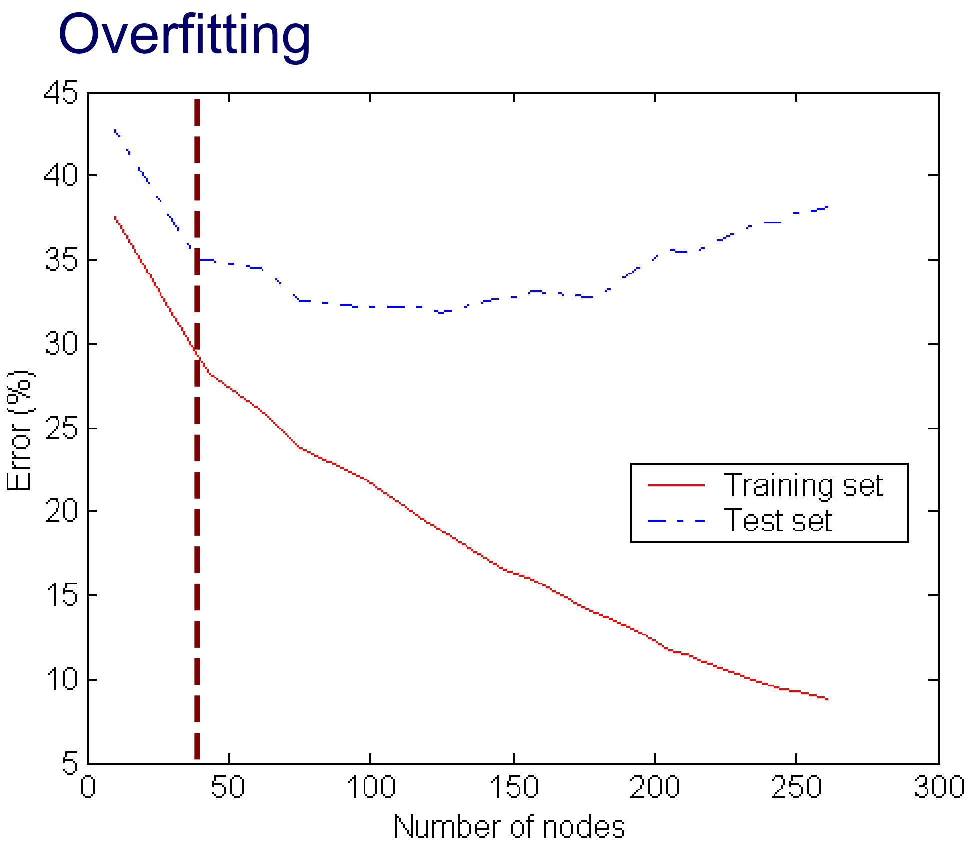
Cross-Validation in RapidMiner




```
clf = KNeighborsClassifier(n_neighbors=3)
scores = cross_val_score(clf, data, target, cv=10)
```

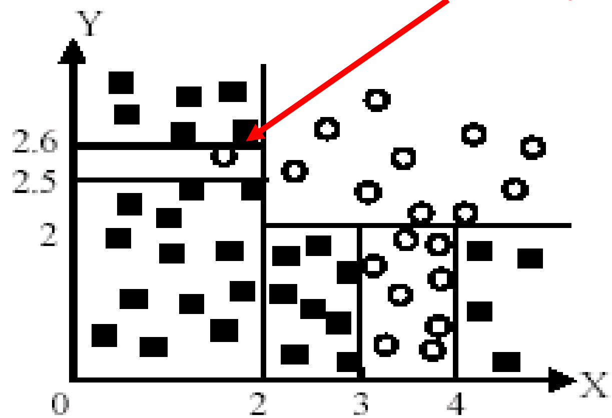
Back to Overfitting

- Overfitting: Good accuracy on training data, but poor on test data.
- Symptoms: Tree too deep and too many branches
- Typical causes of overfitting
  - too little training data
  - noise
  - poor learning algorithm

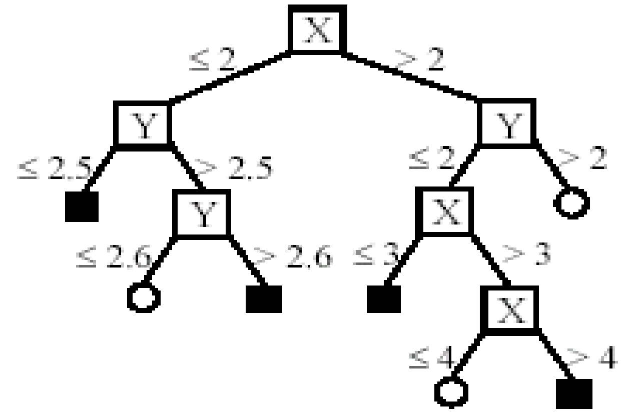


Overfitting and Noise

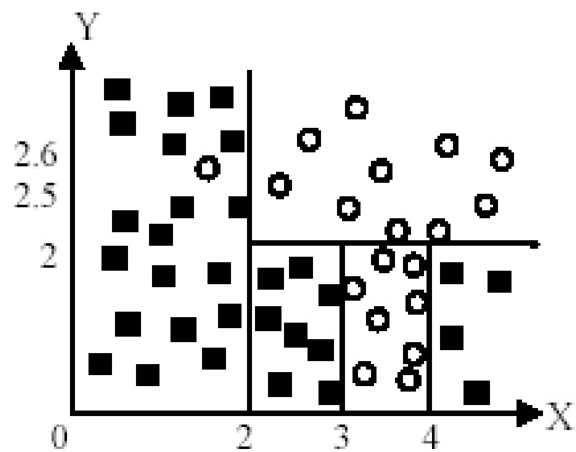
Likely to overfit the data

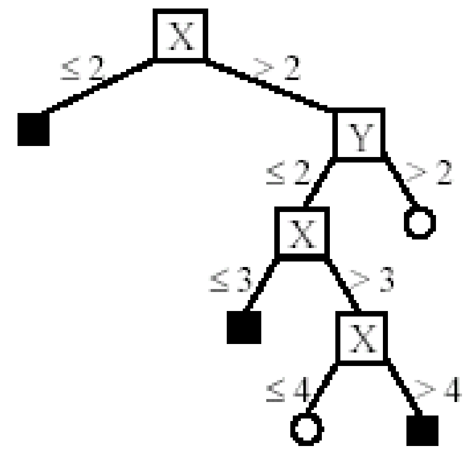


(A) A partition of the data space



(B). The decision tree





How to Address Overfitting?

- Pre-Pruning (Early Stopping Rule)
  - Stop the algorithm before it becomes a fully-grown tree
  - Typical stopping conditions for a node:
    - Stop if all instances belong to the same class
    - Stop if all the attribute values are the same
  - Less restrictive conditions:
    - Stop if number of instances within a node is less than some user-specified threshold
    - Stop if expanding the current node only slightly improves the impurity measure (user-specified threshold)

How to Address Overfitting?

- Post-pruning
  1. Grow decision tree to its entire size
  2. Trim the nodes of the decision tree in a bottom-up fashion
     - using a validation data set
     - or an estimate of the generalization error
  3. If generalization error improves after trimming
     - replace sub-tree by a leaf node
     - Class label of leaf node is determined from majority class of instances in the sub-tree

Training vs. Generalization Errors

- Training error
  - also: resubstitution error, apparent error
  - errors made in training
  - evidence: misclassified training instances
- Generalization error
  - errors made on unseen data
  - evidence: no apparent evidence

- Training error can be computed
- Generalization error must be estimated

Estimating the Generalization Error

- Training errors: error on training (Σ e(t))
- Generalization errors: error on testing (Σ e'(t))
- Methods for estimating generalization errors:
  1. (Too) Optimistic approach: e'(t) = e(t)
  2. Pessimistic approach:
     - For each leaf node: e'(t) = (e(t)+0.5)
       (user-defined 0.5 penalty for large trees)
     - Total errors: e'(T) = e(T) + N $\times$ 0.5
       (N: number of leaf nodes)
     - For a tree with 30 leaf nodes and 10 errors on training
       (out of 1000 instances):
       Training error = 10/1000 = 1%
       Generalization error = (10 + 30$\times$0.5)/1000 = 2.5%
  3. Reduced Error Pruning (REP):
     - use validation data set to estimate generalization error

Example of Post-Pruning

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

Training Error (Before splitting) = 10/30

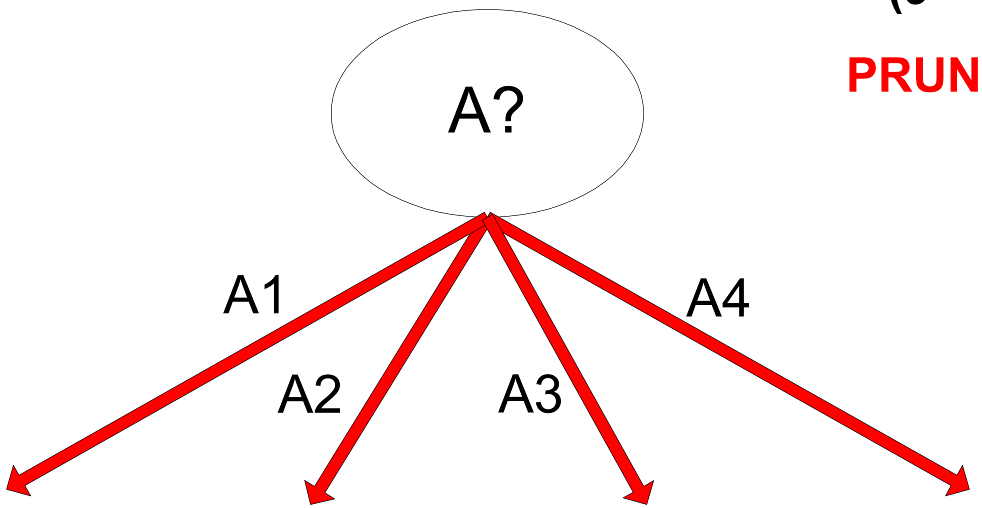
Pessimistic error = (10 + 0.5)/30 = 10.5/30

Training Error (After splitting) = 9/30

Pessimistic error (After splitting)

= (9 + 4 $\times$ 0.5)/30 = 11/30

PRUNE!



Class = Yes	8
Class = No	4

Class = Yes	3
Class = No	4

Class = Yes	4
Class = No	1

Class = Yes	5
Class = No	1

Alternative Classification Methods

- So far, we have seen
  - k-NN
  - Naive Bayes
  - Decision Trees

- There is a whole lot more in RapidMiner & scikit-learn

- Brief intro
  - Artificial Neural Networks
  - Support Vector Machines

Example: Credit Rating

- Consider the following example:
  - and try to build a model
  - which is as small as possible (recall: Occam's Razor)

Person	Employed	Owns House	Balanced Account	Get Credit
Peter Smith	yes	yes	no	yes
Julia Miller	no	yes	no	no
Stephen Baker	yes	no	yes	yes
Mary Fisher	no	no	yes	no
Kim Hanson	no	yes	yes	yes
John Page	yes	no	no	no

Example: Credit Rating

- Smallest model:
  – if at least two of Employed, Owns House, and Balanced Account are yes
    → Get Credit is yes
- Not nicely expressible in trees and rule sets
  – as we know them (attribute-value conditions)

Person	Employed	Owns House	Balanced Account	Get Credit
Peter Smith	yes	yes	no	yes
Julia Miller	no	yes	no	no
Stephen Baker	yes	no	yes	yes
Mary Fisher	no	no	yes	no
Kim Hanson	no	yes	yes	yes
John Page	yes	no	no	no

Example: Credit Rating

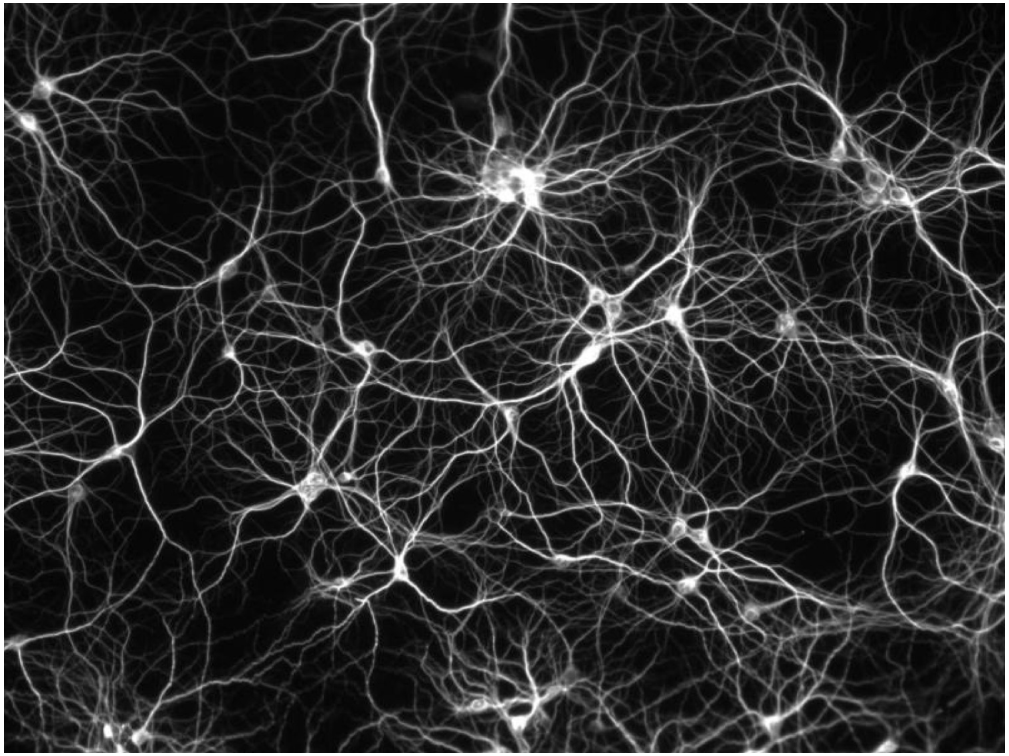
- Smallest model:
  - if at least two of Employed, Owns House, and Balance Account are yes → Get Credit is yes
- As rule set:

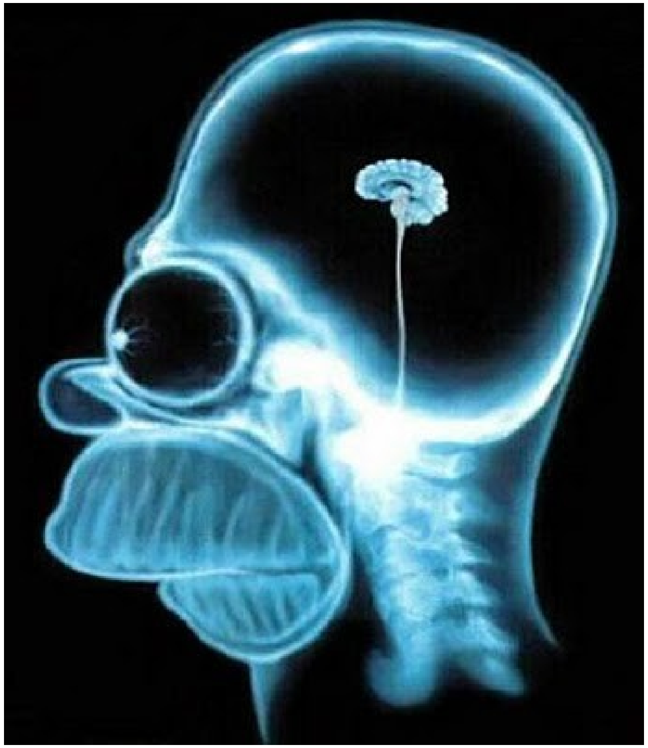
  Employed=yes and OwnsHouse=yes => yes
  Employed=yes and BalanceAccount=yes => yes
  OwnsHouse=yes and BalanceAccount=yes => yes
  => no

- General case:
  - at least m out of n attributes need to be yes => yes
  - this requires $\binom{n}{m}$ rules, i.e., $\frac{n!}{m!\cdot(n-m)!}$
  - e.g., “5 out of 10 attributes need to be yes” requires more than 15,000 rules!

Artificial Neural Networks

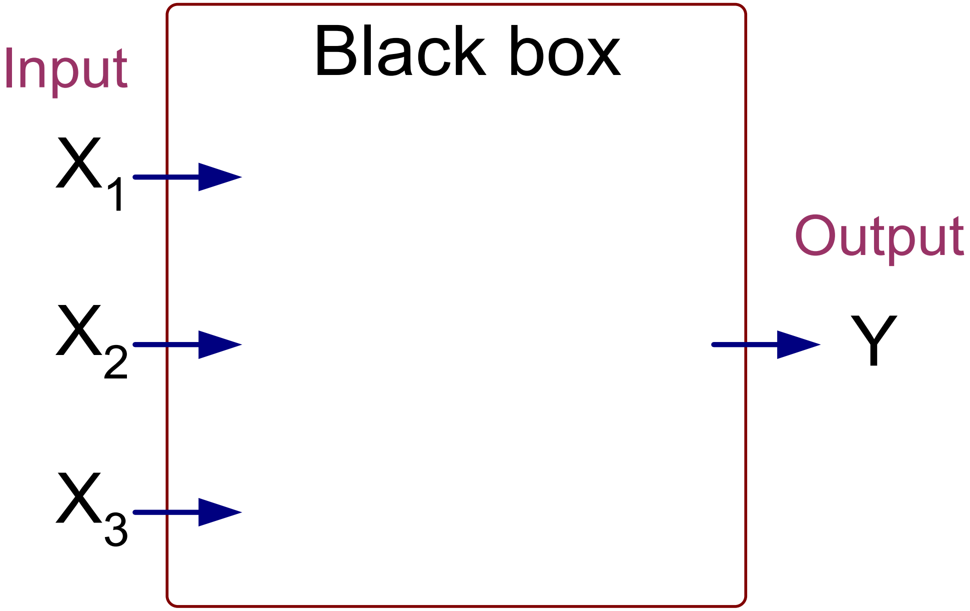
- Inspiration
  - one of the most powerful super computers in the world





Artificial Neural Networks (ANN)

X_1	X_2	X_3	Y
1	0	0	0
1	0	1	1
1	1	0	1
1	1	1	1
0	0	1	0
0	1	0	0
0	1	1	1
0	0	0	0



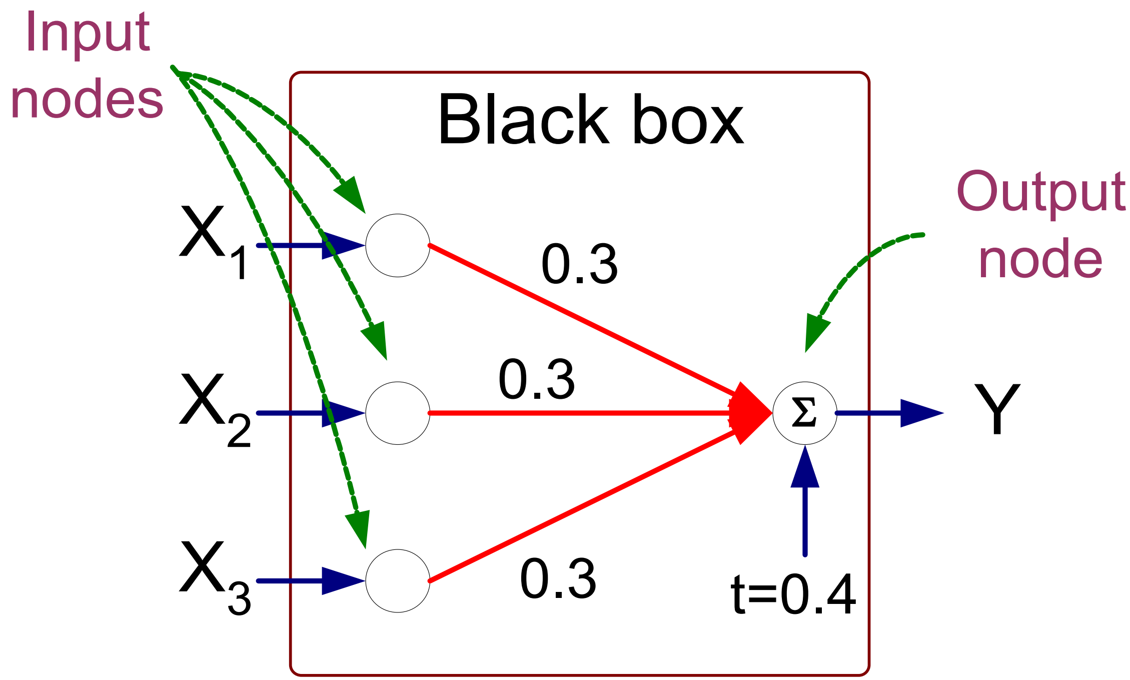
Output Y is 1 if at least two of the three inputs are equal to 1.

Example: Credit Rating

- Smallest model:
  - if at least two of Employed, Owns House, and Balance Account are yes $\rightarrow$ Get Credit is yes
- Given that we represent yes and no by 1 and 0, we want
  - if(Employed + Owns House + Balance Acount)>1.5 $\rightarrow$ Get Credit is yes

Artificial Neural Networks (ANN)

X_1	X_2	X_3	Y
1	0	0	0
1	0	1	1
1	1	0	1
1	1	1	1
0	0	1	0
0	1	0	0
0	1	1	1
0	0	0	0

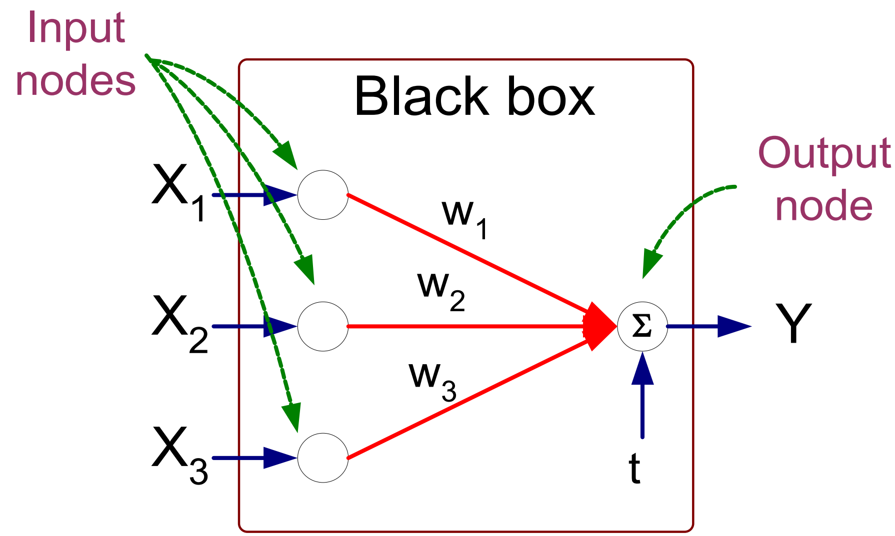


$$Y = I(0.3X_1 + 0.3X_2 + 0.3X_3 - 0.4 > 0)$$

$$\text{where } I(z) = \begin{cases} 1 & \text{if } z \text{ is true} \\ 0 & \text{otherwise} \end{cases}$$

Artificial Neural Networks (ANN)

- Model is an assembly of inter-connected nodes and weighted links
- Output node sums up each of its input value according to the weights of its links
- Compare output node against some threshold t

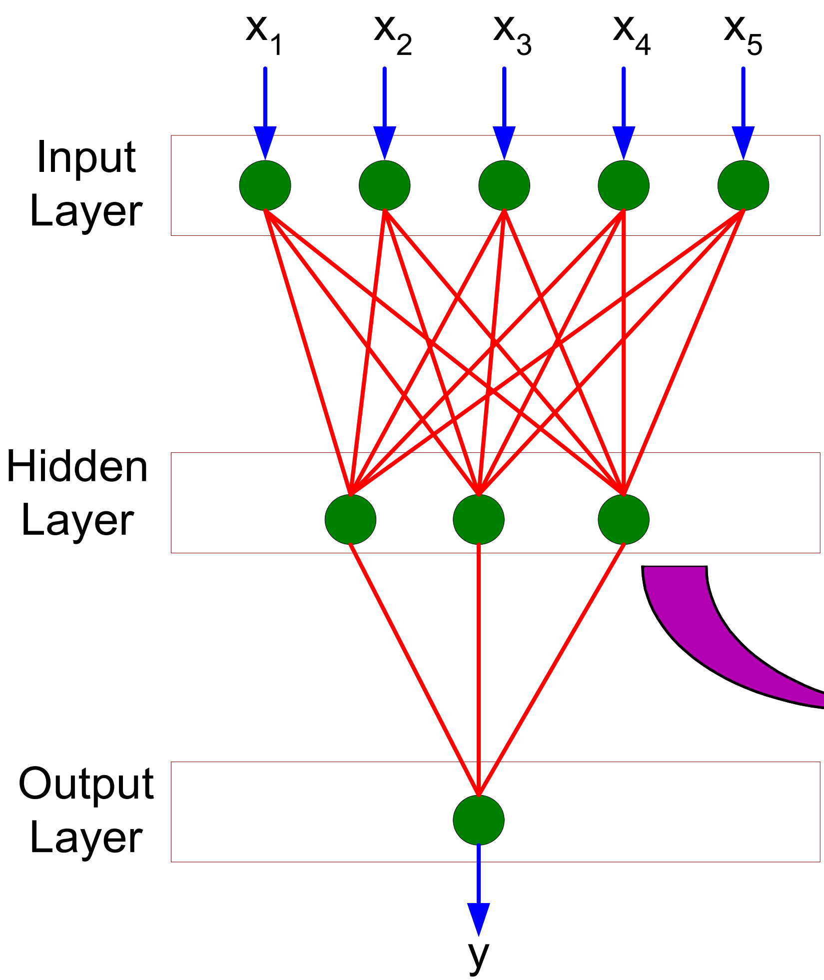


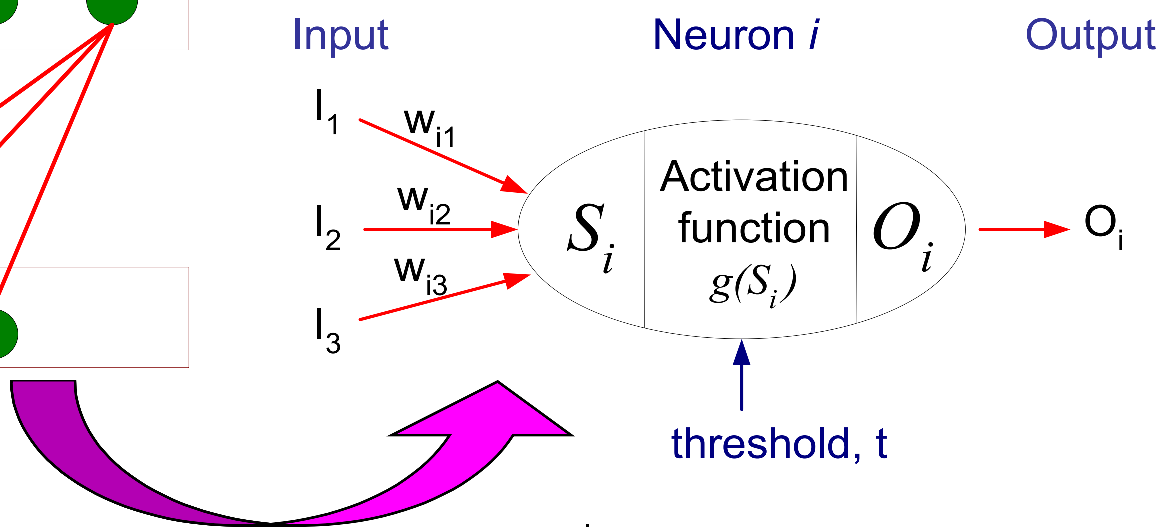
Perceptron Model

$$Y = I(\sum_i w_i X_i - t) \quad \text{or}$$

$$Y = sign(\sum_i w_i X_i - t)$$

General Structure of ANN





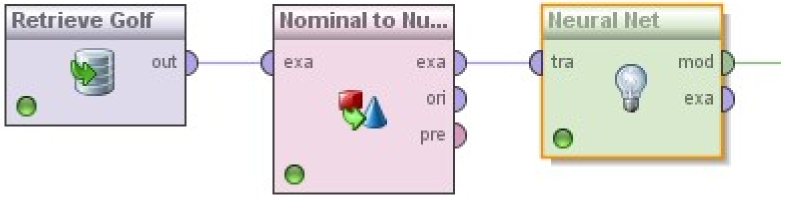
Training ANN means learning the weights of the neurons

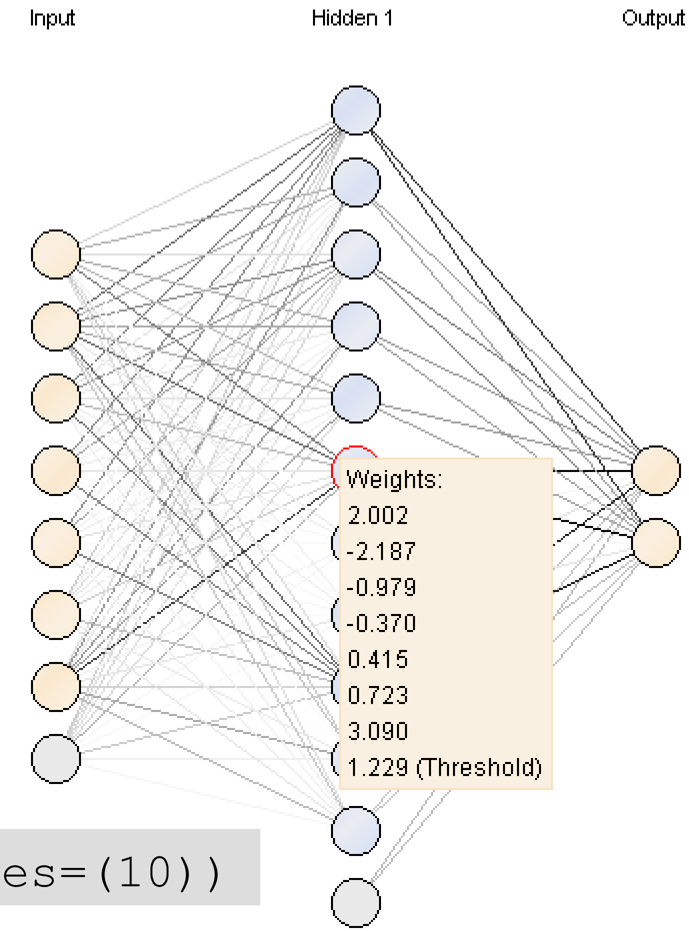
Algorithm for learning ANN

- Initialize the weights (w_0, w_1, …, w_k), e.g., all with 1

- Adjust the weights in such a way that the output of ANN is consistent with class labels of training examples
  - Objective function: $$E = \sum_i \left[Y_i - f(w_i, X_i) \right]^2$$
  - Find the weights w_i's that minimize the above objective function
    - e.g., back propagation algorithm (see books)

ANN in RapidMiner & Python

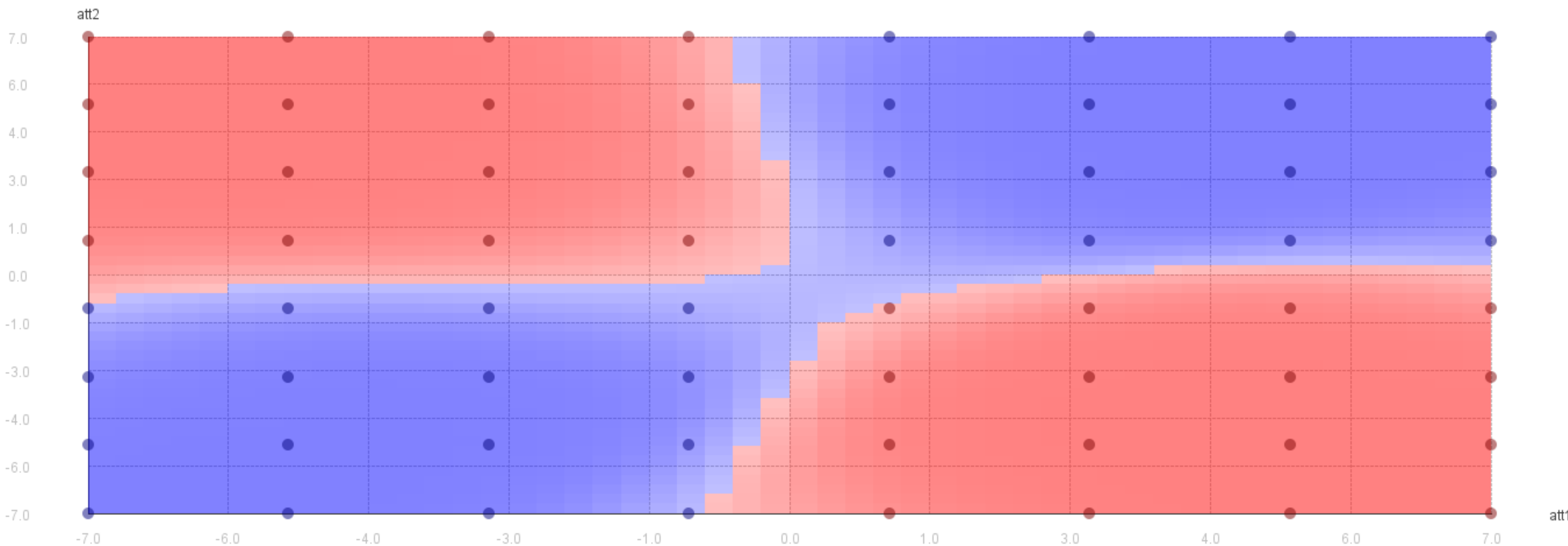





```
clf = MLPClassifier(hidden_layer_sizes=(10))
```

Decision Boundaries of ANN

- Arbitrarily shaped objects
- Fuzzy boundaries



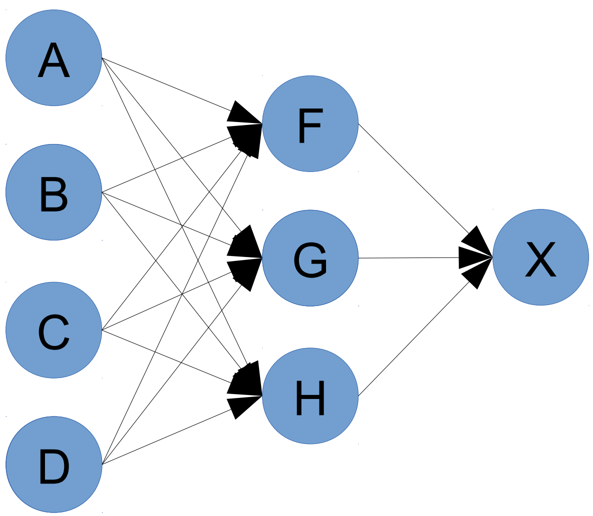
More Exotic Problems

- Consider
  - Four binary features A,B,C,D
  - Goal: Classify true if the number of TRUE values is even (i.e., 0, 2, or 4)

- Very hard for classic machine learning problems
  - Approximate solution can be learned with neural network

More Exotic Problems

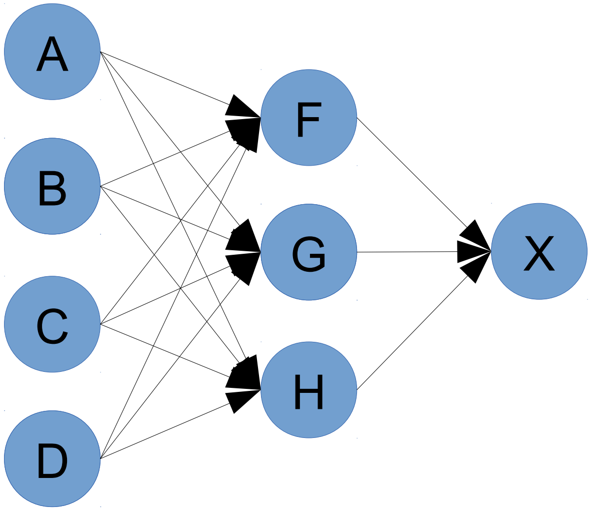
- Consider
  - Four binary features A,B,C,D
  - Goal: Classify true if the number of TRUE values is even (i.e., 0, 2, or 4)



$$F = A + B + C - D < 3$$
$$G = A + B + C - D < 2$$
$$H = A + B + C - D < 1$$

$$X = F + G - H < 2$$

More Exotic Problems



A	B	C	D	F	G	H	X	C
0	0	0	0	1	1	1	TRUE	TRUE
1	0	0	0	1	1	0	FALSE	FALSE
0	1	0	0	1	1	0	FALSE	FALSE
0	0	1	0	1	1	0	FALSE	FALSE
0	0	0	1	1	1	1	TRUE	FALSE
1	1	0	0	1	0	0	TRUE	TRUE
0	1	1	0	1	0	0	TRUE	TRUE
0	0	1	1	1	1	1	TRUE	TRUE
1	0	0	1	1	1	1	TRUE	TRUE
1	0	1	0	1	0	0	TRUE	TRUE
0	1	0	1	1	1	1	TRUE	TRUE
1	1	1	0	0	0	0	TRUE	FALSE
1	1	0	1	1	1	0	FALSE	FALSE
1	0	1	1	1	1	0	FALSE	FALSE
0	1	1	1	1	1	0	FALSE	FALSE
1	1	1	1	1	0	0	TRUE	TRUE

$F = A + B + C - D < 3$
$G = A + B + C - D < 2$
$H = A + B + C - D < 1$

$X = F + G - H < 2$

Hyperparameter Selection

- A hyperparameter is a parameter which influences the learning process and whose value is set before the learning begins
  - pruning thresholds for trees and rules
  - gamma and C for SVMs
  - learning rate, hidden layers for ANNs
- By contrast, parameters are learned from the training data
  - weights in an ANN, probabilities in Naïve Bayes, splits in a tree
- Many methods work poorly with the default hyperparameters
- How to determine good hyperparameters?
  - manually play around with different hyperparameter settings
  - have your machine automatically test many different settings (hyperparameter optimization)

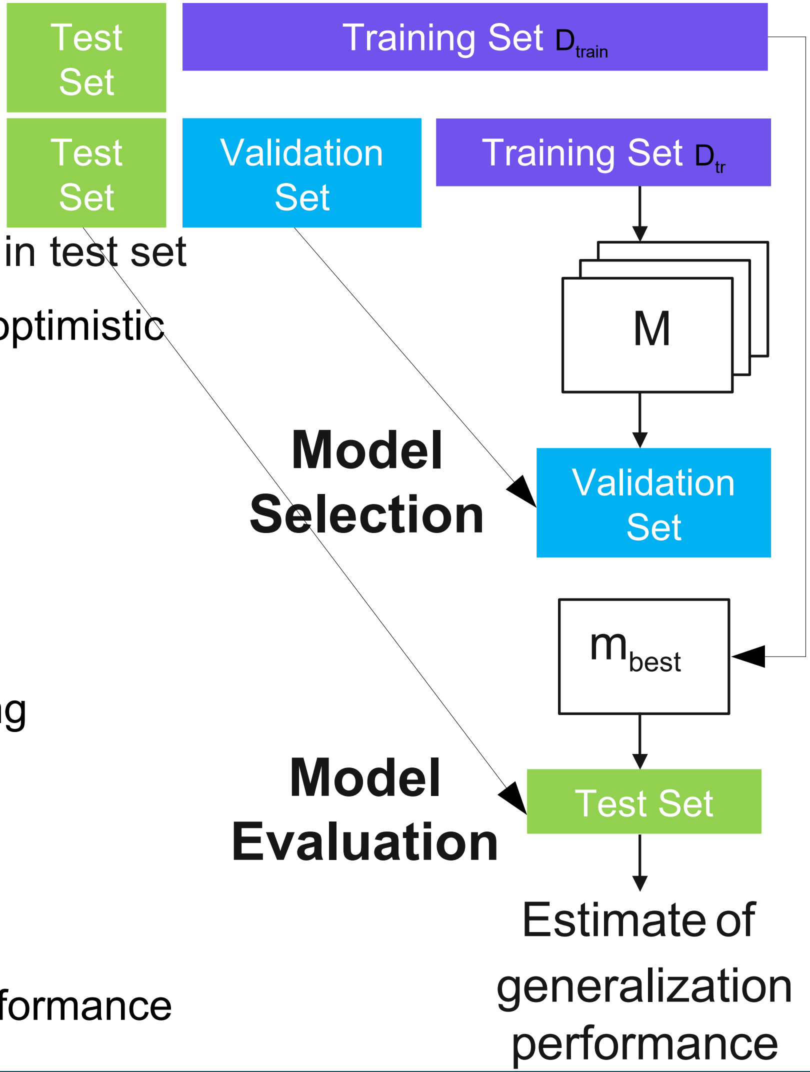
Hyperparameter Optimization

- Goal: Find the combination of hyperparameter values that results in learning the model with the lowest generalization error
- How to determine the parameter value combinations to be tested?
  - Grid Search: Test all combinations in user-defined ranges
  - Random Search: Test combinations of random parameter values
  - Evolutionary Search: Keep specific parameter values that worked well
- Often hundreds of combinations are tested
  - reason for cloud computing

– Model Selection: From all learned models M, select the model m_{best} that is expected to generalize best to unseen records

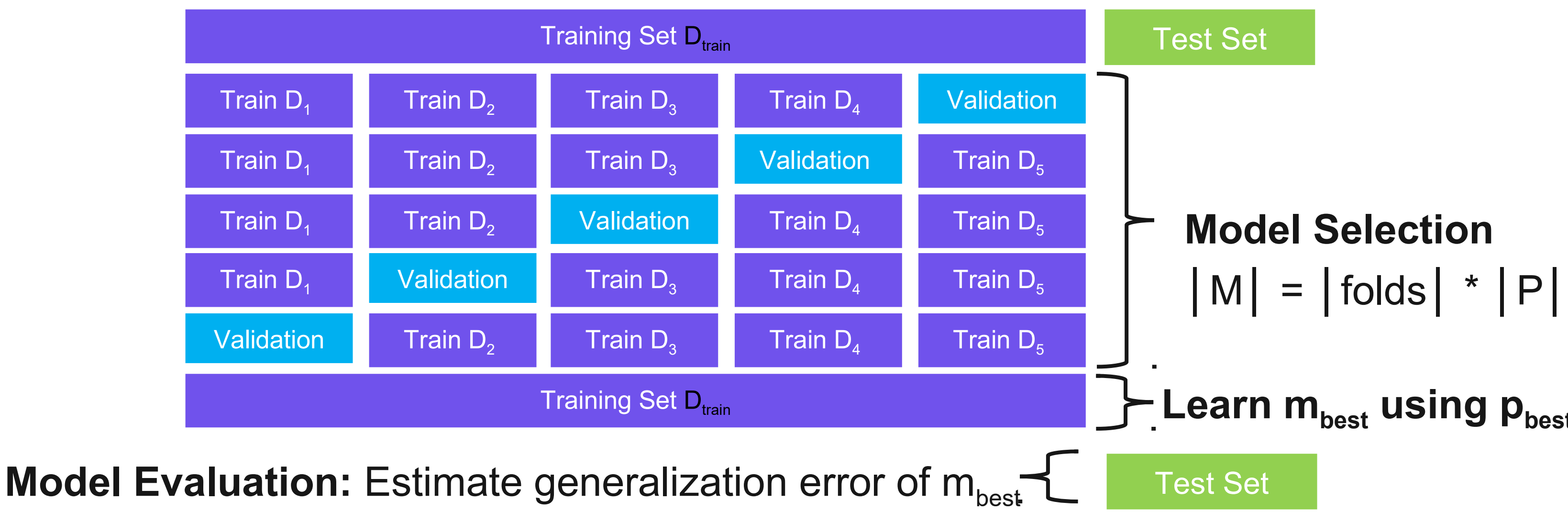
Model Selection Using a Validation Set

- Keep data used for model selection strictly separate from data used for model evaluation, otherwise:
  - selected model m_{best} will overfit to patterns in test set
  – estimate of generalization error will be too optimistic
- Method to find the best model:
  1) Split training set D_{train} into validation set D_{val} and training set D_{tr}
  2) Learn models M on D_{tr} using different hyperparameter value combinations P
  3) Select best parameter values p_{best} by testing each model m_i on the validation set D_{val}
  4) Learn final model m_{best} on complete D_{train} using the parameter values p_{best}
  5) Evaluate m_{best} on test set in order to get an unbiased estimate of its generalization performance



Model Selection using Cross-Validation

- But wait, we want to
  1. make sure that all examples are used for validation once
  2. use as much labeled data as possible for training
- Both goals are met by using cross-validation for model selection



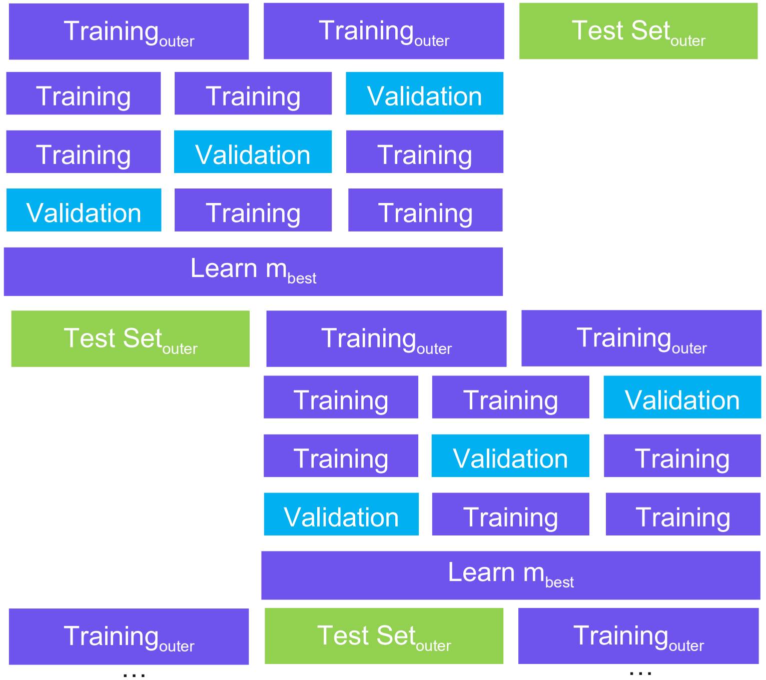
- 5 folds, 100 parameter value sets ➔ 501 models learned

Model Evaluation using Nested Cross-Validation

- Nest two cross-validation loops into each other in order to:
  1. find the best hyperparameter setting (model selection)
  2. get a reliable estimate of the generalization error (model evaluation)

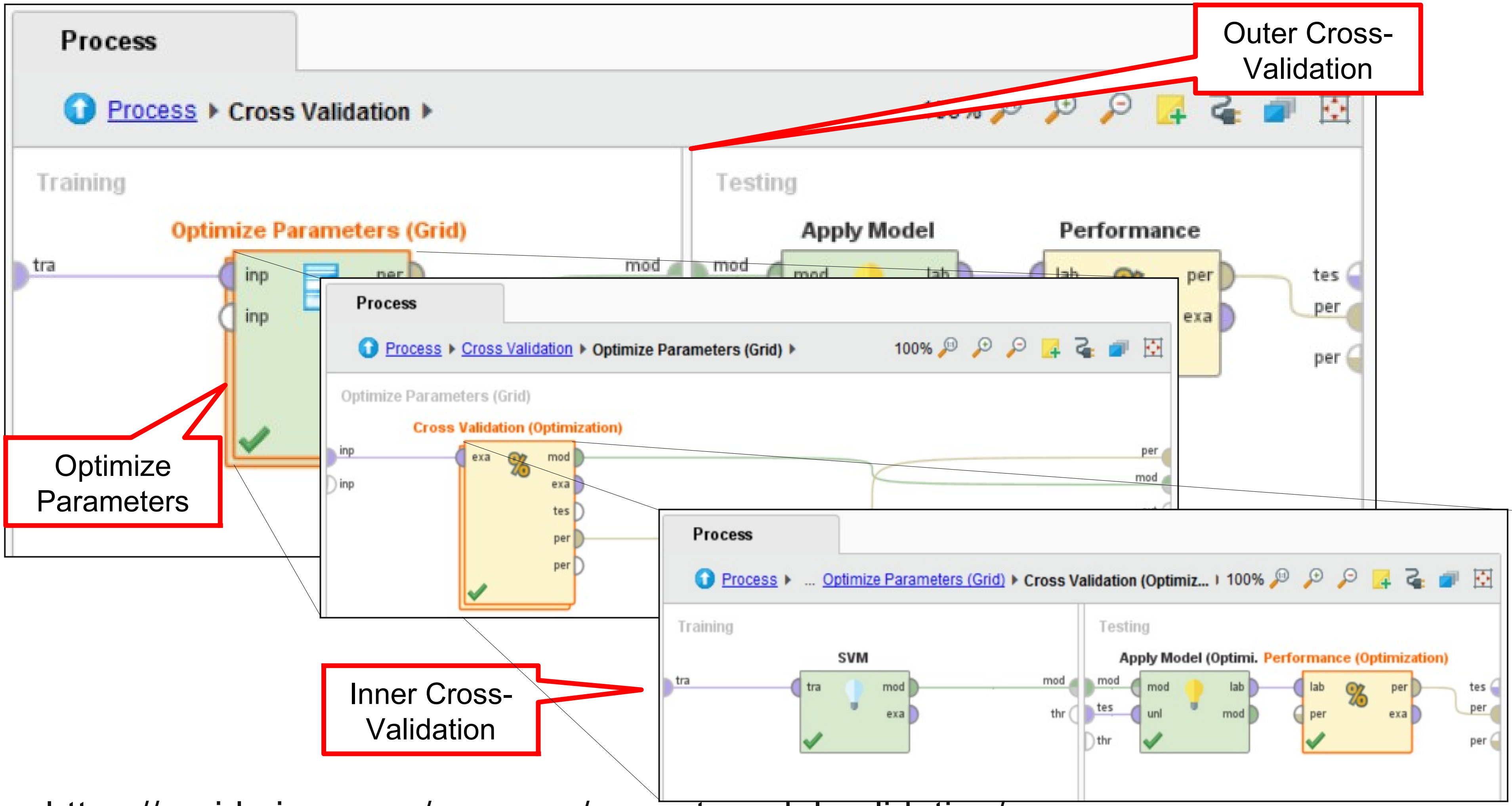
– Outer Cross-Validation
  - estimates generalization error of m_{best}
  - training set is passed on to inner cross-validation in each iteration

– Inner Cross-Validation
  - searches for best parameter combination
  - splits outer training set into inner training and validation set
  - learns model m_{best} using all outer training data



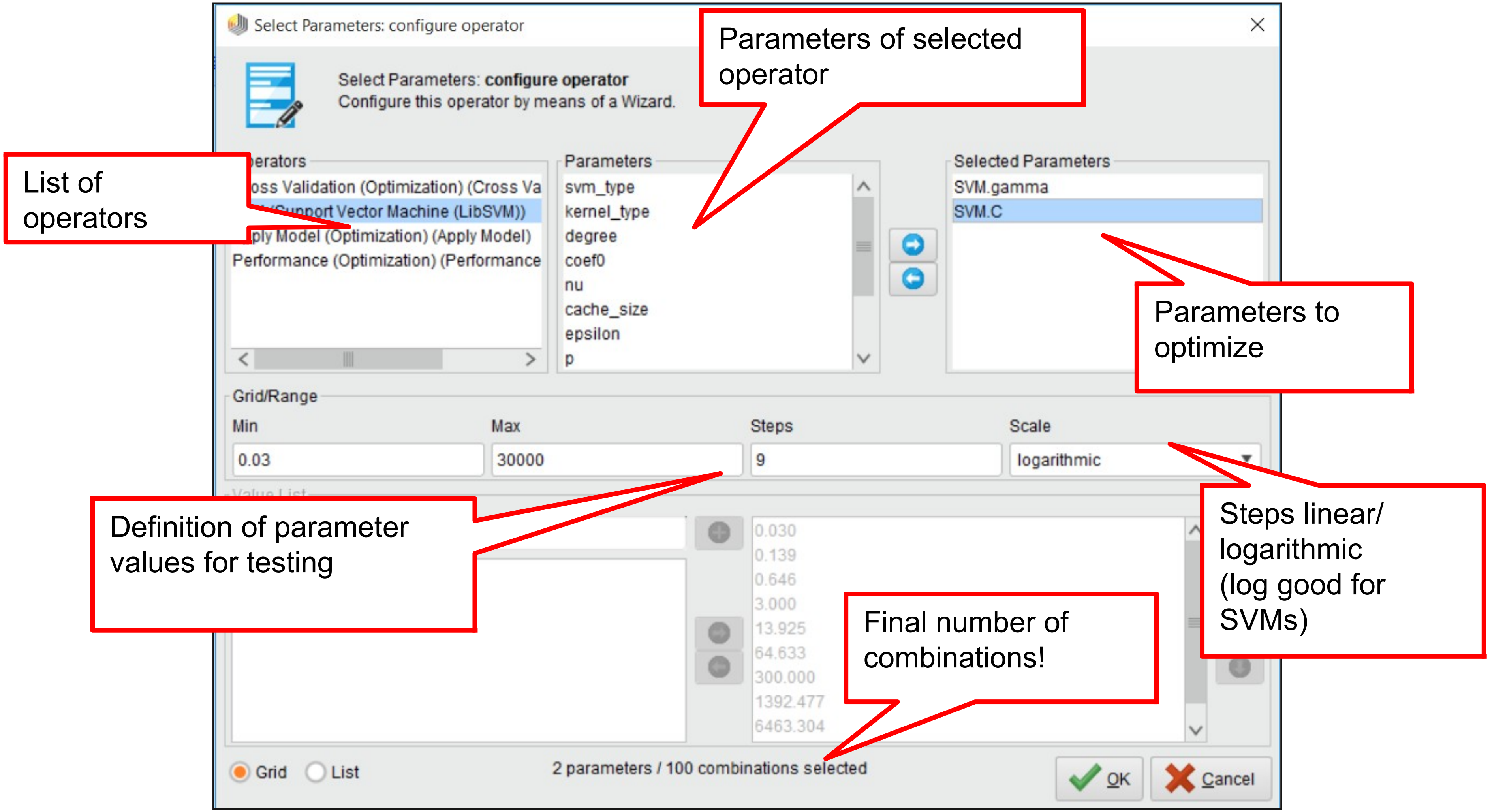
- 5 folds_{Outer}*((5 folds_{Inner}* 100 parameter sets)+1) ➔ 2505 models learned

Nested Cross-Validation in RapidMiner



https://rapidminer.com/resource/correct-model-validation/

Hyperparameter Optimization in RapidMiner



Nested Cross-Validation in Python

```
from sklearn.model_selection import GridSearchCV
from sklearn.model_selection import cross_val_score
from sklearn.svm import SVC

# Specify hyperparameter combinations for search
parameter_grid = {"C": [1, 10, 100, 1000], "gamma": [.001, .01, .1, 1]}

# Create SVM
estimator_svm = SVC(kernel='rbf')

# Create the grid search for model selection
estimator_gs = GridSearchCV(estimator_svm, parameter_grid, scoring='accuracy', cv=5)

# Run nested cross-validation for model evaluation
accuracy_cv = cross_val_score(estimator_gs, dataset, labels, cv=5, scoring='accuracy')
```

Summary

- Classification approaches
  - There are quite a few: Nearest Neighbors, Naive Bayes, Decision Trees, Rules, SVMs, Neural Networks
- Distinctions
  - Lazy vs. eager
  - Performance (accuracy, training time, testing time, model size)
  - Decision Boundaries (theory and practice)
- Issues
  - Overfitting
  - Parameter tuning

Questions?