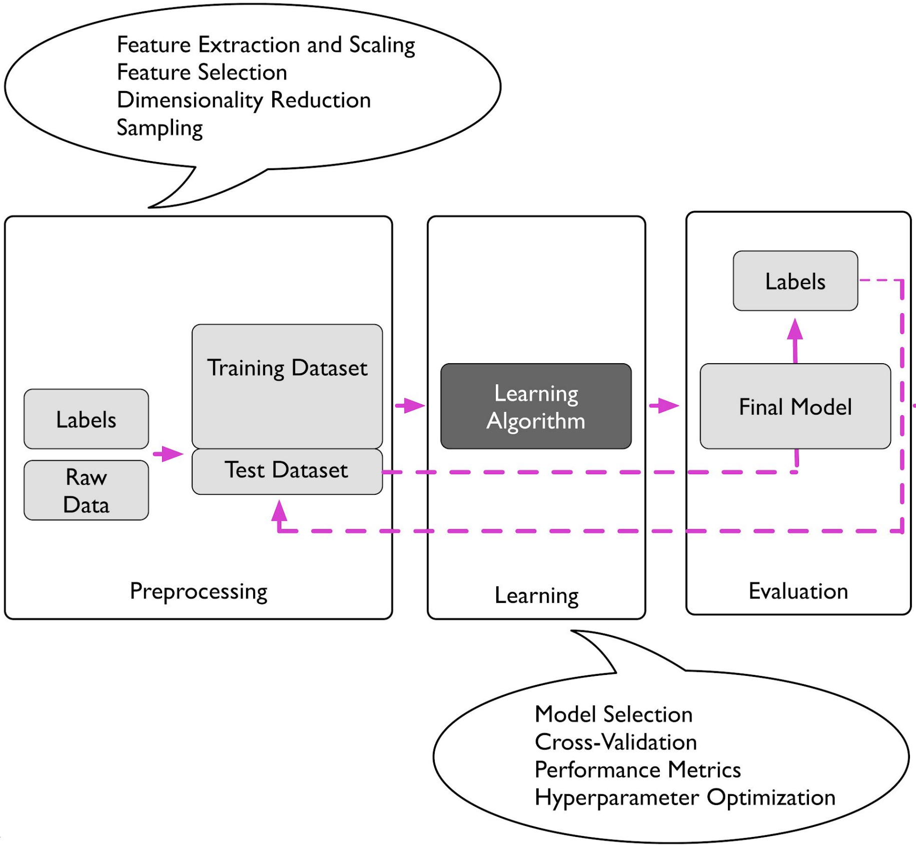
Lecture 12

Decision trees

https://github.com/dalcimar/MA28CP-Intro-to-Machine-Learning
UTFPR - Federal University of Technology - Paraná
https://www.dalcimar.com/

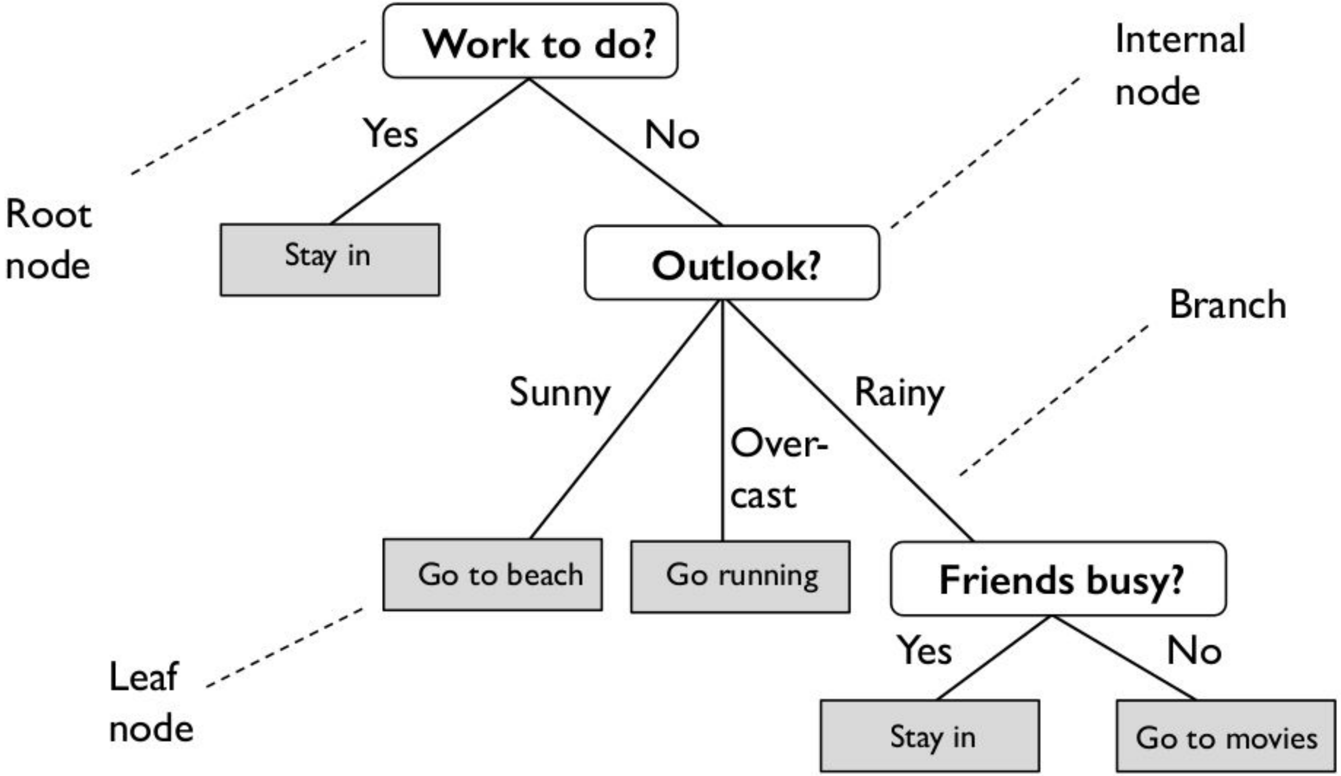
Machine learning pipeline



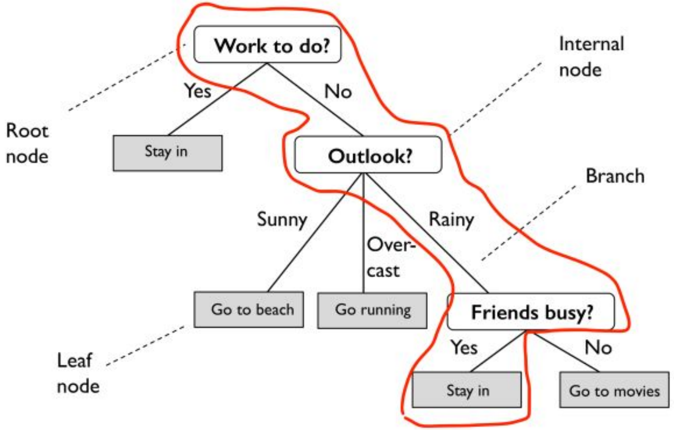
Topics

1. **Intro to decision trees**
2. Recursive and divide & conquer strategy
3. Types of decision trees
4. Splitting criteria
5. Gini & Entropy vs misclassification error
6. Improvements & dealing with overfitting
7. Code example

Decision tree terminology



Decision tree as rulersets



IF ____________________ ___ ____________________

___ ____________________

THEN ________ ___ __________

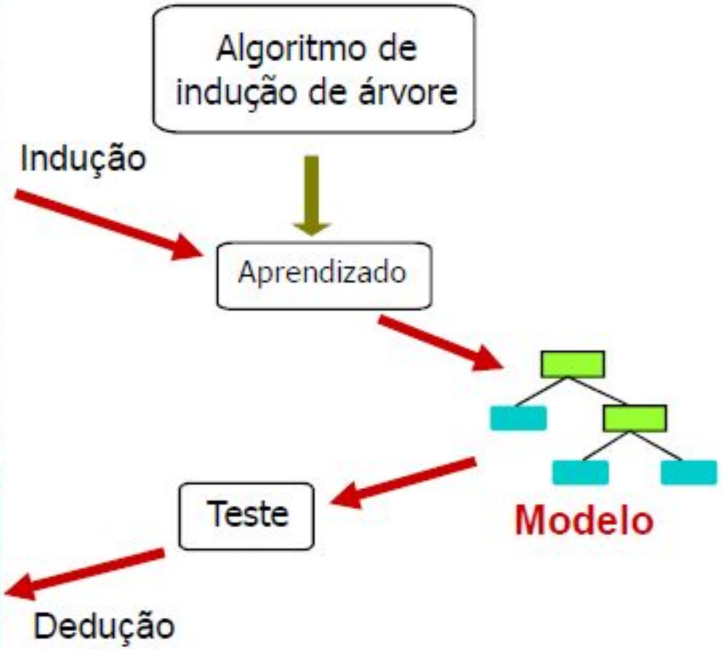
Decision tree pipeline

Conjunto de treinamento

Id	E Credor	Estado Civil	Salário	Calote
1	Sim	Solteiro	125K	Não
2	Não	Casado	100K	Não
3	Não	Solteiro	70K	Não
4	Sim	Casado	120K	Não
5	Não	Divorciado	95K	Sim
6	Não	Casado	60K	Não
7	Sim	Divorciado	220K	Não
8	Não	Solteiro	85K	Sim
9	Não	Casado	75K	Não
10	Não	Solteiro	90K	Sim

Conjunto de teste

Id	E Credor	Estado Civil	Salário	Calote
11	Não	Casado	80K	?
12	Não	Solteiro	100K	?
13	Sim	Solteiro	100K	?
14	Não	Casado	120K	?
15	Sim	Solteiro	80K	?



Training

- Works on categorical (binary, nominal or ordinal) and
- Works also with numeric (continuos) attributes

Id	E Credor	Estado Civil	Salário	Calote
1	Sim	Solteiro	125K	Não
2	Não	Casado	100K	Não
3	Não	Solteiro	70K	Não
4	Sim	Casado	120K	Não
5	Não	Divorciado	95K	Sim
6	Não	Casado	60K	Não
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9	Não	Casado	75K	Não
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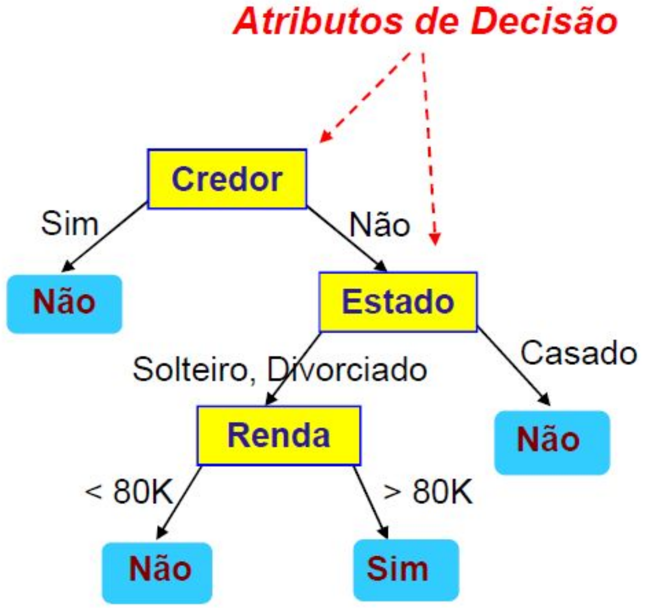
Dados de Treinamento



Modelo: Árvore de Decisão

Training

Id	E Credor	Estado Civil	Salário	Calote
1	Sim	Solteiro	125K	Não
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3	Não	Solteiro	70K	Não
4	Sim	Casado	120K	Não
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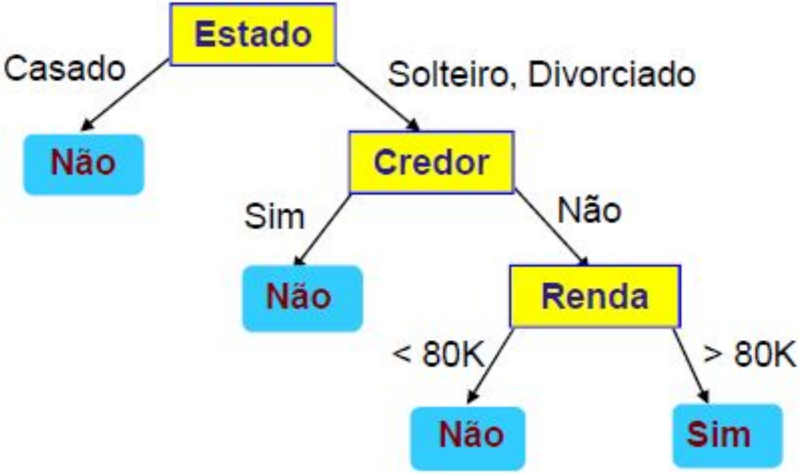
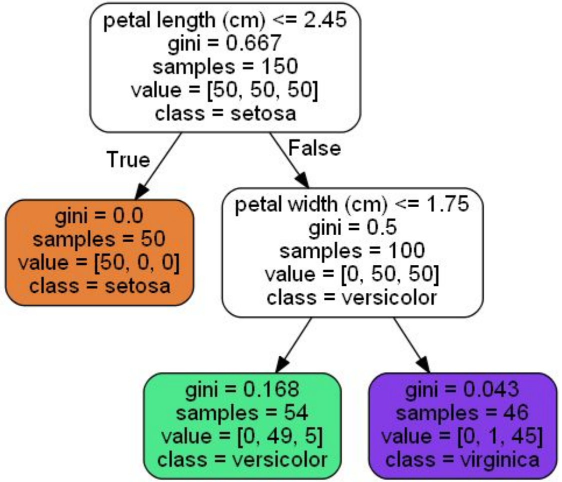


Diferentes árvores podem ser ajustadas para os mesmos dados !

Decision tree on Iris dataset (2 features)



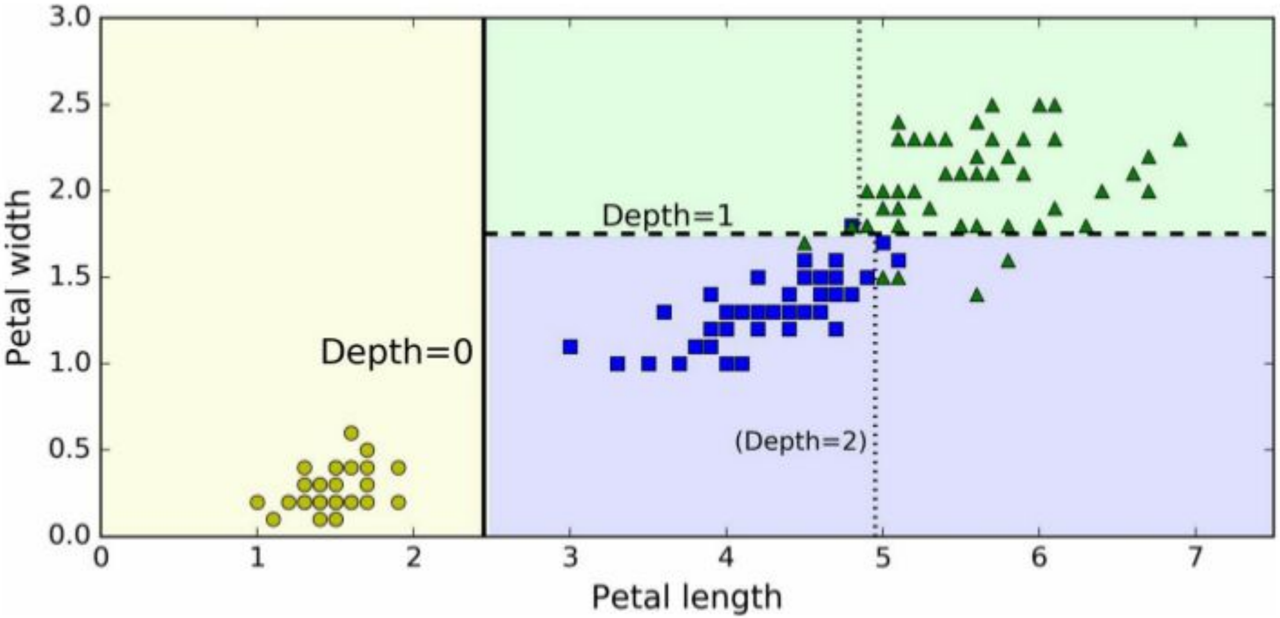
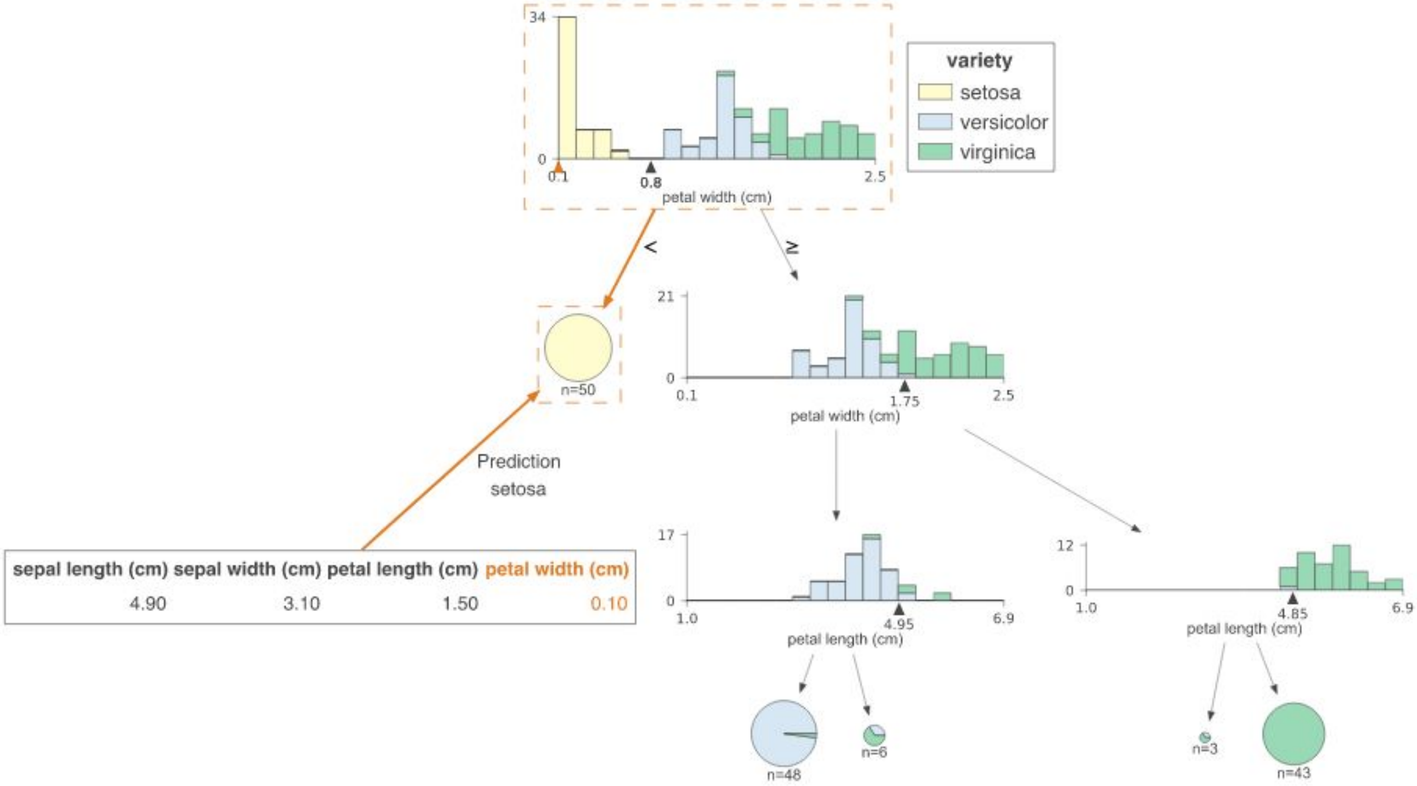


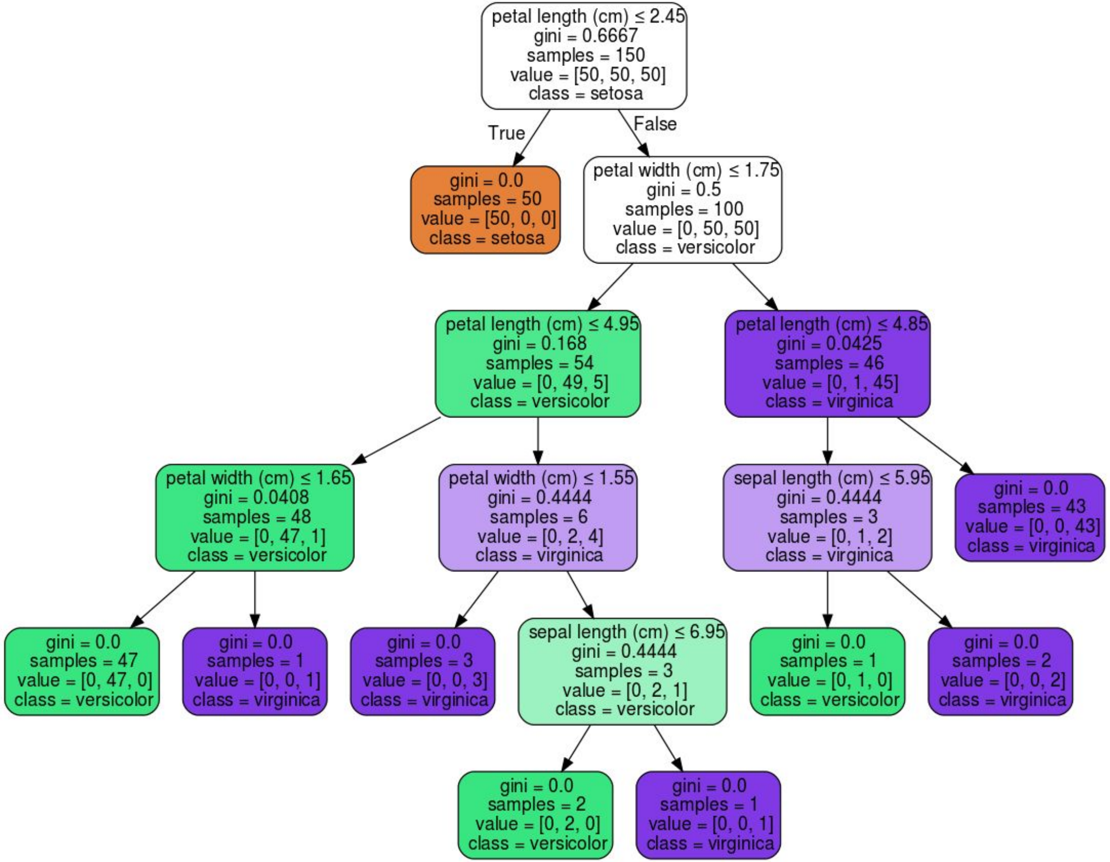
Figure 6-2. Decision Tree decision boundaries

Decision tree on Iris dataset (2 features)

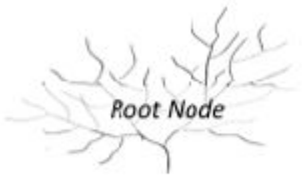


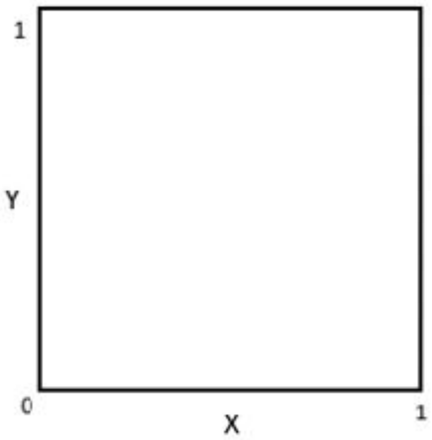
https://explained.ai/decision-tree-viz/images/samples/iris-TD-3-X.svg

Decision tree on Iris dataset (4 features)



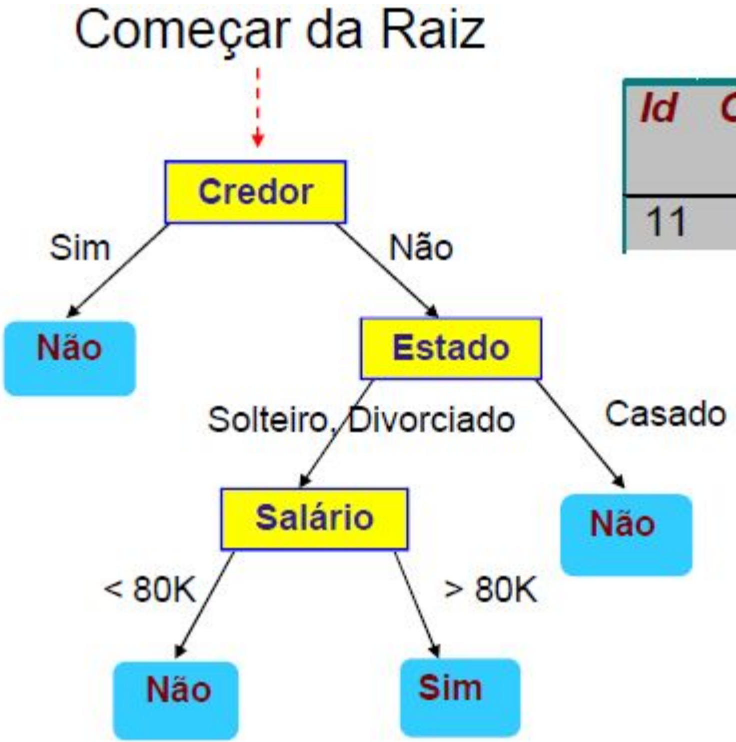
Growing depth process





For more tutorials: annalyzin.wordpress.com

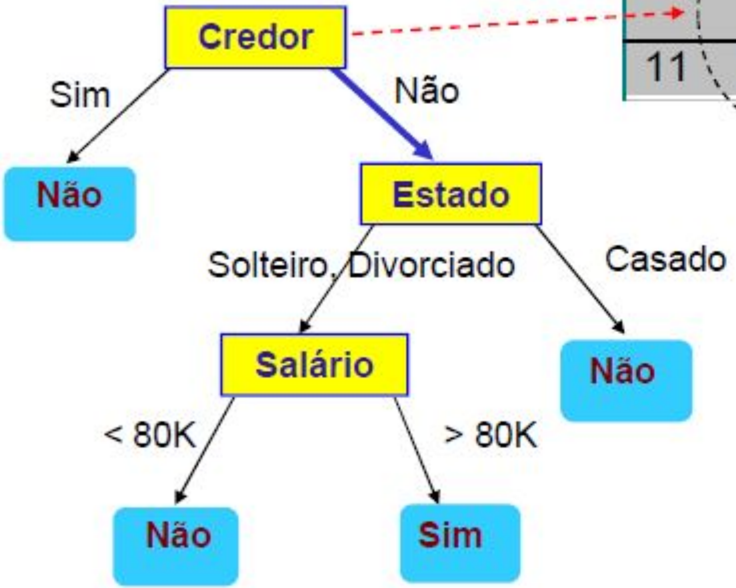
Inference



Dados de Teste

Id	*Credor*	*Estado Civil*	*Salário*	*Calote*
11	Não	Casado	80K	???

Inference



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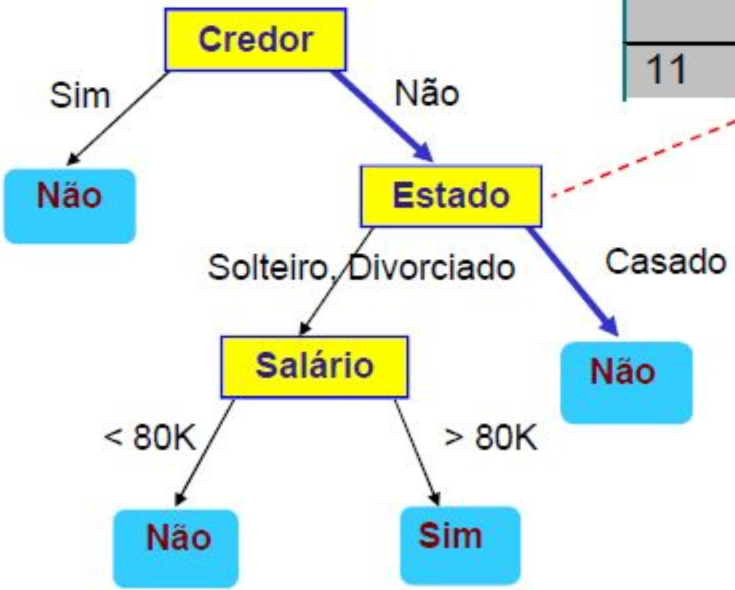

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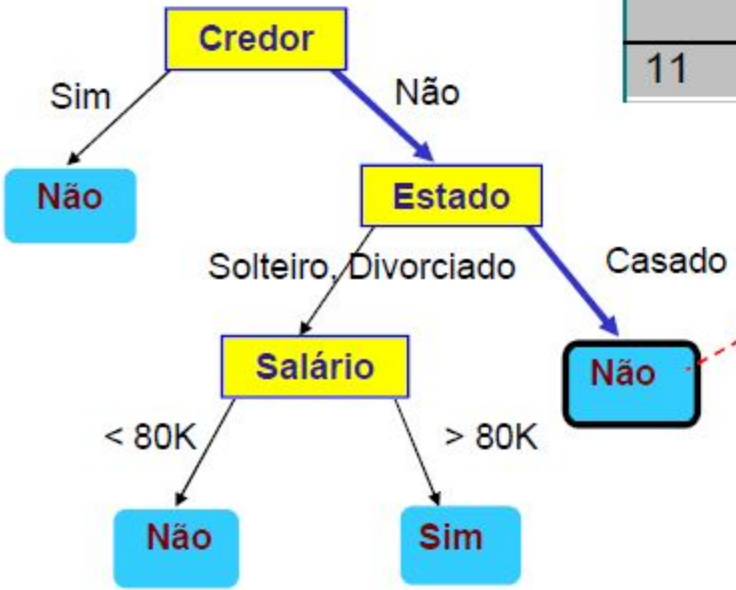

Dados de Teste

Id	*Credor*	*Estado Civil*	*Salário*	*Calote*
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Atribui classe **Não**

Tree depth overfitting

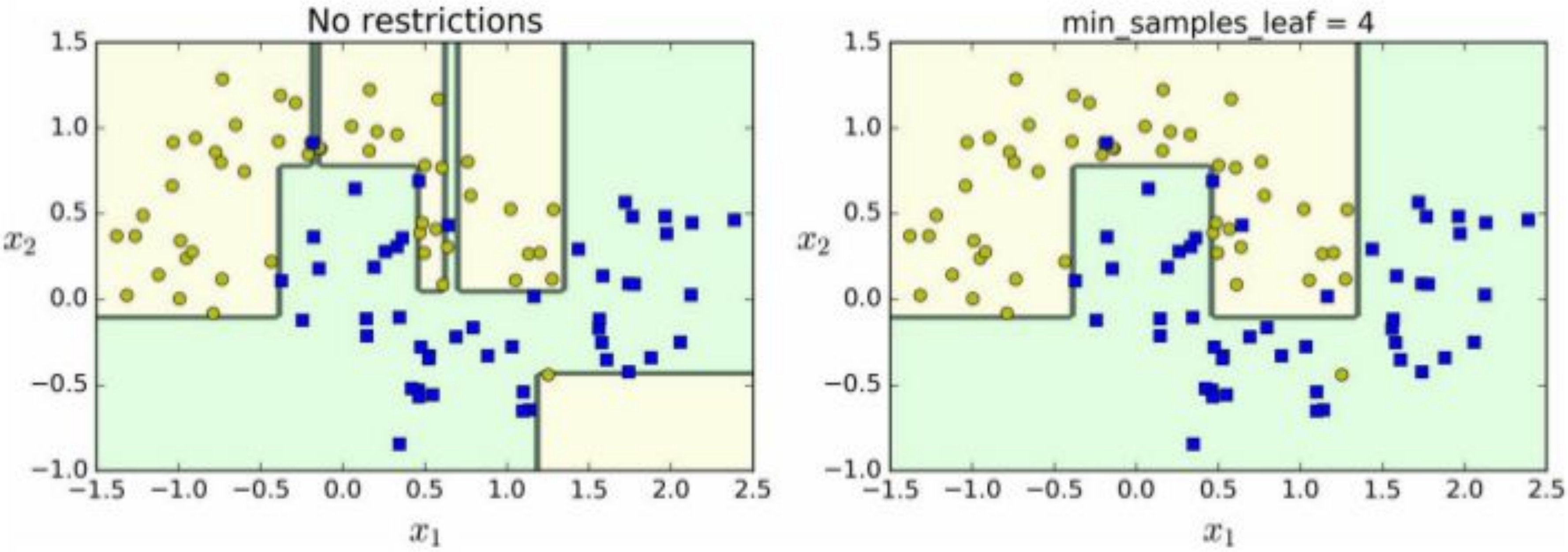

Figure 6-3. Regularization using min_samples_leaf

Animations

Amazing animation of decision tree

http://www.r2d3.us/visual-intro-to-machine-learning-part-1/

Topics

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Recursion / Recursive Algorithms

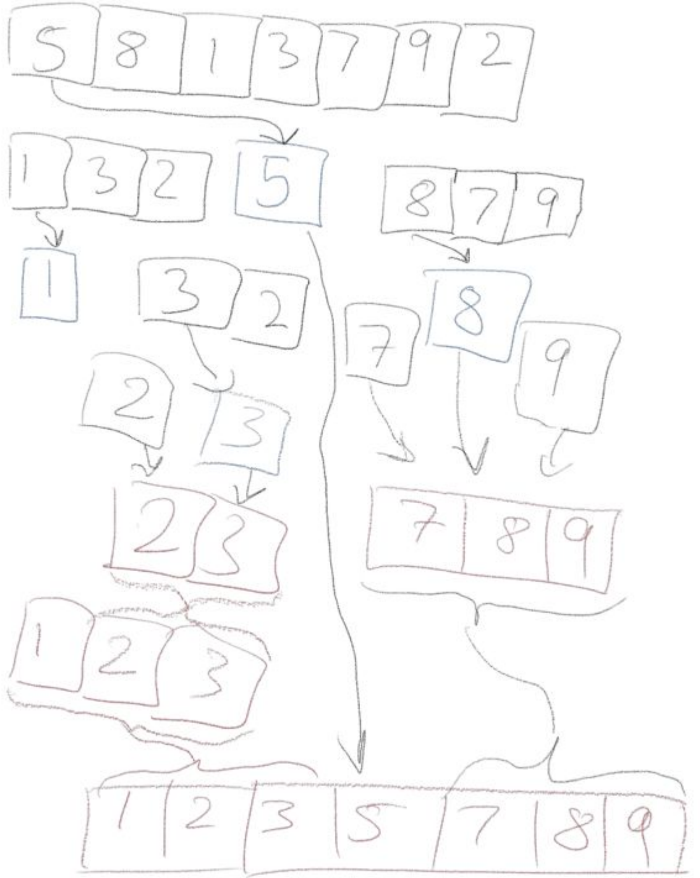
What does this function do?

```
def some_fun(x):
    if x == []:
        return 0
    else:
        return 1 + some_fun(x[1:])
```

Divide & Conquer Algorithms: Quicksort

```
def quicksort(array):
    if len(array) < 2:
        return array
    else:
        pivot = array[0]
        smaller, bigger = [], []
        for ele in array[1:]:
            if ele <= pivot:
                smaller.append(ele)
            else:
                bigger.append(ele)
        return quicksort(smaller) + [pivot] + quicksort(bigger)
```

Divide & Conquer Algorithms: Quicksort

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```

Time complexity of quicksort

O(n log n)

```
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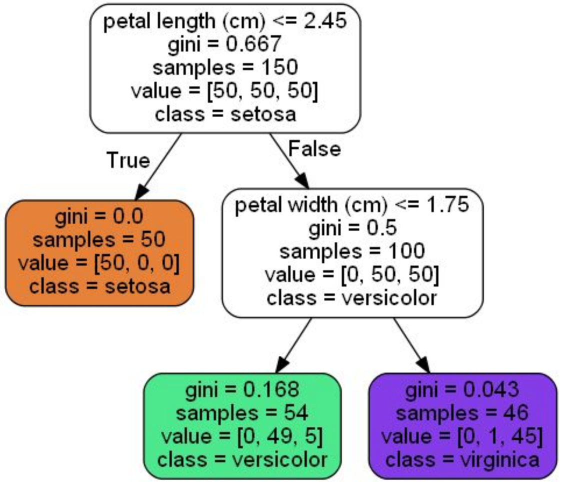
            else:
                bigger.append(ele)
        return quicksort(smaller) + [pivot] + quicksort(bigger)
```

Time and space complexity of sorting algorithms

Algorithm	Time Complexity			Space Complexity
	Best	Average	Worst	Worst
Quicksort	Ω(n log(n))	Θ(n log(n))	O(n^2)	O(log(n))
Mergesort	Ω(n log(n))	Θ(n log(n))	O(n log(n))	O(n)
Timsort	Ω(n)	Θ(n log(n))	O(n log(n))	O(n)
Heapsort	Ω(n log(n))	Θ(n log(n))	O(n log(n))	O(1)
Bubble Sort	Ω(n)	Θ(n^2)	O(n^2)	O(1)
Insertion Sort	Ω(n)	Θ(n^2)	O(n^2)	O(1)
Selection Sort	Ω(n^2)	Θ(n^2)	O(n^2)	O(1)
Tree Sort	Ω(n log(n))	Θ(n log(n))	O(n^2)	O(n)
Shell Sort	Ω(n log(n))	Θ(n(log(n))^2)	O(n(log(n))^2)	O(1)
Bucket Sort	Ω(n+k)	Θ(n+k)	O(n^2)	O(n)
Radix Sort	Ω(nk)	Θ(nk)	O(nk)	O(n+k)
Counting Sort	Ω(n+k)	Θ(n+k)	O(n+k)	O(k)
Cubesort	Ω(n)	Θ(n log(n))	O(n log(n))	O(n)

Decision Tree in Pseudocode



GenerateTree($\mathcal{D}$):

- if $y = 1 \; \forall \; \langle \mathbf{x}, \mathbf{y} \rangle \in \mathcal{D}$ or $y = 0 \; \forall \; \langle \mathbf{x}, y \rangle \in \mathcal{D}$:
  - return Tree
- else:
  - Pick best feature x_j:
    - $\mathcal{D}_0$ at Child$_0$: $x_j = 0 \; \forall \; \langle \mathbf{x}, y \rangle \in \mathcal{D}$
    - $\mathcal{D}_1$ at Child$_1$: $x_j = 1 \; \forall \; \langle \mathbf{x}, y \rangle \in \mathcal{D}$

  return Node(x_j, GenerateTree($\mathcal{D}_0$), GenerateTree($\mathcal{D}_1$))

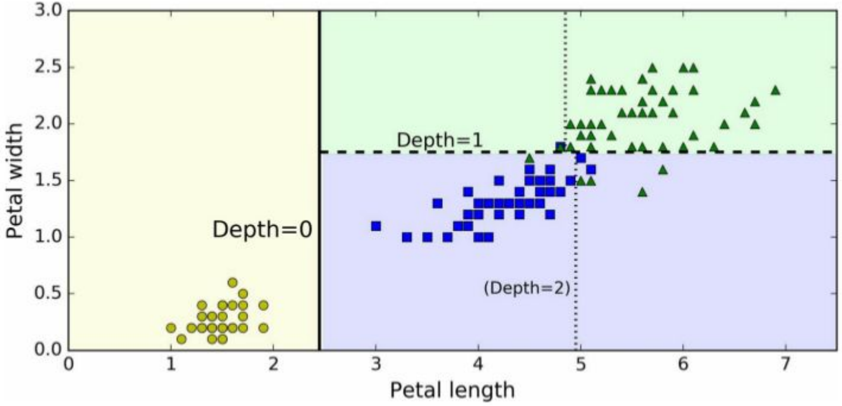


Figure 6-2. Decision Tree decision boundaries

Time complexity decision tree

Growing the tree (**fit()**): $O(m*n^2 \log n)$

- Assuming we have continuous features and perform binary splits, the runtime of the decision tree construction is
- Sorting the values of continuous features helps with determining a decision threshold. If we have n examples, the sorting has time complexity $O(n \log n)$
- If we have to compare sort m features, this becomes $O(m*n \log n)$
- Sorting step up to n/2 times $O(m*n^2 \log n)$

Querying the tree (**predict()**): $O(\log n)$

- depth of $\log_2 n$

Fayyad, Usama Mohammad. "On the induction of decision trees for multiple concept learning." (1992).

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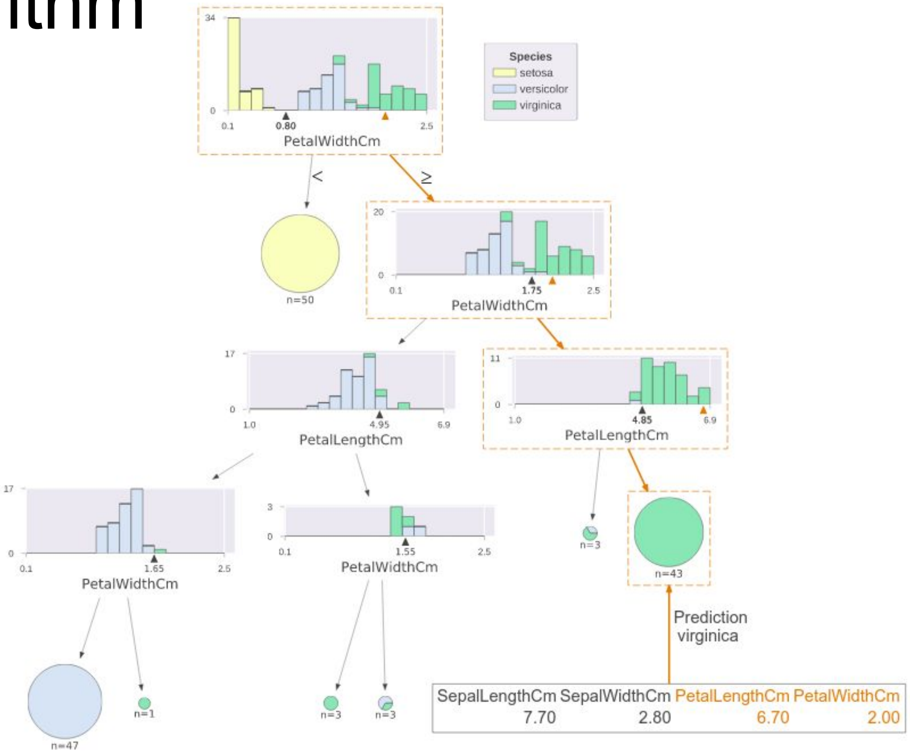
Generic Tree Growing Algorithm



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    - $\mathcal{D}_1$ at Child$_1$: $x_j = 1 \; \forall \; \langle \mathbf{x}, y \rangle \in \mathcal{D}$

  return Node(x_j, GenerateTree($\mathcal{D}_0$), GenerateTree($\mathcal{D}_1$))

Generic Tree Growing Algorithm

1. Pick the feature that, when parent node is split, results in the largest information gain
2. Stop if child nodes are pure or information gain <= 0
3. Go back to step 1 for each of the two child nodes

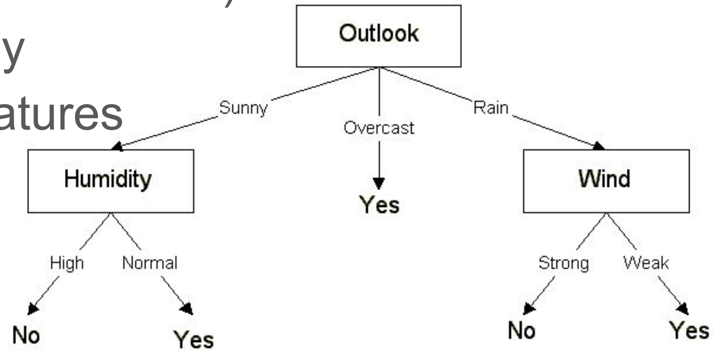
How make predictions of features in dataset not sufficient to make child nodes pure?

Design choices

- What kind of variables
  - Only binary features
  - Only binary or categorical features
  - Numeric features
- How to split
  - what measurement/criterion as measure of goodness
  - binary vs multi-category split
- When to stop
  - if leaf nodes contain only examples of the same class
  - feature values are all the same for all examples
  - statistical significance test

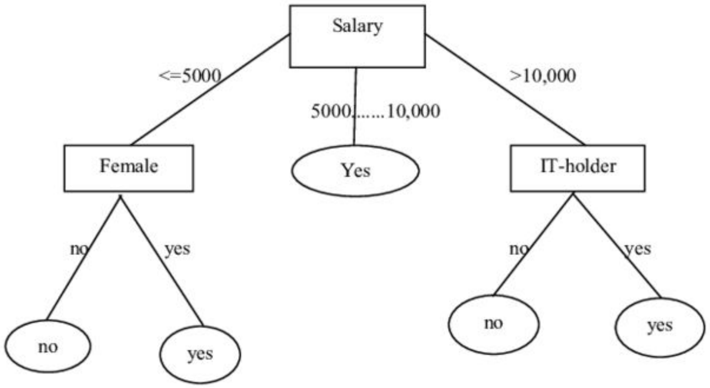
ID3 - Iterative Dichotomizer 3

- Quinlan, J. R. 1986. Induction of Decision Trees. Mach. Learn. 1, 1 (Mar. 1986), 81-106.
- one of the earlier/earliest decision tree algorithms
- **cannot handle numeric features**
- Trees are **grown to their maximum size** and then a **pruning step** is usually applied to improve the ability of the tree to generalise to unseen data
- **multiway tree**, short and wide trees (compared to CART)
- maximizing information gain/minimizing entropy
- discrete features, binary and multi-category features



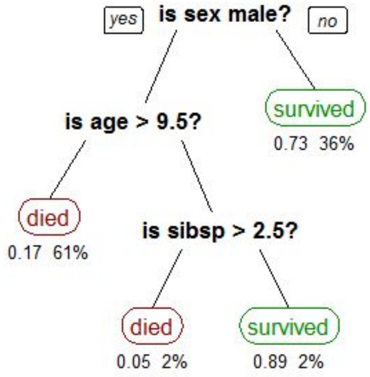
C4.5

- Ross Quinlan 1993, Quinlan, J. R. (1993). C4.5: Programming for machine learning. Morgan Kauffmann, 38, 48.
- **continuous and discrete features**
  - continuous is very expensive, because must consider all possible ranges
- handles missing attributes (ignores them in gain compute)
- **post-pruning** (bottom-up pruning)
- **Gain Ratio**



CART

- Breiman, L. (1984). Classification and regression trees. Belmont, Calif: Wadsworth International Group.
- **continuous and discrete features**
- variance reduction in regression trees
- **strictly binary splits** (taller trees than ID3, C4.5)
  - binary splits can generate better trees than C4.5, but tend to be larger and harder to interpret; k-attributes has a ways to create a binary partitioning
- Gini impurity, twoing criteria in classification trees
- cost complexity pruning



Others

- CHAID (CHi-squared Automatic Interaction Detector); Kass, G. V. (1980). "An exploratory technique for investigating large quantities of categorical data". Applied Statistics. 29 (2): 119–127.
- MARS (Multivariate adaptive regression splines); Friedman, J. H. (1991). "Multivariate Adaptive Regression Splines". The Annals of Statistics. 19: 1
- C5.0 (patented)