Decision Trees for Classification and Regression

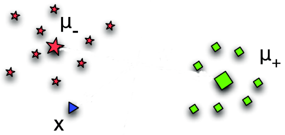
Piyush Rai

Introduction to Machine Learning (CS771A)

August 7, 2018

Recap

Previous class: Looked at Prototype based classification, and nearest neighbor methods



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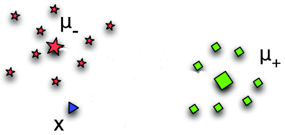

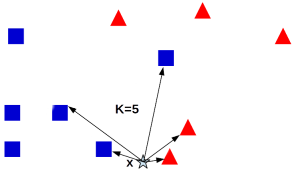

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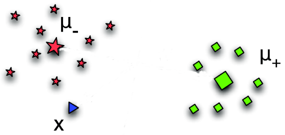

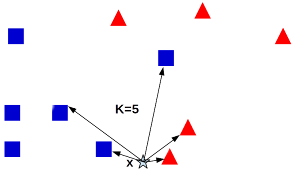

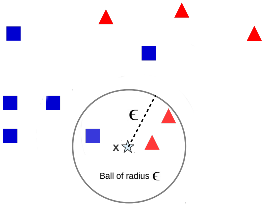

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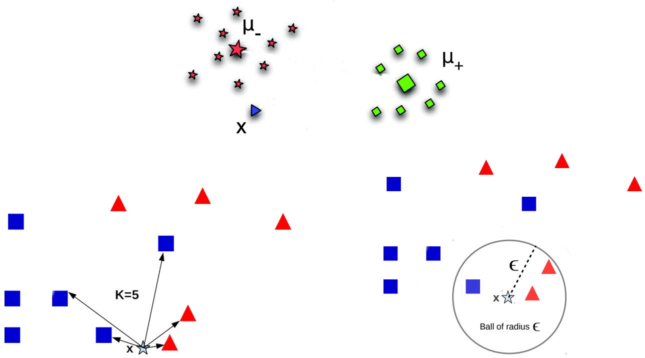
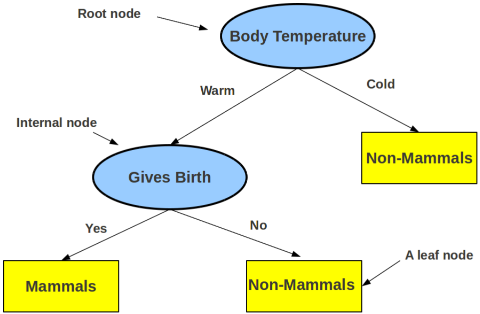


"Local" methods based on distance of the test input with the training inputs (or class prototypes)

Decision Trees
(Another example of a local method)

Decision Tree

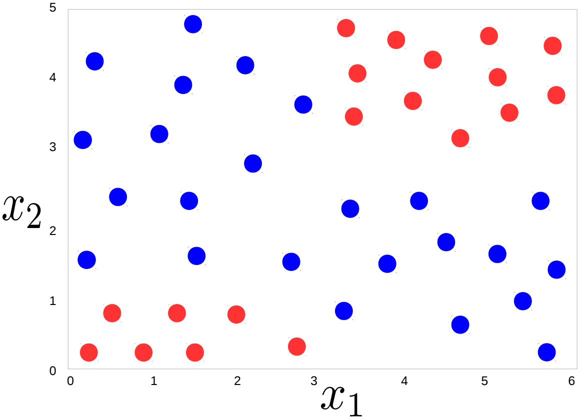
- Defines a tree-structured hierarchy of rules
- Consists of a root node, internal nodes, and leaf nodes



- Root and internal nodes contain the rules
- Leaf nodes define the predictions
- Decision Tree (DT) learning is about learning such a tree from labeled training data

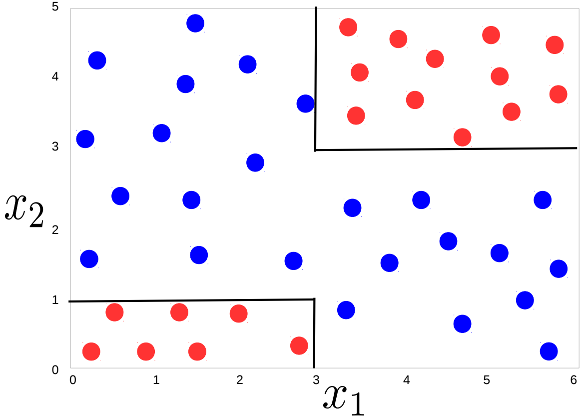
A Classification Problem

Consider binary classification. Assume training data with each input having 2 features (x_1, x_2)



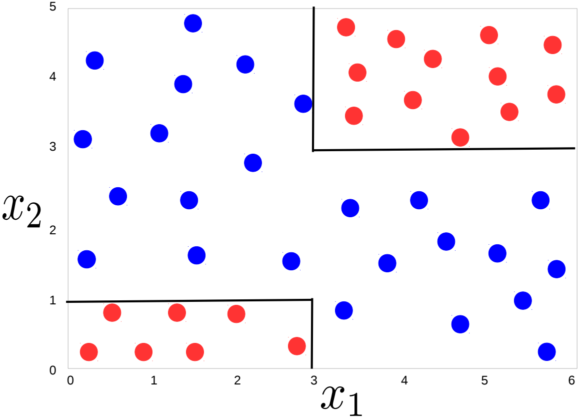
A Classification Problem

The "expected" decision boundary given this training data.



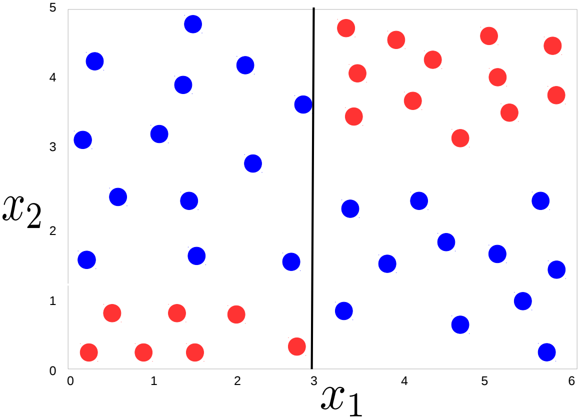
A Classification Problem

The "expected" decision boundary given this training data. Let's learn this!



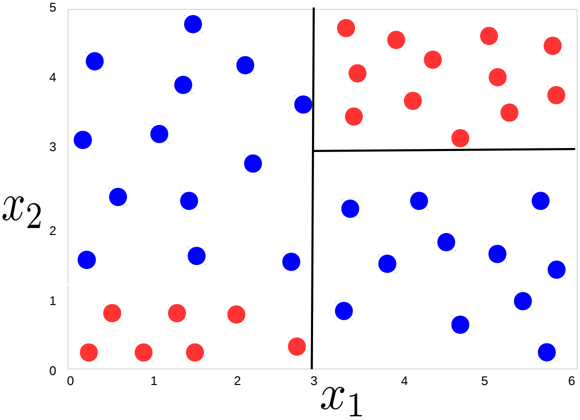
Learning by Asking Questions!

Is x_1 (feature 1) greater than 3 ?



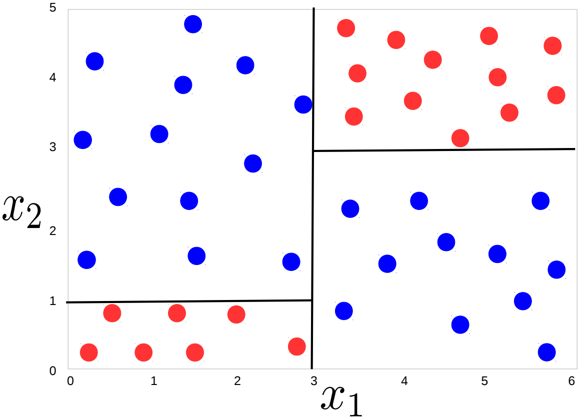
Learning by Asking Questions!

Given $x_1 > 3$, is feature 2 (x_2) greater than 3?



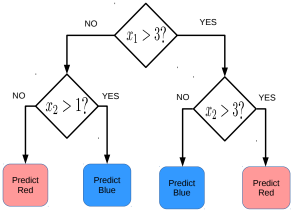
Learning by Asking Questions!

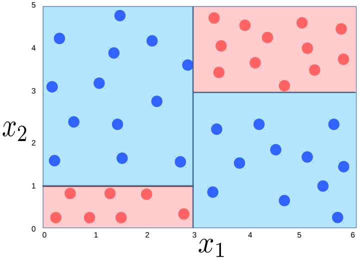
Given $x_1 < 3$, is feature 2 (x_2) greater than 1?



What We Learned

- A Decision Tree (DT) consisting of a set of rules **learned** from training data





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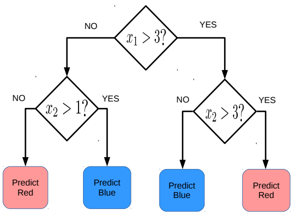

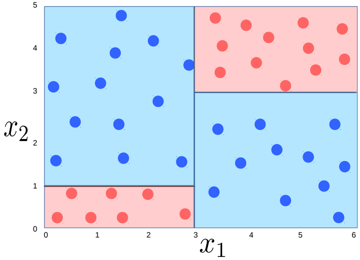

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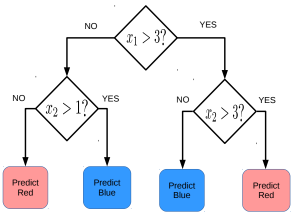

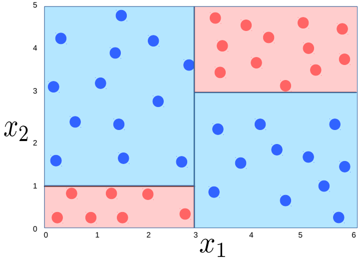

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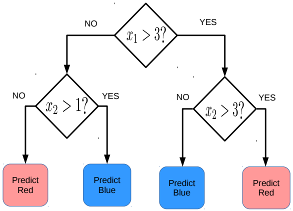

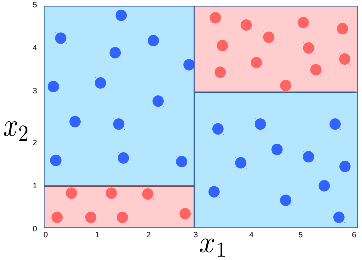

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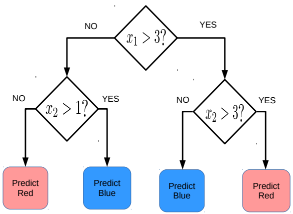

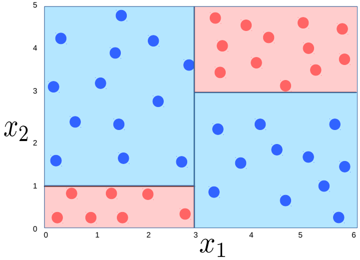

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  - Homogeneous means that the outputs are same/similar for all inputs in that region
- Given a new test input, we can use the DT to predict its label
- A key benefit of DT: Prediction at test time is very fast (just testing a few conditions)

Decision Tree for Classification: Another Example

- Deciding whether to play or not to play Tennis on a Saturday
  - Each input (a Saturday) has 4 categorical features: Outlook, Temp., Humidity, Wind
  - A binary classification problem (play vs no-play)

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1	sunny	hot	high	weak	no
2	sunny	hot	high	strong	no
3	overcast	hot	high	weak	yes
4	rain	mild	high	weak	yes
5	rain	cool	normal	weak	yes
6	rain	cool	normal	strong	no
7	overcast	cool	normal	strong	yes
8	sunny	mild	high	weak	no
9	sunny	cool	normal	weak	yes
10	rain	mild	normal	weak	yes
11	sunny	mild	normal	strong	yes
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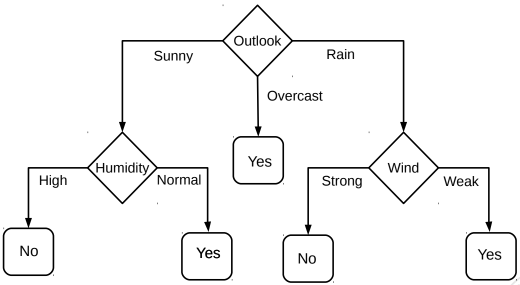

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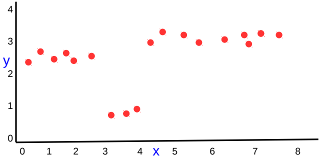
A Decision Tree for Regression

Decision Trees can also be used for regression problems



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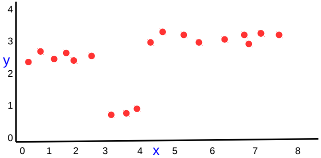

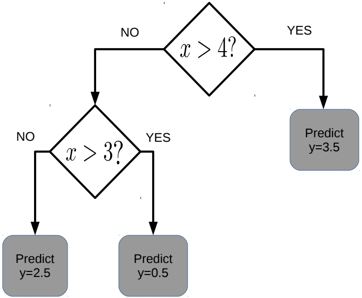

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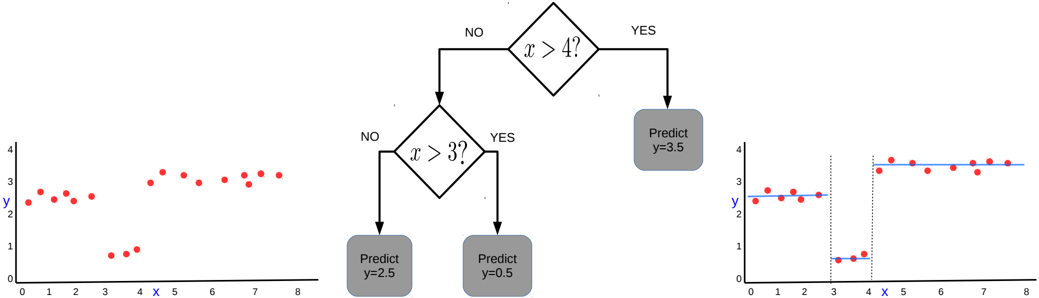

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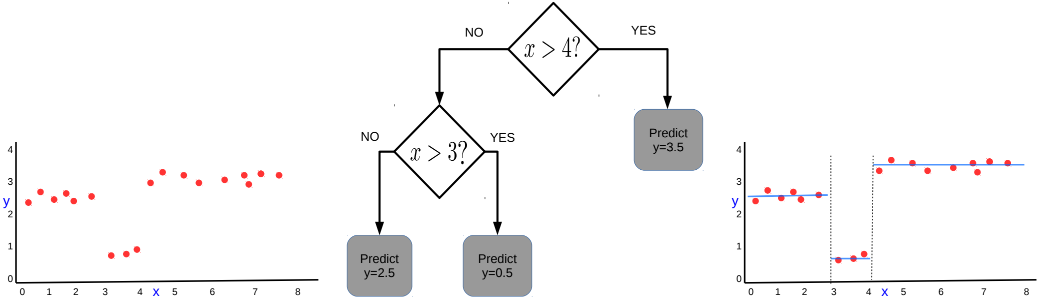
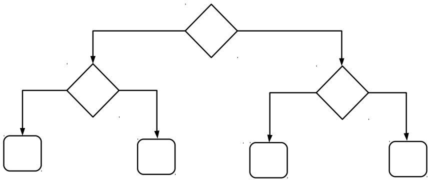


Here too, the DT partitions the training data into homogeneous regions (inputs with similar outputs)

Some Considerations: Shape/Size of DT

- What should be the size/shape of the DT?
  - Number of internal and leaf nodes
  - Branching factor of internal nodes
  - Depth of the tree



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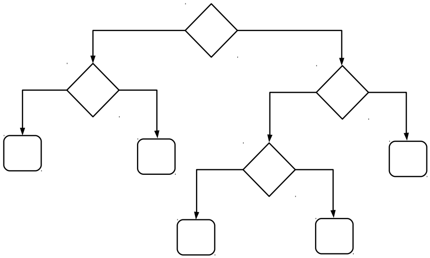

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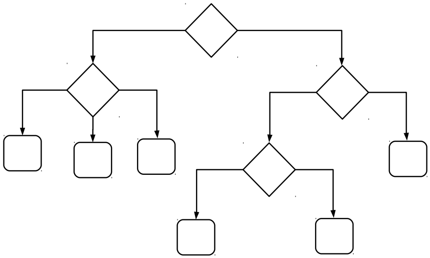

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  - Make a constant prediction (majority/average) for every test input reaching that leaf node?
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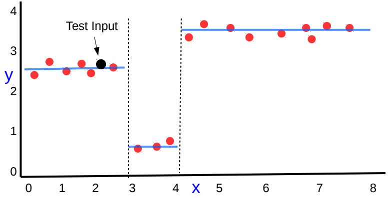

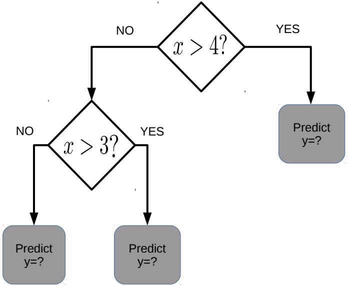

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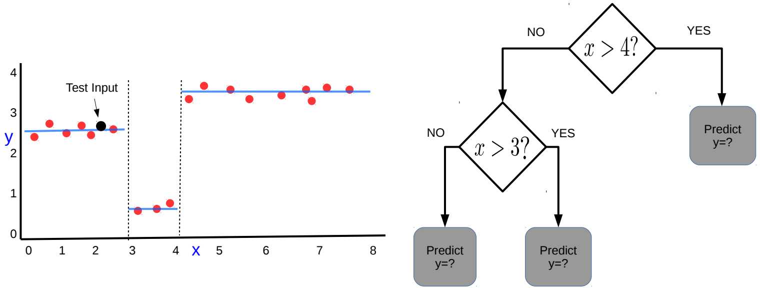

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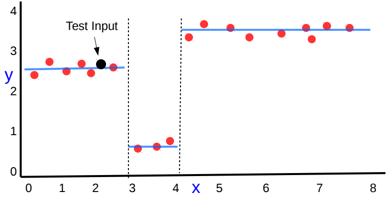

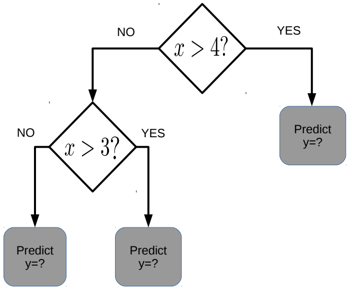

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- Constant prediction is the fastest at test time (and gives a piece-wise constant prediction rule)

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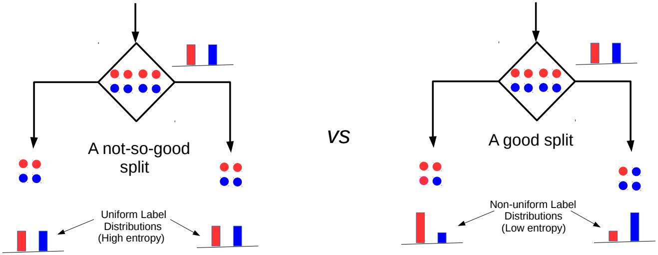

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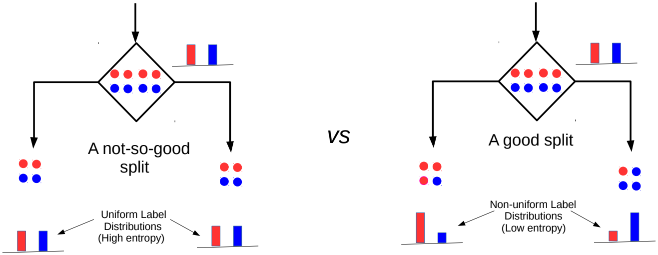

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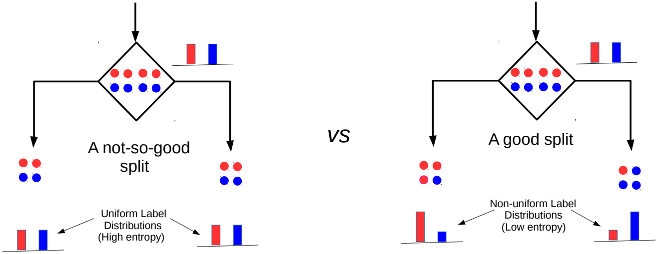

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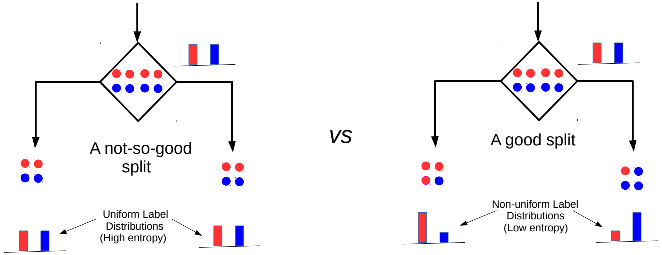

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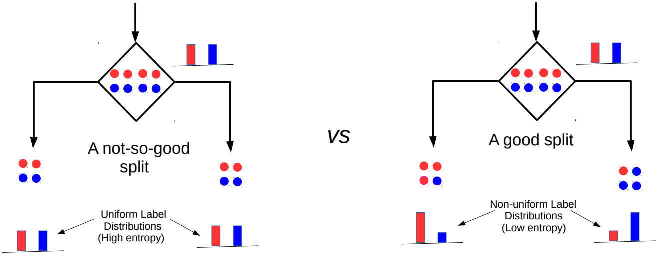

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- For regression, entropy doesn't make sense (outputs are real-valued). Typically variance is used.

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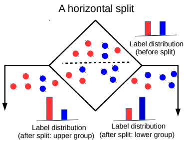

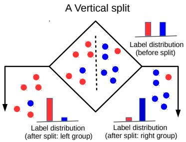

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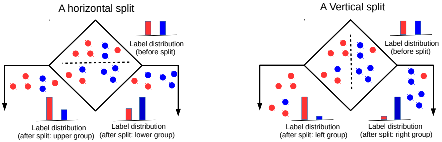
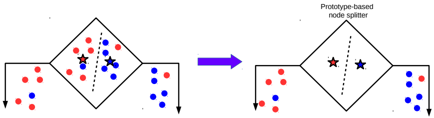


  - Splitting using a classifier learned using data on that node. For example, prototype based classifier



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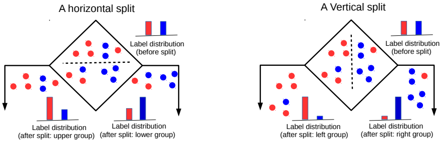

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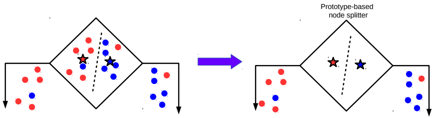

- The same splitting rule will be applied to route a test input that reaches this internal node

Decision Tree Construction

- As an illustration, let's look at one way of constructing a decision tree for some given data
- We will use the entropy/information-gain based splitting criterion for this illustration

day	outlook	temperature	humidity	wind	play
1	sunny	hot	high	weak	no
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3	overcast	hot	high	weak	yes
4	rain	mild	high	weak	yes
5	rain	cool	normal	weak	yes
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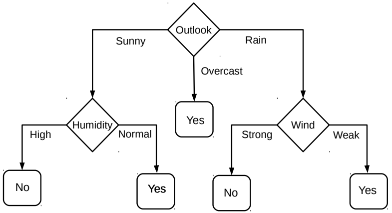

Decision Tree Construction

- As an illustration, let's look at one way of constructing a decision tree for some given data
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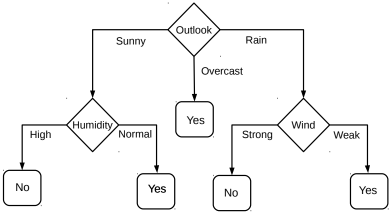

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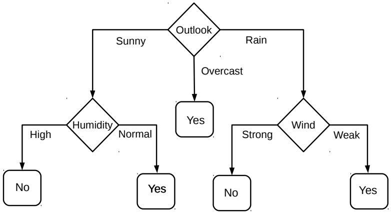

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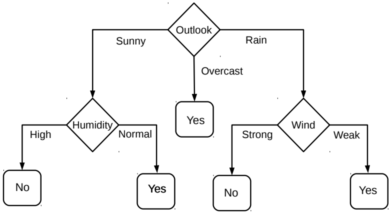

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- **Analogy:** Playing the game 20 Questions (the most useful questions first)

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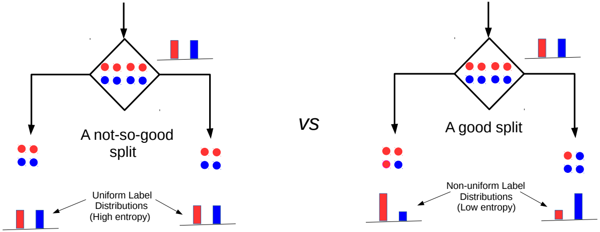
- For DT construction, entropy/IG gives us a criterion to select the best split for an internal node



DT Construction using IG Criterion

- Let's look at IG based DT construction for the Tennis example
- Let's begin with the root node of the DT and compute *IG* of each feature
- Consider feature "wind" $\in$ {weak,strong} and its *IG* at root

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IG(S, \text{wind}) &= H(S) - \frac{|S_{weak}|}{|S|} H(S_{weak}) - \frac{|S_{strong}|}{|S|} H(S_{strong}) \\
&= 0.94 - 8/14 * 0.811 - 6/14 * 1 \\
&= 0.048
\end{aligned}
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Likewise, $IG(S, \text{outlook}) = 0.246$, $IG(S, \text{humidity}) = 0.151$, $IG(S, \text{temperature}) = 0.029 \Rightarrow$ outlook chosen

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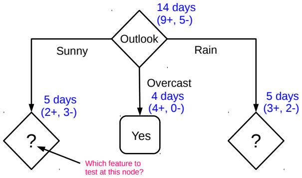

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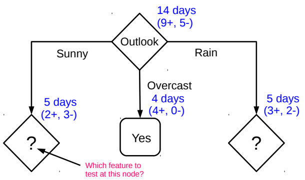

- Proceeding as before, for level 2, left node, we can verify that
  - $IG(S, \text{temperature}) = 0.570$, $IG(S, \text{humidity}) = 0.970$, $IG(S, \text{wind}) = 0.019$ (thus humidity chosen)
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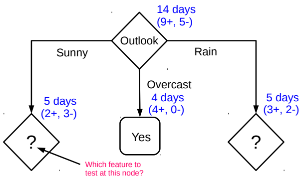

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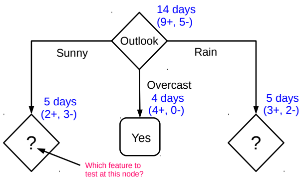

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- No need to expand the middle node (already "pure" - all yes)
- Can also verify that wind has the largest IG for the right node
- Note: If a feature has already been tested along a path earlier, we don't consider it again

When to Stop Growing?

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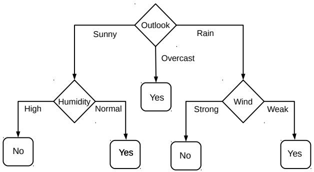

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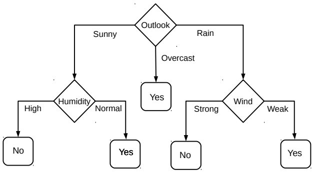

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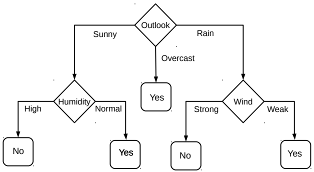

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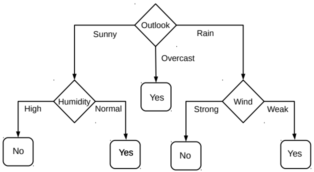

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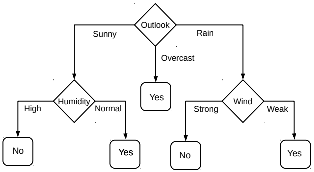
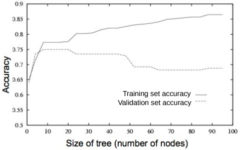


- Stop expanding a node further when
  - It consist of examples all having the same label (the node becomes "pure")
  - We run out of features to test along the path to that node
  - The DT starts to overfit (can be checked by monitoring the validation set accuracy)



Avoiding Overfitting: Decision Tree Pruning

- Desired: a DT that is not too big in size, yet fits the training data reasonably
- Note: An example of a very simple DT is "decision-stump"
  - A decision-stump only tests the value of a single feature
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  - Use model selection methods, such as Minimum Description Length (MDL); more on this later

Decision Tree: Some Comments

- Other alternatives to entropy for judging feature informativeness in DT classification?
  - Gini-index $\sum_{c=1}^{C} p_c(1 - p_c)$ is another popular choice

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Some Aspects about Decision Trees

Some key strengths:

- Simple and each to interpret
- Do not make any assumption about distribution of data
- Easily handle different types of features (real, categorical/nominal, etc.)
- Very fast at test time (just need to check the features, starting the root node and following the DT until you reach a leaf node)
- Multiple DTs can be combined via ensemble methods (e.g., Decision Forest)
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Some key weaknesses:

- Learning the optimal DT is NP-Complete. The existing algorithms are heuristics (e.g., greedy selection of features)
- Can sometimes become very complex unless some pruning is applied