COMS30035, Machine learning: Regresssion and Classification Trees

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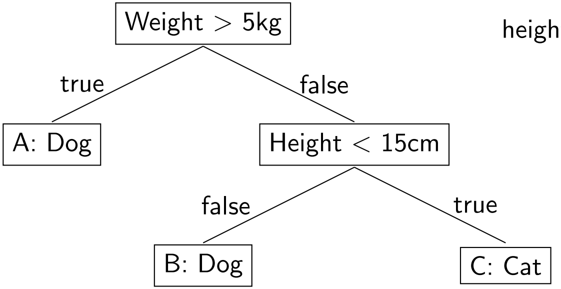
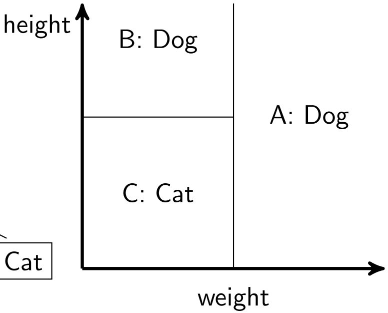
3rd September 2024

Acknowledgement

- These slides are adapted from ones originally created by Edwin Simpson.

Decision Trees





Decision Trees as Partitioning Input Space

- One model is responsible for assigning a decision for each region of input space;
- The correct model for an input $\boldsymbol{x}$ is chosen by traversing the binary decision tree, following the path from the top to a leaf.
- Leaf node is responsible for assigning a decision, such as a:
  - Class label;
  - Probability distribution over class labels;
  - Scalar value (for regression tasks).

Learning the Tree Structure

- Which input variable to use at each node?
- What threshold to set for the split at each node?
- Classification and Regression Trees (CART): one of many possible learning algorithms
- Objective: greedily minimise the error
  - Regression: sum-of-squares
  - Classification: cross-entropy as used in neural networks or Gini impurity

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Learning the Tree Structure

- Number of possible solutions grows combinatorially with the number of input variables
- Greedy algorithm: add nodes one-at-a-time, choosing the best split at each point

1. Start from the root node
2. Run *exhaustive search* over each possible variable and threshold for a new node. For each variable and threshold:
    - Compute average of the target variable for each leaf of the proposed node
    - Compute the error if we stop adding nodes here
3. Choose the variable & threshold that minimise the error
4. Add a new node for the chosen variable and threshold.
5. Repeat step 2 until there are only n data points associated with each leaf node.
6. Prune back the tree to remove branches that do not reduce error by more than a small tolerance value, ϵ.

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Pruning

- Balance residual training-set error against model complexity
- Start with a tree T_0
- Consider pruning each node in T_0 by combining the branches to obtain tree T
- Compute a criterion $C(T) = \sum_{\tau=1}^{|T|} e_\tau(T) + \lambda|T|$
- If $C(T) \leq C(T_0)$ keep the pruned tree, else reinstate the pruned node.

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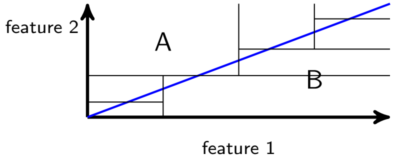
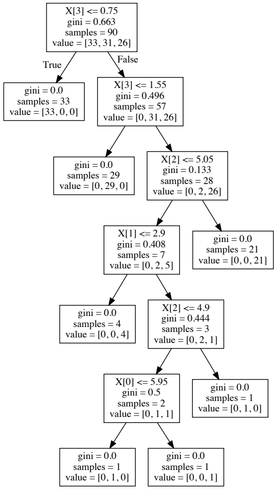
Interpretability

- The sequence of decisions is often easier to interpret than other methods (think of neural networks);
- However, sometimes small changes to the dataset cause big changes to the tree;
- If the optimal decision boundary is not aligned with the axes of an input variable, we need a lot of splits.


feature 2
A
B
feature 1


X[3] <= 0.75
gini = 0.663
samples = 90
value = [33, 31, 26]
True
False
gini = 0.0
samples = 33
value = [33, 0, 0]
X[3] <= 1.55
gini = 0.496
samples = 57
value = [0, 31, 26]
gini = 0.0
samples = 29
value = [0, 29, 0]
X[2] <= 5.05
gini = 0.133
samples = 28
value = [0, 2, 26]
X[1] <= 2.9
gini = 0.408
samples = 7
value = [0, 2, 5]
gini = 0.0
samples = 21
value = [0, 0, 21]
gini = 0.0
samples = 4
value = [0, 0, 4]
X[2] <= 4.9
gini = 0.444
samples = 3
value = [0, 2, 1]
X[0] <= 5.95
gini = 0.5
samples = 2
value = [0, 1, 1]
gini = 0.0
samples = 1
value = [0, 1, 0]
gini = 0.0
samples = 1
value = [0, 1, 0]
gini = 0.0
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