Lectures 5 & 6 Module 3. Decision Tree

COMP 551 Applied machine learning

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Outline

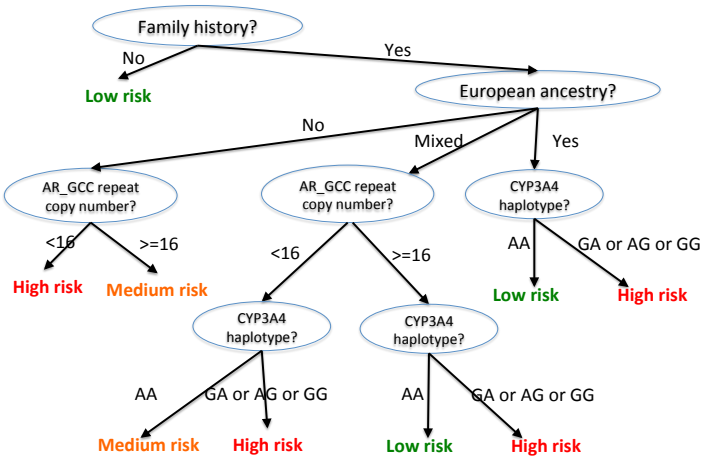
Learning objectives

Understanding the following concepts

- DT prediction
- Cost functions
- DT training algorithm
- Overfitting in DT

Outline

Decision Tree (DT) aka Classification And Regression Tree (CART)



A toy DT for diagnosing non-small cell lung cancer

Pros:

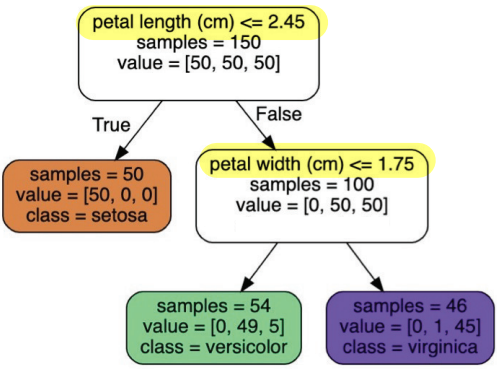
- Easy to interpret
- Handle mixed discrete and continuous inputs
- Insensitive to scaling
- Built-in variable selection
- Non-linear approach

Cons:

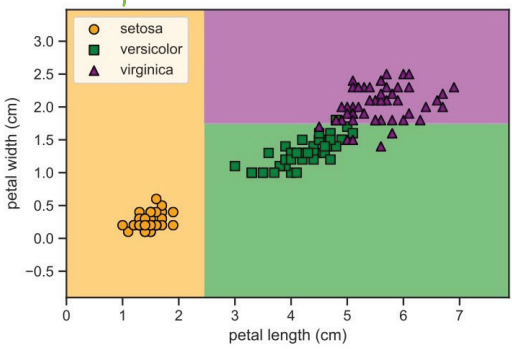
- Produce coarse grained probabilities especially at low tree depth
- Prone to overfitting at high tree depth

DT trained on Iris flower data for multi-class prediction

An example of classifying Iris flower using a classification tree (Murphy22 Figure 18.3):



* You can use the same feature multiple times



Notation review for general supervised learning problem

Our dataset $\mathcal{D}$ consists of N pairs of input vector and target variable:

$$\mathcal{D} = \{(\mathbf{x}^{(n)}, y^{(n)}\}_{n=1}^{N}$$

Target variable

- Classification: $y^{(n)} \in \{1, \ldots, C\}$
- Regression: $y^{(n)} \in \mathbb{R}$

Input features

- Continuous feature i: $x_i^{(n)} \in \mathbb{R}$
- Categorical feature j: $x_j^{(n)} \in \{1, \ldots, C_j\}$

One-hot-encoding

For computational convenience, we often represent the categorical variable using **one-hot encoding** by creating C_j binary input features from variable j (although this is not necessary for DT to work):

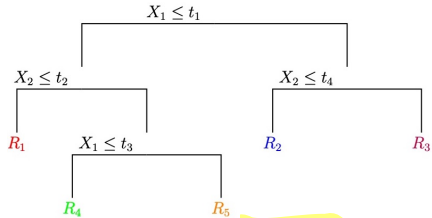
$$x_{j,1}^{(n)}, \ldots, x_{j,C_j}^{(n)} \in \{0, 1\}$$

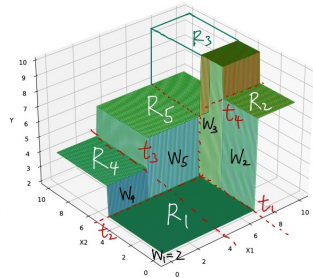
Data	Color
$x^{(1)}$	Red
$x^{(2)}$	Green
$x^{(3)}$	Blue

$\Rightarrow$

Variable	Red	Green	Blue
$x^{(1)}$	1	0	0
$x^{(2)}$	0	1	0
$x^{(3)}$	0	0	1

A simple illustration of a regression tree





- Divide the training data into 5 regions $R_k \in \{R_1, \ldots, R_5\}$ by the thresholds $t_1, \ldots, t_4$. For instance, $R_1 = \{\mathbf{x}_1 \le t_1, \mathbf{x}_2 \le t_2\}$.
- The height of a region (i.e., regression weight) is the *average* target values in region k:

$$w_k = \frac{\sum_{n=1}^{N} y^{(n)} \mathbb{I}[\mathbf{x}^{(n)} \in R_k]}{\sum_{n=1}^{N} \mathbb{I}[\mathbf{x}^{(n)} \in R_k]} = \frac{1}{N_k} \sum_{n \in \mathcal{S}_k} y^{(n)} \quad (\mathcal{S}_k \text{ is the set of data indices in Region } k)$$

- The predicted value of a new data point $\mathbf{x}^{(*)}$ is set to the weight of the region it belongs:

$$\hat{y}^{(*)} \equiv f(\mathbf{x}^{(*)}; \theta) = \sum_{k=1}^{K} w_k \mathbb{I}[\mathbf{x}^{(*)} \in R_k] \quad (\theta \text{ denotes the trained tree and its regression weights})$$

↳ belongs to region

Prediction per region in classification

Most frequent label in region k (i.e., the mode):

$$w_k = \arg\max_c \sum_{n \in \mathcal{S}_k} \mathbb{I}[y^{(n)} = c]$$

take class from highest training example

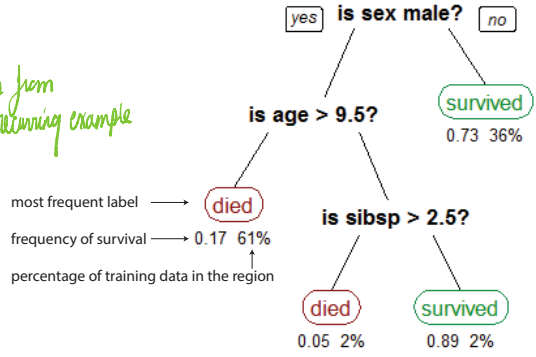
$$\hat{y}^{(*)} = \sum_{k=1}^{K} w_k \mathbb{I}[\mathbf{x}^{(*)} \in R_k]$$

Class probability in region k (i.e., proportion of class c in region k):

$$p(y = c | R_k) = \frac{1}{N_k} \sum_{n \in \mathcal{S}_k} \mathbb{I}[y^{(n)} = c] \equiv \pi_k(c)$$

frequency of survival

$$p(\hat{y}^{(*)} = c) = \sum_{k=1}^{K} \pi_k(c) \mathbb{I}(\mathbf{x}^{(*)} \in R_k)$$



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Survived is the positive label and death is the negative label in the above DT trained on the Titanic dataset.

Two main questions to be answered in this learning module

1. How to split data at each tree node?
   - How to evaluate quality of a split?
   - How to choose feature & threshold?
2. How to decide when to stop the tree from splitting?

1. Evaluate each split by a **cost function**
2. Choose feature and threshold that **minimize** the cost
3. Use a validation set to choose tree depth

Outline

A common cost function for regression is *Mean Squared Error (MSE)*

Our prediction on the training data points in region k is their average target values:

$$w_k = \frac{1}{N_k} \sum_{n \in \mathcal{S}_k} y^{(n)}$$

Note: each training data point falls in exactly one of the regions.
Sum of squared error (SSE) and Mean squared error per region k are:

$$\text{SSE}(R_k, \mathcal{D}; w_k) = \sum_{n \in \mathcal{S}_k} (y^{(n)} - w_k)^2, \quad \text{MSE}(R_k, \mathcal{D}; w_k) = \frac{1}{N_k} \text{SSE}(R_k, \mathcal{D}; w_k)$$

SSE and MSE over all K regions (i.e., all training data points) are:

$$SSE(\mathcal{D}; \theta) = \sum_{k=1}^{K} \text{SSE}(R_k, \mathcal{D}; w_k) = \sum_{k=1}^{K} \sum_{n \in \mathcal{S}_k} (y^{(n)} - w_k)^2, \quad MSE(\mathcal{D}; \theta) = \frac{1}{N} SSE(\mathcal{D}; \theta)$$

↳ sum of all regions

Measuring classification cost using *Misclassification Rate*

Most frequent label in region k (i.e., the mode):

$$w_k = \arg\max_c \sum_{n \in \mathcal{S}_k} \mathbb{I}[y^{(n)} = c]$$

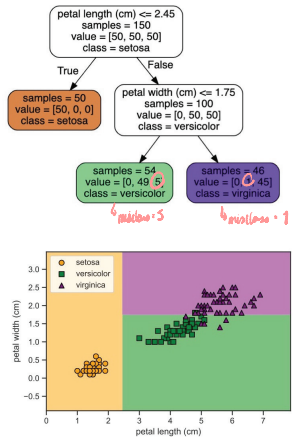
Cost per region k:

$$\text{cost}(R_k, \mathcal{D}; w_k) = \sum_{n \in \mathcal{S}_k} \mathbb{I}[y^{(n)} \neq w_k]$$

Total cost is the overall misclassification rate:

$$\text{total cost}(\mathcal{D}; \theta) = \sum_{k=1}^{K} \text{cost}(R_k, \mathcal{D}; w_k)$$

$$\text{misclassification rate} = \frac{1}{N} cost(\mathcal{D}; \theta)$$

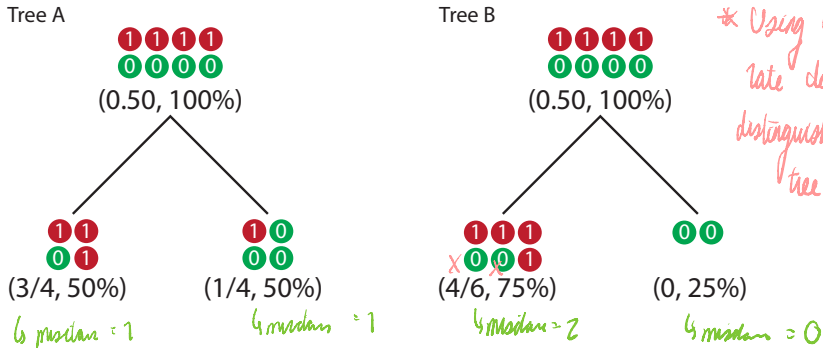


Pop quiz: what's training misclassifcation rate of the above DT?

Answer: $6/150 = 0.04$

Misclassification rate is not sensitive enough

The total misclassification rates are the same for these two trees but the classification cost at each leaf node is different:



$$cost(\mathcal{D}; \theta) = \frac{1}{N} \sum_{k=1}^{K} \sum_{n \in \mathcal{S}_k} \mathbb{I}[y^{(n)} \neq w_k] = 2/8 = 0.25$$

Idea: we need a more sensitive measure of the **model uncertainties** in each region.

Entropy: a measure of uncertainty (the lower the better)

Entropy is the expected amount of information in observing a random variable y:

$$H(y) = -\sum_{c=1}^{C} p(y=c)\log_2 p(y=c)$$

The *less* certain the *higher* the entropy. For example,

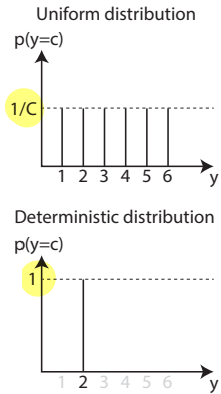
- Uniform distribution where $p(y=c) = \frac{1}{C} \forall c$ has the highest entropy:

$$H(y) = -\sum_{c=1}^{C} \frac{1}{C}\log_2(\frac{1}{C}) = \log_2(C)$$

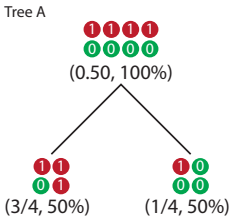
$= -\log_2(C)$

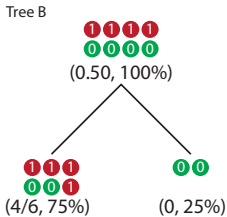
- When $p(y=c) = 1$ and $p(y=c') = 0 \, \forall c' \neq c$ the entropy is the lowest:

$$H(y) = -\log_2(1) = 0$$



Entropy for classification cost





$$H(y;R) = -\sum_c p(y=c;R)\log_2 p(y=c;R)$$

$$= -p(y=0;R)\log_2 p(y=0;R) \quad c=0$$
$$- p(y=1;R)\log_2 p(y=1;R) \quad c=1$$

Tree A

$$H(y;R_{left}) = -\frac{1}{4}\log_2(\frac{1}{4}) - \frac{3}{4}\log_2(\frac{3}{4}) \approx 0.81$$

$$H(y;R_{right}) = -\frac{3}{4}\log_2\frac{3}{4} - \frac{1}{4}\log_2\frac{1}{4} \approx 0.81$$

$$\text{Mean Cost} = \frac{4}{8}H(y;R_{left}) + \frac{4}{8}H(y;R_{right}) = 0.81$$

Tree B

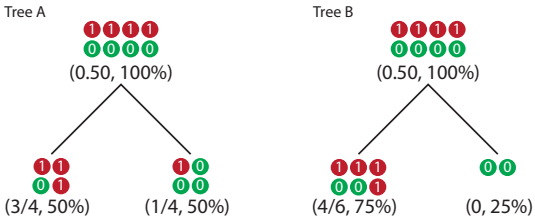
$$H(y;R_{left}) = -\frac{2}{6}\log_2(\frac{2}{6}) - \frac{4}{6}\log_2(\frac{4}{6}) \approx 0.92$$

$$H(y;R_{right}) = -1\log_2 1 - 0 \approx 0$$

$$\text{Mean Cost} = \frac{6}{8}H(y;R_{left}) + \frac{2}{8}H(y;R_{right}) = \mathbf{0.69}$$

Tree B has lower cost than Tree A.

Entropy for classification cost



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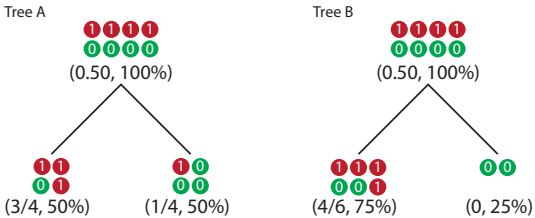
Entropy for classification cost



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$$H(y; R_{right}) = -\frac{3}{4} \log_2 \frac{3}{4} - \frac{1}{4} \log_2 \frac{1}{4} \approx 0.81$$

$$\text{Mean Cost} = \frac{4}{8} H(y; R_{left}) + \frac{4}{8} H(y; R_{right}) = 0.81$$

Tree B

$$H(y; R_{left}) = -\frac{2}{6} \log_2(\frac{2}{6}) - \frac{4}{6} \log_2(\frac{4}{6}) \approx 0.92$$

$$H(y; R_{right}) = -1 \log_2 1 - 0 \approx 0$$

$$\text{Mean Cost} = \frac{6}{8} H(y; R_{left}) + \frac{2}{8} H(y; R_{right}) = \mathbf{0.69}$$

* The lower the mean cost, the lower the entropy
⇒ better efficiency

Tree B has lower cost than Tree A.

Resume here in Lec 6 (Jan 24)

Gini Index (GI): the default cost in DT (the lower the better)

$$p(y = c; R_k) = \frac{1}{N_k} \sum_{n \in \mathcal{S}_k} \mathbb{I}(y^{(n)} = c) \equiv \pi_k(c)$$

$$GI(R_k) = \sum_{c=1}^{C} \pi_k(c)(1 - \pi_k(c)) = \sum_{c=1}^{C} \pi_k(c) - \sum_{c=1}^{C} \pi_k(c)^2 = 1 - \sum_{c=1}^{C} \pi_k(c)^2$$

$$GI = \frac{1}{N} \sum_{k=1}^{K} N_k GI(R_k)$$

* The lower the variance, the more certain the model is

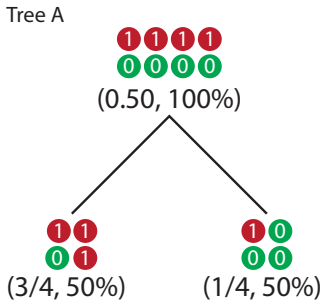
- In theory, $\pi_k(c)(1 - \pi_k(c))$ is the *variance* of the Bernoulli distribution for the Boolean indicator $\mathbb{I}[y = c]$ in region k with rate $\pi_k(c)$ for each class c:

$$y \sim (\pi_k(c))^{\mathbb{I}[y=c]} (1 - \pi_k(c))^{\mathbb{I}[y \neq c]}$$

- Therefore, $\sum_c \pi_k(c)(1 - \pi_k(c))$ measures *the sum of variances* over all classes.
- Therefore, minimizing GI is equivalent to minimizing the expected variance.
- For a "pure" region, where all data points in the region belong to a single class c, $p(y = c; R_k) = 1$ and $p(y = c'; R_k) = 0$ for $c' \neq c$, $GI(R_k) = 0$.

* Cannot further split to improve prediction

Compute GI for the two example trees

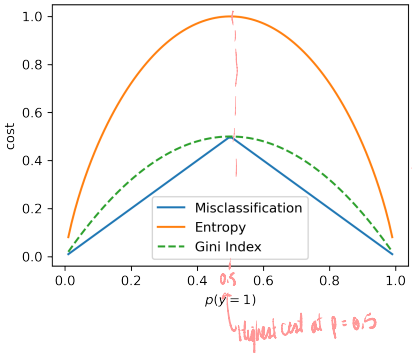


*GI & Entropy will usually give you the same results

$$GI(y; R_{A,left}) = 1 - (0.25^2 + 0.75^2) = 0.375$$
$$GI(y; R_{A,right}) = 1 - (0.75^2 + 0.25^2) = 0.375$$
$$GI(y; TreeA) = \frac{4}{8} GI(y; R_{left}) + \frac{4}{8} GI(y; R_{right}) = 0.375$$

$$GI(y; R_{B,left}) = 1 - ((\frac{2}{6})^2 + (\frac{4}{6})^2) = 0.44$$
$$GI(y; R_{B,right}) = 1 - (1 + 0) = 0$$
$$GI(y; TreeB) = \frac{6}{8} GI(y; R_{left}) + 0 = \mathbf{0.33}$$

Analysis of the 3 *training* cost functions in binary classification (Colab)



Two-class cost as the function $p(y=1) \equiv p$:

$$\text{misclas. rate} = 1 - \max(p, 1-p) = \min(p, 1-p)$$

$$\textit{entropy} = -p\log_2(p) - (1-p)\log_2(1-p)$$

$$\textit{gini index} = p(1-p) + (1-p)p = 2p(1-p)$$

Comments:

- In binary classification, the lower class proportion is the misclassification rate
- We compute gini index each class. In binary classification, the two gini indices are the same.

- All 3 cost functions quantify the "impurity" of a tree node.
- Training a DT involves minimizing one of the cost functions.
- Entropy and Gini Index behave similarly and are usually better choice than misclassification rate as a training cost function because they take into account *the prediction uncertainties* by using prediction probabilities in each leaf node.

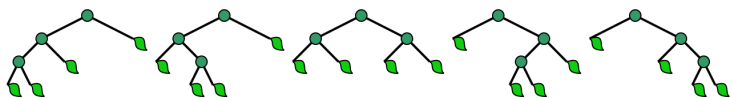
Outline

Combinatorial search space of all possible trees

- **Objective**: find the optimal DT that minimizes the training cost.
- The number of all possible topologies of *full* binary trees with T tests (i.e., T non-leaf nodes) follows the Catalan sequence, where the T^{th} Catalan number is

$$C_T = \frac{1}{T+1}\binom{2T}{T} = \frac{(2T)!}{(T+1)(2T-T)!\,T!} = \frac{(2T)!}{(T+1)!\,T!}$$

For 3 tests, for instance, there are 5 full binary trees to choose from:



- The number of trees grows quite fast as we increase the number of tests. Starting with $T = 0$, the first 12 numbers in the Catalan sequence are: 1, 1, 2, 5, 14, 42, 132, 429, 1430, 4862, 16796, 58786.
- It turns out finding the optimal decision tree is an **NP-hard** combinatorial optimization problem (NP stands for Nondeterministic Polynomial).

Peudocode for greedy heuristic search at each tree node (See Colab)

Algorithm 1 greedy_test(node)

```
1:  min_cost = cost(node.y) // (better than min_cost = ∞
2:  best_feature_index = best_feature_thres = NULL
3:  for each feature d ∈ {1, ..., D} do
4:      for each threshold t ∈ T_d for feature d do // Tests for all unique values of feature d
5:          cost_left = cost(node.y[node.X[:, d] ≤ t])
6:          cost_right = cost(node.y[node.X[:, d] > t])
7:          cost_d = (N_left / N) cost_left + (N_right / N) cost_right
8:          if cost_d < min_cost then
9:              min_cost = cost_d;
10:             best_feature_index = d;
11:             best_feature_thres = threshold
12:         end if
13:     end for
14: end for
15: return min_cost, best_feature_index, best_feature_thres
```

D T N

N: # training examples
D: # features
T: # threshold per feature

Time complexity? O(DTN)

↳ this is only for 1 node

* for continuous data set → take all unique values

Recursively find the best feature and threshold at every node (Colab)

Algorithm 2 `_fit_tree`(node, max_depth, min_leaf_instance)

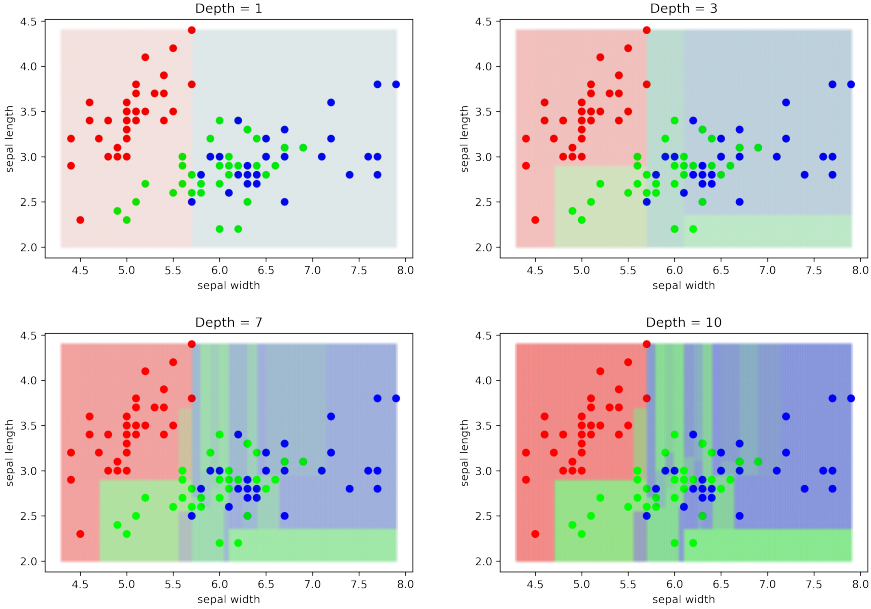
```
1: if node.depth ≤ max_depth and node.X.shape[0] > min_leaf_instance and
   cost(node.y[node.data_indices]) > 0 then
2:     split_cost, split_feat, split_value = greedy_test(node)
3:     node.split_feature = split_feat
4:     node.split_value = split_value
5:     test_logicals = node.X[node.data_indices, split_feat] <= split_value
6:     left_node = Node(data_indices=node.data_indices[test_logical], parent=node)
7:     right_node = Node(data_indices=node.data_indices[!test_logical], parent=node)
8:     _fit_tree(left_node, max_depth, min_leaf_instance)
9:     _fit_tree(right_node, max_depth, min_leaf_instance)
10:    node.left = left_node
11:    node.right = right_node
12: end if
```

Algorithm 3 fit(tree, max_depth, min_leaf_instance=1)

```
1: _fit_tree(tree.root, max_depth, min_leaf_instance)
```

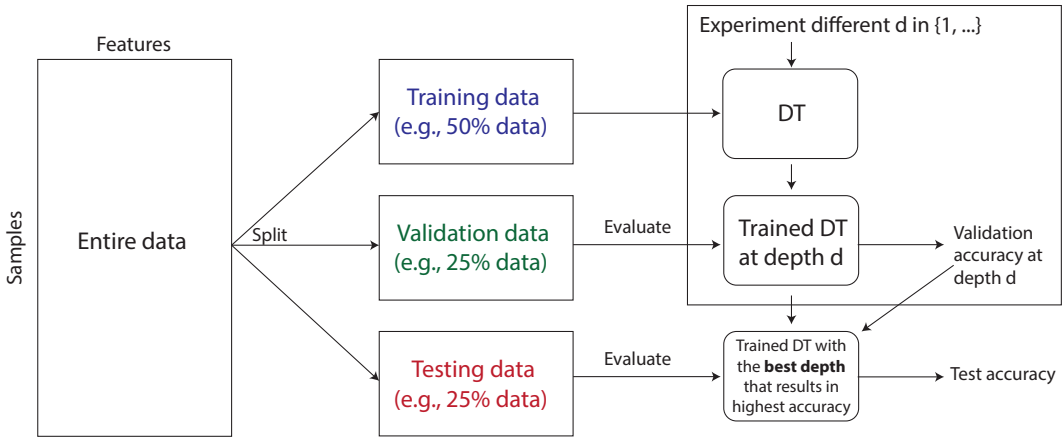
Outline

How to choose maximum tree depth (the hyperparameter for DT)?

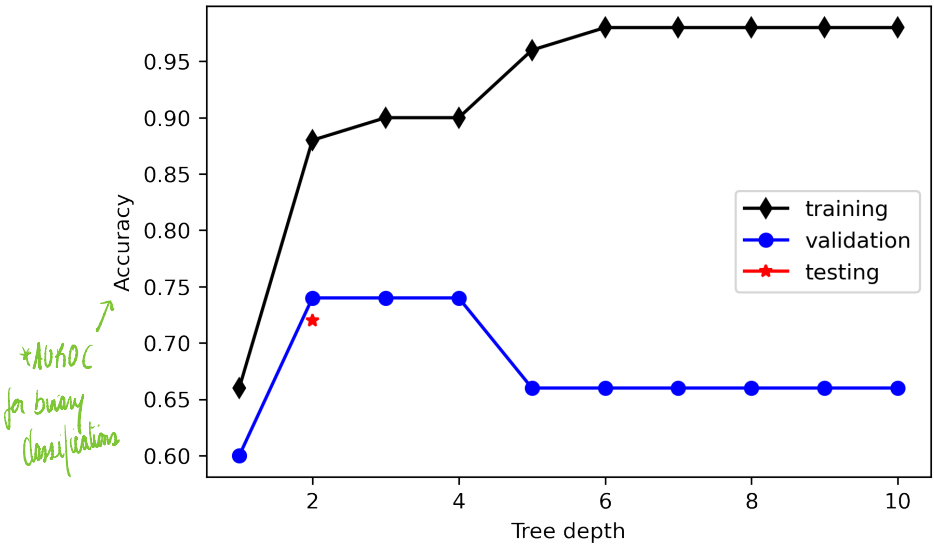


* The more depth, the more decision regions there is going to be

Choose tree depth using a validation set (same as choosing K in KNN)



Choose optimal tree depth using a validation set (Colab)



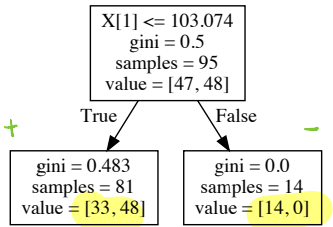
Outline

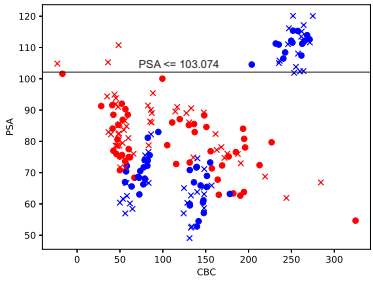
Decision tree using Scikit-Learn

```
1  from sklearn import model_selection,tree
2  import graphviz
3  for depth in range(1,6):
4      dt = tree.DecisionTreeClassifier(max_depth=depth) ← how
5      dt.fit(X_train, y_train)
6      p_train = dt.predict(X_train)
7      p_test = dt.predict(X_test)
8      #plot tree
9      dot_data = tree.export_graphviz(dt, out_file=None)
10     graph = graphviz.Source(dot_data)
11     graph.render("prostate_tree_depth_"+str(depth))
```

Note: Line 9-11 requires installing graphviz: `pip install graphviz`

Decision tree (max_depth = 1)





Training data:

	PN	PP
AN	14	33
AP	0	48

TPR = $48/(48+0) = 1.0$
FPR = $33/(33+14) = 0.7$

Test data:

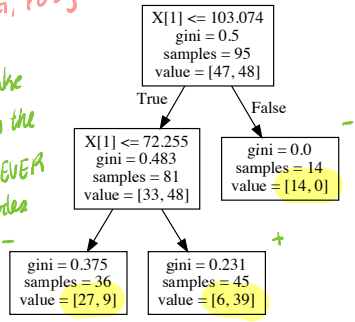
	PN	PP
AN	13	30
AP	3	49

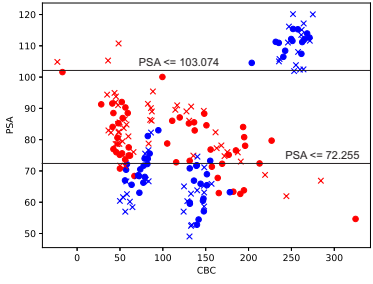
TPR = $49/(49+3) = 0.94$
FPR = $30/(30+13) = 0.7$

Decision tree (max_depth = 2)

[NEG, POS]

* We only make predictions in the leaf nodes, NEVER in internal nodes





Training data:

	PN	PP
AN	41	6
AP	9	39

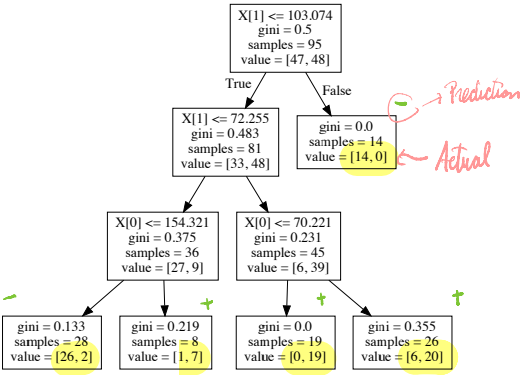
TPR = 39/(39+9) = 0.81
FPR = 6/(6+41) = 0.13

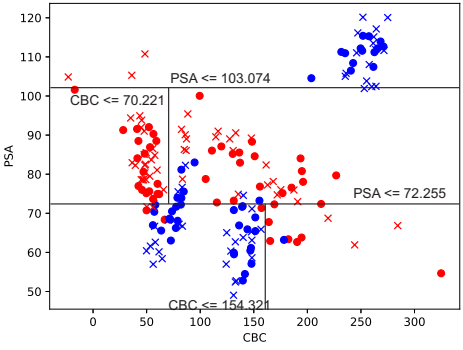
Test data:

	PN	PP
AN	36	7
AP	8	44

TPR = 44/(44+8) = 0.85
FPR = 7/(7+36) = 0.16

Decision tree (max_depth = 3)





* Depending on the thresholds, we will have different TPR and FPR

Training data:

	PN	PP
AN	40	7
AP	2	46

TPR = 46/(46+2) = 0.96
FPR = 7/(7+40) = 0.15

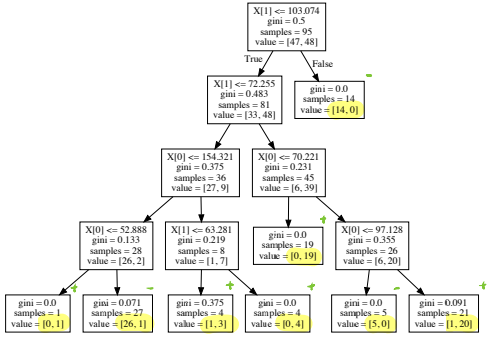
Compute this in midterm (tree will be given)

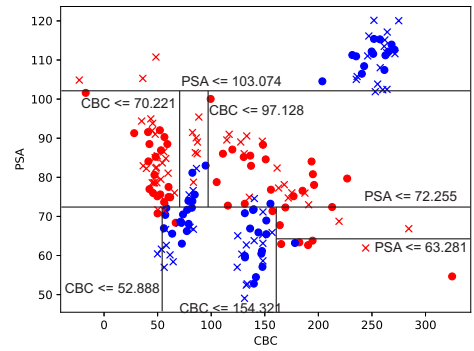
Test data:

	PN	PP
AN	35	8
AP	5	47

TPR = 47/(47+5) = 0.9
FPR = 8/(8+35) = 0.19

Decision tree (max_depth = 4) - overfitting occurs





Training data:

	PN	PP
AN	45	2
AP	1	47

TPR = 47/(47+1) = 0.98
FPR = 2/(2+45) = 0.04

// this is pretty good

Test data:

	PN	PP
AN	37	6
AP	11	41

TPR = 41/(41+11) = 0.79
FPR = 6/(6+37) = 0.14

Decision tree (max_depth = 5 & 6) - more overfitting

Tree depth = 5

Training data:

	PN	PP
AN	46	1
AP	1	47

TPR = 47/(47+1) = 0.98
FPR = 1/(1+46) = 0.02

Test data:

	PN	PP
AN	37	6
AP	11	41

TPR = 41/(41+11) = 0.79
FPR = 6/(6+37) = 0.14

Tree depth = 6

Training data:

	PN	PP
AN	47	0
AP	0	48

TPR = 48/(48+0) = 1.0
FPR = 0/(0+47) = 0.0

Test data:

	PN	PP
AN	37	6
AP	11	41

TPR = 41/(41+11) = 0.79
FPR = 6/(6+37) = 0.14

Outline

Feature importance

- Reduction of the cost (e.g., Gini index) due to the split at node $j \in \{1, \ldots, J\}$:

$$\Delta g_j = \frac{N_j}{N} \times g_j - \frac{N_j^{(left)}}{N} g_j^{(\text{left})} - \frac{N_j^{(right)}}{N} g_j^{(\text{right})}$$

this needs to be reduced to select features

Gini index

where $\frac{N_j}{N}$ is the fraction of samples in node j and g_j is the cost at node j; $\frac{N_j^{(left)}}{N}$ and $\frac{N_j^{(right)}}{N}$ are fractions of samples in the left and right child of node j; $g_j^{(\text{left})}$ and $g_j^{(\text{right})}$ are cost in the left and right child of node j.

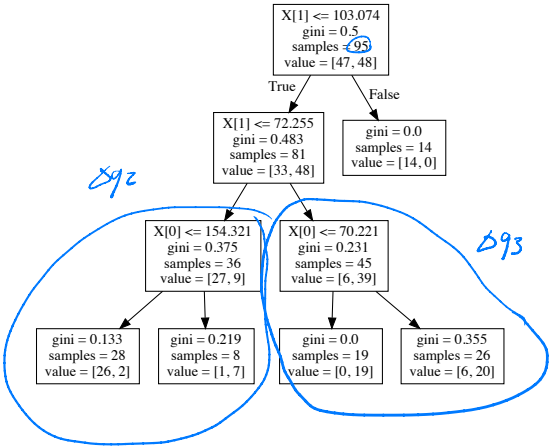
- The feature importance of feature $d \in \{1, \ldots, D\}$ is the total reduction over all the J non-leaf nodes, where feature d is used:

$$r_d = \sum_{j=1}^{J} \Delta g_j \mathbb{I}[v_j = d]$$

where $\mathbb{I}[v_j = d]$ indicates feature d is used in node j. The formula for computing feature importance as one of the optional tasks in Assignment 1 has been updated.

Example: feature importance of x_0 in DT at depth 3

← We're now looking at the internal nodes (it's where you perform the training tests)



- Gini reduction at node 2 (level 3 left node):

$$\Delta g_2 = \frac{36}{95}0.375 - \frac{28}{95}0.133 - \frac{8}{95}0.219 = 0.0844$$

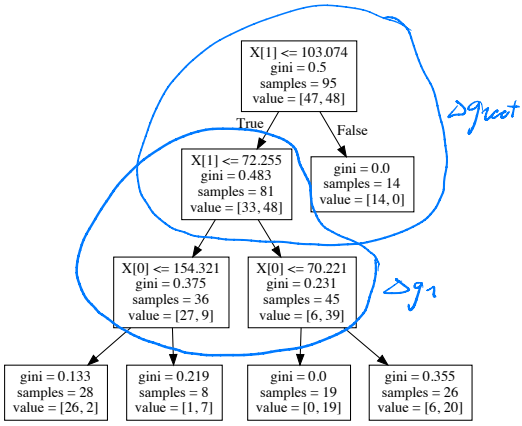
- Gini reduction at node 3 (level 3 right node):

$$\Delta g_3 = \frac{45}{95}0.231 - \frac{19}{95}0 - \frac{26}{95}0.355 = 0.0123$$

- Feature importance of x_0:

$$r_0 = \Delta g_2 + \Delta g_3 = 0.0844 + 0.0123 = \mathbf{0.0967}$$

Example: feature importance of x_1 in DT at depth 3



- Gini reduction at root due to x_1:

$$\Delta g_{root} = \frac{95}{95}0.5 - \frac{81}{95}0.483 - \frac{14}{95}0 = 0.0881$$

- Gini reduction at node 1 (i.e., left child of root) also due to x_1:

$$\Delta g_1 = \frac{81}{95}0.483 - \frac{36}{95}0.375 - \frac{45}{95}0.231 = 0.160$$

- Feature importance of x_1:

$$r_1 = \Delta g_{root} + \Delta g_1 = 0.0881 + 0.160 = \mathbf{0.2481}$$

Therefore, x_1 has more than 2.5 times higher feature importance score than x_0 ($0.2481/0.0967 = 2.566$).

Outline

Summary of DT

- Costs: Misclassification rate, Entropy, Gini index
- DT is a greedy and recursive algorithm that finds the best feature and the best threshold at each tree node to minimize the loss (e.g., Gini index) within the node.
- Compared to KNN, robust to scaling and noise, fast predictions, more interpretable
- Overfitting occurs when the model gets too complicated (i.e., high tree depth in the case of DT) and fits extremely well on the training data but generalizes poorly to the test data.
- Feature importance score derived from a trained DT can be used to rank features.
- DT is the building block of common ensemble learning methods such as Random Forest and XGBoost (Module 6)