

Decision Tree

Random Forest

Decision Tree Example

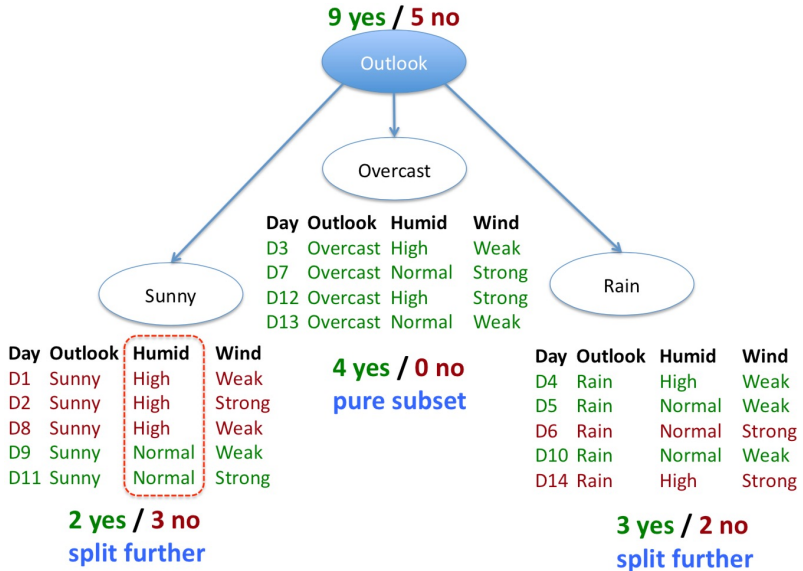
Training examples: 9 yes / 5 no

Day	Outlook	Humidity	Wind	Play
D1	Sunny	High	Weak	No
D2	Sunny	High	Strong	No
D3	Overcast	High	Weak	Yes
D4	Rain	High	Weak	Yes
D5	Rain	Normal	Weak	Yes
D6	Rain	Normal	Strong	No
D7	Overcast	Normal	Strong	Yes
D8	Sunny	High	Weak	No
D9	Sunny	Normal	Weak	Yes
D10	Rain	Normal	Weak	Yes
D11	Sunny	Normal	Strong	Yes
D12	Overcast	High	Strong	Yes
D13	Overcast	Normal	Weak	Yes
D14	Rain	High	Strong	No

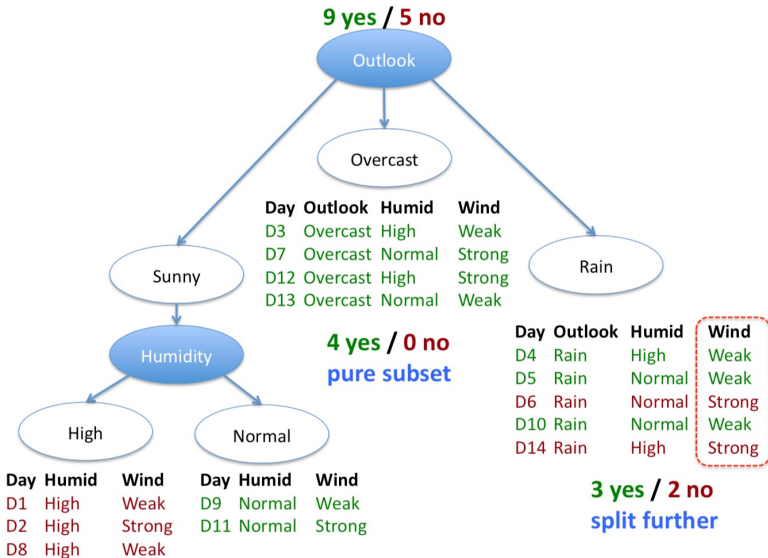
New data:

D15	Rain	High	Weak	?
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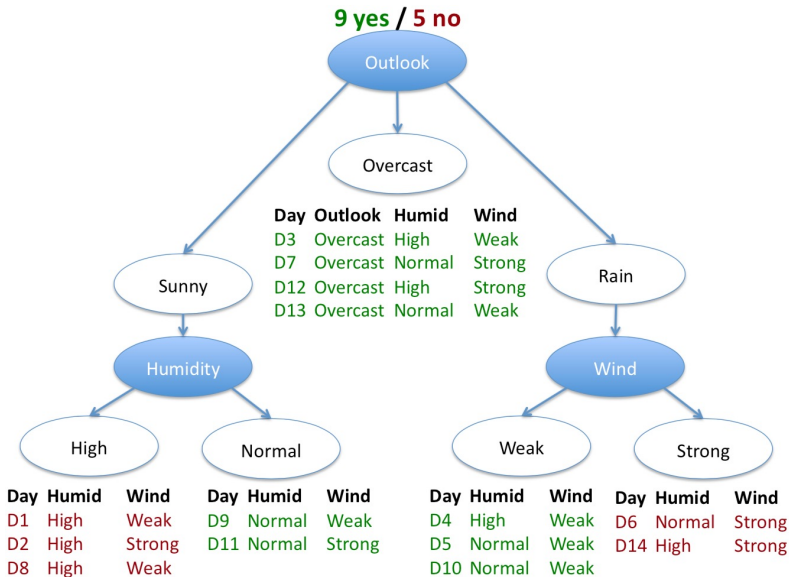
Decision Tree Example



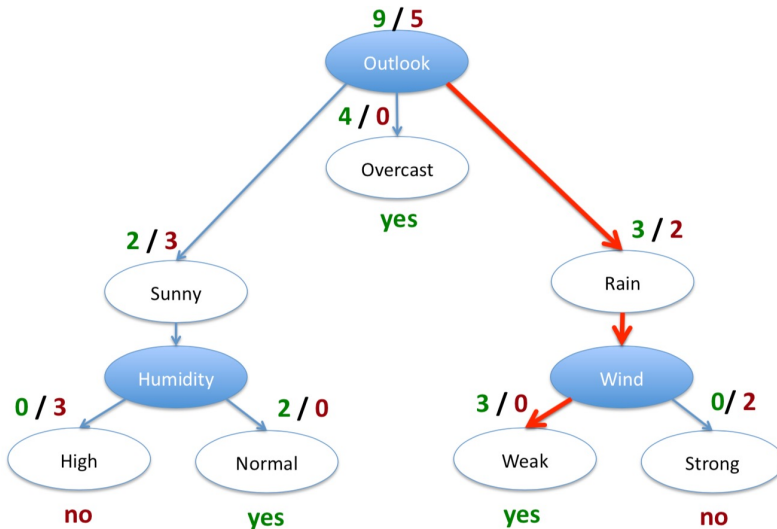
Decision Tree Example



Decision Tree Example



Decision Tree Example



New data:

Day	Outlook	Humid	Wind
D15	Rain	High	Weak

→ Yes

ID3 Algorithm

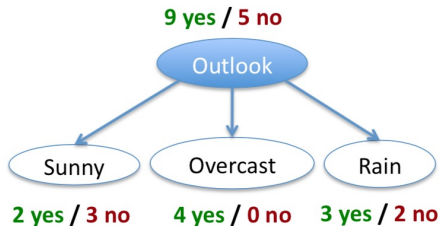
node = Root

examples = Training Set

Split (**node**, {**examples**}):

1. Find A, the **best attribute** for splitting the {**examples**}
2. Create decision nodes for attribute A (i.e., **child nodes** of **node**)
3. Split training {**examples**} to **child nodes**
4. If examples perfectly classified (subset is pure): STOP
else: iterate over new child nodes
 Split (**child_node**, {**subset of examples**})

Find The Best Attribute



- Want to measure “purity” of the split
 - more certain about Yes/No after the split
 - pure set (4 yes / 0 no) => completely certain (100%)
 - impure (3 yes / 3 no) => completely uncertain (50%)
 - can’t use $P(\text{“yes”} \mid \text{set})$:
 - must be symmetric: 4 yes / 0 no as pure as 0 yes / 4 no

Entropy

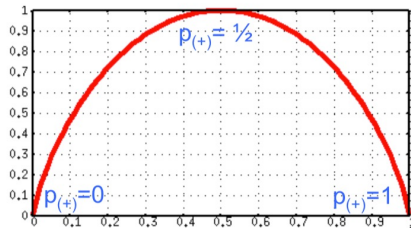
- Entropy: $H(S) = - p_{(+)} \log_2 p_{(+)} - p_{(-)} \log_2 p_{(-)}$ bits
 - S ... subset of training examples
 - $p_{(+)} / p_{(-)}$... % of positive / negative examples in S
- Interpretation: assume item X belongs to S
 - how many bits need to tell if X positive or negative

- impure (3 yes / 3 no):

$$H(S) = -\frac{3}{6} \log_2 \frac{3}{6} - \frac{3}{6} \log_2 \frac{3}{6} = 1 \text{ bits}$$

- pure set (4 yes / 0 no):

$$H(S) = -\frac{4}{4} \log_2 \frac{4}{4} - \frac{0}{4} \log_2 \frac{0}{4} = 0 \text{ bits}$$



Information Gain

- Want many items in pure sets
- Expected drop in entropy after split:

$$Gain(S, A) = H(S) - \sum_{V \in \text{Values}(A)} \frac{|S_V|}{|S|} H(S_V)$$

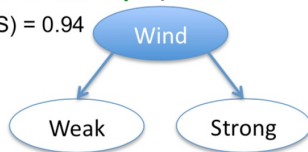
V ... possible values of A
 S ... set of examples $\{X\}$
 S_V ... subset where $X_A = V$

- Mutual Information
 - between attribute A and class labels of S

$$\begin{aligned} \text{Gain}(S, \text{Wind}) &= H(S) - \frac{8}{14} H(S_{\text{weak}}) - \frac{6}{14} H(S_{\text{strong}}) \\ &= 0.94 - \frac{8}{14} * 0.81 - \frac{6}{14} * 1.0 \\ &= 0.049 \end{aligned}$$

$$-\frac{9}{14} \log_2 \frac{9}{14} - \frac{5}{14} \log_2 \frac{5}{14} \quad \mathbf{9 \text{ yes} / 5 \text{ no}}$$

$$H(S) = 0.94$$



$$-\frac{6}{8} \log_2 \frac{6}{8} - \frac{2}{8} \log_2 \frac{2}{8}$$

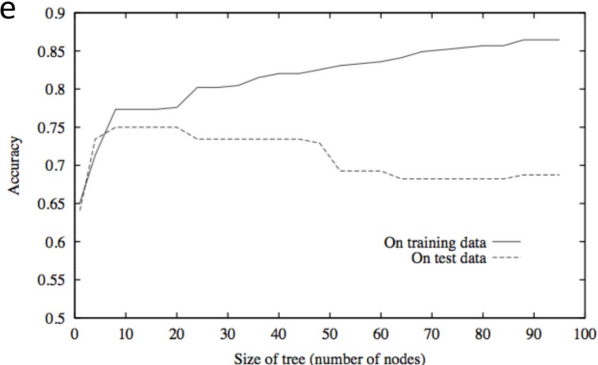
$$H(S_{\text{weak}}) = 0.81$$

$$-\frac{3}{6} \log_2 \frac{3}{6} - \frac{3}{6} \log_2 \frac{3}{6}$$

$$H(S_{\text{strong}}) = 1.0$$

Overfitting in Decision Tree

- Can always classify training examples perfectly
 - keep splitting until each node contains 1 example
 - singleton = pure
- Doesn't work on new data



Avoid Overfitting

How can we avoid overfitting?

- Stop growing when data split is not statistically significant.
- Acquire more training data.
- Remove irrelevant attributes (manual process – not always possible)
- Grow full tree, then post-prune.

How to select “best” tree:

- Measure performance over training data
- Measure performance over separate validation data set
- Add complexity penalty to performance measure

Pre-pruning that stop growing the tree earlier, before it perfectly classifies the training set.

Post-pruning that allows the tree to perfectly classify the training set, and then post prune the tree.

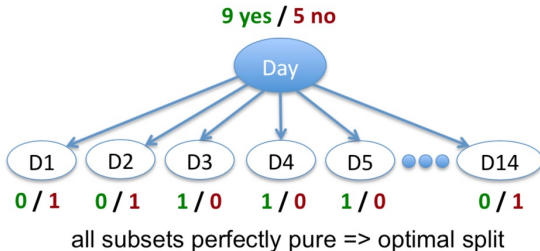
General Structure

Task: classification, discriminative

- Model structure: decision tree
- Score function
 - Information gain at each node
 - Preference for short trees
 - Preference for high-gain attributes near the root
- Optimization / search method
 - Greedy search from simple to complex
 - Guided by information gain

Problem With Information Gain

- Biased towards attributes with many values
- Won't work for new data: D15 Rain High Weak
- Use GainRatio:



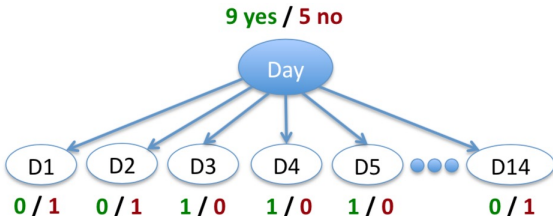
$$SplitEntropy(S, A) = - \sum_{V \in Values(A)} \frac{|S_V|}{|S|} \log \frac{|S_V|}{|S|}$$

A ... candidate attribute
V ... possible values of A
S ... set of examples {X}
 S_V ... subset where $X_A = V$

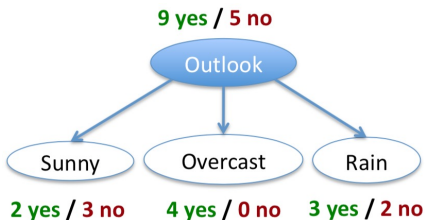
$$GainRatio(S, A) = \frac{Gain(S, A)}{SplitEntropy(S, A)}$$

penalizes attributes
with many values

Problem With Information Gain



$$\begin{aligned} \text{SplitEntropy}(S, \text{Day}) \\ = -14 \left(\frac{1}{14} \log \frac{1}{14} \right) = 3.80 \end{aligned}$$



$$\begin{aligned} \text{SplitEntropy}(S, \text{Outlook}) \\ = -\frac{5}{14} \log \frac{5}{14} - \frac{4}{14} \log \frac{4}{14} - \frac{5}{14} \log \frac{5}{14} = 1.57 \end{aligned}$$

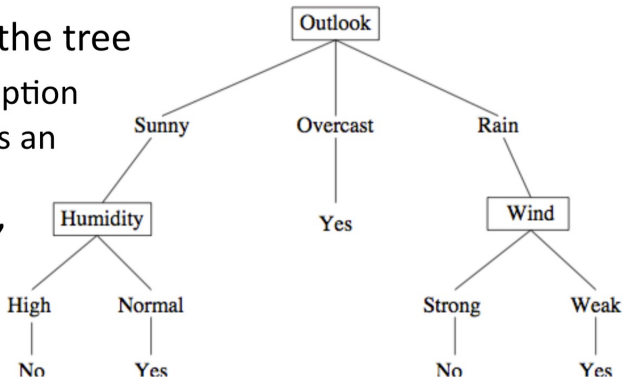
Interpretation of Trees

- Read rules off the tree

- concise description of what makes an item positive

- No “black box”

- important for users

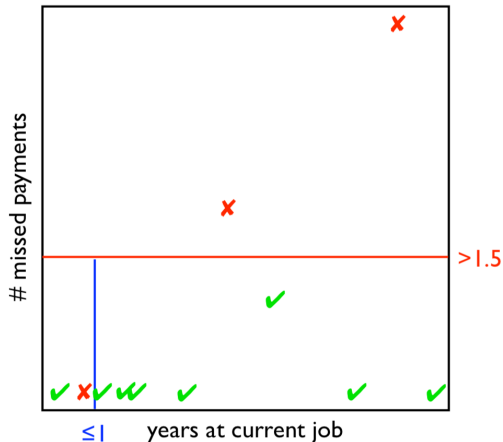


Rule: $(\text{Outlook} = \text{Overcast}) \vee$
 $(\text{Outlook} = \text{Rain} \wedge \text{Wind} = \text{Weak}) \vee$
 $(\text{Outlook} = \text{Sunny} \wedge \text{Humidity} = \text{Normal})$

Continuous Variables

Predicting credit risk

years at current job	# missed payments	defaulted?
7	0	N
0.75	0	Y
3	0	N
9	0	N
4	2	Y
0.25	0	N
5	1	N
8	4	Y
1.0	0	N
1.75	0	N



Continuous Variables

Outlook	Temp	Humidity	Windy	Play
Sunny	85	85	False	No
Sunny	80	90	True	No
Overcast	83	78	False	Yes
Rainy	70	96	False	Yes
Rainy	68	80	False	Yes
Rainy	65	70	True	No
Overcast	64	65	True	Yes
Sunny	72	95	False	No
Sunny	69	70	False	Yes
Rainy	75	80	False	Yes
Sunny	75	70	True	Yes
Overcast	72	90	True	Yes
Overcast	81	75	False	Yes
Rainy	71	80	True	No

Continuous Temperature Attribute

- First, sort the temperature values, including the class labels
- Then, check all the cut points and choose the one with the best information gain.

64	65	68	69	70	71	72	72	75	75	80	81	83	85
Yes	No	Yes	Yes	Yes	No	No	Yes	Yes	Yes	No	Yes	Yes	No

- $Temp < 71.5$: yes = 4, no = 2
- $Temp \geq 71.5$: yes = 5, no = 3

How to compute:

- $H(Temp < 71.5) = ?$
- $H(Temp \geq 71.5) = ?$
- $H(S) = ?$
- $Gain(S, Temp) = ?$

Continuous Temperature Attribute

64	65	68	69	70	71	72	72	75	75	80	81	83	85
Yes	No	Yes	Yes	Yes	No	No	Yes	Yes	Yes	No	Yes	Yes	No

Temp < 71.5: yes = 4, no = 2

Temp ≥ 71.5: yes = 5, no = 3

$$H(Temp < 71.5) = -\frac{4}{6}\log\frac{4}{6} - \frac{2}{6}\log\frac{2}{6} = 0.918$$

$$H(Temp \geq 71.5) = -\frac{5}{8}\log\frac{5}{8} - \frac{3}{8}\log\frac{3}{8} = 0.954$$

$$H(S) = -\frac{9}{14}\log\frac{9}{14} - \frac{5}{14}\log\frac{5}{14} = 0.940$$

$$\begin{aligned} Gain(S, Temp) &= H(S) - \frac{6}{14}H(Temp < 71.5) - \frac{8}{14}H(Temp \geq 71.5) \\ &= 0.940 - \frac{6}{14} * 0.918 - \frac{8}{14} * 0.954 = 0.001 \end{aligned}$$

Continuous Temperature Attribute

- First, sort the temperature values, including the class labels
- Then, check all the cut points and choose the one with the best information gain.

64	65	68	69	70	71	72	72	75	75	80	81	83	85
Yes	No	Yes	Yes	Yes	No	No	Yes	Yes	Yes	No	Yes	Yes	No

- $\text{Temp} < 71.5$: yes = 4, no = 2
- $\text{Temp} \geq 71.5$: yes = 5, no = 3
- Place split points **halfway** between values.
- Able to evaluate all split points in **one pass**.

Information Gain for Humidity

Humidity	Play
65	Yes
70	No
70	Yes
70	Yes
75	Yes
78	Yes
80	Yes
80	Yes
80	No
85	No
90	No
90	Yes
95	No
96	Yes

sort the
attribute
values



Humidity	Play
65	Yes
70	No
70	Yes
70	Yes
75	Yes
78	Yes
80	Yes
80	Yes
<hr/>	
80	No
85	No
90	No
90	Yes
95	No
96	Yes

compute the gain for
every possible split

what is the information
gain if we split here?

Information Gain for Humidity

Humidity	Play	# of Yes	% of Yes	# of No	% of No	Weight	Entropy Left	# of Yes	% of Yes	# of No	% of No	Weight	Entropy Right	Information Gain
65	Yes	1	100.00%	0	0.00%	7.14%	0.00	8.00	0.62	5.00	0.38	92.86%	0.96	0.0477
70	No	1	50.00%	1	50.00%	14.29%	1.00	8.00	0.67	4.00	0.33	85.71%	0.92	0.0103
70	Yes	2	66.67%	1	33.33%	21.43%	0.92	7.00	0.64	4.00	0.36	78.57%	0.95	0.0005
70	Yes	3	75.00%	1	25.00%	28.57%	0.81	6.00	0.60	4.00	0.40	71.43%	0.97	0.0150
75	Yes	4	80.00%	1	20.00%	35.71%	0.72	5.00	0.56	4.00	0.44	64.29%	0.99	0.0453
78	Yes	5	83.33%	1	16.67%	42.86%	0.65	4.00	0.50	4.00	0.50	57.14%	1.00	0.0903
80	Yes	6	85.71%	1	14.29%	50.00%	0.59	3.00	0.43	4.00	0.57	50.00%	0.99	0.1518
80	Yes	7	87.50%	1	12.50%	57.14%	0.54	2.00	0.33	4.00	0.67	42.86%	0.92	0.2361
80	No	7	77.78%	2	22.22%	64.29%	0.76	2.00	0.40	3.00	0.60	35.71%	0.97	0.1022
85	No	7	70.00%	3	30.00%	71.43%	0.88	2.00	0.50	2.00	0.50	28.57%	1.00	0.0251
90	No	7	63.64%	4	36.36%	78.57%	0.95	2.00	0.67	1.00	0.33	21.43%	0.92	0.0005
90	Yes	8	66.67%	4	33.33%	85.71%	0.92	1.00	0.50	1.00	0.50	14.29%	1.00	0.0103
95	No	8	61.54%	5	38.46%	92.86%	0.96	1.00	1.00	0.00	0.00	7.14%	0.00	0.0477
96	Yes	9	64.29%	5	35.71%	100.00%	0.94	0.00	0.00	0.00	0.00	0.00%	0.00	0.0000

Left branch, e.g., < 67.5

Right branch, e.g., ≥ 67.5

Multi-class Classification

Multiclass classification:

- Predict the **best attribute** to split on.
- Entropy:

$$H(S) = - \sum_c p_c \log_2(p_c).$$

- p_c : % of examples of class **c** in S.

Random (Decision) Forest

Training: grow **K** different decision trees:

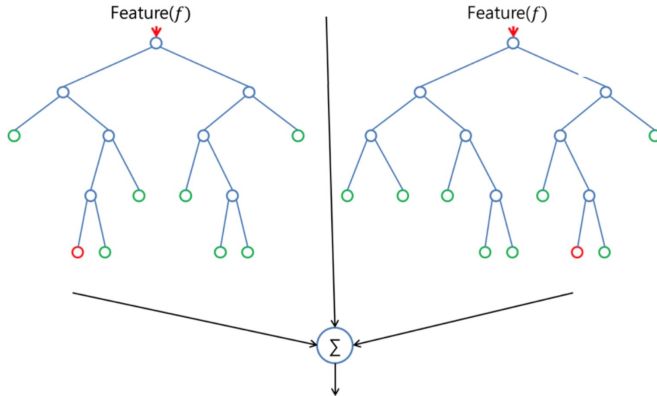
- Pick a **random subset** S_{random} of training examples.
- Grow a full decision tree (no pruning), compute information gain based on S_{random} instead of full set.
- Repeat for **K decision trees**.

Inference: given a new data point X:

- Classify X using each of the K trees.
- Use majority vote: class predicted most often.

Fast, scalable, state-of-the-art performance.

Random (Decision) Forest

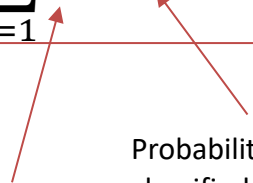


Random forest with majority voting

Gini impurity – An alternative of Entropy

Gini impurity (or **Gini index**) of a dataset D indicates the likelihood of new, random data sample being **misclassified** if the sample is given a random class label **according to the class distribution** in the dataset.

$$Gini(D) = \sum_{i=1}^k p_i(1 - p_i) = 1 - \sum_{i=1}^k p_i^2$$




Probability of the sample
belonging to class i

Probability of the sample **not** being
classified to class i (i.e., misclassified).

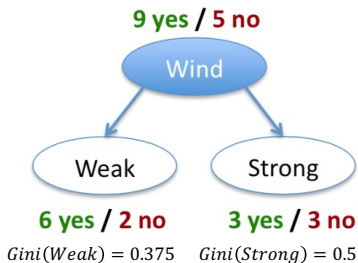
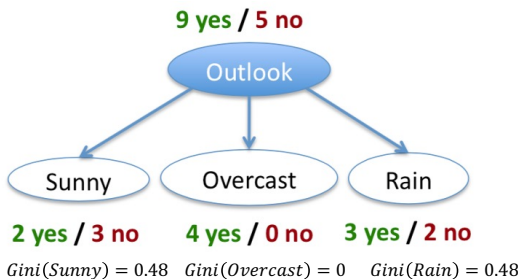
Gini impurity of a dataset

Gini impurity (or **Gini index**) of a dataset D indicates the likelihood of new, random data sample being **misclassified** if the sample is given a random class label **according to the class distribution** in the dataset.

$$Gini(D) = \sum_{i=1}^k p_i(1 - p_i) = 1 - \sum_{i=1}^k p_i^2$$


Probability of the sample belonging to any class is given by $\sum_{i=1}^k p_i = 1$

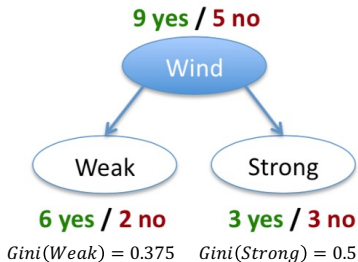
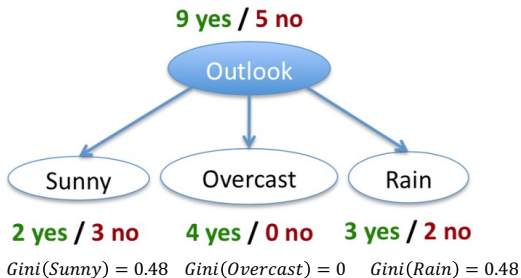
Gini impurity of a dataset



$$Gini(Sunny) = \frac{2}{5} \left(1 - \frac{2}{5} \right) + \frac{3}{5} \left(1 - \frac{3}{5} \right) = 1 - \left(\frac{2}{5} \right)^2 - \left(\frac{3}{5} \right)^2 = 0.48$$

$$Gini(Weak) = \frac{6}{8} \left(1 - \frac{6}{8} \right) + \frac{2}{8} \left(1 - \frac{2}{8} \right) = 1 - \left(\frac{6}{8} \right)^2 - \left(\frac{2}{8} \right)^2 = 0.375$$

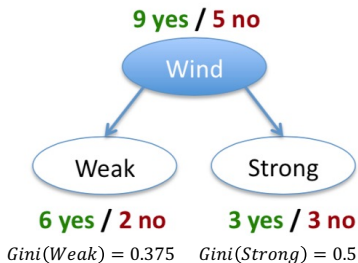
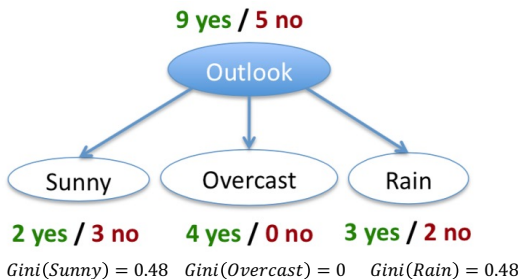
Gini impurity of a dataset



In multi-class classification problem, Gini impurity varies between values 0 and 1 (take an example of 10 data samples and 5 classes):

- Gini = 0: **pure** dataset (e.g., 0/10/0/0/0).
- Gini = 0.5: **equal** distribution over *some* classes (e.g., 5/0/5/0/0).
- Gini = 1: **random** distribution across *all* classes (e.g., 1/2/3/2/2).

Gini impurity of an attribute

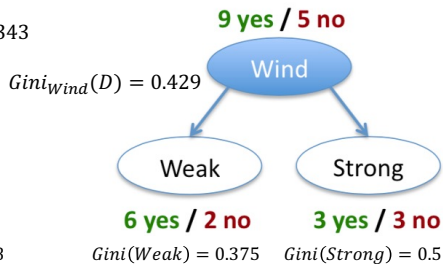
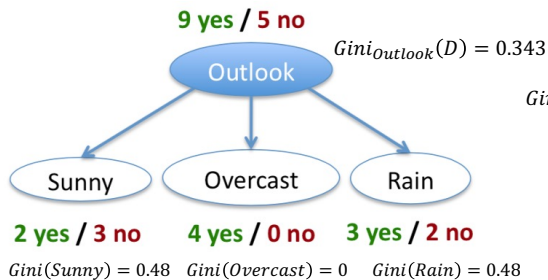


If a dataset D is split on an attribute A into m subsets $\{D_1, \dots, D_m\}$, the Gini impurity can be defined as:

$$Gini_A(D) = \sum_{s=1}^m \frac{|D_s|}{|D|} Gini(D_s)$$

Attribute **minimizing** the Gini impurity is chosen to split the node.

Gini impurity of an attribute



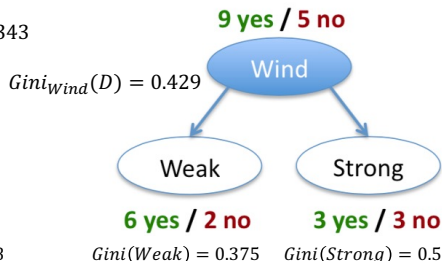
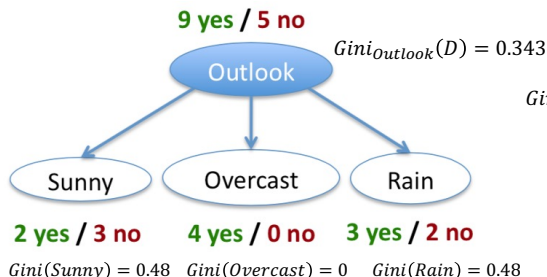
$$Gini_{Outlook}(D) = \frac{5}{14} 0.48 + \frac{4}{14} 0 + \frac{5}{14} 0.48 = 0.343$$

$$Gini_{Wind}(D) = \frac{8}{14} 0.375 + \frac{6}{14} 0.5 = 0.429$$

Outlook is chosen!

Gini information gain

$$Gini(D) = \frac{9}{14} \left(1 - \frac{9}{14}\right) + \frac{5}{14} \left(1 - \frac{5}{14}\right) = 0.459$$



Gini information gain for an attribute (A) is the weighted impurities of the branches is subtracted from the original impurity.

$$\Delta Gini(A) = Gini(D) - Gini_A(D)$$

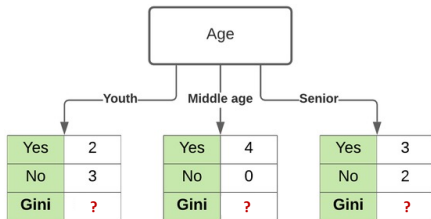
Attribute **maximizing the Gini information gain** is chosen to split.

$$\Delta Gini(Outlook) = 0.459 - 0.343 = 0.116$$

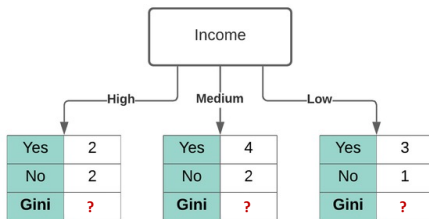
Outlook is chosen!

$$\Delta Gini(Wind) = 0.459 - 0.429 = 0.03$$

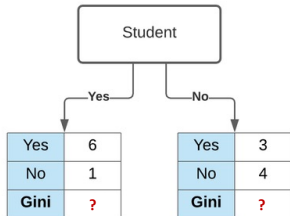
Gini impurity exercise



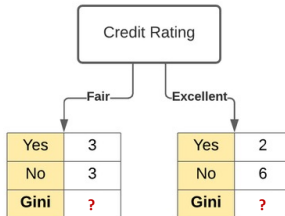
Gini Impurity for Age is ?



Gini Impurity for Income is ?



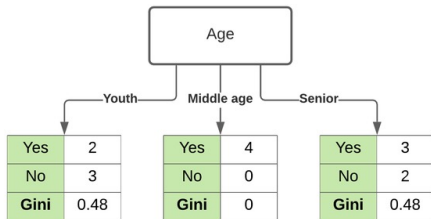
Gini Impurity for Student is ?



Gini Impurity for Credit Rating is ?

What is the best attribute to split?

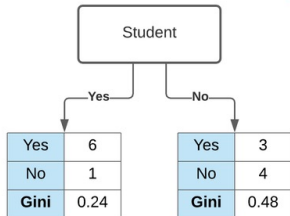
Gini impurity exercise



Gini Impurity for Age is 0.343



Gini Impurity for Income is 0.440



Gini Impurity for Student is 0.367



Gini Impurity for Credit Rating is 0.429

Best

Regression tree

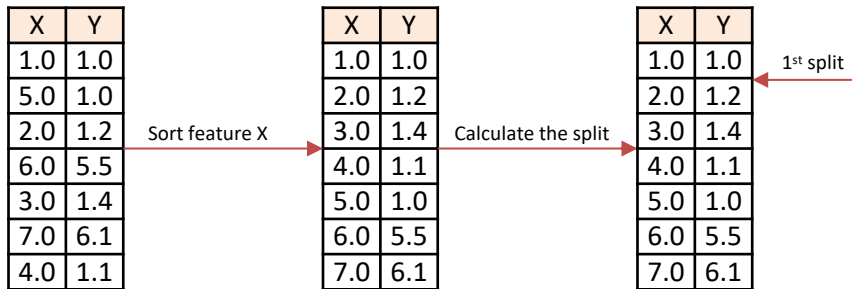
What if the label is not categorical but numeric?

There are two types of decision tree:

- Classification tree: is used when the label is categorical (discrete values).
- Regression tree: is used when the label is numeric (continuous values)

X	Y
1.0	1.0
5.0	1.0
2.0	1.2
6.0	5.5
3.0	1.4
7.0	6.1
4.0	1.1

Regression tree

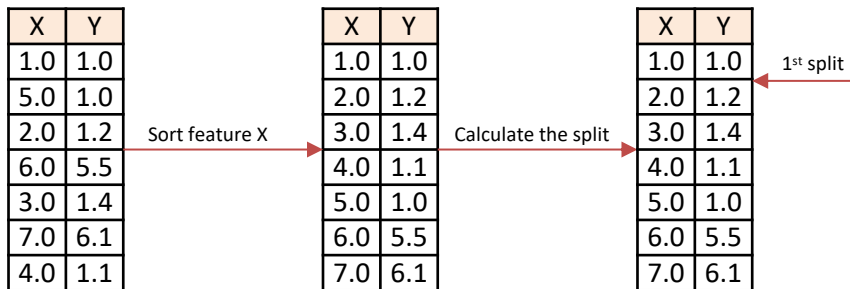


Idea: find the best point to split the dataset into 2 parts so that the Mean Squared Error (MSE) is minimized at that point.

Steps:

- **Sort** the data according to its features (n data samples in total).
- **Brute-force** all possible split points, calculate corresponding MSE values.
- After have n-1 MSE calculated, **choose** the split/threshold of minimum MSE.

Regression tree



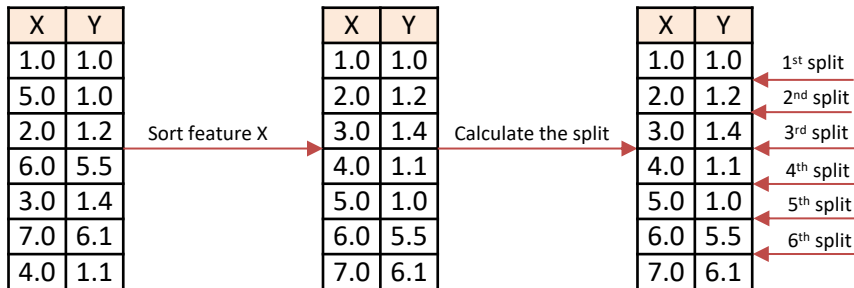
1st split at value $(1+2)/2 = 1.5$. There are two groups:

- Group 1 ($X < 1.5$): $\{(1.0, 1.0)\}$. Average Y value is 1.0 (\hat{y}_{left}).
- Group 2 ($X \geq 1.5$): all other points. Average Y value is 2.72 (\hat{y}_{right}).

Calculate the MSE of the 1st split by (given $n=n_{left}+n_{right}$):

$$\text{MSE}(1^{\text{st}} \text{ split}) = \text{MSE}(1^{\text{st}} \text{ left}) + \text{MSE}(1^{\text{st}} \text{ right}) = \frac{1}{n} \left(\sum_{i=1}^{n_{left}} (y_i - \hat{y}_{left})^2 + \sum_{j=1}^{n_{right}} (y_j - \hat{y}_{right})^2 \right)$$

Regression tree



Similarly calculate MSE of all other possible splits. The chosen split/threshold is the one **having minimum MSE**.

Feature importance - A single decision tree

Idea: calculate a score representing the “importance” of each data feature. The **higher the score**, the **larger the effect** of that feature on the model prediction.

$$I_i = \sum_{n=i} \left(p(n) \text{purity}(n) - \sum_{n_{child}} p(n_{child}) \text{purity}(n_{child}) \right)$$

Importance
of feature i .

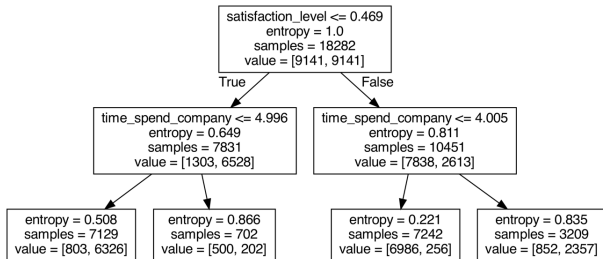
Sum over all
nodes of the
tree that use
feature i .

Probability of using
of a node for a
sample data point.

Purity of a node,
such as Entropy,
Gini, Squared Error.

Feature importance – Example with Entropy

Assume that this is the tree after training



satisfaction_level	0.482504
last_evaluation	0.000000
number_project	0.000000
average_monthly_hours	0.000000
time_spend_company	0.517496
Work_accident	0.000000
promotion_last_5years	0.000000
Department_IT	0.000000
Department_RandD	0.000000
Department_accounting	0.000000
Department_hr	0.000000
Department_management	0.000000
Department_marketing	0.000000
Department_product_mng	0.000000
Department_sales	0.000000
Department_support	0.000000
Department_technical	0.000000
salary_high	0.000000
salary_low	0.000000
salary_medium	0.000000

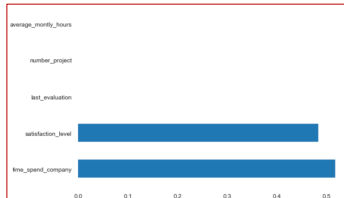
$$\text{satisfaction_level} = 18282/18282 \cdot 1.0 - 7831/18282 \cdot 0.649 - 10451/18282 \cdot 0.811 = 0.2584$$

$$\begin{aligned} \text{time_spend_company} &= (7831/18282 \cdot 0.649 - 7129/18282 \cdot 0.508 - 702/18282 \cdot 0.866) \\ &+ (10451/18282 \cdot 0.811 - 7242/18282 \cdot 0.221 - 3209/18282 \cdot 0.835) \\ &= 0.0466 + 0.2295 = 0.2761 \end{aligned}$$

Then normalize the sum value to 1, we have:

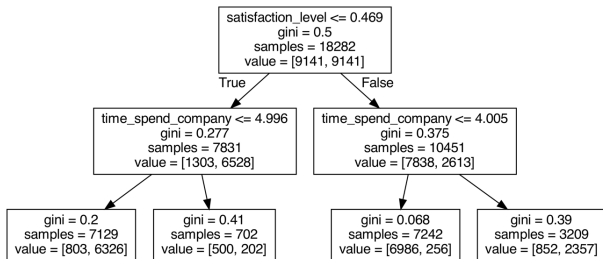
$$\text{satisfaction_level} = 0.2584 / (0.2584 + 0.2761) = \mathbf{0.4834}$$

$$\text{time_spend_company} = 0.2761 / (0.2584 + 0.2761) = \mathbf{0.5166}$$



Feature importance – Example with Gini

Assume that this is the tree after training

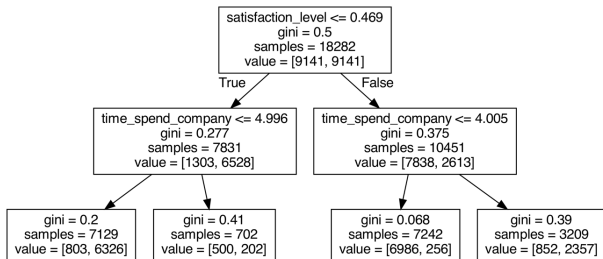


What is the feature importance score of

- `satisfaction_level` = ?
- `time_spend_company` = ?

Feature importance – Example with Gini

Assume that this is the tree after training



$$\text{satisfaction_level} = 18282/18282*0.5 - 7831/18282*0.277 - 10451/18282*0.375 = 0.1670$$

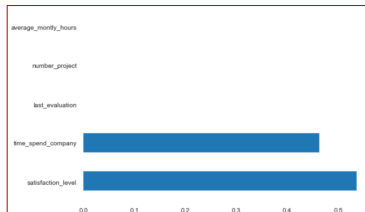
$$\begin{aligned} \text{time_spend_company} &= (7831/18282*0.277 - 7129/18282*0.2 - 702/18282*0.41) \\ &+ (10451/18282*0.375 - 7242/18282*0.068 - 3209/18282*0.39) \\ &= 0.0250 + 0.1190 = 0.1440 \end{aligned}$$

Then normalize the sum value to 1, we have:

$$\text{satisfaction_level} = 0.1670 / (0.1670 + 0.1440) = \mathbf{0.5369}$$

$$\text{time_spend_company} = 0.1440 / (0.1670 + 0.1440) = \mathbf{0.4631}$$

satisfaction_level	0.536586
last_evaluation	0.000000
number_project	0.000000
average_monthly_hours	0.000000
time_spend_company	0.463414
Work_accident	0.000000
promotion_last_5years	0.000000
Department_IT	0.000000
Department_RandD	0.000000
Department_accounting	0.000000
Department_hr	0.000000
Department_management	0.000000
Department_marketing	0.000000
Department_product_mng	0.000000
Department_sales	0.000000
Department_support	0.000000
Department_technical	0.000000
salary_high	0.000000
salary_low	0.000000
salary_medium	0.000000



Feature importance – Random forest

Idea: importance of a feature in a random forest is the sum of importance scores of that feature in all trees in the random forest.

$$I_i = \frac{1}{|B|} \sum_{T \in B} I_i(T)$$

The diagram illustrates the formula for feature importance in a random forest. The formula is enclosed in a red rectangular box. Three red arrows point from descriptive text labels to components of the formula: one from the left variable I_i , one from the denominator $|B|$, and one from the term $I_i(T)$ inside the summation.

Importance of feature i .

Total number of trees in random the forest.

Importance of feature i for a single tree T

Summary

- Decision tree.
- Entropy, information gain, gain ratio.
- Continuous variable in decision tree.
- Random forest.
- Gini impurity of a dataset/attribute, Gini information gain.
- Regression tree.
- Feature importance.

Q&A

Thank you