DECISION TREE AND RANDOM FOREST

1

Decision Tree Algorithm

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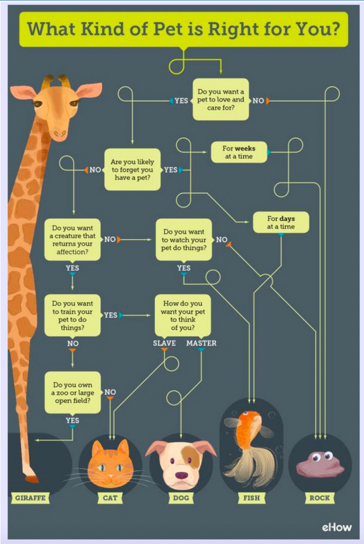
- Similar to how humans make many different decisions
- Decision trees look at one feature/variable at a time



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Decision Tree Algorithm

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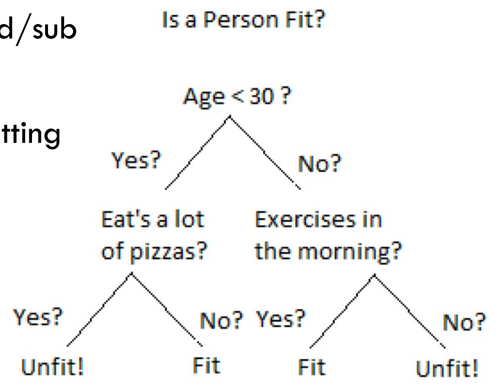
- Root node
- Parent, child/sub nodes
- Branch, splitting
- Leaf nodes



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Decision Tree Algorithm

4

- Training dataset

Day	Outlook	Temp	Humidity	Wind	Tennis?
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
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10	Rain	Mild	Normal	Weak	Yes
11	Sunny	Mild	Normal	Strong	Yes
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13	Overcast	Hot	Normal	Weak	Yes
14	Rain	Mild	High	Strong	No

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Decision Tree Algorithm

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- How can we build a decision tree given a data set?

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Decision Tree Algorithm

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- We will make the best choice at each step
- Identify the best feature/attribute for the each node

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Decision Tree Algorithm

7

- Identify the best feature/attribute for root node
  - Best split: results of each branch should be as homogeneous (or pure) as possible
  - a feature that reduces impurity as much as possible
  - How do we measure the impurity in a set of examples
    - Entropy from information theory
    - Alternatively, use Gini Index

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Decision Tree Algorithm

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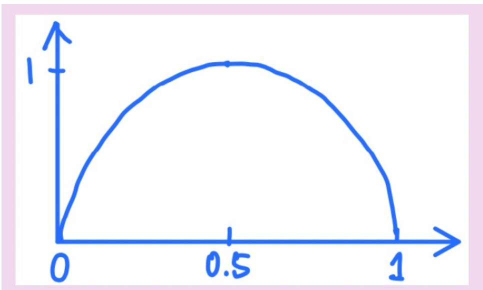
- Entropy for a distribution over two outcomes



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Decision Tree Algorithm

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- Quantifying the information content of a feature
  - entropy of the examples before testing the feature minus the entropy of the examples after testing the feature – Information Gain

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Decision Tree Algorithm

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- Quantifying the information content of a feature
  - Information gain or entropy reduction

$$\text{InfoGain} = I_{\text{before}} - I_{\text{after}}$$

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Decision Tree Algorithm

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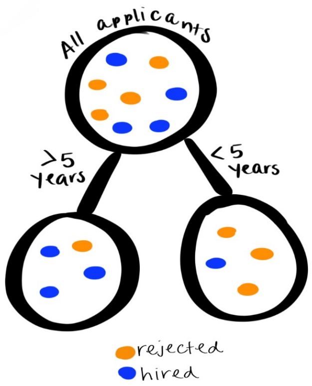
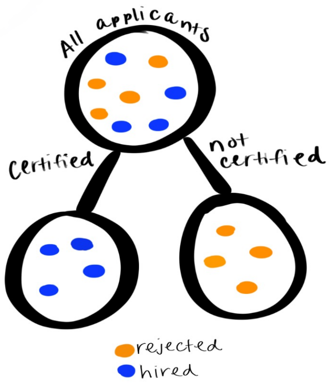
- Information Gain (entropy reduction)





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Decision Tree Algorithm

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- Entropy of the examples before we select a feature for the root node

$$H_{\text{before}} = -\left(\frac{9}{14}\log_2\left(\frac{9}{14}\right) + \frac{5}{14}\log_2\left(\frac{5}{14}\right)\right)$$
$$\approx 0.94$$

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13	Overcast	Hot	Normal	Weak	Yes
14	Rain	Mild	High	Strong	No

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Decision Tree Algorithm

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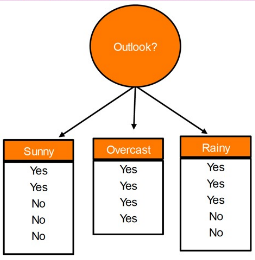
- Information gain if we select Outlook for the root node

$$\text{Outlook} = \begin{cases} \text{Sunny} & 2+ \quad 3- \quad 5 \text{ total} \\ \text{Overcast} & 4+ \quad 0- \quad 4 \text{ total} \\ \text{Rain} & 3+ \quad 2- \quad 5 \text{ total} \end{cases}$$

$$\text{Gain(Outlook)} = 0.94 - \left(\frac{5}{14} \cdot I\left(\frac{2}{5}, \frac{3}{5}\right) + \frac{4}{14} \cdot I\left(\frac{4}{4}, \frac{0}{4}\right) + \frac{5}{14} \cdot I\left(\frac{3}{5}, \frac{2}{5}\right)\right)$$

$$= 0.247$$



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Decision Tree Algorithm

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- Information gain if we select Humidity for the root node

$$\text{Humidity} = \begin{cases} \text{Normal} & 6+ \quad 1- \quad 7 \text{ total} \\ \text{High} & 3+ \quad 4- \quad 7 \text{ total} \end{cases}$$

$$\text{Gain(Humidity)} = 0.94 - \left(\frac{7}{14} \cdot I\left(\frac{6}{7}, \frac{1}{7}\right) + \frac{7}{14} \cdot I\left(\frac{3}{7}, \frac{4}{7}\right)\right)$$

$$= 0.151$$

Day	Outlook	Temp	Humidity	Wind	Tennis?
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
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Decision Tree Algorithm

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- Outlook has the greatest information gain

Gain(**Outlook**) = **0.247** Gain(Humidity) = 0.151
Gain(Temp) = 0.029 Gain(Wind) = 0.048

Day	Outlook	Temp	Humidity	Wind	Tennis?
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Decision Tree Algorithm

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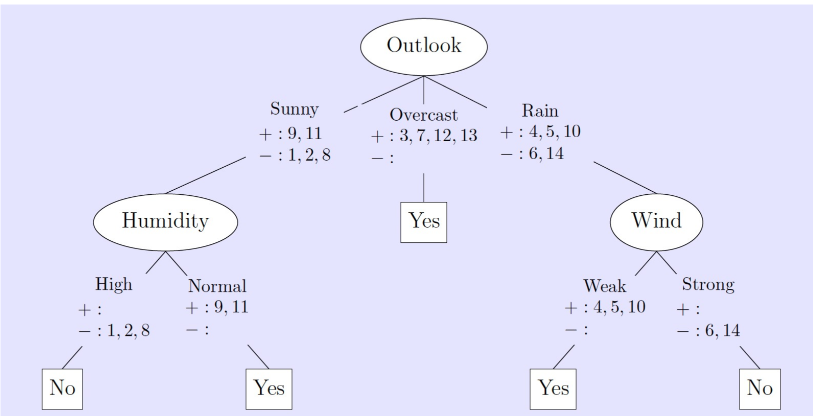
- Outlook has the greatest information gain



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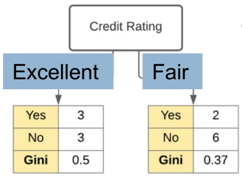
Gini Impurity to Build Decision Trees

	age	income	student	credit_rate	default
0	youth	high	no	fair	no
1	youth	high	no	excellent	no
2	middle_age	high	no	fair	yes
3	senior	medium	no	fair	yes
4	senior	low	yes	fair	yes
5	senior	low	yes	excellent	no
6	middle_age	low	yes	excellent	yes
7	youth	medium	no	fair	no
8	youth	low	yes	fair	yes
9	senior	medium	yes	fair	yes
10	youth	medium	yes	excellent	yes
11	middle_age	medium	no	excellent	yes
12	middle_age	high	yes	fair	yes
13	senior	medium	no	excellent	no

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

$$Gini_A(D) = \frac{n_1}{n} Gini(D_1) + \frac{n_2}{n} Gini(D_2)$$

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



Gini Impurity for Credit Rating is 0.429

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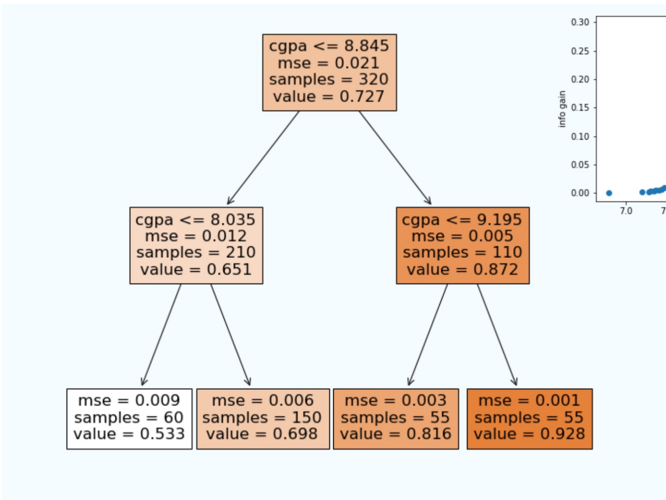
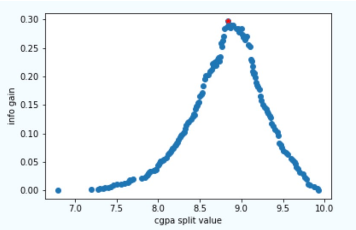
Decision Tree for Regression





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Feature Space

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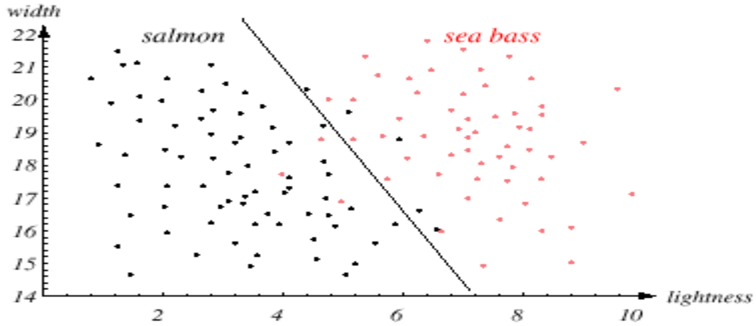
- Two features for classification



Can we improve the performance further? If yes, how?

Image source: Pattern Classification by Duda, Hart and Stork

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Feature Space

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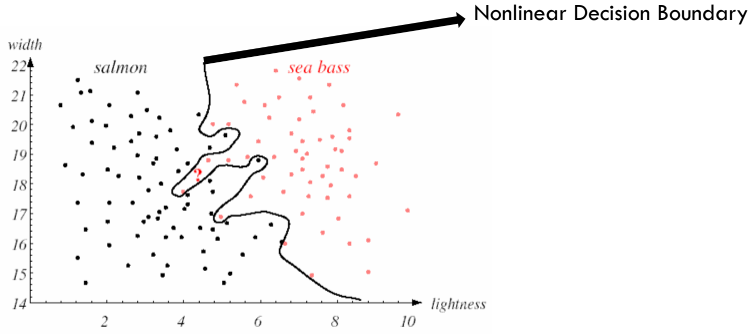
- Two features for classification



Perfect Classification! Is there a catch?

Image source: Pattern Classification by Duda, Hart and Stork

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Generalization

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- Classification Goal: Make accurate predictions for new/unseen data - Good Generalization
- The model should NOT be tuned to the specific characteristics of the training data – Overfitting
- In practice, training data is likely to contain some noise

We are better off with a slightly poorer performance on the training examples if this means that our classifier will have better performance on unseen patterns.

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Generalization

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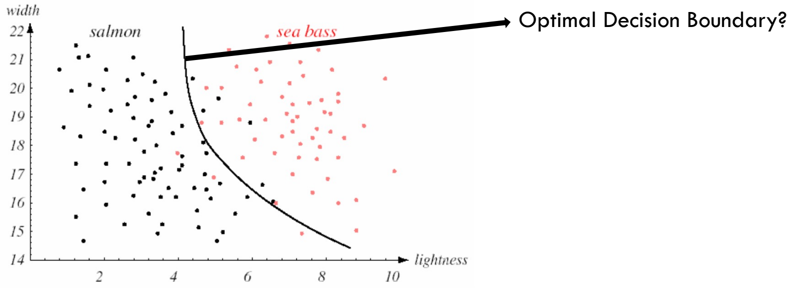
- Classification Goal: Make accurate predictions for new/unseen data - Good Generalization



- A decision boundary that provides an optimal tradeoff between accuracy on the training set and unseen data

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Avoid Overfitting and Achieve Optimal Tradeoff

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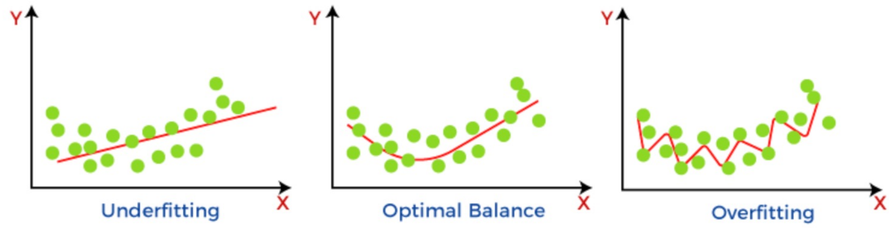

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Feature Space

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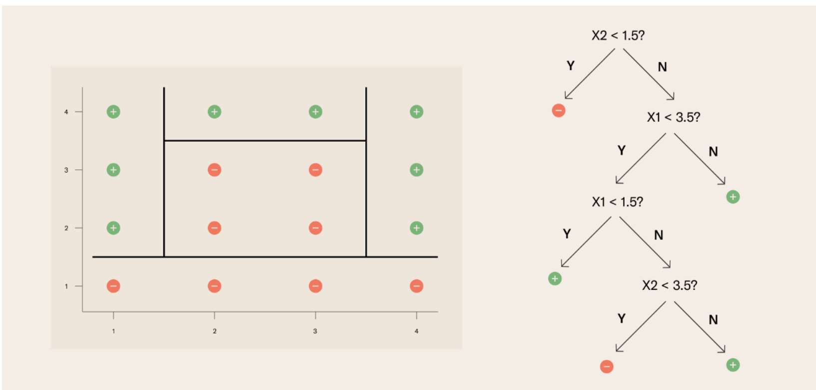
- Decision Boundaries in Decision Tree



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Avoid Overfitting and Achieve Optimal Tradeoff

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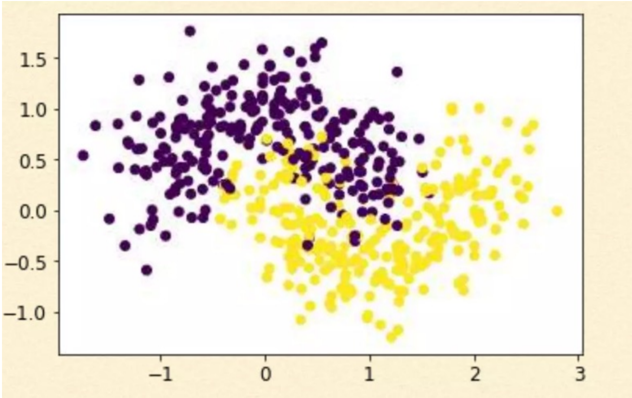
- Decision Tree versus Random Forest



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Avoid Overfitting and Achieve Optimal Tradeoff

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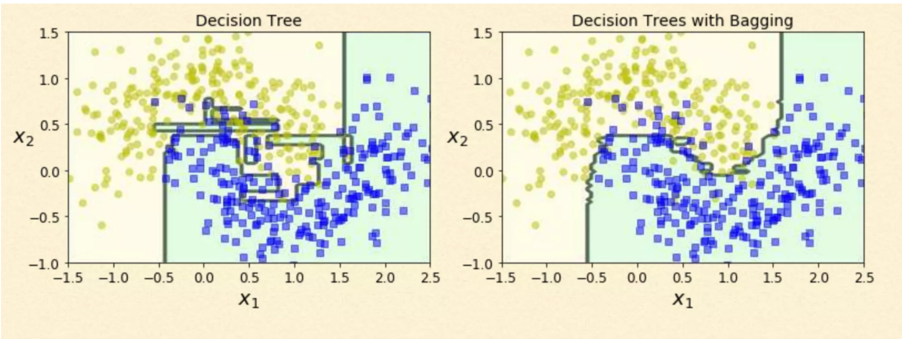
- Decision Tree versus Random Forest



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Random Forest

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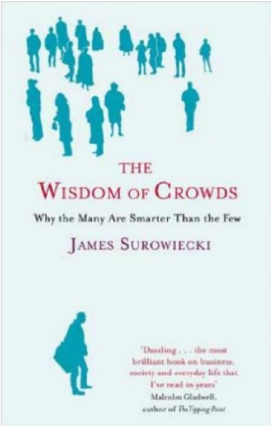
- Ensemble learning is a machine learning technique that aggregates two or more learners to produce better predictions
  - committee-based learning



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Random Forest

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- Base learner, base model, base estimator - refers to the individual models in ensemble algorithms
- consolidating base learner predictions
  - Majority Voting, Averaging

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Random Forest

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- Random forest uses bagging to construct ensembles of randomized decision trees
  - Bagging - bootstrap sampling and aggregation
  - Bootstrap sampling to derive multiple new datasets from one initial training dataset to train multiple base learners

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Bootstrap Sampling

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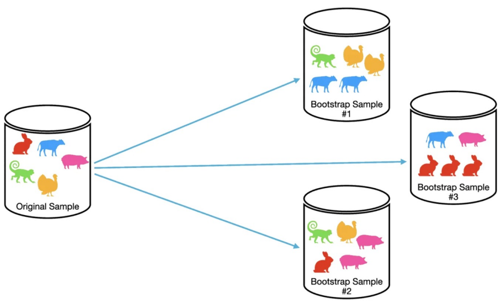
- Random sampling with replacement



- Each bootstrap sample only contains approximately 63.2% of the unique samples from the original dataset

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Random Forest

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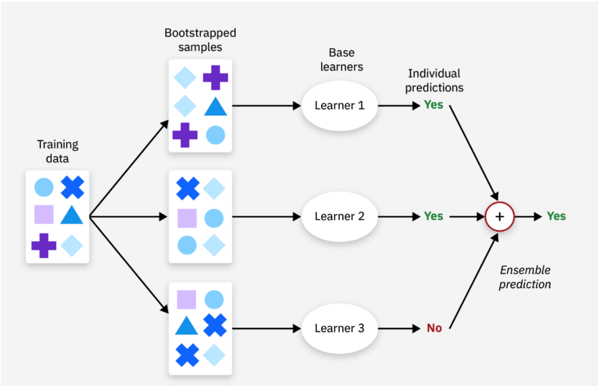
- Random forest uses bagging to construct ensembles of randomized decision trees



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Random Forest

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- Random forest uses bagging to construct ensembles of randomized decision trees
  - considers random subsets of features when splitting a node
  - max_features parameter
- The greater diversity among combined models, the more accurate the resulting ensemble model

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Estimating generalization Performance: Out-of-bag (OOB) error/score

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- Out-of-bag samples as test sets for evaluation
  - Out-of-bag samples are the unique sets of datapoints that are not used for model fitting

  - Each bootstrap sample only contains approximately 63.2% of the unique samples from the original dataset

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Thank You!

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