

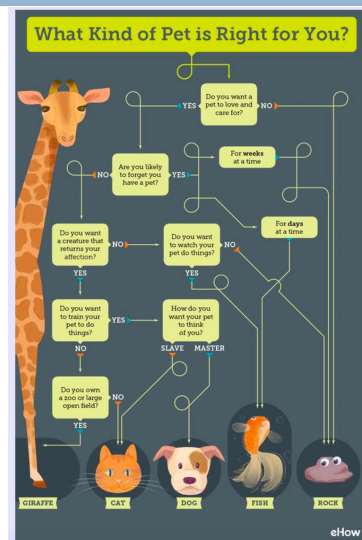
DECISION TREE AND RANDOM FOREST

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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

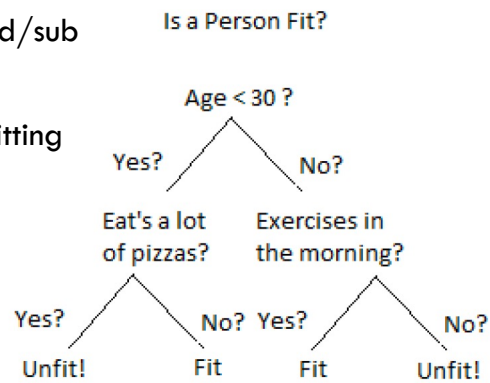


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Decision Tree Algorithm

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



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Decision Tree Algorithm

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- 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
9	Sunny	Cool	Normal	Weak	Yes
10	Rain	Mild	Normal	Weak	Yes
11	Sunny	Mild	Normal	Strong	Yes
12	Overcast	Mild	High	Strong	Yes
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

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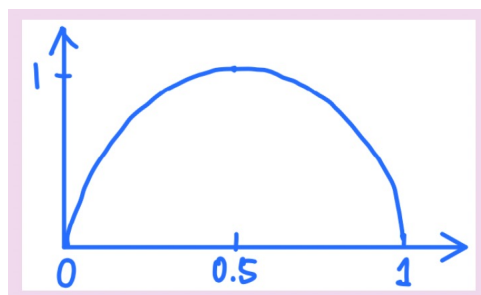
- Identify the best feature/attribute for **root node**
 - Best split: results of each branch should be as **homogeneous** (or **pure**) as possible
 - a feature that reduces **impurity** as much as possible
 - How do we **measure the impurity** in a set of examples
 - **Entropy** from information theory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

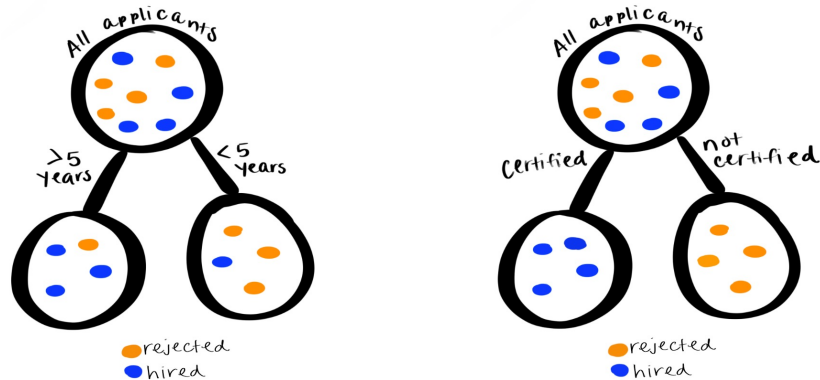
$$\text{InfoGain} = I_{\text{before}} - I_{\text{after}}$$

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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

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

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
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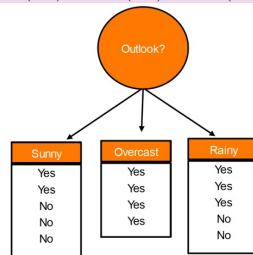
Decision Tree Algorithm

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- Information gain if we select **Outlook** for the **root** node

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

$$\text{Gain}(\text{Outlook}) = 0.94 - \left(\frac{5}{14} \cdot I\left(\frac{2}{5}, \frac{3}{5}\right) + \frac{4}{14} \cdot I\left(\frac{4}{4}, \frac{0}{4}\right) + \frac{5}{14} \cdot I\left(\frac{3}{5}, \frac{2}{5}\right) \right) = 0.247$$



Day	Outlook	Temp	Humidity	Wind	Tennis?
1	Sunny	Hot	High	Weak	No
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3	Overcast	Hot	High	Weak	Yes
4	Rain	Mild	High	Weak	Yes
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13	Overcast	Hot	Normal	Weak	Yes
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Decision Tree Algorithm

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- Information gain if we select **Humidity** for the **root** node

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

$$\text{Gain}(\text{Humidity}) = 0.94 - \left(\frac{7}{14} \cdot I\left(\frac{6}{7}, \frac{1}{7}\right) + \frac{7}{14} \cdot I\left(\frac{3}{7}, \frac{4}{7}\right) \right) = 0.151$$

Day	Outlook	Temp	Humidity	Wind	Tennis?
1	Sunny	Hot	High	Weak	No
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3	Overcast	Hot	High	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

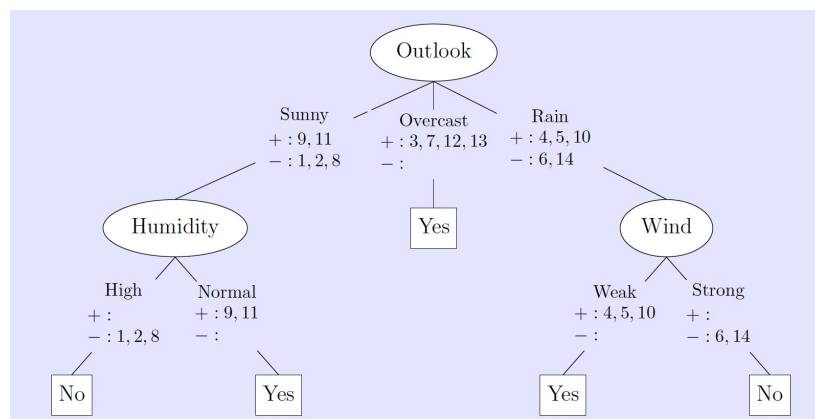
Day	Outlook	Temp	Humidity	Wind	Tennis?
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Decision Tree Algorithm

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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

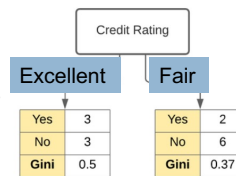
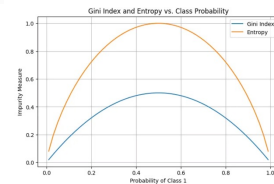
```

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
  
```

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

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

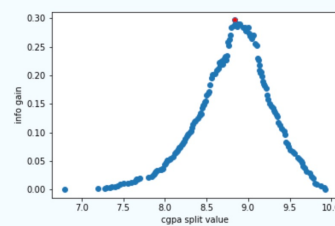
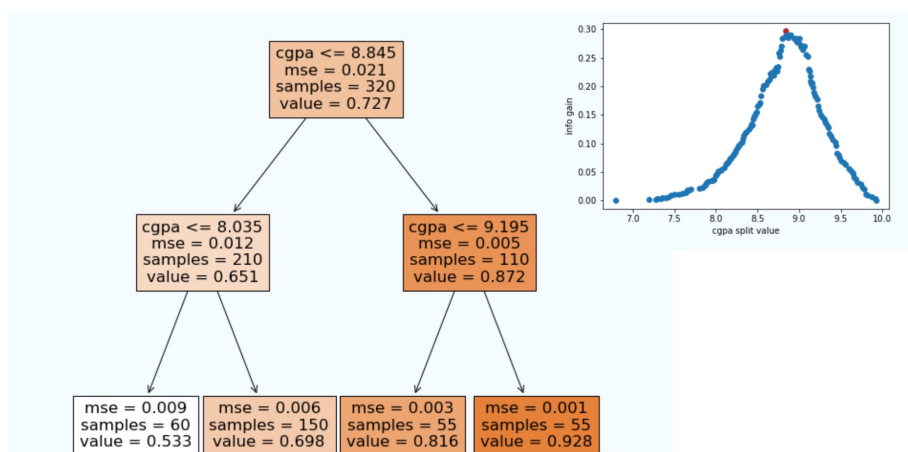
$$\Delta Gini(A) = Gini(D) - Gini_A(D)$$



Gini Impurity for Credit Rating is 0.429

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Decision Tree for Regression



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An example: A Practical Problem

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- A fish-packing plant wants to automate the process of sorting incoming fish according to species
- Problem: Identifying species of a fish on a conveyor belt
 - ▣ Species: Sea bass and salmon

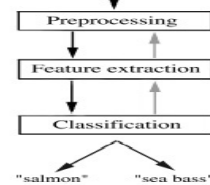


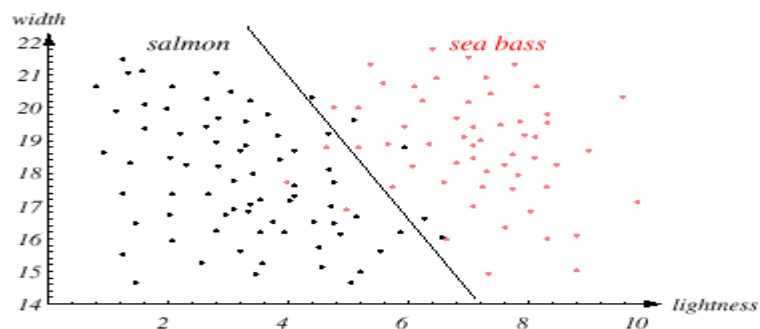
Image source: Pattern Classification by Duda, Hart and Stork

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Feature Space

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- Two features for classification



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

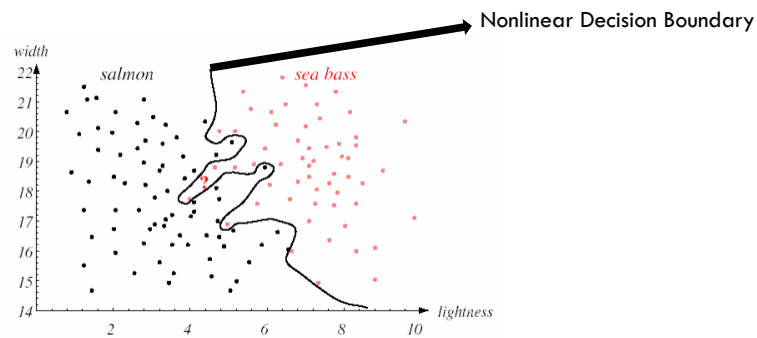
Image source: Pattern Classification by Duda, Hart and Stork

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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

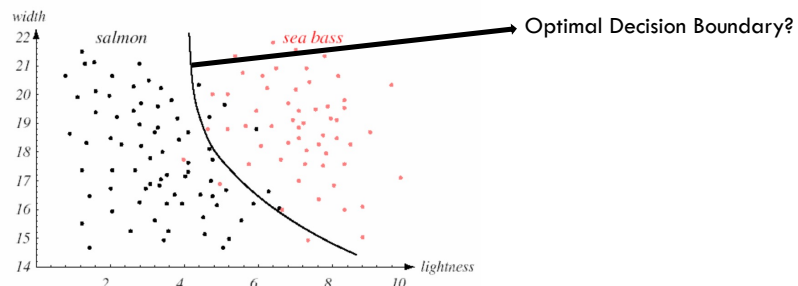
We are better off with a slightly poorer performance on the training examples if this means that our classifier will have better performance on unseen patterns.

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Generalization

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

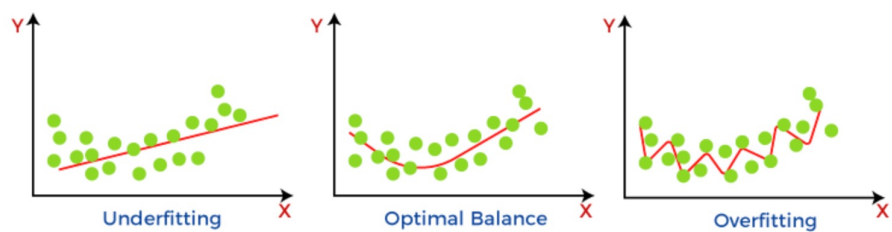


- A decision boundary that provides an **optimal tradeoff** between **accuracy on the training set** and **unseen data**

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Avoid Overfitting and Achieve Optimal Tradeoff

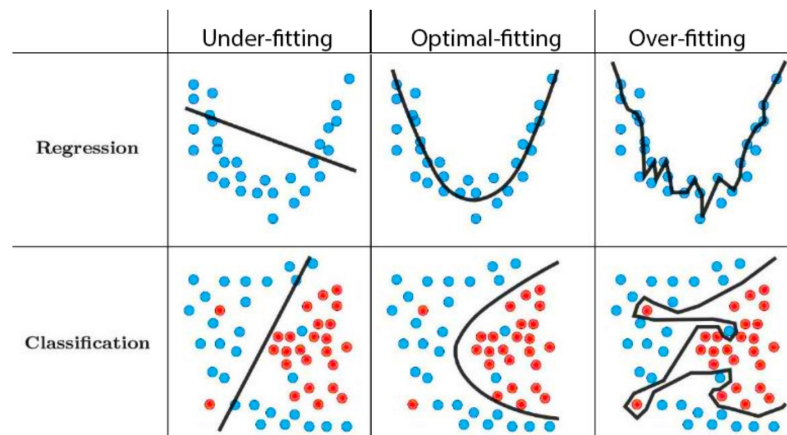
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Underfitting and Overfitting

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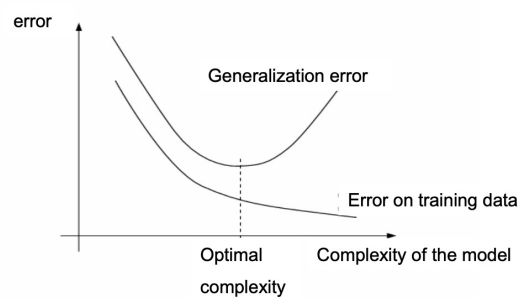


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Fish Classification Problem: Avoid Overfitting and Achieve Optimal Tradeoff

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- Evaluate the classifier model on unseen data – **Validation Set**



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Bias and Variance in Machine Learning

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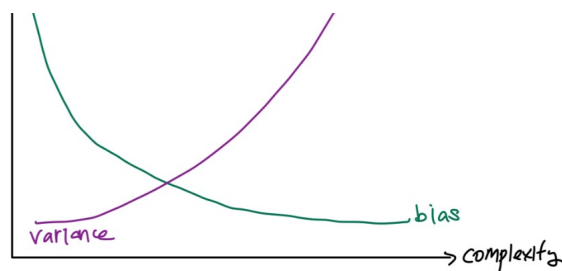
- Bias: The model **makes strong assumptions** about the training data to **simplify the learning process**
 - **Examples:** linear regression algorithms or shallow decision trees, which assume simple relationships even when the data patterns are more complex
- Variance: The **model's sensitivity** to **fluctuations** in the training data (the model's prediction changes as it is trained on different subsets of the training data)

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Bias and Variance in Machine Learning

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- Models with high bias have low variance, and models with low bias have high variance (inverse relationship)



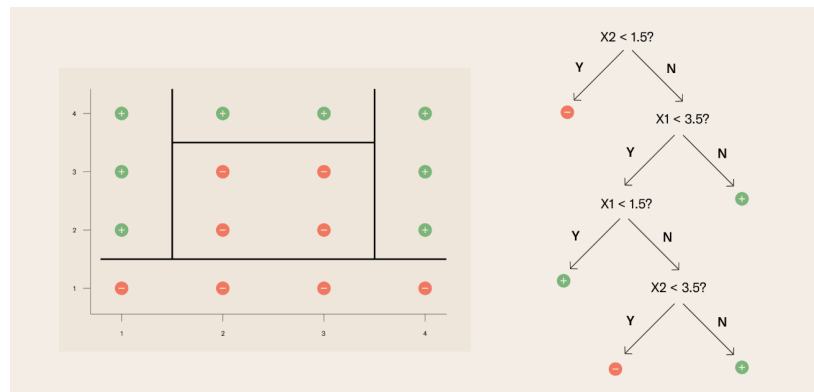
- Bias-variance trade-off: Minimizing errors caused by oversimplification and excessive complication

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Feature Space

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Decision Boundaries in Decision Tree

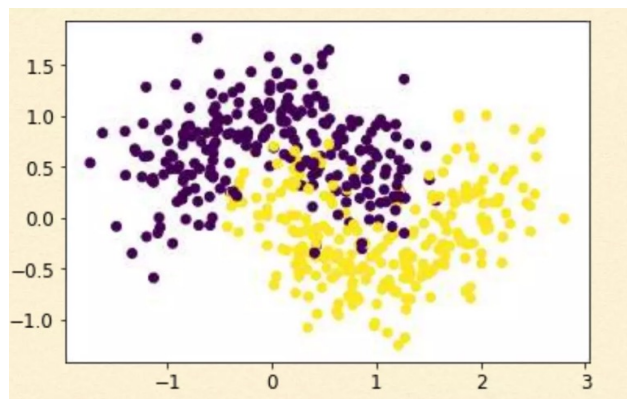


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Avoid Overfitting and Achieve Optimal Tradeoff

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Decision Tree versus Random Forest

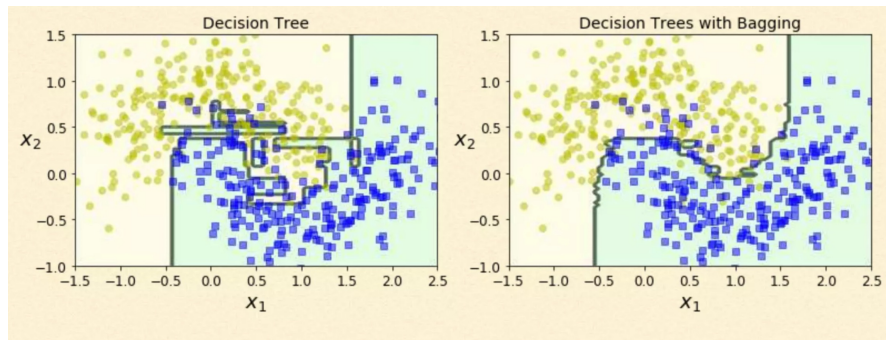


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Avoid Overfitting and Achieve Optimal Tradeoff

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Decision Tree versus Random Forest

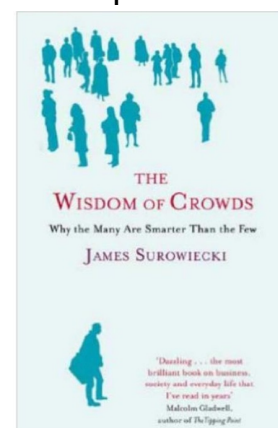


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Random Forest

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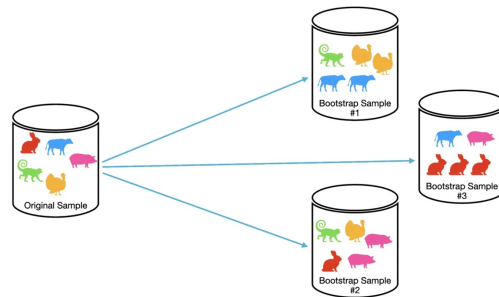
- Random forest uses **bagging** to construct ensembles of **randomized decision trees**
 - Bagging - **bootstrap** sampling and **aggregation**
 - Bootstrap sampling to derive multiple new datasets from one initial training dataset to train multiple base learners

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Bootstrap Sampling

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- Random sampling with replacement



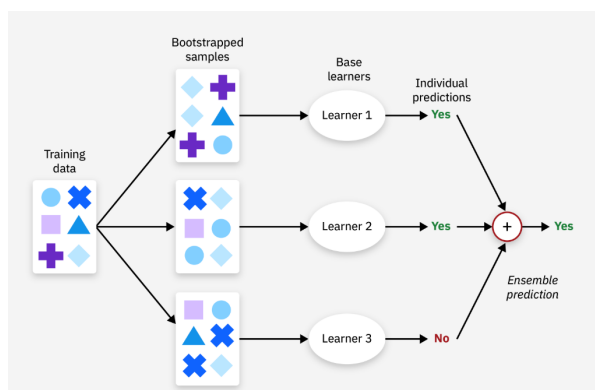
- Each bootstrap sample only contains **approximately 63.2%** of the unique samples from the original dataset

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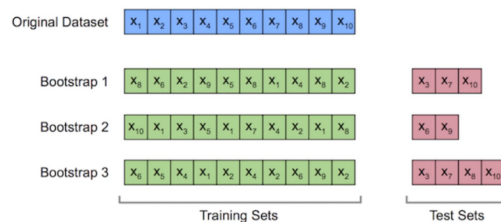
- Random forest uses **bagging** to construct ensembles of **randomized decision trees**
 - considers **random subsets** of features when splitting a node
 - `max_features` parameter
- The **greater diversity** among combined models, the **more accurate** the resulting ensemble model

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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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