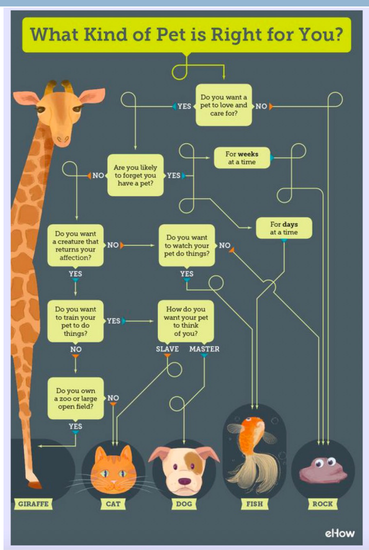
DECISION TREE AND RANDOM FOREST

1

Decision Tree Algorithm

2

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

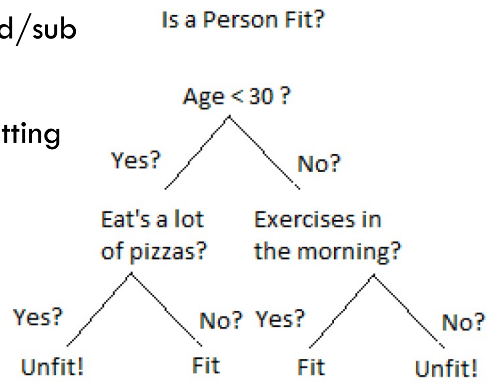


2

Decision Tree Algorithm

3

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



3

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
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

4

Decision Tree Algorithm

5

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

5

Decision Tree Algorithm

6

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

6

Decision Tree Algorithm

7

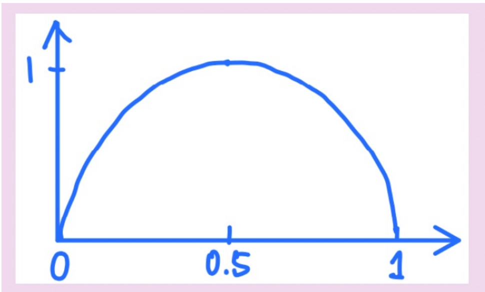
- Identify the best feature/attribute for root node
  - Best split: results of each branch should be as homogeneous (or pure) as possible
  - a feature that reduces impurity as much as possible
  - How do we measure the impurity in a set of examples
    - Entropy from information theory
    - Alternatively,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

7

Decision Tree Algorithm

8

- Entropy for a distribution over two outcomes



8

Decision Tree Algorithm

9

- 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

9

Decision Tree Algorithm

10

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

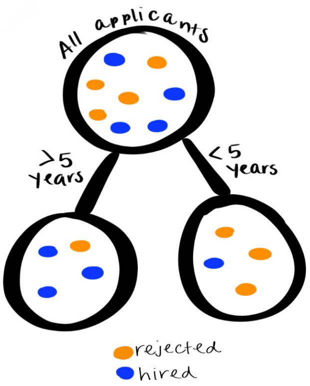
$$\text{InfoGain} = I_{\text{before}} - I_{\text{after}}$$

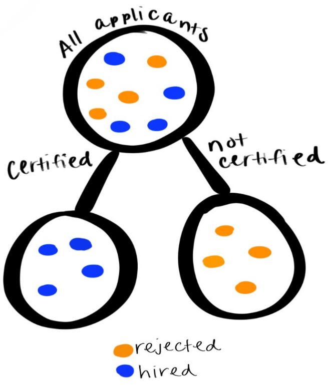
10

Decision Tree Algorithm

11

- Information Gain (entropy reduction)





11

Decision Tree Algorithm

12

- 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
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

12

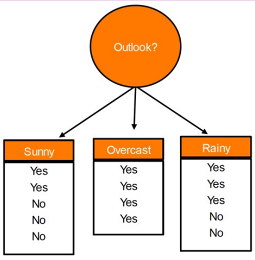
Decision Tree Algorithm

13

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

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

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



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

13

Decision Tree Algorithm

14

- **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
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

14

Decision Tree Algorithm

15

- Outlook has the greatest information gain

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

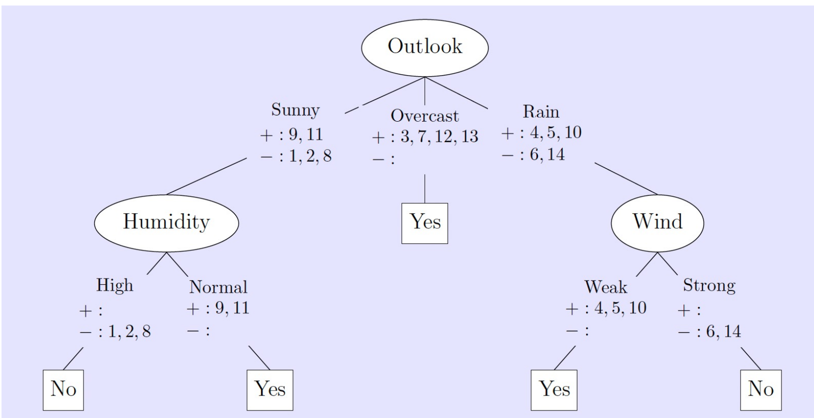
Day	Outlook	Temp	Humidity	Wind	Tennis?
1	Sunny	Hot	High	Weak	No
2	Sunny	Hot	High	Strong	No
3	Overcast	Hot	High	Weak	Yes
4	Rain	Mild	High	Weak	Yes
5	Rain	Cool	Normal	Weak	Yes
6	Rain	Cool	Normal	Strong	No
7	Overcast	Cool	Normal	Strong	Yes
8	Sunny	Mild	High	Weak	No
9	Sunny	Cool	Normal	Weak	Yes
10	Rain	Mild	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

15

Decision Tree Algorithm

16

- Outlook has the greatest information gain



16

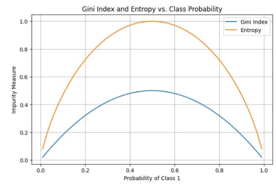
Gini Impurity to Build Decision Trees

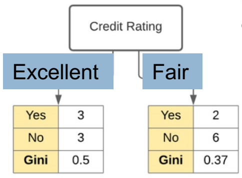
	age	income	student	credit_rate	default
0	youth	high	no	fair	no
1	youth	high	no	excellent	no
2	middle_age	high	no	fair	yes
3	senior	medium	no	fair	yes
4	senior	low	yes	fair	yes
5	senior	low	yes	excellent	no
6	middle_age	low	yes	excellent	yes
7	youth	medium	no	fair	no
8	youth	low	yes	fair	yes
9	senior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

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

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

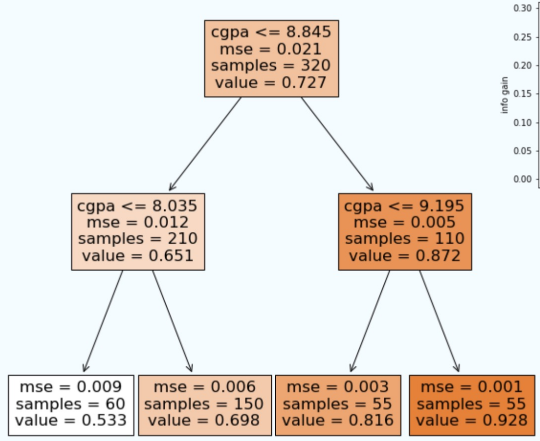
$$\triangle Gini(A) = Gini(D) - Gini_A(D)$$

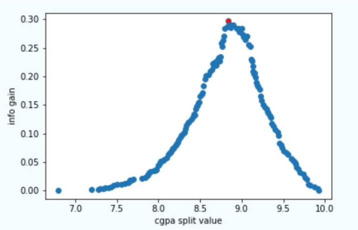




Gini Impurity for Credit Rating is 0.429

Decision Tree for Regression





An example: A Practical Problem

19

- 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

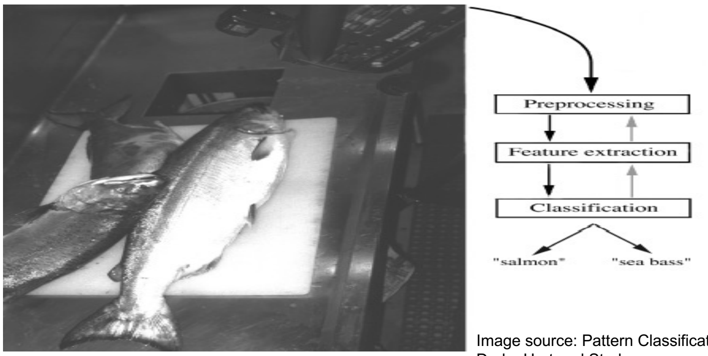


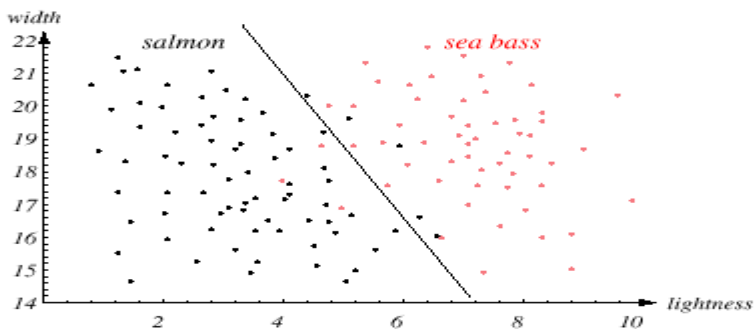
Image source: Pattern Classification by Duda, Hart and Stork

19

Feature Space

20

- Two features for classification



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

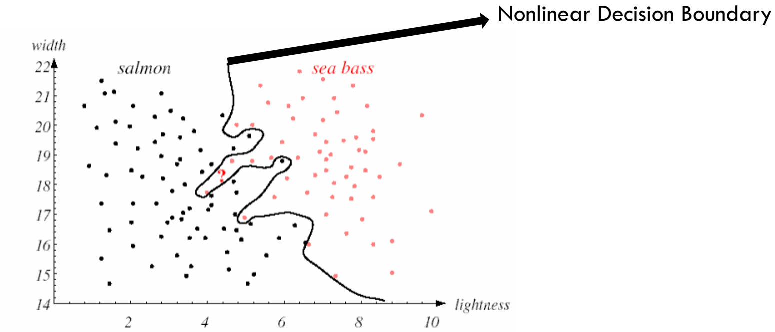
Image source: Pattern Classification by Duda, Hart and Stork

20

Feature Space

21

- Two features for classification



Perfect Classification! Is there a catch?

Image source: Pattern Classification by Duda, Hart and Stork

21

Generalization

22

- 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

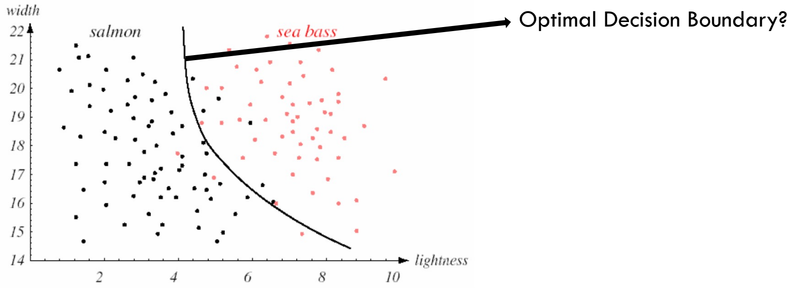
We are better off with a slightly poorer performance on the training examples if this means that our classifier will have better performance on unseen patterns.

22

Generalization

23

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

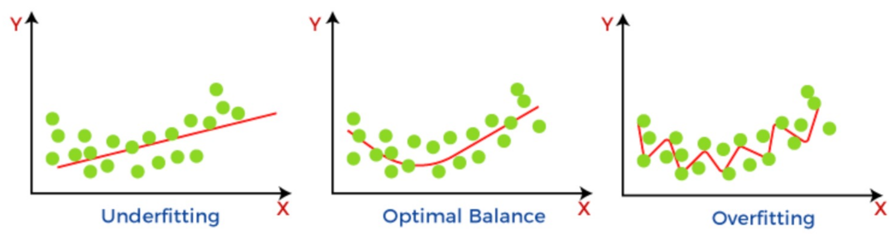


- A decision boundary that provides an optimal tradeoff between accuracy on the training set and unseen data

23

Avoid Overfitting and Achieve Optimal Tradeoff

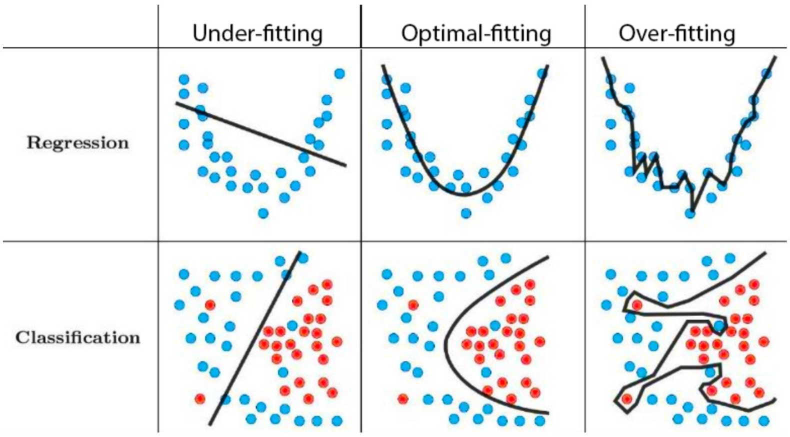
24



24

Underfitting and Overfitting

25

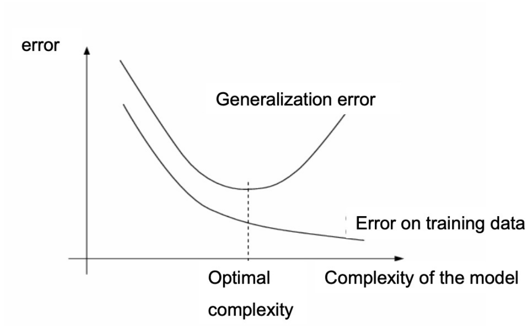


25

Fish Classification Problem: Avoid Overfitting and Achieve Optimal Tradeoff

26

- Evaluate the classifier model on unseen data – Validation Set



26

Bias and Variance in Machine Learning

27

- 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

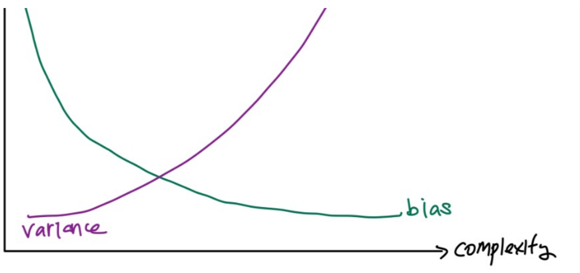
- Variance: The model's sensitivity to fluctuations in the training data (the model's prediction changes as it is trained on different subsets of the training data)

27

Bias and Variance in Machine Learning

28

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



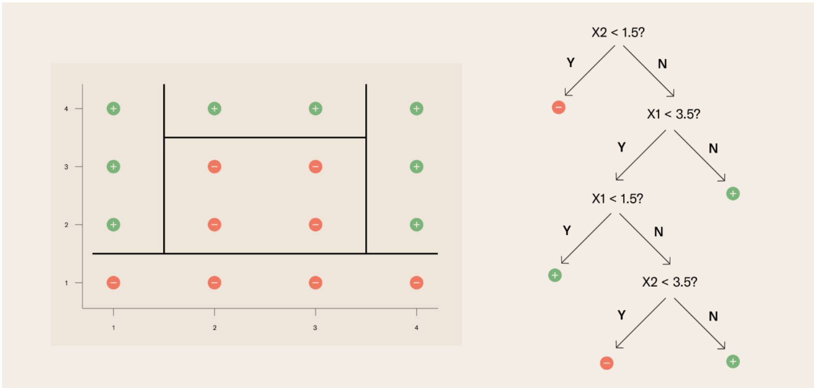
- Bias-variance trade-off: Minimizing errors caused by oversimplification and excessive complication

28

Feature Space

29

- Decision Boundaries in Decision Tree

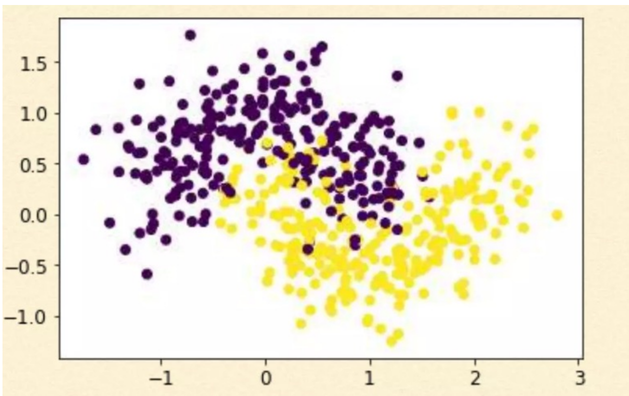


29

Avoid Overfitting and Achieve Optimal Tradeoff

30

- Decision Tree versus Random Forest

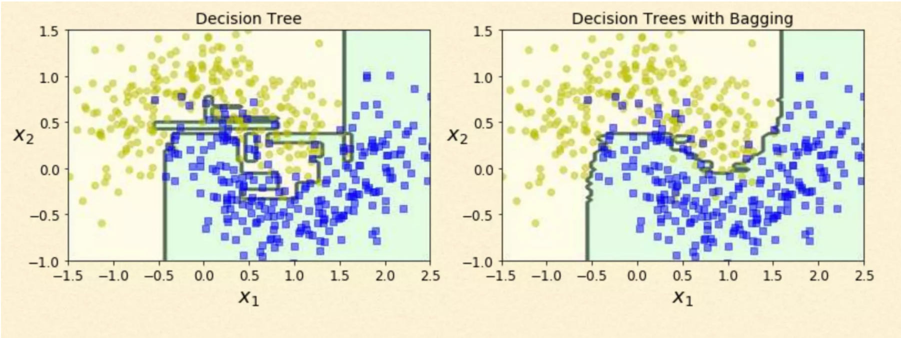


30

Avoid Overfitting and Achieve Optimal Tradeoff

31

- Decision Tree versus Random Forest

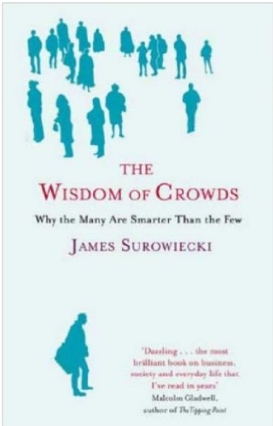


31

Random Forest

32

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



32

Random Forest

33

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

33

Random Forest

34

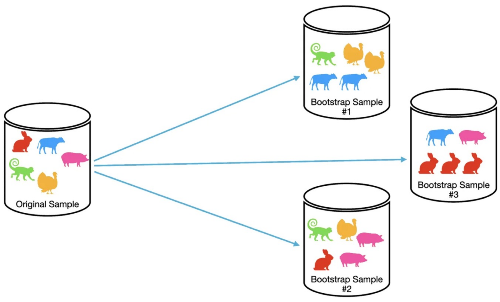
- Random forest uses bagging to construct ensembles of randomized decision trees
  - Bagging - bootstrap sampling and aggregation
  - Bootstrap sampling to derive multiple new datasets from one initial training dataset to train multiple base learners

34

Bootstrap Sampling

35

- Random sampling with replacement



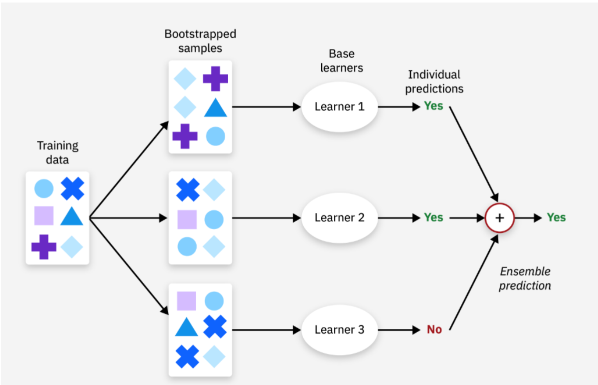
- Each bootstrap sample only contains approximately 63.2% of the unique datapoints from the original dataset

35

Random Forest

36

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



36

Random Forest

37

- 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

37

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

38

- Out-of-bag samples as unseen data 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 data points from the original dataset

38

Thank You!

39