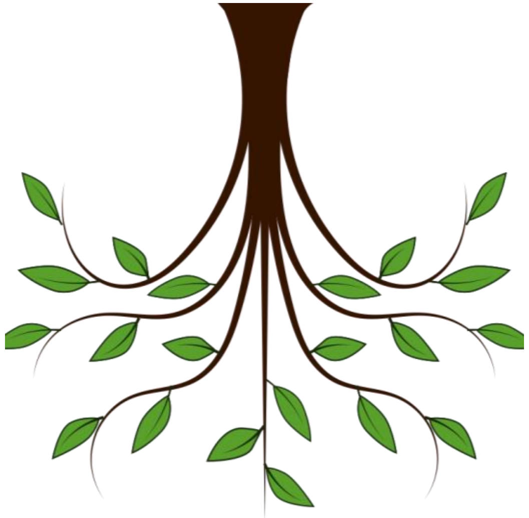
Tree and Ensemble Methods

Making decisions... better



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#MachineLearning

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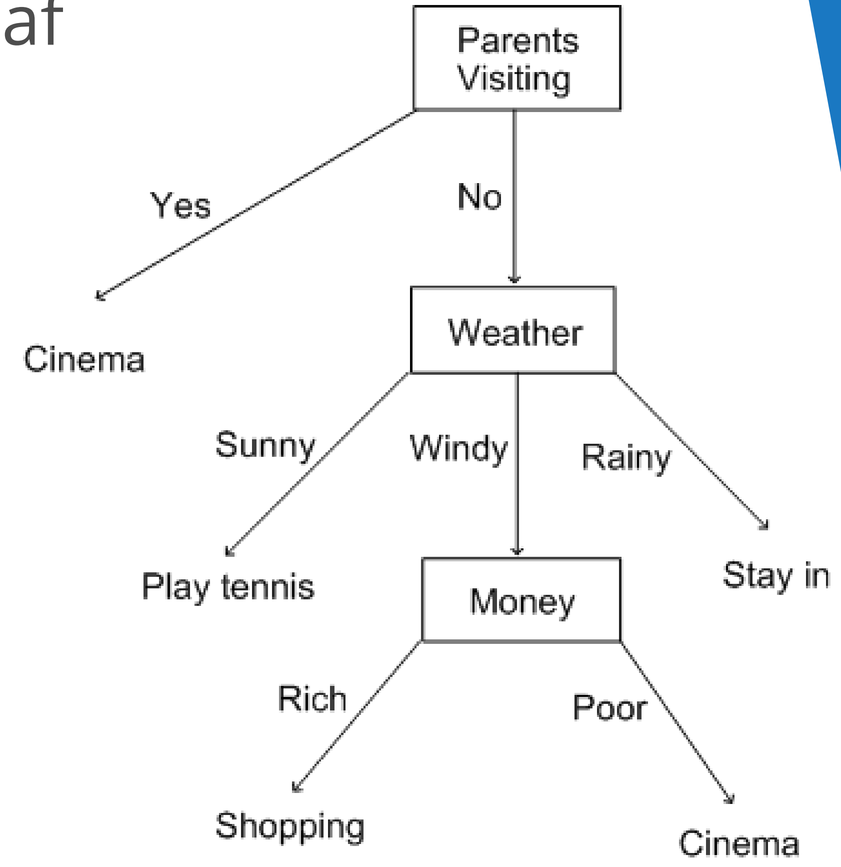
Decision Trees

"To be or not to be..."

Decision Trees

- Can be used for classification or regression
  - **Root**: top node (always a single root)
  - **Leaves**: bottom nodes
  - Getting an answer: path from root to a leaf
- Biggest advantage: easy to interpret
- Answer a series of yes / no questions to get the data model
  - Similar to the way we decide what to do
- We can construct our own decision trees using if-statements
  - Machine learning problem: construct the tree without involving "brain power"

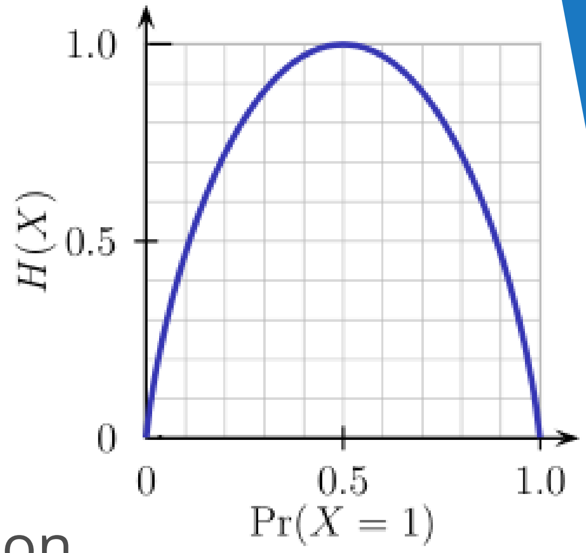


Decision Trees (2)

- Start at the root
- At each step decide how to split the data
  - Choose the feature (column) that results in the largest **information gain** (IG) (example)
- Iterate until every leaf node contains only one class
  - To avoid overfitting ⇒ pruning (limiting the max depth)
- Objective function: maximize IG: $\mathrm{IG}(D_p, f) = I(D_p) - \sum_{j=1}^{m} \frac{N_j}{N_p} I(D_j)$
  - f – feature to perform the split on
  - D_p, D_j – datasets of the parent and child nodes
  - N_p, N_j – number of samples (at parent / child nodes)
  - I – impurity measure
  - More simply, difference between parent and child impurities
    - Greater difference = more IG

Impurity Measures

- Most libraries implement binary decision trees
  - Each node can have 0, 1 or 2 children
  - Reasons: simplicity, reducing the search space
- Three common impurity measures
  - Entropy – measure of classification uncertainty
    - Probability 0 or 1 = no uncertainty
    - Probability $0{,}5$ = max uncertainty
  - Gini index – similar to entropy
    - Criterion to minimize the probability of misclassification
    - We usually use one of the measures, as they provide similar results
  - Misclassification error
    - Linear measure (0 at $p = \{0;1\}$, max at $p = 0{,}5$)
    - **Good for pruning** a tree but worst measure for growing

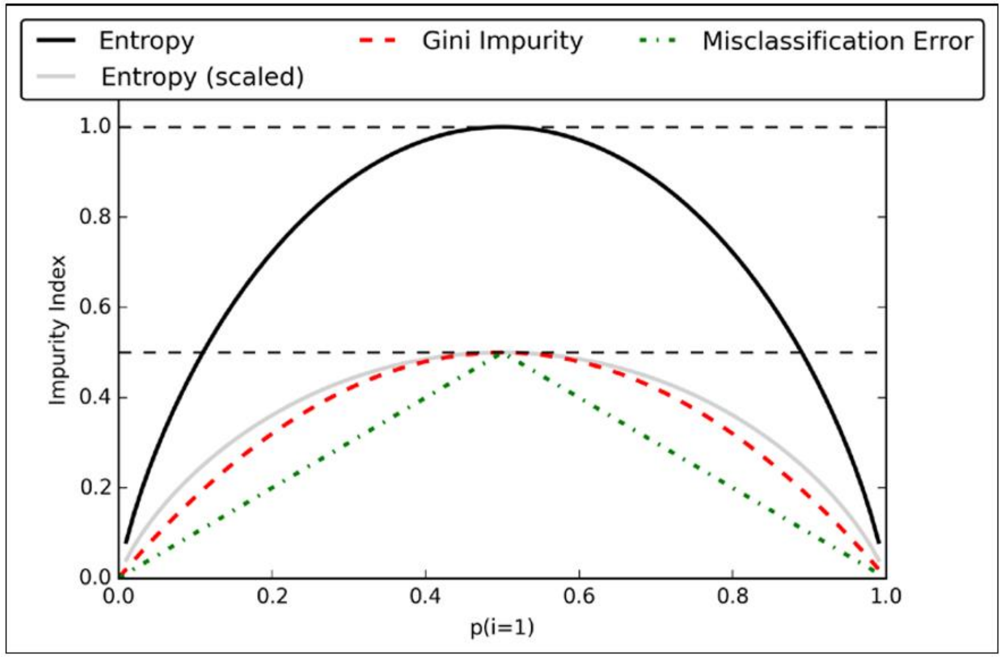


Visualizing Impurity Measures

- For a two-class classifier, visualize the measures
  - Parameter p – probability of class 1 $(0 \le p \le 1)$

```
def entropy(p):
    return -p * np.log2(p) - (1 - p) * np.log2((1 - p))
def gini_index(p):
    return p * (1 - p) + (1 - p) * (1 - (1 - p))
def misclassification_error(p):
    return 1 - np.max([p, 1 - p])
```

  - Scaled entropy:
    entropy / number of classes



- Observations
  - Min: $p = \{0,1\}$, max: $p = 0{,}5$
  - Entropy and Gini are very similar

Decision Trees in `scikit-learn`

- Creating and fitting a classifier – as usual

```
from sklearn.tree import DecisionTreeClassifier
decision_tree = DecisionTreeClassifier()
decision_tree.fit(attributes, labels)
```

- Model hyperparameters
  - `criterion`: `"gini"` (default), `"entropy"`
  - `max_depth`
  - `max_features` (usually we don't change this)
- Outputs
  - `feature_importances_` – Gini scores for all features
  - `n_classes_, n_features_`

Visualizing Decision Tree Boundaries

- For simplicity, let's use the Iris dataset

```python
from sklearn.datasets import load_iris
iris = load_iris()
```

- This method can be applied to all classifiers, not only trees
  - Select 2 features (for a 2D plot)
  - Predict class values for a "mesh" of evenly-spaced samples
  - Plot the test data and predicted values in different colors (classes)

```python
X = iris.data[:, :2] # Sepal length, sepal width
y = iris.target
h = 0.02 # Step size
color_dict = {0: "blue", 1: "lightgreen", 2: "red"}
colors = [color_dict[i] for i in y]

depth_2 = DecisionTreeClassifier(max_depth = 2).fit(X, y)
depth_4 = DecisionTreeClassifier(max_depth = 4).fit(X, y)
titles = ["Max depth = 2", "Max depth = 4"]
```

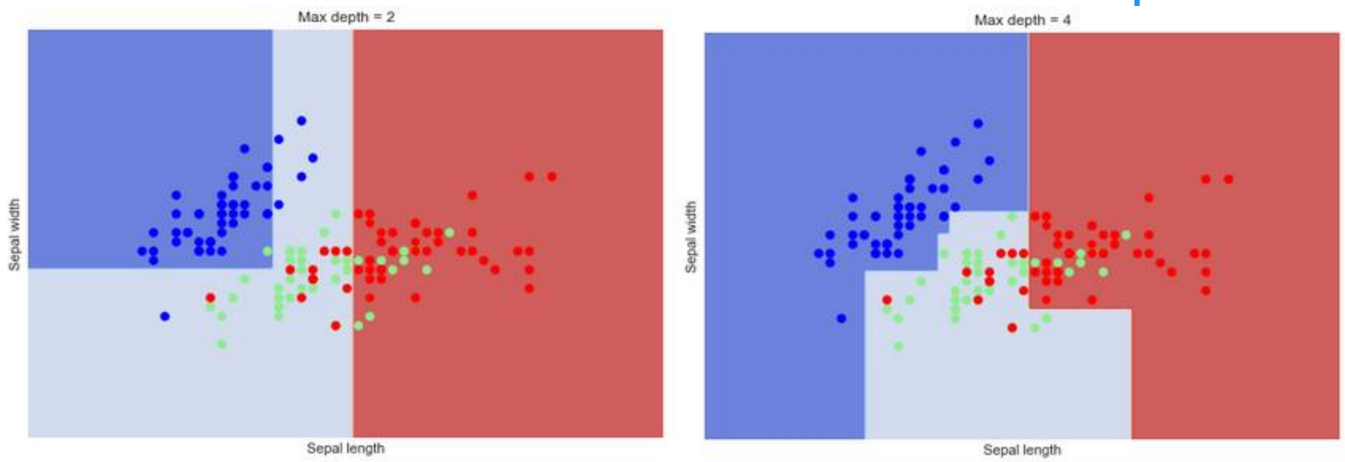
Visualizing Decision Tree Boundaries (2)

- Create a mesh

```
x_min, x_max = X[:, 0].min() - 1, X[:, 0].max() + 1
y_min, y_max = X[:, 1].min() - 1, X[:, 1].max() + 1
xx, yy = np.meshgrid(np.arange(x_min, x_max, h), np.arange(y_min, y_max, h))
```

- Create and evaluate predictions for all classifiers

```
for i, classifier in enumerate((depth_2, depth_4)):
    plt.figure()
    Z = classifier.predict(np.c_[xx.ravel(), yy.ravel()])
    Z = Z.reshape(xx.shape)
    plt.contourf(xx, yy, Z, cmap = plt.cm.coolwarm, alpha = 0.8)
    plt.scatter(X[:, 0], X[:, 1], c = colors)
    plt.xlabel("Sepal length")
    plt.ylabel("Sepal width")
    plt.xlim(xx.min(), xx.max())
    plt.ylim(yy.min(), yy.max())
    plt.xticks(())
    plt.yticks(())
    plt.title(titles[i])
plt.show()
```



Decision Forests

It's even harder to decide...

Random Forests

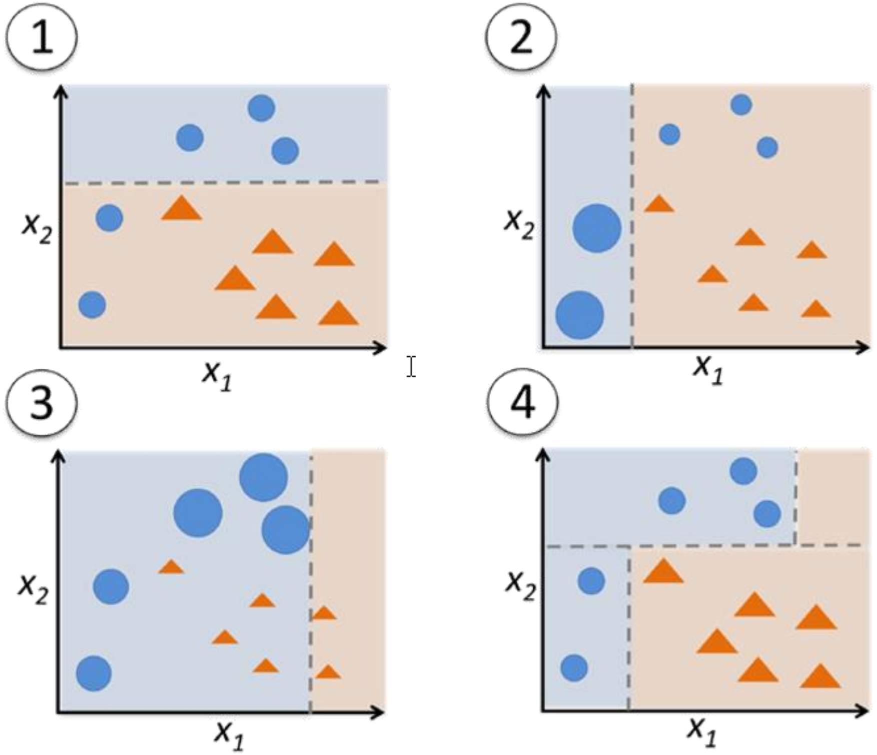
- Combinations (ensembles) of decision trees
- Idea: combine many weak learners (models that perform slightly better than random)
    - Draw a bootstrap sample (random with replacement) of size n
    - Grow k decision trees on the bootstrap sample
        - At each node, randomly select d features and split based on max IG
    - Aggregate the prediction by majority vote
- Differences with decision trees
    - Forests use a random subset of features (trees use all features)
    - A little harder to interpret than decision trees :(
- Advantages :)))
    - Better (lower) generalization error
    - Less susceptible to overfitting
    - Less hyperparameter tuning (in practice, we usually care about k only)

AdaBoost

- Short for "**Ada**ptive **Boost**ing"
    - Another method to combine weak learners into a strong one
- Algorithm
    - Train a weak learner on a random subset (without replacement) of the test data
    - Draw another random subset and add 50% of the previously misclassified samples; train another weak learner on that
    - Find the training samples on which both learners disagree to train a third weak learner
    - Combine the three weak learners via majority voting
- Those algorithms tend to overfit the data
    - We have to check variance carefully

AdaBoost (2)

1. All samples have equal weight
   - First classifier: dashed line minimizes an error function
2. Assign larger weights to misclassified samples, lower weights to correctly classified samples
   - Second classifier: "focuses" on misclassified samples
3. The same as step 2 (we can perform many rounds of boosting)
   - Third classifier
4. End result: combination of all weak learners
   - Resulting classifier: combined results
     - Majority vote



Testing AdaBoost

- Use an AdaBoost classifier to combine 100 "decision stumps" (i.e. decision trees with depth 1)
  - Use the adult income dataset
- Compare the results to only one tree

```
from sklearn.metrics import accuracy_score

# Preprocessing, train / test split

# Single tree
tree = DecisionTreeClassifier(max_depth = 1)
tree.fit(features_train, labels_train)
train_pred = accuracy_score(labels_train, tree.predict(features_train))
test_pred = accuracy_score(labels_test, tree.predict(features_test))
print(
    "Decision tree train / test accuracies: %.3f / %.3f",
    (train_pred, test_pred))
```

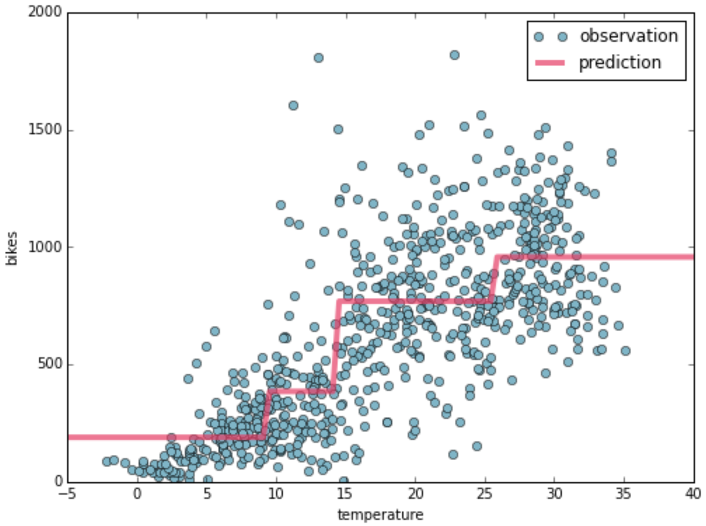
Testing AdaBoost (2)

```python
from sklearn.ensemble import AdaBoostClassifier
# Boosted tree
tree = DecisionTreeClassifier(max_depth = 1)
ada = AdaBoostClassifier(base_estimator = tree,
    n_estimators = 100, learning_rate = 0.1)
ada.fit(features_train, labels_train)
train_pred = accuracy_score(labels_train, ada.predict(features_train))
test_pred = accuracy_score(labels_test, ada.predict(features_test))
print(
    "AdaBoost tree train / test accuracies: %.3f / %.3f",
    (train_pred, test_pred))
```

- Results
  - AdaBoost is better in most cases
    - Predicts the test and train data better
  - AdaBoost has higher variance and reduced bias
    - Better comparison: cross validation; model selection process
      - CV + "hold-out" set

Other Algorithms

- Regression with trees and forests
  - Not commonly used because of the model function
    - Stepwise, not smooth (i.e. no gradients), tends to overfit, etc.
  - [Example]
- Gradient boosting
  - Boosting algorithm (similar to AdaBoost)
  - Trains on the remaining errors
    - Doesn't modify the sampling distribution
  - [Example]
  - **XGBoost** – e**X**treme **G**radient **Boost**ing
    - Usually faster, performs better on large datasets



Summary

- Decision trees
- Ensemble algorithms
  - Random decision forests
  - AdaBoost

Questions?