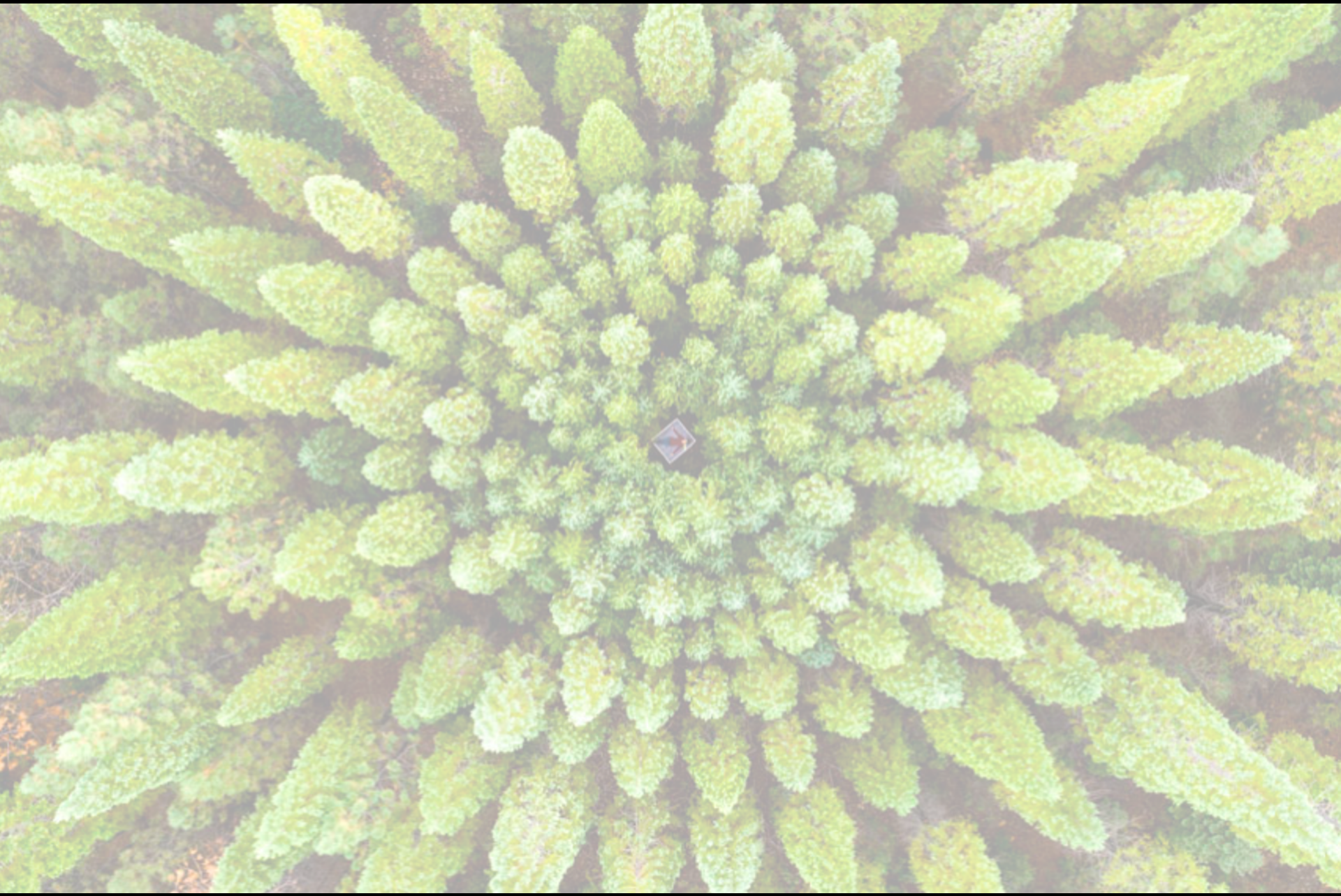
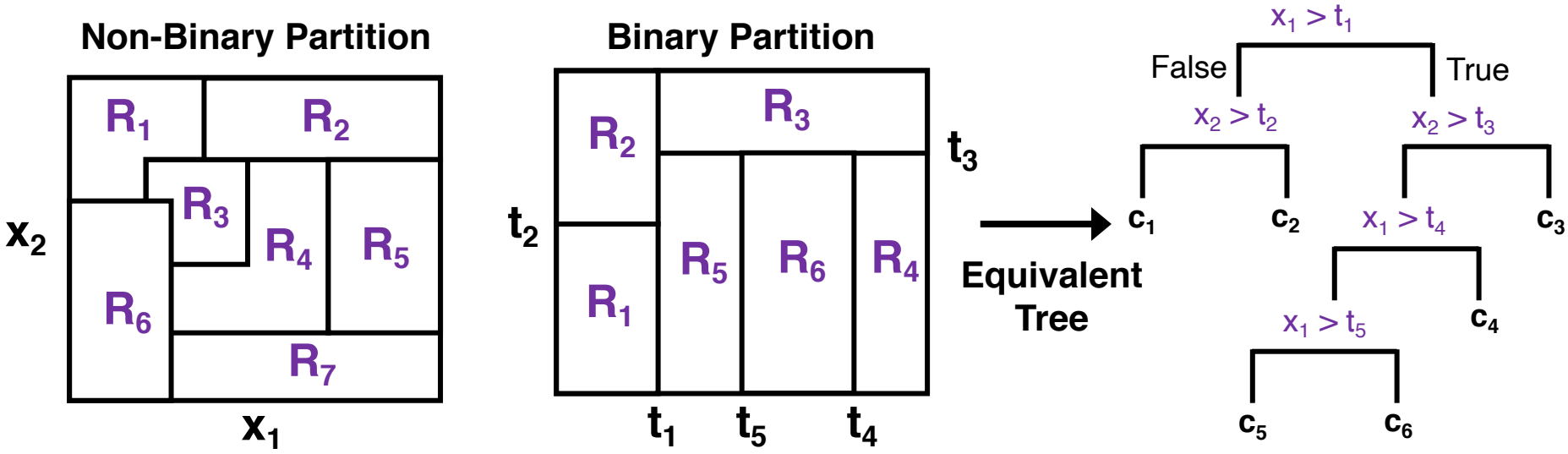
Lecture 15: Decision Trees and Random Forests



Decision Tress - Introduction

• We'll consider a variety known as classification and regression trees (**CART**) originally developed by Brieman (1984), or more commonly just "decision Trees".

• Consider data consisting of a response, **y**, and inputs x_1 and x_2. The idea is to split up the data into regions based on x_1 and x_2. In each region $x \in R_i$ we can model **y** as a constant or category, c_i, depending on the type of **y**.

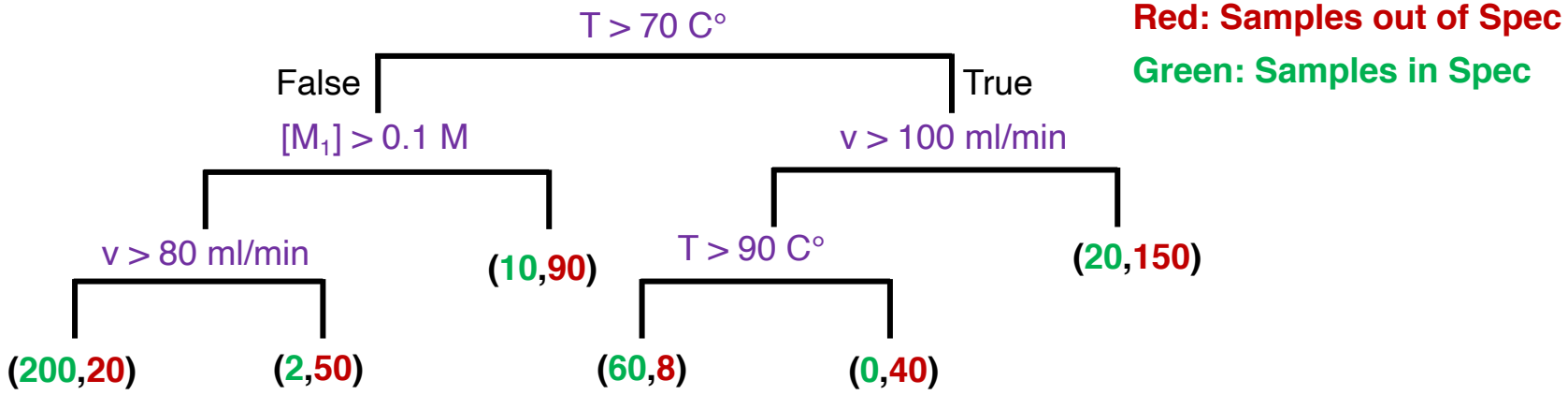


• Even though the model is simple, non-binary splits (left) are difficult to describe computationally. **CART** restricts itself to binary splits of each region with respect to a x_i

Decision Tress - Introduction

• For more than two features, drawing partitions as we did on the previous slide isn't feasible, but the binary tree representation works the same way.

• Let's say our inputs included three continuous features: reactor temperature (T), Reactant concentration (M_1), and volumetric flow rate (v), for a classification task:



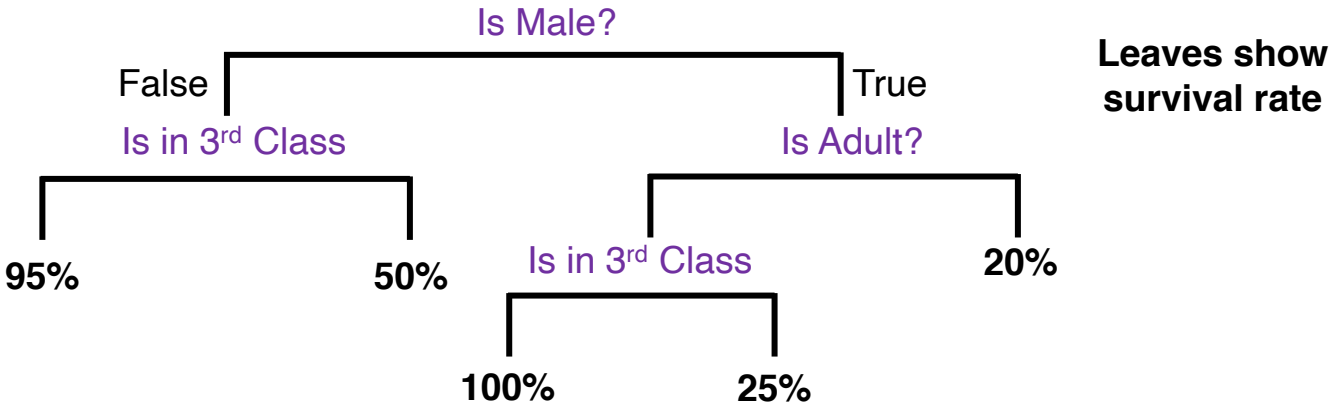
• With our tree in hand, prediction on unseen samples is straightforward: run the **x** for the new sample through the tree starting at the base until you terminate in a leaf. The leaf will tell you your class/value depending on the proportion (classification) or mean (regression).

Decision Tress – Titanic Example

• This is a famous machine learning example that is commonly used to highlight the strength of decision trees and by extension random forests (discussed later).

• Dataset can be downloaded from Kaggle and consists of 891 passengers 11 features (x) and whether or not each survived (y).

Example of decision tree utilizing 3 features:



The example highlights the high interpretability of decision trees. You can identify which features are important, which sub-populations were likely and unlikely to survive, and for what reasons.

Decision Trees – Definitions

Kingsford, C. & Salzberg, S. L. "What are decision trees?" *Nature Biotech.* 26(9), 2008.

Node: A point in DT where a question is asked & a decision must be made

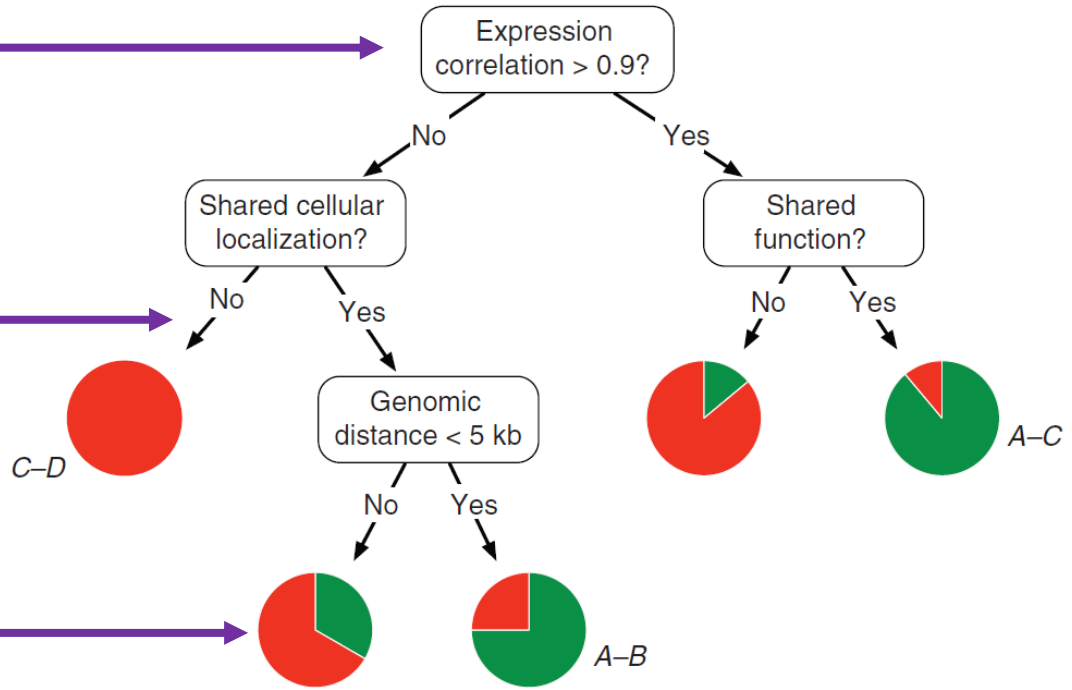
Branch: Represents the decision

Leaf: Final node which yields classification (via proportion)

a

Gene Pair	Interact?	Expression correlation	Shared localization?	Shared function?	Genomic distance
A-B	Yes	0.77	Yes	No	1 kb
A-C	Yes	0.91	Yes	Yes	10 kb
C-D	No	0.1	No	No	1 Mb

b



Decision Trees – Training

• Consider N data, each consisting of a response, y, and k inputs x. That is, (x_i,y_i) for i=1,2…,N with $x_i = (x_1,x_2,\ldots,x_k)$.

• During training we'll need to decide which variables to split on and their split value.

• Suppose we want M regions, $R_1,R_2,\ldots,R_M$ and we model the response in each region as a constant, c_m:

$$f(x) = \sum_{m=1}^{M} c_m I\left(x \in R_m\right)$$

Where I() is an indicator function (1 or 0 for condition)

• If our error is defined as the sum of squares, then the best c_m choice is just the average of y_i in each region:

$$\bar{c}_m = \text{ave}\left(y_i | x_i \in R_m\right)$$

• So far so simple. However, simultaneously optimizing R_m and c_m is infeasible in this way. Instead, we need an algorithm that starts with a single region, tries to optimally split it along some xi, and recursively continues until some termination criteria.

Decision Trees – Training (Regression)

• In the typical greedy **CART** algorithm, we start with all of the data and consider a splitting variable *j* and split point *s*. These will define a pair of half planes:

$$R_1(j,s) = \{X | X_j \leq s\} \qquad R_2(j,s) = \{X | X_j > s\}$$

• We want to find the *j* and *s* that minimize the least-squared error:

$$\min_{j,s} \left[\min_{c_1} \sum_{x_i \in R_1(j,s)} (y_i - c_1)^2 + \min_{c_2} \sum_{x_i \in R_2(j,s)} (y_i - c_2)^2 \right]$$

• The inner minimizations can be solved by taking the average of the y_i in each region:

$$\bar{c}_1 = \text{ave}(y_i | x_i \in R_1(j,s)) \qquad \bar{c}_2 = \text{ave}(y_i | x_i \in R_2(j,s))$$

- The outer minimizations over all *j* and *s* are likewise feasible (ordering tricks can help).
- After finding the best split variable and split value, we recursively repeat on R_1 and R_2.

Decision Trees – Training (Classification)

• For classification, the only changes necessary are to our loss function. We will consider loss functions based on the proportion of observations of a given class, *k*, in R_m:

$$p_{mk} = \frac{1}{N_m} \sum_{x_i \in R_m} I\left(y_i = k\right)$$

• We classify the observations in a node based on the majority proportion:

$$k(m) = \underset{k}{\operatorname{argmax}}\left(p_{mk}\right)$$

• We seek to perform the split such that we minimize the impurity Q of the child nodes:

$$\min_{j,s}\left[\frac{N_1}{N_\mathrm{p}} Q\left(x_i \in R_1(j,s)\right) + \frac{N_2}{N_\mathrm{p}} Q\left(x_i \in R_2(j,s)\right)\right]$$

Where N_1 and N_2 are the samples in the binary child regions and N_p is the number of samples in the parent node.

$$Q = 1 - p_{mk(m)}$$

Misclassification Error

$$Q = \sum_{k=1}^{K} p_{mk}(1 - p_{mk})$$

Gini Index

$$Q = -\sum_{k=1}^{K} p_{mk} \log\left(p_{mk}\right)$$

Cross-Entropy/Deviance

Decision Trees – Training (Classification)

- Misclassification error is not generally desirable for generating trees.

Compare the following splits:

Split A

$$Q = 1 - p_{mk(m)} \rightarrow \frac{400}{800}(1-0.75) + \frac{400}{800}(1-0.75) = 0.25$$

$$Q = \sum_{k=1}^{K} p_{mk}(1-p_{mk}) \rightarrow \frac{400}{800}(0.25(1-0.25)+0.75(1-0.75)) + \frac{400}{800}(0.25(1-0.25)+0.75(1-0.75)) = 0.375$$

$$Q = -\sum_{k=1}^{K} p_{mk}\log(p_{mk}) \rightarrow \frac{400}{800}(-0.75\log(0.75)-0.25\log(0.25)) + \frac{400}{800}(-0.25\log(0.25)-0.75\log(0.75)) = 0.56$$

Split B

$$Q = 1 - p_{mk(m)} \rightarrow \frac{600}{800}(1-0.66) + \frac{200}{800}(1-1) = 0.25$$

$$Q = \sum_{k=1}^{K} p_{mk}(1-p_{mk}) \rightarrow \frac{600}{800}(0.33(1-0.33)+0.66(1-0.66)) + \frac{200}{800}(0.0+0.0) = 0.333$$

$$Q = -\sum_{k=1}^{K} p_{mk}\log(p_{mk}) \rightarrow \frac{600}{800}(-0.33\log(0.33)-0.66\log(0.66)) + \frac{200}{800}(-1.0\log(1.0)-0) = 0.48$$

Both splits exhibit the same misclassification error, but B is intuitively preferable because it produces a “pure” node. Both Gini and Cross-Entropy prefer B (in general, these perform similarly).

Decision Trees – Training (Stopping)

• It is obvious that if we let our tree grow indefinitely, eventually every sample will occupy a pure leave and the data will be perfectly memorized. Several stopping heuristics are variously employed to determine when to stop:

- Is the reduction in error from a split above a threshold? (*not preferred, sometimes split with low reduction will lead to an important split below it*)
- Is the node already pure enough? (*preferred to above, essentially inverse*)
- Has the tree reached a maximum depth?
- Is the number of samples in the children nodes too small?

Decision Trees – Additional Details

• **Why binary splits?** We might consider splitting into more than two child nodes. In general, multiway splits fragment data too quickly and don't leave enough data for lower layers. Also, since a multiway split can be decomposed into a series of binary splits, the latter is preferable.

• Since splits are based on a single feature, XOR type relationships cannot be effectively learned with basic implementations.

Decision Trees – Python Details

.DecisionTreeClassifier() from sklearn.tree

Important hyperparameters:

max_depth: depth to grow tree (important for overfitting)

max_features: number to features to search for split (important for computational efficiency)

min_samples_split: number of samples required to attempt a split

min_samples_leaf: minimum number of samples required to define a leaf.

min_impurity_decrease: minimum impurity decrease to perform a split (Hastie et al say don't use for reasons given above)

Important attributes:

.classes_, **feature_importances_**, <-- useful but not unique

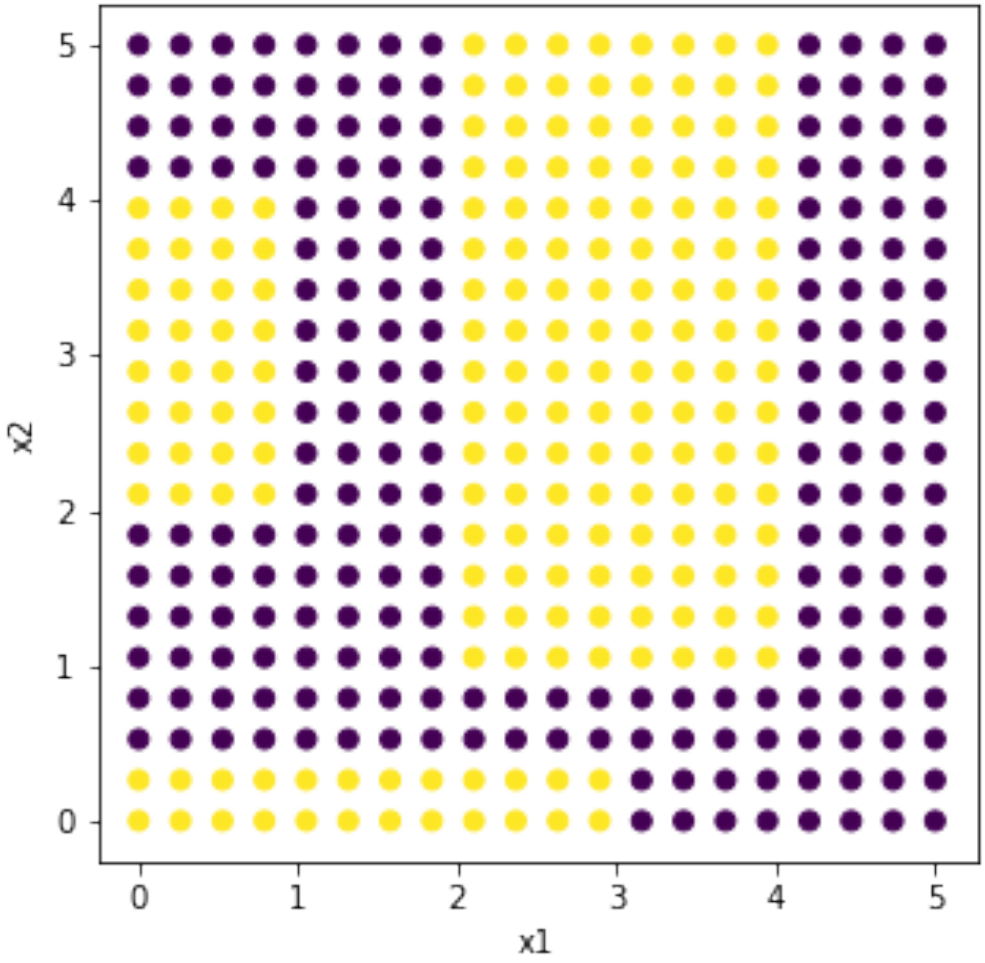
.tree_ <-- stores tree structure

Decision Trees – Python Details

To illustrate some of the details of how decision trees behave, we'll use the following classification problem:

Two features (x1 and x2), one classification (color) with two values (purple, yellow). This could easily map on to a pass/fail type classification

To start we have no noise (this influences hyperparameter selection).



Decision Trees – Python Details

Train the model:

```
from sklearn import tree
model = tree.DecisionTreeClassifier() # default depth and purity criteria
model.fit(X,Y)
```

Illustrate predictions:

```
# Plot decision boundaries
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, 0.01),
np.arange(y_min, y_max, 0.01))
plt.figure(figsize=(5,5))
Z = model.predict(np.c_[xx.ravel(), yy.ravel()])
Z = Z.reshape(xx.shape)
cs = plt.contourf(xx, yy, Z)

# Plot predictions
plt.scatter(X[:,0],X[:,1],edgecolors="k",c=model.predict(X))
plt.xlabel("x1")
plt.ylabel("x2")
plt.show()
```

Note: `np.c_()` is a helper function for reorganizing arrays, `np.r_()` is also a common helper. `plt.contourf()` and `np.meshgrid()` always confuse me personally and I have to experiment with them almost every time that I use them.

Decision Trees – Python Details

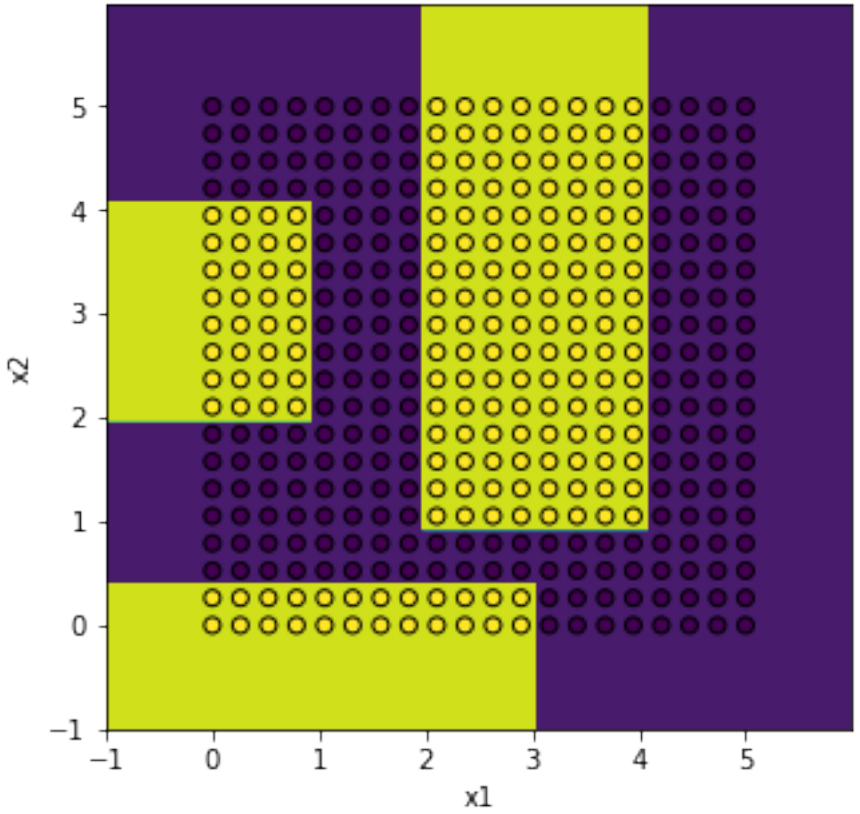
Train the model:

```
from sklearn import tree
model = tree.DecisionTreeClassifier() # default depth and purity criteria
model.fit(X,Y)
```

Illustrate predictions:

Perfect predictions!

It is obvious that if we let our tree grow indefinitely we can always get perfect training predictions, but the model won't generalize



Common stopping criteria:

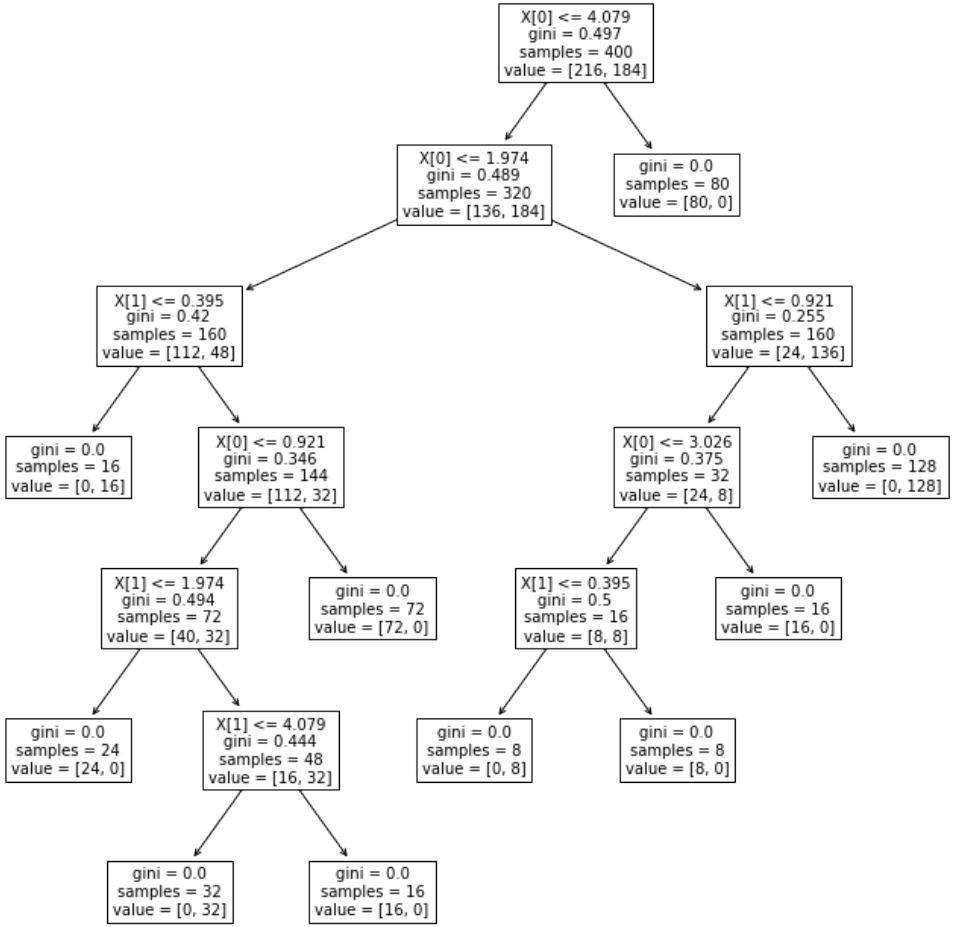
- *Is the node pure enough?*
- *Has the tree reached max depth?*
- *Is the number of samples in the split too small?*

Decision Trees – Python Details

Visualizing the model:

```
# Showing the resulting decision tree
plt.figure(figsize=(12,12))
tree.plot_tree(model, fontsize=10)
plt.show()
```

Note: first split occurs along x1 rather than x2, because it is the only split that allows a pure child leaf:



Decision Trees – Python Details

Varying depth of the tree:

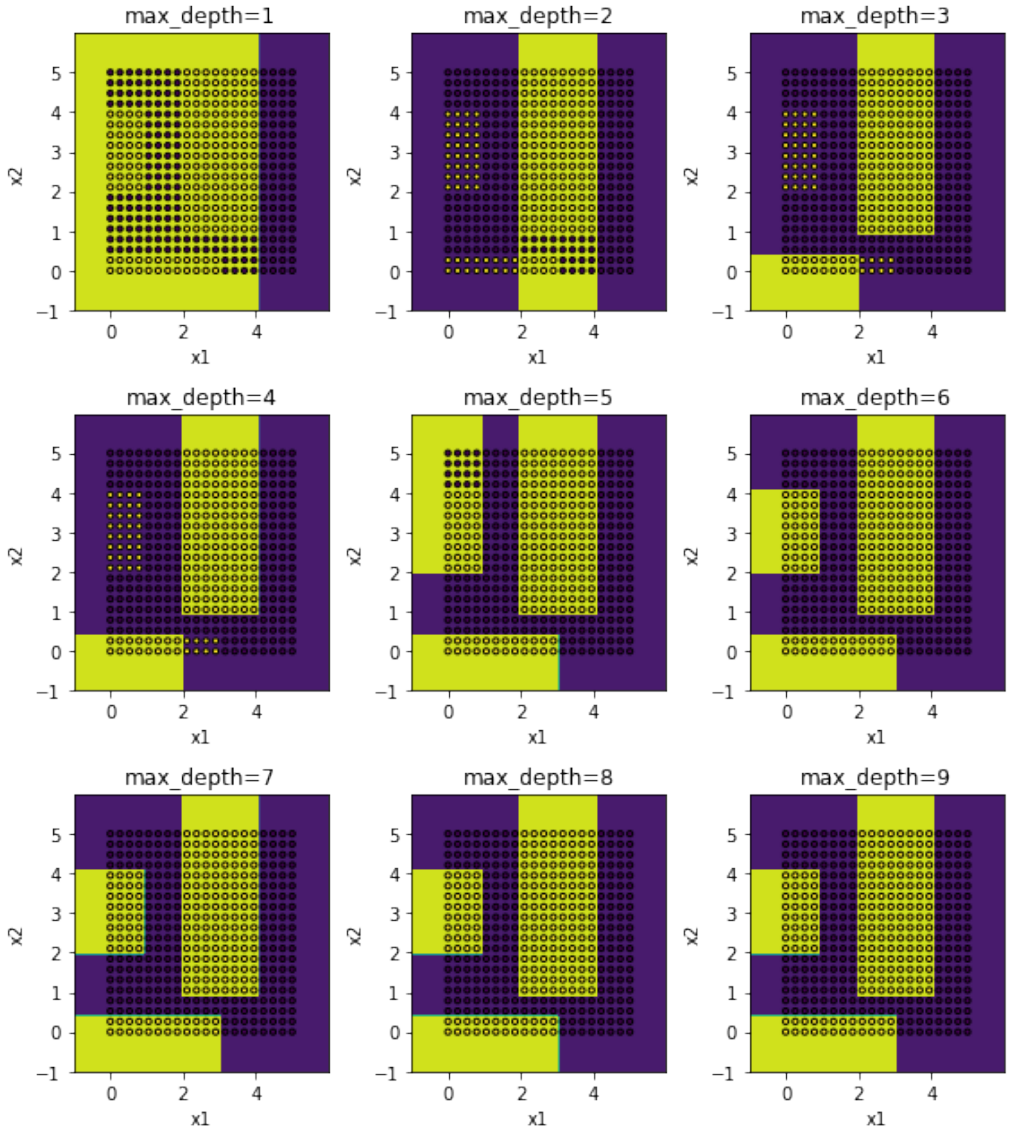
```
# Loop over max_depth and evaluate the results
plt.figure(figsize=(8,9))
for i in range(1,10):
    model = tree.DecisionTreeClassifier(max_depth=i) model.fit(X,Y)
    ax = plt.subplot(3,3,i)
    Z = model.predict(np.c_[xx.ravel(), yy.ravel()])
    Z = Z.reshape(xx.shape)
    ax.contourf(xx, yy, Z)

    # Plot original data
    ax.scatter(X[:,0],X[:,1],s=10,edgecolors="k",c=Y)
    ax.set_xlabel("x1")
    ax.set_ylabel("x2")
    ax.set_title("max_depth={}".format(i))
plt.tight_layout()
plt.show()
```

Decision Trees – Python Details

Varying depth of the tree:

Clearly, adding more complexity after max_depth=6 adds no explanatory power to the model



Decision Trees – Limits of Validation Data

Using validation data to select max_depth:

```
import random
from sklearn.metrics import accuracy_score

# Using validation data to determine an optimal tree depth
inds = list(range(len(X)))
random.shuffle(inds)
train_inds = inds[:int(len(X)*0.8)]
val_inds = inds[int(len(X)*0.8):]
X_train = X[train_inds]
Y_train = Y[train_inds]
X_val = X[val_inds]
Y_val = Y[val_inds]

# Loop over max_depth and evaluate the results
plt.figure(figsize=(8,9))
for i in range(1,10):
    model = tree.DecisionTreeClassifier(max_depth=i)
    model.fit(X_train,Y_train)
    Y_pred = model.predict(X_val)
    acc = accuracy_score(Y_val,Y_pred)
    ax = plt.subplot(3,3,i)
    Z = model.predict(np.c_[xx.ravel(), yy.ravel()])
    Z = Z.reshape(xx.shape)
    ax.contourf(xx, yy, Z)

    # Plot original data
    ax.scatter(X[:,0],X[:,1],s=10,edgecolors="k",c=Y)
    ax.set_xlabel("x1")
    ax.set_ylabel("x2")
    ax.set_title("max_depth={}\nAccuracy:{}".format(i,acc))
plt.tight_layout()
plt.show()
```

Decision Trees – Limits of Validation Data

Using validation data to select max_depth:

Why don't we our validation error eventually increase as we increase the complexity of the tree?

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