Decision Trees

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Data 22100

A closer look at Decision Tree Classifiers

- The code below loads data from the Framingham Heart Disease study and fit it to a decision tree classifier.
- See the review notebook on trees for more details.

Example: the Framingham Heart Disease study dataset

In [35]:
```
import pandas as pd
import numpy as np

%matplotlib inline
import matplotlib.pyplot as plt
plt.style.use('fivethirtyeight')

from sklearn.preprocessing import StandardScaler
from sklearn.model_selection import train_test_split

from sklearn.tree import DecisionTreeClassifier as dec_tr

from sklearn.model_selection import cross_val_score, \
                                    LeaveOneOut, \
                                    RepeatedKFold
from sklearn.metrics import mean_squared_error, \
                            roc_curve, auc, f1_score
```

```
from sklearn.metrics import f1_score, precision_score, \
                            recall_score, accuracy_score

fhd_df = pd.read_csv('data/Framingham_heart_disease.csv')
fhd_df.head()
```

Out[35]:

	male	age	education	currentSmoker	cigsPerDay	BPMeds	prevalentStroke	preva
0	1	39	4.0	0	0.0	0.0	0	
1	0	46	2.0	0	0.0	0.0	0	
2	1	48	1.0	1	20.0	0.0	0	
3	0	61	3.0	1	30.0	0.0	0	
4	0	46	3.0	1	23.0	0.0	0	

In [36]:
```
fhd_df = fhd_df.dropna()
print('# records where TenYearCHD=0 is: %d'%sum(fhd_df.TenYearCHD==0))
print('# records where TenYearCHD=1 is: %d'%sum(fhd_df.TenYearCHD==1))
```

```
# records where TenYearCHD=0 is: 3099
# records where TenYearCHD=1 is: 557
```

There is substantial class imbalance (noted).

Use `sklearn.tree.DecisionTreeClassifier as dec_tr` to predict Coronary Heart Disease risk at 10 years (binary outcome)

- Drop missing values.
- Standardize (relevant) columns.
- Split the data.
- Calculate mean F1 score using cross-validation with the training data.
- Predict for testing data.
- Calculate score using predictions and testing data.

In [37]:
```
from sklearn.model_selection import train_test_split

##############################
# Deal with missing values  #
# (Imputing is mentioned in #
#       the review)         #
##############################

fhd_df = fhd_df.dropna()

#################################
# Standardize numerical columns #
```

```
################################

cat_cols = ['male', 'education', 'currentSmoker', 'BPMeds', \
            'prevalentStroke', 'prevalentHyp', 'diabetes']
num_cols = ['age', 'cigsPerDay', 'totChol', 'sysBP', 'diaBP', \
            'BMI', 'heartRate', 'glucose']
std_cols = ['std '+c for c in num_cols]

scaler = StandardScaler()
scaler.fit(fhd_df[num_cols]) # get all the means and stds

# subtract means and divide by stds
fhd_df[std_cols] = scaler.transform(fhd_df[num_cols])


################################################
# Split data to training and testing datasets #
################################################
predictors = std_cols
outcome = 'TenYearCHD'
X_train, X_test, y_train, y_test = train_test_split(fhd_df[predictors],
                                                    fhd_df[outcome],
                                                    test_size=0.3)


############################################
# Cross validate to get evaluation metircs  #
############################################

model = dec_tr()
k_folds = RepeatedKFold(n_splits=20, n_repeats=5, random_state=1)
scores = cross_val_score(model, X_train, y_train,
                     scoring='f1',
                     cv=k_folds, n_jobs=None) # use one processor to
                                        # succesfully suppress warnings
print(f'Mean F1 score={np.abs(scores).mean():.3f}')


########################################
# Train the model / fit model parameters #
#       and test on testing dataset      #
########################################

model.fit(X_train, y_train)
y_hat = model.predict(X_test)
print(f'F1 score = {f1_score(y_test, y_hat):.3f}')
```

```
Mean F1 score=0.229
F1 score = 0.216
```

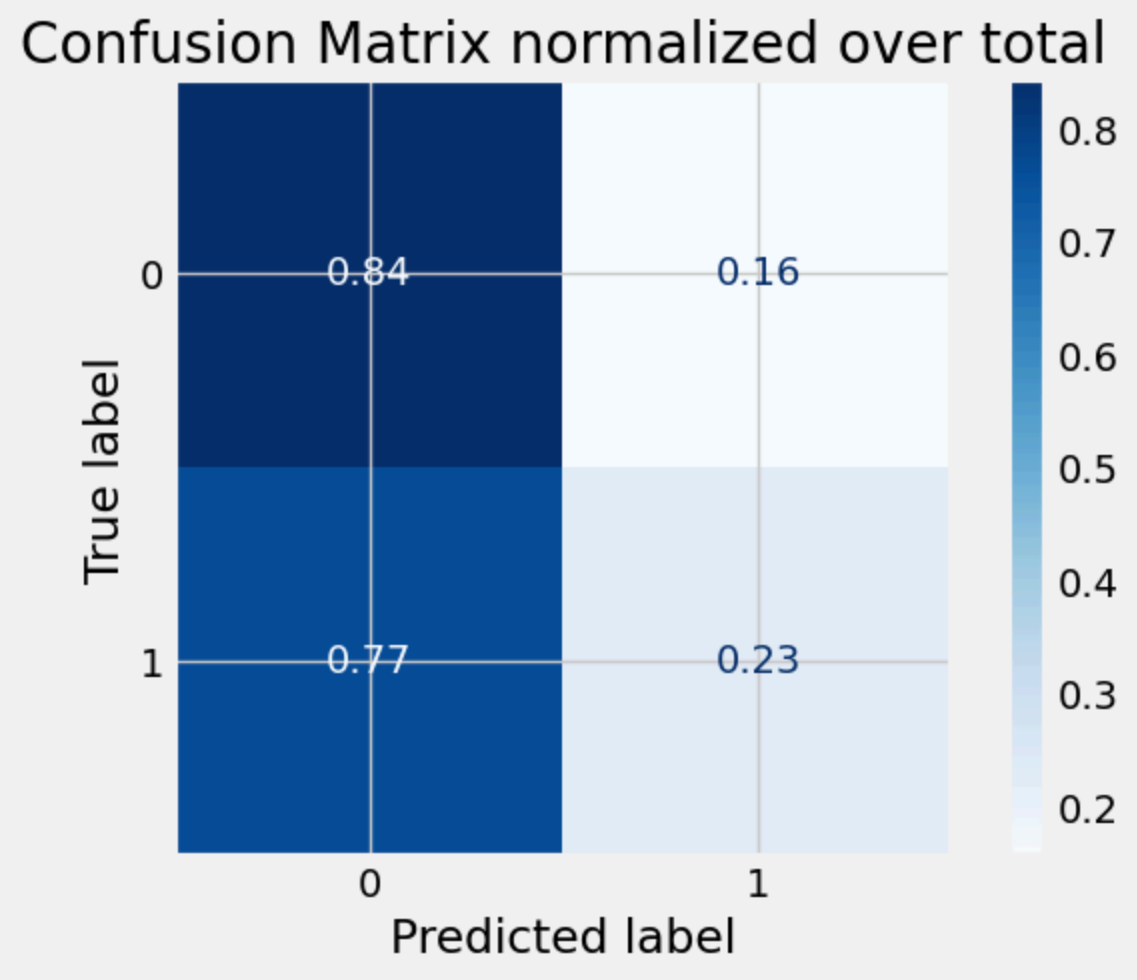
Why if the F2 score low?

In [38]:

```
from sklearn.metrics import confusion_matrix, ConfusionMatrixDisplay

disp = ConfusionMatrixDisplay.from_predictions(
     y_test,
```

```
    y_hat,
    cmap=plt.cm.Blues,
    normalize='true', # Normalized over the true outcomes (rows)
                      # Shows Type II error rates
   )
disp.ax_.set_title('Confusion Matrix normalized over total');
```

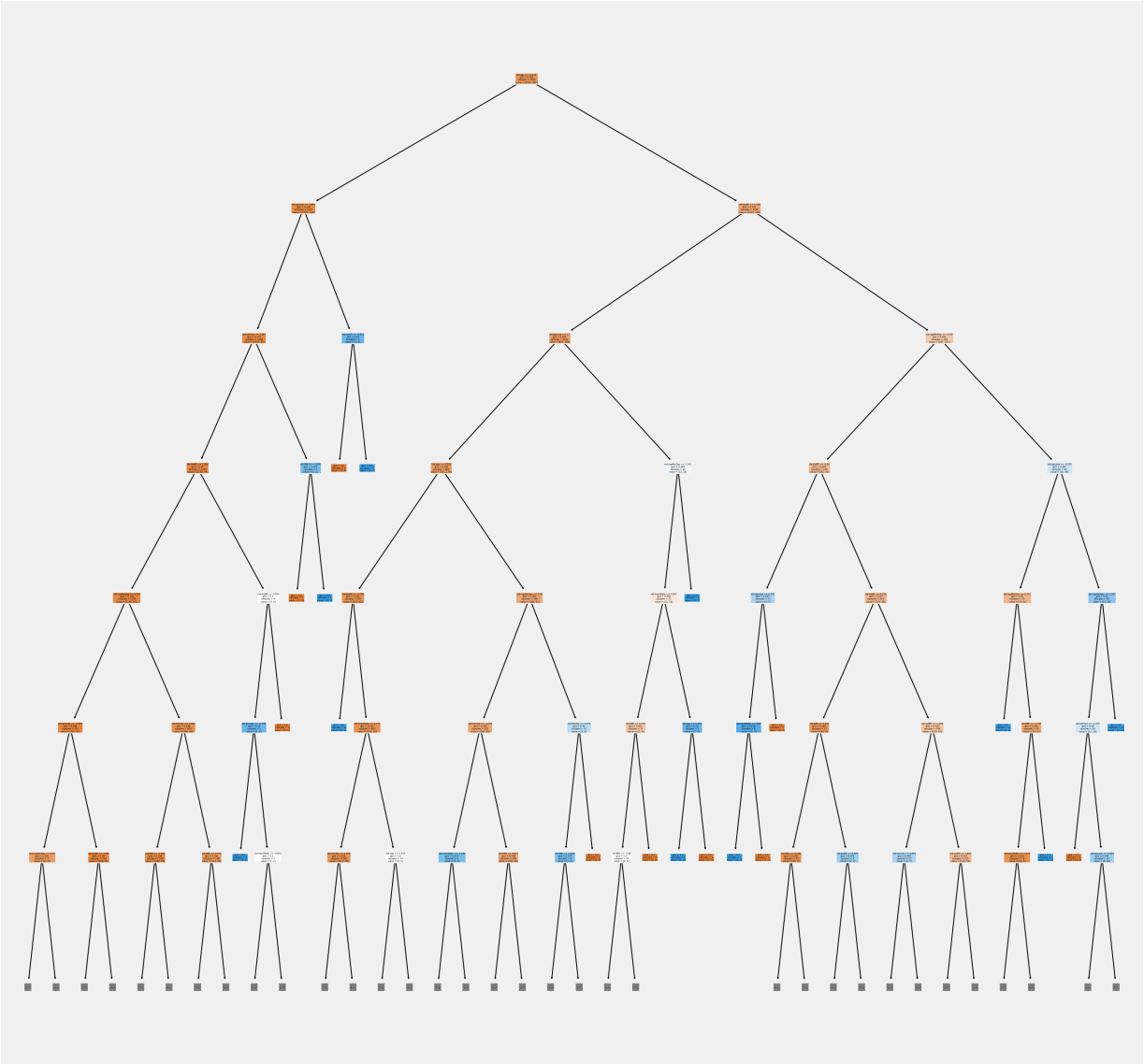


Apparently, there are **not so many true positives**.

What does the decision tree look like?

In [39]:
```
import matplotlib.pyplot as plt
from sklearn import tree

fig, axes = plt.subplots(nrows = 1,ncols = 1,figsize = (10,10), dpi=300)
tree.plot_tree(model,
               feature_names = predictors,
               filled = True,
               max_depth=6);
```



The classes in the FHD dataset are highly imbalanced

(There are ways to **try to** deal with that but they are out of scope).

Why?

- Maybe not all the predictors are relevant?
- Maybe the decisions where chosen poorly?
- Maybe the dataset is not well-suited for decision trees?

How is the decision tree generated?

For instance, is there one 'decision level' per predictor?

In [40]:
```
print('# predictors = %d'%len(predictors))
print('Depth of decision tree = %d'%(model.tree_.max_depth))
```

```
# predictors = 8
Depth of decision tree = 22
```

Apparently, a predictor can be used more than once...

There are several deterministic algorithms for generating a single decision tree

They have names such as ID3, C4.5, or CART.

They vary in some details (binary tree or not, gini or entropy, ...) but share a common logic.

Decision tree algorithm requires an Attribute Selection Measure

---

An **Attribute Selection Measure (ASM)** maps the set of features to a set of scores
given a dataset. The higher the score, the better the feature 'explains' the outcome
in a given dataset. For continuous features, the ASM also determines the splitting point, e.g., `age>30`.

The Decision Tree algorithm

Given a choice of an Attribute Selection Measure:

- Select the best attribute to split the records.
- The selected attribute becomes a **decision node**.
- Breaks the dataset into smaller subsets depending on the value of the decision attribute.
- Repeat this proces (recursively) for each child of the decision node
  until one of the following conditions is true:
  - All remaining records lead to the same decision.
  - The specified (hyperparameter) maximal tree depth was reached.
  - The specified (hyperparameter) minimum number of samples to spilt was reached,
    e.g., a node with less samples will be made a leaf node.
  - No more features/decisions can increase homogeneity.

Example: building a small tree using entropy as an ASM

Entropy can be thought of as a measure of inhomogeneity. The larger it is, the more mixed the sample.

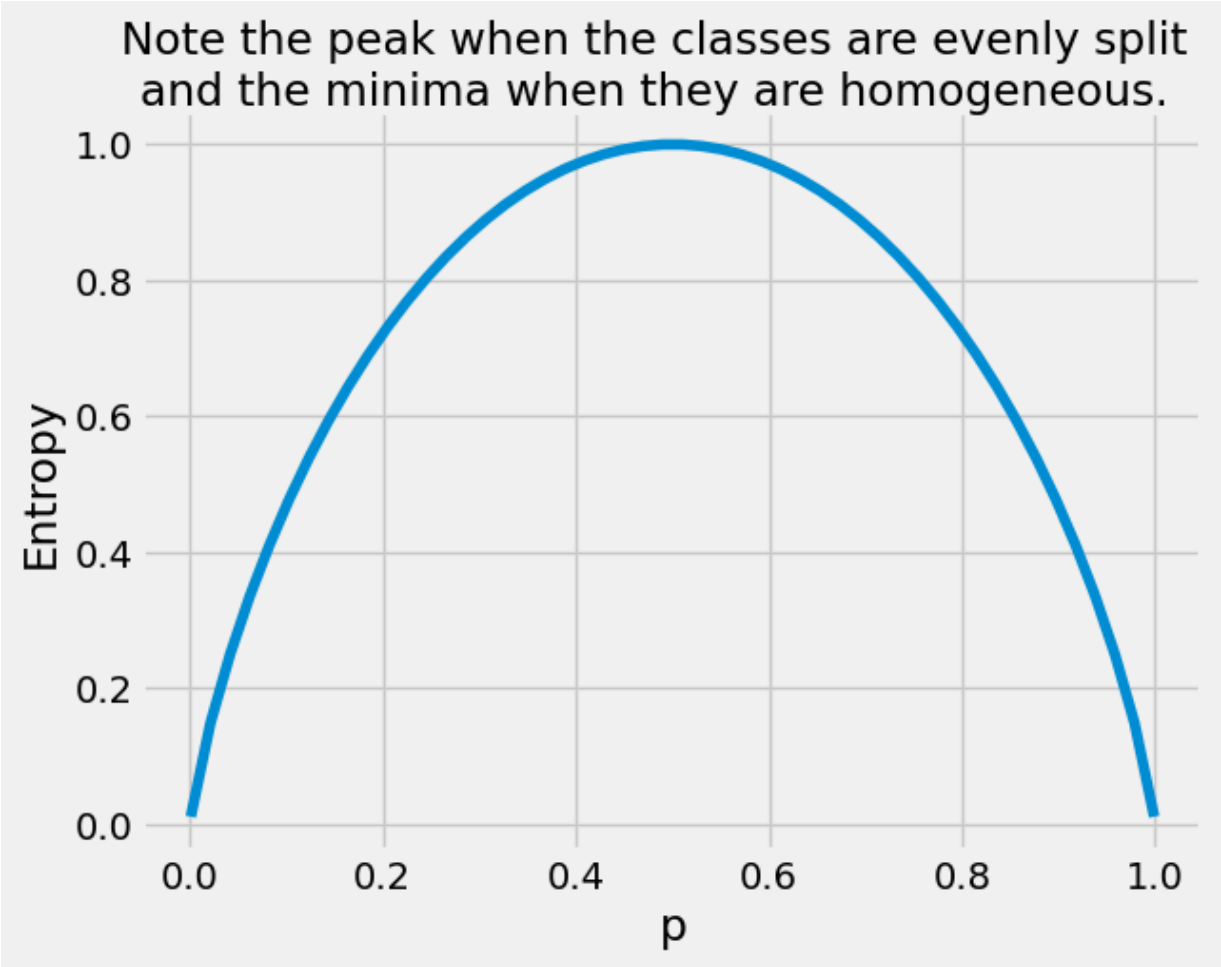
$$\mathcal{E} = -\sum_i p_i \log_2 p_i \tag{1}$$

$$\text{where } p_i = \text{ probability of class}_i = \frac{\text{No. in class}_i}{\text{Total no. in both classes}} \tag{2}$$

$$\text{For two classes:} \quad \mathcal{E} = -\left[p_0 \log_2 p_0 + (1-p_0)\log_2(1-p_0)\right] \tag{3}$$

In [41]:
```
def binary_entropy(p):
    """
    Calculates the entropy of a Bernoulli random variable with
    probability p.
    Uses log base 2.
    """
    return -(p * np.log2(p) +(1-p) * np.log2(1-p))

p = np.linspace(0.001,0.999,50)
plt.plot(p, binary_entropy(p))
plt.xlabel('p')
plt.ylabel('Entropy')
supttl = 'Note the peak when the classes are evenly split\n'
supttl += 'and the minima when they are homogeneous.'
plt.suptitle(supttl);
```



Consider the following fictitious 'dataset':

In [42]:
```
fake_df = pd.DataFrame([[20, 100, 0],
                        [30, 130, 0],
                        [40, 150, 1],
                        [45, 140, 1],
                        [50, 110, 0],
                        [60, 140, 1],
                        [65, 120, 0],
                        [70, 110, 0],
                        [80, 130, 1],
                        [90, 120, 1]], columns=['Age', 'sysBP', 'HD'])
fake_df
```

Out[42]:

	Age	sysBP	HD
0	20	100	0
1	30	130	0
2	40	150	1
3	45	140	1
4	50	110	0
5	60	140	1
6	65	120	0
7	70	110	0
8	80	130	1
9	90	120	1

Proportion of positive cases in the data:

$$P(\text{HD} = 1) = \frac{5}{10} = \frac{1}{2}$$

The entropy of the HD label in the overall data set is:

$$\mathcal{E} = -\left[\frac{1}{2}\log_2\frac{1}{2} + \frac{1}{2}\log_2\frac{1}{2}\right] = 1.0$$

Confirm the above calculation with code:

In [43]:
```
n_1 = (fake_df['HD']==1).sum()
n_0 = (fake_df['HD']==0).sum()
p = n_1 / (n_1 + n_0)
e = binary_entropy(p)

print(f'Number of positive cases (HD=1): n1 = {n_1}')
print(f'Number of negative cases (HD=0): n0 = {n_0}')
print(f'Proportion of positive cases: p = {p}')
print(f'Entropy of HD: E = {e} bits')
```

```
Number of positive cases (HD=1): n1 = 5
Number of negative cases (HD=0): n0 = 5
Proportion of positive cases: p = 0.5
Entropy of HD: E = 1.0 bits
```

Considering a split

What if we split by `Age < 55`?

Proportions and entropies on either side of the split:

$$P(\text{HD}=1 \mid \text{Age}<55)=\frac{2}{5} \qquad P(\text{HD}=1 \mid \text{Age}\geq 55)$$
$$\mathcal{E}_{\text{Age}<55}=-\left[\frac{2}{5}\log_2\frac{2}{5}+\frac{3}{5}\log_2\frac{3}{5}\right]\approx 0.97 \qquad \mathcal{E}_{\text{Age}\geq 55}=-\left[\frac{3}{5}\log_2\frac{3}{5}+\frac{2}{5}\log_2\frac{2}{5}\right]$$

Half the data points are on each side of the split $P(\text{Age}<55)=\frac{5}{10}=\frac{1}{2}$, so the **average entropy** at level 1 would be:

$$\mathcal{E}_1=\frac{1}{2}\mathcal{E}_{\text{Age}<55}+\frac{1}{2}\mathcal{E}_{\text{Age}\geq 55}\approx 0.97$$

Confirm with code:

In [44]:
```
df_split_older = fake_df[fake_df['Age'] >= 55] # older than 55
df_split_younger = fake_df[fake_df['Age'] < 55] # younger than 55

p_older = df_split_older['HD'].mean() # Pr{HD | older}
p_younger = df_split_younger['HD'].mean() # Pr{HD | younger}

e_older = binary_entropy(p_older) # binary entropy of older group
e_younger = binary_entropy(p_younger) # binary entropy of younger group

print(f'Entropy of HD among older: {e_older:.2f} bits')
print(f'Entropy of HD among younger: {e_younger:.2f} bits')

prop_older = (fake_df['Age'] >= 55).mean() # Pr{older}
prop_younger = 1-prop_older # Pr{younger}
e_split = prop_older * e_older + prop_younger * e_younger

print(f'Average entropy of HD at this level: {e_split:.2f} bits')
```

```
Entropy of HD among older: 0.97 bits
Entropy of HD among younger: 0.97 bits
Average entropy of HD at this level: 0.97 bits
```

Considering a different split

What if we instead split by `sysBP < 125`?

Using more general notation for splits:

Proportions and entropies on either side of the split:

$$P(\text{HD}=1 \mid \text{yes})=\frac{1}{5} \qquad P(\text{HD}=1 \mid \text{no})=\frac{4}{5}$$
$$\mathcal{E}_{yes}=-\left[\frac{1}{5}\log_2\frac{1}{5}+\frac{4}{5}\log_2\frac{4}{5}\right]\approx 0.722 \qquad \mathcal{E}_{no}=-\left[\frac{4}{5}\log_2\frac{4}{5}+\frac{1}{5}\log_2\frac{1}{5}\right]\approx 0.7$$

Half the data points are again on each side of the split $P(yes)=\frac{5}{10}=\frac{1}{2}$, so the **average entropy** at level 1 would be:

$$\mathcal{E}_1=\frac{1}{2}\mathcal{E}_{yes}+\frac{1}{2}\mathcal{E}_{no}\approx 0.722$$

Confirm with code:

In [45]:
```
# more general notation:

condition = fake_df['sysBP'] < 125

df_split_1_yes = fake_df[condition] # 'yes': condition satisfied
df_split_1_no = fake_df[~condition] # 'no': condition not satisfied

p_1_yes = df_split_1_yes['HD'].mean() # Pr{HD | yes}
p_1_no = df_split_1_no['HD'].mean()   # Pr{HD | no}

e_yes = binary_entropy(p_1_yes) # binary entropy given 'yes'
e_no = binary_entropy(p_1_no)   # binary entropy given 'no'

print(f'Entropy of HD for yes: {e_yes:.3f} bits')
print(f'Entropy of HD for no: {e_no:.3f} bits')

prop_yes = (condition).mean() # Pr{'yes'} = Pr{condition satisfied}
prop_younger = 1-prop_older # Pr{'no'} = Pr{condition not satisfied}
e_split = prop_yes * e_yes + (1-prop_yes) * e_no

print(f'Average entropy of HD at this level: {e_split:.3f} bits')
```

```
Entropy of HD for yes: 0.722 bits
Entropy of HD for no: 0.722 bits
Average entropy of HD at this level: 0.722 bits
```

Choosing between possible splits

Both splits reduce entropy but the second split is **preferable** because it results in **lower average entropy** than the first.

Information gain (in brief)

$$\boxed{\text{Information Gain} = \text{Entropy}_{\text{parent node}} - \text{Average Entropy}_{\text{child nodes}}}$$

This is what we want to **maximize**.

Choosing the best possible split (i.e., learning)

Coming up with the **split point** is similar:

For each feature:

- The values are sorted
- Mid-points between adjacent values evaluated.
- Best split (best feature/value combination) is chosen.

Another possible criterion: Gini

The **Gini** index can be thought of as a measure of inhomogeneity. The larger it is, the more mixed the sample.

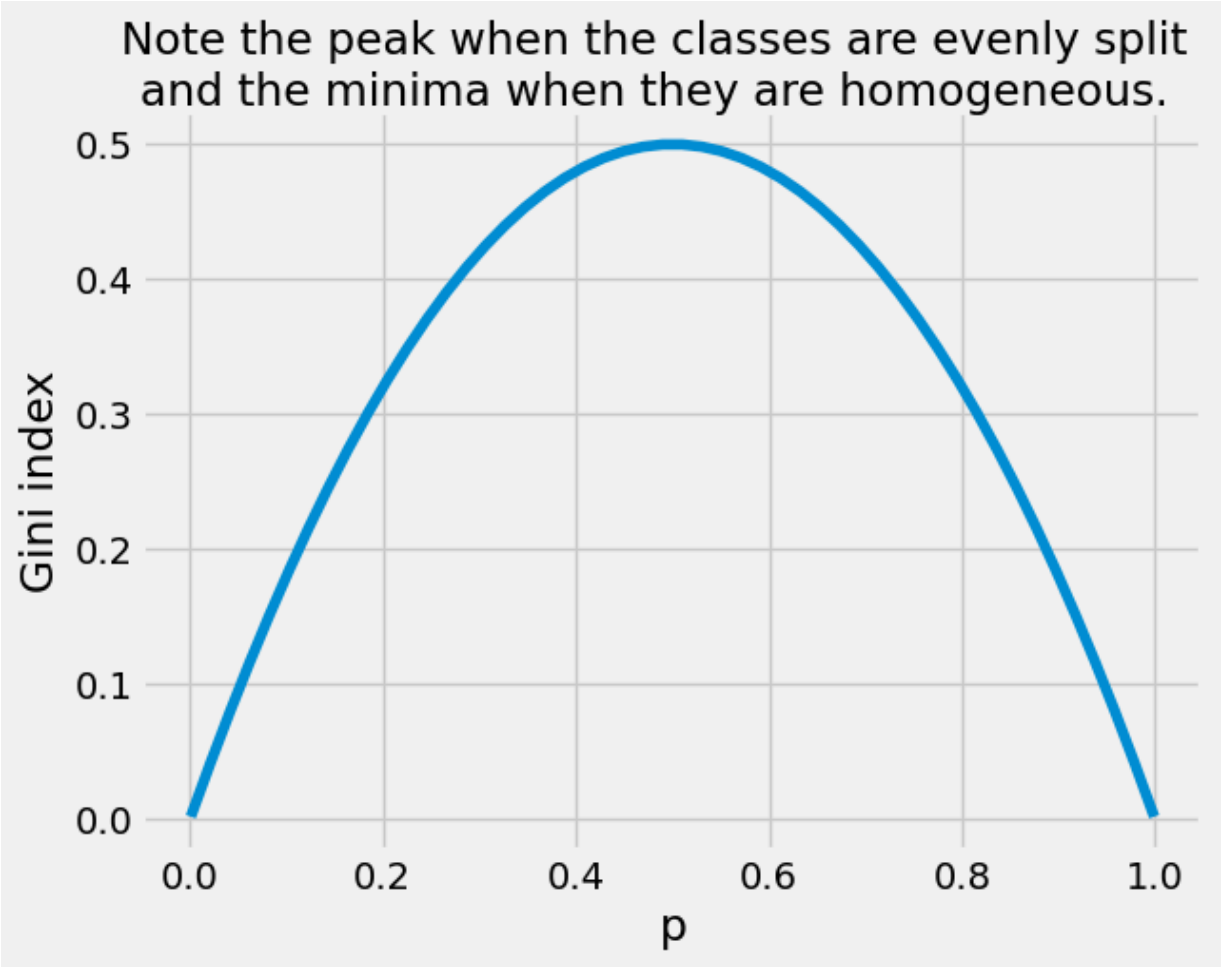
$$\mathcal{E} = 1 - \sum_i p_i^2 \tag{8}$$

$$\text{where } p_i = \text{ probability of class}_i = \frac{\text{No. in class}_i}{\text{Total no. in both classes}} \tag{9}$$

$$\tag{10}$$

$$\text{For two classes: } \mathcal{E} = 1 - \left[p_0^2 + (1-p_0)^2\right] \tag{11}$$

In [46]:
```
p = np.linspace(0.001,0.999,50)
gini = 1 - (p**2 + (1-p)**2)
plt.plot(p, gini)
plt.xlabel('p')
plt.ylabel('Gini index')
supttl = 'Note the peak when the classes are evenly split\n'
supttl += 'and the minima when they are homogeneous.'
plt.suptitle(supttl);
```



Example: Brexit data

This dataset breaks the Brexit vote to 650 constituencies and looks at demographic statistics such as eduction, immigration, race/ethnicity, and income.

Questions the data may address is whether factors such as overall wealth, a multi cultural environment, age, etc. may have influenced the vote.
Or rather, were they good predictors of the vote?

The data breakdown is based on publically available UK government (census-like) data, UK electoral commission data, and the work of a BBC team that matched the different datasets.

The datasets are fairly clean but there is some wrangling necesary

- A few special characters need to be replaced.
- A few naming discrepencies need to be resolved.

In [50]:
```
import pandas as pd
import numpy as np

##############################
```

```
# Rudimentary Data Wrangling #
#    (crude, but will do)    #
#############################

# Read ethnicity data file
ethn_df = pd.read_csv('data/Brexit-Constituency-Ethnicity.csv')

# Rename the constituency column (for later join)
ethn_df.rename({'ConstituencyName': 'Constituency'}, axis=1,
               inplace=True)

# Sort alphabetically by constituency
ethn_df.sort_values(by='Constituency', axis=0, ascending=True,
                    inplace=True, ignore_index=True)

# Correct wrong character
ethn_df.loc[647, 'Constituency'] = 'Ynys Mon'

# Correct name (extra 'South' moved)
ethn_df.loc[117, 'Constituency'] = \
    'Carmarthen West and South Pembrokeshire'

# Read constituency data file
data_df = pd.read_csv('data/Brexit-UK-constituency-data.csv')

# Rename the constituency column (for later join)
data_df.rename({'PCON14NM': 'Constituency'}, axis=1, inplace=True)

# Remove 'England', 'Northern Ireland', 'Scotland', 'UK', 'Wales'
# from constituencies
data_df = data_df[~data_df['Constituency'].isin(\
        ['England', 'Northern Ireland', 'Scotland', 'UK', 'Wales'])]

# Sort alphabetically by constituency
data_df.sort_values(by='Constituency', axis=0, ascending=True,
                    inplace=True, ignore_index=True)

# Correct wrong character
data_df.loc[647, 'Constituency'] = 'Ynys Mon'

# Read results (votes) data file
rslt_df = pd.read_csv('data/Brexit-results.csv')

# Sort alphabetically by constituency
rslt_df.sort_values(by='Constituency', axis=0, ascending=True,
                    inplace=True, ignore_index=True)

# Make sure that constituencies in ethn_df match those in rslt_df
# and that constituencies in data_df match those in rslt_df
for k in range(len(rslt_df)):
    if (rslt_df.Constituency[k] in ethn_df.Constituency[k]) or \
       (ethn_df.Constituency[k] in rslt_df.Constituency[k]):
        ethn_df.loc[k, 'Constituency'] = rslt_df.Constituency.values[k]
    if (rslt_df.Constituency[k] in data_df.Constituency[k]) or \
       (data_df.Constituency[k] in rslt_df.Constituency[k]):
        data_df.loc[k, 'Constituency'] = rslt_df.Constituency.values[k]
```

```
#for c in set(data_df.Constituency) - set(rslt_df.Constituency):
#    idxs = [i for i in rslt_df.Constituency.index if \
#            c in rslt_df.Constituency[i]]
#    jdxs = [j for j in data_df.Constituency.index if \
#            c in data_df.Constituency[j]]
#    if len(idxs)==1 and len(jdxs)==1:
#        data_df.loc[jdxs[0], 'Constituency'] = \
#                    rslt_df.Constituency.values[idxs[0]]

# Check that data_df, rslt_df, and ethn_df have the same lengths
print('Length of dataframes: ', len(rslt_df),
                                 len(data_df), len(ethn_df))

# Check the class balance between constituencies 'for' and 'against'
print('Class Balance: %.1f%% for leaving and %.1f%% against.'%\
                      (100*sum(rslt_df.Leave>'50')/len(rslt_df),
                       100*sum(rslt_df.Leave<'50')/len(rslt_df)))

# Check that data_df, rslt_df, and ethn_df have the same constituencies
print('Constituency name discrepencies:',
      set(rslt_df.Constituency) - set(data_df.Constituency),
      set(data_df.Constituency) - set(rslt_df.Constituency),
      set(rslt_df.Constituency) - set(ethn_df.Constituency),
      set(ethn_df.Constituency) - set(rslt_df.Constituency) )
```

```
Length of dataframes:  650 650 650
Class Balance: 62.9% for leaving and 37.1% against.
Constituency name discrepencies: set() set() set() set()
```

Choosing predictors and dealing with missing values

Here, as opposed to previous datasets, it may make more sense to impute missing demographic statistics than simply drop records with missing values.

- The number of records is not very large to begin with.
- The number of missing values is rather small.
- Statistics such as mean age, income, and education level don't fluctuate wildly for large groups of people (like constituencies).

In [53]:
```
##########################################
# Determine predictor and outcome columns #
#    (and fill in some missing values)    #
##########################################

# Creat a 'Brexit' column:
#    1 for leaving the EU ('yes' to Brexit)
#    0 for staying in the EU ('no' to Brexit)
rslt_df['Brexit'] = (rslt_df.Leave>'50').astype(int)

rslt_df.head(20)
df = rslt_df
df = df.merge(data_df, how='inner')
df = df.merge(ethn_df, how='inner')
```

```
outcome = 'Brexit'
predictors = [
       'salary', 'publicsector', 'degree', 'age', 'nonukborn',
       'health', 'PopTotalConstNum', 'PopWhiteConst%',
       'PopMixedConst%', 'PopAsianConst%', 'PopBlackConst%',
       'PopWhiteReg%',   'PopMixedReg%',   'PopAsianReg%',
       'PopBlackReg%'
    ]

# Convert 'x' (code for missing values) to np.nan
print("Missing values in public sector column (no. of 'x's):",
                                        len(df[df.publicsector=='x']))
df.loc[df.publicsector=='x','publicsector'] = np.nan

# Convert all predictors types to float
df[predictors] = df[predictors].astype(float)

# Replace missing values with the mean value:
from sklearn.impute import SimpleImputer
imp = SimpleImputer(missing_values=np.nan, strategy='mean')
vals2d = df.publicsector.values.reshape(-1, 1)
imp.fit(vals2d) # the imputer fitting function needs a 2d array
df.publicsector = imp.transform(vals2d).reshape(-1) # pandas need a
                                                    # 1d array
print('\nAfter imputing...')
print("Missing values in public sector column (no. of NaNs):",
                                              df.isnull().sum().sum())
```

```
Missing values in public sector column (no. of 'x's): 18

After imputing...
Missing values in public sector column (no. of NaNs): 0
```

Model:

- Split the data.
- Calculate mean F1 score by cross-validating the training data.
- Train/fit the model.
- Predict using the testing data.
- Score the model on the predictions and the testing data.
- Print the number of predictors and the maximal depth of the tree.

In [55]:
```
################################################
# Split data to training and testing datasets #
################################################
X_train, X_test, y_train, y_test = train_test_split(df[predictors],
                                                    df[outcome],
                                                    test_size=0.3)
                                # different splits -> different trees

############################################
# Cross validate to get evaluation metircs  #
############################################
```

```
model = dec_tr()
k_folds = RepeatedKFold(n_splits=20, n_repeats=5, random_state=1)
scores = cross_val_score(model, X_train, y_train,
                     scoring='f1',
                     cv=k_folds, n_jobs=None) # use one processor
                              # to succesfully suppress warnings
print('CV: Mean F1 score=%.2f'%np.abs(scores).mean())


##########################################
# Train the model / fit model parameters #
#       and test on testing dataset      #
##########################################

model.fit(X_train, y_train)
y_train_hat = model.predict(X_train)
y_hat = model.predict(X_test)
print('F1 score for the *training* dataset = %.3f'%\
       f1_score(y_train, y_train_hat))
print('F1 score for the *testing* dataset = %.3f'%\
       f1_score(y_test, y_hat))
print('# predictors = %d'%len(predictors))
print('Depth of the decision tree = %d'%(model.tree_.max_depth))
```

```
CV: Mean F1 score=0.88
F1 score for the *training* dataset = 1.000
F1 score for the *testing* dataset = 0.850
# predictors = 15
Depth of the decision tree = 12
```

The training data score is perfect but the testing data score is not worlds apart and the CV score is similar to the testing score.

Good start!

Still, the model is complicated

- Many predictors (> 10)
- Deep tree (> 10)
- Some overfitting (training score is perfect)

Pruning

Pre-pruning

Stopping the growth of the decision tree early by setting hyperparameters.

In `sklearn`:

- `max_depth` sets the maximal depth of the tree.
- `min_samples_leaf` sets minimum number of samples required to be at a leaf node (default=1).
- `min_samples_split` sets the smallest sample size that can be further split.

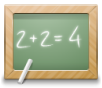
Good values for these hyperparameters can be found with `GridSearchCV` (although there is no guarantee that a better optimum does not exist).

Post pruning (Cost Complexity Pruning)

- Typically, the tree is grown freely and afterwards parts of it are removed (to reduce overfitting).
- In theory, best if every subtree is scored using some classification error metric, e.g., accuracy.
  Subtrees that do not improve the performance of the tree on a CV/test dataset are removed.

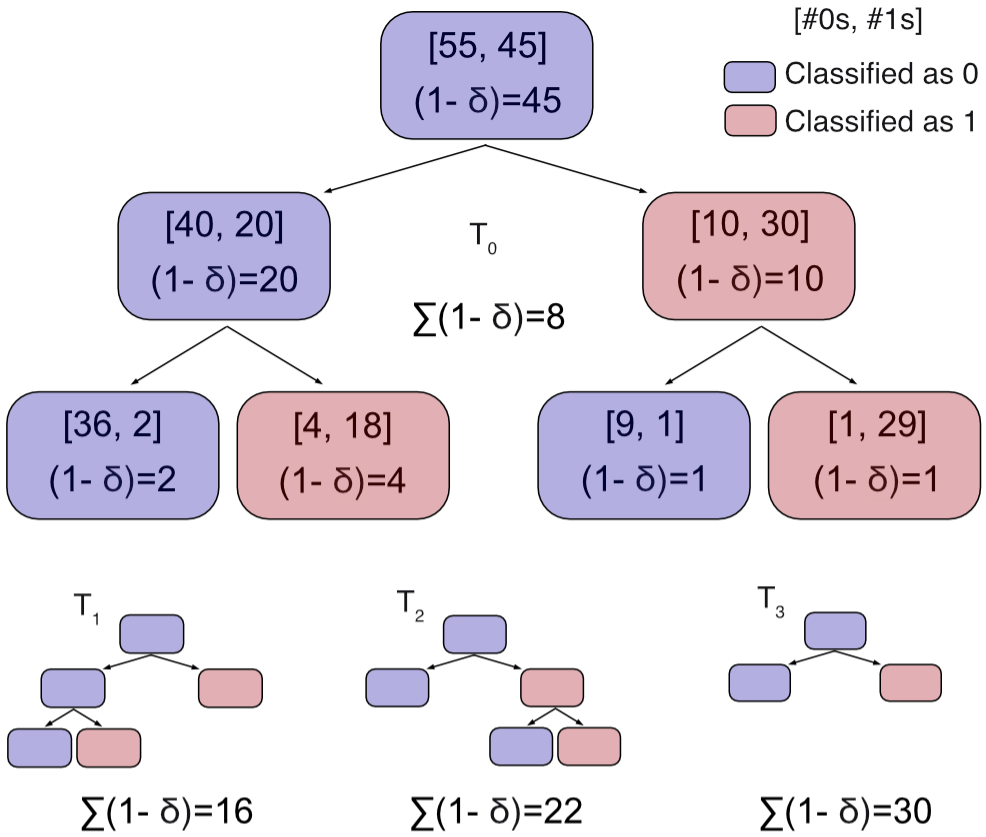
However...

- Systematically evaluating **every subtree** of a complex tree is computationally expensive (it will take forever).
  Cost Complexity Pruning (CCP) is more efficient.
- Similar to Lasso regularization, CCP places an $L1$ **complexity penalty** on the tree.
- The strength of the complexity penalty is tuned using the hyperparameter α.
- An good value for α is found through cross-validation.



The gist of it is demonstrated in the following example:

$$
\begin{aligned}
|T| &= \text{the number of leafs in the tree= 'complexity'} \\
\{k_\ell\} &= \text{indices of all the records (predictors/outcome rows) that lead} \\
y_{k_\ell},\ \hat{y}_{k_\ell} &= \text{actual and predicted outcomes associated with leaf } \ell \\
\delta_{\hat{y},\,y} &= \begin{cases} 1 & \text{if } \hat{y} = y \\ 0 & \text{if } \hat{y} \neq y \end{cases} \\
SE_\ell &= \sum_{k_\ell} \left[1 - \delta_{\hat{y}_{k_\ell},\, y_{k_\ell}}\right] = \text{no. of errors (misclassifications) for leaf } \ell \\
\text{Overall score} &= \sum_{\ell=1}^{|T|} SE_\ell \ + \ \alpha|T| \\
&= \text{total no. of errors summed over all leafs + complexity pena}
\end{aligned}
$$



$T_1 < T_2$ always
--> T_2 is never optimal.

$T_3 < T_1$ when $\alpha > 14$ and $T_3 < T_0$ when $\alpha > 22/2$
--> T_3 is optimal when $\alpha > 14$.

if $\alpha < 14$ then $T_1 < T_0$ when $\alpha > 8$
--> T_1 is optimal when $8 < \alpha < 14$.

if $\alpha < 8$ then T_0 is optimal.

Conclusion: cross-validate with, say, $\alpha = 4, 11, 17$

▶ ← Also...

Cost Complexity Pruning with `sklearn`

- Train your Decision Tree model to its **full depth**
- Compute `ccp_alphas` using `cost_complexity_pruning_path()`

- Compute test/train (or cross-validated) scores for each value in `ccp_alphas`.
- Plot the scores for each value in `ccp_alphas`.

Another way to avoid an overly complicated tree:

Feature selection by Importance (I)

Features can be selected using a feature importance score:

Feature importance is a score assigned to each feature based on how significant they are at predicting the outcome. The score is based on **weighted Gini indices**.

- Feature importance scores can provide insight into the data by pointing to the most relevant features (and the least relevant ones). This could inform further data collection, for instance.
- Feature importance scores can improve the model through feature selection (drop the least important ones).

Calculating feature importances

- **The importance of a Node:**

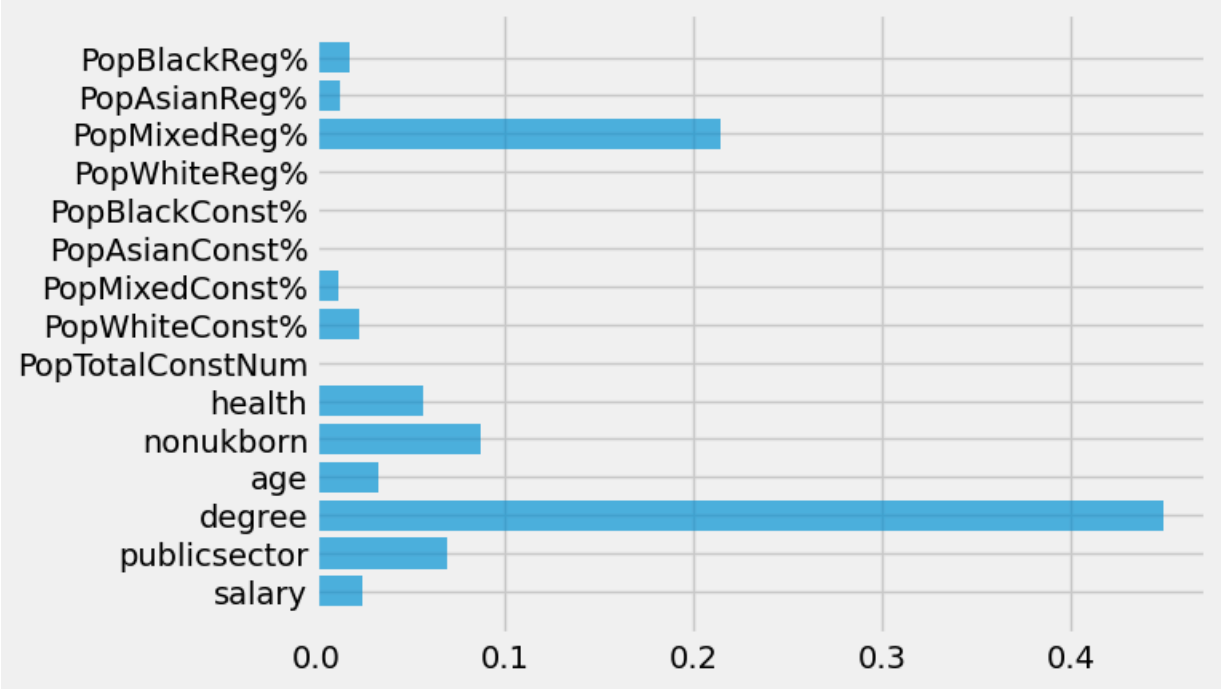
$$\begin{aligned} f(\text{ node }) &= (\%\text{ samples reaching node }) \times (\text{ Gini impurity of} \\ NodeImportance(\text{ node }) &= f(\text{node }) - f(\text{ left child }) - f(\text{ right child }) \\ &\quad (\text{for a leaf: } \%\text{ samples reaching a child } = 0) \end{aligned}$$

- **The importance of a feature:**

$$FeatureImportance(\text{ feature}_k) = \frac{\sum_{\text{nodes splitting on feature}_k} NodeImportance(\text{ n}}{\sum_{\text{all nodes}} NodeImportance(\text{ node })}$$

The sklearn implementation of decision trees calculates `feature_importances_`

In [56]:
```
plt.barh(predictors, model.feature_importances_, alpha=0.67);
```



Train an 'extensive tree' and calculate the Cost Complexity Alphas:

In [57]:

```
################################################
# Split data to training and testing datasets #
################################################
X_train, X_test, y_train, y_test = train_test_split(df[predictors],
                                                    df[outcome],
                                                    test_size=0.3)
                                # different splits -> different trees

################################################
# Initialize an instance of the model object #
################################################
model = dec_tr()

########################################
# Train the model / fit model parameters #
#       and test on testing dataset      #
########################################

model.fit(X_train, y_train)
y_train_hat = model.predict(X_train)
y_hat = model.predict(X_test)
print('Depth of the decision tree = %d'%(model.tree_.max_depth))
print('The no. of leaves in the decision tree = %d'%\
      (model.get_n_leaves()) )
print('F1 score for the *training* dataset = %.3f'%\
      f1_score(y_train, y_train_hat))
print('F1 score for the *testing* dataset = %.3f'%\
      f1_score(y_test, y_hat))

######################
# Compute ccp_alphas #
######################
```

```
path = model.cost_complexity_pruning_path(X_train,y_train)
alphas = path['ccp_alphas']
alphas
```

```
Depth of the decision tree = 11
The no. of leaves in the decision tree = 45
F1 score for the *training* dataset = 1.000
F1 score for the *testing* dataset = 0.899
```

Out[57]:
```
array([0.        , 0.00173718, 0.00212422, 0.00217338, 0.0029304 ,
       0.0032406 , 0.0032967 , 0.0035964 , 0.00376766, 0.00384615,
       0.0040293 , 0.00417436, 0.00417977, 0.0043956 , 0.00494505,
       0.00497964, 0.00544223, 0.00561661, 0.00603792, 0.00633176,
       0.00956891, 0.02812628, 0.08163842, 0.1949952 ])
```

Calculate and plot accuracy scores for each Cost Complexity Alpha:

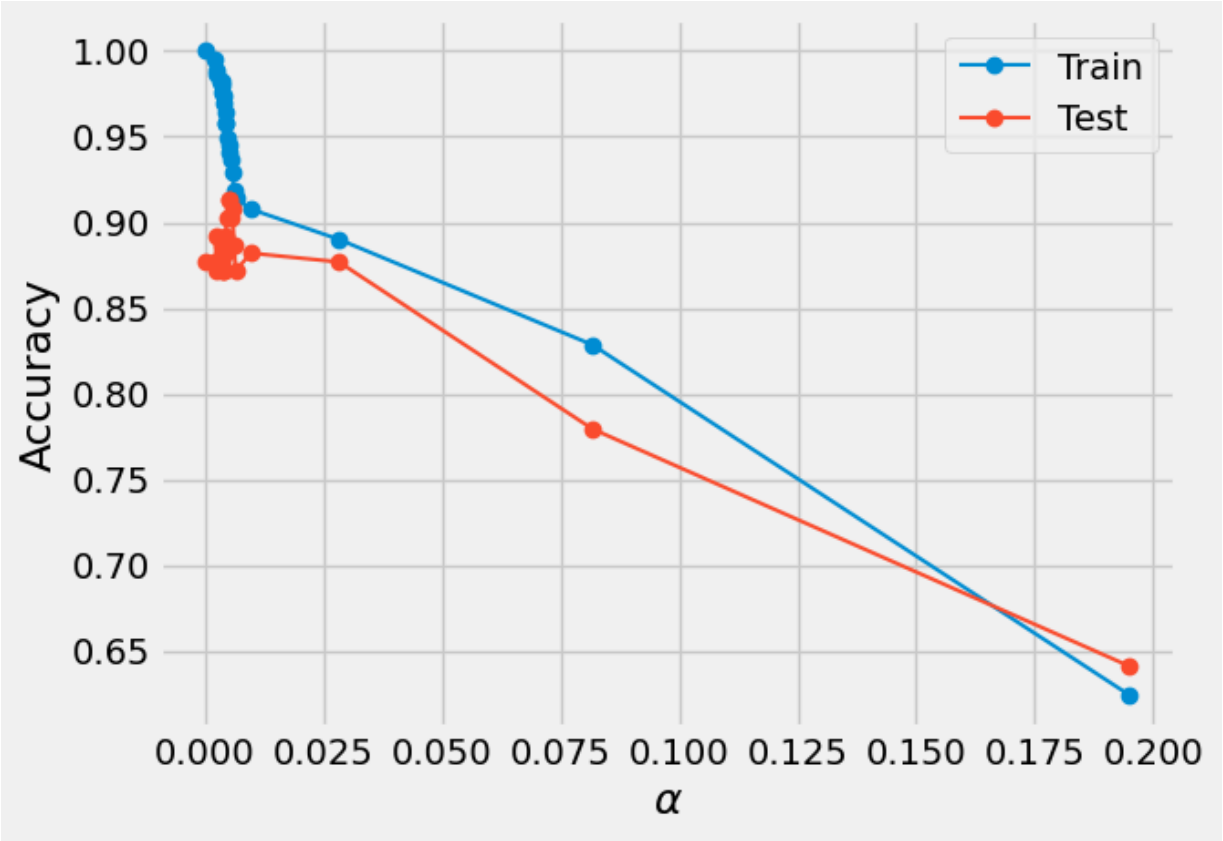
In [58]:
```
############################################################
# Compute test/train scores for each value in ccp_alphas #
############################################################

accuracy_train, accuracy_test = [], []

for alpha in alphas:
    model_alpha = dec_tr(ccp_alpha=alpha)
    model_alpha.fit(X_train, y_train)
    y_train_hat = model_alpha.predict(X_train)
    y_hat = model_alpha.predict(X_test)

    # (BTW, Instead of one test/train score, its more time-consuming
    #  but more stable to save cross-validation scores, or run this
    # code with several test_train_splits and look at a few
    #   'best' alphas)
    accuracy_train.append(accuracy_score(y_train, y_train_hat))
    accuracy_test.append(accuracy_score(y_test, y_hat))

plt.plot(alphas, accuracy_train, color='C0', marker='o', linewidth=1.5)
plt.plot(alphas, accuracy_test, color='C1', marker='o', linewidth=1.5)
plt.xlabel(r'$\alpha$')
plt.ylabel('Accuracy')
plt.legend(['Train', 'Test']);
```



Choose an α value that performs well on the testing data and fit the model:

In [59]:
```
##########################################
# Train the model / fit model parameters #
#       with the best alpha              #
##########################################

best_alpha = 0.02
model_alpha = dec_tr(ccp_alpha=best_alpha)
model_alpha.fit(X_train, y_train)
y_train_hat = model_alpha.predict(X_train)
y_hat = model_alpha.predict(X_test)

print('Depth of the decision tree = %d'%(model_alpha.tree_.max_depth))
print('The no. of leaves in the decision tree = %d'%\
      (model_alpha.get_n_leaves()) )
print('F1 score for the *training* dataset = %.3f'%\
      f1_score(y_train, y_train_hat))
print('F1 score for the *testing* dataset = %.3f'%\
      f1_score(y_test, y_hat))
```

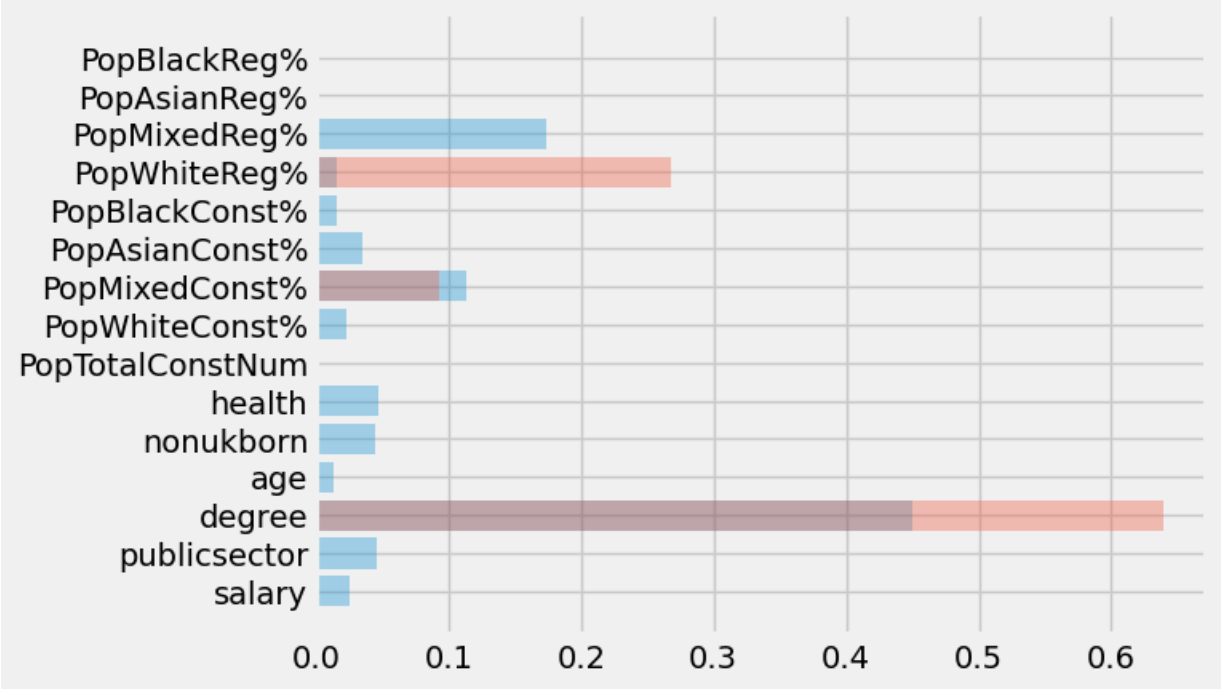
```
Depth of the decision tree = 3
The no. of leaves in the decision tree = 4
F1 score for the *training* dataset = 0.928
F1 score for the *testing* dataset = 0.910
```

Note:

- The result is a much simpler model!
- Overfitting the training data is considerably reduced.
- Performance on the testing dat didn't suffer...

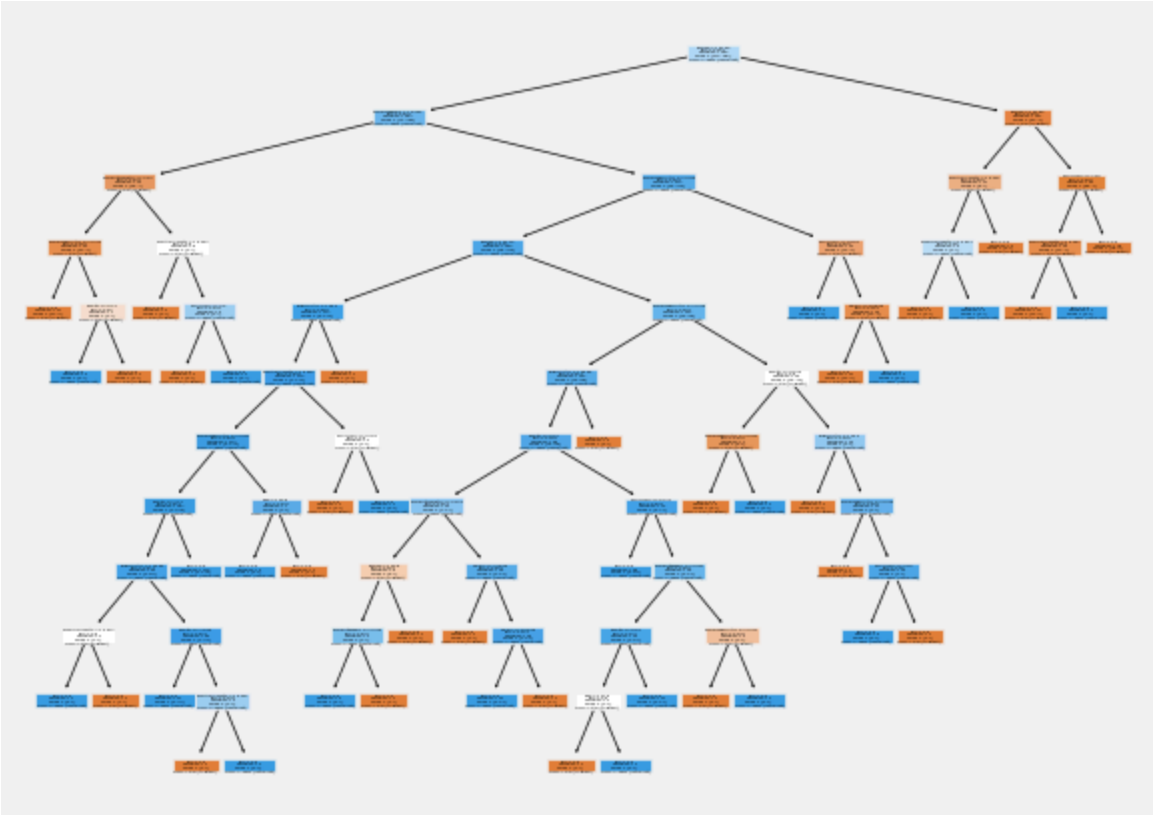
Pruned trees have different importance scores, of course:

In [60]:
```
plt.barh(predictors, model.feature_importances_, alpha=0.33)
plt.barh(predictors, model_alpha.feature_importances_, alpha=0.33);
```

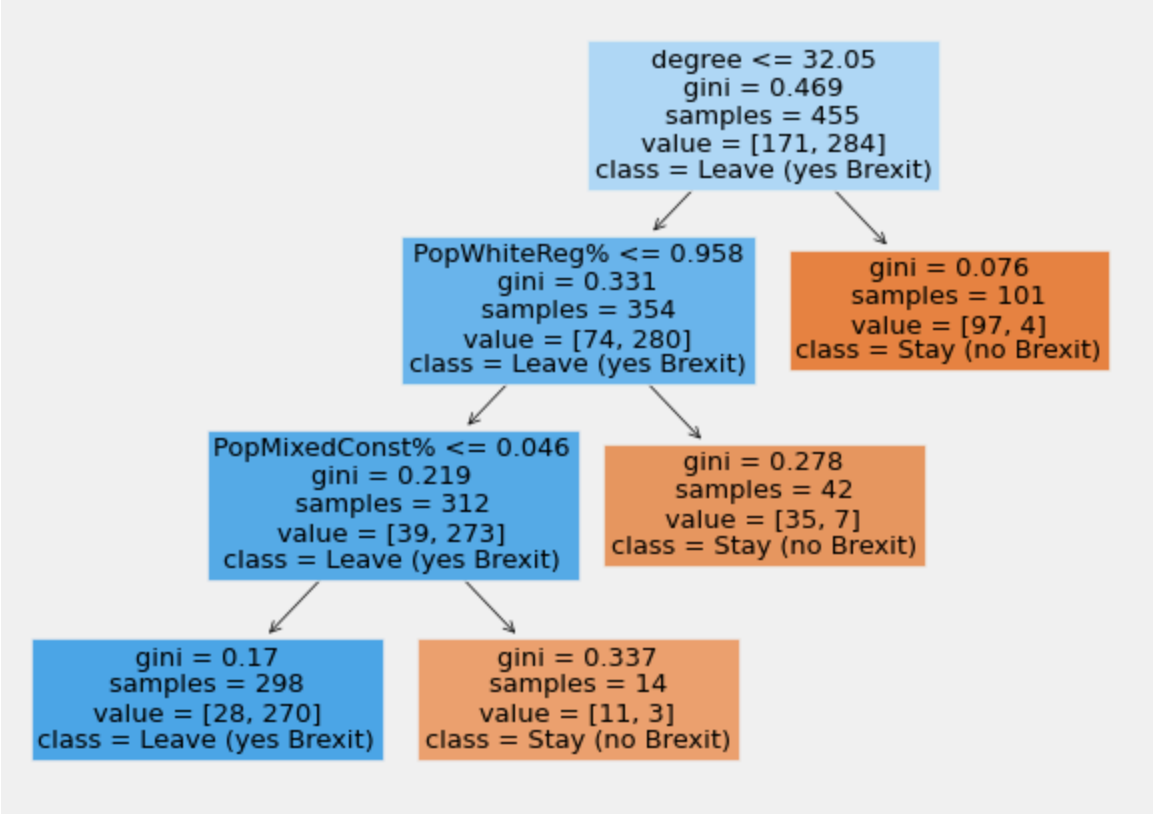


Visualizing the original and the pruned trees:

In [61]:
```
# Original:
tree.plot_tree(model,
               feature_names = predictors,
               class_names=['Stay (no Brexit)', 'Leave (yes Brexit)'],
               filled = True);
```



In [62]:
```
# Pruned:
tree.plot_tree(model_alpha,
               feature_names = predictors,
               class_names=['Stay (no Brexit)', 'Leave (yes Brexit)'],
               filled = True);
```



Finally, it is typically more stable to use cross-validated scores for choosing α:

In [69]:
```
%%time

#####################################################################
# Compute cross-validated scores for each value in ccp_alphas #
#####################################################################

accuracy_CV = []

for alpha in alphas:
    model_alpha = dec_tr(ccp_alpha=alpha)
    model_alpha.fit(X_train, y_train)
    y_train_hat = model_alpha.predict(X_train)
    y_hat = model_alpha.predict(X_test)

    k_folds = RepeatedKFold(n_splits=20, n_repeats=5, random_state=1)
    scores = cross_val_score(model, X_train, y_train,
                    scoring='accuracy',
                    cv=k_folds, n_jobs=None)
    accuracy_CV.append(scores.mean())
```

```
CPU times: user 10.7 s, sys: 100 ms, total: 10.8 s
Wall time: 11.5 s
```

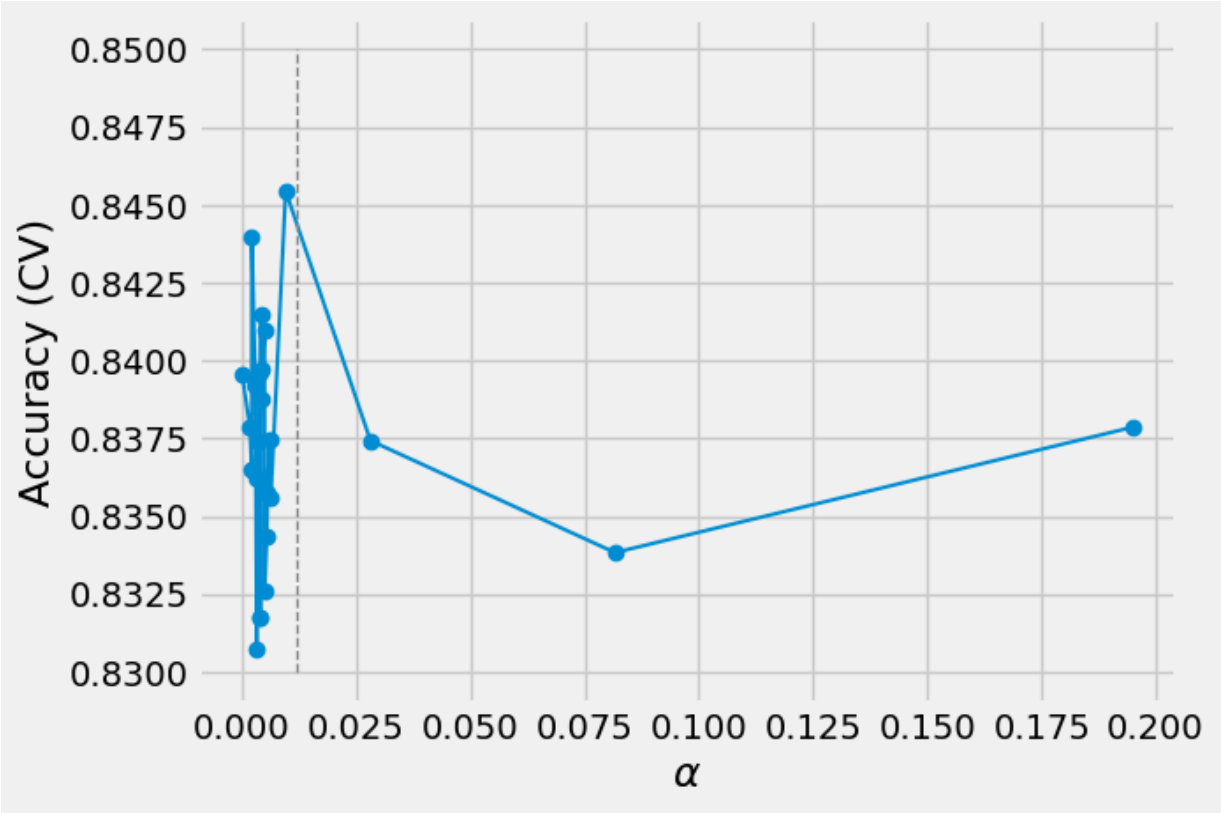
In [72]:
```
best_alpha = 0.012

plt.plot(alphas, accuracy_CV, color='C0', marker='o', linewidth=1.5)
plt.xlabel(r'$\alpha$')
plt.ylabel('Accuracy (CV)')
plt.plot([best_alpha, best_alpha], [0.83, 0.85], linestyle='dashed',
         color='C4', linewidth=1);

model_alpha = dec_tr(ccp_alpha=best_alpha)
model_alpha.fit(X_train, y_train)
y_train_hat = model_alpha.predict(X_train)
y_hat = model_alpha.predict(X_test)

print('Depth of the decision tree = %d'%(model_alpha.tree_.max_depth))
print('The no. of leaves in the decision tree = %d'%\
      (model_alpha.get_n_leaves()) )
print('F1 score for the *training* dataset = %.3f'%\
      f1_score(y_train, y_train_hat))
print('F1 score for the *testing* dataset = %.3f'%\
      f1_score(y_test, y_hat))
```

```
Depth of the decision tree = 3
The no. of leaves in the decision tree = 4
F1 score for the *training* dataset = 0.928
F1 score for the *testing* dataset = 0.910
```



Ensemble methods

Single trees are **sensitive to sample size:**

- Small datasets are particularly prone to overfitting.
- Large ones can result in overly complex trees.

Using **multiple (weak) learners** can yield better predictions.

In [ ]: