Decision Trees

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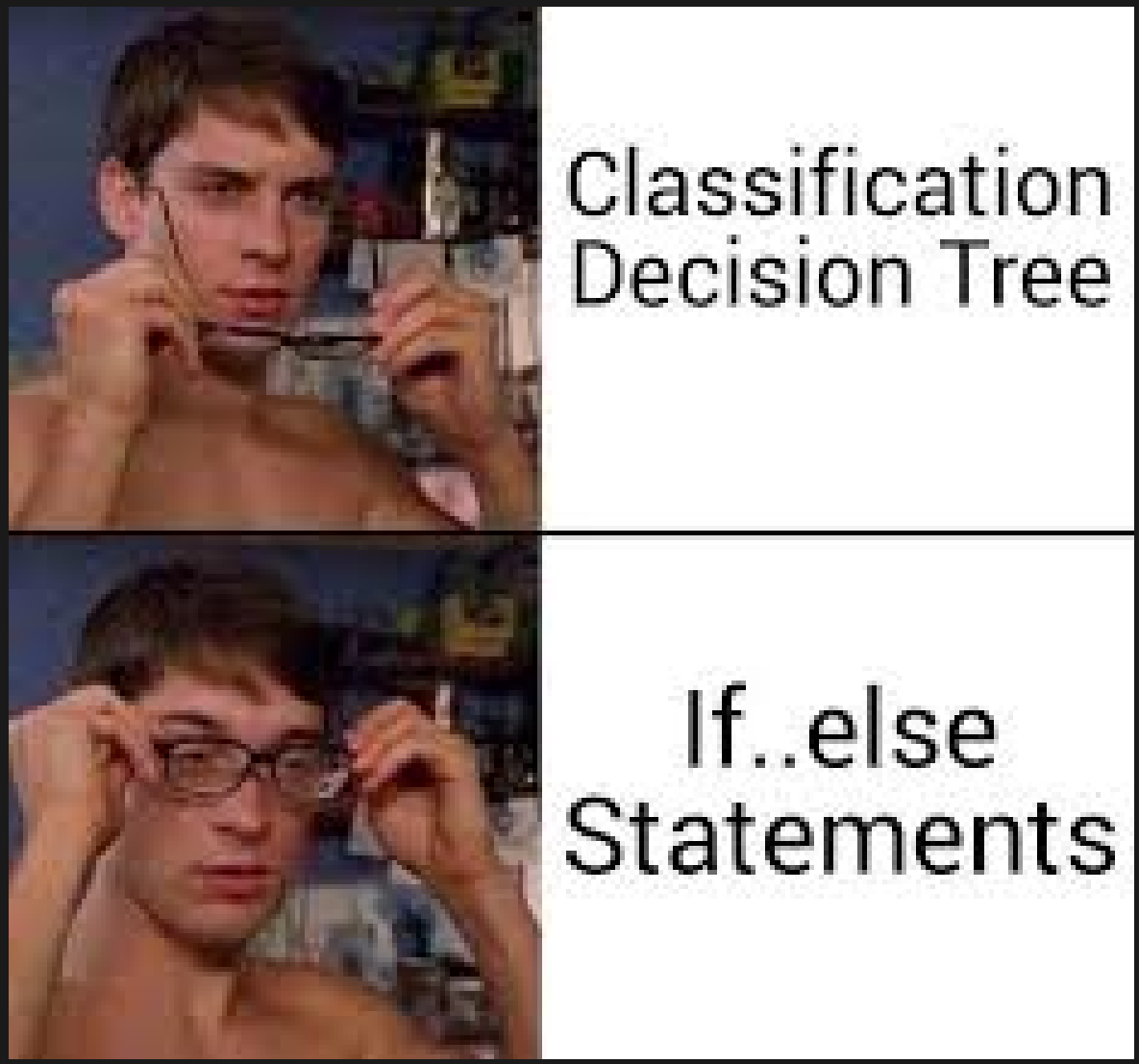
Lecture 06.1 (v3.0.0)



neuralnetmemes on IG

Signposting

- - This is the final set of key classification tools: Decision Trees and Random Forests.
  - We'll also cover regression trees.
- The Workshop covers using them in practice.

Questions

- Which splits should we make in a tree?
- When should we stop splitting?
- How can we combine multiple trees?

Trees, Forests, Decisions

- **Decision trees**: are extremely flexible and can fit highly non-linear spaces.
  - They can capture arbitrary complexity in the training data
  - They tend to overfit
  - They have overly-regular shapes, aligned to features
- **Random Forests**: Combining many random, decision trees
  - Randomization fights overfitting
  - Averaging creates smoother decision boundaries
  - Remarkable predictive performance.

Some data, before we start

```
from sklearn.model_selection import train_test_split

X_train, X_test, y_train, y_test = train_test_split(
    features_pd, labels, train_size=0.8, test_size=0.2)
```

Decision Tree

- A decision tree is a sequence of conditionally evaluated tests:
- If c_1 then:
  - If c_{11} then:
    - ...
  - Else $!c_{11}$ so:
    - ...
- Else $!c_1$ so:
  - If c_{21} then:
    - ...
  - Else $!c_{21}$ so:
    - ...
- The conditions need to be chosen appropriately. How to decide?

Decision Tree Algorithm: CART

- **Classification and Regression Trees** (CART)[1]
- Consider a decision tree for C classes.
- For each **feature** $j \in [1, \cdots, J]$, we evaluate the **best-split** location in the feature space...
  - i.e. the one that **Minimises** the "Gini impurity":

$$G_j = 1 - \sum_{c=1}^{C} p_{jc}^2 = \sum_{c=1}^{C} p_{jc}(1 - p_{jc}).$$

  - The assignment probability p_{jc} is the probability that class c is found at this leaf of the tree, if we use feature j.
  - We choose the "best" (induces many $p \to 0$ or $p \to 1$) feature as the next split.

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[1] CART = Classification and Regression Trees. Breiman, Leo; Friedman, J. H.; Olshen, R. A.; Stone, C. J. (1984). Classification and regression trees. See Wei-Yin Loh's Review

Gini index example

```
def sq(y):
    return y * y
sq = np.vectorize(sq)
def gini(x):
    return 1-sq(x/x.sum()).sum()
```

Gini index example

```
test=pd.DataFrame()
test["size0"]=np.array([100,100,100])
test["size1.1"]=np.array([50,50,50])
test["size1.2"]=np.array([50,50,50])
test["size2.1"]=np.array([100,0,0])
test["size2.2"]=np.array([0,100,100])
```

Gini index example

```
test=pd.DataFrame()
test["size0"]=np.array([100,100,100])
test["size1.1"]=np.array([50,50,50])
test["size1.2"]=np.array([50,50,50])
test["size2.1"]=np.array([100,0,0])
test["size2.2"]=np.array([0,100,100])

print("Gini index initial value    =",gini(test["size0"]))
print("Gini reduction from split 1 =",gini(test["size0"]) -
  (gini(test["size1.1"])/2+gini(test["size1.2"])/2))
print("Gini reduction from split 2 =",gini(test["size0"]) -
  (gini(test["size2.1"])*1/3+gini(test["size2.2"])*2/3))
```

Gini index example

```
test=pd.DataFrame()
test["size0"]=np.array([100,100,100])
test["size1.1"]=np.array([50,50,50])
test["size1.2"]=np.array([50,50,50])
test["size2.1"]=np.array([100,0,0])
test["size2.2"]=np.array([0,100,100])

print("Gini index initial value    =",gini(test["size0"]))
print("Gini reduction from split 1 =",gini(test["size0"]) -
  (gini(test["size1.1"])/2+gini(test["size1.2"])/2))
print("Gini reduction from split 2 =",gini(test["size0"]) -
  (gini(test["size2.1"])*1/3+gini(test["size2.2"])*2/3))
```

```
Gini index initial value    = 0.666666666667
Gini reduction from split 1 = 0.0
Gini reduction from split 2 = 0.333333333334
```

Decision Tree Algorithm: ID3

- But is Gini Index *right*?
- ID3[2] (Iterative Dichotomiser 3) **Maximises** the "information gain", by **Minimising**:

$$H_j = -\sum_{c=1}^{C} p_{jc} \log(p_{jc})$$

  - The difference is how each probability is weighted.
  - We still define "best" feature as one that makes many $p \to 0$ and $p \to 1$.
  - Gini punishes large absolute-value mistakes whilst information punishes large log-scale mistakes.
  - The difference is important for a tree but usually unimportant for the classifier.

[2] ID = Iterative Dichotomiser. Quinlan, J. R. 1986. Induction of Decision Trees. Mach. Learn. 1, 1 (Mar. 1986), 81-106.

ID3

```
def ylogy(y): # CAREFUL!
    ty=[max(1e-10,x) for x in y]
    return y * np.log(ty)
def id3(x):
return -ylogy(x/x.sum()).sum()
```

ID3

```
def ylogy(y): # CAREFUL!
    ty=[max(1e-10,x) for x in y]
    return y * np.log(ty)
def id3(x):
return -ylogy(x/x.sum()).sum()

print("ID3 index initial value    =",id3(test["size0"]))
print("ID3 reduction from split 1 =",id3(test["size0"]) -
  (id3(test["size1.1"])/2+id3(test["size1.2"])/2))
print("ID3 reduction from split 2 =",id3(test["size0"]) -
  (id3(test["size2.1"])*1/3+id3(test["size2.2"])*2/3))
```

ID3

```
def ylogy(y): # CAREFUL!
    ty=[max(1e-10,x) for x in y]
    return y * np.log(ty)
def id3(x):
return -ylogy(x/x.sum()).sum()

print("ID3 index initial value    =",id3(test["size0"]))
print("ID3 reduction from split 1 =",id3(test["size0"]) -
  (id3(test["size1.1"])/2+id3(test["size1.2"])/2))
print("ID3 reduction from split 2 =",id3(test["size0"]) -
  (id3(test["size2.1"])*1/3+id3(test["size2.2"])*2/3))

ID3 index initial value    = 1.0986122886681096
ID3 reduction from split 1 = 0.0
ID3 reduction from split 2 = 0.6365141682948128
```

Decision Tree pruning (Information Criteria)

- Decision trees **overfit** to the data.
- Penalisation is often used:
  - Minimise $\mathcal{L}' = \mathcal{L}(\mathbf{y}, \hat{\mathbf{y}}) + \alpha|T|$
  - Where $|T|$ is the number of bipartitions in the tree, and $\mathcal{L}$ is a log-loss.
  - All the usual caveats of Information Criteria apply.
  - Tree search is usually performed by a greedy brute force approach:
    - Evaluate $\mathcal{L}'$ for every branch in the tree
    - Choose the sub-tree with the lowest value
    - Repeat until no cuts improve the loss
  - Alternative search approaches exist for large trees

Decision Tree pruning (Cross Validation)

- To avoid the problems with Information Criteria, Cross-validation can be used
- Choose the **sub-tree** that has the best **out of sample** predictive power.
  - With a single left-out dataset (risks overfitting),
  - Or random sets (higher variance)
- Now we have to re-compute the entire model each pruning
- Search is a computational concern

Regression Trees (simple version)

- Regression trees are constructed identically to classification trees
- Decision can follow information or squared loss
- Prediction is the average $\hat{y}_i|\{i \in c_j\} = \bar{y}_{c_j}$ inside the leaf j
- Comparing to classification: if $y \in \{0, 1\}$ this reduces to:

$$R_j = \frac{1}{N_j} \sum_{i \in c_j} (y_i - \hat{y}(x_i))^2 \quad (1)$$

$$= \frac{1}{N_j} \sum_{i \in c_j} \left(y_i^2 - 2 y_i \hat{y}(x_i) + \hat{y}(x_i)^2 \right) \quad (2)$$

- Which since $\hat{y} = \bar{y}$, simplifies to:

$$R = \bar{y} - 2\bar{y}^2 + \bar{y}^2 \quad (3)$$

$$= \bar{y}(1 - \bar{y}) \quad (4)$$

Comparing Regression Trees to Classification Trees

- Similarly the Gini index is:

$$G = \sum_{j=1}^{J} p_j(1 - p_j) \tag{5}$$

$$= \bar{y}(1 - \bar{y}) \tag{6}$$

- So regression trees and classification trees use equivalent loss functions in CART.

General Regression Trees

- Within each decision node (leaf) we fit a model
- This is typically a **constant** model, i.e. the average
- Why?
  - The piecewise constant model fit can be arbitrarily good (number of splits scales with data volume)
  - Making non-constant models consistent is computationally costly
- Why not?
  - Computational cost grows with tree depth
  - Often locally the structure is linear
- Leads to Local Regression Trees [3]
  - Complex if we ensure that the local regressions meet up

[3] Karalic A, "Employing Linear Regression in Regression Tree Leaves" (1992) ECAI-92

Decision tree notes

- In practice, **bagging** (bootstrapping the data) is important, to prevent overfitting and for smoothing the output
- The choice of feature space directly affects the decisions that are examined. So **LDA** or similar could usefully be applied to obtain "orthogonal" feature space, **reducing depth**.
- There are parameters, e.g. depth/stopping criterion/split rule, which could be chosen by cross-validation.

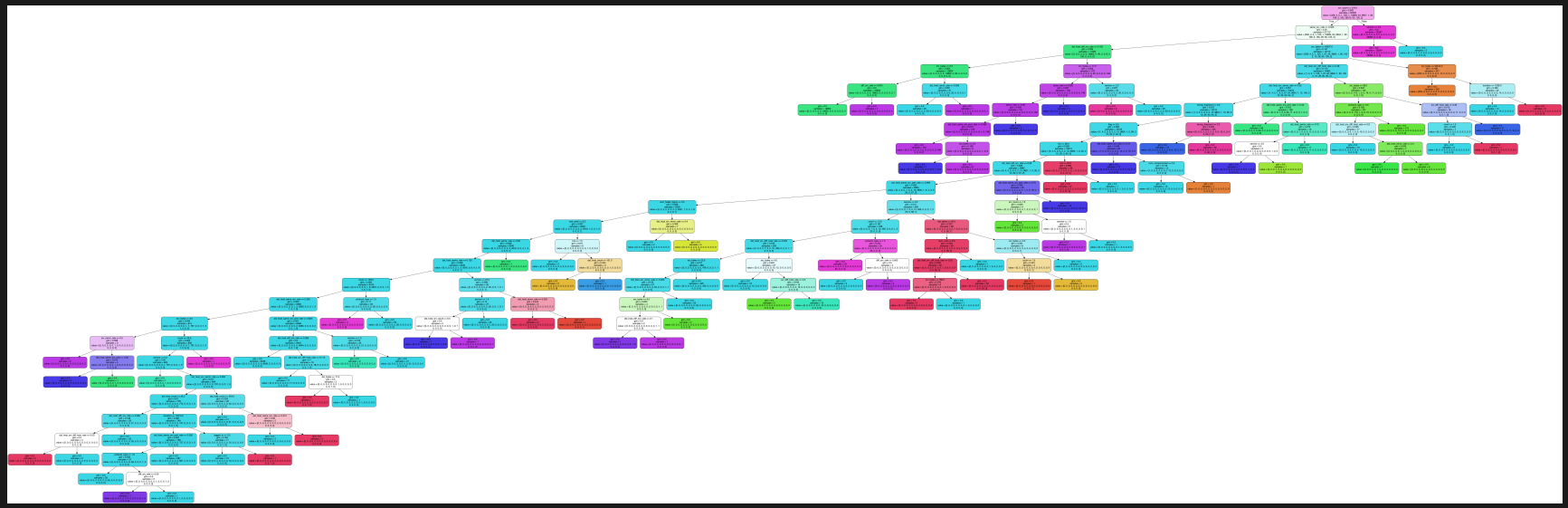
Fitting a Decision Tree in Python

```
from sklearn import tree
cldt = tree.DecisionTreeClassifier()

trained_model_d= cldt.fit(X_train, y_train)
y_pred_d = cldt.predict(X_test)
error_d = zero_one_loss(y_test, y_pred_d)
```

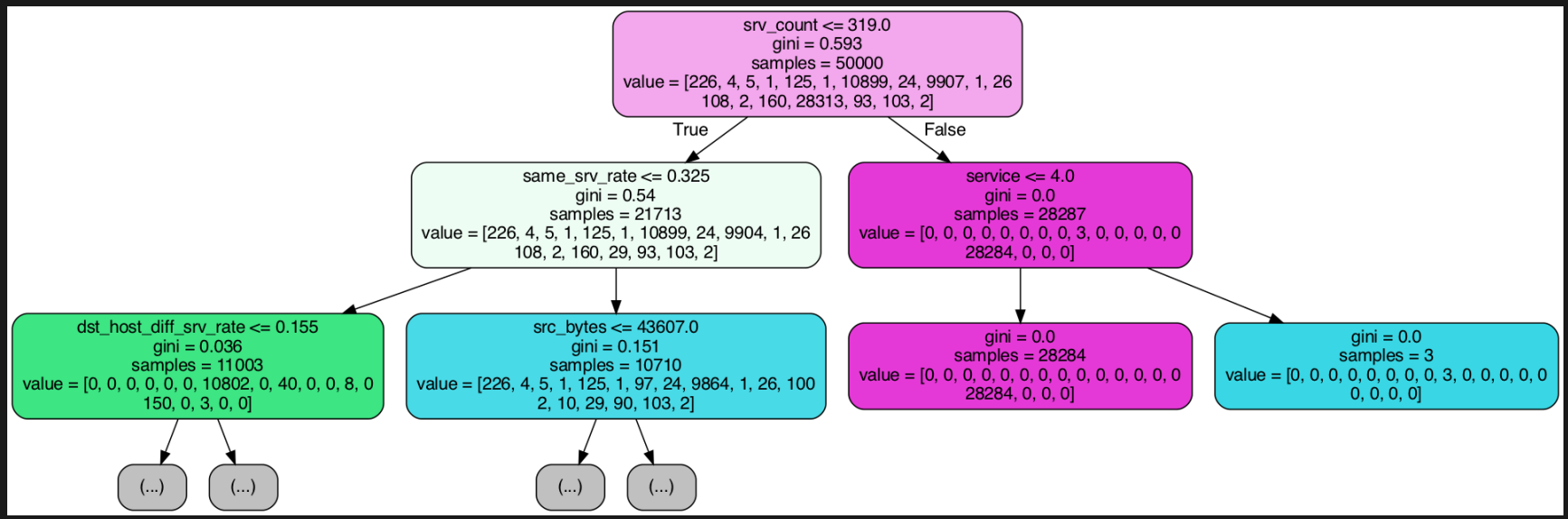
Plot a Decision Tree in Python

```
from sklearn.externals.six import StringIO
from IPython.display import Image
from sklearn.tree import export_graphviz
import pydotplus
dot_data = StringIO()
export_graphviz(cldt, out_file=dot_data,max_depth=2,
                feature_names=X_train.columns.values,
                filled=True, rounded=True)
graph = pydotplus.graph_from_dot_data(
    dot_data.getvalue())
Image(graph.create_png())
```

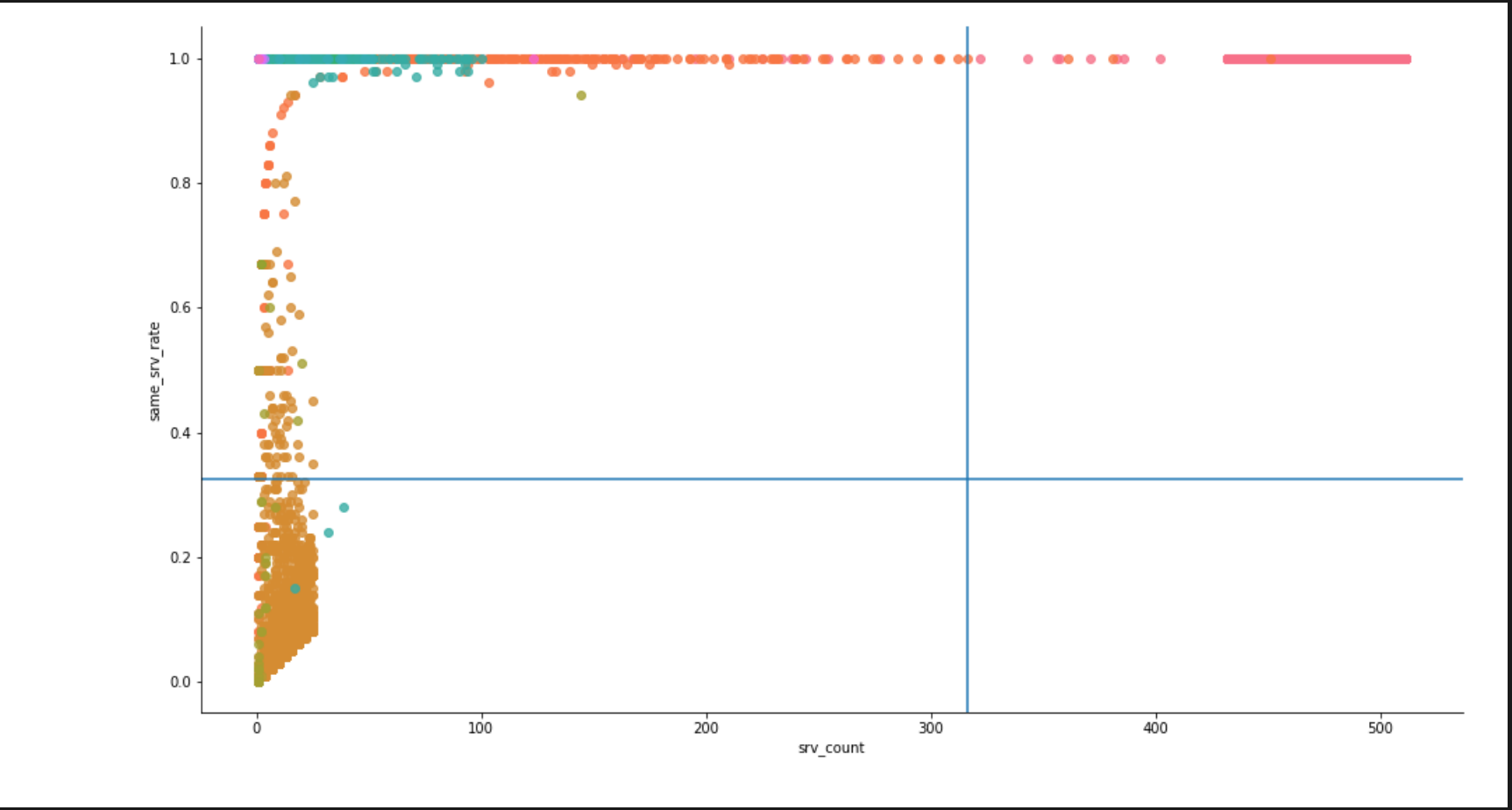
Decision Tree (whole)



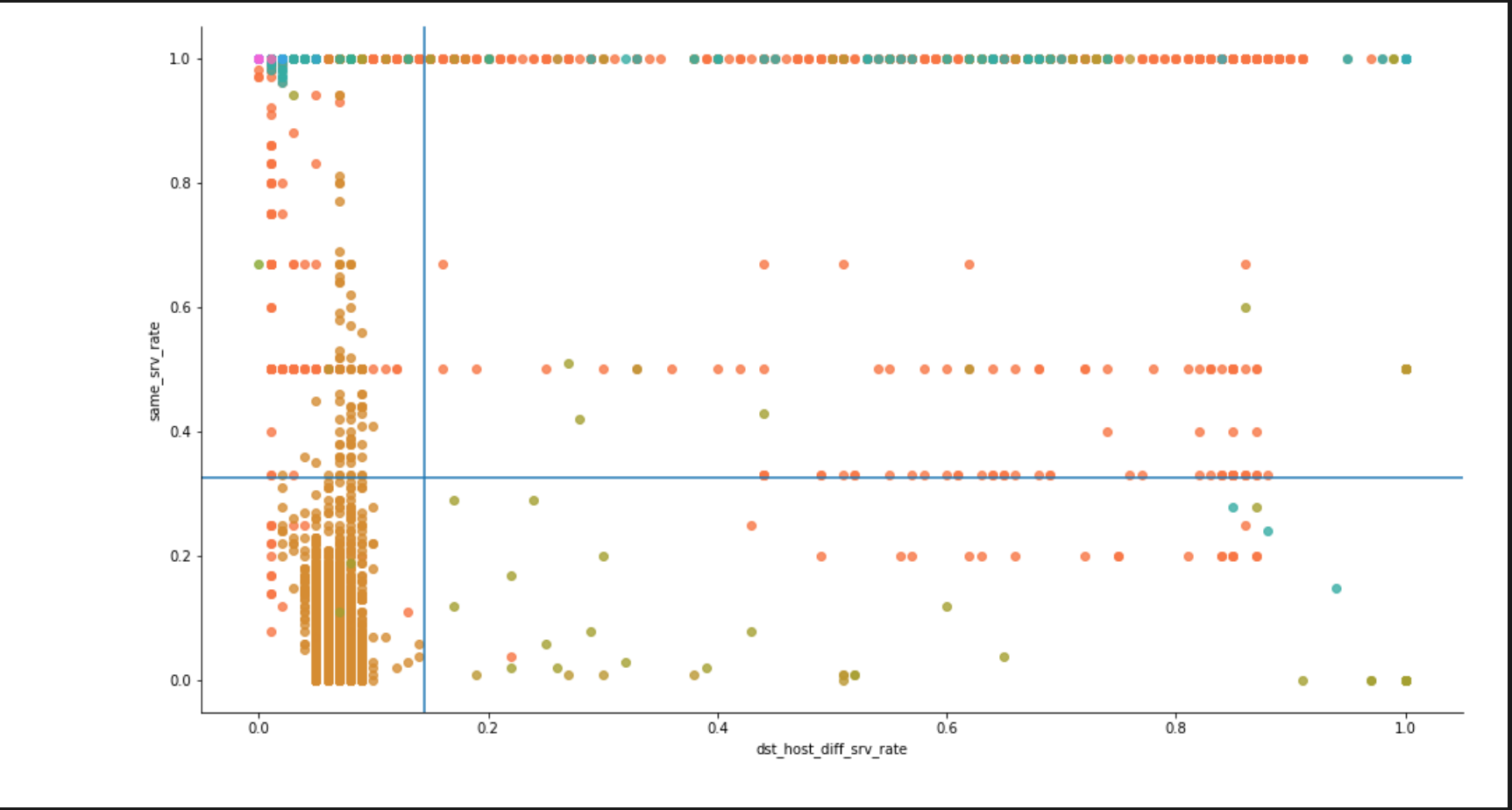
Decision Tree (root)



Decision Tree in feature space (1)



Decision Tree in feature space (2)



Boosted decision tree

- As noted previously, adaboost is using a **sequence of decisions** to make a boosted classifier.
- By default it uses a boosted depth=1 decision tree, i.e. classifiers were just the features. This is called a **decision stump**.
- You can use deeper trees, eg. with xgboost[4]; usually the depth is limited to control learning cost and complexity
- Boosting in theory doesn't need trees so the difference is about **learning rate** and **computational complexity**

[4] J. Elith, J. Leathwick, and T. Hastie "A working guide to boosted regression trees" (2008). British Ecological Society.

LightGBM and Histogram Boosting

- LightGBM[5] is a popular, efficient implementation of boosted decision trees
  - It uses a histogram approach to speed up learning
  - It is very fast, and can be faster than random forests
- Speed and efficiency comes from:
  - Binning continuous features into discrete bins
  - Binning categorical features into **binary** bins (no one-hot encoding)
  - Using a leaf-wise tree growth algorithm (over depth-wise)

[5] LightGBM: A Highly Efficient Gradient Boosting Decision Tree (2017) Microsoft Research, url.

Random Forest

- A **random forest** is a set of **decision trees** that are combined together to perform classification.
- For each of T trees, the following steps are run:
  a) Choose which of J variables to include:
  - Choose m_f **random features**. The canonical choice is $m_f = \sqrt{J}$.
  - Like **bagging for features**? (downsampling **without** replaceme
  b) Learn a Tree classifier independently as above.

Random Forest outputs

- The Random Forest **combines decision trees** into a classification by:
  - Weighting each tree according to its performance
  - Report the weighted vote
- It is also possible to extract **feature importance**:
  - How much a feature decreases the score, averaged over all trees
  - Features that are never used will get a score of 0
  - Features that are important in every tree in which they appear will get a high score
  - Features that are correlated will often split their importance

Random Forest vs boosted decision tree

- Gradient Boosting Machine (GBM) is the go-to boosted decision tree
- GBM and RF differ in the way the trees are built, the order, and the way the results are combined
- RF can be trivially paralellized
- GBMs seem to outperform RFs under competition conditions, but do worse when their parameters are untuned[6]

[6] http://fastml.com/what-is-better-gradient-boosted-trees-or-random-forest/

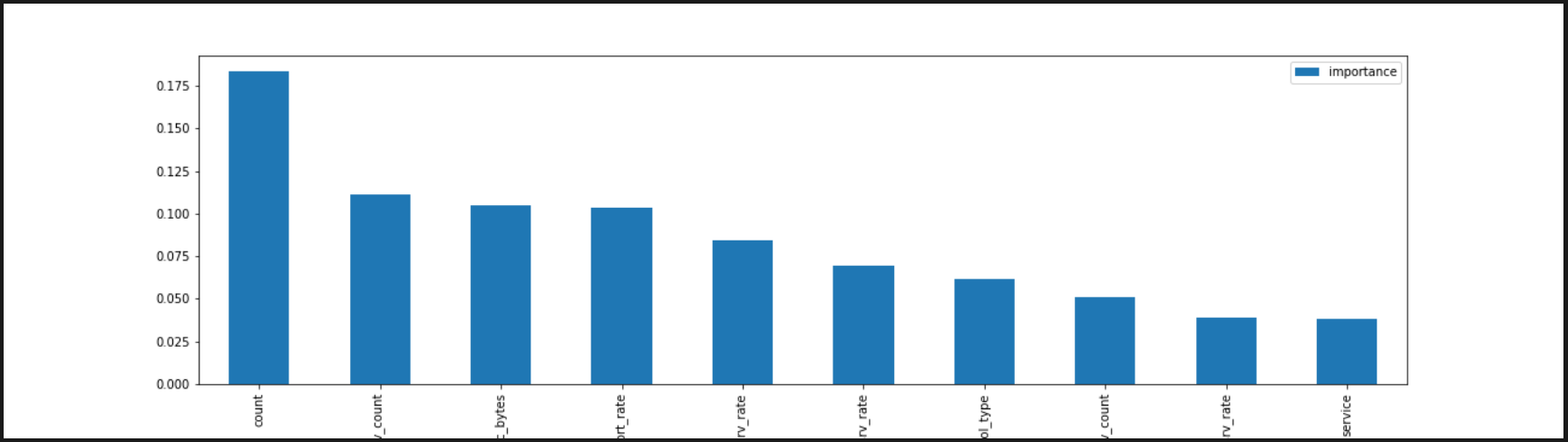
Random Forest algorithm

```
from sklearn.ensemble import RandomForestClassifier
clf= RandomForestClassifier(n_jobs=-1,
    random_state=3, n_estimators=102)
trained_model= clf.fit(X_train, y_train)
clf_score=trained_model.score(X_train, y_train)
y_pred = clf.predict(X_test)
```

Random Forest Feature Importance

```
feature_importances = pd.DataFrame(clf.feature_importances_,
    index = X_train.columns,
    columns=['importance']).sort_values('importance',
    ascending=False)

feature_importances.nlargest(10,
    columns=['importance']).plot(kind='bar',figsize=(18, 5))
```

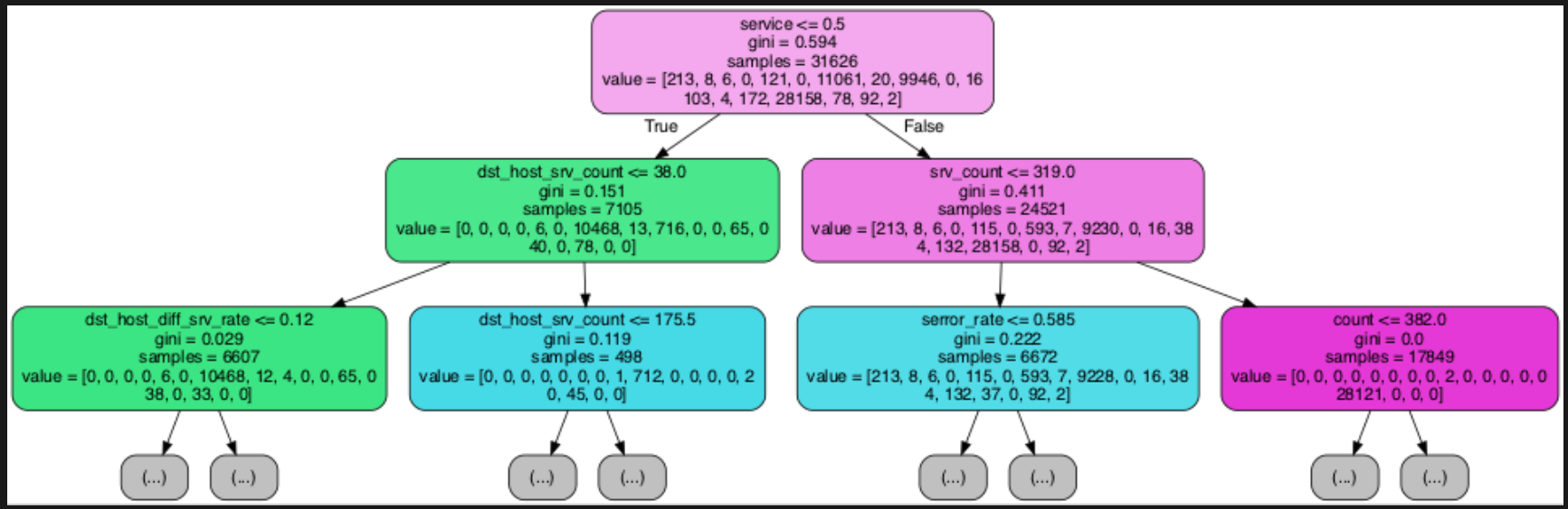
Random Forest Feature Importance



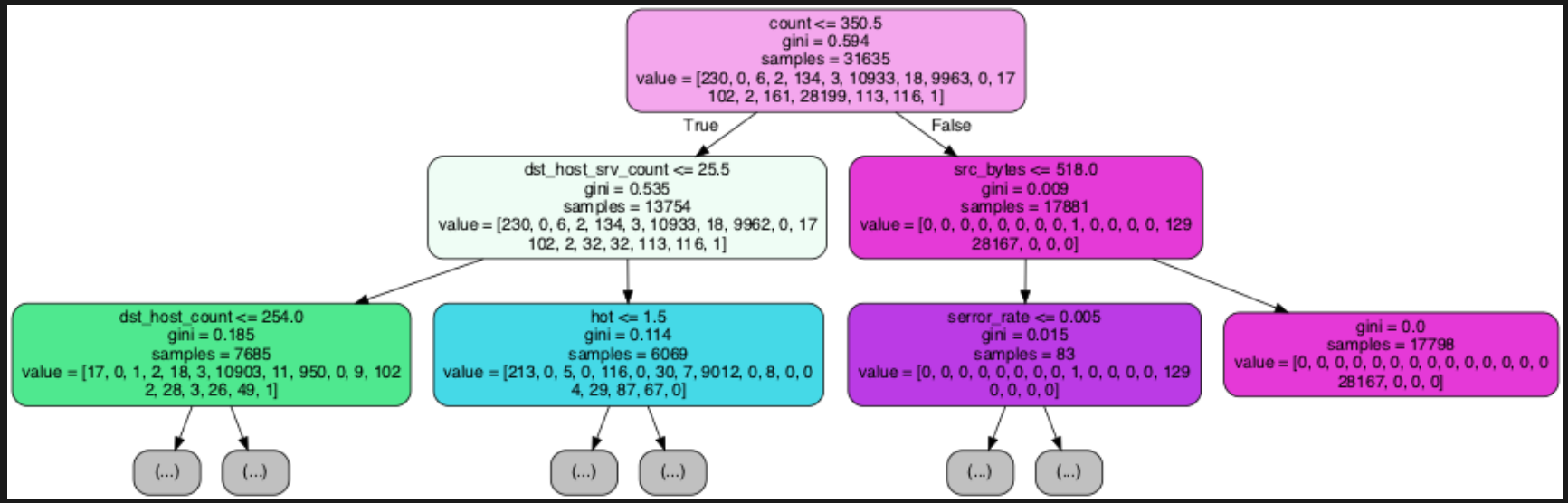
Random Forest Extract single trees

```
estimator5 = clf.estimators_[5]

dot_data = StringIO()
export_graphviz(estimator5, out_file=dot_data,max_depth=2,
                feature_names=X_train.columns.values,
                filled=True, rounded=True)

graph = pydotplus.graph_from_dot_data(dot_data.getvalue())
Image(graph.create_png())
```

Random Forest Feature Trees



Random Forest Feature Trees



Final thoughts

- In what sense are decision trees “interpretable”?
- In what sense are decision trees “AI”?

Signposting

- **References**:
- Tree methods:
  - Chapter 9.2 of The Elements of Statistical Learning: Data Mining, Inference, and Prediction (Friedman, Hastie and Tibshirani).
  - Penn State U Applied Data Mining and Statistical Learning How to prune trees
  - Decision Tree Algorithms: Deep Math ML
- Regression Trees:
  - Karalic A, "Employing Linear Regression in Regression Tree Leaves" (1992) ECAI-92

Signposting

- **References (2)**:
- Boosted Decision Trees:
  - J. Elith, J. Leathwick, and T. Hastie "A working guide to boosted regression trees" (2008). British Ecological Society.
- CART:
  - CART = Classification and Regression Trees. Breiman, Leo; Friedman, J. H.; Olshen, R. A.; Stone, C. J. (1984). Classification and regression trees.
  - Wei-Yin Loh's 2011 Review is popular.
- ID3: Quinlan, J. R. 1986. Induction of Decision Trees. Mach. Learn. 1, 1 (Mar. 1986), 81-106.

Signposting

- In the practical we'll implement these models in R and Python; compare implementations, and to previous results.
- Next semester we'll start with the "other" LDA (Latent Dirichlet Allocation), Topic Modelling, and Modelling Documents.
- **References**:
  - Chapter 15 of The Elements of Statistical Learning: Data Mining, Inference, and Prediction (Friedman, Hastie and Tibshirani).
  - Implement a Random Forest From Scratch in Python
  - A Gentle Introduction to Random Forests at CitizenNet
  - DataDive on Selecting good features
  - Cosma Shalizi on Regression Trees
  - Gilles Louppe PhD Thesis: Understanding Random Forests