

Welcome to the Jungle

@__mharrison__

PyCon Colombia 2018





About Me

- Corporate Trainer
- Author (*Illustrated Guide to Python 3, Guide to Learning the Pandas Library*)
- Python since 2000



Outline

- Machine Learning in a Nutshell
- Which algorithm to use?
- The Titanic
- Decision Trees
- Random Forests
- Conclusion

Machine Learning

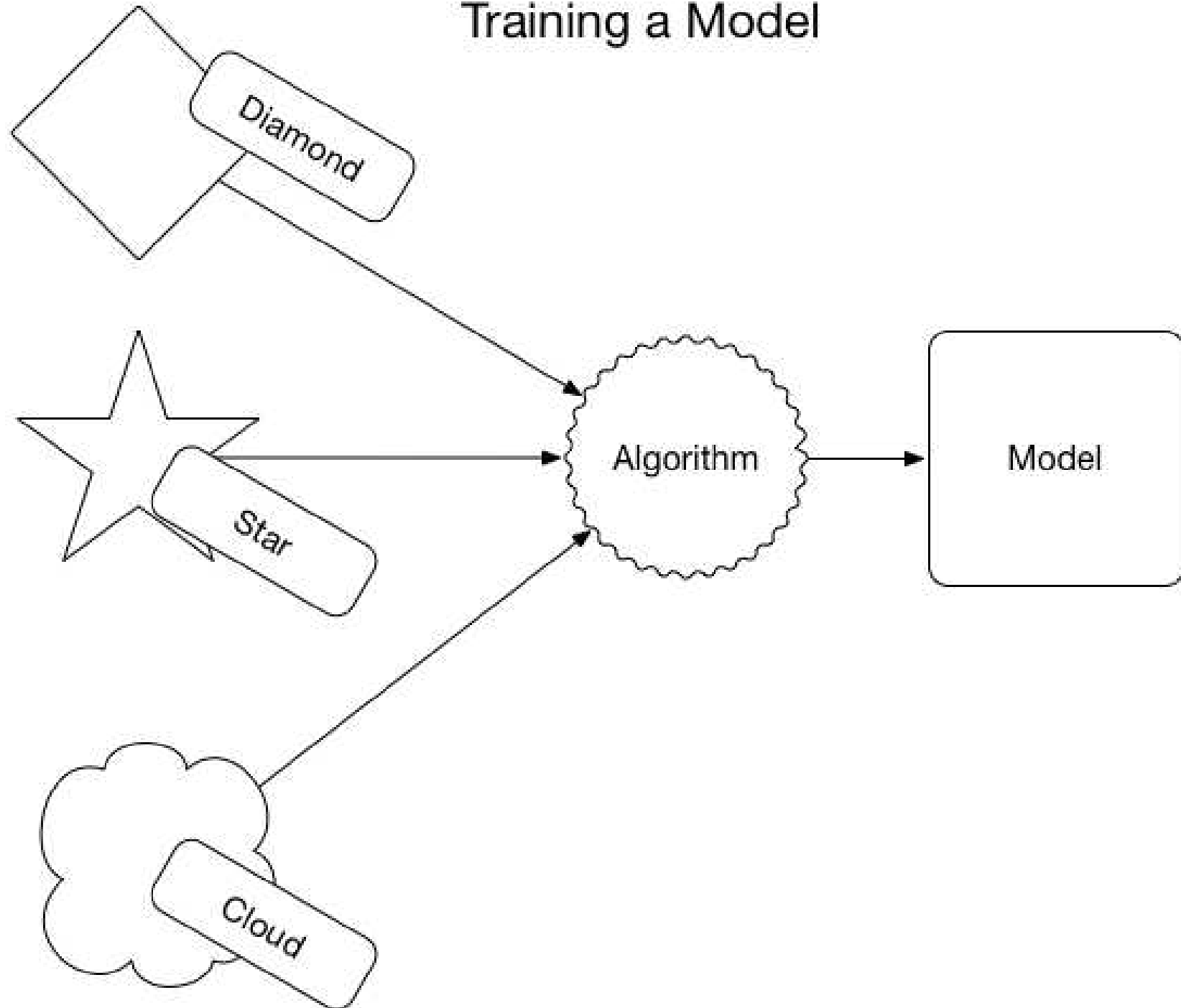
Supervised Classification

Sometimes called "Predictive Modeling."

1. Identify patterns from labeled examples.
(Training Set => Model)
2. Based on those patterns, try to guess labels for other examples. (Predict)

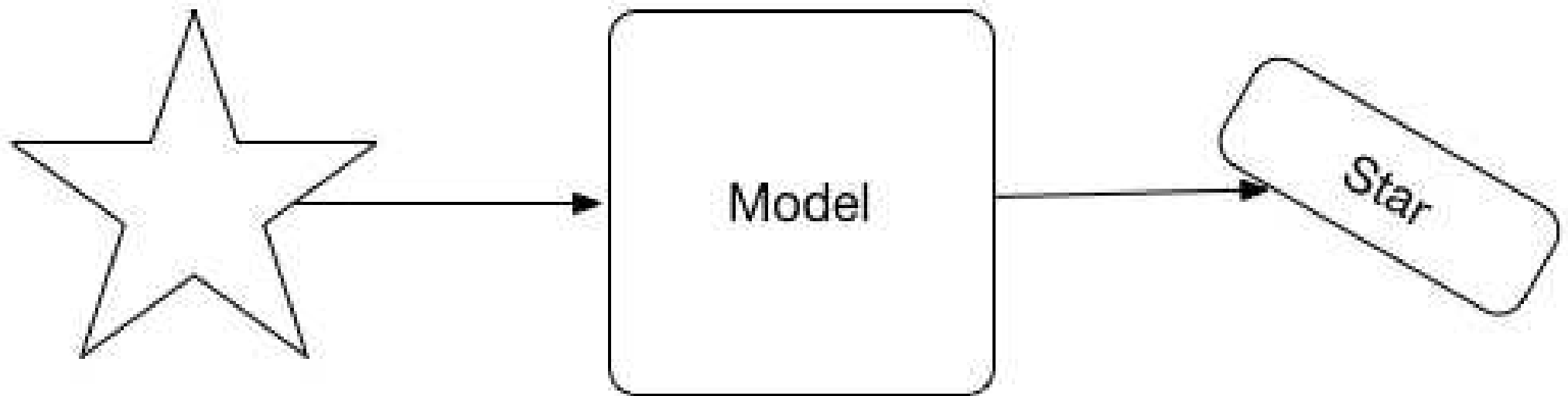
Labeled Data

Training a Model



Predicting a Label

Unlabeled Data



Examples

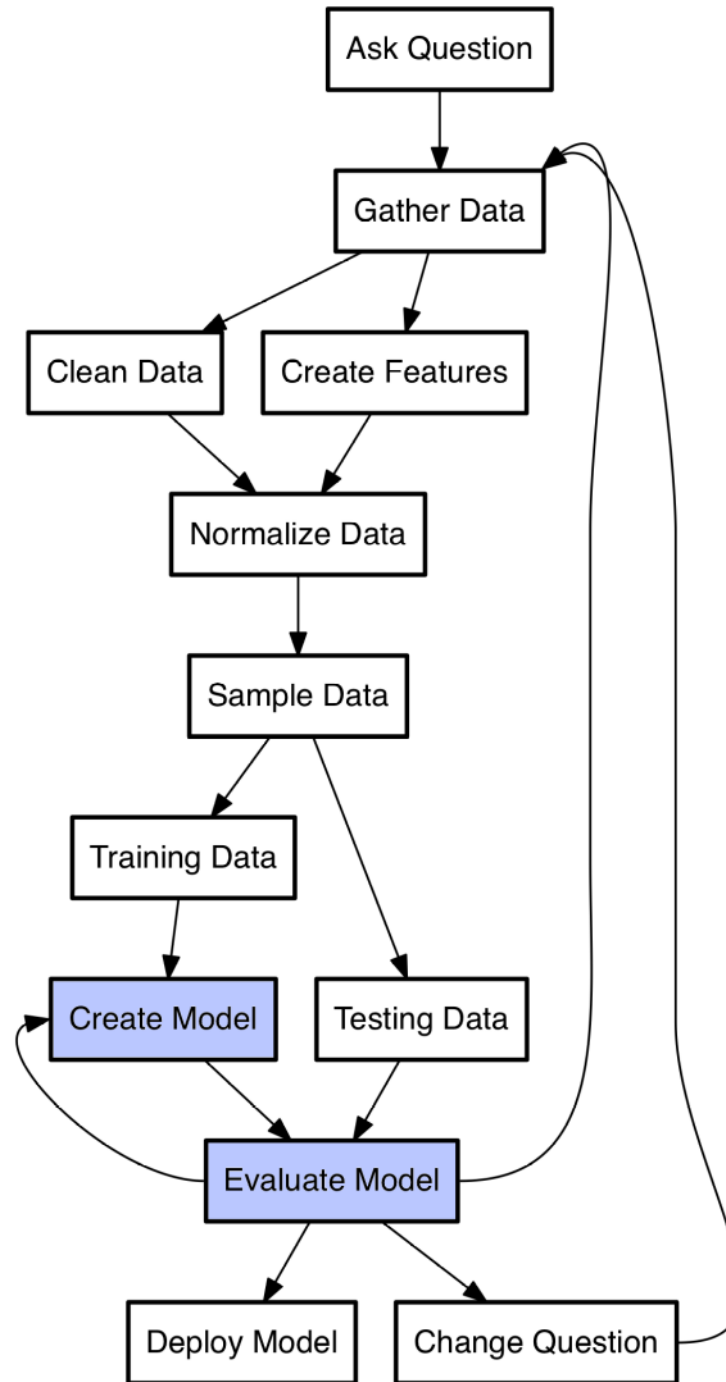
Binary Classification

- Is this student at high risk for dropping out?
- Is this individual at high risk for defaulting on a loan?
- Is this person at high risk for becoming infected with a certain disease?

Multi-class Classification

- What is the most likely disease given this individual's current symptoms?
- Which ad is the user most likely to click on?





Machine Learning Process

So which algorithm
should I use to build a
model?

No Free Lunch

If an algorithm performs well on a certain class of problems then it necessarily pays for that with degraded performance on the set of all remaining problems.

David Wolpert and William Macready. No Free Lunch Theorems for Optimization. IEEE Transactions on Evolutionary Computation, 1:67, 1997.

No Free Lunch

No single algorithm will build the best model on every dataset.

Which algorithm?

- What is your background discipline? (statistics, computer science, AI)
- Which classifiers are you aware of?
- Is there an implementation of this classifier in your project language?
- Do you understand the parameters well enough to tune them?
- Does it work with your data?

Premise

Manuel Fernández-Delgado, Eva Cernadas, Senén Barro, and Dinani Amorim. Do we Need Hundreds of Classifiers to Solve Real World Classification Problems? *Journal of Machine Learning Research*, 15(Oct):3133–3181, 2014.

<http://jmlr.csail.mit.edu/papers/v15/delgado14a.html>

Premise

It turns out that Random Forests are usually a good place to start.

Premise

Thunderdome with:

- 179 classifiers from 17 classifier families
- 121 datasets from the UCI repository

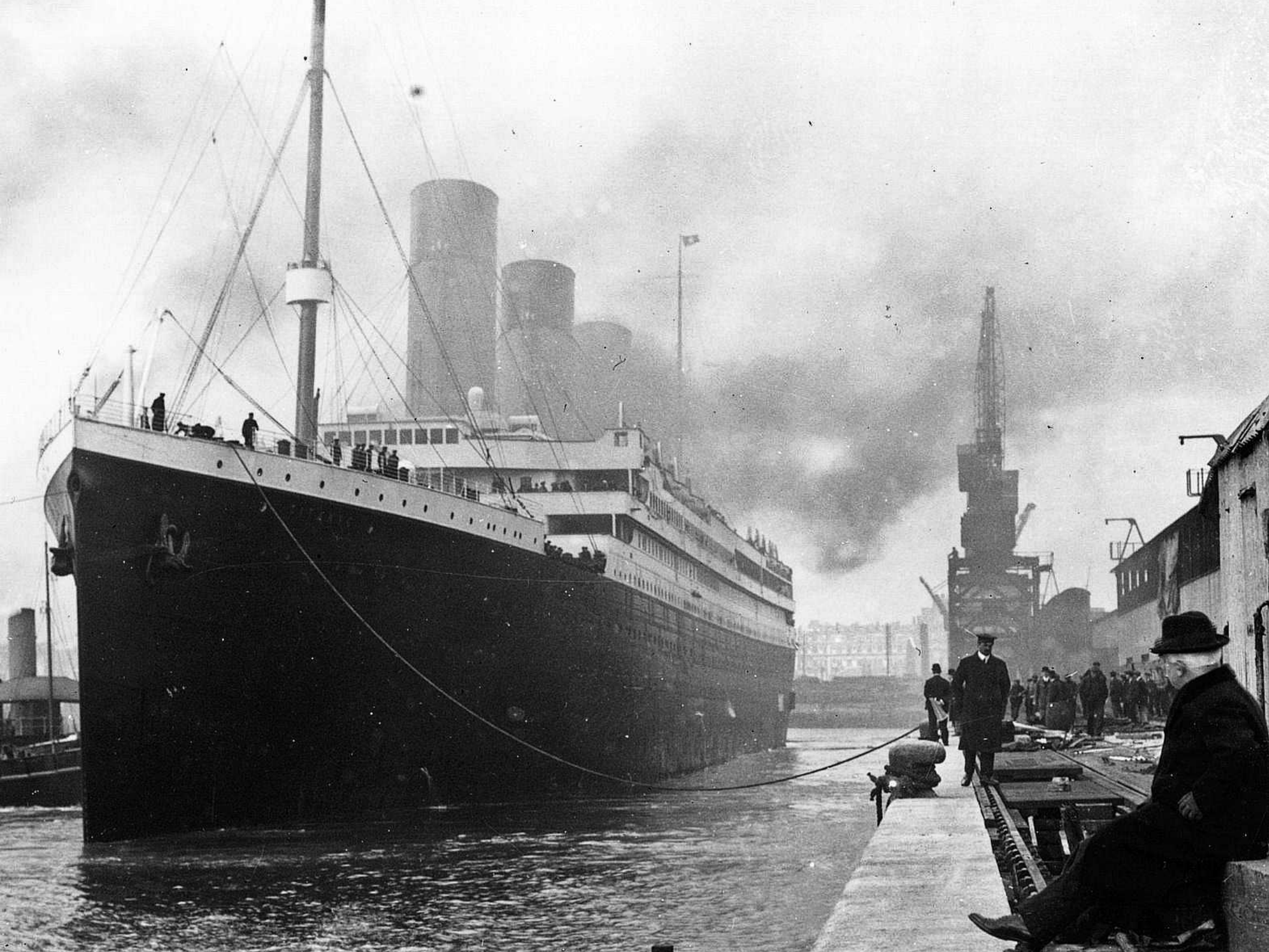
Premise

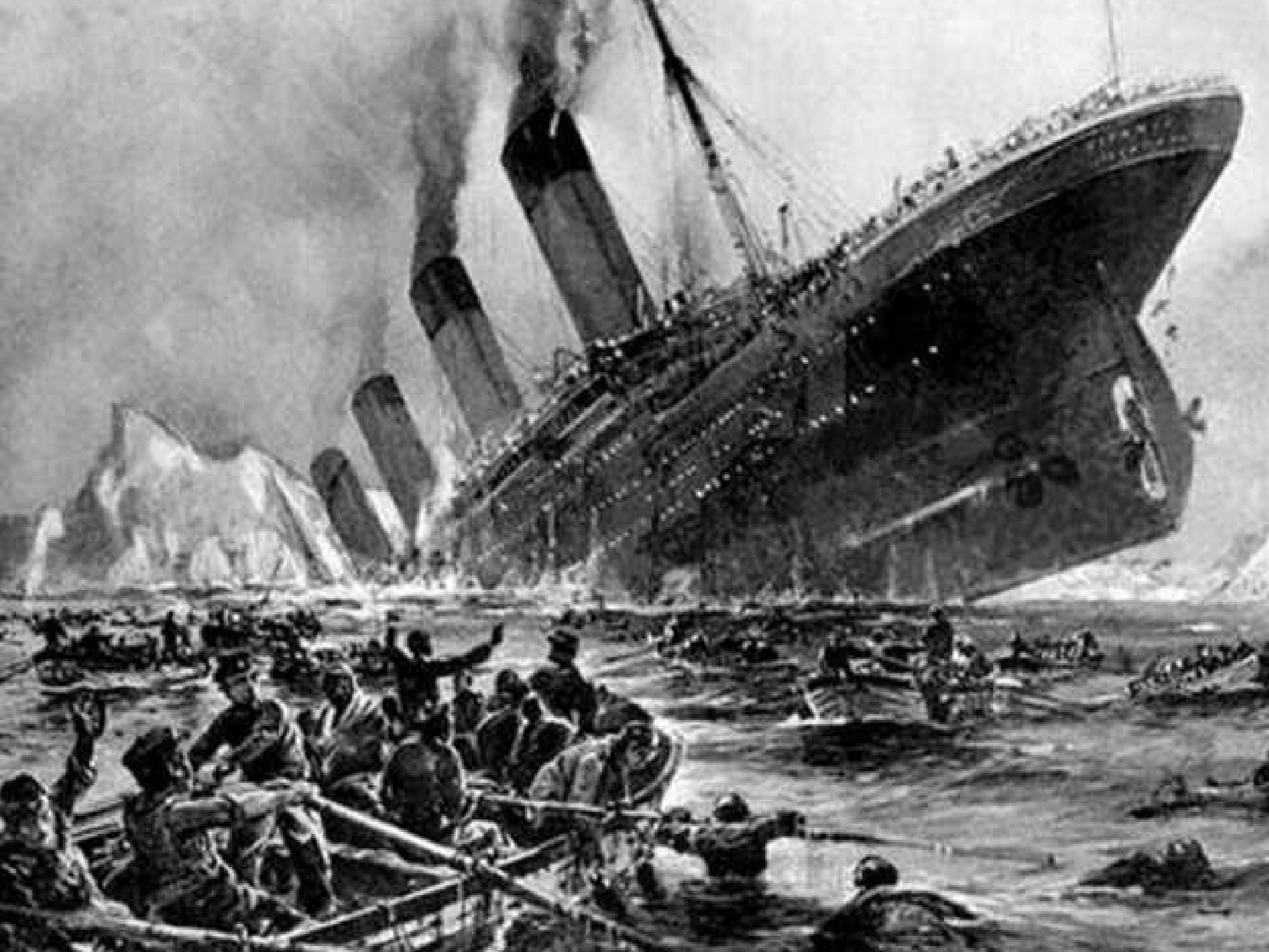
"The Random Forest is clearly the best family of classifiers, followed by SVM, neural networks, and boosting ensembles."

- On average, RF achieved 94.1% of the theoretical maximum accuracy for each dataset.
- RF achieved over 90% of maximum accuracy in 84.3% of datasets.

The RMS Titanic







Classification Task

Predict who did and did not survive the disaster on the Titanic

Classification Task

Predict who did and did not survive the disaster on the Titanic

(and see if we can get some idea of *why* it turned out that way)

Get Data

```
>>> import pandas as pd  
>>> df = pd.read_excel('data/titanic3.xls')
```

<http://biostat.mc.vanderbilt.edu/wiki/pub/Main/DataSets/titanic3.xls>

Columns

- class: Passenger class (1 = first; 2 = second; 3 = third)
- name: Name
- sex: Sex
- age: Age
- sibsp: Number of siblings / spouses aboard
- parch: Number of parents / children aboard
- ticket: Ticket number
- fare: Passenger fare
- cabin: Cabin
- embarked: Port of embarkation (C = Cherbourg; Q = Queenstown; S = Southampton)
- boat: Lifeboat (if survived)
- body: Body number (if did not survive and body was recovered)

Label Column

The column giving the label for our classification task:

- survival: Survival (0 = no; 1 = yes)

Exploring

```
>>> df.shape
```

```
(1309, 14)
```

```
>>> df.embarked.value_counts()
```

```
S      914
```

```
C      270
```

```
Q      123
```

```
Name: embarked, dtype: int64
```

Exploring

```
>>> df.cabin.value_counts()
```

```
C23 C25 C27      6
```

```
B57 B59 B63 B66    5
```

```
G6      5
```

```
B96 B98      4
```

```
F2      4
```

```
F4      4
```

```
C22 C26      4
```

```
F33      4
```

```
D        4
```

```
C78      4
```

```
E101     3
```

```
B58 B60     3
```

```
...
```

```
Name: cabin, dtype: int64
```

Question

Can we build a model that will predict survival?

Assignment

Load Data

Decision Trees

Decision Trees

```
>>> from sklearn import tree
>>> model = tree.DecisionTreeClassifier(random_state=42)
>>> ignore =
set('boat,body,home.dest,name,ticket'.split(','))
>>> cols = [c for c in df.columns if c != 'survived' and c
not in ignore]
>>> X = df[cols]
>>> y = df.survived
>>> model.fit(X, y)
Traceback (most recent call last):
...
ValueError: could not convert string to float: 'S'
```

Create Dummy Variables

```
>>> dummy_cols = 'pclass,sex,cabin,embarked'.split(',')
>>> df2 = pd.get_dummies(df, columns=dummy_cols)

>>> model = tree.DecisionTreeClassifier(random_state=42)
>>> ignore =
set('boat,body,home.dest,name,ticket'.split(','))
>>> cols = [c for c in df2.columns if c != 'survived' and c
...         not in ignore and c not in dummy_cols]
>>> X = df2[cols]
>>> y = df2.survived
```


Try Again

```
>>> model.fit(X, y)
```

```
Traceback (most recent call last):
```

```
...
```

```
ValueError: Input contains NaN, infinity  
or a value too large for  
dtype('float32').
```

Imputing

Fancy term for filling in values. Mean is a good choice for decision trees as it doesn't bias the splitting, whereas 0 would

Try Again

```
>>> X = X.fillna(X.mean())
```

```
>>> X.dtypes
```

age	float64
sibsp	int64
parch	int64
fare	float64
pclass_1	float64
pclass_2	float64
pclass_3	float64
sex_female	float64
sex_male	float64
cabin_A10	float64
cabin_A11	float64
cabin_A14	float64

Assignment

Convert to numeric

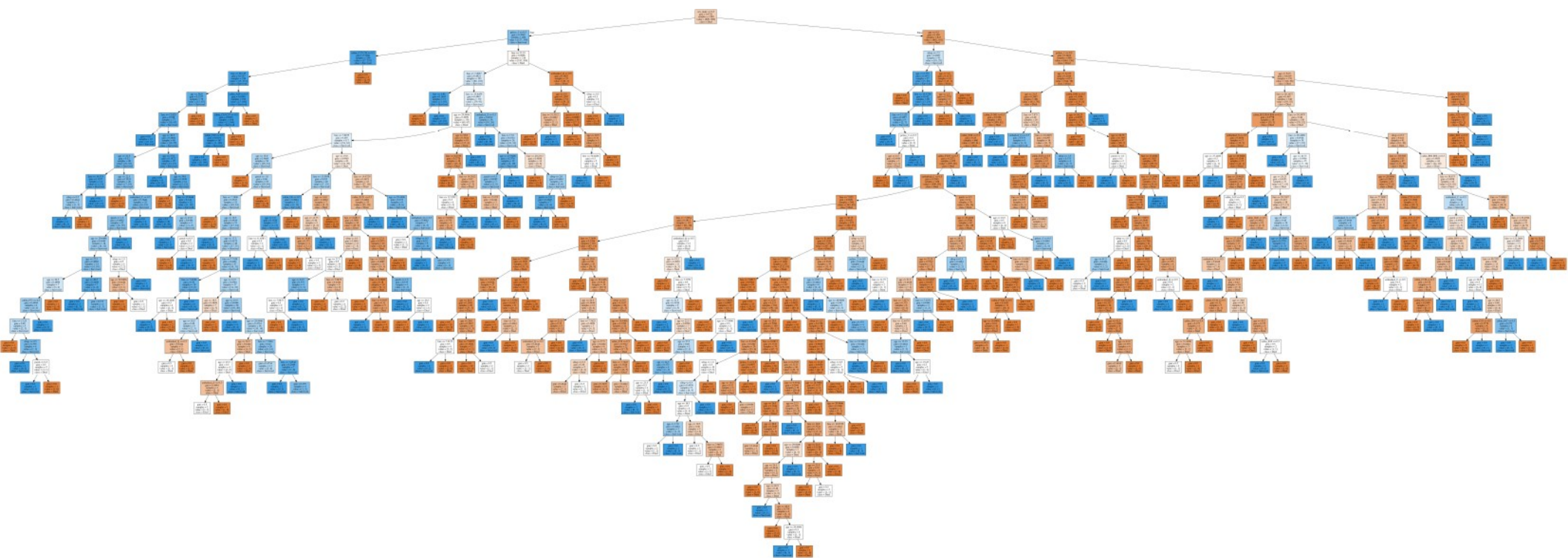
Try Again

```
>>> model.fit(X, y)
```

```
DecisionTreeClassifier(class_weight=None,  
                        criterion='gini', max_depth=None,  
                        max_features=None, max_leaf_nodes=None,  
                        min_samples_leaf=1, min_samples_split=2,  
                        min_weight_fraction_leaf=0.0,  
                        presort=False, random_state=42,  
                        splitter='best')
```

What Does the Tree Look Like?

```
>>> tree.export_graphviz(model,  
...     out_file='/tmp/tree1.dot',  
...     feature_names=X.columns,  
...     class_names=['Died', 'Survived'],  
...     filled=True)  
  
>>> import subprocess  
>>> _ = subprocess.check_output(  
...     'dot -Tpng -oimg/tree1.png /tmp/tree1.dot'.split())
```



Assignment

Decision Tree

Does it Generalize?

Need a Test Set

```
>>> from sklearn import model_selection
>>> X_train, X_test, y_train, y_test = \
...     model_selection.train_test_split(
...     X, y, test_size=.3, random_state=42)

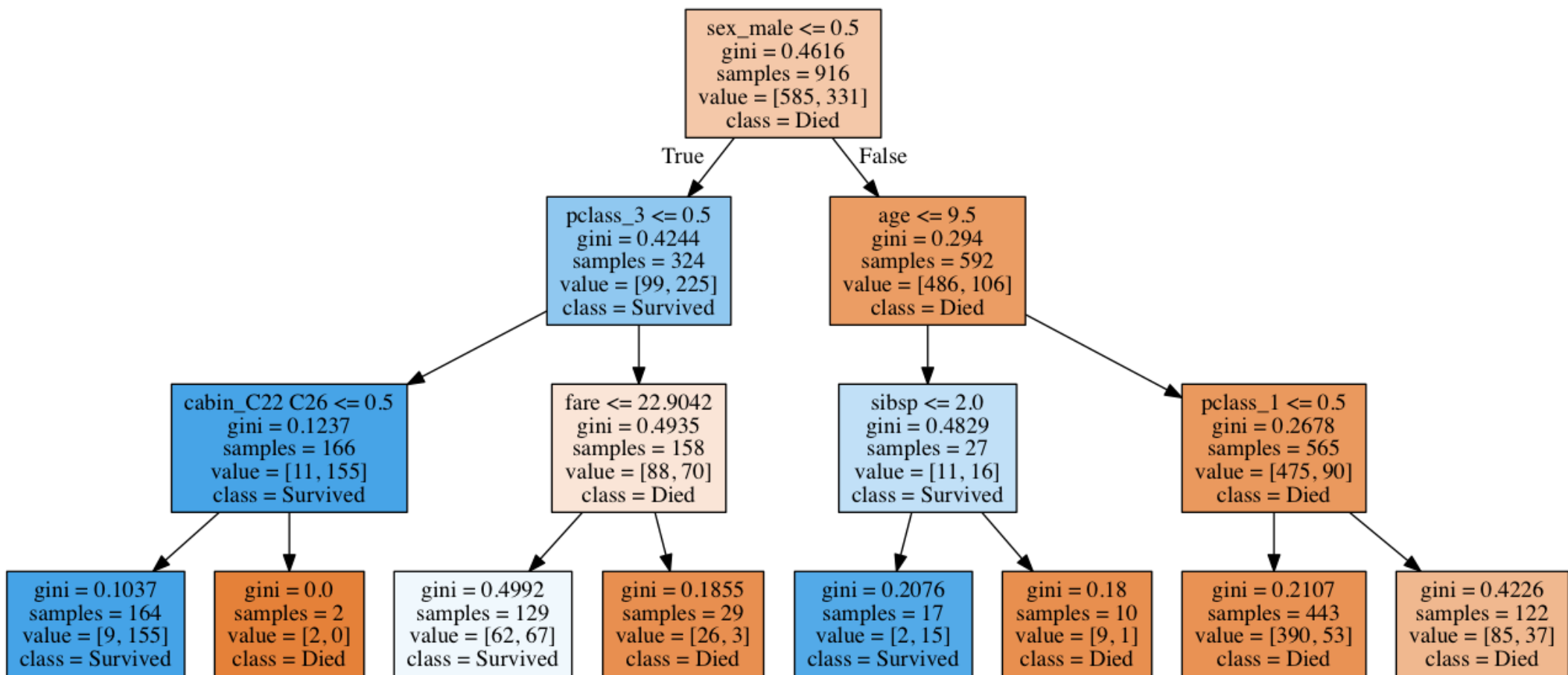
>>> _ = model.fit(X_train, y_train)
>>> model.score(X_test, y_test)
0.76844783715012721
```

Another Model

```
>>> model2 = tree.DecisionTreeClassifier(  
...     random_state=42, max_depth=3)  
>>> _ = model2.fit(X_train, y_train)  
>>> model2.score(X_test, y_test)  
0.81424936386768443
```

What Does the Tree Look Like?

```
>>> tree.export_graphviz(model2,  
...     out_file='/tmp/tree2.dot',  
...     feature_names=X.columns,  
...     class_names=['Died', 'Survived'],  
...     filled=True)  
  
>>> import subprocess  
>>> _ = subprocess.check_output(  
...     'dot -Tpng -oimg/tree2.png /tmp/tree2.dot'.split())
```



Assignment

Training / Testing & Generalization

Another Performance Measure

ROC Curve

Receiver Operating Characteristic - area indicates performance

ROC

```
>>> from sklearn.metrics import auc, confusion_matrix, roc_curve

>>> def fig_with_title(ax, title, figkwargs):
...     if figkwargs is None:
...         figkwargs = {}
...     if not ax:
...         fig = plt.figure(**figkwargs)
...         ax = plt.subplot(111)
...     else:
...         fig = plt.gcf()
...     if title:
...         ax.set_title(title)
...     return fig, ax
```

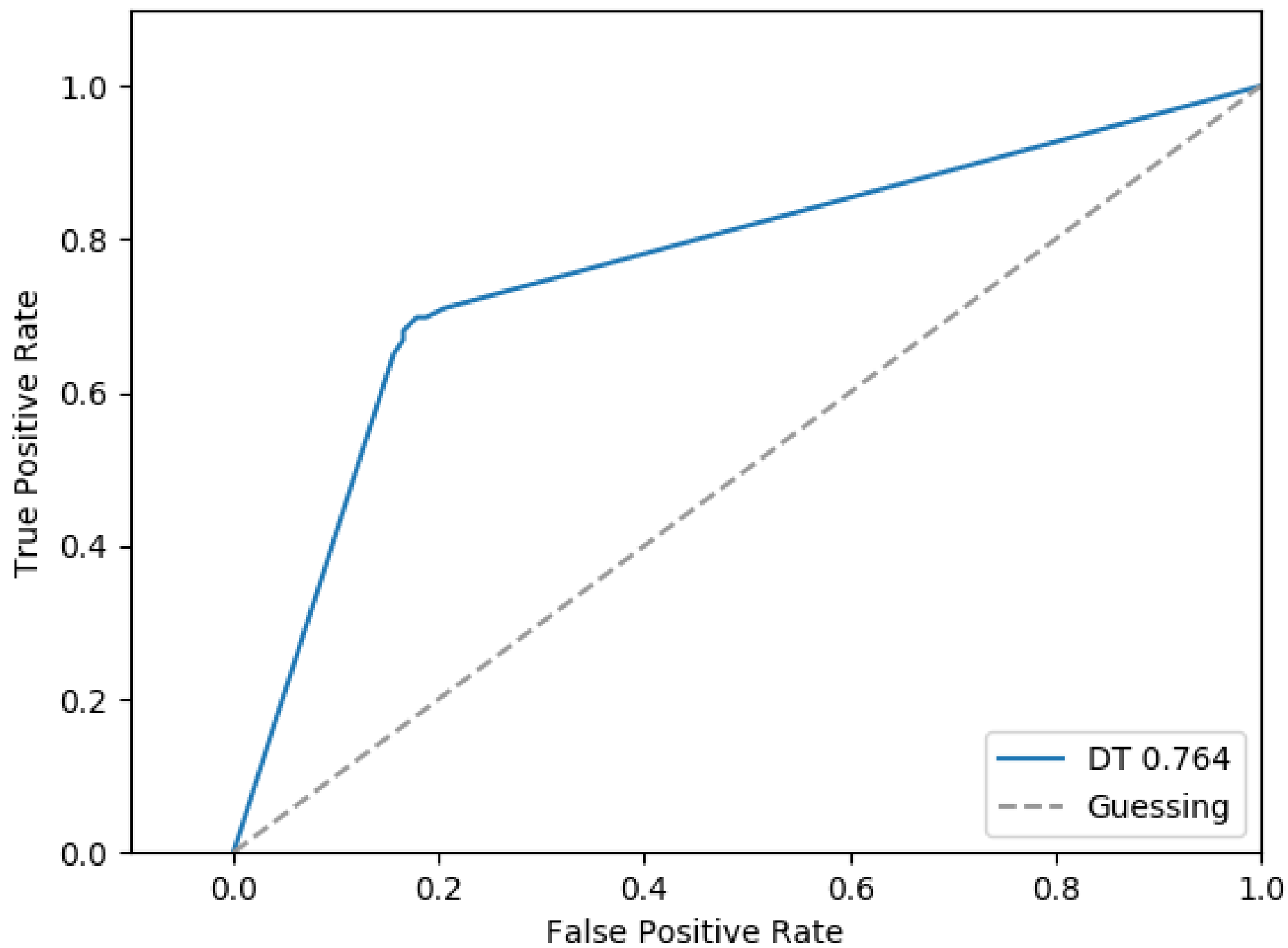
ROC

```
>>> def plot_roc_curve_binary(clf, X, y, label='ROC Curve (area={area:.3f})',
...                           title="ROC Curve", pos_label=None, sample_weight=None,
...                           ax=None, figkwargs=None, plot_guess=False):
...     ax = ax or plt.subplot(111)
...     ax.set_xlim([-0.1, 1])
...     ax.set_ylim([0, 1.1])
...     y_score = clf.predict_proba(X)
...     if y_score.shape[1] != 2 and not pos_label:
...         warnings.warn("Shape is not binary {} and no pos_label".format(y_score.shape))
...         return
...     try:
...         fpr, tpr, thresholds = roc_curve(y, y_score[:,1], pos_label=pos_label,
...                                         sample_weight=sample_weight)
...     except ValueError as e:
...         if 'is not binary' in str(e):
...             warnings.warn("Check if y is numeric")
...             raise
...
...     roc_auc = auc(fpr, tpr)
...     fig, ax = fig_with_title(ax, title, figkwargs)
...
...     ax.plot(fpr, tpr, label=label.format(area=roc_auc))
...     if plot_guess:
...         ax.plot([0, 1], [0, 1], '--', color=(0.6, 0.6, 0.6), label='Guessing')
...     ax.set_xlabel('False Positive Rate')
...     ax.set_ylabel('True Positive Rate')
...     ax.legend(loc="lower right")
...     return fig, ax
```

ROC

```
>>> from matplotlib import pyplot as plt
>>> plt.clf()
>>> fig, ax = plot_roc_curve_binary(
...     model, X_test, y_test,
...     'DT {area:.3}', plot_guess=1)
>>> fig.savefig('img/ml-roc.png')
```

ROC Curve



Assignment

ROC Curve

Pros / Cons Decision Trees

Pros:

- Easy to explain

Cons:

- Tends to overfit

Random Forest

Random Forest

Created by Tin Kam Ho (1995), Leo Breiman, and Adele Cutler (2001).

Condorcet's Jury Theorem

From 1785 *Essay on the Application of Analysis to the Probability of Majority Decisions*. If each member of jury has $p > .5$ of predicting correct choice, adding more jury members increases probability of correct choice.

Random Forest

Algorithm:

- Sample from training set N (random WITH REPLACEMENT - lets us do OOB)
- Select m input variables (subset of M total input variables)
- Grow a tree
- Repeat above (create *ensemble*)
- Predict by aggregation predictions of forest (votes for classification, average for regression)

Random Forest

```
>>> from sklearn import ensemble
>>> model3 = ensemble.RandomForestClassifier(random_state=42)
>>> model3.fit(X_train, y_train)
RandomForestClassifier(bootstrap=True, class_weight=None,
                        criterion='gini', max_depth=None, max_features='auto',
                        max_leaf_nodes=None, min_samples_leaf=1,
min_samples_split=2,
                        min_weight_fraction_leaf=0.0, n_estimators=10, n_jobs=1,
                        oob_score=False, random_state=None, verbose=0,
                        warm_start=False)

>>> model3.score(X_test, y_test)
0.75572519083969469
```

Feature Importance

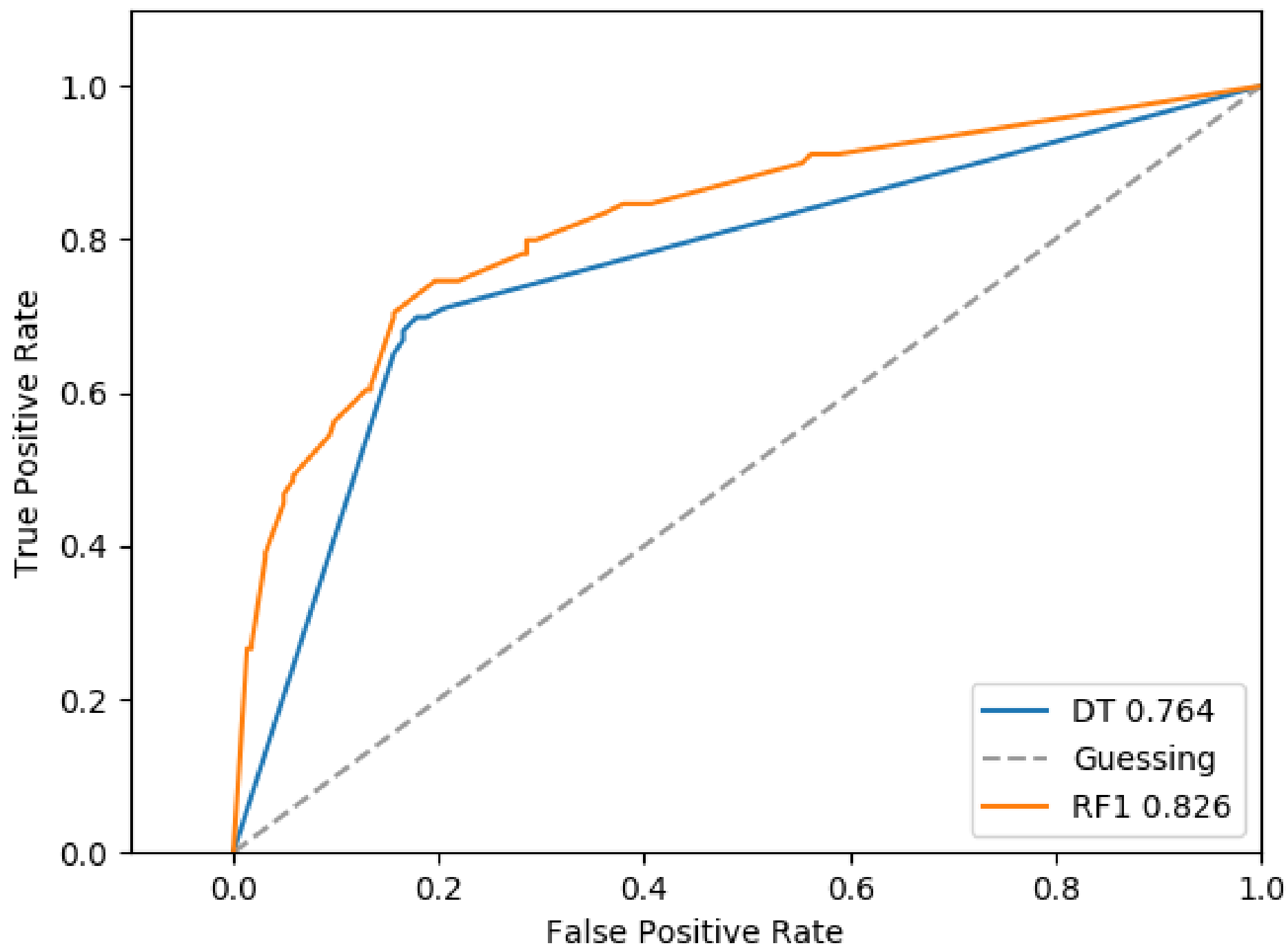
Most important features at the top of the decision trees

```
>>> print(sorted(zip(X.columns, model3.feature_importances_),  
...               key=lambda x: x[1], reverse=True))  
[('age', 0.22344483424840464), ('fare', 0.19018725802080991),  
 ('sex_male', 0.12990057398621174), ('sex_female',  
 0.12860349870512569), ('pclass_3', 0.051127382589271984),  
 ('parch', 0.042403381656923547), ('sibsp',  
 0.041437135835858306), ('pclass_1', 0.026146920495887703),  
 ('embarked_S', 0.016952460872998475), ('pclass_2',  
 0.014536895778953276), ('embarked_C', 0.011974575978148253),  
 ('embarked_Q', 0.0066746190486480592), ('cabin_D56',  
 0.0050674850086476347), ('cabin_C22 C26',  
 0.0038209715167321157), ('cabin_F E57',
```

ROC

```
>>> fig, ax = plot_roc_curve_binary(  
...     model3, X_test, y_test,  
...     'RF1 {area:.3}')  
>>> fig.savefig('img/ml-roc3.png')
```

ROC Curve



Assignment

Random Forest

Confusion Matrix

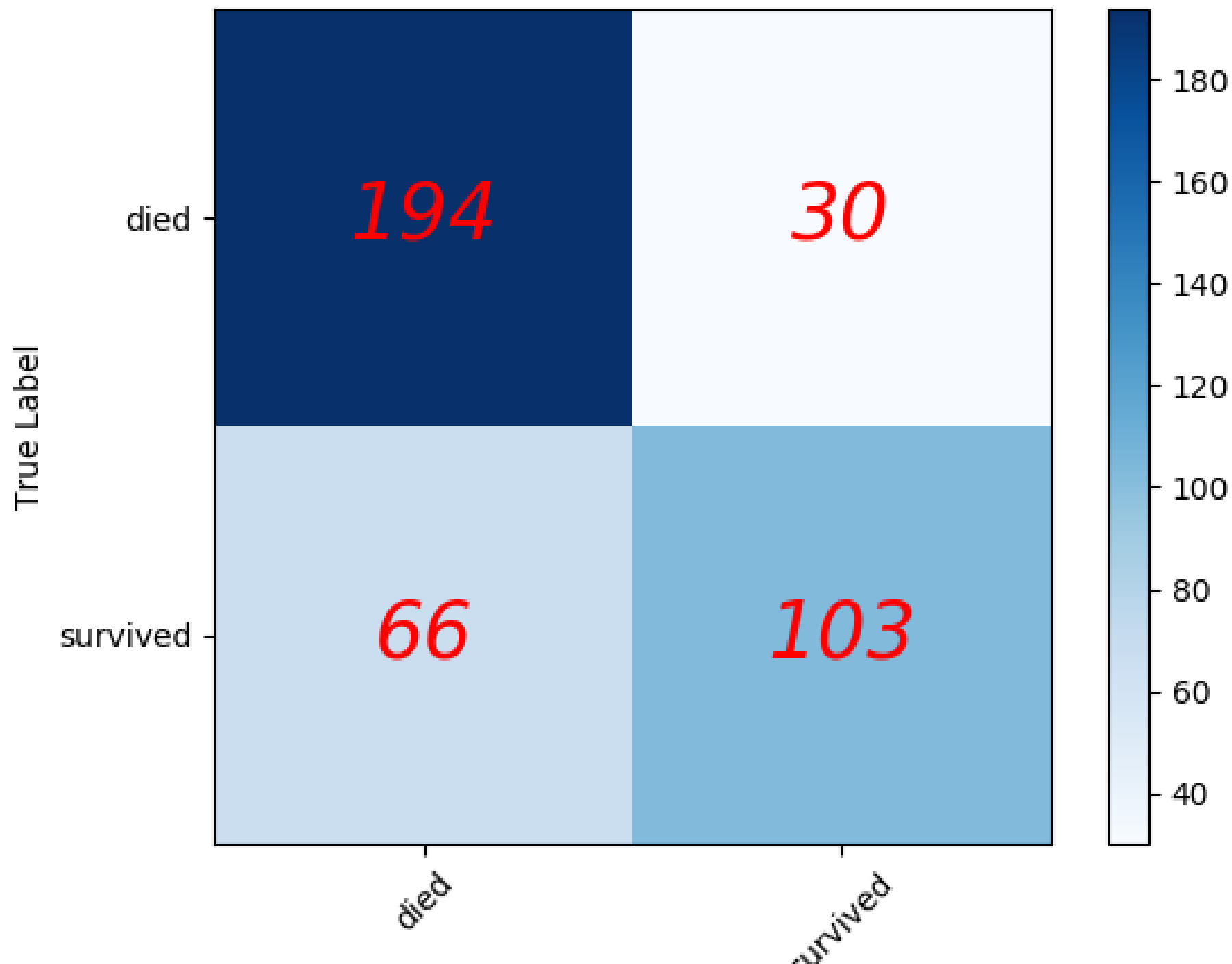
Confusion Matrix

```
>>> def plot_confusion_matrix(clf, X, y, labels, random_state=42, annotate=True,
...                             cmap=plt.cm.Blues,
...                             title="Confusion Matrix", ax=None, figkwargs=None):
...     fig, ax = fig_with_title(ax, title, figkwargs)
...     #X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=random_state)
...     y_pred = clf.predict(X)
...     cm = confusion_matrix(y, y_pred)
...     im = ax.imshow(cm, interpolation='nearest', cmap=cmap)
...     fig.colorbar(im)
...     ax.set_xticks(range(len(labels)))
...     ax.set_xticklabels(labels, rotation=45)
...     ax.set_yticks(range(len(labels)))
...     ax.set_yticklabels(labels)
...     ax.set_ylabel('True Label')
...     ax.set_xlabel('Predicted Label')
...     if annotate:
...         for x in range(len(labels)):
...             for y in range(len(labels)):
...                 plt.annotate(str(cm[x][y]),
...                             xy=(y,x),
...                             ha='center', va='center', color='red', fontsize=25, fontstyle='oblique')
...     return fig, ax
```

Confusion Matrix

```
>>> plt.clf()
>>> fig, ax = plot_confusion_matrix(
...     model3, X_test, y_test,
...     ['died', 'survived'])
>>> fig.savefig('img/ml-conf.png')
```

Confusion Matrix



Assignment

Plot a Confusion Matrix

Calibration Curves

Calibration Curves

Another mechanism to see how a classifier behaves

<https://jmetzen.github.io/2015-04-14/calibration.html>

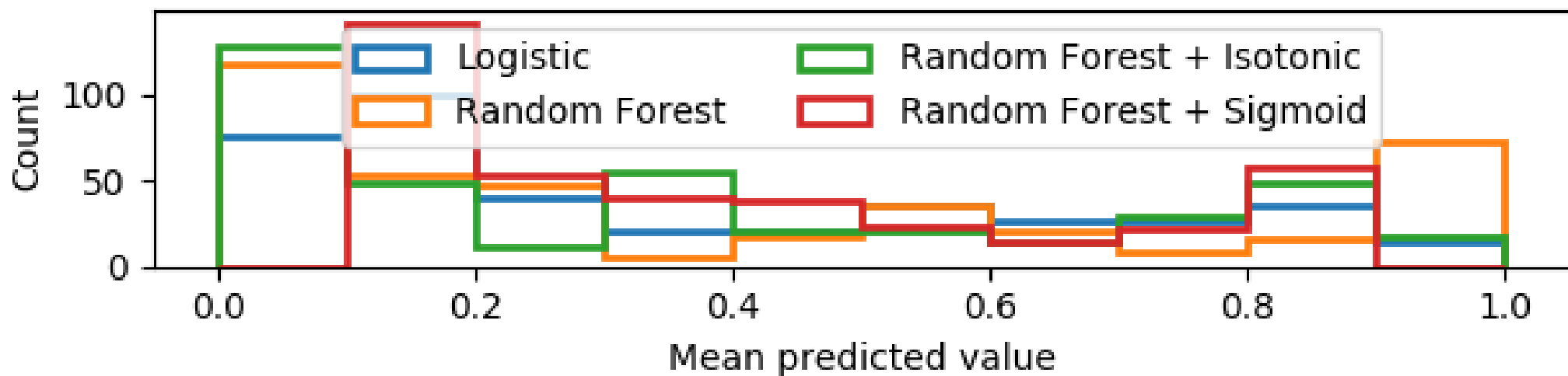
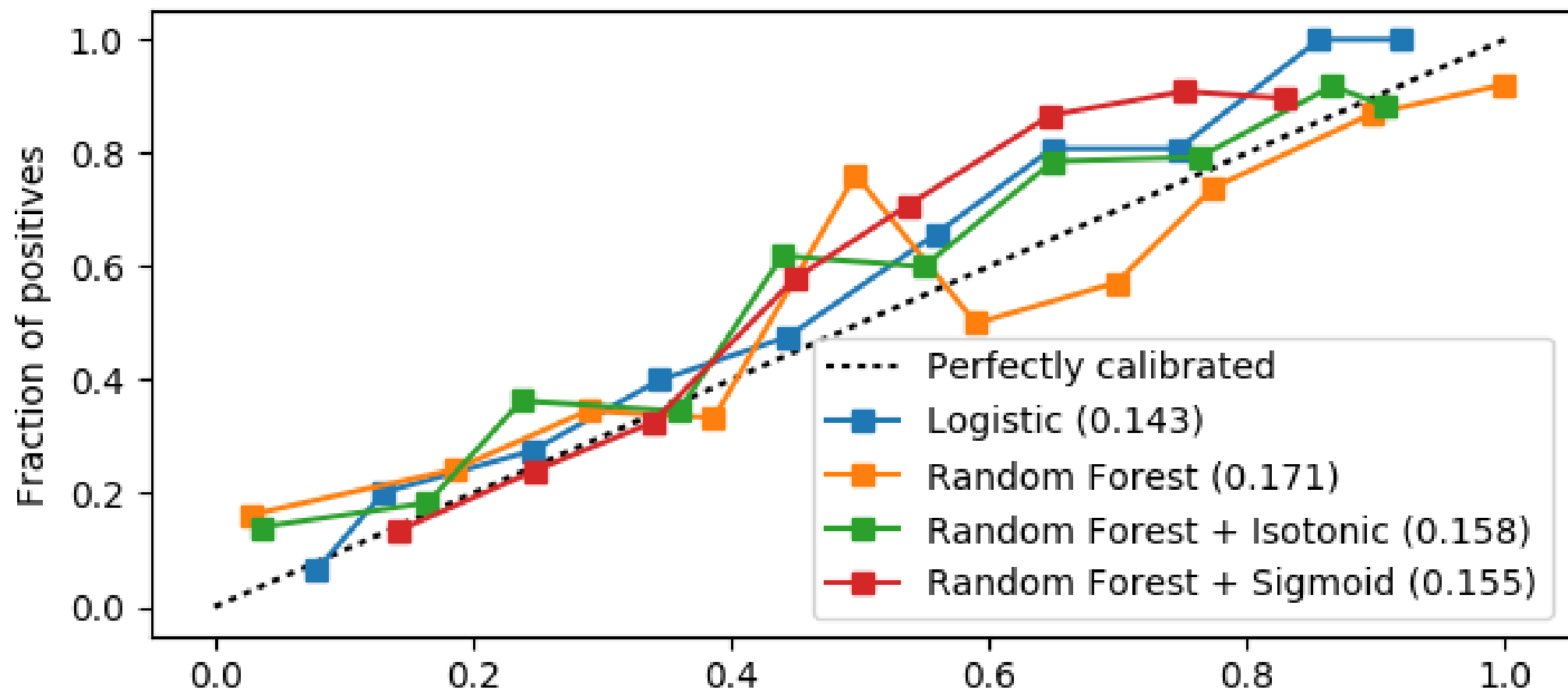
Calibration Curves

```
>>> from sklearn.calibration import CalibratedClassifierCV, calibration_curve
>>> from sklearn.linear_model import LogisticRegression
>>> from sklearn.metrics import (brier_score_loss, precision_score, recall_score,
...                               f1_score)
...
>>> def plot_calibration_curve(est, name, fig_index,
...                             X_train, X_test, y_train, y_test):
...     """Plot calibration curve for est w/o and with calibration. """
...     # Calibrated with isotonic calibration
...     isotonic = CalibratedClassifierCV(est, cv=2, method='isotonic')
...
...     # Calibrated with sigmoid calibration
...     sigmoid = CalibratedClassifierCV(est, cv=2, method='sigmoid')
...
...     # Logistic regression with no calibration as baseline
...     lr = LogisticRegression(C=1., solver='lbfgs')
...
...     fig = plt.figure(fig_index, figsize=(10, 10))
...     ax1 = plt.subplot2grid((3, 1), (0, 0), rowspan=2)
...     ax2 = plt.subplot2grid((3, 1), (2, 0))
...
...     ax1.plot([0, 1], [0, 1], "k:", label="Perfectly calibrated")
...     for clf, name in [(lr, 'Logistic'),
...                       (isotonic, name + ' + Isotonic'),
...                       (sigmoid, name + ' + Sigmoid')]:
...         clf.fit(X_train, y_train)
...         y_pred = clf.predict(X_test)
...         if hasattr(clf, "predict_proba"):
...             prob_pos = clf.predict_proba(X_test)[:, 1]
...         else: # use decision function
...             prob_pos = clf.decision_function(X_test)
...             prob_pos = \
...                 (prob_pos - prob_pos.min()) / (prob_pos.max() - prob_pos.min())
...
...         clf_score = brier_score_loss(y_test, prob_pos, pos_label=y.max())
...         print("%s: % name)
...         print("\tBrier: %1.3f" % (clf_score))
...         print("\tPrecision: %1.3f" % precision_score(y_test, y_pred))
...         print("\tRecall: %1.3f" % recall_score(y_test, y_pred))
...         print("\tF1: %1.3f" % f1_score(y_test, y_pred))
...         print("\tScore: %1.3f" % clf.score(X_test, y_test))
...
...         fraction_of_positives, mean_predicted_value = \
...             calibration_curve(y_test, prob_pos, n_bins=10)
...
...         ax1.plot(mean_predicted_value, fraction_of_positives, "s-",
...                  label="%s (%1.3f)" % (name, clf_score))
...
...         ax2.hist(prob_pos, range=(0, 1), bins=10, label=name,
...                  histtype='step', lw=2)
...
...     ax1.set_ylabel("Fraction of positives")
...     ax1.set_ylim([-0.05, 1.05])
...     ax1.legend(loc='lower right')
...     ax1.set_title('Calibration plots (reliability curve)')
...
...     ax2.set_xlabel("Mean predicted value")
...     ax2.set_ylabel("Count")
...     ax2.legend(loc='upper center', ncol=2)
...
...     plt.tight_layout()
...     return fig, [ax1, ax2]
```

Calibration Curves

```
>>> fig, axs = plot_calibration_curve(  
...     model3, 'Random Forest', 1,  
...     X_train, X_test, y_train, y_test)  
>>> fig.savefig('img/ml-cc.png')
```


Calibration plots (reliability curve)



Tuning

Overfitting & Underfitting

- Overfitting - memorizing data
- Underfitting - not flexible enough (cannot capture trend)

Tuning

Fancy term *regularization* - attempt to prevent *overfitting*

Tuning

- `max_features` - Don't want to use all of the features (all tree will look the same). By taking samples of features, you reduce bias and correlation among trees
- `n_estimators` - More is better, but diminishing returns (don't need too many jurors, takes a longer time to train, lots of memory)
- `max_depth` - too tall, overfitting. Can't know ahead of time what good size could be. Can use these parameters to constrain depth as well:
- `min_samples_leaf` - smaller is more prone to overfitting (capturing noise)
- `max_leaf_nodes` - Can't be more than this many leaves
- `min_weight_fraction_leaf` - The minimum weighted fraction of the input samples required to be at a leaf node. Note: this parameter is tree-specific.

Adjusting Parameters

Adjust Parameters

Adjust min_samples_leaf:

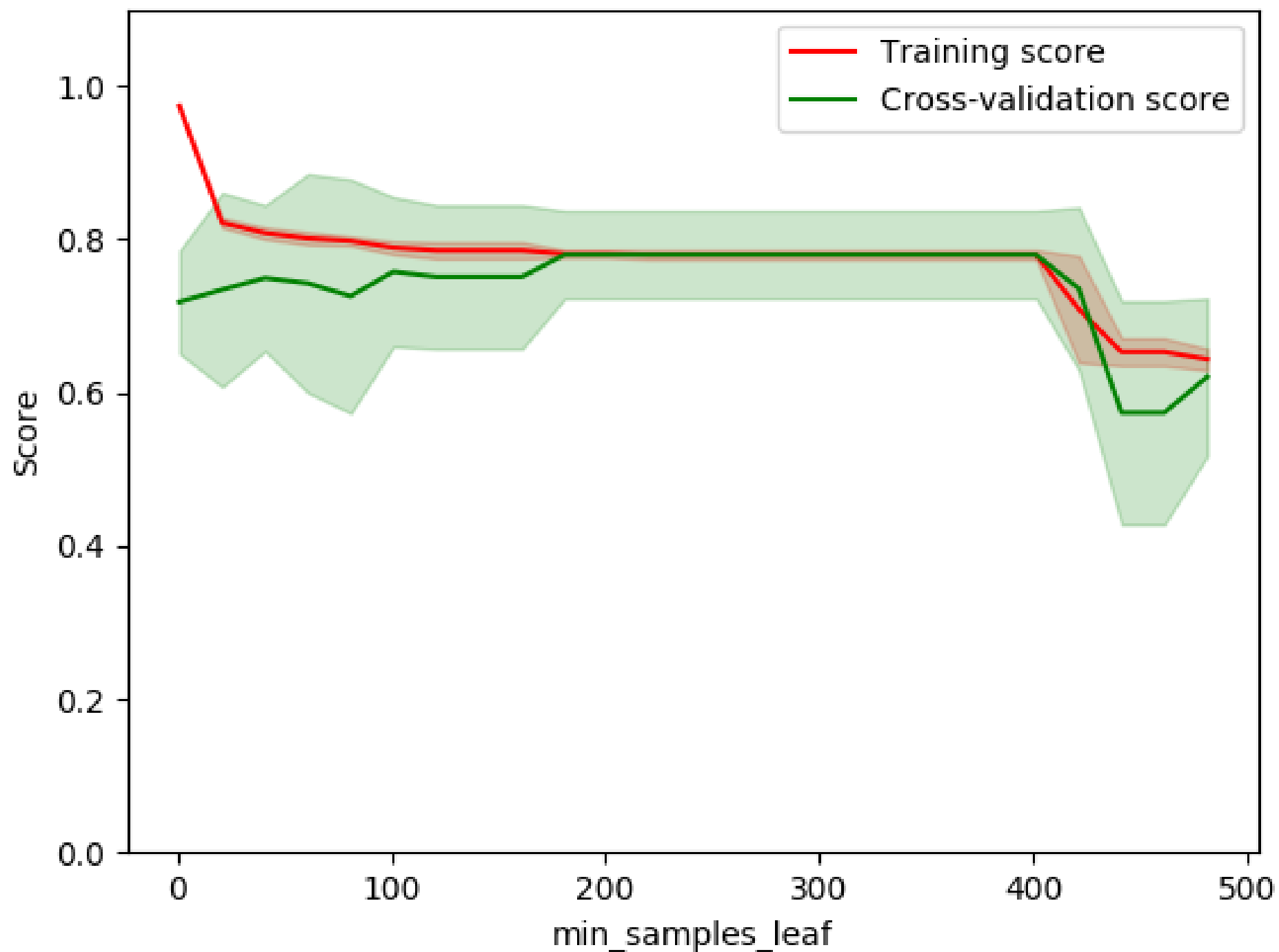
```
>>> import numpy as np
>>> from sklearn.model_selection import validation_curve
>>> model3 = tree.DecisionTreeClassifier(random_state=42)
>>> param_range = np.arange(1, 500, 20)
>>> param_name = 'min_samples_leaf'
>>> train_scores, test_scores = validation_curve(
...     model3, X, y, param_name=param_name,
...     param_range=param_range,
...     cv=10, scoring="accuracy", n_jobs=1)
>>> train_scores_mean = np.mean(train_scores, axis=1)
>>> train_scores_std = np.std(train_scores, axis=1)
>>> test_scores_mean = np.mean(test_scores, axis=1)
>>> test_scores_std = np.std(test_scores, axis=1)
```

Plot Validation Curve

```
>>> import matplotlib.pyplot as plt
>>> fig = plt.figure()
>>> ax = fig.add_subplot(111)
>>> plt.title("Validation Curve with Decision Tree")
>>> plt.xlabel(param_name)
>>> plt.ylabel("Score")
>>> plt.ylim(0.0, 1.1)
>>> plt.plot(param_range, train_scores_mean, label="Training score", color="r")
>>> plt.fill_between(param_range, train_scores_mean - train_scores_std,
...                  train_scores_mean + train_scores_std, alpha=0.2, color="r")
>>> plt.plot(param_range, test_scores_mean, label="Cross-validation score",
...          color="g")
>>> plt.fill_between(param_range, test_scores_mean - test_scores_std,
...                  test_scores_mean + test_scores_std, alpha=0.2, color="g")
>>> plt.legend(loc="best")

>>> fig.savefig('img/ml-dt-param-features.png')
>>> #plt.clf()
```


Validation Curve with Decision Tree



Grid Search

Grid Search

```
>>> from sklearn.model_selection import GridSearchCV
>>> model5 = ensemble.RandomForestClassifier()
>>> params = {'max_features': [.1, .3, .5, 1],
...           'n_estimators': [10, 20, 50],
...           'min_samples_leaf': [3, 5, 9],
...           'random_state': [42]}
>>> cv = GridSearchCV(model5, params).fit(X, y)
>>> cv.best_params_
{'max_features': 0.1, 'min_samples_leaf': 3,
'n_estimators': 20, 'random_state': 42}
```

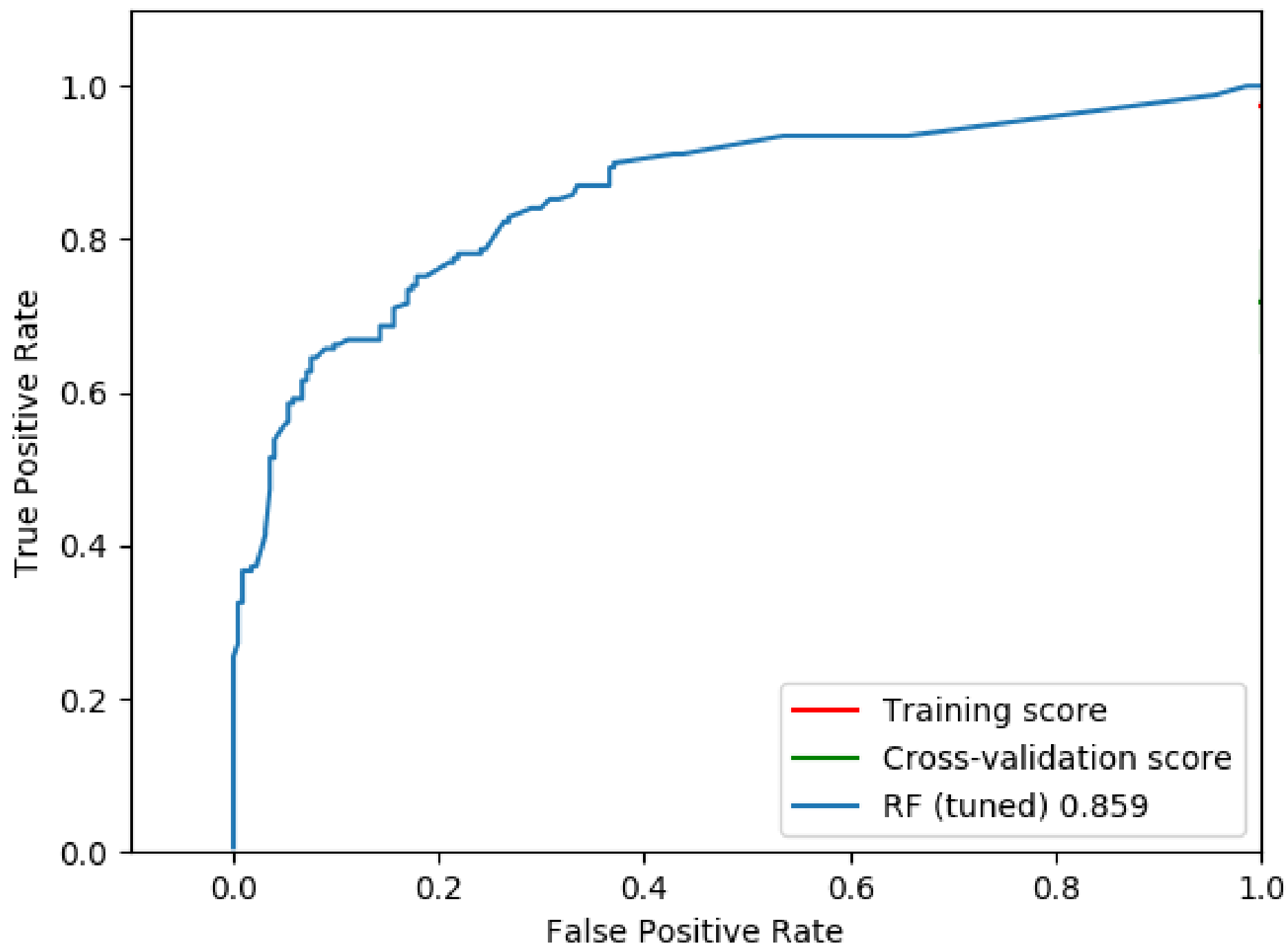
Grid Search

```
>>> model6 = ensemble.RandomForestClassifier(  
...     **cv.best_params_)  
>>> model6.fit(X_train, y_train)  
>>> model6.score(X_test, y_test)  
0.77608142493638677
```

ROC

```
>>> fig, ax = plot_roc_curve_binary(  
...     model6, X_test, y_test,  
...     'RF (tuned) {area:.3}')(  
>>> fig.savefig('img/ml-roc6.png')
```

ROC Curve



Assignment

Optimizing Models

How Much Data Do We Need?

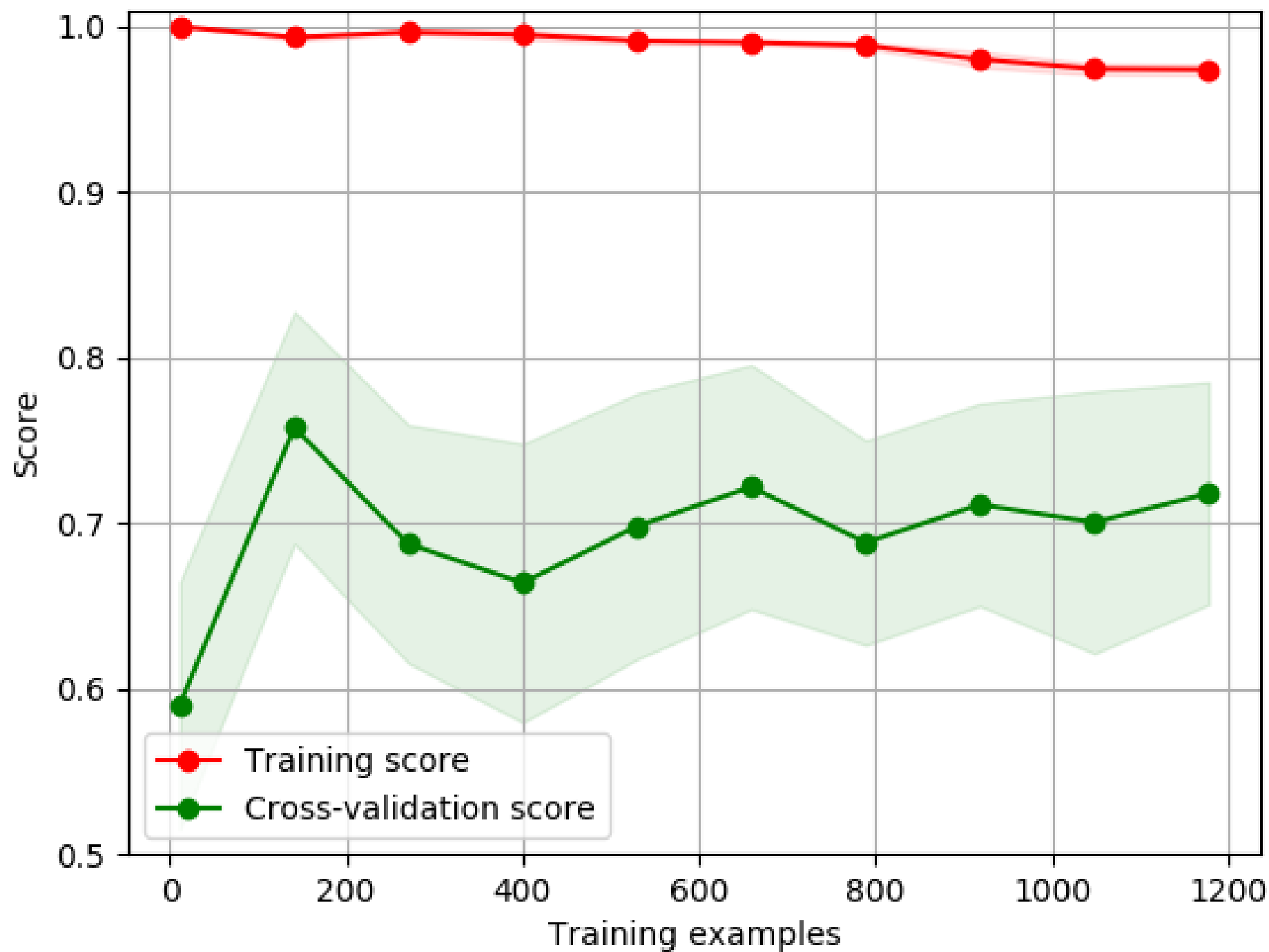
Learning Curve

```
>>> from sklearn.model_selection import learning_curve
>>> def plot_learning_curve(estimator, title, X, y, ylim=None, cv=None,
...                          n_jobs=1, train_sizes=np.linspace(.01, 1.0, 10)):
...     fig = plt.figure()
...     plt.title(title)
...     if ylim is not None:
...         plt.ylim(*ylim)
...     plt.xlabel("Training examples")
...     plt.ylabel("Score")
...     train_sizes, train_scores, test_scores = learning_curve(
...         estimator, X, y, cv=cv, n_jobs=n_jobs, train_sizes=train_sizes)
...     train_scores_mean = np.mean(train_scores, axis=1)
...     train_scores_std = np.std(train_scores, axis=1)
...     test_scores_mean = np.mean(test_scores, axis=1)
...     test_scores_std = np.std(test_scores, axis=1)
...     plt.grid()
...
...     plt.fill_between(train_sizes, train_scores_mean - train_scores_std,
...                      train_scores_mean + train_scores_std, alpha=0.1,
...                      color="r")
...     plt.fill_between(train_sizes, test_scores_mean - test_scores_std,
...                      test_scores_mean + test_scores_std, alpha=0.1, color="g")
...     plt.plot(train_sizes, train_scores_mean, 'o-', color="r",
...              label="Training score")
...     plt.plot(train_sizes, test_scores_mean, 'o-', color="g",
...              label="Cross-validation score")
...
...     plt.legend(loc="best")
...     return fig, plt
```

Plot it

```
>>> title = "Learning Curves (Decision Tree)"
>>> fig, plt = plot_learning_curve(model,
...     title, X, y, ylim=(0.5, 1.01), cv=10, n_jobs=4)
>>> fig.savefig('img/ml-1c.png')
```

Learning Curves (Decision Tree)



Assignment

Learning Curves

Summary

Summary

- Scalable (can build trees per CPU)
- Reduces variance in decision tree
- No normalization of data (don't want money range (\$0 - \$10,000,000) overriding age (0-100))
- Feature importance (look at "mean decrease of impurity" where this node appears)
- Helps with missing data, outliers, and dimension reduction
- Works with both regression and classification
- Sampling allows "out of bag" estimate, removing need for test set

Why Python?

- Efficient algorithm
- Close to metal, 3000+ lines of Cython
- Faster than OpenCV (C++), Weka (Java), RandomForest (R / Fortran)

Attribution

- <https://www.flickr.com/photos/eeekim/2375990831>
- Leonardo from internet

Thanks

@__mharrison__