Survey of Machine Learning Methods

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Overview

- Short theoretical review of each method
- Strong and weak points of each method
- Compare out of the box performance on Rate My Professor

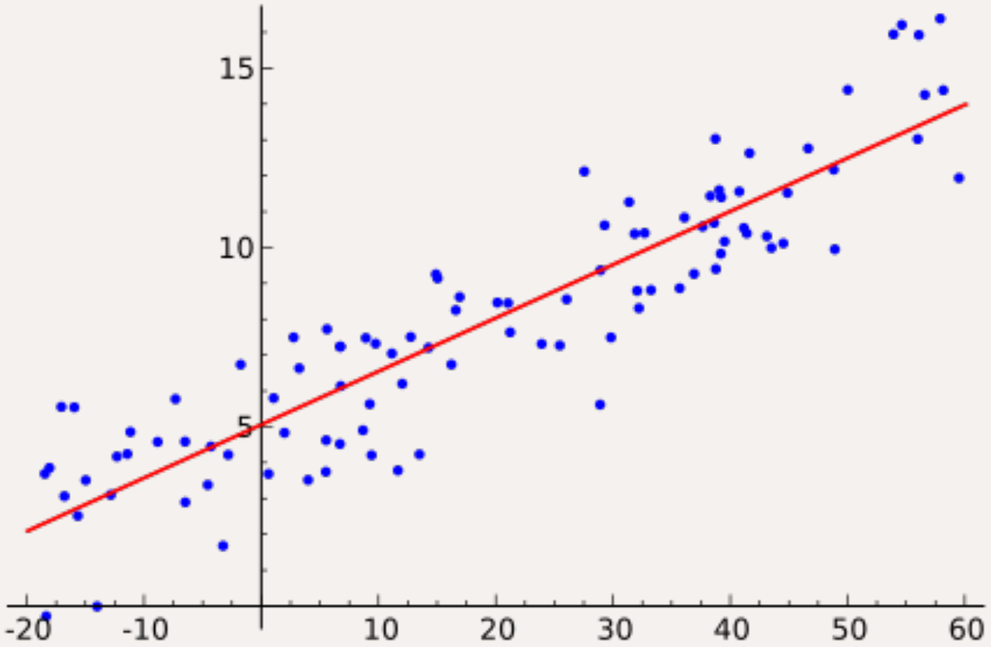
Models

- Linear Models
- Decision Trees
- Random Forests
- X is training data (design matrix), y is targets

Linear Regression

Linear Regression

Find coefficients w such that the mean squared error is minimized:



Objective Function

$$\min_{w} ||Xw - y||_2^2$$

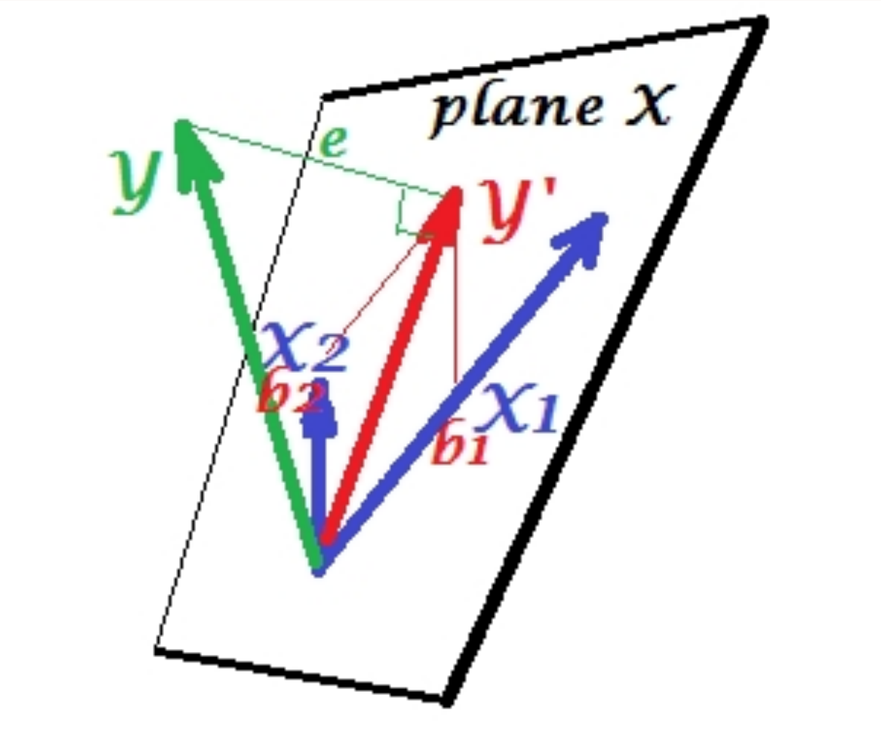
- Where could this go wrong?

Correlation in Design Matrix

- What if there are correlated variables in X?
- The matrix X would be nearly singular
- Singular matrix equivalent to determinant equal to zero

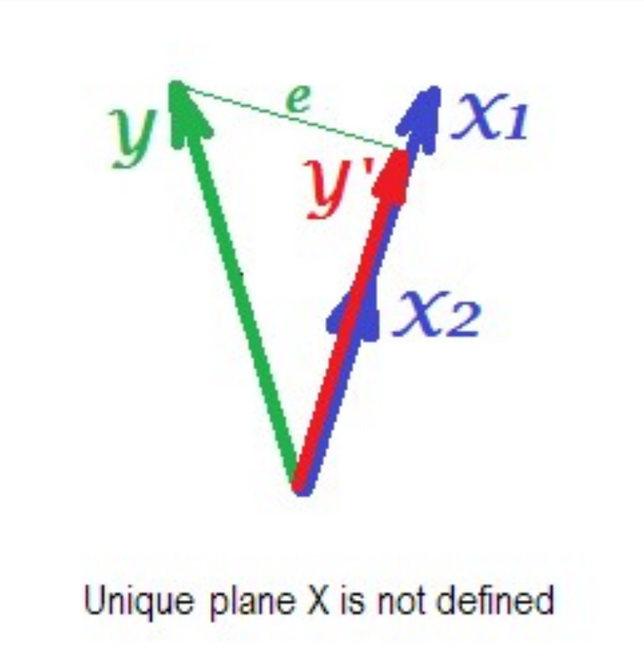
$$\begin{bmatrix} 0 & 0 \\ 1 & 1 \end{bmatrix}$$

Slight Correlation in X



- The plane X is well defined

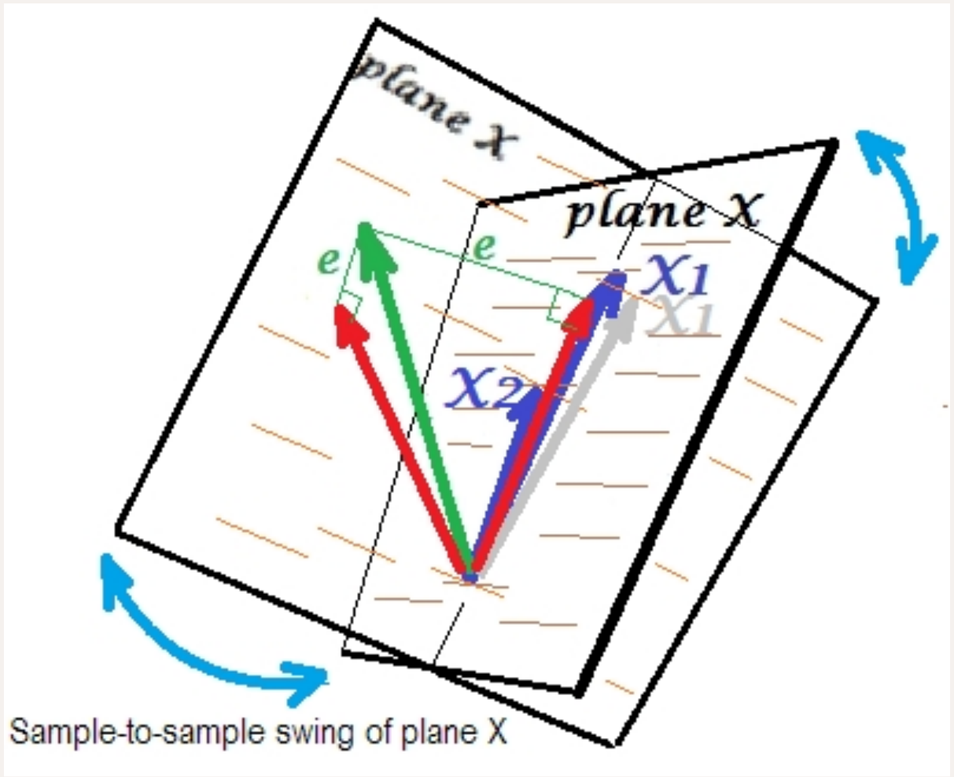
Perfect Correlation in X



- The plane X disappears since only one variable is needed to explain y

Near Perfect Correlation in X

- Slight divergence in X_1 causes large shift in plane X



Example

Even a very slight perturbation in X causes a huge shift

```
In [1]: from sklearn.linear_model import LinearRegression
In [2]: m = LinearRegression(fit_intercept=False)
In [3]: m.fit([[0, 0], [1, 1]], [1, 1])
Out[3]: LinearRegression(copy_X=True, fit_intercept=False, n_jobs=1, normalize=False)

In [4]: m.coef_
Out[4]: array([ 0.5,  0.5])

In [17]: m.fit([[.001, 0], [1, 1]], [1, 1])
Out[17]: LinearRegression(copy_X=True, fit_intercept=False, n_jobs=1, normalize=False)

In [18]: m.coef_
Out[18]: array([ 1000.,  -999.])
```

Fixing This

- The problem is that there are no other optimization constraints
- Next two models impose constraints
  - Ridge Regression
  - Lasso Regression

Ridge Regression

Ridge Regression

- Optimizes the same least squares problem as linear regression with a penalty on size of coefficients

$$\min_{w} ||Xw - y||_2^2 + \alpha||w||_2^2$$

Example

```
In [1]: from sklearn.linear_model import Ridge
In [2]: r = Ridge(fit_intercept=False)
In [3]: r.fit([[0, 0], [1, 1]], [1, 1])
In [4]: r.coef_
Out[4]: array([ 0.33333333,  0.33333333])

In [5]: r.fit(np.array([[.001, 0], [1, 1]]), [1, 1])
In [6]: r.coef_
Out[6]: array([ 0.33399978,  0.33300011])
```

Lasso Regression

Lasso Regression

- Optimize least squares with penalty for too many important coefficients
- Prefers models with fewer parameter values due to l_1 norm

$$\min_w \frac{1}{2n} ||Xw - y||_2^2 + \alpha ||w||_1$$

Compare on Rate My Professor

```
import pandas as pd
from sklearn.cross_validation import train_test_split
from sklearn.feature_extraction.text import CountVectorizer
from sklearn.pipeline import Pipeline
from sklearn.grid_search import GridSearchCV
from sklearn.metrics import mean_squared_error
from sklearn.linear_model import LinearRegression, Ridge, Lasso

data = pd.read_csv('train.csv')
data['comments'] = data['comments'].fillna('')
train, test = train_test_split(data, train_size=.3)

 def test_model(model, ngrams):
    pipeline = Pipeline([
            ('vectorizer', CountVectorizer(ngram_range=ngrams)),
            ('model', model)
    ])

    cv = GridSearchCV(pipeline, {}, scoring='mean_squared_error')
    cv = cv.fit(train['comments'], train['quality'])
    validation_score = model.best_score_
    predictions = model.predict(test['comments'])
    test_score = mean_squared_error(test['quality'], predictions)
    return validation_score, test_score
```

Compare on Rate My Professor

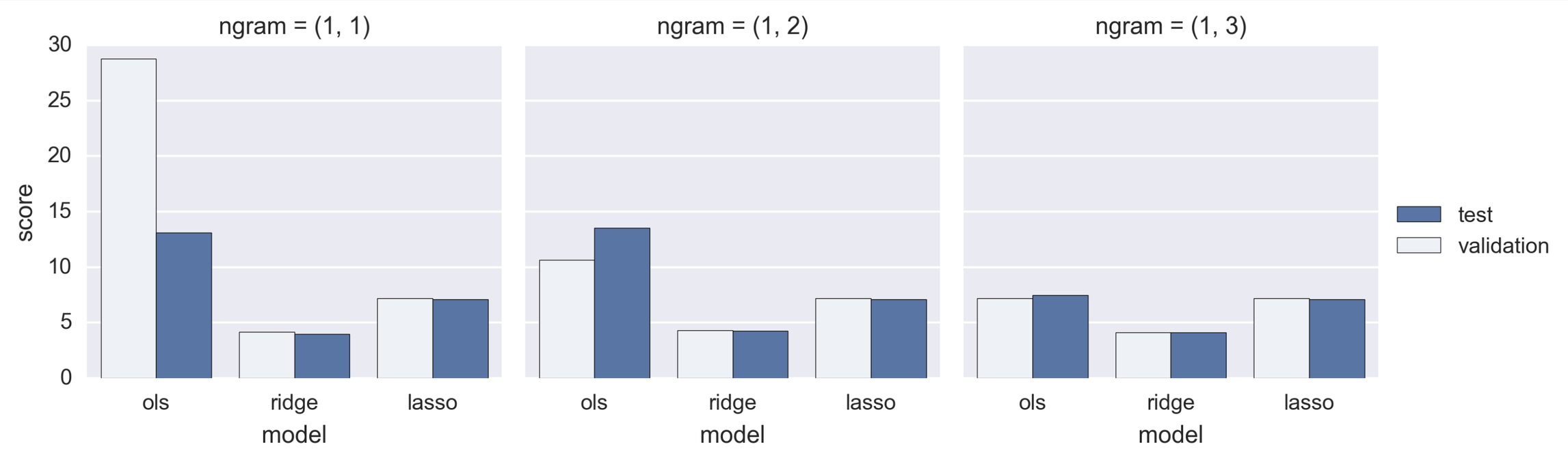
```
import itertools

models = [('ols', LinearRegression()), ('ridge', Ridge()), ('lasso', Lasso())]
ngram_ranges = [(1, 1), (1, 2), (1, 3)]

scores = []
for m, ngram in itertools.product(models, ngram_ranges):
    name = m[0]
    model = m[1]
    validation_score, test_score = test_model(model, ngram)
    scores.append({'score': -validation_score, 'model': name, 'ngram': str(ngram), 'fold': 'validation'})
    scores.append({'score': test_score, 'model': name, 'ngram': str(ngram), 'fold': 'test'})

import seaborn as sb
df = pd.DataFrame(scores)
```

RMP: Dimensionality

Using `CountVectorizer` with 1, 2, and 3 grams

- 20% of training data
- 1-gram: ~50,000
- 2-gram: ~650,000
- 3-gram: ~2,500,000
- Can you guess which model did the best?

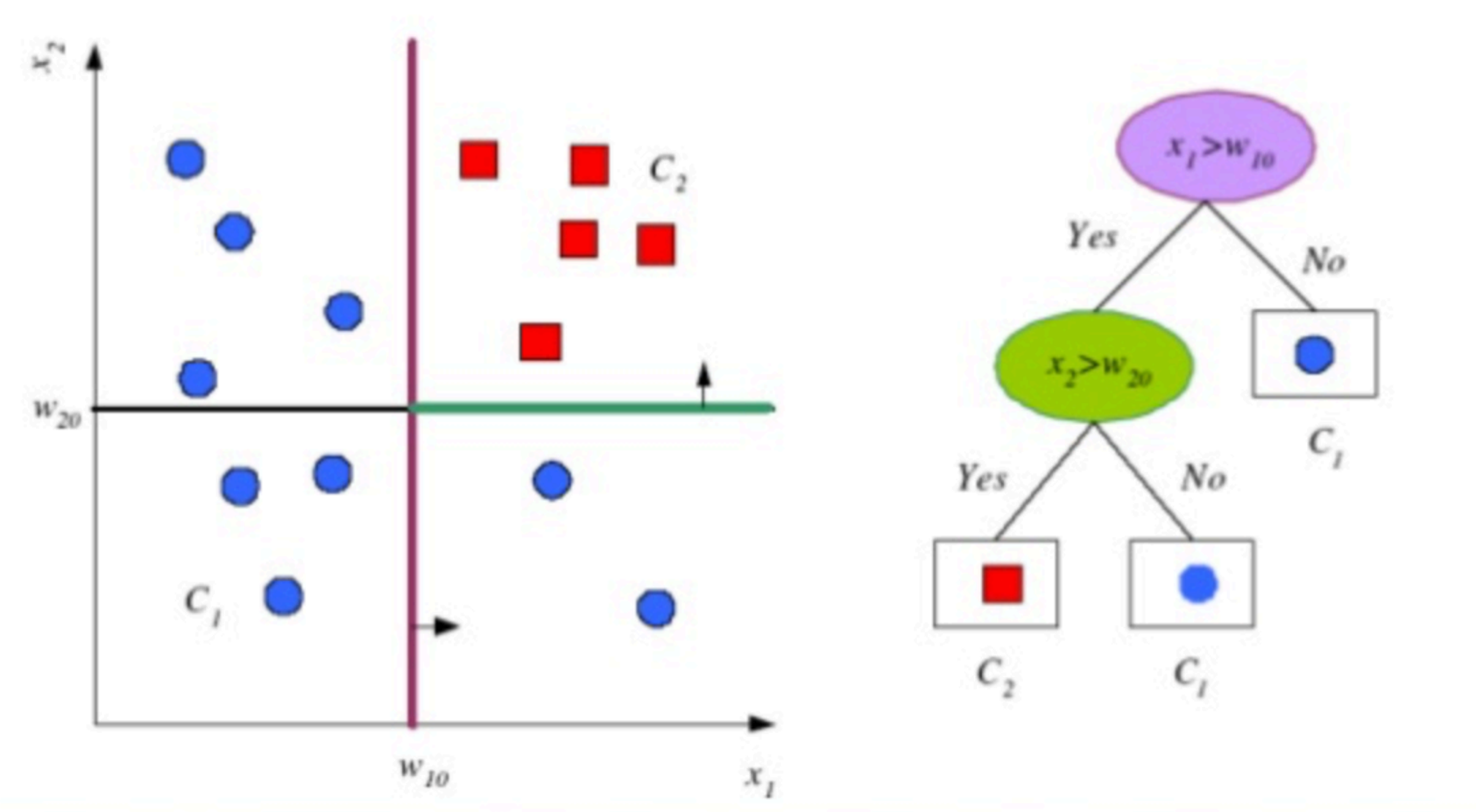
Comparison of Models



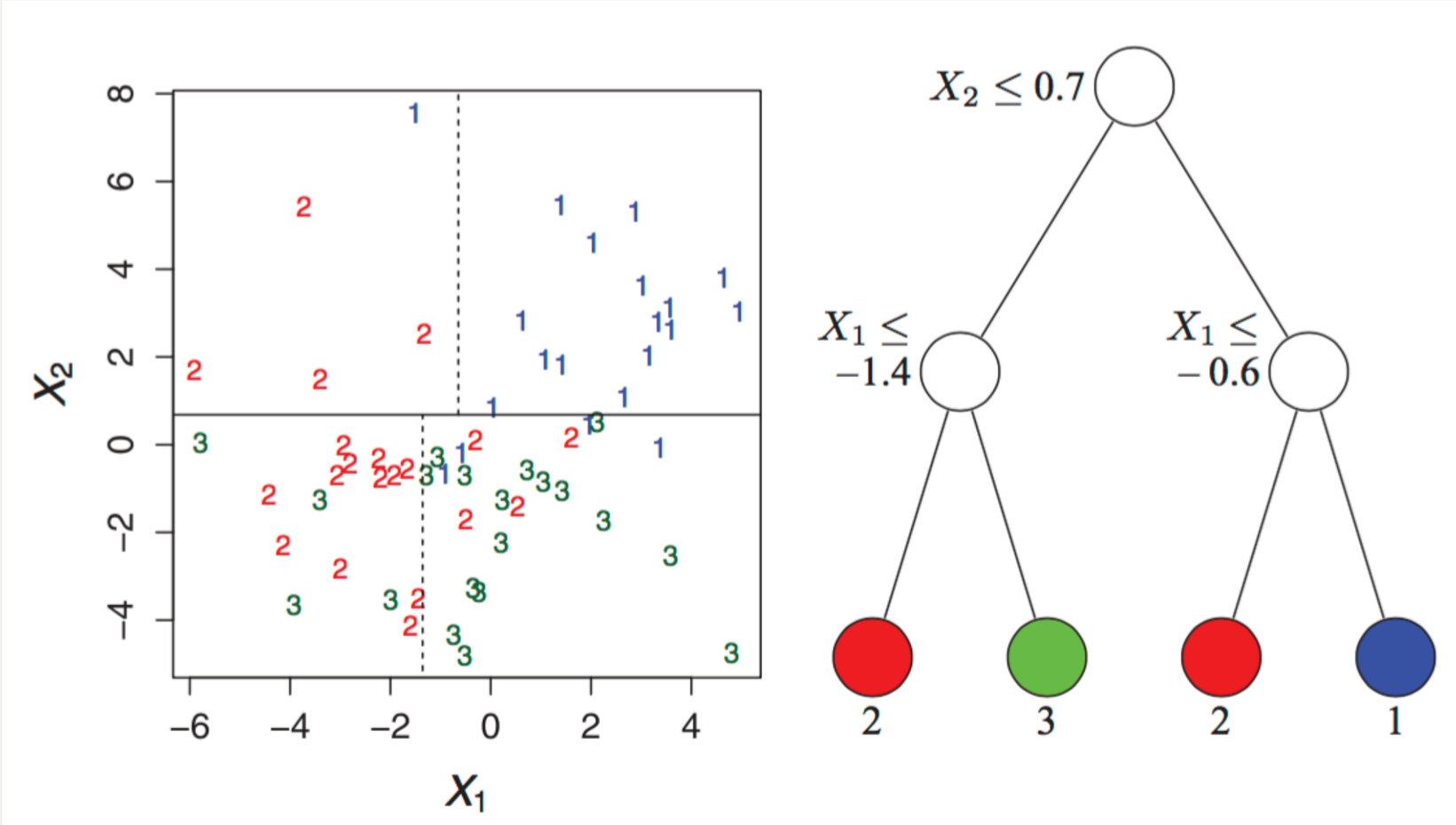
- Ideas on why?

Decision Trees

Decision Trees: Classification



Decision Trees: Classification



Decision Trees

- Recursively: pick the x_i which best splits the data and create a split
- Stop when the data is pure or knowledge gain is small/zero

Gini Impurity

- Randomly assign classes according to frequency of labels
- How often a randomly selected element has wrong class
- f_i: fraction of items labeled with class i
- $i \in \{1, 2, \ldots, J\}$, J is the number of classes

$$I_g(f) = \sum_{i=1}^{J} f_i(1 - f_i)$$

Example

- Suppose $J = 2$
- $f_1 = .5$ and $f_2 = .5$ then $I_g(f) = .5^2 + .5^2 = .5$
- $f_1 = .1$ and $f_2 = .9$ then $I_g(f) = .1 \cdot .9 + .1 \cdot .9 = .18$
- Pick the variable which produces the highest Gini Impurity
- There are other similar metrics

Decision Trees for Regression

- No classes, numeric target
- How can we adapt to this using a similar idea?

Decision Trees for Regression

- Switch Gini Impurity with Standard Deviation Reduction
- Find splits that minimize the sum of squared errors (promote homogeneity)
- $\bar{y_i}$ is mean target in set S_i

$$SSE = \sum_{i \in S_1} (y_i - \bar{y_1})^2 + \sum_{i \in S_2} (y_i - \bar{y_2})^2$$

Growing a Regression Tree

- Split the data on each attribute
- Categorical is simple, Ordinal values: sort and split values of attribute
- Calculate the change in standard deviation
- Find the attribute that reduces standard deviation the most

More complete explanation by CMU[12]

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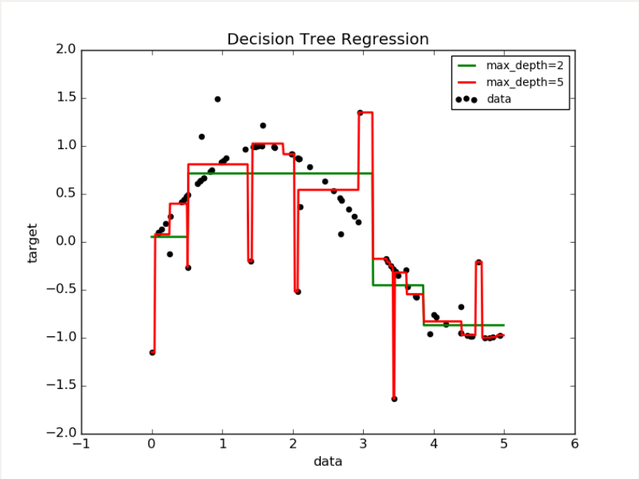
[1] Regression Tree Notes

[2] Additional Notes

Challenges with Decision Trees

- Prone to overfitting: low bias, very high variance
- Bias: trees find the relevant relations
- Variance: Sensitive to noise/variance in training set



Tree Overfitting on RMP

```
from sklearn.tree import DecisionTreeRegressor
tree_scores = []
for i in [5, 50, 100, 150, 200, 250, 300, 350]:
    validation_score, test_score = test_model(DecisionTreeRegressor(max_depth=i), (1, 1))
    tree_scores.append({'Max Depth': i, 'score': -validation_score, 'fold': 'validation'})
    tree_scores.append({'Max Depth': i, 'score': test_score, 'fold': 'test'})

tree_df = pd.DataFrame(tree_scores)
g = sb.barplot(x='Max Depth', y='score', hue='fold', data=tree_df, ci=None)
plt.legend(loc='upper left')
plt.ylabel('MSE Score')
g.savefig('plot-tree-overfitting.png', format='png', dpi=300)
```

Tree Overfitting on RMP

Random Forests

Random Forests

- Use predictive power of decision trees without issue of overfitting
- Idea: fit many trees on different subsets of features and training examples then vote on the answer
- Generally one of the best off-the-shell learning methods

Tree Bagging

- $X = x_1, \ldots, x_n$ with $Y = y_1, \ldots, y_n$
- Given B bags

```
for b in range(B):
    # sample with replacement n training examples: Xb, Yb
    # Train a decision tree fb on Xb, Yb

# Save all the trees for later
```

Tree Bagging and Random Forests

After training, predictions for new x' are made using a vote

$$\hat{f} = \frac{1}{B}\sum_{b=1}^{B}\hat{f}_b(x')$$

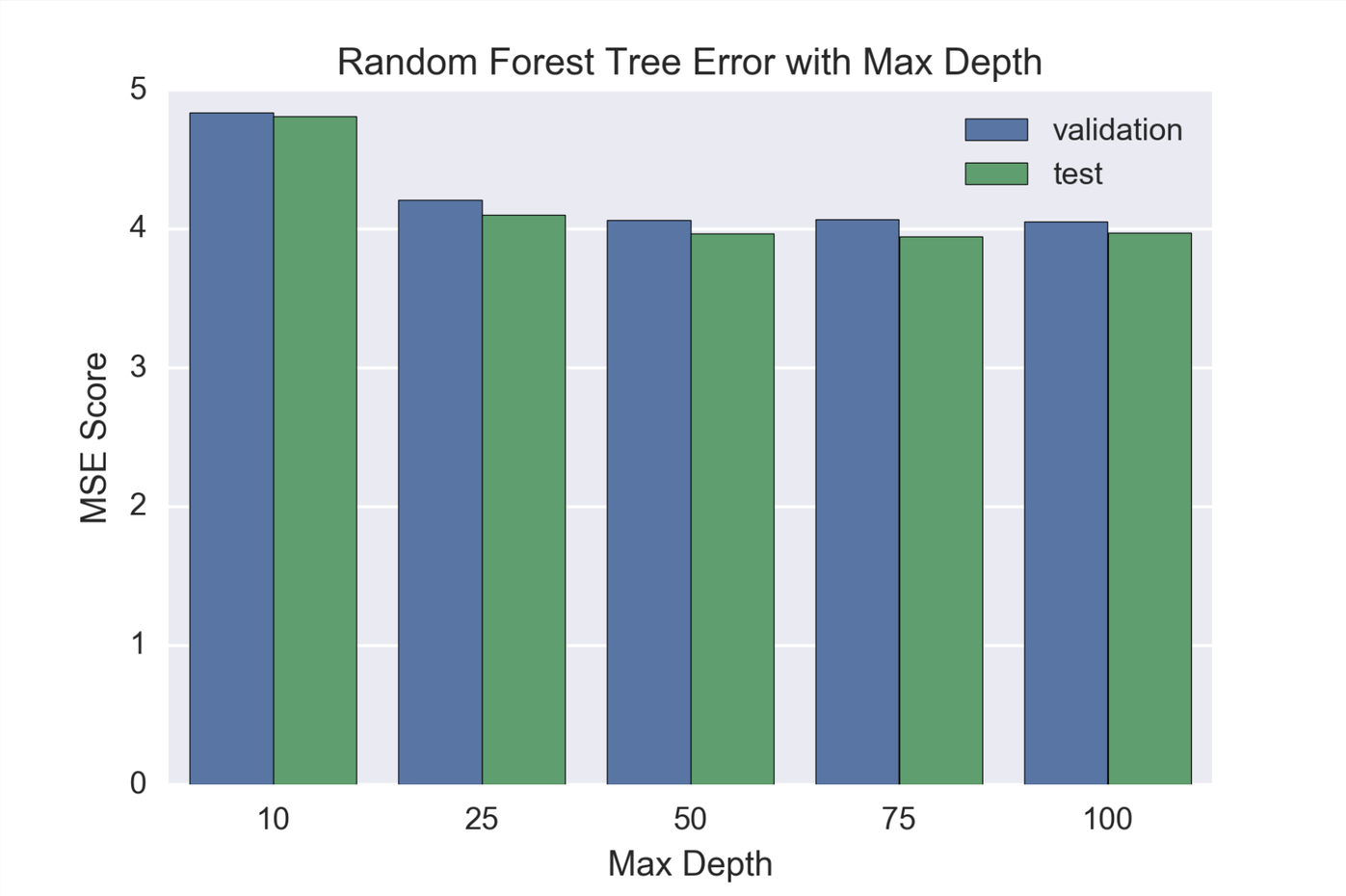
- Creating random subsets of features for each tree results in a Random Forest

Random Forests on RMP

```
from sklearn.ensemble import RandomForestRegressor

rf_scores = []
for i in [10, 25, 50, 75, 100]:
    validation_score, test_score = test_model(
        RandomForestRegressor(max_depth=i, n_jobs=-1),
        (1, 1)
    )
    rf_scores.append({'Max Depth': i, 'score': -validation_score, 'fold': 'validation'})
    rf_scores.append({'Max Depth': i, 'score': test_score, 'fold': 'test'})
```

Random Forests on RMP



Summary

- Linear Models: Ordinary Least Squares, Ridge, and Lasso
- Decision Trees
- Random Forests
- Code examples of all of these using 20% data as training
- Best out-of-box model: Random Forests (~4.0)

Questions?

- More About Pedro Rodriguez: pedrorodriguez.io
- github.com/Entilzha
- Colorado Data Science Team: codatascience.github.io
- Code at github.com/CoDataScience/rate-my-professor