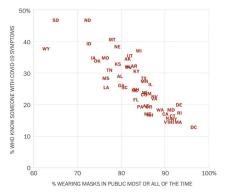
Building a Robot Judge: Data Science for Decision-Making

5. Classification

Week 2 Review: Four Types of Confounders

Masking up

Fewer covid-19 symptoms reported in states with higher rates of mask use (data as of October 19, 2020)



Source: Delphi COVIDCast, Carnegie Mellon University THE WASHINGTON POST

https://twitter.com/ASlavitt/status/

Recall that there are four types of confounders. Based on the first letter your last name, think of an example confounder for this proposed causal relationship.

- 1. [A-G] positively correlated with outcome, positively correlated with treatment
- 2. [H-M] positively correlated with outcome, negatively correlated with treatment
- 3. [N-S] negatively correlated with outcome, positively correlated with treatment
- [T-Z] negatively correlated with outcome, negatively correlated with treatment

Write it down privately. Which direction is the bias of the estimate (up or down), relative to the true causal effect (if this is the only confounder)? (3 minutes)

Week 3 Review: What line # has a bug?

Write it down (90 seconds)

```
1 X_train, X_test, y_train, y_test = train_test_split(X,y_true)
2 lasso = Lasso()
3 lasso.fit(X_train, y_train)
4 y_pred = lasso.predict(X)
5 mae = mean_absolute_error(y_true,y_pred)
```

Note: mean absolute error $(\sum |y - \hat{y}|)$ is an alternative regression metric that is less sensitive to outliers than mean squared error $(\sum (y - \hat{y})^2)$.

Week 4 Review: Confounding factors for a tax cut (3 minutes)

- Imagine that cantons Zurich and Zug each enact a tax cut and you estimate a negative effect on local employment using two-way fixed-effects regression. What are some potential confounding factors that would bias this estimate?
 - write them down privately.

Another on Correlation vs Causation

https://www.sciencedaily.com/releases/2022/08/220825120349.htm

Science News

from research organizations

Study uncovers differences in saliva bacteria of students with recent suicidal thoughts

Date: August 25, 2022

Source: University of Florida

Summary: Adding to a growing body of research on mental health and the human microbiome, a

new study compared the bacteria in the saliva of students with and without recent

thoughts of suicide, called suicidal ideation.

Share:

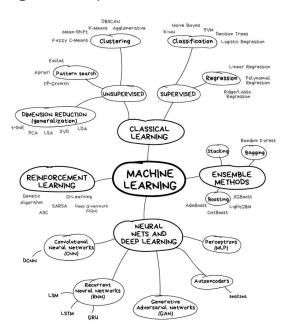




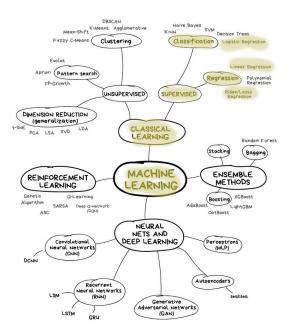


Controlling for the influence of other factors known to impact mental health, such as diet and sleep, the researchers found that students with recent suicidal thoughts had higher levels of bacteria associated with periodontal disease and other inflammatory health conditions. They also found that these students had lower levels of Alloprevotella rava, a bacterium known to produce a compound that promotes brain health. These students also shared a genetic variation that the researchers found may influence the presence of Alloprevotella rava in the mouth.

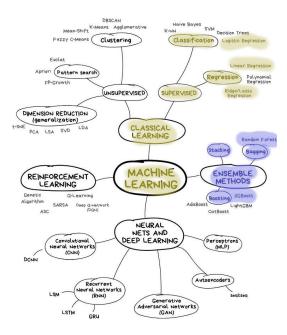
The Machine Learning Landscape



What we have done so far



What we will do today



Outline

Binary Classifier Metrics

Multi-Class Models

Ensemble Learning with XGBoost

Response Essays

Machine learning metrics

► For regression, evaluation is relatively straightforward – we have mean squared error, mean absolute error, or R-squared (see Week 3 slides).

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- ▶ For classification, things are more complicated.
- ► As a (good) baseline, we have:
 - ▶ accuracy = (# correct test-set predictions) / (# of test-set observations)

Machine learning metrics

- For regression, evaluation is relatively straightforward we have mean squared error, mean absolute error, or R-squared (see Week 3 slides).
- For classification, things are more complicated.
- ► As a (good) baseline, we have:
 - ightharpoonup accuracy = (# correct test-set predictions) / (# of test-set observations)
- ▶ But what if one of the outcomes is rare e.g., one out of 20?
 - ▶ Then I can guess the modal class and get 95% accuracy.
- ► As we will see, there are a range of other useful metrics besides accuracy for evaluating classifier performance.

Confusion Matrix

A nice way to visualize classifier performance:

		Predicted Class	
		Negative	Positive
True Class	Negative	# True Negatives	# False Positives
	Positive	# False Negatives	# True Positives

Cell values give counts in the test set.

```
from sklearn.metrics import confusion_matrix
confusion_matrix(y_test,y_pred)
```

$$\mathsf{Accuracy} = \frac{\mathsf{True}\;\mathsf{Positives}\;+\;\mathsf{True}\;\mathsf{Negatives}}{\mathsf{True}\;\mathsf{Positives}\;+\;\mathsf{False}\;\mathsf{Positives}\;+\;\mathsf{False}\;\mathsf{Negatives}\;+\;\mathsf{True}\;\mathsf{Negatives}}$$

Precision and Recall

		Predicted Class		
		Negative	Positive	
True Class	Negative	# True Negatives	# False Positives	
	Positive	# False Negatives	# True Positives	

```
from sklearn.metrics import precision_score, recall_score
precision_score(y_test,y_pred)
recall_score(y_test,y_pred)
```

Precision and Recall

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$$\frac{\text{Precision (for positive class)} = \frac{\text{True Positives}}{\text{True Positives} + \text{False Positives}}$$

Precision decreases with false positives. "When I guess this outcome, I tend to guess correctly."

Precision and Recall

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recall_score(y_test,y_pred)

$$Precision (for positive class) = \frac{True Positives}{True Positives + False Positives}$$

Precision decreases with false positives. "When I guess this outcome, I tend to guess correctly."

Recall (for positive class) =
$$\frac{\text{True Positives}}{\text{True Positives} + \text{False Negatives}}$$

▶ Recall decreases with false negatives. "When this outcome occurs, I don't miss it."

Note: sckit-learn will produce precision/recall for Y = 1 by default

Trading off precision and recall

- Recall our decision framework:
 - a decision-maker who has to make a decision W, that will produce some value or benefit, conditional on the value of Y:

$$V = u(W, Y)$$

ightharpoonup One can imagine decision contexts where precision/recall should be valued asymmetrically. This is part of the function u(W, Y).

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- One can imagine decision contexts where precision/recall should be valued asymmetrically. This is part of the function u(W, Y).
- For these decisions, would you prefer high precision or high recall?
 - 1. deciding "send to prison" in court
 - 2. detecting bombs during flight screening

Balanced Accuracy and F1 Score

- ▶ If labels are (almost) balanced, then accuracy (share correct predictions) is a decent metric.
 - ▶ If not (say 90% in one category), accuracy will be uninformative/misleading.

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Balanced Accuracy =
$$\frac{1}{2} \left(\frac{TP}{TP + FN} + \frac{TN}{TN + FP} \right)$$

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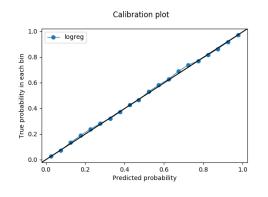
- ightharpoonup ightharpoonup equal to accuracy when classes are balanced, or performance is the same across classes.
- \triangleright Another standard metric is F_1 score = the harmonic mean of precision and recall:

$$F_1 = \frac{2}{\frac{1}{\text{precision}} + \frac{1}{\text{recall}}} = 2 \times \frac{\text{precision} \times \text{recall}}{\text{precision} + \text{recall}}$$

penalizes both false positives and false negatives. still ignores true negatives.

from sklearn.metrics import balanced_accuracy_score, f1_score
balanced_accuracy_score(y_test,y_pred)
f1_score(y_test,y_pred) # gives values for both classes

Evaluating Classification Models: Calibration Curves



- ► Plotting the binned fraction in a category (Y axis) against the predicted probability in a category (X axis):
- ▶ Provides evidence of whether the classifer is replicating the conditional distribution of the outcome.

```
from seaborn import regplot
regplot(y_test, y_pred, x_bins=20)
```

ROC Curve and AUC

ROC Curve Plot Perfect Skill Classifier True Positive Rate **ROC Curve ROC Curve** for a Skillful for a No Skill Classifier Classifier Worse than no skill

False Positive Rate

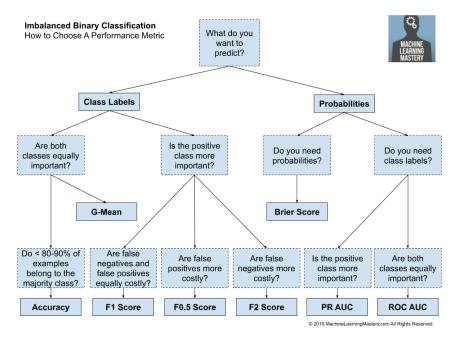
AUC = area under the (ROC) curve

provides an aggregate measure of performance across all possible classification thresholds.

Interpreting AUC:

= probability that the model (correctly) ranks a random positive example more highly than a random negative example.

from sklearn.metrics import roc_auc_score
roc_auc_score(y_test,y_pred)



See details in "Tour of evaluation metrics for imbalanced classification" (on syllabus).

Outline

Binary Classifier Metrics

Multi-Class Models

Ensemble Learning with XGBoost

Response Essays

Multi-Class Models

Many interesting machine learning problems involve multiple un-ordered categories:

- categorizing a case by area of law.
- predicting the political party of a speaker in a multi-party system.
- predicting authorship from documents
- ▶ image classification / object detection

Multiple Classes: Setup

▶ The outcome is $y_i \in \{1,...,k,...,n_y\}$ output classes, which can also be represented as a one-hot vector

$$\mathbf{y}_i = {\mathbf{1}[y_i = 1], ..., \mathbf{1}[y_i = n_y]}$$

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$$\mathbf{y}_i = {\mathbf{1}[y_i = 1], ..., \mathbf{1}[y_i = n_y]}$$

We want to learn a vector function

$$\mathbf{y} = \mathbf{h}(\mathbf{x}, \theta)$$

outputing a vector of probabilities across outcomes as a function of the inputs:

$$\hat{\mathbf{y}} = {\{\hat{y}^1, ..., \hat{y}^{n_y}\}, \hat{y}^k \in [0, 1] \ \forall k}$$

for prediction, select the highest-probability class:

$$\tilde{\mathbf{y}} = \arg\max_{k} \hat{\mathbf{y}}_{[k]}$$

Categorical Cross Entropy

► The standard loss function in multinomial classification is **categorical cross entropy**:

$$L(\theta) = -\sum_{k=1}^{n_y} \boldsymbol{y}_{[k]} \log(\hat{\boldsymbol{y}}_{[k]}(\boldsymbol{x}, \theta))$$

measures dissimilarity between the true label distribution y and the predicted label distribution \hat{y} .

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- measures dissimilarity between the true label distribution y and the predicted label distribution \hat{y} .
- Since there is just one true class $(y = 1 \text{ for one class } k^*$, and zero for others), simplifies to

$$L(\theta) = -\log(\hat{\boldsymbol{y}}_{[k^*]}(\boldsymbol{x}, \theta))$$

- Rewards putting higher probability on the true class, ignores distribution of probabilities on other classes.
- function is convex \rightarrow gradient descent will find the optimum.

Multinomial Logistic Regression

Multinomial logistic regression computes probabilities for each class k using the softmax transformation

$$\hat{y}_k(\mathbf{x}_i) = \Pr(y_i = k) = \frac{\exp(\theta'_k \mathbf{x}_i)}{\sum_{l=1}^{n_y} \exp(\theta'_l \mathbf{x}_i)}$$

- ightharpoonup softmax is the multiclass generalization of sigmoid. can then interpret \hat{y} as probabilities.
- ▶ n_x features and n_y output classes \rightarrow there is a $n_y \times n_x$ parameter matrix Θ , where the parameters for each class θ_k are stored as rows.
- ▶ the prediction $y_i \in \{1,...,n_y\}$ is determined by the highest-probability category.

Regularized Multinomial Logistic

▶ The L2-penalized logistic regression loss (the default in sklearn) is

$$\mathcal{L}(\theta) = -\frac{1}{n_D} \sum_{i=1}^{n_D} \log \frac{\exp(\theta'_{k^*} \mathbf{x}_i)}{\sum_{j=1}^{n_y} \exp(\theta'_j \mathbf{x}_i)} + \lambda \sum_{j=1}^{n_x} \sum_{k=1}^{n_y} (\theta_{[j,k]})^2$$

- λ = strength of L2 penalty (could also add lasso penalty)
- ▶ as before, predictors should be scaled to the same variance.

```
from sklearn.linear_model import LogisticRegression
logit = LogisticRegression()
logit.fit(X,y)
```

if y is categorical, sklearn automatically uses multinomial logistic

Multi-Class Confusion Matrix

		Predicted Class		
		Class A	Class B	Class C
True Class	Class A	Correct A	A, classed as B	A, classed as C
	Class B	B, classed as A	Correct B	B, classed as C
	Class C	C, classed as A	C, classed as B	Correct C

▶ More generally, can have a confusion matrix M with items M_{ij} (row i, column j).

Multi-Class Performance Metrics

Confusion matrix M with items M_{ij} (row i, column j).

Precision for
$$k = \frac{\text{True Positives for } k}{\text{True Positives for } k + \text{False Positives for } k} = \frac{M_{kk}}{\sum_{l} M_{lk}}$$
Recall for $k = \frac{\text{True Positives for } k}{\text{True Positives for } k + \text{False Negatives for } k} = \frac{M_{kk}}{\sum_{l} M_{kl}}$

$$F_1(k) = 2 \times \frac{\operatorname{precision}(k) \times \operatorname{recall}(k)}{\operatorname{precision}(k) + \operatorname{recall}(k)}$$

in sklearn, syntax is the same as binary case.

Metrics for whole model

Balanced Accuracy =
$$\frac{1}{n_y} \sum_{k} \text{Recall for } k$$

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▶ Macro-averaging: average of the per-class precision, recall, and F1, e.g.

$$F_1 = \frac{1}{n_y} \sum_{k=1}^{n_y} F_1(k)$$

weights all classes equally

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- weights all classes equally
- Both of these approaches up-weight frequent classes:
 - ▶ **Micro-averaging**: Compute model-level sums for true positives, false positives, and false negatives; compute precision/recall from model sums.
 - "Weighted": computed like macro-averaging, but classes are weighted by true frequency.

"Rookie data science mistakes invalidates a dozen medical studies"

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their amazement, Vandewiele's team discovered that the authors of the too-good-to-be-true studies were performing oversampling before splitting the dataset into two. Because the split was done randomly, this had the devastating side-effect of the same datapoints ending up in both the training and testing set. In effect, the models were being shown the questions they were to be assessed on well before the exam! No wonder their results were suspiciously great.

Nested Sample Splits

Nested Sample Splits

To do evaluations in the full data, use nested cross-validation:

- ▶ split data into K folds, e.g. 5.
- ▶ for each fold $k \in \{1, 2, ..., K\}$:
 - ightharpoonup train and tune model in rest of data $\neg k$
 - ightharpoonup evaluate metrics (e.g. MSE, balanced accuracy) in k.
- Report mean and s.d. of metrics across folds.

Outline

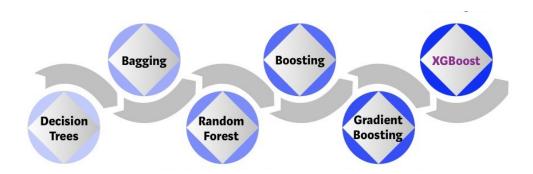
Binary Classifier Metrics

Multi-Class Models

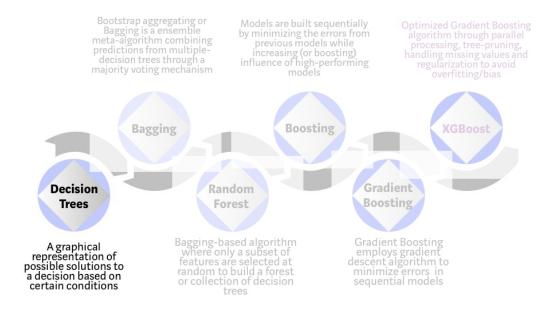
Ensemble Learning with XGBoost

Response Essays

XGBoost: Overview

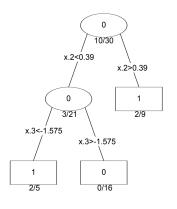


XGBoost Ingredients: Decision Trees



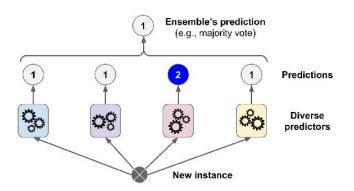
Decision Trees

Classification Tree



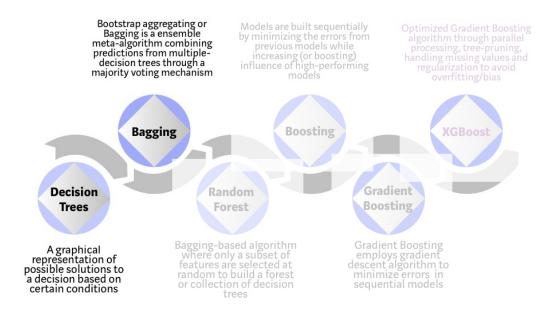
- ▶ Decision trees learn a series of binary splits in the data based on hard thresholds.
 - if yes, go right; if no, go left.
- Can have additional splits as you move through the tree.
- fast and interpretable, but performance is often poor.

Voting Classifiers



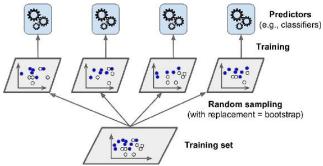
- voting classifiers (ensembles of different models that vote on the prediction) generally out-perform the best classifier in the ensemble.
 - more diverse algorithms will make different types of errors, and improve your ensemble's robustness.

XGBoost Ingredients: Bootstrapping



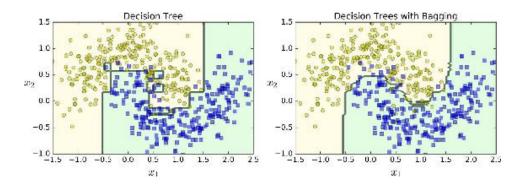
Bootstrapping

▶ Rather than use the same data on different classifiers, one can use different subsets of the data on the same classifier:



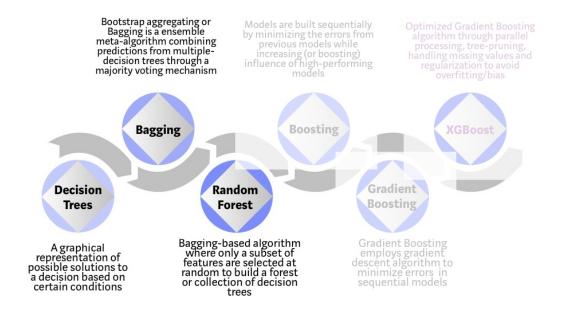
can also use different subsets of features across subclassifiers.

Bootstrapping Benefits



- ▶ A bootstraped ensemble generally has a similar bias but lower variance than a single predictor trained on all the data.
- ▶ Predictors can be trained in parallel using separate CPU cores.

XGBoost Ingredients: Random Forests



Random Forests are optimized ensembles of bootstrapped decision trees:

```
from sklearn.ensemble import RandomForestClassifier
rfc = RandomForestClassifier()
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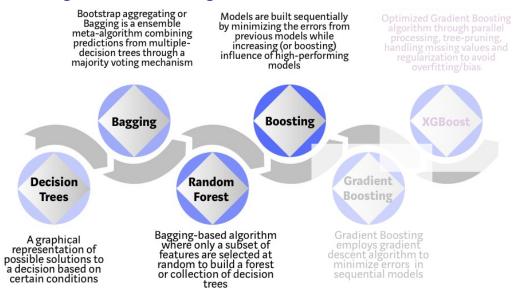
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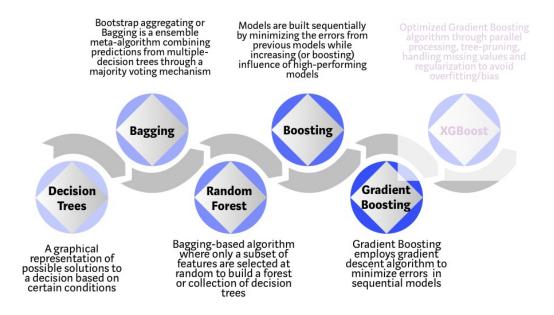
- 1. Each voting tree gets its own sample of data.
- 2. At each tree split, a random sample of features is drawn, only those features are considered for splitting.
- 3. For each tree, error rate is computed using data outside its bootstrap sample.

XGBoost Ingredients: Boosting



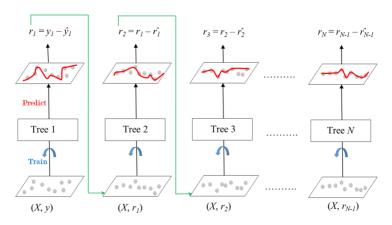
▶ works by sequentially adding predictors to an ensemble – fits the new predictor to the residual errors made by the previous predictor to gradually improve the model.

XGBoost Ingredients: Gradient Boosting



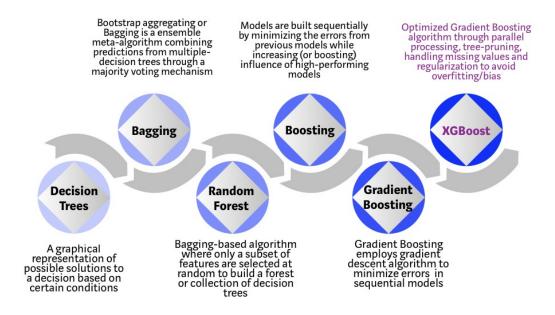
Gradient Boosting Machines

▶ Gradient boosting refers to an additive ensemble of trees:



Adds additional layers of trees to fit the residuals of the first layers

XGBoost Ingredients



XGBoost

- ► Feurer et al (2018) find that XGBoost beats a sophisticated AutoML procedure with grid search over 15 classifiers and 18 data preprocessors.
- ► A good starting point for any machine learning task:
 - easy to use
 - actively developed
 - efficient / parallelizable
 - provides model explanations
 - takes sparse matrices as input

Complicated in Theory, Easy in practice

```
from xgboost import XGBClassifier
model = XGBClassifier()
model.fit(X train, y train,
          early stopping rounds=10,
          eval metric="logloss",
          eval set=[(X eval, y eval)]
y pred = model.predict(X test)
accuracy = accuracy score(y test, y pred)
```

▶ See more detailed examples/explanation in the "XGBoost Explained" reading, and this week's example code notebook.

Early Stopping with Validation Set

- Early stopping is an elegant regularization technique, used in xgboost and in neural nets:
 - pradually train the model gradients while checking fit in a held-out validation set.
 - for xgboost, this means adding more layers of trees to fit the residuals.
 - when model starts overfitting, stop training.

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 - for xgboost, this means adding more layers of trees to fit the residuals.
 - when model starts overfitting, stop training.
- Requires user to specify two additional parameters:
 - eval_set = validation set (separate from training set and test set)
 - early_stopping_rounds: stop training if we have done this many epochs without improving validation set performance.

```
from sklearn.model_selection import train_test_split
X_val_train, X_test, y_val_train, y_test = train_test_split(X, y)
X_train, X_val, y_train, y_val = train_test_split(X_val_train, y_val_train)
```

Early Stopping with Validation Set

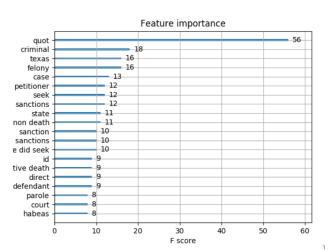
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X_train, X_val, y_train, y_val = train_test_split(X_val_train, y_val_train)

from xgboost import XGBClassifier
xgb = XGBClassifier(eval_set = [X_val, y_val], early_stopping_rounds=10)
xgb.fit(X_train, y_train)
y_pred = xgb.predict(X_test)
balanced_accuracy_score(y_test, y_pred)
```

Feature Importance

```
from xgboost import plot_importance
plot_importance(xgb_reg, max_num_features=20)
<IPython.core.display.Javascript object>
```



➤ XGBoost provides a metric of feature importance that summarizes how well each feature contributes to predictive accuracy. (will return to this in week 9)

Outline

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Response Essays

First Response Essay due Friday

https://docs.google.com/document/d/1Q0BuQdVl2azNy_ 2RsIvE4PSPwFNsCHXQ2gIc6hOqUoQ/edit?usp=sharing

- Critically read and review an application paper.
- ▶ 300 words is the minimum for a passing grade but 500+ words would be expected for high grade.
- ▶ Please anonymize your submission put your name in the filename, but not anywhere in the file. Submit as TXT or PDF.

What can I write about?

Any "Applications" reading from weeks 1 through 5.

Or another article applying tools from one of the first topics (machine learning, causal inference with linear regression, fixed effects models, or classification). Please confirm with me by email by tomorrow.

What to think about

Questions to ask in reading responses

- 1. What is the research question?
- 2. What is interesting about the data? Is it the right dataset to answer the research question?
- 3. Did they provide sufficient visuals and descriptive statistics to provide trust in the data and its usefulness for the stated purpose?
- 4. What is the goal of the data analysis?
 - a. What are they trying to measure?
 - b. What are they trying to predict or learn?
- 5. Given the answer to #4, is the right model being used? What other models could they have tried?
- 6. Did they provide validation that the model is delivering on the stated goals (#4)?
- 7. How were the model predictions/statistics used in a social-science analysis? What results seemed incomplete or non-robust?
- 8. Did they answer the research question (#1)? Highlight limitations and open questions.
- Annotated examples from previous years are available here: http://bit.ly/BRJ_essay-examples.