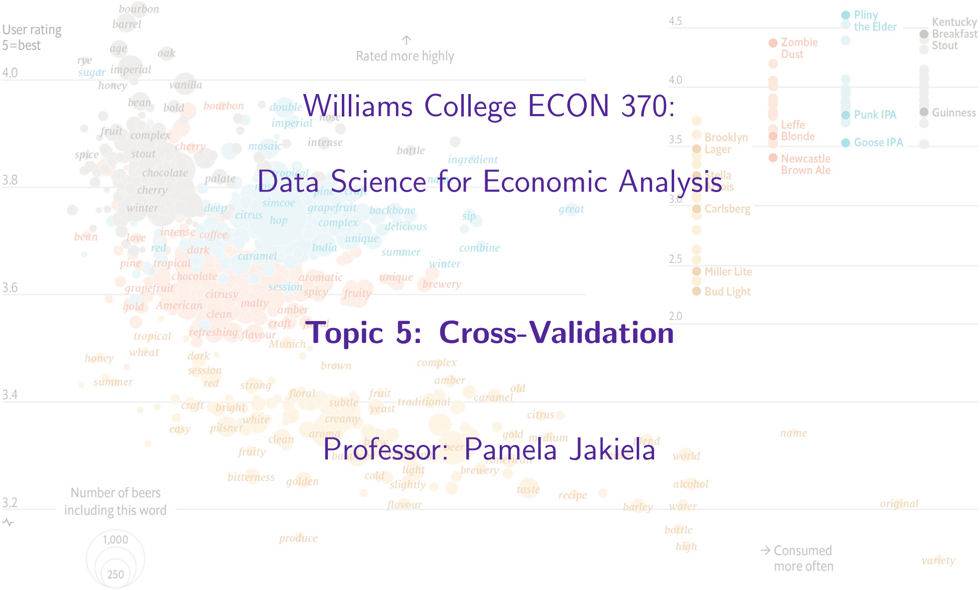

Williams College ECON 370:

Data Science for Economic Analysis

Topic 5: Cross-Validation

Professor: Pamela Jakiela

Thought Experiment: 100 True Null Hypotheses

Let Y and $X_1, \ldots, X_{100}$ be column vectors containing $N = 20$ draws from iid standard normals.

Suppose you run 100 regressions, regressing Y on each X_i variable (individually).

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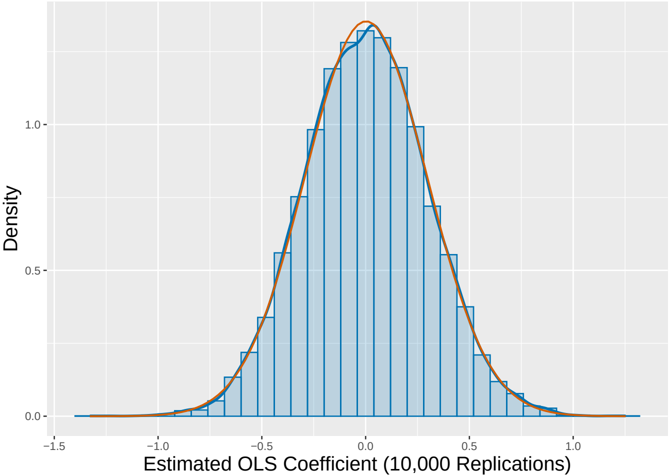
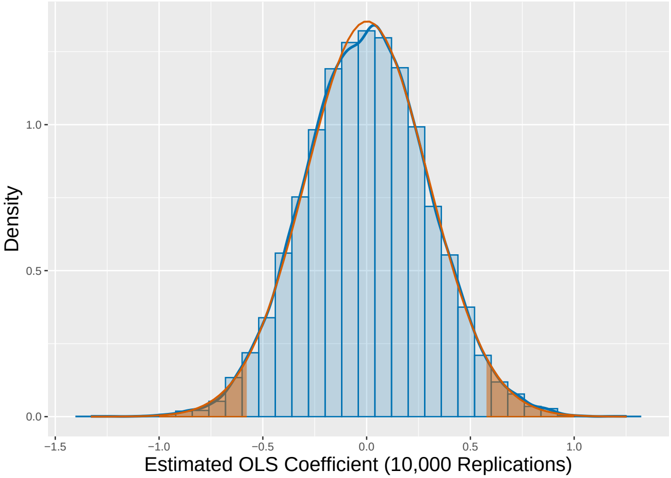
What if we ran 10,000 regressions? How many significant X_i variables should we expect?

$\hat{\beta}_{OLS} \sim N(\beta_0, \tilde{\sigma}_{OLS})$: OLS Coefficients Are Normally Distributed About β_0



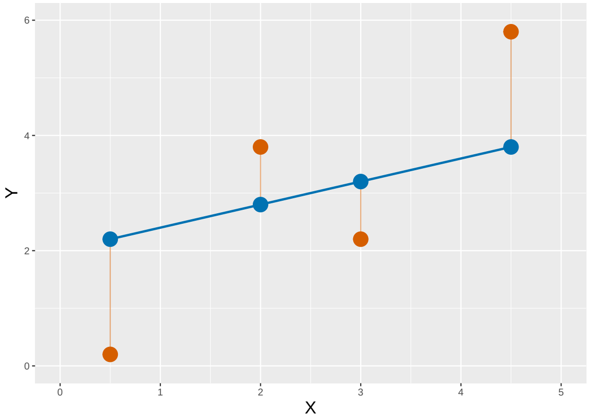
A Test Size of 0.05 Means. . .



Strong Associations Occur by Chance (with 10,000 Replications)

Top 3 | Middle 3 | Bottom 3

OLS Is Fitting the Noise (and the True Model)



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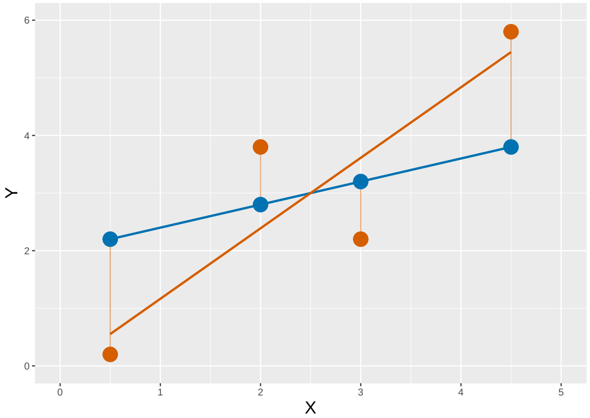

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Over-fitting becomes a serious concern with many data science techniques that make use of very large data sets (including not just large Ns but many variables) and very flexible models

- (Aside about prediction vs. inference/causality and statistics/CS vs. economics here)

Another Thought Experiment: 100 True Null Hypotheses

Let Y and $X_1, \ldots, X_{100}$ be column vectors containing $N = 20$ draws from iid standard normals.

Split the data in half into Data Set 1 ($N = 10$) and Data Set 2 ($N = 10$).

Run 100 regressions, regressing Y on each X_i variable (individually) using only Data Set 1.

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How many of the estimated OLS coefficients should we expect to be statistically significant?

How many of the X_i variables that are statistically significant predictors of Y in Data Set 1 will also be statistically significant predictors of Y in Data Set 2?

The Validation Set Approach to Specification Selection

OLS minimizes the residual sum of squares (RSS) or, equivalently, the mean squared error (MSE), but if we care about prediction then we want to minimize the MSE in new data

- OLS will never tell you that you have included too many (non-collinear) variables

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We don't always care about prediction, but when we do we need a strategy to avoid over-fitting

- One approach is to randomly partition a data into a **training** sample and a **test** sample
  - The training sample is used to choose or fit the model
  - The test sample is used to run the model, calculate the RSS or MSE
- The validation set approach builds on the intuition from the thought experiment: random noise in the training, test data sets is uncorrelated, so if we fit the model on the training data and then calculate the MSE on the test data, there is no (ok, much less) over-fitting

The Validation Set Approach in Practice: Baseball Data

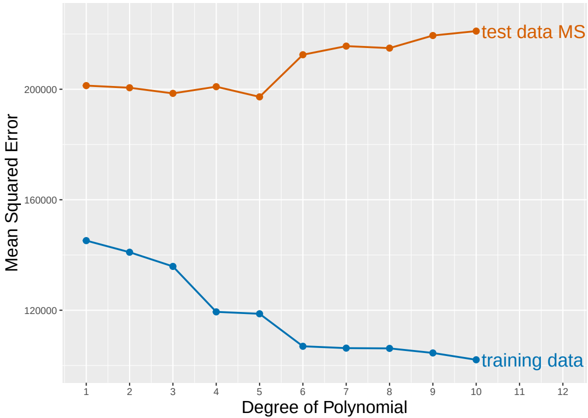
Data from 263 major league baseball players active in 1986 and 1987

- Variables include salary in 1987 (Y) and runs scored in 1986

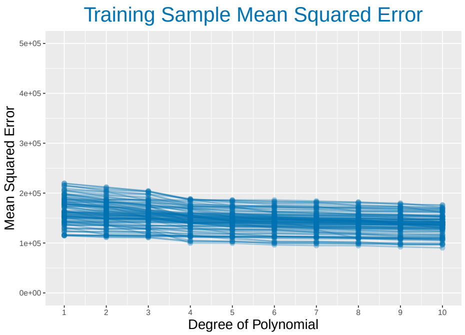
We're going to fit a linear regression of salary on runs, runs^2, runs^3, runs^4 etc.

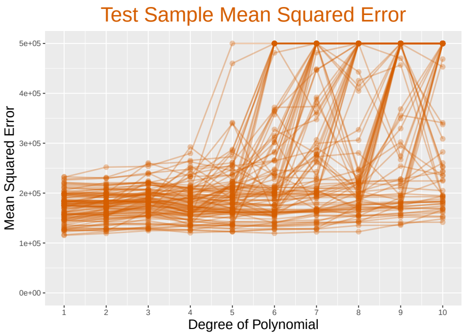
- Our goal is to determine the degree of polynomial that we should include in the regression

The Validation Set Approach in Practice: Baseball Data

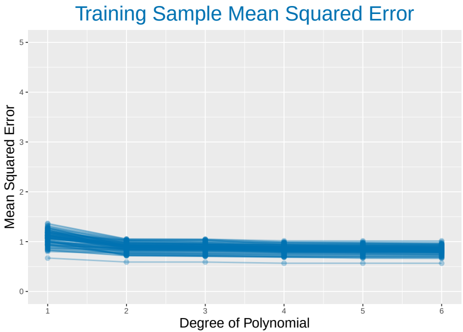


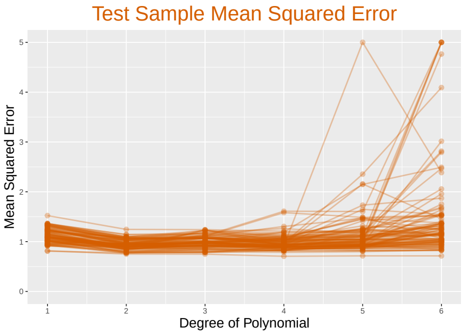
The Validation Set Approach in Practice: Baseball Data (100 Replications)





Validation Set Approach Correct 43% of Time in Simulated Data*





data-generating process: $Y = 0.8X + 0.4X^2 + \varepsilon$ where $X \sim N(0,1)$, $\varepsilon \sim N(0,1)$, $N = 240$

*This is just one example, but the validation set approach is often noisy

Cross-Validation

In **cross-validation**, we run the validation set approach multiple times and average the results

- Each observation only appears in the test data set once
- In each cut of the data, all the observations that are not test data are training data

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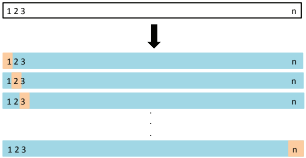
Two types of cross-validation, defined by the way we construct the test data sets:

- Leave-One-Out Cross-Validation (LOOCV): each observation is a singleton test data set
- k-Fold Cross-Validation: partition the data into k **folds**, each a test data set

Leave-One-Out Cross-Validation

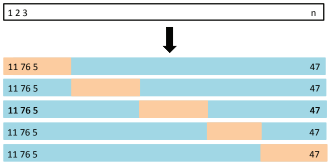


source: James et al. (2021)

Leave-One-Out Cross-Validation (LOOCV): each observation is a singleton test data set

- Run the validation set approach N times using all other observations as training data
- Calculate the squared prediction error for each observation, average to calculate MSE
- LOOCV may be computationally costly (when using models more complicated than OLS)

k-Fold Cross-Validation

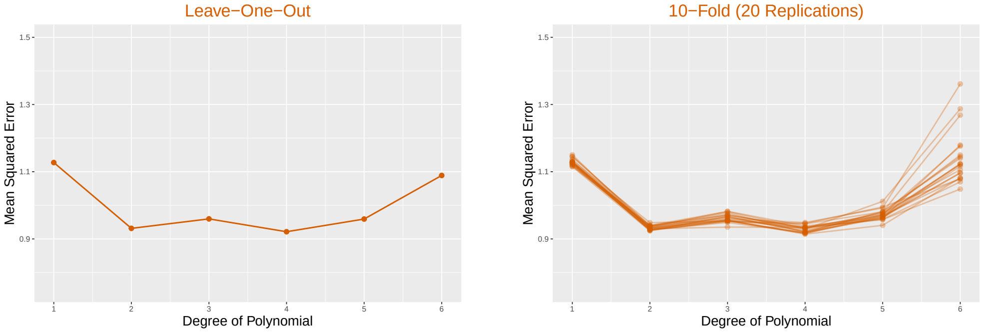


source: James et al. (2021)

k-Fold Cross-Validation:

- Randomly partition the sample into k distinct test data sets (aka folds)
- Run the validation set approach k times using the observations in fold k as the test data and the remainder of the data (i.e. everything but fold k) as the associated training data
- Calculate the mean squared prediction error in each old, average across folds

Comparing Test MSE: Leave-One-Out CV vs. *k*-Fold CV



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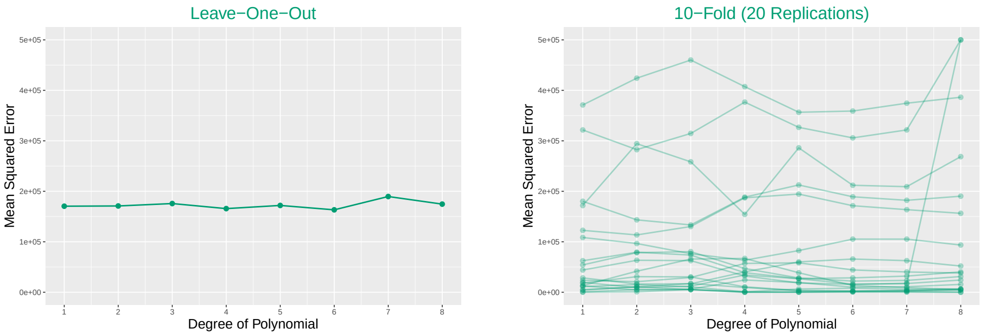

data source: Hitters data from James et al. (2021)

Summary: Cross-Validation to Choose an OLS Specification

- Randomize observations into k distinct groups (folds), make sure to set the seed
  - Skip this step in LOOCV
- For each of the k (in k-fold) or N (in LOOCV) partitions of the data into training vs. test:
  - Estimate each candidate specification j in the training data
  - Use the estimate coefficients to predict outcomes in test data in fold k
  - Calculate squared residuals, MSE in fold k for candidate specification j
- Calculate test MSE for specification j by averaging across folds (or test data sets)
- If graph of test MSEs has a flat bottom, tend toward most parsimonious specification