# Class 4: Resampling and Boosting

MSA 8150: Machine Learning for Analytics

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# Introduction

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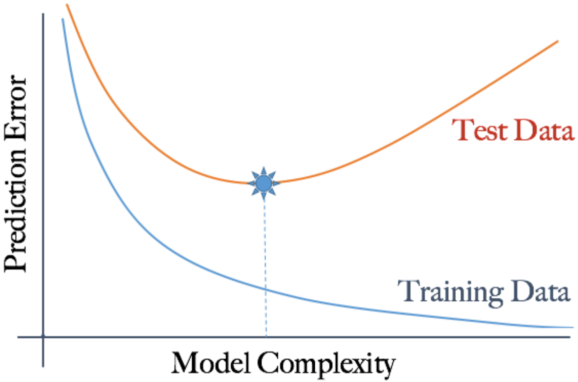
- To produce justifiable model reliability arguments, the test data should not be used in the training
- If the model is evaluated against the training data the results can be very distracting
- The training error rate is often quite different from the test error rate, and in particular the former can dramatically underestimate the latter (recall the accuracy vs complexity chart)

# Training vs Test Model Evaluation

Recall this plot from the first session



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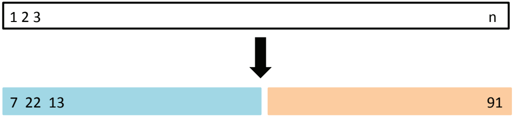
- We are interested in a class of methods that estimate the test error by holding out a subset of the training observations from the fitting process, and then applying the statistical learning method to those (held out) observations



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- The model is fit on the training set, and the fitted model is used to predict the responses for the observations in the validation set
- The error with reference to the hold-out set is an approximation of the test error

# example

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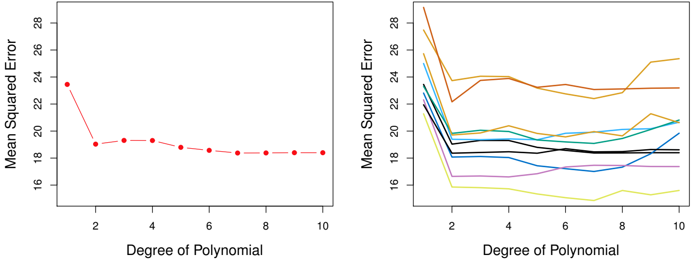
- We randomly split the 392 observations into two sets, a training set containing 196 of the data points, and a validation set containing the remaining 196 observations.



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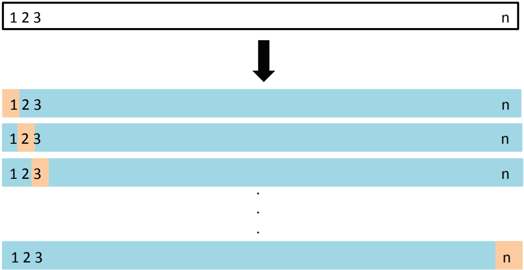
- Since a large portion of the data need to be held aside, the model fits are not accurate enough

# Leave-One Out Cross-Validation (LOOCV)

- We have $n$ data points $(x_1, y_1), \cdots, (x_n, y_n)$, we use $n-1$ for the training and one instance for the test
- Of course a single test point is no where close to the true test error, but this process is repeated $n$ times, every time $n-1$ points used for training and one point left out for the test
- Considering $MSE_1 = (y_1 - \hat{y}_1)^2, \cdots MSE_n = (y_n - \hat{y}_n)^2$, an approximation of the test error is

$$CV_n = \frac{1}{n} \sum_{i=1}^{n} MSE_i$$



# Cons & Pros with LOOCV

- It has a very small bias compared to the validation set approach (it almost uses as much data as possible to fit the model)
- The test error overestimation is less than the validation set approach (because of what we mentioned above)
- Its results are reproducible unlike the validation set approach which uses a random subset of the data for test evaluation
- It can be computationally very expensive (requires running the algorithm $n$ times)
- For linear models there is a shortcut to calculate $CV_n$ that only requires fitting the model once with the entire data (but **this shortcut only applies to linear models**)

$$CV_n = \frac{1}{n}\sum_{i=1}^{n}\left(\frac{y_i - \hat{y}_i}{1 - h_i}\right)^2$$

where $\hat{y}_i$ are the fitted values of the original least squares problem and $h_i$ are only data dependent

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- Often $K = 5$ or $K = 10$ is what is considered in application

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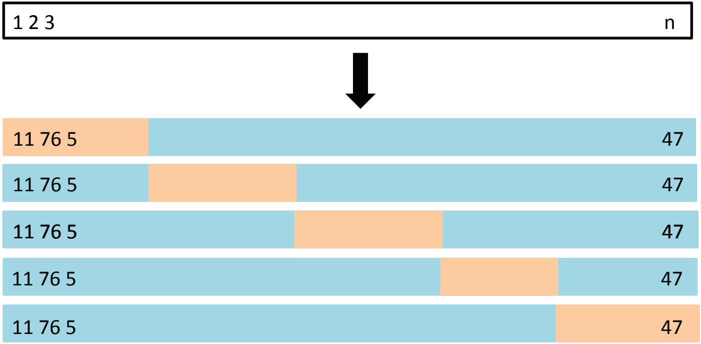

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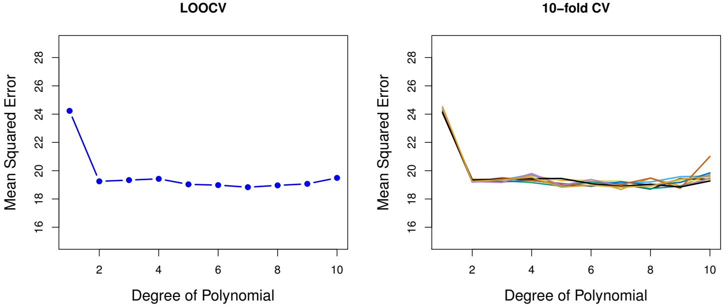
- LOOCV is a special case of $K$-fold CV for $K = n$
- In general $K$-fold CV is much cheaper than LOOCV because it only requires $K$ model fits vs $n$ model fits
- For model selection, $K$-fold CV often gives us similar outcomes at a much lower computational cost



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# K-Fold Cross Validation and LOOCV

- Aside form the computational issues, even surprisingly K-Fold CV produces better test estimates than the LOOCV
- LOOCV has a lower bias compared to the K-fold CV, since it uses more data to fit the model
- But K-fold CV has a lower variance compared to the LOOCV, since LOOCV is the sum of $n$ highly correlated random variables while the correlation between the MSEs in K-fold CV is lower, recall

$$var(X+Y) = var(X) + var(Y) + 2cov(X,Y)$$

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- Compute

$$CV_K = \frac{1}{K} \sum_{k=1}^{K} Err_k$$

where

$$Err_k = \frac{1}{\#\text{ elements in } C_k} \sum_{i \in C_k} I(y_i \neq \hat{y}_i)$$

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- It can provide an estimate of the standard error of a coefficient, or a **confidence interval for that coefficient**, regardless of how complex the derivation of that coefficient is

# Bootstrap via an Example

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- To minimize the risk, we want to minimize $var(\alpha X + (1-\alpha)Y)$
- We can show that (in the class we do it) that the minimizer is

$$\alpha = \frac{var(Y) - cov(X,Y)}{var(X) + var(Y) - 2cov(X,Y)}$$

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- However in a real-world we only have one sample set to use
- Bootstrap yet allows us to generate good estimates of $\alpha$ **using only one sample set!**

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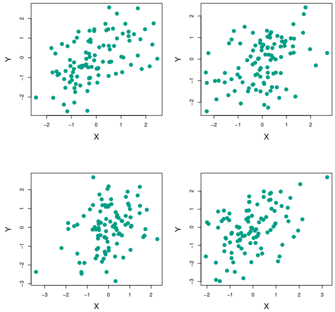
- We generate 1000 sample sets each containing 100 pairs of $X, Y$
- For the synthetic data generated $var(X) = 1, var(Y) = 1.25$ and $cov(X, Y) = 0.5$ which yield an optimal value of $\alpha = 0.6$



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– To get the left panel we generate 1000 synthetic sample sets, for each obtain $\hat{\alpha}$ and plot the histogram and calculate

$$\bar{\alpha} = \frac{1}{1000}\sum_{i=1}^{1000}\hat{\alpha}_i, \quad SE(\alpha) = \sqrt{\frac{1}{999}\sum_{i=1}^{1000}(\hat{\alpha}_i - \bar{\alpha})^2}$$

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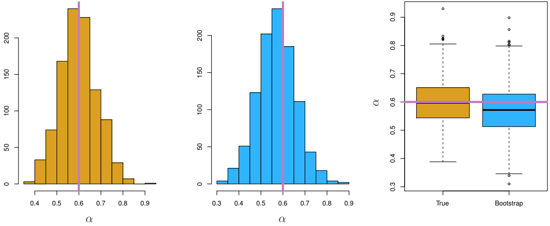
- Surprisingly, the results are very close



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- We estimate the standard error of these bootstrap estimates using the formula

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- This serves as an estimate of the standard error of $\alpha$ estimated from the original data set!

# Programming Exercise

In the remainder of the session we go through some programming exercise over the following topics

- Linear models, data splitting, confidence intervals, etc
- Some classification examples
- Some cross validation and bootstrap exercise

**Questions?**

# References


- https://www.alsharif.info/iom530, 2013.
- J. Friedman, T. Hastie, and R. Tibshirani.
  **The elements of statistical learning.**
  Springer series in statistics, 2nd edition, 2009.
- G. James, D. Witten, T. Hastie, and R. Tibshirani.
  **https://lagunita.stanford.edu/c4x/HumanitiesScience/StatLearning/asset/cv_boot.pdf, 2013.**
- G. James, D. Witten, T. Hastie, and R. Tibshirani.
  **An introduction to statistical learning: with applications in R, volume 112.**
  Springer, 2013.