8: Resampling Methods (K-fold Cross Validation)

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$ echo "Data Science Institute"
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Activity (15 minutes)

Watch this video about k-Fold Cross-Validation: https://www.youtube.com/watch?v=wjILv3-UGM8&t=439s

k-Fold Cross-Validation

k-fold cross validation involves randomly dividing the set of observations into k approximately equally sized groups. Then,

- Fit the model using the observations from all but one of the groups.

- Make predictions for the response of the observations in the remaining group.

- Compute the validation set error.

- Repeat this process for each group.

k-Fold Cross-Validation

The k-fold cross validation estimate of the test error is the average of the k validation set errors.

$$CV_{(k)} = \frac{1}{k} \sum_{i=1}^{k} MSE_i$$

LOOCV is a special case of the k-fold cross validation approach using $k = n$ ($n = $ number of observations).

Breakout Room

Based on what you learned so far, how does LOOCV compare to k-fold CV?

Comparing LOOCV and k-fold CV

- The ♦ ***computational time/effort for k-fold CV for $k < n$ is less*** ♦ since we are fitting fewer models in the process.

- ♦ ***LOOCV is less biased*** ♦ in its estimation of the test error rate since it trains the model on more observations.

- ♦ ***LOOCV has a test error estimate that has higher variance*** ♦ than k-fold CV ($k < n$)

- the models in the LOOCV process are fit with nearly identical training sets

Comparing LOOCV and k-fold CV

- thus, each test error result is much more correlated with one another than they would be for k-fold CV

- averaging highly correlated quantities has a higher variance than if they were not correlated

Thus, there is a bias-variance trade-off when it comes to choosing k for k-fold cross-validation. Typically $k = 5$ or $k = 10$ is used.

Exercises: k-fold CV

Open the k-fold CV Jupyter Notebook file.

- Go over the "k-fold CV" section together as a class.

- Questions should be completed at home if time does not allow.

References

Chapter 5 of the ISLP book:

James, Gareth, et al. "Resampling Methods." An Introduction to Statistical Learning: with Applications in Python, Springer, 2023.