DS 3010

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Module 2: Statistical Decision Theory

Part 2: Cross Validation

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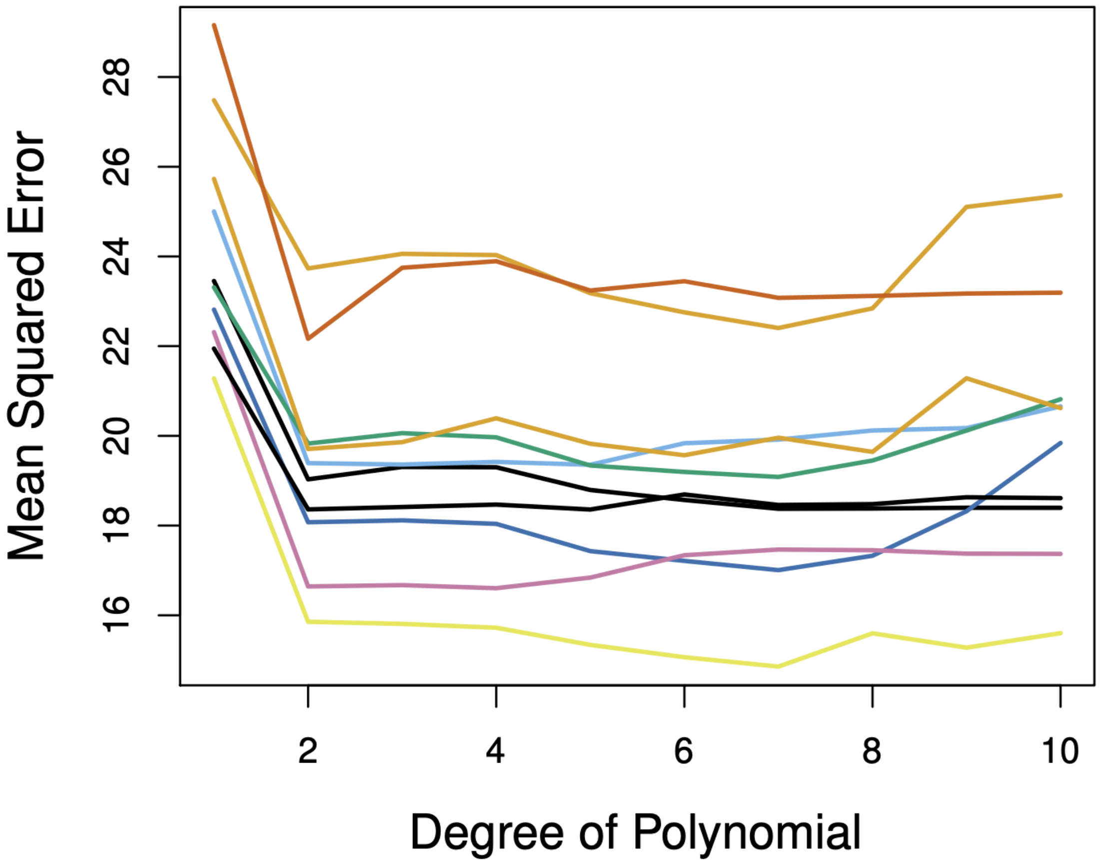
How have we estimated test MSE so far?

Training data	50%
Testing data	50%

Validation Set Approach:

Randomly split data into training data (50%) and testing data (50%)

How have we estimated test MSE so far ?



Problems:

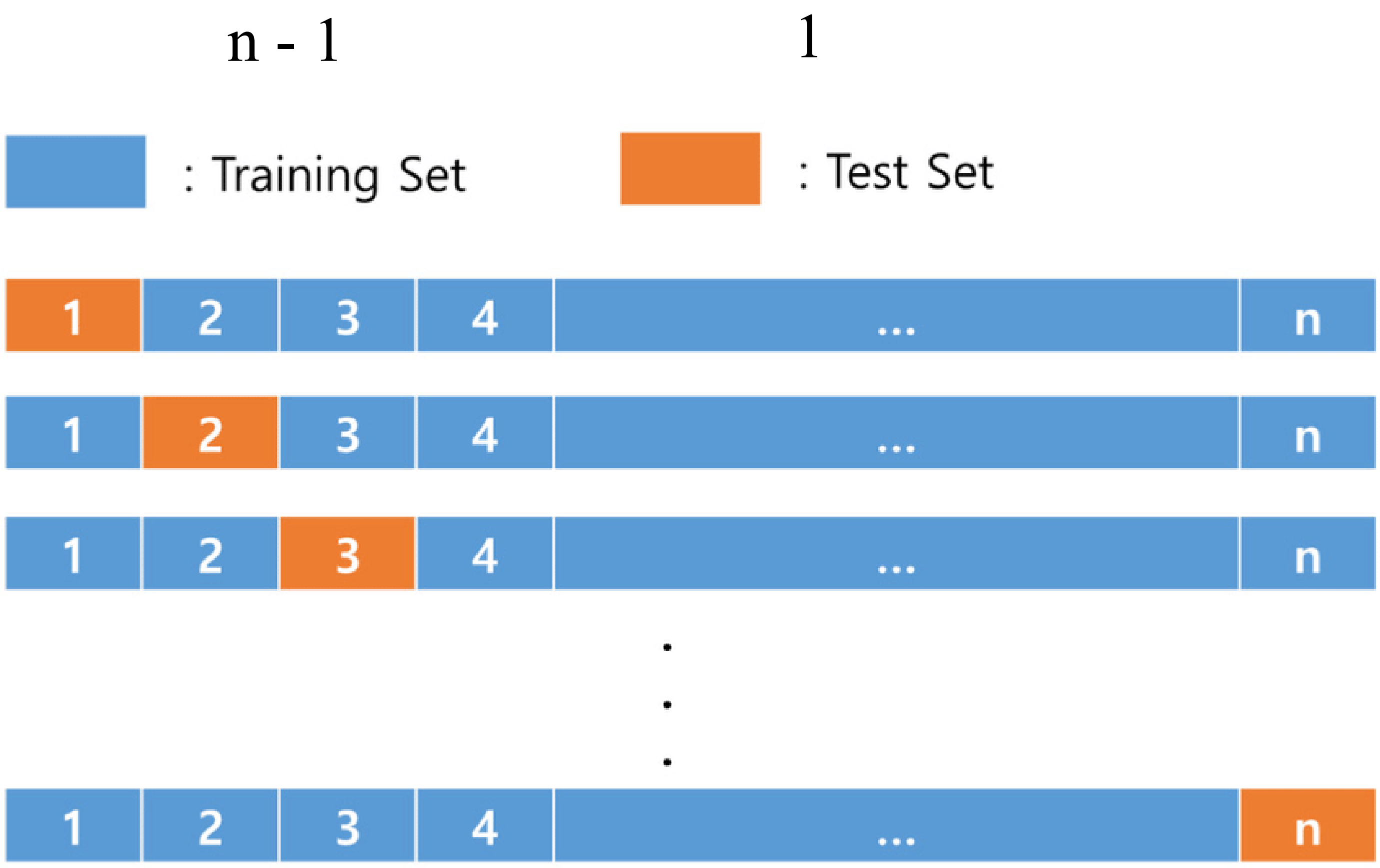
- **Highly variable:** depending on precisely which observations are included in the training set and which observations are included in the validation set.

Can you think of a better way to create a training and testing dataset ?

What is Cross-Validation ?

Cross validation is a technique used in machine learning to evaluate the performance of a model on unseen data. It involves dividing the available data into **multiple folds or subsets**, using **one of these folds** as a validation set, and training the model on the remaining folds.

Leave-one-out cross-validation (LOOCV)



Leave-one-out cross-validation (LOOCV)

Testing data: a single observation (x_1, y_1)

Training data: observations {(x_2,y_2), . . . , (x_n,y_n)} make up the training set.

$$MSE_1 = (y_1 - \hat{y}_1)^2$$

Repeat the procedure by selecting (x_2,y_2), for the validation data

$$MSE_2 = (y_2 - \hat{y}_2)^2$$

……..

Repeating this approach **n** times produces n squared errors, $\mathrm{M}SE_1$, $\mathrm{M}SE_2$, ….. $MSEn$

Leave-one-out cross-validation (LOOCV)

The LOOCV estimate for the test MSE:

$$\mathrm{CV}_{(n)} = \frac{1}{n}\sum_{i=1}^{n} \mathrm{MSE}_i.$$

Leave-one-out cross-validation (LOOCV)

$$\mathrm{CV}_{(n)} = \frac{1}{n}\sum_{i=1}^{n}\mathrm{MSE}_i.$$

Lower Bias: LOOCV trains the model on **n - 1 observations** (almost the entire dataset), it provides a more accurate estimate of the test error compared to the validation set approach, which typically uses **half size** of the data set.

Consistency: LOOCV is **deterministic**—it always gives the same result when repeated, unlike the validation set approach, which can vary depending on how the data is randomly split.

Leave-one-out cross-validation (LOOCV)

This process can be **computationally expensive**

- when: **n is large**.
- **Fitting the model is slow** (e.g., complex models)

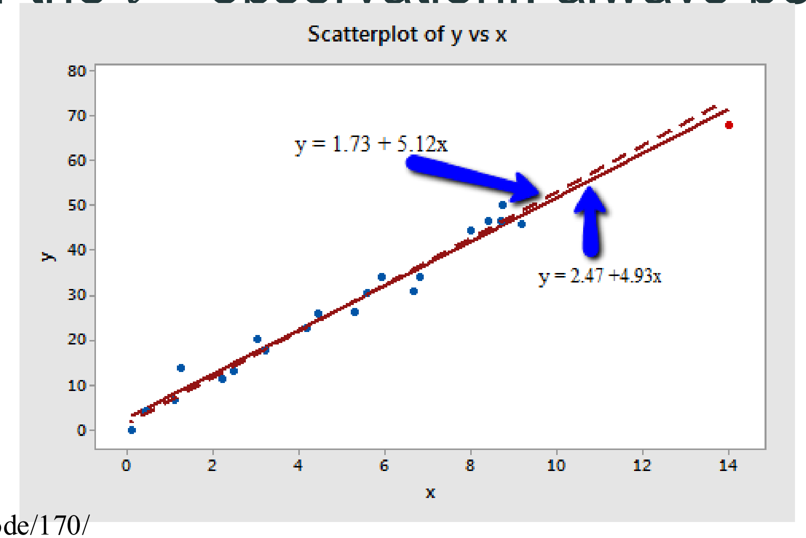
PRESS (Predicted Residual Sum of Squares)

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

$\hat{y}_i$ is the i^{th}fitted value

y_1 is the true value

h_i: the leverage fmeasures how much an observation influences its own fitted valueor the i^{th} observation., always between **1/n** and **1**.



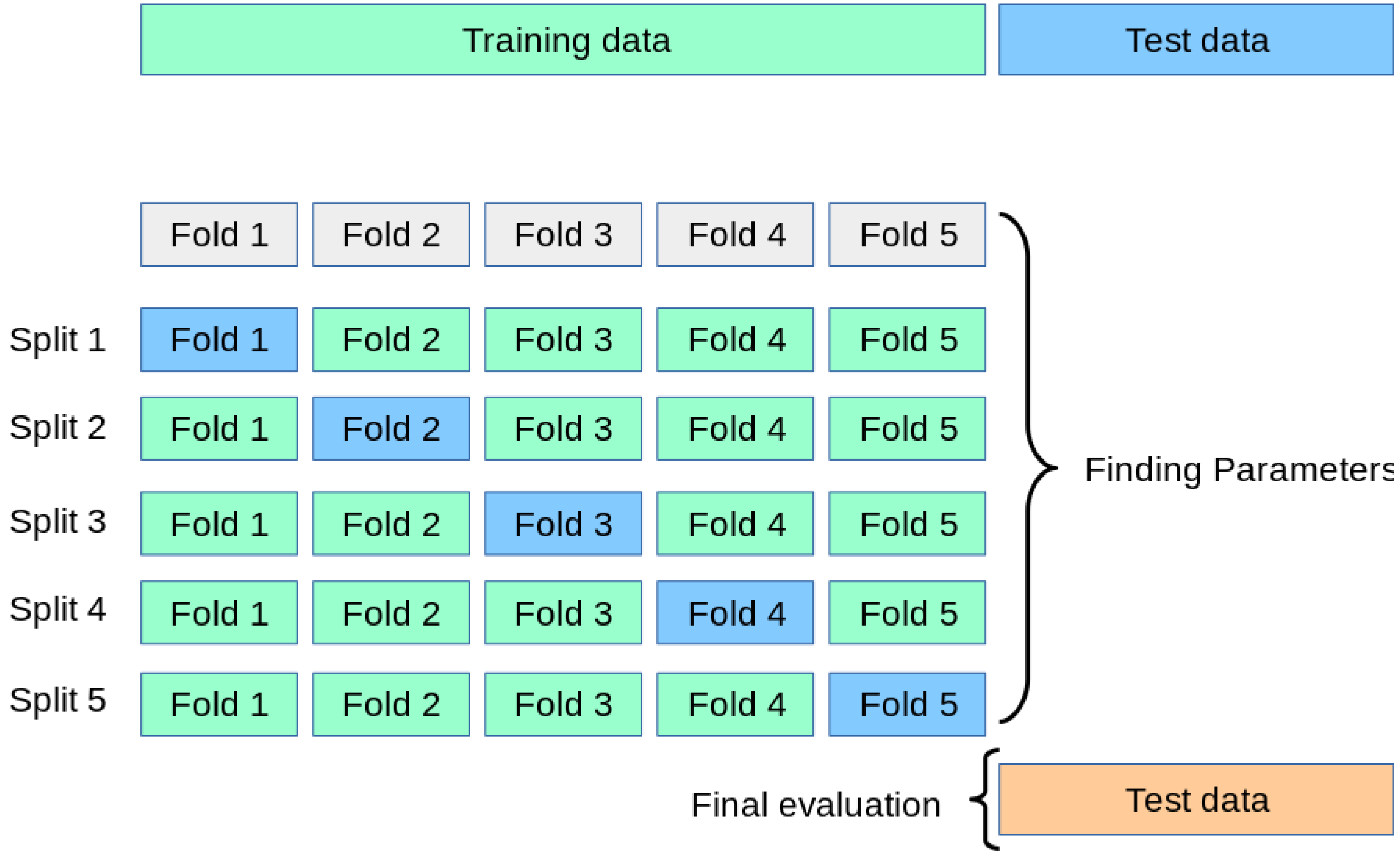
[1]https://online.stat.psu.edu/stat462/node/170/

PRESS

Faster Computation: PRESS uses a shortcut formula involving leverage values, making it as fast as fitting the model **once**, while **LOOCV** requires fitting the model **n times**.

Same Result: For linear regression, **PRESS** gives the **same result as LOOCV**, but is computationally efficient.

k-fold cross-validation



- Randomly dividing the set of observations into **k groups**, or *folds*, of approximately equal size.
- The **k-th fold** is treated as a validation set, and the method is fit on the remaining **k − 1 folds**.

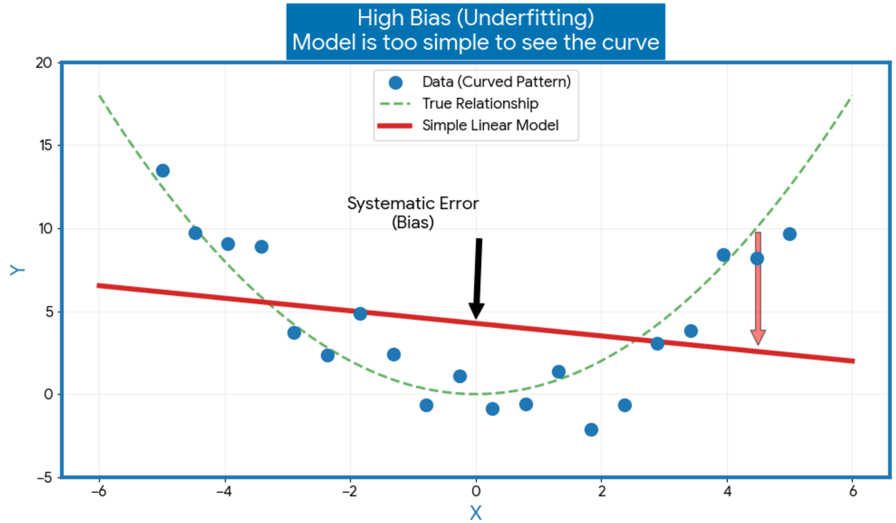
k-fold cross-validation

$$\mathrm{CV}_{(k)} = \frac{1}{k}\sum_{i=1}^{k} \mathrm{MSE}_i .$$

Bias and Variance of the Model (True Prediction Performance)

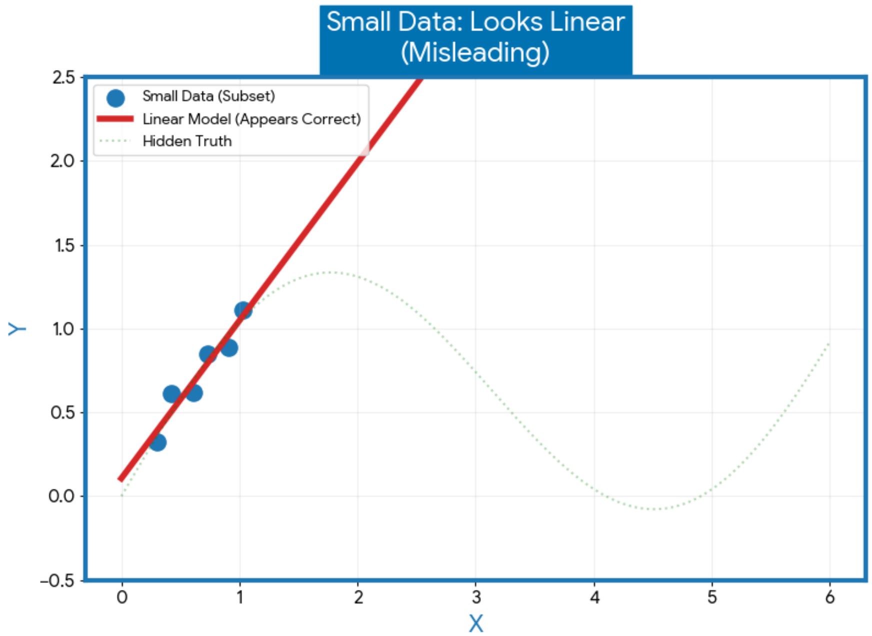
Bias : Measures how far off the model's predictions are on average from the true relationship.

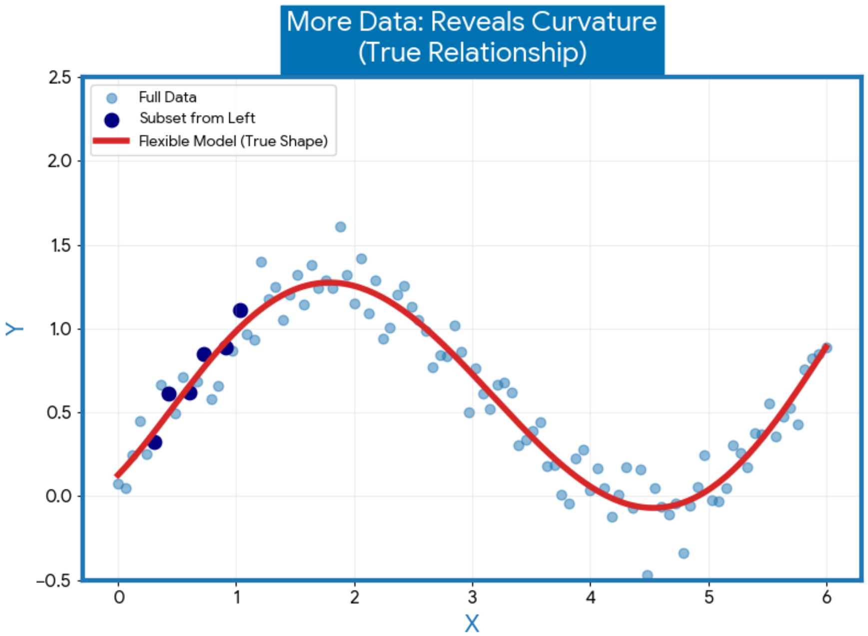
High bias → The model is too simple, underfits the data, and makes systematic errors.



Variance : Measures how much the model's predictions would vary if we trained it on different datasets.

High variance → The model is too sensitive to the training data, and small changes in the data lead to large changes in predictions.





High bias

Low bias

Bias-variance trade-off k-fold CV

Validation Set Approach (50%):

High bias because the training set is smaller, leading to underfitting.

LOOCV (n-1):

Low bias because each training set uses almost the entire dataset (n - 1 observations).

k-Fold Cross-Validation (k-1/k):

Intermediate bias (lower than the validation set approach but higher than LOOCV).

Method	Training data	Bias
Validation Set Approach	50%	High
LOOCV	n-1	Low
k-Fold CV	(k-1)/k	Medium

Bias-variance trade-off k-fold CV

Therefore, from the perspective of bias reduction it is clear that Loocv is to be preferred to k-fold.