MANIPAL
ACADEMY of HIGHER EDUCATION
(Institution of Eminence Deemed to be University)

Linear Regression Models

Segment 4 – Model Diagnostics

Topic 2 – Cross Validation

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Topics

1. Basic Idea of Cross Validation
2. K-fold Cross Validation
3. Leave-one-out Cross Validation
4. Train-Test-Validation Split vs. Cross Validation

Basic Idea of Cross Validation

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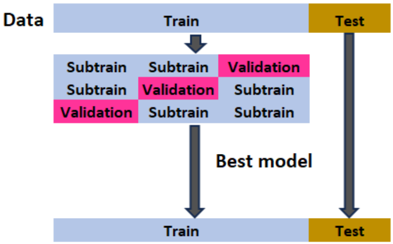

Data

Train | Test

Subtrain	Subtrain	Validation
Subtrain	Validation	Subtrain
Validation	Subtrain	Subtrain

Best model

Train | Test

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- This is an example of a 3-fold cross validation as the training data is split into 3 subsets.

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- This means, the K-fold cross validation procedure will result in an overestimation of the true prediction error of the model obtained using the entire training data.
- On the other hand, the K-fold cross validation procedure will result in an estimate of the true prediction error (of the model obtained using the entire training data) which will not be too sensitive to the subtrain data used to train the models.

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- The leave-one-out cross validation procedure makes use of almost the entire training data for model-building which results in an almost unbiased estimate of the true prediction error.
- On the other hand, the leave-one-out cross validation procedure will result in an estimate of the true prediction error that is very sensitive to the subtrain data used to train the models.
- K is typically chosen to be 5 or 10 to strike a balance between computational efficiency and a reliable estimate of the true prediction error.

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- In this case, if the computational cost is not too high, it would be better to use a cross validation procedure as it would yield a reliable (low-variance) estimate of the generalization error.
- On the other hand, if there is a separate test set with a substantial number of samples that will be used for model evaluation, it would be better to use a train-validation split procedure which will lead to an unbiased estimate of the generalization error.

Summary

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- Describe cross validation and its necessity.

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- Compare and contrast different cross validation approaches.