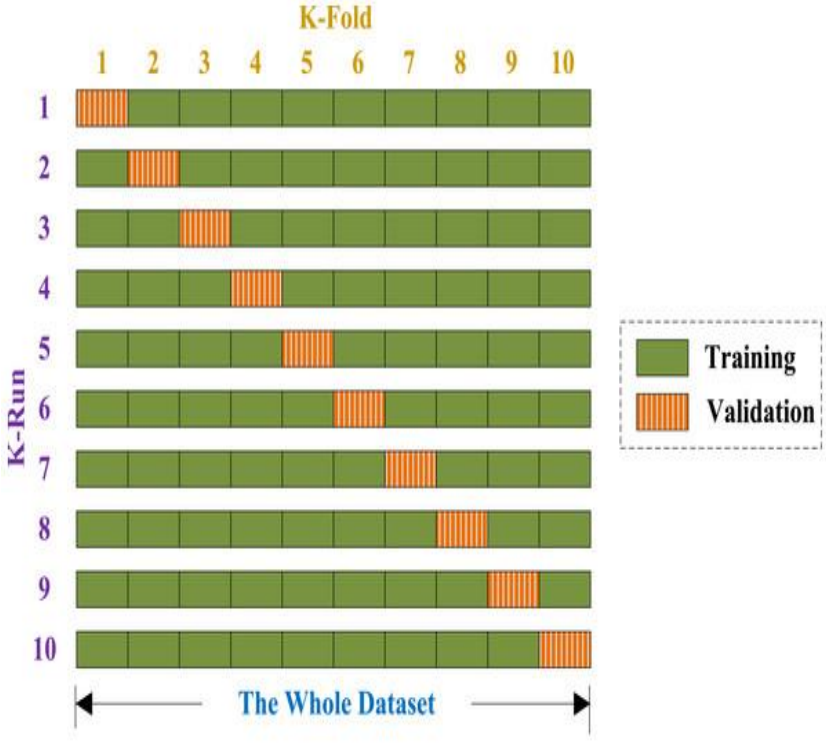
Multiple Linear Regression

Cross Validation - II

Contents

K-Fold Cross Validation



- In k-fold cross-validation the data is first partitioned into k equally (or nearly equally) sized segments or folds
- Then k iterations of training and testing are performed such that each time one fold is kept aside for testing and model is developed using k-1 folds

- Model performance measure is aggregate measure based on above iterations

K-Fold Cross Validation in R

```
#Creating ‘k’ Folds
kfolds<-trainControl(method="cv",number=4)
```

- *trainControl() controls the computational nuances of the train function.*
- *method=“cv” tells R to use Cross Validation method.*
- *number= specifies the number of folds.*

```
#Testing
model<-
train(claimamt~vehage+CC+Length,data=motor,method="lm",trControl=k
folds)
model
```

- *train() fits predictive models over different tuning parameters.*
- *It performs a number of classification and regression routines, fits each model and calculates a resampling based performance measure.*
- *method=lm fits a linear regression*
- *trControl= specifies the train function.*

K-Fold Cross Validation in R

```
# Output
```

```
Linear Regression

1000 samples
   3 predictor

No pre-processing
Resampling: Cross-Validated (4 fold)
Summary of sample sizes: 751, 749, 750, 750
Resampling results:

  RMSE      Rsquared   MAE
  11445.19  0.7319599  9004.326
```

Interpretation :

- *R^2 of the original model is 73.19%*
- *RMSE for the original is model is 11444.51*
- *Comparing the RMSE values, we can say that the model is stable*

Repeated K-Fold Cross Validation

- As the name suggests, repeated k-fold cross validation technique **undertakes cross validation and repeats the process m-number of times**
- This ensures that more robust measure of model performance is generated
- **K-fold** is repeated m times with different randomization in each repetition

For instance,

- Five repeats of 10-fold cross validation will generate 50 total resamples.
- These results are again averaged to produce a single estimate
- This is not the same as 50-fold cross validation

Repeated K-Fold Cross Validation in R

```
#Creating ‘k’ Folds and ‘m’ repeats

kfolds<-trainControl(method="repeatedcv",number=4,repeats=5)
```

- *trainControl() control the computational nuances of the train function.*
- *method=“repeatedcv” tells R to use Repeated Cross Validation method.*
- *number= specifies the number of folds.*
- *repeats= specifies the number of repeats.*

```
#Testing

model<-
train(claimamt~vehage+CC+Length,data=motor,method="lm",trControl=k
folds)

model
```

Repeated K-Fold Cross Validation in R

```
# Output
```

```
Linear Regression

1000 samples
   3 predictor

No pre-processing
Resampling: Cross-Validated (4 fold, repeated 5 times)
Summary of sample sizes: 749, 749, 751, 751, 749, 751, ...
Resampling results:

  RMSE      Rsquared   MAE
  11527.31  0.7305732  9043.351
```

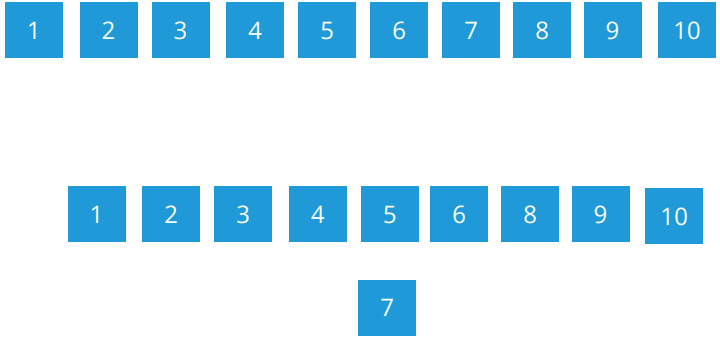
Interpretation :

- *R^2 of the original model is 73.19%*
- *RMSE for the original is 11444.51*
- *RMSE values of the cross validated model indicates stability.*

Leave One Out Cross Validation (LOOCV)

- **LOOCV** is a special case of k-fold cross validation where **k equals the sample size (n)**
- Each time one observation is kept aside and the model is developed on the remaining data.
- The left out observation is predicted using the model.
- This process is repeated n times
- RMSE is computed based on these predicted residuals

- Sample size is 10 and one observations (say 7) is chosen to be kept aside
- The model is developed on the new sample with n=9 and observation 7 is predicted



LOOCV in R

```
#Creating ‘k’ Folds
kfolds<-trainControl(method="LOOCV")
```

- *trainControl() control the computational nuances of the train function.*
- *method=“LOOCV” tells R to use Leave One Out Cross Validation process.*
- *No other arguments need to be included in the command.*

```
#Testing
model<-
train(claimamt~vehage+CC+Length,data=motor,method="lm",trControl=k
folds)
model
```

LOOCV in R

```
# Output
```

```
Linear Regression

1000 samples
   3 predictor

No pre-processing
Resampling: Leave-One-Out Cross-Validation
Summary of sample sizes: 999, 999, 999, 999, 999, 999, ...
Resampling results:

  RMSE      Rsquared   MAE
  11515.85  0.7294088  9039.582
```

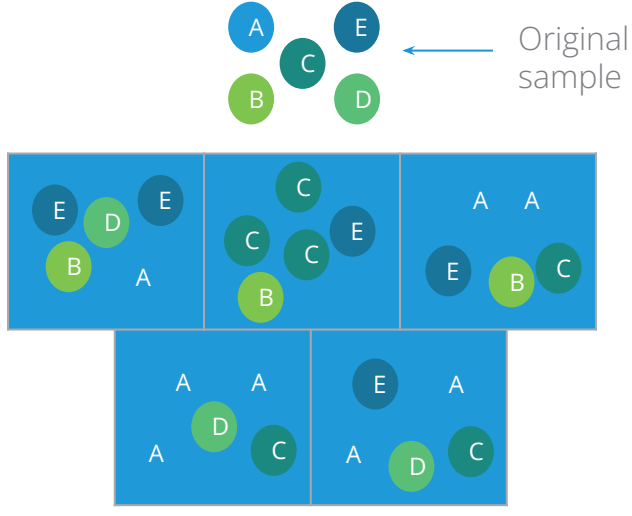
Interpretation :

- *R^2 of the original model is 73.19%*
- *Not much difference in RMSE values compared to that of the original model*
- *Thus model can be considered stable*

Resampling Validation (Bootstrapping)

- Bootstrapping is a technique by which a **random sample with replacement is repeatedly drawn from the original sample and the size of the random sample is the same as original** (Therefore having some observations appear more than once)
- Bootstrapping essentially allows us to simulate repeated statistical experiments
- Generally, 100-500 bootstrap samples are considered adequate for evaluating precision of a model

- Suppose our sample size is 5
- Number of bootstrap samples is 5
- 5 samples of size 5 are drawn
- Model is fit on each of the samples and average of all results is considered to measure model performance



Bootstrapping in R

```
#Creating ‘k’ Folds

kfolds<-trainControl(method="boot")
```

- *trainControl() control the computational nuances of the train function.*
- *method=“boot” tells R to use bootstrapping approach to resampling.*

```
#Testing

model<-
train(claimamt~vehage+CC+Length,data=motor,method="lm",trControl=k
folds)
model
```

Bootstrapping in R

```
# Output
```

```
Linear Regression

1000 samples
   3 predictor

No pre-processing
Resampling: Bootstrapped (25 reps)
Summary of sample sizes: 1000, 1000, 1000, 1000, 1000, 1000, ...
Resampling results:

  RMSE   Rsquared   MAE
  11400  0.7354236  8967.069
```

Interpretation :

- *R^2 of the original model is 73.19%*
- *RMSE for the original is 11444.51*
- *Comparing the RMSE values of the cross validated model, we can say model is stable.*

Quick recap

This session illustrated five most important **model validation techniques:**

K-Fold Cross Validation	• Data is first partitioned into **k** equally (or nearly equally) sized segments or folds • Then k iterations of training and testing are performed such that each time one fold is kept aside for testing and model is developed using **k-1** folds
Repeated K-Fold Cross Validation	• This is an extension of k-fold method wherein the process is repeated **m** number of times

Quick Recap

Leave One Out Cross Validation (LOOCV)	• Special case of k-fold cross validation where **k** equals the sample size (n), observation number **i** is kept aside and the model is developed on remaining data after which error is calculated • This process is repeated **n** times, for all i's • RMSE is computed based on these predicted residuals
Resampling Cross Validation (Bootstrapping)	• Random sample with replacement is repeatedly drawn from the original sample and the size of the random sample is same as original • Model is fit on each sample and average results are considered for measuring model validity
Validation in R	• Package **caret** has all functions needed to carry out different types of validation • **`createDataPartition()`, `trainControl()`** and **`train()`** are the most important functions • Depending on the validation technique, **`method=`** needs to be specified in **`trainControl()`**