

# Resampling Methods.

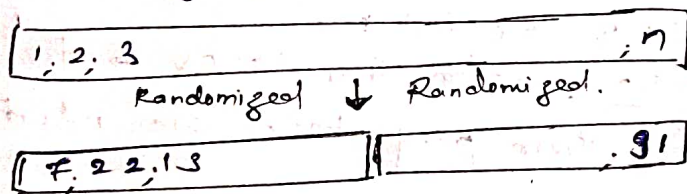
## \* Introduction:

- Resampling method: repeatedly drawing samples from a training set and fitting a model at interest on each sample in order to obtain additional information about the model.
- cross validation: can be used to estimate the test error associated with a given statistical learning method in order to evaluate its performance or to select appropriate level of flexibility.
- model assessment: process of evaluating a model's performance
- model selection: process of selecting the proper level of flexibility.
- bootstrap: used in several contexts, most commonly to provide a measure of accuracy of a parameter estimate or of a given statistical learning method

## 1. Cross validation.

### 5.1.1: The validation set approach.

- it involves randomly dividing the available set of observations into two parts: training set (used for model fitting) & a validation set / hold-out set (prediction & calculating estimate of test error)



Drawbacks

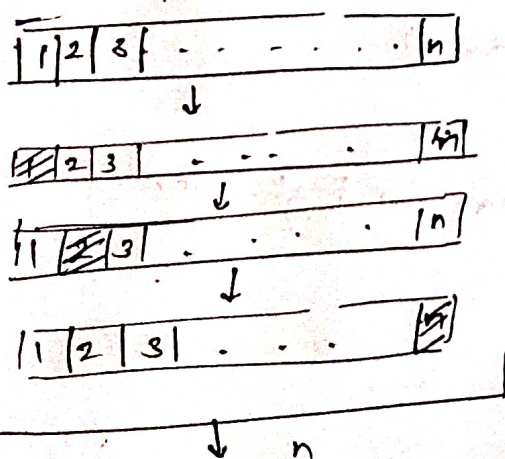
- \* validation estimate of the test error rate can be highly variable, depending on which observations included in train & test.

- \* if training set small - model may perform bad & validation set error

may tend to overestimate the test error rate.

### 5.1.2 Leave one out cross validation (LOOCV)

attempts to address drawbacks of ~~validation set~~ validation set approach.



$MSE_i = \frac{1}{n-1} \sum_{j \neq i} (y_j - \hat{y}_j)^2$  → not included in validation set the  $i$ th observation.

→ consider all  $\binom{n}{1} = n$  possible leave one out ~~validation~~ validation sets then get the average: that is the required estimation.

- \* Advantages - less bias (on repetitions).
- does not overestimate test error.
- no randomness involved in the train-validation split.

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

Note: LOOCV has potential to be expensive for implementation.

For least squares linear / polynomial regression:

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

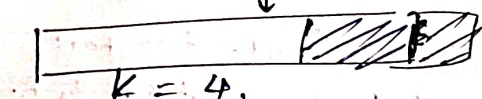
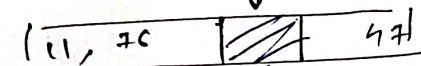
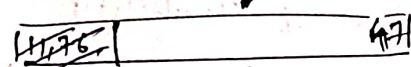
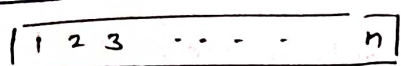
This formulae does not hold true in general!

where:

$\hat{y}_i$ :  $i$ th fitted value from the original least squares fit.

$$h_i: \text{leverage} = \frac{1}{n} + \frac{(x_i - \bar{x})^2}{\sum_{i=1}^n (x_i - \bar{x})^2}$$

5.1.3: k-fold cross validation: (1) Randomly split into  $k$  many ~~non~~ overlapping groups of equal size.

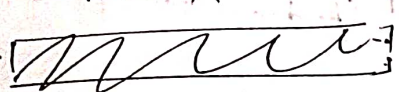


(2)  $i$ th group held out as validation set. remaining ' $k-1$ ' used for training model.

(3) repeat process for holding out each group  $i: i = 1(1)k$

Formula:  $CV(k) = \frac{1}{k} \sum_{i=1}^k MSE_i$

generally:  $k = 5$  or  $10$  (computation perspective)



→ very less variability compared to validation set approach

5.1.4. Bias - Variance Trade Off for k-Fold Cross-Validation.

-  $k$  fold CV gives more accurate estimate of the test error.

- no. of observations in  $k$  fold is  $\frac{(k-1)n}{k}$ . → more than LOOCV but less than validation set approach ⇒ from perspective of bias reduction LOOCV is preferred to  $k$ -fold CV.

- LOOCV has higher variance than does  $k$ -fold CV with  $k < n$ .

→ LOOCV: training sets almost identical. - highly truly correlated. - averaging output of these  $n$  fitted outputs.

$k$  fold: - less overlap in training sets ⇒ less correlated

$$\therefore \text{var}(\text{mean of } n \text{ uncorr. data}) < \text{var}(\text{mean of } n \text{ highly correlated data})$$

$$\Rightarrow \text{Var}(k \text{ fold}) < \text{Var}(LOOCV)$$

\* for  $k$  fold CV with  $k=5$  or  $10$ : ~~not~~ no high bias nor high variance



S.1.5 Cross validation on classification Problems.

- Regression: MSE, classification: error rate / ~~fraction~~ fraction of misclassified objects.

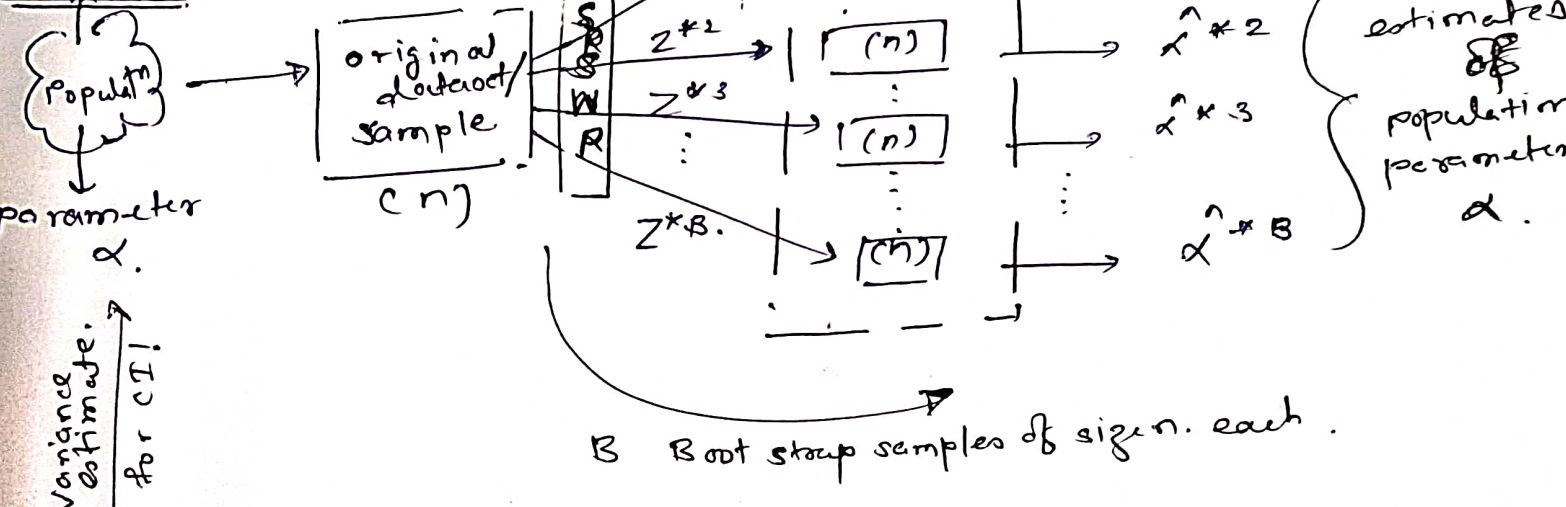
For LOOCV:  $CV_{err} = \frac{1}{n} \sum_{i=1}^n Err_i$  where  $Err_i = I(y_i \neq \hat{y}_i)$

For K fold CV:  $CV_{err} = \frac{1}{K} \sum_{i=1}^K Err_i$

\* 2. Bootstrap.

- widely applicable & extremely powerful statistical tool that can be used to quantify the uncertainty associated with a given estimator or statistical learning method.
- used when measure of variability is hard to obtain.
- rather than repeatedly obtaining independent data sets from the population we instead obtain distinct data sets by repeatedly sampling observations from the original data set.

Unknown!



$SE_B(\hat{\alpha}) = \sqrt{\frac{1}{B-1} \sum_{r=1}^B \left( \hat{\alpha}^{*r} - \frac{1}{B} \sum_{r=1}^B \hat{\alpha}^{*r} \right)^2}$

\* Advantage: - Can be used in almost all situations.  
 - No complicated mathematical ~~situation~~ formulae required.