Resampling Methods

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1. Cross Validation

2. Bootstrap

About Resampling

- Pretending the data as population,
- repeatedly draw sample from the data,
- refitting a model of interest on each sample.
- Main task: assess the validity/accuracy of statistical methods and models.
  - **Cross-validation**: estimate the *test error* of models
  - **Bootstrap**: quantify the *uncertainty* of estimators

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- because of possibility of over-fit, it cannot be used to properly assess test error.
- Test error would be also easily computable, if test data are well designated.
- Normally we are just given ... data.
- Shall have to create "test data" for the purpose of computing test error.

The validation set approach

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- The "test data" here should be more accurately called *validation data* or hold out data,
- meaning that they not used in training.
- Model fitting only uses the training data.

Ideal scenario for performance assessment

- In a "data-rich" scenario, we can afford to separate the data into three parts:
    - *training data*: used to train various models.
    - *validation data*: used to assess the models and identify the best.
    - *test data*: test the results of the best model.

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    - *training data*: used to train various models.
    - *validation data*: used to assess the models and identify the best.
    - *test data*: test the results of the best model.
- Usually, people also call validation data or hold-out data as test data.

Validation and Cross validation

- Validation set approach.
- LOOCV (Leave-one-out cross valiation)
- K-fold cross validation.

Validation set approach

A set of n observations are *randomly* split into

- **a training set**
  – shown in blue, containing observations 7, 22, and 13, among others,
- **a validation set**
  – shown in beige, and containing observation 91, among others).

Figure: 5.1. A schematic display of the validation set approach. The statistical learning method is fit on the training set, and its performance is evaluated on the validation set.

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- Only a subset of the observations–the training set are used to fit the model.
- Statistical methods tend to perform worse when trained on fewer observations.

Drawback of validation set approach

- Our ultimate goal is to produce the best model with best prediction accuracy.
- Validation set approach has a drawback of using ONLY training data to fit model.
- The validation data do not participate in model building but only model assessment.
- A "waste" of data.
- We need more data to participate in model building.

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- We need more data to participate in model building.
- We need to improve it.

Cross Validation.

The leave-one-out cross-validation

Suppose the data contain n data points: $(\mathbf{x}_1, y_1), \cdots, (\mathbf{x}_n, y_n)$.

- *Pick data point 1 as validation set, the rest as training set.*
  - Fit the model on the training set,
  - evaluate the test error on the validation set, $\text{MSE}_1 = (y_1 - \hat{y}_1)^2$.

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- *Pick data point 2 as validation set, the rest as training set.*
  - Fit the model on the training set,
  - evaluate the test error on the validation set, $\mathrm{MSE}_2 = (y_2 - \hat{y}_2)^2$.

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  - Fit the model on the training set,
  - evaluate the test error on the validation set, $\text{MSE}_1 = (y_1 - \hat{y}_1)^2$.
- *Pick data point 2 as validation set, the rest as training set.*
  - Fit the model on the training set,
  - evaluate the test error on the validation set, $\text{MSE}_2 = (y_2 - \hat{y}_2)^2$.
- ..... (repeat the procedure for all data point.)
- Obtain an estimate of the test error by combining the MSE_i, $i =, ..., n$.

The LOOCV estimate for the test MSE is

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

LOOCV

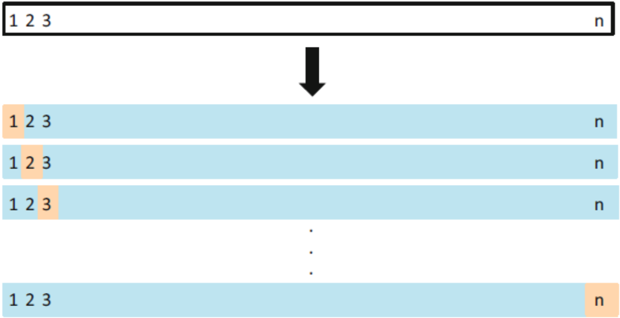

Figure: 5.3. A schematic display of LOOCV.

A set of n data points is repeatedly split into

- a *training* set (shown in blue): containing all but one observation,
- a *validation* set (shown in beige): contains only that observation.

Pros and cons of LOOCV

Advantages:

- Far less bias, since the training data size $(n-1)$ is close to the entire data size (n).
- One single test error estimate (thanks to the averaging), without the variablity validation set approach.

Disadvantage:

- could be computationally expensive since the model need to be fit n times.
- The MSE_i may be too much correlated.

Complexity of LOOCV in linear model?

- Consinder linear model:

$$y_i = \mathbf{x}_i^T \beta + \epsilon_i, \qquad i = 1, .., n$$

  and the fitted values $\hat{y}_i = \mathbf{x}_i^T \hat{\beta}$, where $\hat{\beta}$ is the least squares estimate of β based on all data $(\mathbf{x}_i, y_i), i = 1, ..., n$.
- Using LOOCV, the

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

- Looks to be complicated to compute least squares estimate n times.

Recall: Leverage

- Recall the hat matrix

$$\mathbf{H} = \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T \quad \text{as } \hat{y} = \mathbf{H}y.$$

  Let $h_{ij} = \mathbf{x}_i^T(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{x}_j$ be the (i, j) elements of $\mathbf{H}$.
- The leverage of the i-th observation is just the i-th diagonal element of $\mathbf{H}$, denoted as h_{ii}.
- A high leverage implies that observation is quite influential. Note that the average of h_{ii} is $(p+1)/n$.
- E.g., if h_{ii} is greater than $2(p+1)/n$, twice of the average, is generally considered large.

Simple Formula of LOOCV in linear model

- Easy formula:

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

where $\hat{y}_i$ is the fitted values of least squares method based on all data. h_i is the leverage.

Fast computation of cross-validation I

- The leave-one-out cross-validation statistic is given by

$$CV = \frac{1}{n}\sum_{i=1}^{n} e_{[i]}^2,$$

where $e_{[i]} = y_i - \hat{y}_{[i]}$, the observations are given by $y_1, \ldots, y_n$, and $\hat{y}_{[i]}$ is the predicted value obtained when the model is estimated with the ith case deleted.

- Suppose we have a linear regression model $\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{e}$. The $\hat{\boldsymbol{\beta}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y}$ and $\mathbf{H} = \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T$ is the hat matrix. It has this name because it is used to compute $\hat{\mathbf{Y}} = \mathbf{X}\hat{\boldsymbol{\beta}} = \mathbf{HY}$. If the diagonal values of $\mathbf{H}$ are denoted by $h_1, \ldots, h_N$, then the leave-one-oout cross-validation statistic can be computed using

$$CV = \frac{1}{N}\sum_{i=1}^{N}[e_i/(1-h_i)]^2,$$

where $e_i = y_i - \hat{y}_i$ is predicted value obtained when the model is estimated with all data included.

Fast computation of cross-validation II

Proof

- Let $\mathbf{X}_{[i]}$ and $\mathbf{Y}_{[i]}$ be similar to $\mathbf{X}$ and $\mathbf{Y}$ but with the ith row deleted in each case. Let $\mathbf{x}_i^T$ be the ith row of $\mathbf{X}$ and let

$$\hat{\boldsymbol{\beta}}_{[i]} = (\mathbf{X}_{[i]}^T \mathbf{X}_{[i]})^{-1} \mathbf{X}_{[i]}^T \mathbf{Y}_{[i]}$$

  be the estimate of $\boldsymbol{\beta}$ without the ith case. Then $e_{[i]} = y_i - \mathbf{x}_i^T \hat{\boldsymbol{\beta}}_{[i]}$.

- Now $\mathbf{X}_{[i]}^T \mathbf{X}_{[i]} = (\mathbf{X}^T \mathbf{X} - \mathbf{x}_i \mathbf{x}_i^T)$ and $\mathbf{x}_i^T (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{x}_i = h_i$. So by the Sherman-Morrison-Woodbury formula,

$$(\mathbf{X}_{[i]}^T \mathbf{X}_{[i]})^{-1} = (\mathbf{X}^T \mathbf{X})^{-1} + \frac{(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{x}_i \mathbf{x}_i^T (\mathbf{X}^T \mathbf{X})^{-1}}{1 - h_i}.$$

Fast computation of cross-validation III

Proof

- Also note that $\mathbf{X}_{[i]}^T \mathbf{Y}_{[i]} = \mathbf{X}^T \mathbf{Y} - \mathbf{x} y_i$. Therefore

$$\begin{aligned}
\hat{\boldsymbol{\beta}}_{[i]} &= \left[(\mathbf{X}^T\mathbf{X})^{-1} + \frac{(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{x}_i\mathbf{x}_i^T(\mathbf{X}^T\mathbf{X})^{-1}}{1-h_i} \right] (\mathbf{X}^T\mathbf{Y} - \mathbf{x}_i y_i) \\
&= \hat{\boldsymbol{\beta}} - \left[\frac{(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{x}_i}{1-h_i} \right] [y_i(1-h_i) - \mathbf{x}_i^T \hat{\boldsymbol{\beta}} + h_i y_i] \\
&= \hat{\boldsymbol{\beta}} - (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{x}_i e_i/(1-h_i)
\end{aligned}$$

- Thus

$$\begin{aligned}
e_{[i]} &= y_i - \mathbf{x}_i^T \hat{\boldsymbol{\beta}}_{[i]} \\
&= y_i - \mathbf{x}_i^T \left[\hat{\boldsymbol{\beta}} - (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{x}_i e_i/(1-h_i) \right] \\
&= e_i + h_i e_i/(1-h_i) = e_i/(1-h_i)
\end{aligned}$$

Simplicity of LOOCV in linear model

- One fit (with all data) does it all!
- The prediction error rate (in terms of MSE) is just weighted average of the least squares fit residuals.
- High leverage point gets more weight in prediction error estimation.

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- Repeat the procedures over every subset.
- Average over the above K estimates of the test errors,

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- LOOCV is a special case of K-fold cross validation, actually n-fold cross validation.

K-fold cross validation

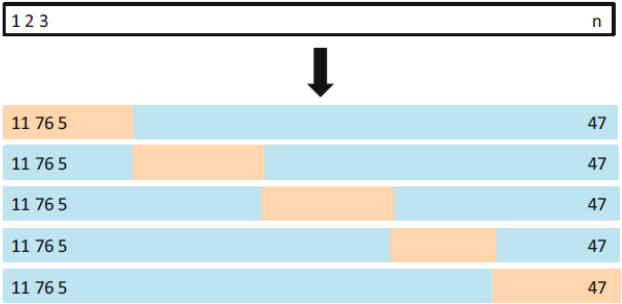

Figure: 5.5. A schematic display of 5-fold CV.

A set of n observations is randomly split into five non-overlapping groups.

- Each of these fifths acts as a validation set (shown in beige),
- the remainder as a training set (shown in blue).

K-fold cross validation

- Common choices of K: $K = 5$ or $K = 10$.
- Advantage over LOOCV:
  1. computationally lighter, espeically for complex model with large data.
  2. Likely less variance (to be addressed later).
- Advantage over validation set approach:
  Less variability resulting from the data-split, thanks to the averaging.

Bias variance trade-off

- In terms of bias of estimation of test error:
  - Validation set approach has more bias due to smaller size of training data;
  - LOOCV is nearly unbiased;
  - K-fold (e.g, $K = 5$ or 10) has intermediate bias.
- K-fold cross validation has smaller variance than that of LOOCV.
  - The n traing sets LOOCV are too similar to each other. As a result, the trained models are too postively correlated.
  - The K training sets of K-fold cross validation are much less similar to each other.
- The K-fold cross validation generally has less variance than LOOCV.

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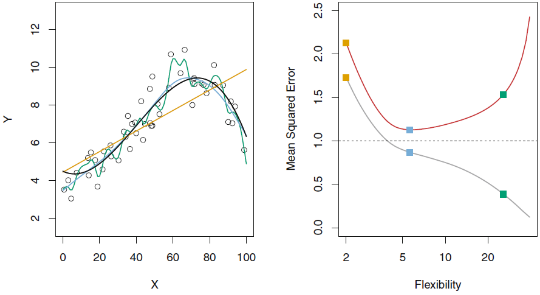
- MSE is a popular criterion to measure predition/estimation accuracy for regression. There are other criteria.
- For classification with qualitative response, a natural choice is:
  - 1 for incorrect classification,
  - 0 for correct classification.
- For LOOCV,
  - Let $y_i^{(i)}$ is the classification of i-th observation based on model fitted not using i-th observation,
    $$\mathrm{Err}_i = I(y_i \neq \hat{y}_i^{(i)}).$$
  - The average number of incorrect classification
    $$\mathrm{CV}_{(n)} = \frac{1}{n}\sum_{i=1}^{n} Err_i.$$



- Training error declines in general when model complexity increases. Some times even reaches 0.
- Test error general declines first and then increases.
- 10-fold cross validation provides reasonable estimate of the test error, with slight under-estimation.

Bootstrap as a resampling procedure.

- Suppose we have data $x_1, ..., x_n$, representing the ages of n randomly selected people in Wuhan.
- Use sample mean $\bar{x}$ to estimate the population mean μ, the avearge age of all residents of Wuhan.

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  - They rely on normality assumption or central limit theorm.
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- Is there another reliable way?
- Just bootstrap.

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- Use the distribution of $\bar{x}_1^* - \bar{x}, ..., \bar{x}_M^* - \bar{x}$ to approximate that of $\bar{x} - \mu$.

Example

- X and Y are two random variables. Then minimizer of $\mathrm{var}(\alpha X + (1-\alpha)Y)$ is

$$\alpha = \frac{\sigma_Y^2 - \sigma_{XY}}{\sigma_X^2 + \sigma_Y^2 - 2\sigma_{XY}}.$$

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- Data: $(X_1, Y_1), ..., (X_n, Y_n)$.
- We can compute sample variances and covariances.
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- Use Bootstrap.

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- Repeat this procedure, and we have $\hat{\alpha}^*_1, ..., \hat{\alpha}^*_M$ for a large M.
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- Repeat this procedure, and we have $\hat{\alpha}_1^*, ..., \hat{\alpha}_M^*$ for a large M.
- Use the distribution of $\hat{\alpha}_1^* - \hat{\alpha}, ..., \hat{\alpha}_M^* - \hat{\alpha}$ to approximate the distribution of $\hat{\alpha} - \alpha$.
- For example, we can use
$$\frac{1}{M}\sum_{j=1}^{M}(\hat{\alpha}_j^* - \hat{\alpha})^2$$
to estimate $E(\hat{\alpha} - \alpha)^2$.

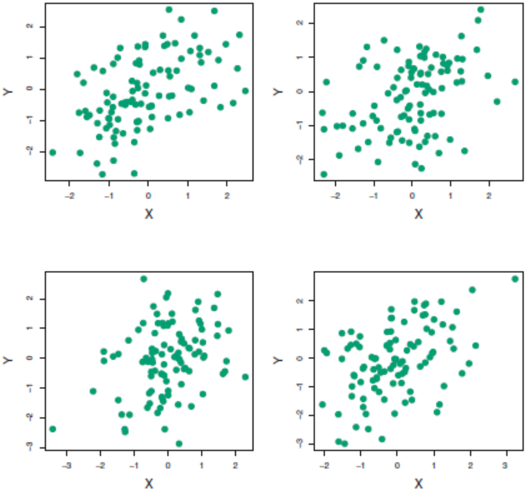
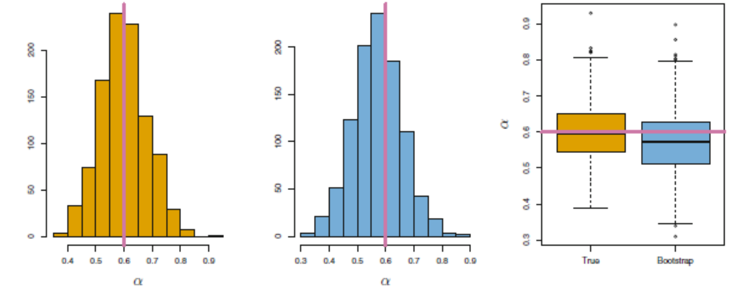


Figure: 5.9. Each panel displays 100 simulated returns for investments X and Y. From left to right and top to bottom, the resulting estimates for α are 0.576, 0.532, 0.657, and 0.651.



- **Left**: A histogram of the estimates of α obtained by generating 1,000 simulated data sets from the true population.
- **Center**: A histogram of the estimates of α obtained from 1,000 bootstrap samples from a single data set.
- **Right**: The estimates of α displayed in the left and center panels are shown as boxplots. In each panel, the pink line indicates the true value of α.