# Linear and Generalized Linear Models (4433LGLM6Y)

## Model selection

Meeting 8

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# Model selection (Fox: chapter 22, Faraway PRA: chapter 10)

Model selection and criteria

Model validation

Collinearity

# Model Selection: Caution!

- Suppose we have many predictor variables, not all necessarily related to the response variable.
- We want to select the "best" subset of predictors.
- The following problems may appear (according to Fox):

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  - Problem of simultaneous inference.

Also look at the CI

  - What does “failing to reject a null hypothesis” mean?
  - Impact of large samples on hypothesis tests: trivially small effects become statistically significant if dataset is large.

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  - Exaggerated precision. ⇒ low variance

## General strategies

- Addressing these concerns (according to Fox):
  - Use alternative model-selection criteria instead of statistical significance.

    补偿
  - Compensate for simultaneous inference, e.g., by Bonferroni adjustments,
  - Validate a statistical model selected by another approach.
  - Model averaging
  - Avoid model selection. Specify maximally complex and flexible model without trying to simplify it. Issues here?

# Model Selection

- Reasons for selecting "best" subset of regressors:
  - We can explain the data in simplest way, removing redundant predictors.

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    - Principle of Occam's Razor (parsimony) : among several plausible explanations for phenomenon, simplest is best.
  - Unnecessary predictors will add noise to the estimation of other quantities that are of interest,
    - degrees of freedom are wasted.
  - Collinearity is caused by having too many variables doing same job.
    - Remove excess predictors.

# Types of variable selection

- Two main types of variable selection:
  - Stepwise approach, comparing successive models
    - Backwards
    - Forward
    - Stepwise (mixed)

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    - Stepwise approach may use hypothesis testing to select the next step, but other criteria may be used too.
  - Criterion approach, finding a model that optimizes some measure of goodness of fit.

- Marginality principle: keep lower order terms in the model, if higher order term is important.

- Model selection is conceptually simplest if the goal is prediction
  - Example: develop regression model that will predict new data as accurately as possible.

## Stepwise procedures

- Backward elimination vs Forward elimination
- Both procedures can be implemented using `step()` command in R.
- Stepwise selection (mixed)
- Stepwise procedures may also be used in combination with other criteria, e.g., AIC (see `stepAIC()`).

# Stepwise procedures: Backward Elimination

$(X^TX)^{-1}$ $k>n$ $\text{rank}[(X^TX)^{-1}]<k$

model may not exist

- Backward Elimination

  1. Start with all predictors in model (full model).
  2. Remove a predictor with the highest p-value, greater than threshold p-value-to-stay $\alpha_{crit}$
  3. Refit the model and repeat the step 2.
  4. Stop if all p-values of terms remaining in the model are smaller than $\alpha_{crit}$.

e.g., 0.05

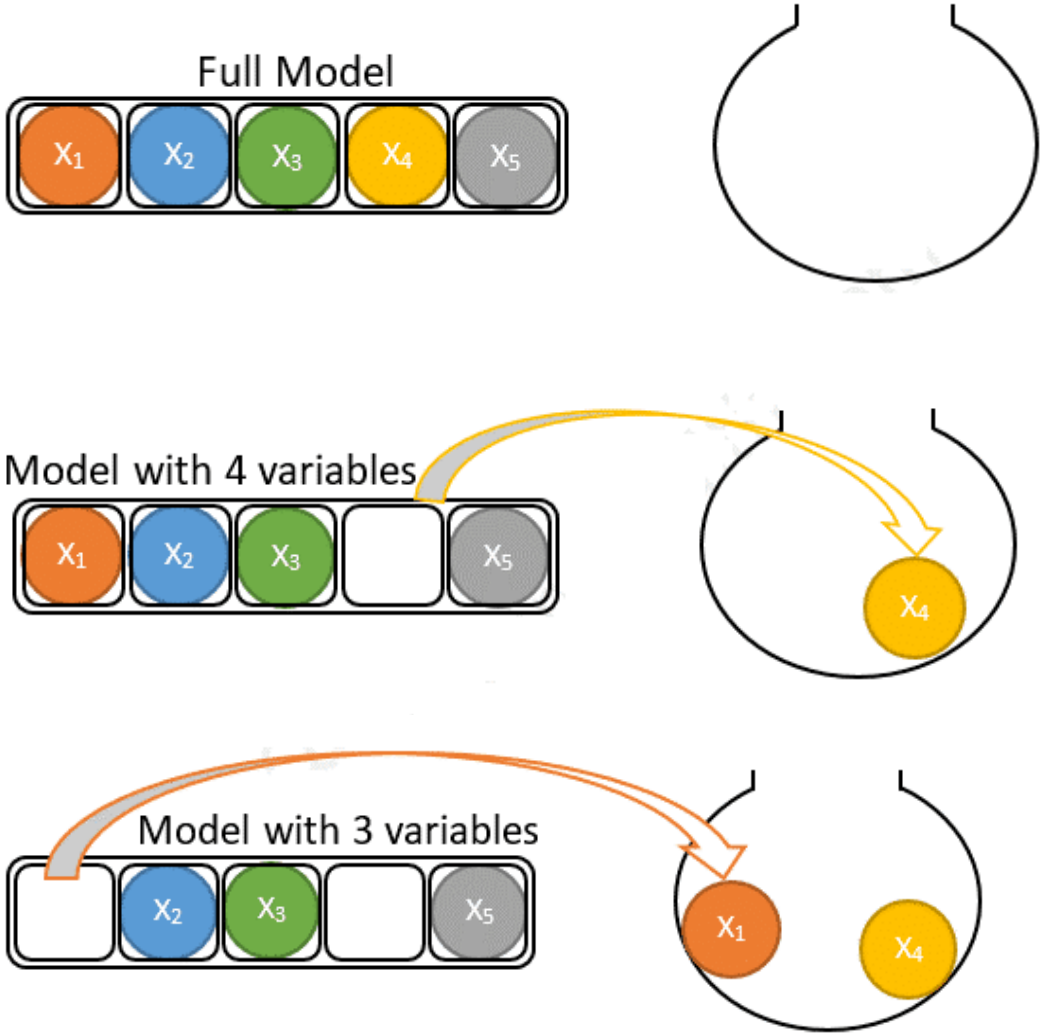
- What is the main drawback of this approach?

Other criteria may be used here as well, e.g., *AIC.*

# Stepwise procedures: Backward Elimination with 5 predictors

- Backward Elimination

  1. Start with all 5 predictors in model (full model).
  2. Remove a predictor with the least significant predictor (e.g., $X_4$)
  3. Refit the model and repeat the step 2.
  4. Keep removing the least significant predictors until all of them are significant (or running out of predictors).



## Example: Life expectancy dataset

- Examine the relationship between life expectancy and other socio-economic variables for the U.S. states.

```
> statedata <- read.csv("statedata.csv", header = TRUE)
> head(statedata)
  life.exp population income illiteracy murder highSchoolGrad frost   area
1    69.05       3615   3624        2.1   15.1           41.3    20  50708
2    69.31        365   6315        1.5   11.3           66.7   152 566432
3    70.55       2212   4530        1.8    7.8           58.1    15 113417
4    70.66       2110   3378        1.9   10.1           39.9    65  51945
5    71.71      21198   5114        1.1   10.3           62.6    20 156361
6    72.06       2541   4884        0.7    6.8           63.9   166 103766
```

- There is an easier way to do this in **R**, but let's try manually first.

- See using `step()` or `stepAIC()` commands.

# Example: Life expectancy dataset

```
> statreg <- lm(life.exp ~ ., data = statedata)
> coef(summary(statreg))
                   Estimate   Std. Error     t value     Pr(>|t|)
(Intercept)     7.094322e+01 1.747975e+00 40.58594017 2.510609e-35
population      5.180036e-05 2.918703e-05  1.77477309 8.318351e-02
income         -2.180424e-05 2.444256e-04 -0.08920603 9.293422e-01
illiteracy      3.382032e-02 3.662799e-01  0.09233464 9.268712e-01
murder         -3.011232e-01 4.662073e-02 -6.45899735 8.679582e-08
highSchoolGrad  4.892948e-02 2.332328e-02  2.09788176 4.197175e-02
frost          -5.735001e-03 3.143230e-03 -1.82455682 7.518682e-02
area           -7.383166e-08 1.668163e-06 -0.04425927 9.649075e-01
> summary(statreg)$r.squared
[1] 0.7361563
```

"area" shows the highest p-value above the threshold (e.g., 0.05), i.e., the least significant predictor.

# Example: Life expectancy dataset

```
> statreg <- update(statreg, ~ . -area, data = statedata)
> coef(summary(statreg))
                    Estimate   Std. Error     t value     Pr(>|t|)
(Intercept)    70.9893185176 1.387454e+00 51.16515405 3.694989e-40
population      0.0000518827 2.878768e-05  1.80225346 7.851808e-02
income         -0.0000244403 2.342908e-04 -0.10431609 9.174036e-01
illiteracy      0.0284588124 3.416329e-01  0.08330231 9.339978e-01
murder         -0.3018231392 4.334432e-02 -6.96338357 1.453868e-08
highSchoolGrad  0.0484723220 2.066727e-02  2.34536620 2.369166e-02
frost          -0.0057757582 2.970228e-03 -1.94455035 5.838883e-02
> summary(statreg)$r.squared
[1] 0.736144
```

- Next, “illiteracy” shows the highest p-value above the threshold.

```
> statreg <- update(statreg, ~ . -illiteracy, data = statedata)
> coef(summary(statreg))
                    Estimate   Std. Error    t value     Pr(>|t|)
(Intercept)     7.106575e+01 1.0289414512 69.0668559 1.659665e-46
population      5.114856e-05 0.0000270945  1.8877836 6.566097e-02
income         -2.477076e-05 0.0002315986 -0.1069555 9.153104e-01
murder         -3.000077e-01 0.0370418231 -8.0991613 2.907482e-10
highSchoolGrad  4.775797e-02 0.0185907897  2.5689048 1.367027e-02
frost          -5.909864e-03 0.0024677801 -2.3948100 2.095338e-02
> summary(statreg)$r.squared
[1] 0.7361014
```

- “income” shows the highest p-value above the threshold.

# Example: Life expectancy dataset

```
> statreg <- update(statreg, ~ . -income, data = statedata)
> coef(summary(statreg))
                    Estimate   Std. Error   t value     Pr(>|t|)
(Intercept)     7.102713e+01 9.528530e-01 74.541541 8.612596e-49
population      5.013998e-05 2.512002e-05  1.996017 5.200514e-02
murder         -3.001488e-01 3.660946e-02 -8.198669 1.774520e-10
highSchoolGrad  4.658225e-02 1.482706e-02  3.141704 2.968091e-03
frost          -5.943290e-03 2.420875e-03 -2.455017 1.801778e-02
> summary(statreg)$r.squared
[1] 0.7360328
```

- Next, “population” shows the highest p-value above the threshold.

```
> statreg <- update(statreg, ~ . -population, data = statedata)
> coef(summary(statreg))
                    Estimate  Std. Error   t value     Pr(>|t|)
(Intercept)    71.036378813 0.983262169 72.245614 5.253889e-49
murder         -0.283065168 0.036731323 -7.706370 8.039156e-10
highSchoolGrad  0.049948704 0.015201124  3.285856 1.950415e-03
frost          -0.006911735 0.002447477 -2.824025 6.987727e-03
> summary(statreg)$r.squared
[1] 0.7126624
```

- The procedure stops here.

# Stepwise procedures: Forward Selection with 5 predictors

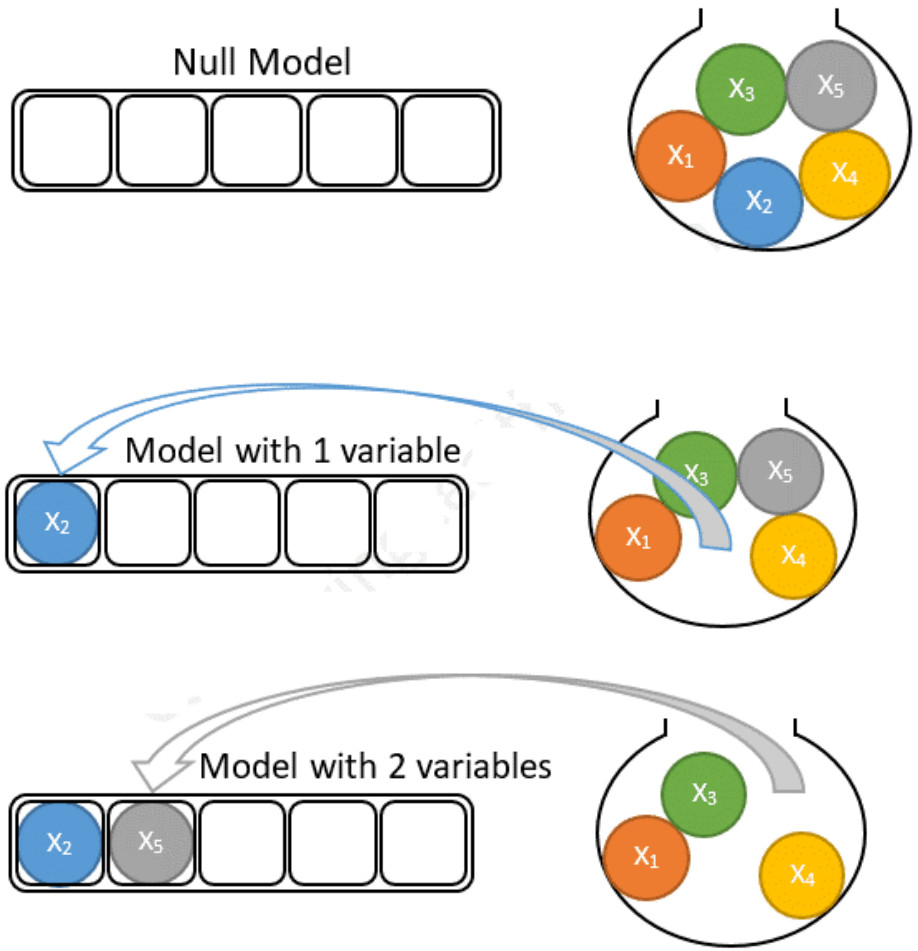
- Forward Selection

    1. Start with no predictor in model (null model).
    2. Enter a predictor with the smallest p-value, smaller than threshold p-value-to-enter $\alpha_{crit}$.
    3. Refit the model and repeat the step 2.
    4. Stop if all p-values of terms not in the model are higher than $\alpha_{crit}$ .

# Stepwise procedures: Forward Selection

- Forward Selection

  1. Start with no predictor in model (null model).
  2. Enter the most significant predictor (e.g., $X_2$)
  3. Refit the model and repeat the step 2.
  4. Keep adding the most significant predictors until those not in the model are not significant.



## Stepwise procedures: Stepwise (or mixed) selection

- This is a combination of backward elimination and forward selection. After entering variable, all variables in model are candidate for removal.
- Thresholds p-value-to-enter and p-value-to-stay need to be specified.

- Drawback related to earlier mentioned caveats:
  - “Optimal” model may be missed due to adding / dropping of single variables.
  - Stepwise selection tends to pick models smaller than desirable for prediction purposes.
  - If using p-values: don’t treat p-values literally! (recall multiple testing problem)
  - Procedures are not linked to final objective of prediction or explanation.

## Criterion-Based Procedures

- Criterion-based procedures typically compare all possible models (i.e., all possible “subsets regression”)
- A model with $k$ regressors has $2^k$ possible sub-models! (why?)

- Different criteria may be used, e.g.:
  - $R^2_{adj}$ ($R^2$ - adjusted)
  - Mallow’s $C_p$
  - Predicted residual error sum of squares (PRESS) and Cross-Validation
  - Akaike information criterion (AIC)
  - Bayesian (sometimes Schwarz's Bayesian) information criterion (BIC)

# Criterion-Based Procedures: $R^2_{adj}$

- Recall

$$R^2 = \frac{RegSS}{TSS} = 1 - \frac{RSS}{TSS}.$$

- Why can't we use $R^2$ as a model selection criterion?

$\hat{\sigma}^2_{Null}$ is the estimate of error variance based on the "empty" model (intercept only).

- Instead, we use the adjusted $R^2$:

$$R^2_{adj} = 1 - \frac{RSS/(n-p)}{TSS\ /(n-1)} = 1 - \frac{\hat{\sigma}^2_{Model}}{\hat{\sigma}^2_{Null}}$$

- $R^2_{adj}$ will only increase by changing a model, if the estimate of error variance based on new model $\hat{\sigma}^2_{Model}$ decreases. It will only decrease, if the "change" in RSS is compensated by change in residual df.

## Criterion-Based Procedure

- Good model should predict well, so total prediction MSE (on population level) should be small.
- The scalled (normalized) MSE is:

$$\frac{1}{\sigma_\epsilon^2}\sum_{i=1}^{n} E\left(\hat{Y}_i - E(Y_i)\right)^2 = \frac{1}{\sigma_\epsilon^2}\sum_{i=1}^{n}\left\{V\left(\hat{Y}_i\right) + \left(E\left(\hat{Y}_i\right) - E(Y_i)\right)^2\right\}.$$

- There are two components: variance $V\left(\hat{Y}_i\right)$ and squared bias $\left(E\left(\hat{Y}_i\right) - E(Y_i)\right)^2$.

- Bias-variance trade-off: by removing a variable, the decrease in variance offsets any increase in bias

## Criterion-Based Procedure: Mallow's $C_p$

$$\hat{\sigma}_\epsilon^2 = \frac{RSS_p}{n-p} = \frac{\sum E_i^2}{n-p}$$

- Prediction MSE is estimated by Mallow's $C_p$:

$$C_p = \frac{RSS_p}{\hat{\sigma}_\epsilon^2} + 2p - n$$

$\hat{\sigma}_\epsilon^2$ is from the full model, and $RSS_p$ from current model (with $p$ parameters).

- Good model should have $C_p$ close to or below $p$. Model with a bad fit has $C_p$ much bigger than $p$.

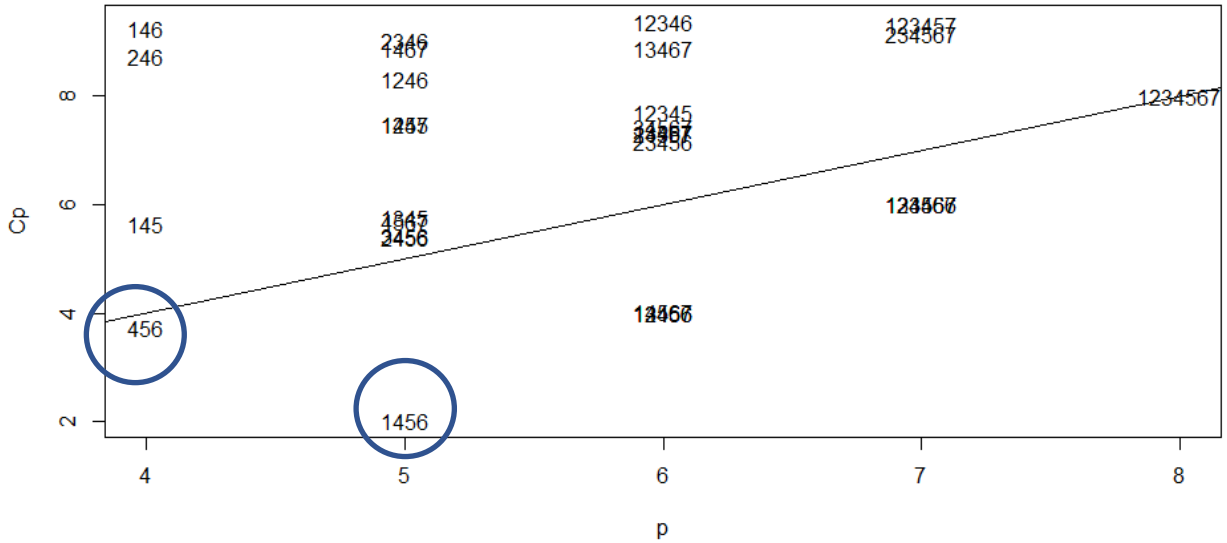
- For full model, we have $C_p = p$ (why?).

$$C_p = \frac{RSS_p}{RSS_p/(n-p)} + 2p - n = n - p + 2p - n = p$$

# Mallow's $C_p$ : Example

- In practice, we plot $C_p$ against p and look for models with small $p$ and with $C_p$ around or less than p.

```
> library(leaps)
> statreg <- lm(life.exp ~ ., data = statedata)
> x <- model.matrix(statreg)[,-1]
> y <- statedata$life.exp
> statregCP <- leaps(x,y)
> Cpplot(statregCP)
```




- We have $k = 7$ predictors
- How many models are there, in total?
- Good options are the models “456” and “1456”. Smaller model is more parsimonious, but larger models fits slightly better.

# Criterion-Based Procedure: $R^2_{adj}$

- Now, let's check the model selection with $R^2_{adj}$.

```
> adjr <- leaps(x, y, method = "adjr2")
> maxadjr(adjr, 8)
    1,4,5,6   1,2,4,5,6   1,3,4,5,6   1,4,5,6,7 1,2,3,4,5,6 1,3,4,5,6,7
      0.713       0.706       0.706       0.706       0.699       0.699
1,2,4,5,6,7       4,5,6
      0.699       0.694
```

- Model with largest $R^2_{adj}$ is "1456".
- What about the best 3-predictor model ?
- Variable selection methods are sensitive to outliers, influential points, and transformations.

## Criterion-Based Procedure: Cross-Validation

- $PRESS$ = Predicted REsidual Sum of Squares (Leave-one-out cross-validated residuals):

$$PRESS = \sum_{i=1}^{n} \left(\hat{Y}_{-i} - Y_i\right)^2.$$

Use i-th obs to predict, use obs without i-th to fit

- $\hat{Y}_{-i}$ is the prediction for $i$-th observation, using a model fitted <u>without the $i$-th observation</u>.

- Cross-validation criterion estimates the mean-squared error of prediction as:

$$CV \equiv \frac{\sum_{i=1}^{n} \left(\hat{Y}_{-i} - Y_i\right)^2}{n} = \frac{PRESS}{n}$$

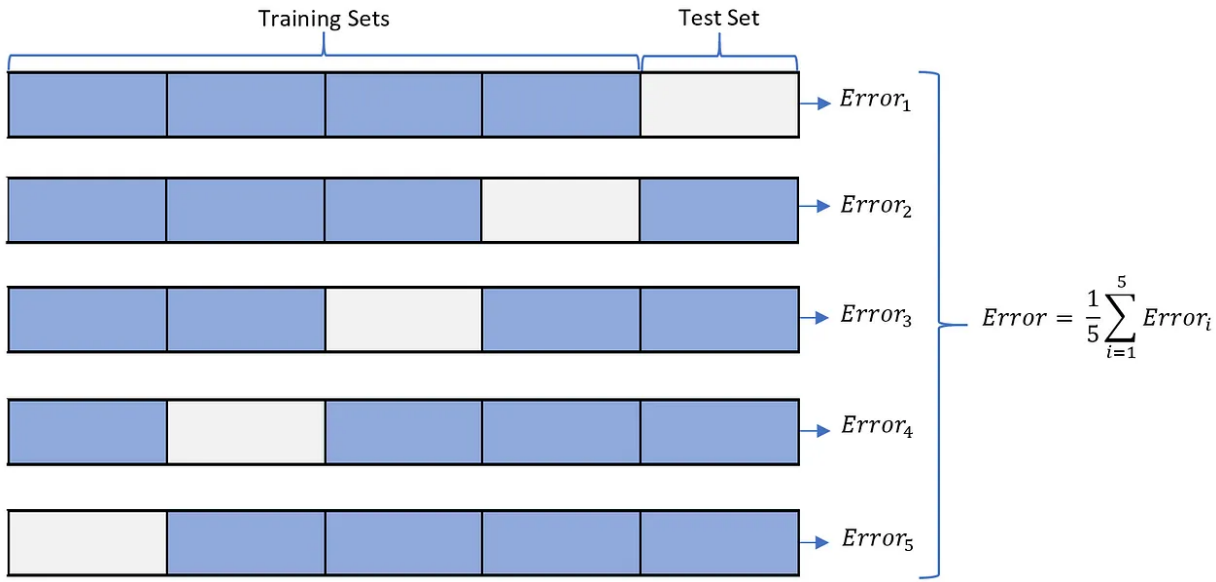
What is the drawback of LOOCV?

- We prefer the model with the smallest value of CV or PRESS.

# Criterion-Based Procedure: PRESS and Cross-Validation

- Alternative is $k$-fold cross validation:

  1. Divide the data into small number of subsets or folds (e.g., 5 or 10) of roughly equal size
  2. Fit a model omitting each subset in turn (i.e., use only the training data)
  3. Obtain the fitted values for all observations in omitted subset (i.e., the test data).



## Criterion-Based Procedure: *AIC* and *BIC*

- Penalized model-fit statistics:

$$-2\log L(\hat{\theta}) \; + \; penalty$$

  - $\theta$ is the vector of parameters of the model, including the regression coefficients and the error variance. Here, $\hat{\theta}$ is the m.l.e.
  - $L(\hat{\theta})$ is the maximized likelihood under current model.
  - $penalty \; \equiv \; c \times p$ ($c$ is a scaling parameter).

- The magnitude of a criterion is not interpretable, but differences are.
- Model with the smallest value of information criterion is preferred.

## Criterion-Based Procedure: *AIC* and *BIC*

- Most popular criteria are

$$AIC = -2\log L(\hat{\theta}) + 2p, \text{ thus } c = 2$$

$$BIC = -2\log L(\hat{\theta}) + p\log(n), \text{ thus } c = \log(n)$$

- When the sample size $n$ is small, there is a high chance that AIC will select models that have too many parameters (i.e., AIC will overfit). In this case, the corrected AIC can be used:

$$AICc = AIC + \frac{2p^2 + 2k}{n - k - 1}$$

# Example: Life expectancy dataset

```
> statreg <- lm(life.exp ~ ., data = statedata)
> stepres<-step(statreg, steps = 2)
Start:  AIC=-22.18
life.exp ~ population + income + illiteracy + murder + highSchoolGrad +
    frost + area

                 Df Sum of Sq    RSS     AIC
- area            1    0.0011 23.298 -24.182
- income          1    0.0044 23.302 -24.175
- illiteracy      1    0.0047 23.302 -24.174
<none>                         23.297 -22.185
- population      1    1.7472 25.044 -20.569
- frost           1    1.8466 25.144 -20.371
- highSchoolGrad  1    2.4413 25.738 -19.202
- murder          1   23.1411 46.438  10.305
```

What would be the AIC value, if the predictor is removed.

```
Step:  AIC=-24.18
life.exp ~ population + income + illiteracy + murder + highSchoolGrad +
    frost

                 Df Sum of Sq    RSS     AIC
- illiteracy      1    0.0038 23.302 -26.174
- income          1    0.0059 23.304 -26.170
<none>                         23.298 -24.182
- population      1    1.7599 25.058 -22.541
- frost           1    2.0488 25.347 -21.968
- highSchoolGrad  1    2.9804 26.279 -20.163
- murder          1   26.2721 49.570  11.569

Step:  AIC=-26.17
life.exp ~ population + income + murder + highSchoolGrad + frost
```

The variables are removed step-by-step, and AIC is checked at each step.

# Summary model selection

- Stepwise procedures:
  - Search through space of potential models.
  - Testing-based procedures use dubious hypothesis testing.
- Criterion-based procedures:
  - search through a wider space of models (“all possible subsets regression")
  - compare the models using a particular criterion.

- Criterion based procedures are usually preferred.

## Summary model selection

- The aim of variable selection is to construct a model that predicts well or explains relationships in data well.
- It is part of process of model building, like identification of outliers and in influential points, and variable transformation.
- Automatic selections are not guaranteed to be consistent. Use methods as guide only.

- Accept possibility that several models are suggested which fit equally well. Then consider:
  - Do models have similar qualitative consequences?
  - Do they make similar predictions?
  - What is cost of measuring predictors?
  - Which has best diagnostics?

# Model validation

- Model validation: split dataset into training subsample and validation subsample:
  - Training subsample is used to specify the statistical model.
  - Validation subsample is used to evaluate the fitted model.

- Cross-validation is an application of this idea where the roles of training and validation subsamples are interchanged.

- Statistical modeling: iterative sequence of data exploration, model fitting, model criticism, model re-specification.

- Variables may be dropped, interactions may be incorporated or deleted, variables may be transformed, unusual data may be corrected, removed, or otherwise accommodated.

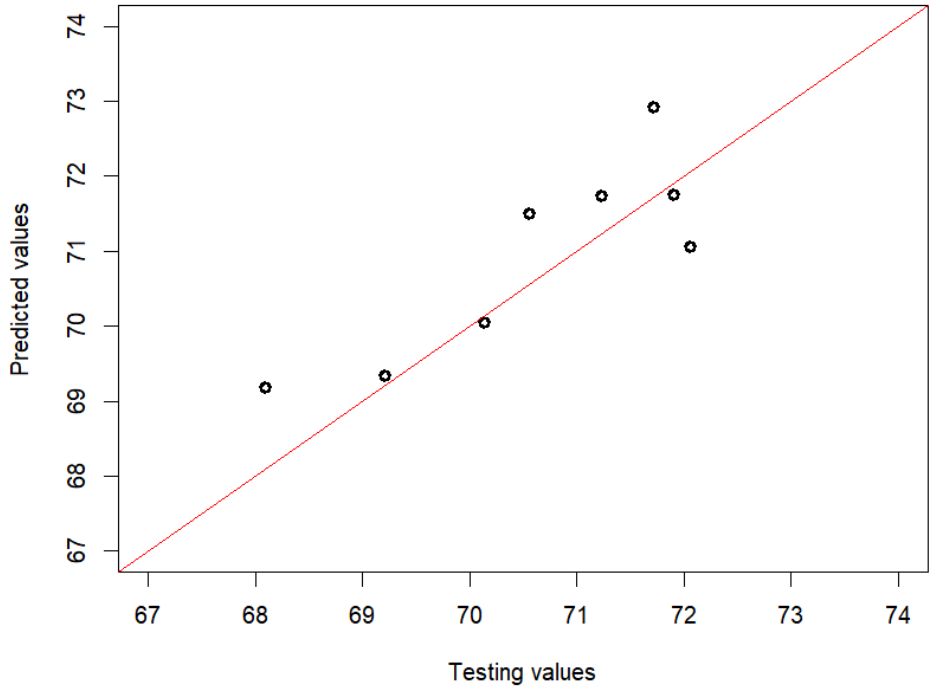
# Example: Model validation


```
> library(caret)
> set.seed(123)
> # creating training data as 80% of the dataset
> random_sample <- createDataPartition(statedata$life.exp, p = 0.8, list = FALSE)
> # training dataset from the random_sample
> training_dataset  <- statedata[random_sample, ]
> # testing dataset from rows which are not  included in random_sample
> testing_dataset <- statedata[-random_sample, ]
```

```
> # Building the model on the training data
> statereg <- lm(life.exp  ~., data = training_dataset)
> # predicting the target variable
> predictions <- predict(statereg, testing_dataset)
```

# Example: Model validation

```
> plot(predictions ~ testing_dataset$life.exp,
+      xlab="Testing values", ylab = "Predicted values",
+      lwd= 3, xlim = c(67, 74), ylim=c(67,74))
> abline(a=0, b=1, col="red")
```




- Evaluation is usually done using Pearson's correlation or Root mean squared error (RMSE) metrics. ??

```
> # computing model performance metrics
> (R2 <- R2(predictions, testing_dataset$life.exp))
[1] 0.720348
> (RMSE <- RMSE(predictions, testing_dataset$life.exp))
[1] 0.7794504
```

- Usually, several random partition is used.

# Model validation

- Resulting model should accurately reflect the principal characteristics of your data.
- Danger: overfitting and overstating strength of results.

- Ideal solution: collect new data with which to validate model (often not possible).

- Model validation simulates the collection of new data by randomly dividing data into two parts:
  - First, for exploration and model formulation,
  - second for checking adequacy of model, formal estimation, and testing.

## Collinearity

- If a perfect linear relationship among regressors exist, least-squares coefficient are no longer uniquely defined.
- Strong, but less-than-perfect linear relationship among $X$'s causes least-squares coefficients to be unstable:
  - large standard errors of coefficients,
  - broad confidence intervals,
  - hypothesis tests with low power.

## Collinearity and Remedies

- Small changes in data can greatly change the coefficients.
- Large changes in coefficients coincide with only very small changes in residual sum of squares.
- This is problem is known as collinearity or multicollinearity.
  - Collinearity is relatively rare problem in social-science applications of linear models.
  - Methods employed as remedies for collinearity may be worse than the disease.
  - Usually, it is impossible to redesign study to decrease correlations between $X$'s.

## Detecting Collinearity

- Suppose a perfect linear relationship exists between $X$'s:

$$c_1 X_{i1} + c_2 X_{i2} + \ldots + c_k X_{ik} = c_0.$$

- Then, the matrix $\mathbf{X}'\mathbf{X}$ is singular (why?),
- Therefore.
  - least squares normal equations do not have unique solution
  - sampling variances of regression coefficients are infinite.

- Perfect collinearity is often a product of some error in formulating linear model
  - e.g., too many dummies.

# Detecting Collinearity

- The sampling variance of the slope $B_j$ is

$$V(B_j) = \frac{1}{1 - R_j^2} \times \frac{\sigma_\epsilon^2}{(n-1)S_j^2}$$

Here, $R_j^2$ is the $R^2$ for regression of $X_j$ on other $X$'s .

$S_j^2$ is the sample variance of $X_j$.

- The first term is called Variance Inflation Factor:

$$VIF = \frac{1}{1 - R_j^2}$$

- $VIF$ indicates directly the impact of collinearity on precision of $B_j$.

- $VIF$ is a basic diagnostic for collinearity.

- A rule of thumb: $VIF$ is greater than 10 (very strong) or 5 (strong) (why these values?).

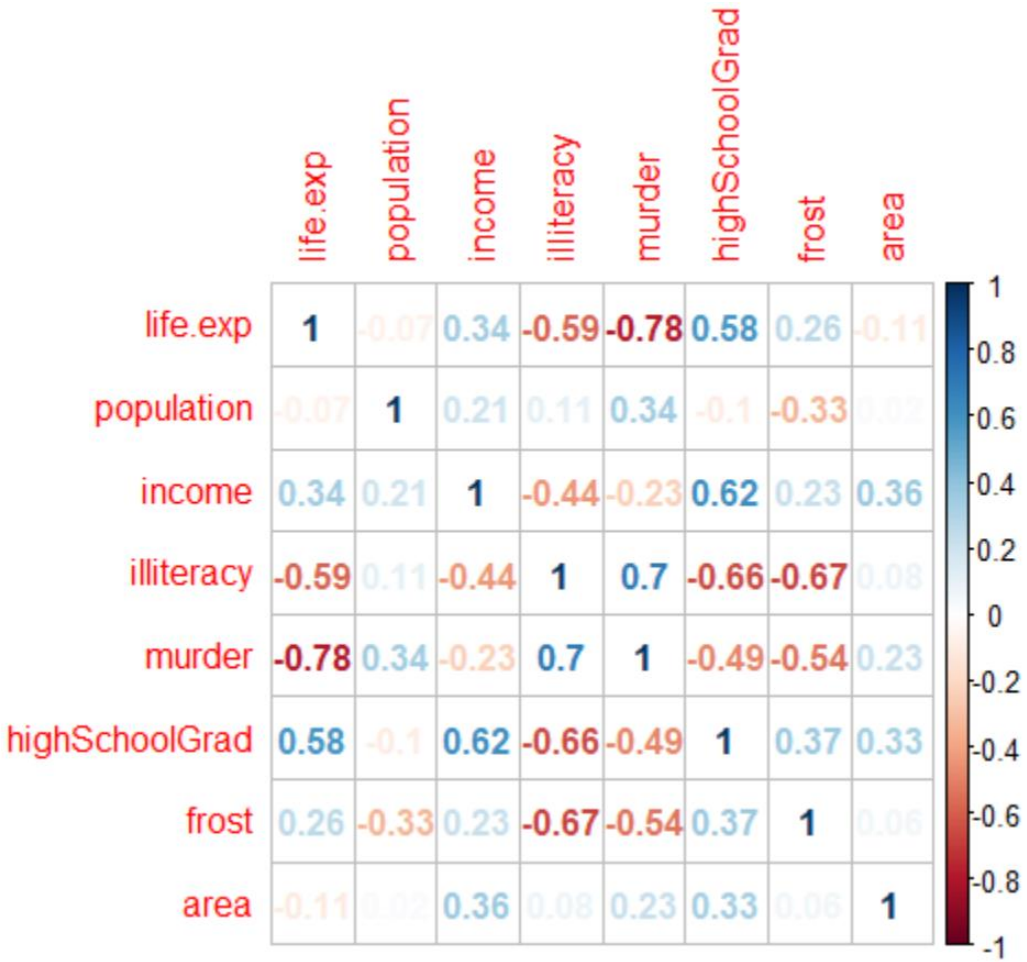
# Detecting Collinearity (Optional)

- Ways for detecting collinearity besides looking at the VIF's.
  - Examination of the correlation matrix of predictors:
  - Regress $X_i$ on all other $X$'s and repeat this for all predictors. $R_i^2$ close to one indicates the problem.
  - Examine the eigenvalues $\lambda_i$ of $\mathbf{X}'\mathbf{X}$: small eigenvalues indicate problem.
  - Large condition numbers $\kappa(\mathbf{X}'\mathbf{X}) = \sqrt{\lambda_1/\lambda_p}$ ($\kappa > 30$ is considered large).
  - Also check the values of condition index $\sqrt{\lambda_1/\lambda_i}$

# Detecting Collinearity: Example

```
> statreg <- lm(life.exp ~ ., data = statedata)
> vif(statreg)
    population         income     illiteracy
      1.499915       1.992680       4.403151
        murder highSchoolGrad          frost
      2.616472       3.134887       2.358206
          area
      1.789764
```

- What is your opinion?



# Collinearity: No Quick Fix

- Collinearity leads to
  - imprecise estimates of $\beta$; even the signs of coefficients may be misleading.
  - t-tests fail to reveal significant factors.
- Coping With Collinearity
  - Model re-specification.
  - Variable Selection.
  - Biased Estimation: e.g., Ridge Regression..
  - Prior Info About Regression Coefficients: e.g., Bayesian approaches.

# Geometric interpretation of collinearity (Optional)

- Imagine a table: as two diagonally opposite legs are moved closer together, the table becomes increasing
- no collinearity (a), complete collinearity (b) and strong collinearity