# Math 5305 Notes

## Diagnostics and Remedial Measures

Jesse Crawford

Department of Mathematics
Tarleton State University

# Model Assumptions

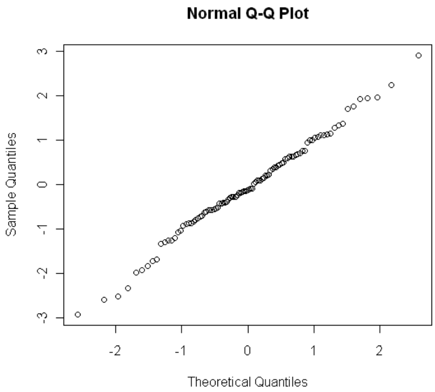
- $Y = X\beta + \epsilon$
- $p < n$ and $X$ has full rank.
- $\epsilon \perp\!\!\!\perp X$
- $\epsilon_1, \ldots, \epsilon_n$ are independent
- $E(\epsilon) = 0$
- $\text{Var}(\epsilon_i) = \sigma^2$ for all $i$
- $\epsilon_1, \ldots, \epsilon_n$ are normally distributed

# Outline

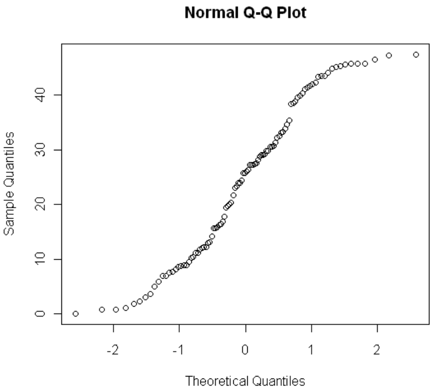
1. Error Term Assumptions
2. Transformations of $Y$
3. Functional Form
4. Model Building

# Normality of Errors Diagnostics

Quantile-Quantile Plot of residuals.




Normally Distributed Residuals



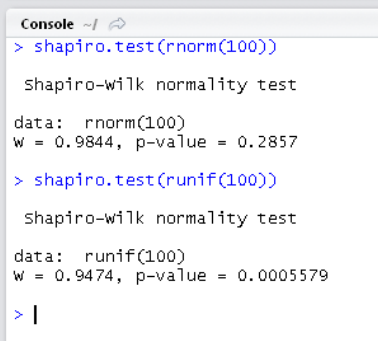

Uniformly Distributed Residuals

R Command: `qqnorm(e)`

# Normality of Errors Diagnostics

## Shapiro-Wilks Test on Residuals

- Null hypothesis is that the $\epsilon_i$'s are normally distributed.
- Command: `shapiro.test(e)`, where `e` is the vector of residuals.



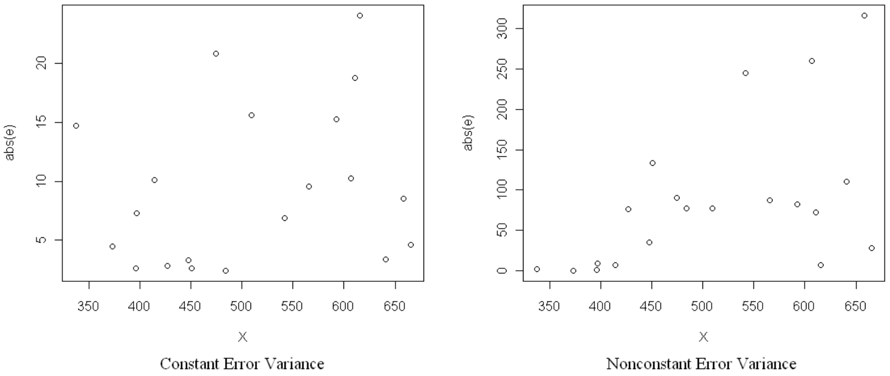
```
Console ~/
> shapiro.test(rnorm(100))

 Shapiro-Wilk normality test

data:  rnorm(100)
W = 0.9844, p-value = 0.2857

> shapiro.test(runif(100))

 Shapiro-Wilk normality test

data:  runif(100)
W = 0.9474, p-value = 0.0005579

> |
```

- Reject $H_0$ if *p*-value is less than $\alpha$.

# Normality of Errors Remedial Measures

- Transform $Y$

Plot $|e|$ vs. $\hat{Y}$ or $X_j$.



# Constancy of Error Variance Diagnostics

Brown-Forsythe Test

- The null hypothesis is $\text{Var}(\epsilon_1) = \cdots = \text{Var}(\epsilon_n) = \sigma^2$.
- Divide all observations into two groups based on whether $\hat{Y}$ (or $X_j$) is above or below a certain value.
- Define $e_{i1} =$ $i$th residual in group 1 and $e_{i2} =$ $i$th residual in group 2.
- Let $n_1$ and $n_2$ be the groups sizes, $n = n_1 + n_2$, and $\tilde{e}_1$ and $\tilde{e}_2$ be the medians of the residuals in each group.
- Define $d_{i1} = |e_{i1} - \tilde{e}_1|$ and $d_{i2} = |e_{i2} - \tilde{e}_2|$ for each $i$.
- Perform a two-sample $t$-test using the $d_{i1}$'s and $d_{i2}$'s.

# Constancy of Error Variance Diagnostics

Brown-Forsythe Test (cont)

- $$t = \frac{\overline{d}_1 - \overline{d}_2}{s_p\sqrt{\frac{1}{n_1} + \frac{1}{n_2}}}$$

- $$s_p^2 = \frac{\sum_{i=1}^{n_1}(d_{i1} - \overline{d}_1)^2 + \sum_{i=1}^{n_2}(d_{i2} - \overline{d}_2)^2}{n - 2}$$

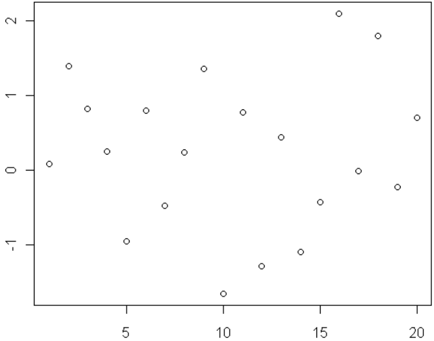
- Reject $H_0$ if $|t| > t_{\alpha/2}(n - 2)$.

# Constancy of Error Variance Remedial Measures

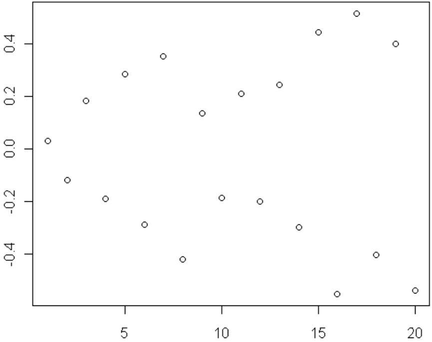
- Transform $Y$
- Use GLS

# Independence of Errors Diagnostics

- Were the data collected in time order?
- Durbin-Watson Test
- Sequence plot: plot $\epsilon_1, \ldots, \epsilon_n$ vs. $1, \ldots, n$.



No Auto Correlation



Autocorrelated Residuals

# Independence of Errors Remedial Measures

- If data were collected in time order, and the Durbin-Watson test/sequence plot show evidence of autocorrelation, use time series analysis.
- If there is a structural reason to believe the $\epsilon_i$'s are dependent, use GLS.

# Outline

# MLE for the OLS Model

## Theorem

- *Consider an OLS model* $Y = X\beta + \epsilon$.
- *Ch4 assumptions hold and* $\epsilon$ *is normally distributed.*
- *Then the maximum likelihood estimators for* $\beta$ *and* $\sigma^2$ *are*

$$\hat{\beta} = (X'X)^{-1}X'Y \text{ and}$$

$$\tilde{\sigma}^2 = \frac{1}{n}\|e\|^2.$$

- *If L is the likelihood function, then*

$$-2\ln(L(\hat{\beta}, \tilde{\sigma}^2)) = n\ln(2\pi) + n\ln(\|e\|^2) - n\ln(n) + n$$

- *For linear models with normal disturbance terms, maximizing likelihood is equivalent to minimizing residual sum of squares,* $\|e\|^2$.

# Transformations of $Y$

- Problem: error terms not normal or have nonconstant variance.
- Possible solution: transform $Y$
- Assuming values of $Y$ are **nonnegative**, possible transformations include

$$\tilde{Y}_i = \sqrt{Y_i}$$

$$\tilde{Y}_i = \ln Y_i$$

$$\tilde{Y}_i = \frac{1}{Y_i}$$

- We would then fit the model

$$\tilde{Y} = X\beta + \epsilon$$

# Box-Cox Transformations

- Assume $Y$ values are nonnegative. If not, add a constant to all $Y$ values.
- Given a power parameter $\lambda \in \mathbb{R}$, the Box-Cox transformation is

$$\tilde{Y} = \begin{cases} Y^{\lambda}, & \text{if } \lambda \neq 0 \\ \ln(Y), & \text{if } \lambda = 0 \end{cases}$$

- The model becomes

$$\tilde{Y} = X\beta + \epsilon$$

- $\lambda$ is estimated with maximum likelihood (least squares).

- Consider a range of values for $\lambda$, such as $-2, -1.9, -1.8, \ldots, 1.8, 1.9, 2.0$.
- For each value of $\lambda$ in this range, perform the following steps.
  - Standardize $Y$ as follows:

$$W_i = \begin{cases} K_1(Y_i^\lambda - 1), & \text{if } \lambda \neq 0 \\ K_2(\ln(Y_i)), & \text{if } \lambda = 0, \end{cases}$$

    where

$$K_2 = \left( \prod_{i=1}^{n} Y_i \right)^{\frac{1}{n}}$$

$$K_1 = \frac{1}{\lambda K_2^{\lambda - 1}}.$$

  - Fit the model $W = X\beta + \epsilon$ and compute $\|e\|^2$.
- The value of $\lambda$ leading to the smallest value of $\|e\|^2$ is the MLE.

# Outline

# Overall Measures of Fit

- $$R^2 = 1 - \frac{\|e\|^2}{\|Y - \overline{Y}\|^2}$$
- Adjusted $R^2$
$$R_a^2 = 1 - \frac{n-1}{n-p}\frac{\|e\|^2}{\|Y - \overline{Y}\|^2} = 1 - \frac{\hat{\sigma}^2}{\mathrm{Var}(Y)}$$
- Aikake Information Criterion
$$\mathrm{AIC} = 2p - 2\ln(L) = 2p + n\ln(2\pi) + n\ln(\|e\|^2) - n\ln(n) + n$$
- How R calculates AIC for linear models
$$2p + n\ln(\|e\|^2) - n\ln(n)$$

# Measures of Fit Based on Cross-validation

Leave One Out Cross-validation (LOOCV)

- For each $i = 1, \ldots, n$, fit a model based on the other observations $1, \ldots, i-1, i+1, \ldots, n$.
- Use this model to predict $Y_i$, and call this prediction $\hat{Y}_i$.
- Find the prediction sum of square errors (PRESS)

$$\text{PRESS} = \sum_{i=1}^{n} (Y_i - \hat{Y}_i)^2.$$

# Measures of Fit Based on Cross-validation

Delete-*d* Cross-validation

- Choose an integer $d$ between 1 and $n$. A value that has been suggested by Shao (1997) is

$$d = n(1 - (\ln(n) - 1)^{-1}).$$

- Repeat the following process a large number (say 1000) times:
  - Randomly select $d$ rows of the data and remove them.
  - Fit a model to the remaining $n - d$ rows.
  - Use this model to predict the values of $Y_i$ for the removed rows.
  - Find the prediction sum of square errors

$$\text{PRESS} = \sum_{\text{Removed Rows}} (Y_i - \hat{Y}_i)^2.$$

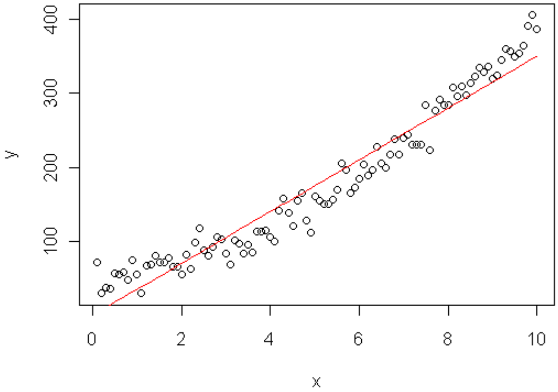
- Finally, average all of these PRESS values to find a single overall PRESS value.

# Diagnostics and Remedial Measures for Curvature

- Diagnostics
  - Plot $Y$ vs. $X_j$
  - Plot $e$ vs. $\hat{Y}$ or $X_j$
  - Compare original model to a model with higher order terms using an $F$-test or using overall measures of fit.
- Remedial Measures
  - Transform $X_j$ or add higher order terms.

# Example Involving Curvature

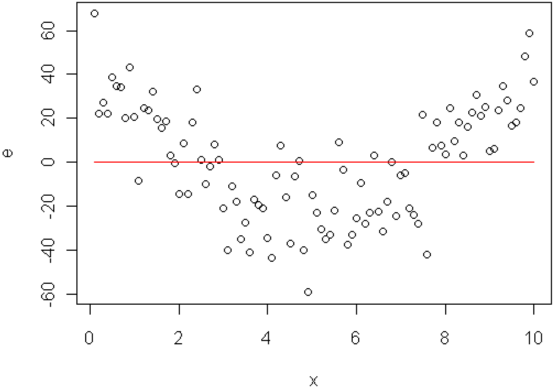
- Scatterplot of $Y$ vs. $X$




- Do we need higher order terms?

# Example Involving Curvature

- Scatterplot of *e* vs. *X*

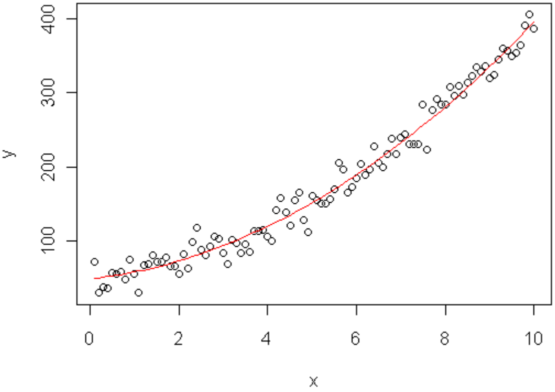



- Trend in residual plot indicates functional form is wrong.

# Example Involving Curvature

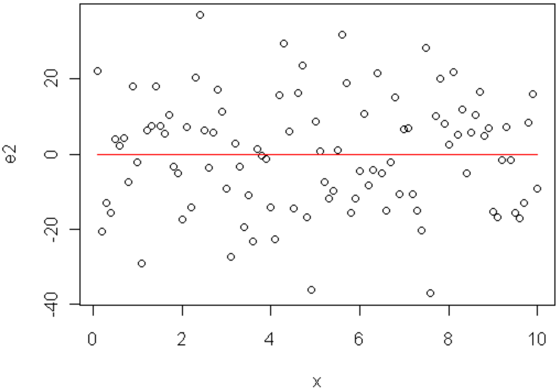
- Fitting quadratic model

$$Y_i = \beta_1 + \beta_2 X_i + \beta_3 X_i^2 + \epsilon_i$$



# Example Involving Curvature

- Scatterplot of *e* vs. *X* for quadratic model




- Lack of trend in residual plot indicates functional form is right.

# Two Models

- True Model:

$$Y_i = 50 + 5X_i + 3X_i^2 + \epsilon_i$$

- Model 1:

$$Y_i = \beta_1 + \beta_2 X_i + \epsilon_i$$

- Model 2:

$$Y_i = \beta_1 + \beta_2 X_i + \beta_3 X_i^2 + \epsilon_i$$

# Two Models

- True Model:

$$Y_i = 50 + 5X_i + 3X_i^2 + \epsilon_i$$

```
Call:
lm(formula = y ~ x)

Residuals:
    Min      1Q  Median      3Q     Max 
-59.411 -21.309   0.998  20.750  67.615 

Coefficients:
            Estimate Std. Error t value Pr(>|t|)    
(Intercept)   0.7928     5.2482   0.151     0.88    
x            34.8783     0.9022  38.657   <2e-16 ***
---
```

Model 1

```
Call:
lm(formula = y ~ x + I(x^2))

Residuals:
     Min       1Q   Median       3Q      Max 
-37.0814 -11.7763   0.8271   9.0966  36.9520 

Coefficients:
            Estimate Std. Error t value Pr(>|t|)    
(Intercept)  49.2248     4.6405  10.608  < 2e-16 ***
x             6.3889     2.1208   3.012  0.00331 ** 
I(x^2)        2.8207     0.2034  13.865  < 2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.
```

Model 2

# Comparing the Models with an $F$-test

- Model 1:
$$Y_i = \beta_1 + \beta_2 X_i + \epsilon_i$$
- Model 2:
$$Y_i = \beta_1 + \beta_2 X_i + \beta_3 X_i^2 + \epsilon_i$$
- $$\texttt{ftest(model1,model2)} = 9.59 \times 10^{-25}$$
- So, we reject Model 1 in favor of Model 2.

# Comparing the Models with Measures of Overall Fit

- $R^2$ (higher is better)
  - Model 1: 0.9385
  - Model 2: 0.9794
- Adjusted $R^2$ (higher is better)
  - Model 1: 0.9378
  - Model 2: 0.9789
- AIC (lower is better)
  - Model 1: 653.94
  - Model 2: 546.67
- Leave One Out PRESS (lower is better)
  - Model 1: 69572.47
  - Model 2: 23633.27
- SSE ($\|e\|^2$)
  - Model 1: 66474.03
  - Model 2: 22293.14

# Interaction Terms

- Consider the regression model

$$Y_i = \beta_1 X_{i1} + \cdots + \beta_p X_{ip} + \epsilon_i$$

- An *interaction term* is a term of the form

$$\beta_{j_1 j_2} X_{ij_1} X_{ij_2}$$

## Example

- Consider the regression model

$$\text{BloodPressure}_i = \beta_0 + \beta_1 \text{Gender}_i + \beta_2 \text{Cholesterol}_i + \epsilon_i$$

- Here is the same model with an added interaction term for Gender and Cholesterol

$$\begin{aligned}\text{BloodPressure}_i =& \beta_0 + \beta_1 \text{Gender}_i + \beta_2 \text{Cholesterol}_i \\ &+ \beta_{12} \text{Gender}_i \text{Cholesterol}_i + \epsilon_i\end{aligned}$$

# Diagnostics and Remedial Measures for Interactions

- Diagnostics
  - Plot $e$ vs. interaction term.
  - Compare original model to a model with the interaction term using an $F$-test or using overall measures of fit.
- Remedial Measures
  - Include the interaction term if necessary.

# Outline

# General Guidelines

- Data should be screened for errors.
- Rule of thumb: Sample size should be about 6 to 10 times as large as the number of variables in the pool of potential variables.
- Variables may need to be eliminated if they
  - are not clinically relevant
  - have large measurement errors
  - duplicate other variables
- Clinical considerations should be taken into account. Subject matter experts should be consulted.

# Model Building Overview

- Data cleaning/checking
- Split Data into a training sample and a validation sample (this step is not necessary if it is possible to generate new data).
  - Univariate Analyses
    - Quantitative variables can be checked for curvature.
    - Appropriate categories can be considered for categorical variables.
  - Variable Selection
  - Diagnostics and Remedial Measures
- Model Validation: Can be done by comparing model to
  - New data
  - Data from the validation sample

# Variable Selection Methods

- Manually
- Stepwise Method

```
d=data.frame(Y=Y,X=X)
bigmodel=lm(Y~.,data=d)
stepmodel=step(bigmodel)
```

- Best Subsets Method

```
library(bestglm)
Xy=as.data.frame(cbind(x1,x2,x3,x4,x5,x6,Y))
bestglm(Xy,family=gaussian,IC="AIC")
bestglm(Xy,family=gaussian,IC="CV",t=10)
```

- Combination: Use stepwise to narrow the list of variables and then apply best subsets to the remaining variables.

# Model Validation

- Models are validated by assessing their performance on a new data set.
- The new data set can actually be newly collected data or can be the validation sample that was set aside at the beginning of model building.
- Diagnostics should be used to determine if the fitted model is consistent with the new data.
- The Mean Squared Prediction Error (MSPR) should be determined
  - Let $Y_i$, $i = 1, \ldots, n^\star$ be the new data set.
  - For each $i$, use the model fitted to the training to data to predict $Y_i$.
  - Call the predicted value $\hat{Y}_i$.
  - The MSPR is

$$MSPR = \frac{\sum_{i=1}^{n^\star}(Y_i - \hat{Y}_i)^2}{n^\star}.$$

# Example with Stepwise/Best Subsets Methods

```
X=matrix(runif(5000),100,50)

X0=cbind(rep(1,100),X[,1:3])
beta=c(50,5,10,30)
epsilon=rnorm(100,0,1)
Y=X0%*%beta+epsilon
```

True Model:

$$Y_i = 50 + 5X_{i1} + 10X_{i2} + 30X_{i3} + \epsilon_i, \text{ for } i = 1, \ldots, 100.$$

Variables $X_{i4}, \ldots, X_{i50}$ are just noise.

True Model:

$$Y_i = 50 + 5X_{i1} + 10X_{i2} + 30X_{i3} + \epsilon_i, \text{ for } i = 1, \ldots, 100.$$

```
x1=X0[,2]
x2=X0[,3]
x3=X0[,4]

model=lm(Y~x1+x2+x3)
summary(model)
```

```
Coefficients:
            Estimate Std. Error t value Pr(>|t|)    
(Intercept)  50.2288     0.3242  154.95   <2e-16 ***
x1            4.1198     0.3828   10.76   <2e-16 ***
x2            9.9273     0.3749   26.48   <2e-16 ***
x3           30.2708     0.3708   81.63   <2e-16 ***
```

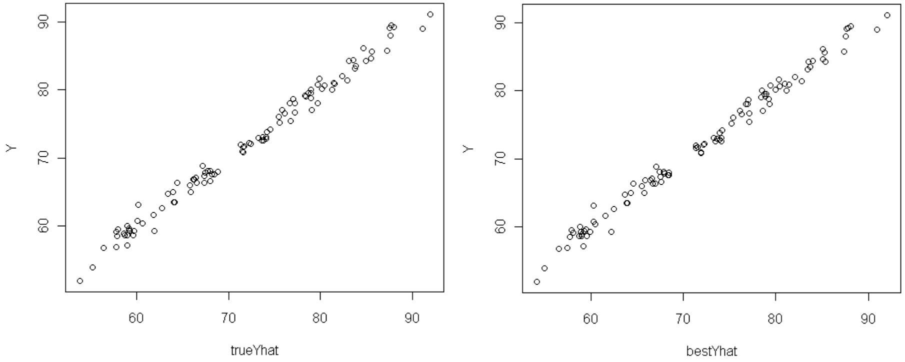
```
d=data.frame(Y=Y,X=X)
bigmodel=lm(Y~.,data=d)

stepmodel=step(bigmodel)
summary(stepmodel)
```

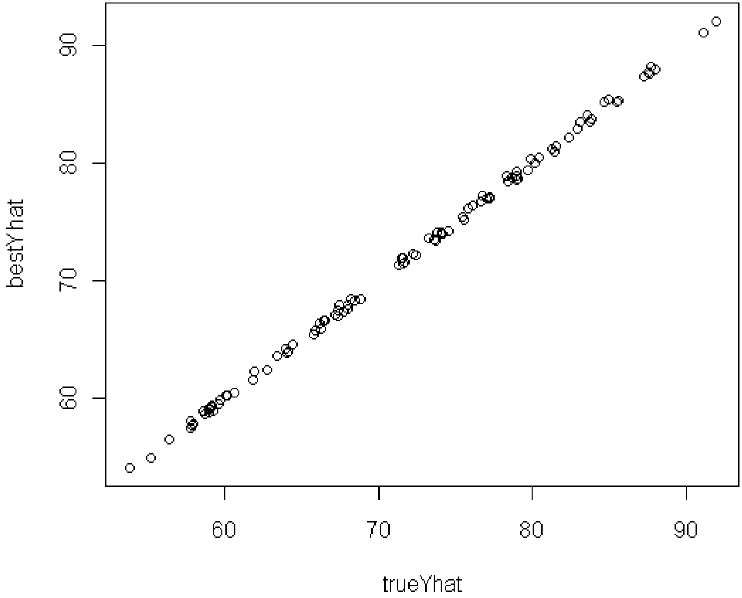
```
Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  47.6880     0.8455  56.404  < 2e-16 ***
X.1           3.8129     0.3426  11.129  < 2e-16 ***
X.2          10.1911     0.3503  29.095  < 2e-16 ***
X.3          30.6207     0.3688  83.021  < 2e-16 ***
X.4           0.6246     0.3961   1.577  0.11891
X.6           0.7788     0.3333   2.337  0.02203 *
X.14          0.6239     0.3617   1.725  0.08848 .
X.15          0.9363     0.3304   2.834  0.00584 **
X.16         -0.5682     0.3289  -1.727  0.08807 .
X.21         -0.6973     0.3601  -1.936  0.05644 .
X.23          0.6019     0.3580   1.681  0.09671 .
X.27          0.4442     0.3254   1.365  0.17614
X.28         -0.6381     0.3559  -1.793  0.07684 .
X.30          0.9224     0.3210   2.874  0.00522 **
X.35         -0.8150     0.3805  -2.142  0.03532 *
X.37          0.9491     0.3569   2.659  0.00949 **
X.41          0.9769     0.3812   2.563  0.01231 *
X.42          0.9704     0.3344   2.902  0.00481 **
X.43         -1.0106     0.3639  -2.777  0.00686 **
X.47         -0.4945     0.3286  -1.505  0.13642
X.48          0.5735     0.3797   1.511  0.13496
X.50          0.6709     0.3698   1.814  0.07352 .
```

```
Xy=as.data.frame(cbind(X[,c(1,2,3,4,6,14,15,16,21,23,2
                                42,43,47,48,50)],Y))

bestmodel=bestglm(Xy,IC="CV",family=gaussian,t=10)
summary(bestmodel$BestModel)
```

```
Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  49.7149     0.3706 134.153   <2e-16 ***
V1            4.0777     0.3719  10.963   <2e-16 ***
V2            9.8833     0.3643  27.128   <2e-16 ***
V3           30.4825     0.3689  82.634   <2e-16 ***
V15           0.9209     0.3508   2.625   0.0101 *
```

```
truemodel=lm(Y~x1+x2+x3)
trueYhat=predict(truemodel)

bestYhat=predict(bestmodel$BestModel)
```




bestYhat
trueYhat
60
70
80
90
60
70
80
90

# Additional Reading

Kutner et. al. (2005). *Applied Linear Statistical Models, 5th ed.* McGraw-Hill/Irwin, New York, N.Y.