Lecture 13: Regression Diagnostics II

Ailin Zhang

2023-06-13

Week 6 - 8 Plans

- Week 6: Lec 13, 14 (in person); Lec 15 (online)
- Week 7 (Dragon Boat Festival): Lec 16 (+quiz), Lec 17 (Scope of Midterm)
- Week 8: Tue (RC by TA), Lec 18 (online), Midterm on Friday
- Distribute project guidlines after the midterm

Recap: Regression Diagnostics

- Regression diagnostics are used after fitting to check if a fitted mean function ($E(Y|X)$) and assumptions are consistent with observed data.
- To fit a model with least square estimates and perform statistical analysis rely on the regression assumptions:
    - Assumptions about the model form
        - The relationship between the response (Y) and the predictors ($X_1, \dots, X_p$) is linear
    - Assumptions about the errors
        - The errors are independent, with mean zero and constant variance. The errors can be normally distributed (optional)
    - Assumptions about the predictors
        - The predictors are non-random, measured without error, and linearly independent
    - Assumptions about the observations
        - All observations are equally reliable and have an approximately equal role in determining the regression results and in influencing conclusions

Recap: Leverage

$\hat{Y} = X\hat{\beta} = X(X^TX)^{-1}X^TY = HY$ (where H is called the hat matrix or the projection matrix)

- Recall in SLR, we can solve H analytically:

$$h_{ij} = \frac{1}{n} + \frac{(x_i - \bar{x})(x_j - \bar{x})}{\sum\limits_{k=1}^{n}(x_k - \bar{x})^2}$$

And the leverage in SLR is given by

$$h_{ii} = \frac{1}{n} + \frac{(x_i - \bar{x})^2}{\sum\limits_{k=1}^{n}(x_k - \bar{x})^2}$$

Recap: Leverage

- If the leverage of i-th observation, h_{ii}, is large (close to 1), then this i-th observation is called a leverage point. It means the prediction of $\hat{y}_i$ depends a lot on the observation y_i itself and relatively less on other observations.

Other properties:

1. $\frac{1}{n} \leq h_{ii} \leq 1$
2. $\sum h_{ii} = p + 1$
3. Thus, on average, $h_{ii} \approx (p+1)/n$

   We can look for values far from this as rough screen for high leverage points.

Recap: Three Types of Residuals

- The raw residual of the i-th observation is defined to be

$$e_i = y_i - \hat{y}_i = \text{observed } y_i - \text{predicted } y_i$$

  We call this as (raw) residuals.

- Standardized residual or internally studentized residuals:

$$r_i = \frac{e_i}{\hat{\sigma}\sqrt{1-h_{ii}}}$$

- Externally studentized residuals or studentized residuals are defined as:

$$r_i^* = \frac{e_i}{\hat{\sigma}_{(i)}\sqrt{1-h_{ii}}}$$

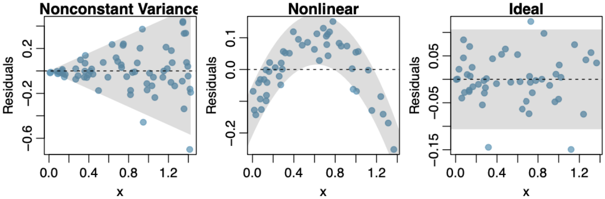
Recap: Comparisons of 3 Types of Residuals

- e_i's add up to 0, r_i's and r_i^*'s do not add up to 0
- e_i's have unequal variance, r_i's and r_i^*'s have variance 1
- r_i^*'s has a t-distribution with df=n-p-2, but r_i does not have a t-distribution.
- With a large enough sample, r_i's and r_i^*'s are approximately $N(0, 1)$
- None of the 3 types of residuals are strictly independent, but the dependence can be ignored with large enough samples

Recap: Various Kinds of Residual Plots

- Residuals v.s. fitted values
- Residuals v.s. each predictor
- Residuals v.s. potential predictors not yet included in the model
- Residuals v.s. several predictors using `ggplot()`
- Residuals v.s. time if the data are collected over time
- Residuals v.s. . . .

In all the plots above, points should scatter evenly above and below the zero line in a band of constant width.



Agenda

- Revisit Regression Assumptions
- Leverage
- Types of Residuals
- Residual Plots
- Graphical Methods (Today)
- Influential Points and Outliers
- Measure of Influence

Checking Assumptions with Graphs

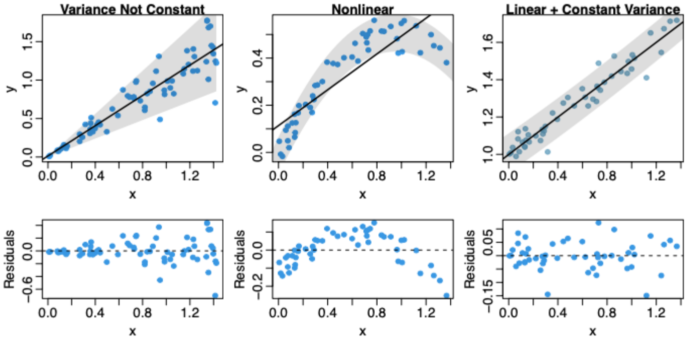
Graphs are useful to: - Detect errors in the data - Recognize patterns in the data (e.g., clusters, outliers, gaps, etc.) - Explore relationships among variables - Discover new phenomena - Confirm or negate assumptions - Assess the adequacy of a fitted model - Suggest remedial actions (e.g., transform the data, redesign the experiment, collect more data, etc.) - Enhance numerical analysis in general

Checking Assumptions for SLR Using Graphs

For SLR, one can plot

Y against X, Residuals against X, or Residuals against Y

and spot problems (nonlinearity, nonconstant variability, outliers)



Checking Assumptions for MLR Using Graphs

For MLR, it is more difficult to check whether the linear form $Y = \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p$ is correctly specified.

We need to check the following:

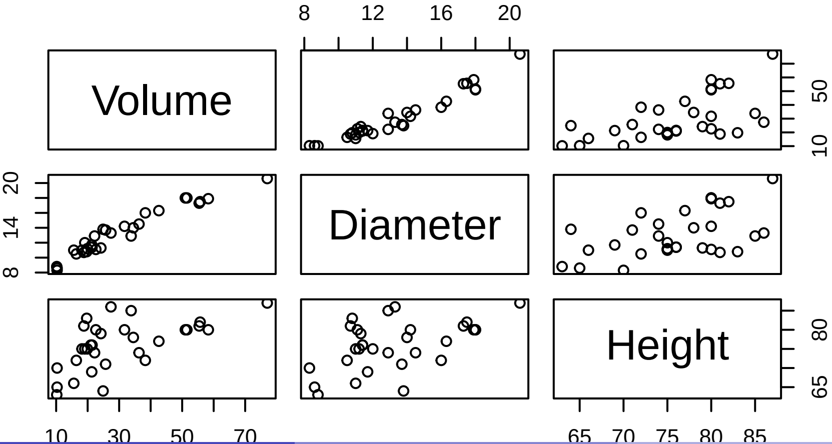
- Is Y is linear X_j given other X_k's?
- Do we miss any important predictor, any interactions?
- Does each X_i have linear effect on Y given other predictors?

Tools:

- Pairwise scatterplots = Scatterplot Matrix
- Multi-panel scatterplots using `facet` feature in ggplot
- Plotting residuals against each predictors and potential predictors not in the model
- Normal probability plot
- Added variable plots
- Residual plus component plots

Pairwise Scatterplots

```r
data("trees")
colnames(trees) = c("Diameter", "Height", "Volume")
pairs(Volume ~ Diameter + Height, data=trees)
```

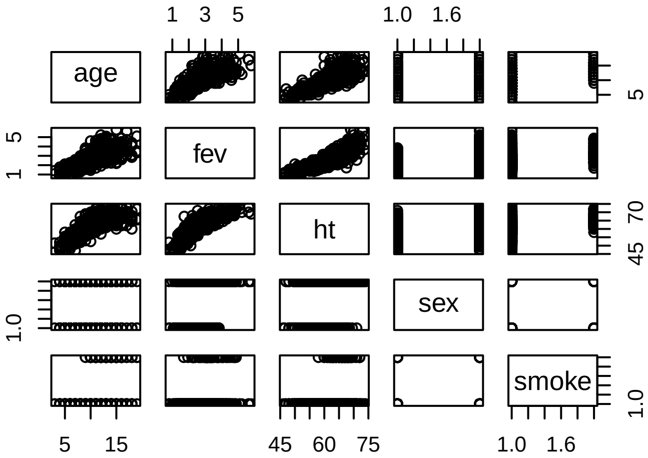


Pairwise Scatterplots

- Explore the relationships between each pair of variables and to identify general patterns
- Pairwise scatterplots only allow us the inspect the relations between variables pairwisely, but not 3 or more variables at the same time.
- When there are many predictors, people usually pick the ones with large correlation between the response to begin with.

Pairwise Scatterplots?

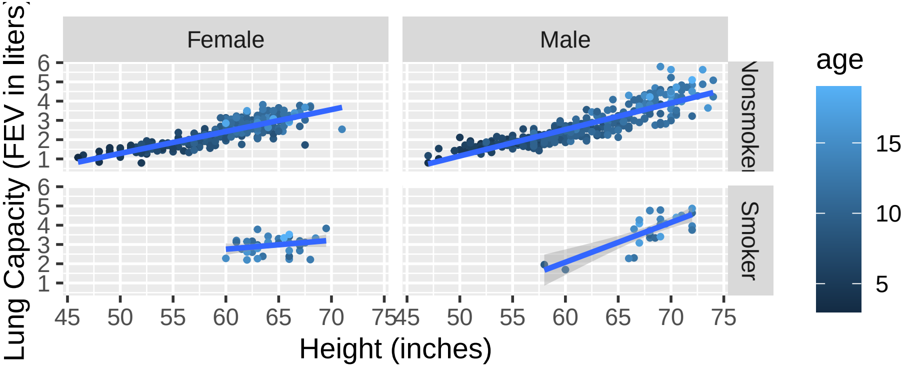
```
fevdata = read.table("fevdata.txt", header=TRUE)
fevdata$sex = factor(fevdata$sex, labels=c("Female","Male"))
fevdata$smoke = factor(fevdata$smoke, labels=c("Nonsmoker","Smoker"))
pairs(fevdata, oma = c(2,2,2,2))
```



Multi-panel scatterplots

```r
library(ggplot2)
ggplot(fevdata, aes(x = ht, y = fev, color=age)) +
geom_point(cex=0.7) + facet_grid(smoke~sex) + geom_smooth(method='lm') +
labs(x="Height (inches)", y="Lung Capacity (FEV in liters)")
```

```
## `geom_smooth()` using formula 'y ~ x'
```

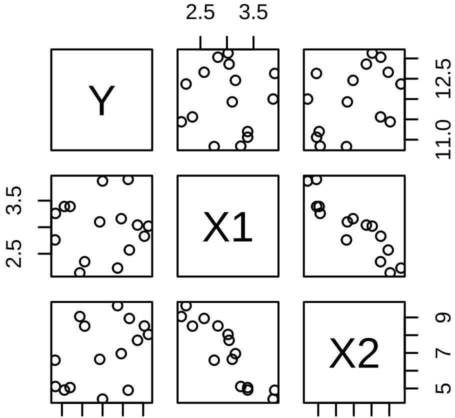


Multi-panel scatterplots with ggplot

- ggplot are more useful in inspecting the relations between 3 or more variables as the the plot on the previous page
- In multiple regression, the scatter plots of Y versus each predictor variable may or may not show linear patterns. Where the presence of a linear pattern is reassuring, the absence of such a pattern does not imply that our linear model is incorrect.

Hamilton's Data (Regression Analysis By Example page 103)

```r
hamilton = read.table("hamilton.txt", h = T)
pairs(hamilton, oma=c(2,2,2,2))
```



Hamilton's Data

```
summary(lm(Y ~ X1, data=hamilton))$coef
```

```
##                Estimate Std. Error     t value     Pr(>|t|)
## (Intercept) 11.988755072  1.2668907 9.463132626 3.399903e-07
## X1           0.003747477  0.4160825 0.009006571 9.929506e-01
```

```
summary(lm(Y ~ X1, data=hamilton))$r.squared
```

```
## [1] 6.239832e-06
```

```
summary(lm(Y ~ X2, data=hamilton))$coef
```

```
##               Estimate Std. Error   t value     Pr(>|t|)
## (Intercept) 10.6319366  0.8109425 13.110593 7.178282e-09
## X2           0.1954562  0.1125087  1.737254 1.059593e-01
```

```
summary(lm(Y ~ X2, data=hamilton))$r.squared
```

```
## [1] 0.1884157
```

When X1 or X2 is the only predictor, neither of them is significant

Hamilton's Data

```
summary(lm(Y ~ X1+X2, data=hamilton))$coef
```

```
##               Estimate  Std. Error   t value     Pr(>|t|)
## (Intercept) -4.515414 0.061141807 -73.85149 2.527961e-17
## X1           3.097008 0.012274433 252.31373 1.010771e-23
## X2           1.031859 0.003684173 280.07891 2.888447e-24
```

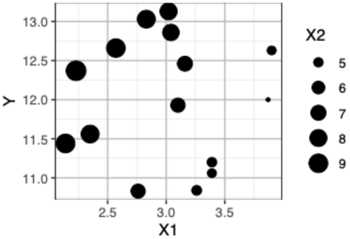
```
summary(lm(Y ~ X1+X2, data=hamilton))$r.squared
```

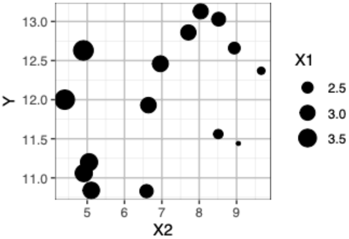
```
## [1] 0.999847
```

X1 and X2 become highly significant when both are included

ggplots Can Show X2 Effect on Y After Accounting For X1

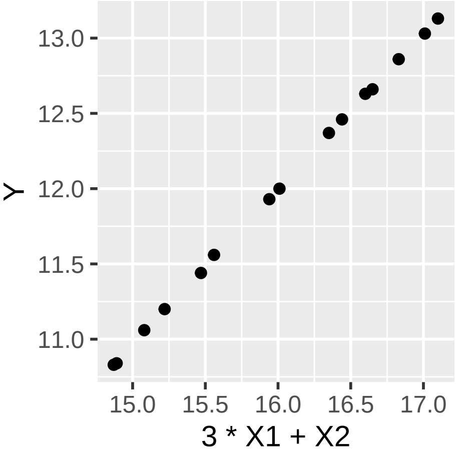
```
ggplot(hamilton, aes(x = X1, y = Y, size=X2)) + geom_point()
ggplot(hamilton, aes(x = X2, y = Y, size=X1)) + geom_point()
```





- For points with similar X1, points with larger size (higher values of X2) have larger Y values. Hence we can see X2has an effect on Y after accounting for X1.
- Recall β_2 is the effect of X2 on Y when X1 is hold constant.

```
ggplot(hamilton, aes(x = 3*X1+X2, y = Y)) + geom_point()
```



In fact, Y and `3*X1+X2` are highly correlated.

Check Interactions of Two Numerical Variables

The model

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \epsilon$$

No interaction assumes that

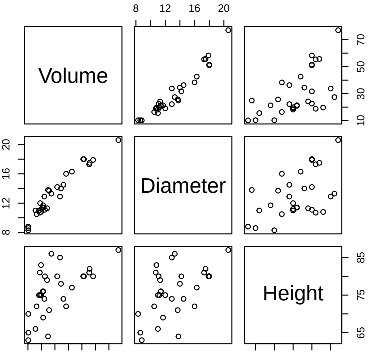
- Y is linear in X_1 for each given X_2 and the slope of X_1 doesn't change with X_2
- Y is linear in X_2 for each given X_1 and the slope of X_2 doesn't change with X_1

Revist the trees data

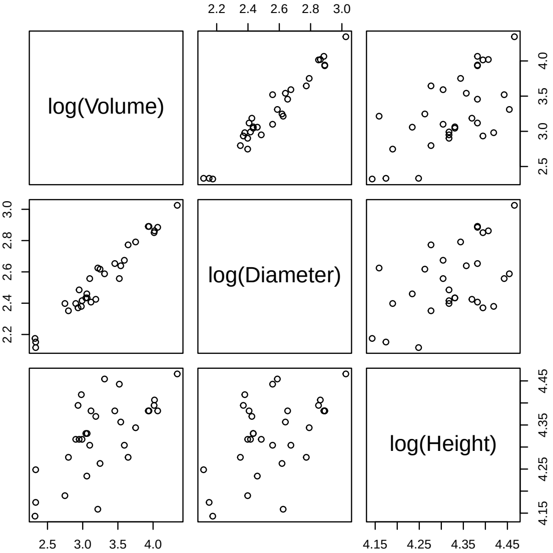
Recall the trees data are measurements of the diameter, height and volume of timber in 31 felled black cherry trees. The variables are

- Girth: Tree diameter in inches measured at 4 ft 6 in above the ground
- Height: Height in ft
- Volume: Volume of timber in cubic ft

```r
data("trees")
trees$Diameter = trees$Girth
pairs(Volume ~ Diameter + Height, data=trees, oma = c(2,2,2,2))
```



```r
pairs(log(Volume) ~ log(Diameter) + log(Height),
      data=trees, oma = c(2,2,2,2))
```



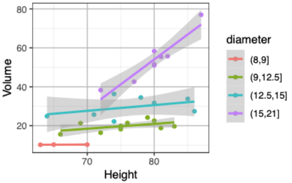
Model Comparison

From the pairwise scatter plots above, the two models below don't seem to differ too much.

- The model $V = \beta_0 + \beta_1 D + \beta_2 H + \epsilon$ implies the slope of H stay the same for each level of D.

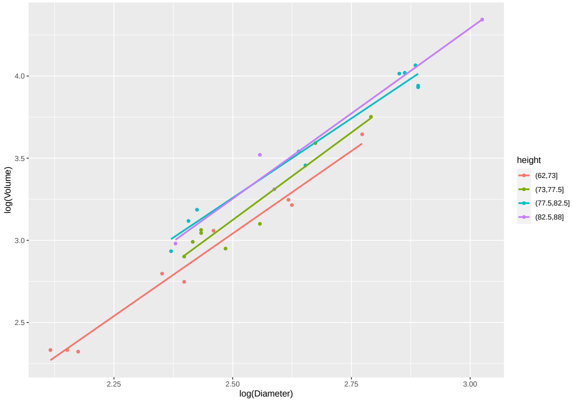
```
trees$diameter = cut(trees$Diameter, breaks=c(8,9,12.5,15,21))

ggplot(trees, aes(x=Height, y=Volume, color=diameter)) +
  geom_point() + geom_smooth(method='lm', formula='y~x')
```



Observe the slopes of Height increases as Diameter increases, which means the model $V = \beta_0 + \beta_1 D + \beta_2 H + \epsilon$ isn't appropriate.

```
trees$height = cut(trees$Height, breaks=c(62,73,77.5,82.5,88))
ggplot(trees, aes(x=log(Diameter), y=log(Volume), color=height
```



The model $\log(V) = \beta_0 + \beta_1 \log(D) + \beta_2 \log(H) + \epsilon$

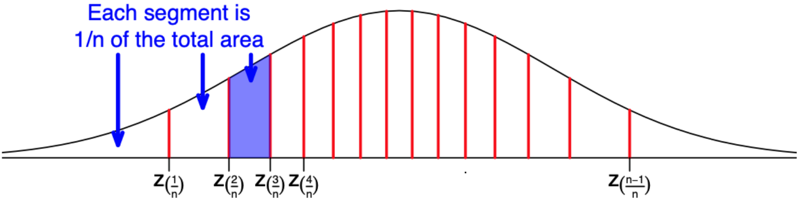
is more appropriate since the slopes of `log(Height)` don't change with Diameter as much as before the log-transformation

Normal Probability Plot

- Histogram of the residuals: if normal, should be bell-shaped
  - Pros: simple, easy to understand
  - Cons: for a small sample, histogram may not be bell-shaped even though the sample is from a normal distribution
- Normal probability plot of the residuals
  - also called normal QQ plot, QQ stands for "quantile-quantile"
  - best tool to assess normality

Theory of Normal Probability Plot

- Data: $y_1, y_2, \dots, y_n$
- Sorted Data: $y_{(1)} \le y_{(2)} \le \cdots \le y_{(n)}$, which are called the sample Quantiles
- Theoretical Quantiles of the $N(0,1)$: $z_{(1/n)}, z_{(2/n)}, \dots, z_{(n-1)/n}$ where, $z_{(k/n)}$ is a value such that $P(Z \le z_{(k/n)}) = k/n$ for $Z \sim N(0,1)$.


Each segment is
1/n of the total area
$\mathbf{z}_{(\frac{1}{n})}$
$\mathbf{z}_{(\frac{2}{n})}$
$\mathbf{z}_{(\frac{3}{n})}$
$\mathbf{z}_{(\frac{4}{n})}$
$\mathbf{z}_{(\frac{n-1}{n})}$

Theory of Normal Probability Plot

- If $Y \sim N(\mu, \sigma^2)$ and we observed $Y_1, Y_2, \ldots, Y_n$
- We expected k/n of the observations to be $\leq \mu + \sigma z_{(k/n)}$
- If the data are indeed $N(\mu, \sigma^2)$, we will expect that

$$y_{(k)} \approx \mu + \sigma z_{(k/n)}$$

- If one plots the Sample Quantiles $y = \{y_{(k)}\}$ against the Theoretical Quantiles $z = \{z_{(k/n)}\}$, points would fall on the straight line:

$$y = \mu + \sigma z$$

A Technical Remark

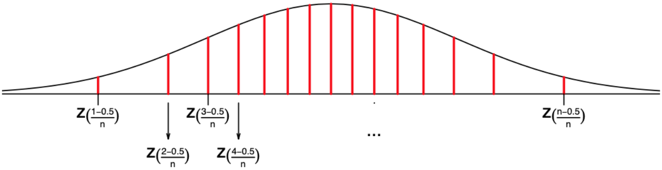
R actually uses the Theoretical Quantiles:

$$z_{\frac{1-0.5}{n}}, z_{\frac{2-0.5}{n}}, \ldots, z_{\frac{n-0.5}{n}}$$

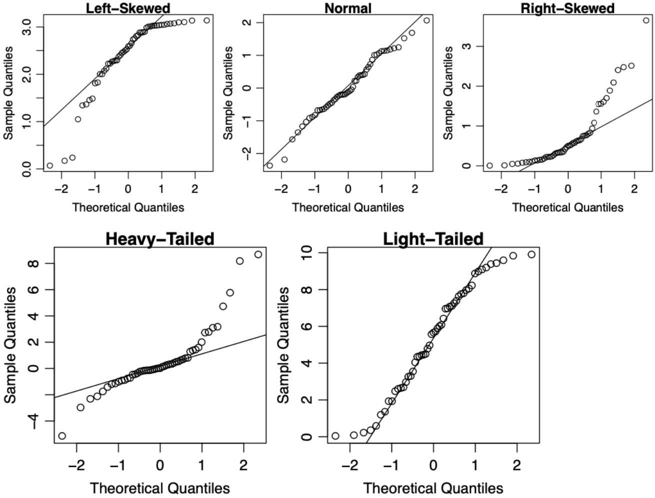
instead of

$$z_{\frac{1}{n}}, z_{\frac{2}{n}}, \ldots, z_{\frac{n}{n}}$$

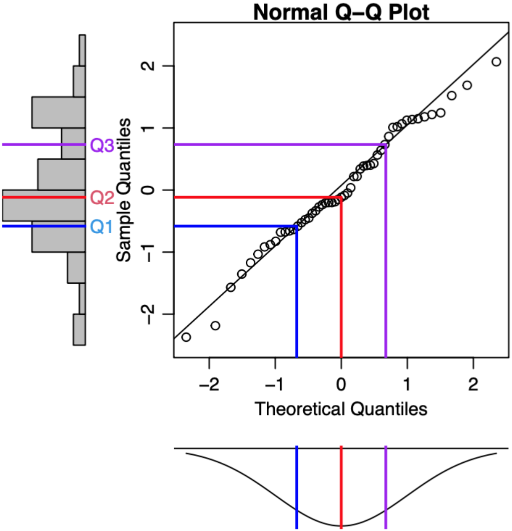
since $z_{(n/n)} = \infty$.



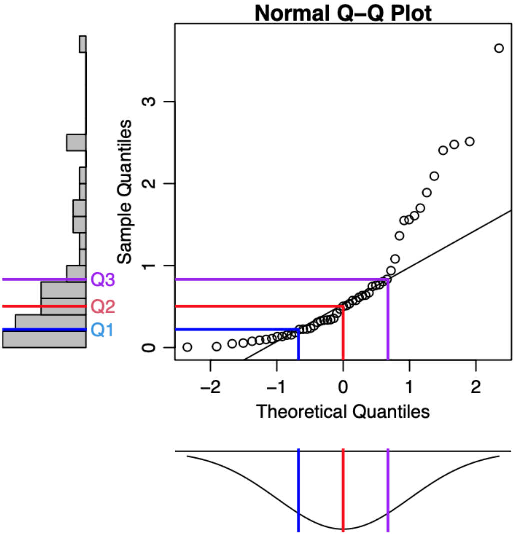
Different QQ Plots



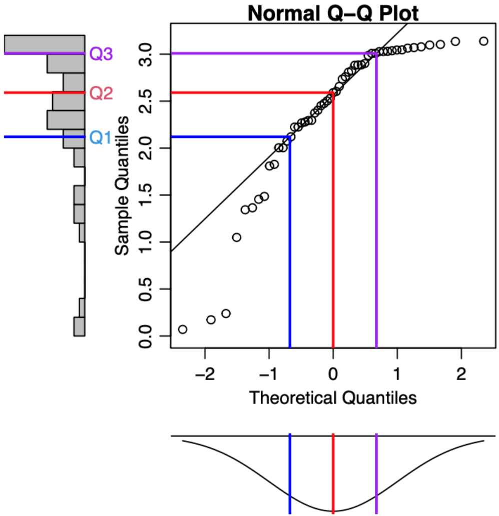
Normal QQ Plot — Normal Data



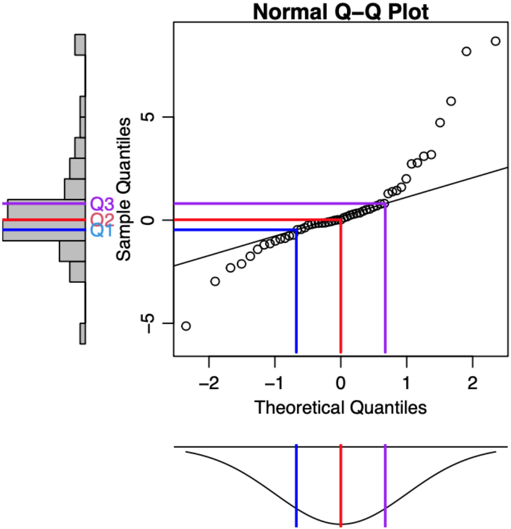
Normal QQ Plot — Right-Skewed Data



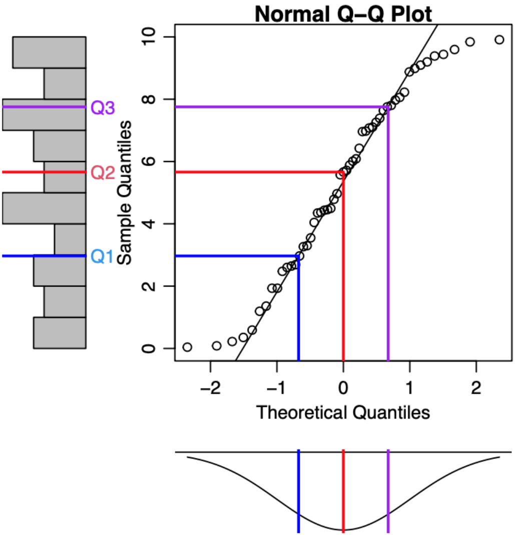
Normal QQ Plot — Left-Skewed Data



Normal QQ Plot — Heavy-Tailed Data



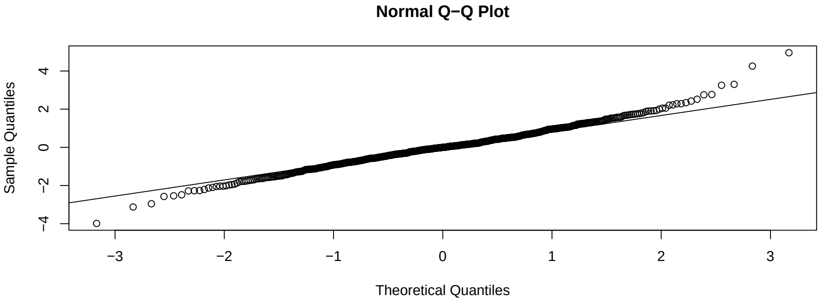
Normal QQ Plot — Light-Tailed Data



Normal QQ Plots in R

The R command qqnorm() can make normal QQ plots. The qqline() command will add a straight line to the normal QQ plot to help gauging normality.

```
lm1=lm(fev ~ ht + sex, data = fevdata)
qqnorm(rstudent(lm1))
qqline(rstudent(lm1))
```



Other Normality Tests

- Shapiro–Wilk test Compute test statistics $W = \frac{b^2}{SS}$, where

  $b = \sum_{i=1}^{m} a_i(x_{n+1-i} - x_i)$ weight a_i can be referenced from the table.

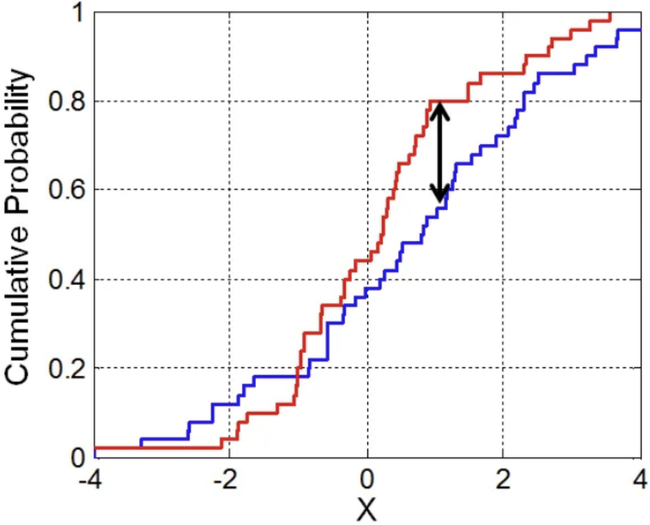
  $SS = \sum_{i=1}^{n}(x_i - \bar{x})^2$

- Kolmogorov–Smirnov test

  Measure the greatest vertical distance between the two distributions and calculate the test statistic where m and n are the sample sizes

  $D_{n,m} = \sup_x |F_{1,n}(x) - F_{2,m}(x)|$

Kolmogorov–Smirnov Test



Residual Plus Component Plot

A Residual Plus Component Plot is a scatterplot of

$$(e + \hat{\beta}_j X_j) \quad \text{versus} \quad X_j$$

where e and $\hat{\beta}_j$ are from the regression of Y on all predictors, including X_j.

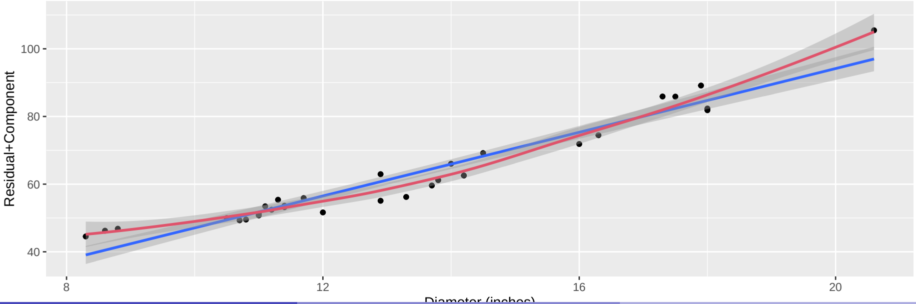
- The slope of the graph is $\hat{\beta}_j$
- This plot is useful to detect non-linearity in the partial relationship between Y and X_j.
- It adds a line indicating where the line of best fit lies

Residual Plus Component Plot (Trees Data)

For the model `lmtrees1 = lm(Volume ~ Diameter + Height, data=trees)`, the Residual Plus Component plot below for Diameter shows clear **nonlinearity**.

```
lmtrees1 = lm(Volume ~ Diameter + Height, data=trees)
ggplot(trees, aes(x=Diameter,
                  y=lmtrees1$res+lmtrees1$coef[2]*Diameter))+
  geom_point() + geom_smooth(method='lm') +
  geom_smooth(method='loess', col=2) +
  labs(x="Diameter (inches)", y="Residual+Component")
```

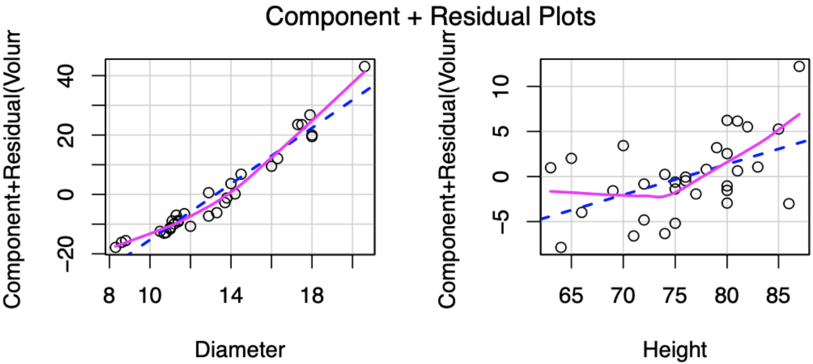
```
## `geom_smooth()` using formula 'y ~ x'
## `geom_smooth()` using formula 'y ~ x'
```



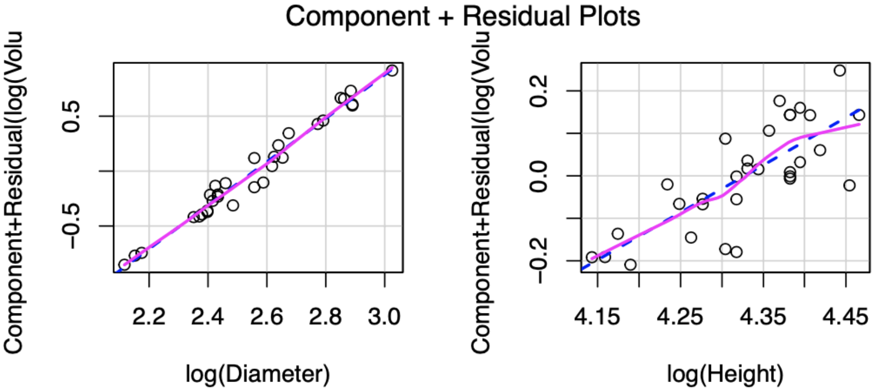
crPlots() in the car Library

The `crPlots()` function in the `car` library can produce residual plus component plots automatically

```
library(car)
crPlots(lmtrees1)
```



```r
lmtrees2 = lm(log(Volume) ~ log(Diameter) + log(Height), data=
crPlots(lmtrees2)
```



Both plots look linear, meaning the model

$\log(V) = \beta_0 + \beta_1 \log(D) + \beta_2 \log(H) + \epsilon$ is appropriate.

crPlots() doesn't work if the model includes interactions

```r
lm2 = lm(fev ~ age*smoke + age*sex + ht, data=fevdata)
#crPlots(lm2, "ht")
# not work since lm2 includes interactions
```