Linear Models

	Rain	Yield
[1,]	9.6	24.5
[2,]	12.9	33.7
[3,]	9.9	27.9
[4,]	8.7	27.5
[5,]	6.8	21.7
[6,]	12.5	31.9
[7,]	13.0	36.8
[8,]	10.1	29.9
[9,]	10.1	30.2
[10,]	10.1	32.0
[11,]	10.8	34.0
[12,]	7.8	19.4
[13,]	16.2	36.0
[14,]	14.1	30.2

….

Estimate Yield when Rain=10.1

Approach 1:

Mean(29.9,30.2,32.0) = 30.7

Approach 2:

Postulate: mean(Y/X=x) = f(x)

Simple Linear Regression

Consider the Corn Rain (X) and Corn Yield (Y) data discussed earlier. Denote the individual paired observations by: $(X_i, Y_i), i = 1, \cdots, n$.

Given $X = x$, let the expected value of Y be

$$\mu_{Y/x} = \beta_o + \beta_1 x$$

for any (X_i, Y_i), one has the simple linear regression model:

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

where ϵ_i are assumed to be uncorrelated random variables, with mean 0 and unknown variance σ^2.

Under the above formulation, the main objectives of regression analysis are:

- To find reasonable estimates of the unknown parameters
- To make inference about the unknown parameters, and
- To assess model adequacy.

Estimation: OLS

Let

$$Q(\beta_o, \beta_1) = \sum_{j=1}^{n} (Y_j - \beta_o - \beta_1 X_j)^2.$$

Then the least squares estimators $\hat{\beta}_0$ and $\hat{\beta}_1$ are such that

$$Q(\hat{\beta}_o, \hat{\beta}_1) = min$$

$$\hat{\beta}_1 = \frac{\Sigma_{j=1}^{n}(X_j - \bar{X})(Y_j - \bar{Y})}{\Sigma_{j=1}^{n}(X_j - \bar{X})^2}$$

and

$$\hat{\beta}_o = \bar{Y} - \hat{\beta}_1 \bar{X}$$

Properties of OLS Estimators

Theorem 1. Under the model assumptions, the OLS estimators are the best, linear unbiased estimators (BLUE).

A reasonable estimator of the error variance, σ^2 is given by

$$\hat{\sigma}^2 = \frac{\Sigma_{j=1}^{n}(Y_j - \hat{Y}_j)^2}{n-2}$$

where $\hat{Y}_j = \hat{\beta}_o + \hat{\beta}_1 X_j$ is the fitted value.

Goodness-of-fit measures

It can be shown that:

$$\sum_{j=1}^{n}(Y_j - \bar{Y})^2 = \sum_{j=1}^{n}(\hat{Y}_j - \bar{Y})^2 + \sum_{j=1}^{n}(Y_j - \hat{Y}_j)^2.$$

Then a measure of goodness of fit is:

$$R^2 = 1 - \frac{\Sigma_{j=1}^{n}(Y_j - \hat{Y}_j)^2}{\Sigma_{j=1}^{n}(Y_j - \bar{Y}_j)^2}$$

Values of R^2 close to 1 indicate good fit, while values near 0 suggest lack of fit.

Inference

$$H_o : \beta_1 = c$$

against the alternative

$$H_1 : \beta_1 > c$$

A reasonable test statistic is given by

$$T = \frac{\hat{\beta}_1 - c}{SE(\hat{\beta}_1)}$$

where

$$SE(\hat{\beta}_1) = \frac{\hat{\sigma}}{\sqrt{\Sigma_{j=1}^{n}(X_j - \bar{X})^2}}$$

Under the above assumptions, T has a $t_{(n-2)}$ distribution when H_o holds.

Inference

A $100(1-\alpha)\%$ confidence interval for β_1 is given by

$$\hat{\beta}_1 \pm t_{\alpha/2,n-2} SE(\hat{\beta}_1)$$

Similar results may be obtained for the intercept.

```
corn.reg <- lm(corn.yield ~ corn.rain)
summary(corn.reg)
```

```
Coefficients:
                  Value Std. Error t value Pr(>|t|)
(Intercept) 23.5521  3.2365      7.2771  0.0000
  corn.rain  0.7755  0.2939      2.6391  0.0122

Residual standard error: 4.049 on 36 degrees of
Multiple R-Squared: 0.1621
```

Departures from Assumptions

1. Functional form

Diagnosis:

- Look at the scatter plot of the data
- Compute R^2
- Plots of residuals versus X

Corrective measures

- Simple transformations, e.g., log
- Non-linear model
- Other predictors

Departures from Assumptions

2. Non-constancy of the Error Variance

Impact

- OLS estimators not optimal
- Associated inferential results unreliable

Diagnosis

- Plot residuals vs. X, and see whether error variance changes with X
- Variance homogeneity test to the residual variances based on data divided into two groups by values of X.

Corrective measures

- Transformation
- Build variance structure into model: WLS

Departures from Assumptions

3. Non-normality

Impact

- p-values and confidence intervals may not be reliable.

Diagnosis

- Simple graphical displays, e.g., histograms, qqnorm of the residuals
- Goodness-of-t tests, e.g., the Kolmogorov-Smirnov or Shapiro-Wilk test, on the residuals.

Corrective measures

- Transformation
- Robust regression methods

Departures from Assumptions

4. Correlated Errors

Impact

- p-values and confidence intervals may not be reliable.

Diagnosis

- Plot data over time/Look at design of study
- Durbin-Watson test for 1st order AR

Corrective measures

- Transformation: Cochrane-Orcutt Procedure
- Use models that incorporate the correlation structure
  - Generalized Estimating Equations (GEE)

To construct the Durbin-Watson test, let

$$\epsilon_j = \rho\epsilon_{j-1} + u_j$$

where u_j is $N(0, \sigma^2)$, and $\rho = cor(\epsilon_j, \epsilon_{j-1})$. We wish to test

$$H_o : \rho = 0$$

against

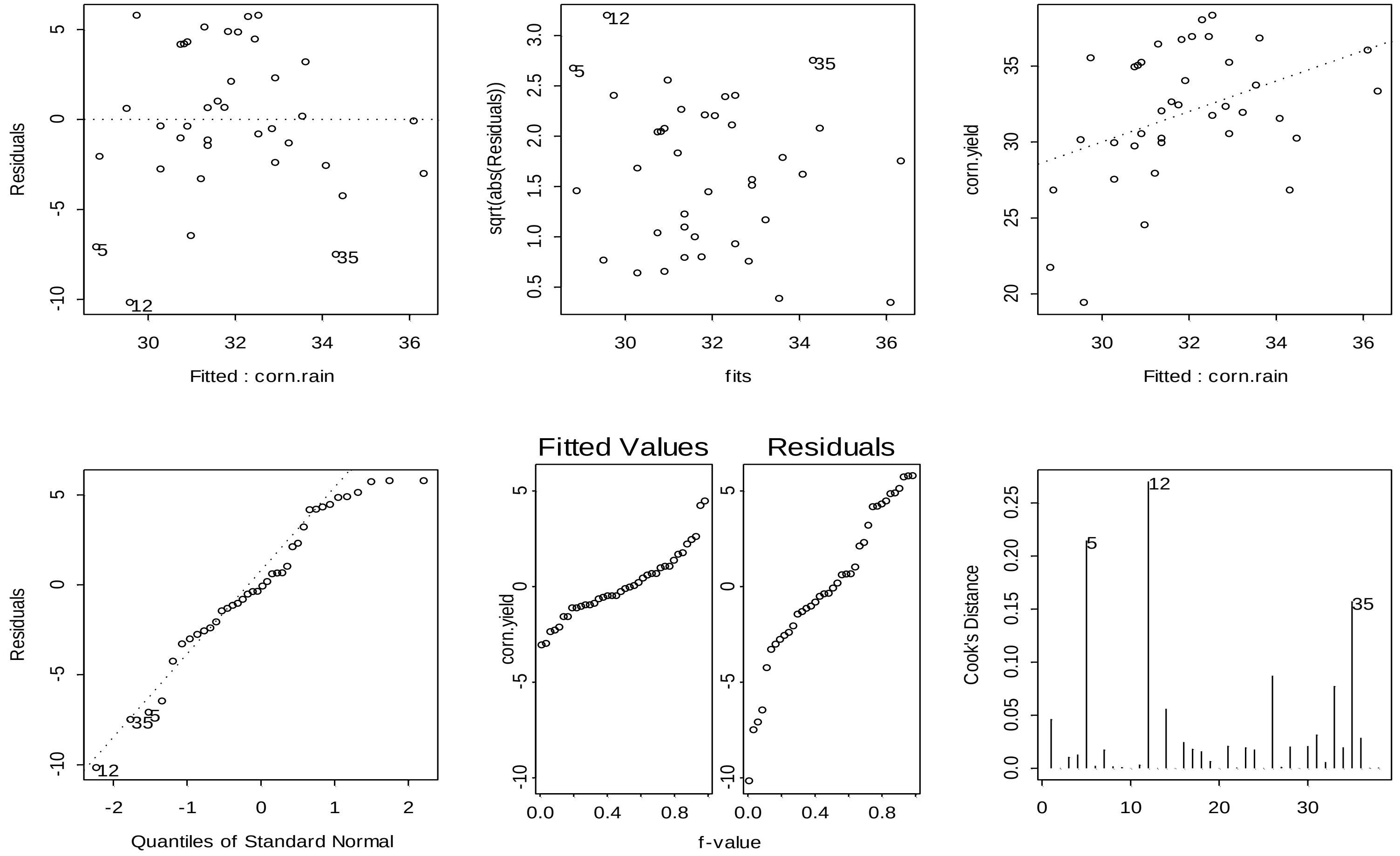
$$H_1 : \rho > 0$$

Put

$$D = \frac{\Sigma_{j=2}^{n}(\hat{\epsilon}_j - \hat{\epsilon}_{j-1})^2}{\Sigma_j \hat{\epsilon}^2_{j=1}}$$

The Durbin-Watson test rejects H_o when D is too small. Tables of critical values are available

```
> corn.reg <- lm(corn.yield~corn.rain)
> plot(corn.reg)
```



Estimation and Prediction

Let x_o be a value of the explanatory variable.

Then an estimator of the mean of Y corresponding to $X = x_o$ is

$$\hat{Y}_o = \hat{\beta}_o + \hat{\beta}_1 x_o$$

and has estimated SE given by

$$\hat{\sigma}\sqrt{\left(1/n + \frac{(x_o - \bar{X})^2}{\Sigma(X_i - \bar{X})^2}\right)}$$

Estimation and Prediction

Next suppose we wish to predict a future value of Y corresponding to $X = x_{new}$. This is given by

$$\hat{Y}_{new} = \hat{\beta}_o + \hat{\beta}_{\mathbf{1}} x_{new}$$

and has estimated SE given by

$$\hat{\sigma}\sqrt{\left(1 + 1/n + \frac{(x_o - \bar{X})^2}{\Sigma(X_i - \bar{X})^2}\right)}$$

Regression Through the Origin

An appropraite model is

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

$$\hat{\beta}_1 = \frac{\Sigma_i X_i Y_i}{\Sigma_i X_i^2}$$

$$\hat{\sigma}^2 = \frac{\Sigma_i \epsilon_i^2}{n-1}$$

.

It follows that

$$SE(\hat{\beta}) = \frac{\hat{\sigma}}{\sqrt{\Sigma_i X_i^2}}$$

Inverse Prediction (Calibration)

Given a new observation Y_{new}, we wish to estimate the corresponding X_{new}. Under normality, the MLE is given by

$$\hat{X}_{new} = (Y_{new} - \hat{\beta}_o)/\hat{\beta}_{\mathbf{1}}$$

The variance is estimated by

$$\hat{\sigma}^2_{\hat{X}_{new}} = \frac{\hat{\sigma}^2}{\hat{\beta}^2_{\mathbf{1}}}[1 + 1/n + \frac{(\hat{X}_{new} - \bar{X})^2}{\Sigma_i(X_i - \bar{X})^2}$$

Multiple Regression

Given Y, a dependent variable, and $X_1, \cdots, X_p$, p explanatory variables, the mean of Y given $X_j = x_j, j = 1, \cdots, p$, may be expressed, under the linear model assumption, as

$$\mu_{Y|x_1,\cdots,x_p} = \beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p$$

Let $(Y_i, X_{i,1}, \cdots, X_{i,p})$, $i = 1, \cdots, n$, be a random sample. It is often convenient to use the corresponding matrix formulations for the model:

$$\mathbf{Y} = \mathbf{X}\beta + \epsilon,$$

where $\mathbf{Y}$ is $n \times 1$, β is $p+1 \times 1$, $\mathbf{X}$ is $n \times p+1$, and ϵ is $n \times 1$. As in the simple linear model case, the error terms are assumed to be uncorrelated, with mean 0 and constant variance σ^2.

Then under the model assumptions, the LS estimators are obtained as solutions to the normal equations:

$$\mathbf{X}'\mathbf{X}\beta = \mathbf{X}'\mathbf{Y}$$

When $\mathbf{X}$ is full rank, the BLUE is given by

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

The Gauss-Markov Theorem.

Under the model assumptions, OLSE is UMVUE in the class of linear unbiased estimators.

Assume **X** (n x p+1) is of full rank. Then

$$Var(\hat{\beta}) = (\mathbf{X}'\mathbf{X})^{-\mathbf{1}}\sigma^{\mathbf{2}}$$

The distribution of $\hat{\beta}$ is (p+1) variate normal

As in the simple linear model case, a reasonable estimator of σ^2 is

$$\hat{\sigma}^2 = \frac{\Sigma_{j=1}^{n}(Y_j - \hat{Y}_j)^2}{n-p-1}$$

Inference

Consider the testing problem of $H_0 : \beta_k = \beta_{k,0}$

$$T = \frac{(\hat{\beta}_k - \beta_{k,0})}{SE(\hat{\beta}_k)}$$

Null distribution?

Similarly, a $100(1-\alpha)\%$ confidence interval for β_k is given by

$$\hat{\beta}_k \pm T_{n-p-1,\alpha/2} SE(\hat{\beta}_k)$$

Outliers and Influential Points

$$\mathbf{H} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'$$

$$\mathbf{h} = \mathbf{diag}(\mathbf{H})$$

The hat matrix plays an important role in model diagnostics.

h_{ii} is sometimes referred to as the leverage of the ith case. Recall that $0 \leq h_{ii} \leq 1$, and $\Sigma_i h_{ii} = p + 1$. When h_{ii} is large, i.e., $h_{ii} > 2(p+1)/n$, the ith case is said to have a high leverage in determining $\hat{Y}_i$.

$$var(\hat{\epsilon}_j) = (1 - h_{jj})\sigma^2$$

Outliers and Influential Points

- Semi-studentized residuals

  Let

  $$T_j^* = \frac{\hat{\epsilon}_j}{\hat{\sigma}}$$

  Large values of T_j^* may indicate outliers in the Y values.

- Studentized Residuals

  Define

  $$T_j = \frac{\hat{\epsilon}_j}{\hat{\sigma}\sqrt{1 - h_{jj}}}$$

Deleted Residuals

Let $\hat{Y}_{(i)}$ be the fitted value obtained after deleting the ith record. It can be shown that the deleted residual

$$\hat{\epsilon}_{(i)} = \frac{\hat{\epsilon}_i}{\sqrt{1 - h_{ii}}}$$

with

$$SE(\hat{\epsilon}_{(i)}) = \frac{\hat{\sigma}_{(i)}}{\sqrt{1 - h_{ii}}}$$

$$(n - p - 1)\hat{\sigma}^2 = (n - p - 1)\hat{\sigma}^2_{(i)} - \frac{\hat{\epsilon}_i^2}{(1 - h_{ii})}$$

Studentized deleted residuals

$$
\begin{aligned}
T_{(i)} &= \frac{\hat{\epsilon}_{(i)}}{SE(\hat{\epsilon}_{(i)})} \\
&= \frac{\hat{\epsilon}_i}{\hat{\sigma}_{(i)}\sqrt{1 - h_{ii}}}
\end{aligned}
$$

The following Bonferroni confidence set may be used to identify Y-outliers:

$$| T_{(i)} | > t_{\alpha/2n, n'-p-1}$$

where $n' = n - 1$.

DIFFTS

The influence of the ith observation on the fitted value $\hat{Y}_i$ may be assessed based on

$$DFFITS_i = \frac{\hat{Y}_i - \hat{Y}_{(i)}}{\hat{\sigma}_{(i)}\sqrt{h_{ii}}}$$
$$= T_{(i)} \left(\frac{h_{ii}}{1 - h_{ii}} \right)^{1/2}$$

The ith case is considered influential if $|DFFITS_i| > 1$ for small to medium n, and exceeds $2\sqrt{\frac{p+1}{n}}$ for large n.

Cook's Distance

An aggregate measure of influence

Cook's Distance, defined as

$$D_i = \frac{(\hat{\mathbf{Y}} - \hat{\mathbf{Y}}_{(\mathbf{i})})'(\hat{\mathbf{Y}} - \hat{\mathbf{Y}}_{(\mathbf{i})})}{(p+1)\hat{\sigma}^2}$$

which is distributed as $F_{p+\mathbf{1},n-p-\mathbf{1}}$. The ith case is said to be an influential point over all the n fitted values, if $D_i > F_{\alpha,p+\mathbf{1},n-p-\mathbf{1}}$.

DFBETAS

$$DFBETAS_{k(i)} = \frac{\hat{\beta}_k - \hat{\beta}_{k(i)}}{\hat{\sigma}_{(i)}\sqrt{c_{kk}}}$$

where c_{kk} is the kth diagonal element of $\mathbf{(X'X)^{-1}}$

Large values of $|DFBETAS_{k(i)}|$ indicate the influence of the i^{th} case on the k^{th} regression coefficient estimate.

Typically > 1 or 2/sqrt(n), depending on n

```
> fit1 <-lm(Y~x1+x2)
> summary(fit1)
Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) -0.94425    4.11174  -0.230 0.839714
x1           3.22012    0.33886   9.503 0.010893 *
x2           6.05792    0.08339  72.643 0.000189 ***
```

```
> lmi <- lm.influence(fit1)

> names(lmi)
[1] "coefficients" "sigma"        "hat"
```

```
> names(lms)
 [1] "call"         "terms"        "residuals"    "coefficients" "sigma"
 [6] "df"           "r.squared"    "fstatistic"   "cov.unscaled" "correlation"

>lms <- summary(fit1)
```

```
 e <- resid(fit1)
 s <-lms$sigma
 si <-lmi$sigma
xxi <-diag(lms$cov.unscaled)
 h <-lmi$hat
```

```
coef(lmi)
 (Intercept)          x1           x2
1 -15.0108430  0.20726437  0.468425836
2  -3.8149505  0.28318345  0.058954961
3  11.7849186 -1.70357945 -0.184475162
4   0.4542068 -0.02554101 -0.007153742
5   2.3582137 -0.08404465 -0.044319891
```

```
bi <- coef(fit1)-t(coef(lmi))
dfbetas  <- bi/t(si%o%xxi^0.5)
 stand.resid <- e/(s*(1-h)^0.5)
student.resid <-  e/(si*(1-h)^0.5)
DFFITS <- h^0.5*e/(si*(1-h))
```

Problem Set 4

Reading Assignment:

Chapter 7,8, and 10: The Statistical Sleuth: A Course in Methods of Data Analysis. Ramsey & Schafer

1. Chapter 8, Exercise 18 (Chernobyl Fallout). In addition to (a)-(d), assess the validity of the following underlying assumptions, and suggest remedial measures in case they are not satisfied.
   - Linearity/functional form
   - Normality
   - Homoscedasticity
   - Uncorrelated error

2. Consider the data set 'stackloss' in R, consisting of data on:

   [,1] 'Air Flow' Flow of cooling air

   [,2] 'Water Temp' Cooling Water Inlet Temperature

   [,3] 'Acid Conc.' Concentration of acid [per 1000, minus 500]

   [,4] 'stack.loss' Stack loss

a) Fit a multiple linear regression model of Stack Loss on the three explanatory variables.
b) State and assess the validity of the underlying assumptions, and check for outliers and influential points.