Regression

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Inference in Regression Analysis

Let $y = \beta_0 + \beta_1 x + \epsilon$ be a simple linear regression model with $\epsilon \sim N(0, \sigma^2)$ and ϵ_i are independent then

- b_0 and b_1 have normal distributions.
- b_0 and b_1 are unbiased estimators of β_0 and β_1 respectively
- $Var(b_0) = \sigma^2 \left(\frac{1}{n} + \frac{\overline{x}^2}{S_{xx}}\right)$
- $Var(b_1) = \frac{\sigma^2}{S_{xx}}$

where σ^2 is the variance of ϵ_i
Note that $s^2 = \frac{1}{n-2}\sum_{i=1}^{n}(y_i - \widehat{y_i})^2$ is called the mean square error(MSE) or residual mean square. Therefore,

$$MSE = \frac{SSE}{n-2}$$

It can be shown for a simple linear regression model that MSE is an unbiased estimator of σ^2.

Conducting a Residual Analysis and Prediction

Conducting a Residual Analysis

The residuals are obtained using the `residuals` function in R. However these residuals don't have the same variance(heteroscedastic). We therefore use the studentized residuals, which have the same variance.

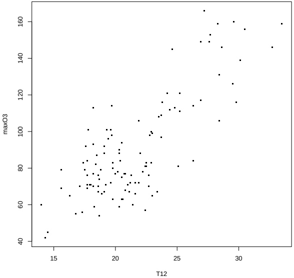
Predicting a new Value

Once a simple regression is developed we can use it to predict the corresponding y value for a given value of x. However the predicted value is of little interest without its corresponding confidence interval. We can use the R code `predict` to make a prediction.

Example

Air Pollution is currently one of the most serious public health worries worldwide. Many epidemiological studies have proved that some chemical compounds such as sulphur dioxide (SO_2), nitrogen dioxide (NO_2), ozone (O_3) or other air-borne dust particles can have on our health. Link below contains 112 observations recorded during Summer 2001 in Rennes (France). Measurements for many variables including the ozone concentration(O3) and midday temperature (T12) are provided. We would like to study the relationship between the ozone level and the midday temperature.
http://www.agrocampus-ouest.fr/igagrocampus-ouest.fr/math/RforStat/ozone.txt

```
>ozone=read.table("http://www.agrocampus-ouest.fr/igagrocampus-ouest.fr/math/RforStat/ozone.txt", header=T)
>plot(maxO3~T12, data=ozone, pch=15, cex=0.5)
```



Example-Ozone

We will study the ozone data using R code below:

```
>ozone=read.table("http://www.agrocampus-ouest.fr/igagrocampus-ouest.fr/math/RforStat/ozone.txt", header=T)
```

```
>model=lm(maxO3~T12, data=ozone)
>summary(model)
>coef(model)
>residuals<-residuals(model)
>res.simple<-residuals(model)
>plot(res.simple, pch=16, ylab="Residuals")
>abline(h=c(-2,0,2),lty=c(2,1,2))
>xnew<-20
>xnew=as.data.frame(xnew)
>colnames(xnew)<-"T12"
>predict(model, xnew, interval="pred")
```

The Analysis of Variance

Once we fit a model we want to check

- Does x, the regressor variable, truly influence y, the response?
- Is there an adequate fit of the data to the model?
- Will the model adequately predict the response?

In the first case, success can be quite often be achieved in answering the question through hypothesis testing on the slope β_1. We would like to test

$$\begin{aligned} H_0 &: \beta_1 = 0 \\ H_a &: \beta_1 \neq 0 \end{aligned}$$

Of course if H_0 is true, the implication is that the model reduces to $E(y) = \beta_0$, suggesting that the regressor variable doesn't influence the response(at least through the linear model). Rejection of H_0 in favor of H_a leads one to conclude that x significantly influence the response.

The Analysis of Variance

A simple F-test produced through the computation outlined in the ANOVA table can be used. Since we have

$$\frac{SS_{Reg}/1}{SS_{Res}/n-2} = \frac{MSR}{s^2} \sim \frac{\chi_1^2/1}{\chi_{(n-2)}^2/(n-2)}$$

under H_0, we have MS_{Reg}/s^2 follows the $F_{1,n-2}$ under H_0 and is thus a candidate for a test statistic for testing the hypothesis. Below is a standard ANOVA table

Source	*Sum of Squares*	*df*	*Mean Square*	*F*
Regression	$SS_{Reg} = \sum(\widehat{y}_i - \overline{y})^2$	1	$SS_{Reg}/1$	$F = \frac{MS_{Reg}}{MSE}$
Residual	$SS_{Res} = \sum(y_i - \widehat{y}_i)^2$	$n-2$	$MSE = s^2$	
Total	$SS_{Total} = \sum(y_i - \overline{y})^2$	$n-1$		

Remark: For a given α level, the F test of $H_0 : \beta_1 = 0$ Vs. $H_1 : \beta_1 \neq 0$ is equivalent to the two-tailed t-test.

Example

Table below provides data on the boiling point of water (in ^oF) and barometric pressure (inches of mercury)

Boiling Point	Barometric Pressure	Boiling Point	Barometric Pressure
199.5	20.79	201.9	24.02
199.3	20.79	201.3	24.01
197.9	22.40	203.6	25.14
198.4	22.67	204.6	26.57
199.4	23.15	209.5	28.49
199.9	23.35	208.6	27.76
200.9	23.89	210.7	29.64
201.1	23.99	211.9	29.88
		212.2	30.06

Example

```
>T<-c(199.5,201.9,199.3,201.3,197.9,203.6,198.4,204.6,199.4,209.5,199.9,208.6,200.9,210.7,201.1,211.9,212.2)
>P<-c(20.79,24.02,20.79,24.01,22.40,25.14,22.67,26.57,23.15,28.49,23.35,27.76,23.89,29.64,23.99,29.88,30.06)
> model=lm(P~T)
> model

Call:
lm(formula = P ~ T)
Coefficients:
(Intercept)            T
   -95.7572       0.5937

> anova(model)
Analysis of Variance Table
Response: P
          Df Sum Sq Mean Sq F value    Pr(>F)
T          1 141.65 141.654  226.04 1.879e-10 ***
Residuals 15   9.40   0.627
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1
```

For the given data we have the following ANOVA table

Source	*SS*	*df*	*MS*	*F*	$Pr > F$
Regression	141.65393	1	141.65393	226.04	< 0.0001
Error	9.40008	15	0.62667		
Total	151.05401	16			

Decision: Since $p < \alpha$ we reject the null hypothesis that $\beta_1 = 0$, which means there is a strong relationship between the temperature and the barometric pressure

Quality of Fitted Model

To answer

- Is there an adequate fit of the data to the model?
- Will the model adequately predict the response?

We compute the coefficient of Determination.

The coefficient of determination, often is denoted by R^2 and is defined by

$$R^2 = \frac{SS_{Reg}}{SS_{Total}} = \frac{\sum(\widehat{y}_i - \overline{y})^2}{\sum(y_i - \overline{y})^2}$$

which also can be written as

$$R^2 = 1 - \frac{SS_{Res}}{SS_{Total}}$$

It is clear that

$$0 \leq R^2 \leq 1$$

We may interpret R^2 as the proportion of variation in the response data that is explained by the model. Thus, the larger R^2 is, the more the total variation of y is reduced by introducing the predictor variable x. When all the observation fall on the fitted regression line then $SS_{Res} = 0$ and $R^2 = 1$ whereas when the fitted regression line is horizontal so that $b_1 = 0$ then $SS_{Res} = SS_{Total}$ and $R^2 = 0$.

Adjusted R^2

Adjustment is made for complexity of the model (i.e. penalty for higher number of variables). The Formula for adjusted R^2 is

$$R^2_{Adj.} = 1 - \frac{MS_{Res}}{MS_{Total}}$$

It should be noted that R^2 is a measure of the <u>linear</u> association between y and x. A small R^2 does not always imply a poor relationship between y and x.

Example

```
> x1<-c(10,8,13,9,11,14, 6, 4,12, 7, 5)
> y1<-c(8.04,6.95,7.58,8.81,8.33,9.96,7.24,4.26,10.84, 4.82, 5.68)
> x2<-c(10,8, 13, 9,11,14, 6, 4,12, 7, 5)
> y2<-c(9.14, 8.14,8.74,8.77,9.26,8.10,6.13,3.10,9.13,7.26,4.74)
> x3<-c(10,8,13,9,11,14,6,4,12,7, 5)
> y3<-c(7.46, 6.77,12.74,7.11,7.81,8.84,6.08,5.39, 8.15,6.42,5.73)
> x4<-c(8,  8,  8 , 8 , 8 , 8 , 8 ,19 , 8,  8,  8)
> y4<-c(6.58, 5.76, 7.71, 8.84,8.47,7.04,5.25,12.50,5.56,7.91,6.89)

>par(mfrow=c(2,2))
>par(mfrow=c(2,2),oma=c(0,0,2,0))
>plot(x1,y1,main=" Scatter plot of Data Set 1")
>plot(x2,y2,main=" Scatter plot of Data Set 2" )
>plot(x3,y3,main=" Scatter plot of Data Set 3")
>plot(x4,y4, main="Scatter plot of Data Set 4")
```

A Look at Residuals

We would like to see what type of information can be gained from the ordinary residuals which is given by $e_i = y_i - \widehat{y}_i$ called as the errors of fit. The residuals may be regarded as the observed error, in distinction to the unknown true error ϵ_i in the regression model:

$\epsilon_i = y_i - E(y_i)$

We know that from the normal theory assumption ϵ_i are assumed to be independent normal random variables with mean 0 and variance σ^2. If the model is appropriate for the data at hand, the observed residuals e_i should reflect the properties assumed for ϵ_i. This is the basic idea of residual analysis, a highly useful means of examining the aptness of a statistical model.

Properties of Residuals:

a. We have

$$\overline{e} = \frac{\sum e_i}{n} = 0$$

so it provides no information as to whether the true errors ϵ_i have expected value $E(\epsilon_i) = 0$.

b. We have

$$Var(e_i) = \frac{\sum_i (e_i - \overline{e})^2}{n-2} = \frac{\sum e_i^2}{n-2} = \frac{SSE}{n-2} = MSE$$

Diagnostics of Residuals

Graphical analysis of residuals is very effective to investigate the adequacy of the fit of the regression model and to check the underlying assumptions. We look at the following plots of residuals in order to check the model assumptions

- Plots of the residuals against predictor variable.
- Plot of absolute or squared residuals against predictor variables
- Plots of residuals against fitted values.
- Box plots of residuals
- Normal probability plots of residuals.

If the simple linear regression model is not appropriate it may occur due to

- Nonlinearity of Regression function
- Nonconstancy of Error Variance
- Nonindependence of Error terms
- Nonnormality of Error terms
- Omission of important predictor variable
- Outlying Observations

Example

```
 > x1<-c(10,8,13,9,11,14, 6, 4,12, 7, 5)
>  y1<-c(8.04,6.95,7.58,8.81,8.33,9.96,7.24,4.26,10.84, 4.82, 5.68)
>  x2<-c(10,8, 13, 9,11,14, 6, 4,12, 7, 5)
>  y2<-c(9.14, 8.14,8.74,8.77,9.26,8.10,6.13,3.10,9.13,7.26,4.74)
>  x3<-c(10,8,13,9,11,14,6,4,12,7, 5)
>  y3<-c(7.46, 6.77,12.74,7.11,7.81,8.84,6.08,5.39, 8.15,6.42,5.73)
>  x4<-c(8,  8,  8 , 8 , 8 , 8 , 8 ,19 , 8,  8,  8)
>  y4<-c(6.58, 5.76, 7.71, 8.84,8.47,7.04,5.25,12.50,5.56,7.91,6.89)
>  model1= lm(y1~x1)
>  model2=lm(y2~x2)
>  model3=lm(y3~x3)
>  model4= lm(y4~x4)
>  res1=resid(model1) # It computes the residules of the first model
>  res2=resid(model2)
>  res3=resid(model3)
>  res4=resid(model4)
>  fit1=fitted(model1) # It computes the Fitted values of the first model
>  fit2=fitted(model2)
>  fit3=fitted(model3)
>  fit4=fitted(model4)
>  par(mfrow=c(2,2))
>  plot(fit1,res1,main="Data Set 1: Fitted VS Residual plot")
>  plot(fit2,res2,main="Data Set 2: Fitted VS Residual plot")
>  plot(fit3,res3,main="Data Set 3: Fitted VS Residual plot")
>  plot(fit4,res4,main="Data Set 4: Fitted VS Residual plot")
```

Box-Cox Transformation

If the simple linear regression model is not appropriate for the data set there are two choices

a) Abandon the simple linear regression model and develop and use a more appropriate model,

b) Employ some transformation on the data so that the simple linear regression model is appropriate for the transformed data.

Box-Cox Transformation or power transformation:

It is often difficult to determine from the scatter plot which transformation is most appropriate for correcting the skewness of the distributions of error terms, unequal error variance and the nonlinearity of the regression function. The box cox transformation is given by

$$g(y_i) = \frac{y_i^\lambda - 1}{\lambda}$$

If $\lambda = 1$, no transformation is needed and we analyze the original data. If $\lambda = -1$ we analyze the reciprocal $1/y_i$. If $\lambda = 1/2$, we analyze the the $\sqrt{y_i}$. And we analyze $\ln(y_i)$ if $\lambda = 0$

The maximum likelihood estimator of λ minimizes $SSE(\lambda)$ where $SSE(\lambda)$ is the residuals sum of squares from fitting the regression model with transformed response

Example

```
x<-c(0, 0, 0, 0, 0, 1, 1, 1, 1, 1, 2, 2, 2, 2, 2, 3, 3, 3, 3, 3, 4, 4, 4, 4, 4)
y<-c(13.44, 12.84, 11.91, 20.09, 15.60, 10.11, 11.38, 10.28,  8.96,  8.59,  9.83,  9.00,
  8.65,  7.85,  8.88,  7.94,  6.01,  5.14, 6.90,  6.77,  4.86,  5.10,  5.67,  5.75,6.23)

>model1<-lm(y~x)
> par(mfrow=c(2,2)) # We need to specify this  dimension
> plot(model1)

>library(MASS)
>b=boxcox(model1) #  It will search the value of the parameter [-2,2]
>b=boxcox(model1, lambda=seq(0,3, by=0.01)) # for any positive value in [0,3]
>y1<-y^(-0.5)
> model2=lm(y1~x)
>par(mfrow=c(2,2))
> plot(model2)


>library(moments)
>skewness(model1$resid)
>skewness(model2$resid)
```

Regression Through the Origin

In practice sometimes one might be interested in building a model with no intercept. For example in chemical experiment the yield of a chemical process is zero when the temperature is zero.
The no intercept model is

$$y = \beta_1 x_i + \epsilon$$

Let b_1 be the estimator of β_1. Given n observations $(x_i, y_i), i = 1, 2, \cdots, n$ the least square function is

$$SSE = \sum_{i=1}^{n} (y_i - b_1 x_i)^2$$

The only normal equation is

$$b_1 \sum_{i=1}^{n} x_i^2 = \sum_{i=1}^{n} x_i y_i$$

Therefore, the least square estimator of the slope is

$$b_1 = \frac{\sum_{i=1}^{n} x_i y_i}{\sum_{i=1}^{n} x_i^2}$$

Example

Data below measures the temperature(x) vs. the chemical product yield (y).

Temp(x)	95	100	105	110	115	125	135	140	145	150	155
Yield(y)	8	10	9	10	11	13	10	11	12	13	11

```
> x=c(95, 100, 105, 110, 115, 125, 135, 140, 145, 150, 155)
> y=c(8, 10,  9, 10, 11, 13, 10, 11, 12, 13, 11)
> model1<-lm(y~x)
> model1
Call:
lm(formula = y ~ x)# Intercept model
Coefficients:
(Intercept)            x
    4.33838      0.05111
> model2<-lm(y~-1+x) # No intercept model
> model2
Call:
lm(formula = y ~ -1 + x)
Coefficients:
      x
0.08493
```

Simple Linear Regression Model in Matrix Terms

Let us consider a simple linear regression model

$$y_i = \beta_0 + \beta_1 x_i + \epsilon_i, \quad i = 1, 2, \cdots, n$$

This implies

$$\begin{aligned} y_1 &= \beta_0 + \beta_1 x_1 + \epsilon_1 \\ y_2 &= \beta_0 + \beta_1 x_2 + \epsilon_2 \\ &\vdots \\ y_n &= \beta_0 + \beta_1 x_n + \epsilon_n \end{aligned}$$

Let $\mathbf{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}$, $\mathbf{x} = \begin{pmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{pmatrix}$, $\boldsymbol{\beta} = \begin{pmatrix} \beta_0 \\ \beta_1 \end{pmatrix}$ and $\boldsymbol{\epsilon} = \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{pmatrix}$

Note that $\mathbf{x} = \begin{pmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{pmatrix}$ is called the design matrix.

Then we write the model as $\mathbf{y} = \mathbf{x}\boldsymbol{\beta} + \boldsymbol{\epsilon}$