清华大学统计学辅修课程

Design and Analysis of Experiments

Lecture 7 – Experiment Data Analysis via Regression

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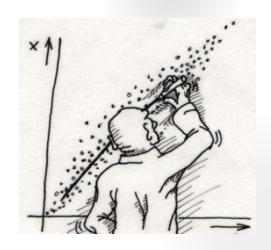
http://www.stat.tsinghua.edu.cn

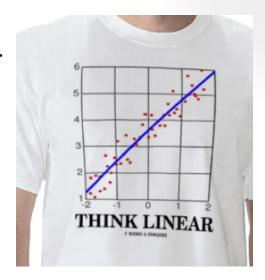




Outline

- ► Experiments with a single quantitative factor
 - > Regression model vs. fixed effects model
 - Model with non-linear terms
- ▶ One Quality Factor & One Quantitative Factor
 - > Regression on each level of one factor







Experiments with a Single Quantitative Factor

► Elements:

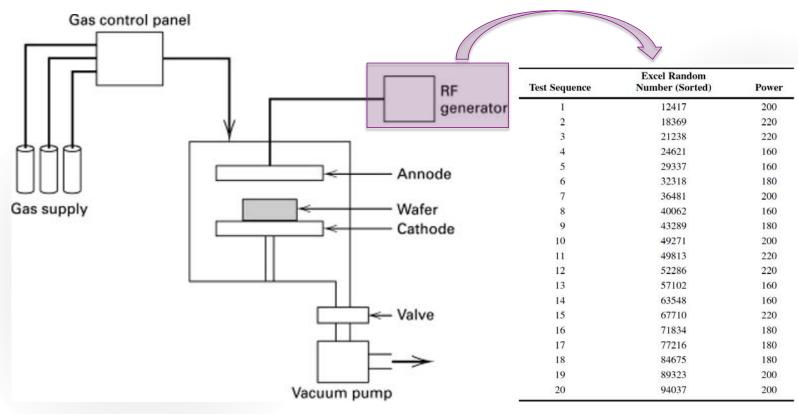
- > Quantitative factor A with a levels
- \triangleright Response Y

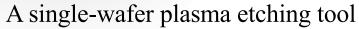
► Goals:

- > Evaluate the impact of factor A to response Y
- > Find the best choice of A
- ► Analysis strategies:
 - > Treat a levels of A as nominal variables (i.e., fixed effects)
 - > Fit a regression model of A & Y



Single Factor Experiment: An Example







Data from the Experiment

Power							
(W)	1	2	3	4	5	Totals	Averages
160	575	542	530	539	570	2756	551.2
180	565	593	590	579	610	2937	587.4
200	600	651	610	637	629	3127	625.4
220	725	700	715	685	710	3535	707.0

Etch Rate Data (in Å/min) from the Plasma Etching Experiment)



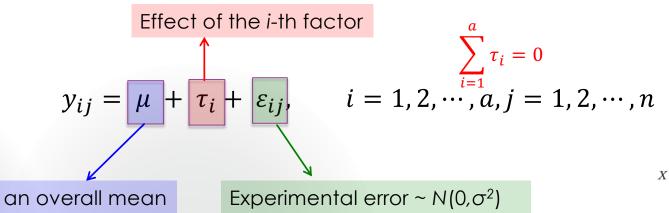
1 1 0 0

1 0 0 1

1 0 0 1

Fixed Effects Model (FEM)

► Statistical model



► Equivalent regression model

$$y = X\beta + \varepsilon, \beta = \begin{pmatrix} \mu \\ \tau_1 \\ \dots \\ \tau_a \end{pmatrix},$$

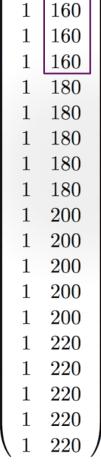


Power		(
(W)	1	2	3	4	5	Totals	Averages
160	575	542	530	539	570	2756	551.2
180	565	593	590	579	610	2937	587.4
200	600	651	610	637	629	3127	625.4
220	725	700	715	685	710	3535	707.0

X =

► Regression model with a different coding

$$y = X\beta + \varepsilon, \beta = \begin{pmatrix} \beta_0 \\ \beta_1 \end{pmatrix}$$



X =

► Statistical model

The data can be divided into 5 groups with same structure

> 3 levels are good enough to study a linear effect

Linear effect of factor A $y_{ij} = \beta_0 + \beta_1 x_i + \epsilon_{ij}, \qquad i = 1, 2, \dots, a, j = 1, 2, \dots, n$

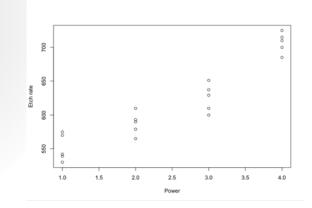
$$i=1,2,\cdots$$
 , $a,j=1,2,\cdots$, n

Grand mean

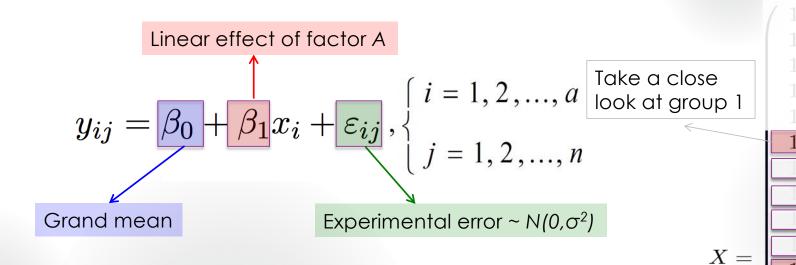
Experimental error ~ $N(0, \sigma^2)$

► In the matrix form

$$y = X\beta + \varepsilon$$







Power		(Observation	ıs			
(W)	1	2	3	4	5	Totals	Averages
160	575	542	530	539	570	2756	551.2
180	565	593	590	579	610	2937	587.4
200	600	651	610	637	629	3127	625.4
220	725	700	715	685	710	3535	707.0



Transform the Data for Better Performance

Power			Observation	ns	
(W)	1	2	3	4	5
160	575	542	530	539	570
180	565	593	590	579	610
200	600	651	610	637	629
220	725	700	715	685	710

$$y_{ij} = \beta_0 + \beta_1 x_i + \varepsilon_{ij}$$

$$X = \begin{pmatrix} 1 & 180 \\ 1 & 200 \\ 1 & 220 \end{pmatrix}$$

$$y_{ij} = \beta_0 + \beta_1 \left(\frac{x_i - \bar{x}}{\Delta}\right) + \varepsilon_{ij}$$
$$X^* = \begin{pmatrix} 1 & -1 \\ 1 & 0 \\ 1 & +1 \end{pmatrix}$$

Orthogonal vectors

Estimation & Hypothesis Testing of Linear Model



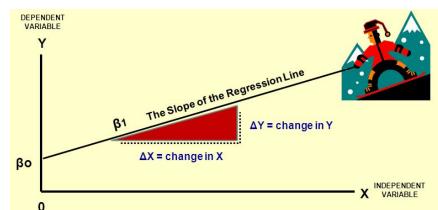
► Least square estimates:

$$\hat{\beta} = (X^T X)^{-1} X^T y$$

$$\hat{y} = X\hat{\beta} = X(X^TX)^{-1}X^Ty = Hy$$

$$\Rightarrow e = y - \hat{y} = y - Hy$$

$$\hat{\sigma}^2 = \frac{e^T e}{n - p}$$

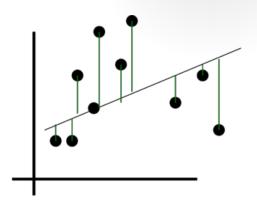


- ► Hypothesis testing:
 - > t-test for one coefficient

$$H_0: \beta_j = 0$$
 vs $H_1: \beta_j \neq 0$, $j = 0$ or 1

> *F*-test for the whole model

$$H_0: \beta_0 = \beta_1 = 0$$
 vs $H_1: \beta_0^2 + \beta_1^2 \neq 0$



Regression Model vs. Fixed Effects Model

$$y_{ij} = \beta_0 + \beta_1 x_i + \varepsilon_{ij}$$

$$y_{ij} = \mu + \tau_i + \varepsilon_{ij}$$

Advantages

- ► Fewer parameters
- ► More df to estimate σ^2
- ► Needs no replicates
- ► Can be used for prediction

Limitations

► Sensitive to linear assumption

of free parameters in regression model is 3:

$$\beta_0, \beta_1, \sigma^2$$

of free parameters in fixed effect model is (a+1):

$$\mu$$
, τ_1 , τ_2 , ..., τ_{a-1} , σ^2

Fit the Etching Data via Linear Regression

Power		•					
(W)	1	2	3	4	5	Totals	Averages
160	575	542	530	539	570	2756	551.2
180	565	593	590	579	610	2937	587.4
200	600	651	610	637	629	3127	625.4
220	725	700	715	685	710	3535	707.0

Etch Rate Data (in Å/min) from the Plasma Etching Experiment)

> mod <- lm(Rate ~ as.numeric(Power), data=Etch)

> summary(mod)

Estimate Std. Error t value Pr(>|t|)

(Intercept) 491.400 11.799 41.65 < 2e-16 ***

x 50.540 4.308 11.73 7.26e-10 ***

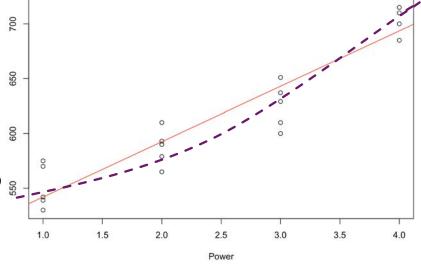
Residual standard error: 21.54 on 18 degrees of freedom

Multiple R-squared: 0.8843, Adjusted R-squared: 0.8779

F-statistic: 137.6 on 1 and 18 DF, p-value: 7.263e-10

l: 0.8779 -10





Adding a Quadratic Term

- \rightarrow x <- as.numeric(Etch\$Power); x2 <- x^2
- ightharpoonup > summary(lm(Rate ~ x + x2, data=Etch))
- Or simply

ightharpoonup > summary(lm(Rate ~ x + I(x^2), data=Etch))

Coefficients:

Estimate Std. Error t value Pr(>|t|)
(Intercept) 548.150 22.949 23.886 1.61e-14 ***

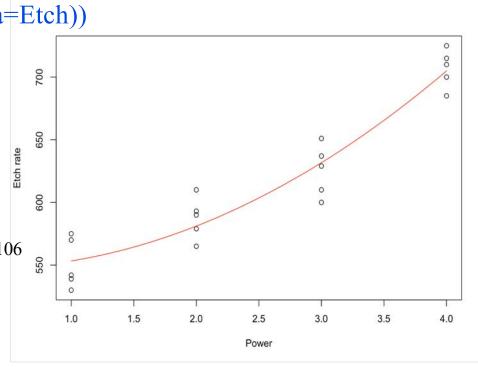
x -6.210 20.936 -0.297 0.7703

x2 11.350 4.122 2.754 0.0136 *

Residual standard error: 18.43 on 17 degrees of freedom

Multiple R-squared: 0.92, Adjusted R-squared: 0.9106

F-statistic: 97.76 on 2 and 17 DF, p-value: 4.74e-10





Numerical Proof of Improvement

- ▶ We use the anova() function to further quantify the extent to which the quadratic fit is superior to the linear fit
- > x <- as.numeric(Etch\$Power);
- $ightharpoonup > modf <- lm(Rate ~ x + I(x^2), data=Etch)$
- ightharpoonup > mod <- lm(Rate ~ x , data=Etch)
- > anova(mod, modf)

```
Analysis of Variance Table
```

```
Model 1: Rate ~ as.numeric(Power)
```

Model 2: Rate $\sim x + I(x^2)$

Res.Df RSS Df Sum of Sq F Pr(>F)

1 18 8352

2 17 5776 1 2576 7.58 0.014 *

Note: Model Comparisons by R

► Regression Model

$$y_{ij} = \beta_0 + \beta_1 x_i + \varepsilon_{ij}$$

► Fixed Effect Model

$$y_{ij} = \mu + \tau_i + \varepsilon_{ij}$$

summary(lm(Rate ~ Power, data=Etch))

Coefficients:

Estimate Std. Error t value Pr(>|t|) (Intercept) 491.400 11.799 41.65 < 2e-16 *** as.numeric(Power) 50.540 4.308 11.73 7.26e-10 ***

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: <u>21.54</u> on 18 degrees of freedom Multiple R-squared: 0.8843, Adjusted R-squared: 0.8779

F-statistic: 137.6 on 1 and 18 DF, p-value: 7.263e-10

Coefficients:

Estimate Std. Error t value Pr(>|t|)

(Intercept) 551.200 8.169 67.471 < 2e-16 ***
Power180 36.200 11.553 3.133 0.00642 **

Power200 74.200 11.553 6.422 8.44e-06 ***

Power220 155.800 11.553 13.485 3.73e-10 ***

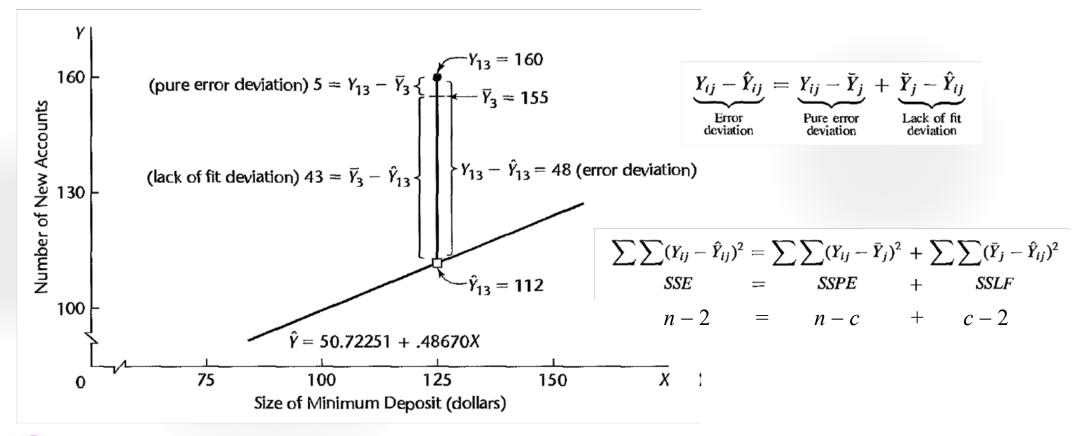
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 18.27 on 16 degrees of freedom

Multiple R-squared: 0.9261, Adjusted R-squared: 0.9122

F-statistic: 66.8 on 3 and 16 DF, p-value: 2.883e-09

Illustration of Decomposition of Error Deviation





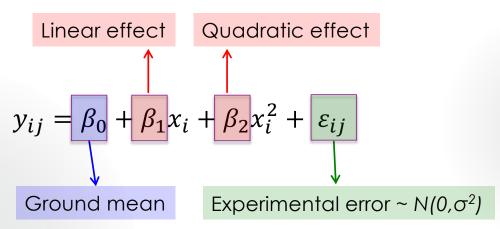
ANOVA Table

▶ For testing lack of fit of simple linear regression function

Source of Variation	SS	đf	MS
Regression	$SSR = \sum \sum (\hat{Y}_{ij} - \bar{Y})^2$	1	$MSR = \frac{SSR}{1}$
Error	$SSE = \sum \sum (Y_{ij} - \hat{Y}_{ij})^2$	n-2	$MSE = \frac{SSE}{n-2}$
Lack of fit	$SSLF = \sum \sum (\bar{Y}_j - \hat{Y}_{ij})^2$	a-2	$MSLF = \frac{SSLF}{c_1 - 2}$
Pure error	$SSPE = \sum \sum (Y_{ij} - \bar{Y}_j)^2$	$n-\alpha$	$MSPE = \frac{SSPE}{n - c_{l}}$
Total	$SSTO = \sum \sum (Y_{ij} - \tilde{Y})^2$	n-1	•

Model with Non-linear Terms

► Naive model



► A better model with transformed data

$$y_{ij} = \beta_0 + \beta_1 x_i \left(\frac{x_i - \bar{x}}{\Delta}\right) + \beta_2 \left(\frac{x_i - \bar{x}}{\Delta}\right)^2 + \varepsilon_{ij}$$

Data Transformation in Quadratic Model

\overline{x}	$x-ar{x}$	$rac{x-ar{x}}{\Delta}$	$z=(rac{x-ar{x}}{\Delta})^2$	$z-ar{z}$
180	-20	-1	1	+1/3
200	0	0	0	-2/3
220	+20	+1	1	+1/3

$$y_{ij} = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \varepsilon_{ij} \qquad y_{ij} = \beta_0 + \beta_1 \left(\frac{x_i - \bar{x}}{\Delta}\right) + \beta_2 \left(\frac{x_i - \bar{x}}{\Delta}\right)^2 + \varepsilon_{ij}$$



$$X = \begin{pmatrix} 1 & 180 & 180^2 \\ 1 & 200 & 200^2 \\ 1 & 220 & 220^2 \end{pmatrix}$$

$$X^* = \begin{pmatrix} 1 & -1 & +1 \\ 1 & 0 & -2 \\ 1 & +1 & +1 \end{pmatrix}$$

Orthogonal vectors

D-Optimal Design

Definition

- ► Regression model $y = X\beta + \varepsilon$
- Least square estimate $\hat{\beta} = (X^T X)^{-1} X^T y$

$$Cov(\hat{\beta}) = \sigma^2(X^TX)^{-1}$$

- ► Let $D = |X^T X|$, we have $|Cov(\hat{\beta})| = \sigma^2/D$
- ▶ Design X that maximizes D, and thus minimizes $|Cov(\hat{\beta})|$ is called the D-optimal design

D-Optimal Design for Simple Linear Regression

► Regression model:

$$y = \beta_0 + \beta_1 x + \varepsilon$$

- ► Assume $x \in [-1, 1]$
- ▶D-optimal design is: half data points take −1, half take 1
- ► This can be easily proved based on the facts below:

$$X^{T}X = \begin{pmatrix} N & \sum x_{i} \\ \sum x_{i} \sum x_{i}^{2} \end{pmatrix} \qquad D = |\mathbf{X}^{T}\mathbf{X}| = N\sum x_{i}^{2} - (\sum x_{i})^{2}$$

D-Optimal Design for Quadratic Regression

► Regression model:

$$y = \beta_0 + \beta_1 x + \beta_2 x^2 + \varepsilon$$

- ► Assume $x \in [-1, 1]$
- ▶D-optimal design is: 1/3 take -1, 1/3 take 0, 1/3 take 1
- ► This can be proved similarly by checking:

g:
$$X^{T}X = \begin{pmatrix} N & \sum x_{i} & \sum x_{i}^{2} \\ \sum x_{i} & \sum x_{i}^{2} & \sum x_{i}^{3} \\ \sum x_{i}^{2} & \sum x_{i}^{3} & \sum x_{i}^{4} \end{pmatrix}$$

One Quality Factor & One Quantitative Factor

▶ Elements:

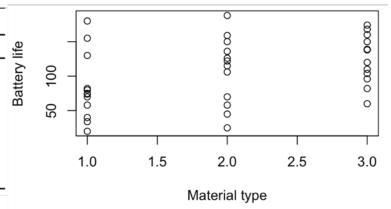
- > Quality factor A with a levels
- > Quantitative factor B with b levels
- \triangleright Response Y

► Goals:

- > Evaluate the impact of factor A & B to response Y
- > Find the best combination of A & B
- ► Analysis strategies:
 - > Treat levels of A & B as nominal variables (i.e., fixed effects)
 - > Fit a regression model of B & Y for each level of A separately

The Battery Life Experiment: An Example

Material			Temper	ature (°F)		
Туре	1	5	7	0	1	25
1	130	155	34	40	20	70
	74	180	80	75	82	58
2	150	188	136	122	25	70
	159	126	106	115	58	45
3	138	110	174	120	96	104
	168	160	150	139	82	60



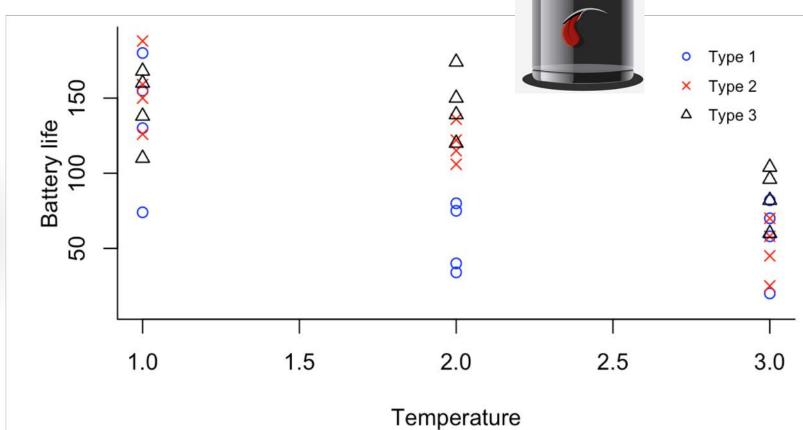
Factor A= Material type (a = 3); Factor B= Temperature (b = 3); n = 4

- Q1. What **effects** do material type & temperature have on life?
- Q2. Is there a choice of material that would give long life *regardless of temperature*(a **robust** product)?



Linear Regression done by R

ightharpoonup See the data grouped by each level of A





Linear Regression done by R

- ► > mod <- lm(Life ~ Type, data= Battery)
- > summary(mod)

Coefficients:

Estimate Std. Error t value Pr(>|t|)83.17 13.00 6.396 3.03e-07 *** (Intercept)

Type2 25.17 18.39 1.368 0.1804

Type3 41.92 18.39 2.279 0.0292 *

Residual standard error: 45.05 on 33 degrees of freedom

Multiple R-squared: 0.1376, Adjusted R-squared:

0.08533

F-statistic: 2.633 on 2 and 33 DF, p-value: 0.08695





$$\hat{\mu}_1 = 83.17$$

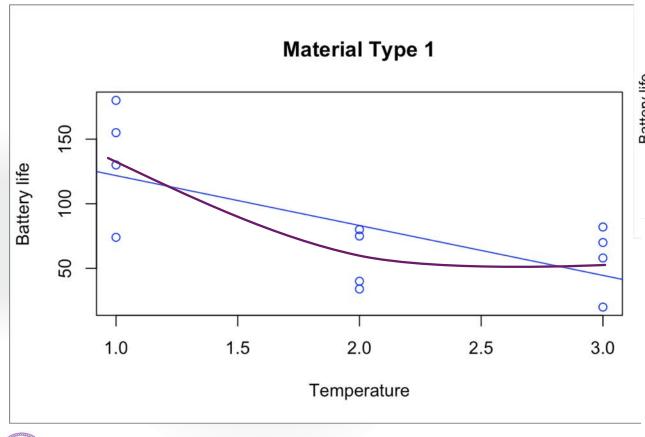
$$\hat{\mu}_2 = 83.17 + 25.17$$

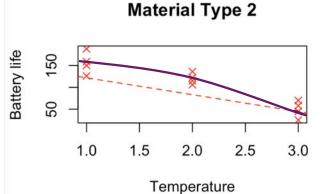
$$\hat{\mu}_3 = 83.17 + 41.92$$

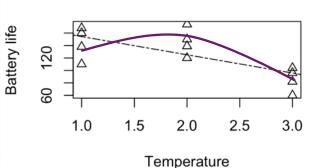


Linear Regression done by R: Separate Lines

► > mod1 <- lm(Life ~ as.numeric(Temp), data=Battery[Type==1,])



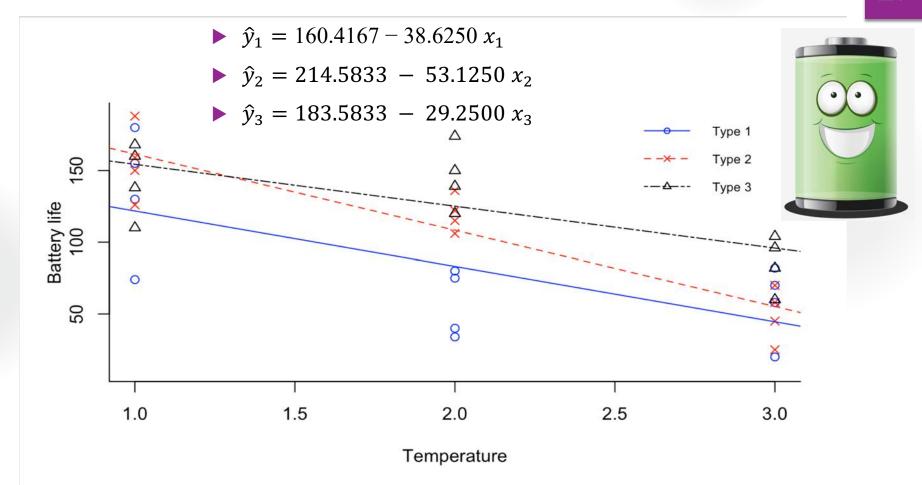




Material Type 3



Linear Regression by R: All 3 in 1 Plot





Quadratic Regression by R

 $\hat{y}_1 = 57.2 - 109.2x_1 + 311.0x_1^2$

Estimate Std. Error t value Pr(>|t|)

(Intercept) 160.4 28.6 5.61 0.00023 ***

x -38.6 13.2 -2.92 0.01540 *

Residual standard error: 37.5 on 10 degrees of freedom

Multiple R-squared: 0.46, Adjusted R-squared: 0.406

F-statistic: 8.5 on 1 and 10 DF, p-value: 0.0154

Estimate Std. Error t value Pr(>|t|)

(Intercept) 57.2 16.7 3.43 0.0075 **

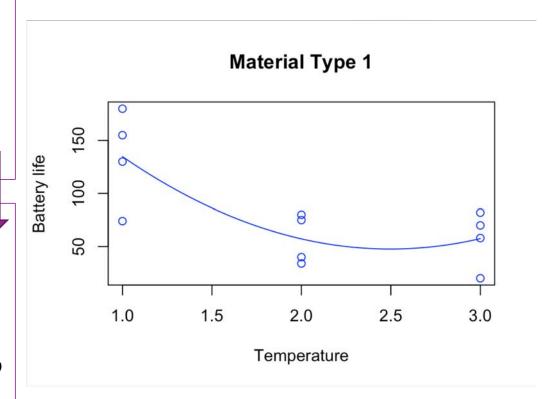
x -109.2 33.3 -3.28 0.0096 **

 $I(x^2)$ 311.0 163.3 1.90 0.0893.

Residual standard error: 33.3 on 9 degrees of freedom

Multiple R-squared: 0.615, Adjusted R-squared: 0.529

F-statistic: 7.18 on 2 and 9 DF, p-value: 0.0137





Full Regression Model

$$y_{ijk} = \beta_{i0} + \beta_{i1}x_{ijk} + \beta_{i2}x_{ijk}^2 + \varepsilon_{ijk}$$

 \triangleright Separate regressions on each of the *a* levels of factor *A*

$$y_{1jk} = eta_{10} + eta_{11} x_{1jk} + eta_{12} x_{1jk}^2 + eta_{1jk}$$
 $y_{2jk} = eta_{20} + eta_{21} x_{2jk} + eta_{22} x_{2jk}^2 + eta_{2jk}$
 \dots
 $y_{ajk} = eta_{a0} + eta_{31} x_{ajk} + eta_{a2} x_{ajk}^2 + eta_{ajk}$



$$\hat{y}_1 = 83.17$$

 $\hat{y}_2 = 83.17 + 25.17$
 $\hat{y}_3 = 83.17 + 41.92$

Main effects of A Linear & quadratic effects of B Experimental error $\sim N(0,\sigma^2)$

▶ Parameters:
$$(\overrightarrow{\beta}_1, \overrightarrow{\beta}_2, \dots, \overrightarrow{\beta}_a, \sigma^2)$$
 $\overrightarrow{\beta}_i = (\beta_{i0}, \beta_{i1}, \beta_{i2})$

▶ #Parameters:
$$3 \times a + 1 < a \times b$$

$$\hat{y}_1 = 160.4167 - 38.6250 x_1$$

$$\hat{y}_2 = 214.5833 - 53.1250 x_2$$

$$\hat{y}_3 = 183.5833 - 29.2500 x_3$$



Note: Interpreting the Intercept

- > > data1 <- Battery[Type==1,]</pre>
- > data1\$x <- with(data1,as.numeric(Temp)-mean(as.numeric(Temp)))
- \rightarrow mod11 <- lm(Life~ x, data=data1)
- ► > summary(mod11)
- ► Coefficients:

$$\hat{y}_1 = 83.17$$

Estimate St	td.	Error	t value	Pr(> t)

(Intercept) 83.17 10.81 7.690 1.66e-05 ***

x -38.62 13.25 -2.916 0.0154 *





Interpreting the Intercept

$$\hat{y}_1 = 57.2 - 109.2x_1 + 311.0x_1^2$$

- 33
- \triangleright > summary(lm(Life ~ poly(x, 2), data=Battery[Type==1,]))
- ightharpoonup > summary(lm(Life ~ x + I(x^2), data=Battery[Type==1,]))

Coefficients:

Estimate Std. Error t value Pr(>|t|) (Intercept) 83.17 9.62 8.64 1.2e-05 *** poly(x, 2)1 -109.25 33.34 -3.28 0.0096 ** poly(x, 2)2 63.48 33.34 1.90 0.0893 .

```
Estimate Std. Error t value Pr(>|t|) (Intercept) 57.2 16.7 3.43 0.0075 ** x -109.2 33.3 -3.28 0.0096 ** I(x^2) 311.0 163.3 1.90 0.0893 .
```

Residual standard error: 33.3 on 9 degrees of freedom Multiple R-squared: 0.615, Adjusted R-squared: 0.529

F-statistic: 7.18 on 2 and 9 DF, p-value: 0.0137

Residual standard error: 33.3 on 9 degrees of freedom

Multiple R-squared: 0.615, Adjusted R-squared: 0.529

F-statistic: 7.18 on 2 and 9 DF, p-value: 0.0137



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Test Various Effects

$$y_{ijk} = \beta_{i0} + \beta_{i1}x_{ijk} + \beta_{i2}x_{ijk}^2 + \varepsilon_{ijk}$$

► Test main effects of factor A:

$$H_0$$
: $\beta_{10} = \beta_{20} = \dots = \beta_{a0} = 0$ vs H_1 : any of them $\neq 0$

► Test linear effects of factor *B*:

$$H_0$$
: $\beta_{11} = \beta_{21} = \dots = \beta_{a1} = 0$ vs H_1 : any of them $\neq 0$

► Test quadratic effects of factor *B*:

$$H_0$$
: $\beta_{12} = \beta_{22} = \dots = \beta_{a2} = 0$ vs H_1 : any of them $\neq 0$

$$y_{1jk} = \beta_{10} + \beta_{11}x_{1jk} + \beta_{12}x_{1jk}^2 + \varepsilon_{1jk}$$

$$y_{2jk} = \beta_{20} + \beta_{21}x_{2jk} + \beta_{22}x_{2jk}^2 + \varepsilon_{2jk}$$

$$\cdots$$

$$y_{ajk} = \beta_{a0} + \beta_{31}x_{ajk} + \beta_{a2}x_{ajk}^2 + \varepsilon_{ajk}$$

► Test interaction of factor A & B:

$$H_0$$
: $\beta_{11} = \beta_{21} = \cdots = \beta_{a1} = \beta_1$ vs H_1 : any pair are different

$$H_0$$
: $\beta_{12} = \beta_{22} = \cdots = \beta_{a2} = \beta_2$ vs H_1 : any pair are different



The hierarchy principle indicates that if a model contains a high-order term, it should also contain all of the lower order terms that compose it

R Code

- ▶ full <- lm(Life ~ Type * poly(as.numeric(Temp), 2), Battery)
- ► r1 <- lm(Life ~ poly(as.numeric(Temp), 2), Battery)
- ► r2 <- lm(Life ~ Type * I(as.numeric(Temp)^ 2), Battery)
- ► r3 <- lm(Life ~ Type * as.numeric(Temp), Battery)
- ► r4 <- lm(Life ~ Type + poly(as.numeric(Temp), 2), Battery)
- ▶ anova(r1, full)
- ▶ anova(r2, full)
- ▶ anova(r3, full)
- anova(r4, full)

