Design of Experiments (Math 556)

MWF 8:00am-9:30am, WH 329
May 2, Tuesday meet Friday class !!
Office: WH 132
Office hours: M, T 7-8pm. Through Zoom
https://binghamton.zoom.us/j/8265526594?pwd=d3l6OGx1cmZ4M3cxZEJwVGd1RGcrUT09
Meeting ID: 826 552 6594
Passcode: 031320
Textbook: Statistics for Experimenters (2nd ed.)
by George Box, J Stuart Hunter and William G. Hunter
Quiz: Once a week at a random day,
quiz problems: formulas for Math 447-448 (see my website)
Midterm: March 20 (M)
Final May 11 5:40-7:40pm CW 314 **Changed to WH329 !!**
Each is allowed to bring a piece of paper with anything you prefer on it.
Homework assigned during a week is due next Wednesday before 8:00am.
Email me at qyu@math.binghamton.edu before 8:00am on Wednesday.
HW is on my website: http://www.math.binghamton.edu/qyu/qyu_personal
Remind me if you do not see it by Saturday morning !
Try to use Latex in homework. Otherwise, take a picture and convert it to a pdf file.

There will be homework due this Friday, as well as quiz !!!

The lecture note is also on my website
http://www.math.binghamton.edu/qyu/qyu_personal
note and note2 are updated one,
Grading Policy: 40% hw and quizzes +60% exams,
B = 70 ±

Chapter 1. Introduction

Self-reading.

Chapter 2. Basic

All concepts in this chapter have been introduced in 501, except autocorrelation.
Recall
X and Y are random variables, with observations (X_i, Y_i), $i = 1, ..., n$.
Population covariance and correlation:
$Cov(X,Y) = E(XY) - E(X)E(Y)$,
$\rho = \rho_{X,Y} = \frac{Cov(X,Y)}{\sigma_X \sigma_Y}$,
Sample Covariance $\hat{Cov}(X,Y) = \overline{XY} - \overline{X} \cdot \overline{Y}$
Sample correlation $\hat\rho = r = \frac{\overline{XY} - \overline{X} \cdot \overline{Y}}{\hat\sigma_X \hat\sigma_Y}$, where $\hat\sigma^2_X = \overline{XX} - (\overline{X})^2$,
Note that the sample variance of X is often refer to $S^2 = \frac{1}{n-1}\sum_{i=1}^n (X_i - \overline{X})^2$
(S^2 is also denoted by s^2 in the textbook. **Which is a better notation ?**)
Definition. The lag-k sample autocorrelation coefficient of Y_i's is

$$r_k = \frac{\sum_{i>k}^n (Y_i - \overline{Y})(Y_{i-k} - \overline{Y})}{\sum_{i=1}^n (Y_i - \overline{Y})^2}, \ k = 1, 2, ...$$

It measures the serial dependence of the data in time.

If $r_k \neq 0$, are the data i.i.d. ?

If $r_k > 0$ significantly, are the data i.i.d. ?

```
> x=rnorm(20)
> cor(x[1:19],x[2:20])                    [1] -0.1431549
> cor.test(x[1:19],x[2:20])
t = -0.59639, df = 17, p-value = 0.5588
cor -0.1431549
```

Theorem 1. If X_1, ..., X_n are i.i.d. from $N(\mu, \sigma^2)$, then
(a) $\overline{X} \perp S^2$;
(b) $\overline{X} \sim N(\mu, \sigma^2/n)$;
(c) $(n-1)S^2/\sigma^2 = n\hat{\sigma}^2/\sigma^2 \sim \chi^2(n-1)$.

Chapter 3. Comparing Two Entities

3.1. Consider the test for the difference of the means of two random samples X_i's and Y_j's.

H_o: $\mu_Y - \mu_X = \delta$ v.s. H_1: $\mu_Y - \mu_X > \delta$.

Two-samples test: Under the assumption that (1) two samples are independent, (2) X_i's are from $N(\mu_X, \sigma^2)$ and (3) Y_j's are $N(\mu_Y, \sigma^2)$, then a common test is

$$\phi = \mathbf{1}(t > t_{\alpha, n_Y+n_X-2}), \text{ where} \qquad (1)$$

$$t = \frac{\overline{Y} - \overline{X} - \delta}{s_p\sqrt{1/n_X + 1/n_Y}} \text{ and } s_p^2 = \frac{\sum_{i=1}^{n_X}(X_i - \overline{X})^2 + \sum_{j=1}^{n_Y}(Y_j - \overline{Y})^2}{n_Y + n_X - 2}.$$

This is due to

(a) $T = \frac{N(0,1)}{\sqrt{\chi^2(\nu)/\nu}} \sim$ distribution ?, where $N(0,1) \perp \chi^2(\nu)$

(b) $t = \frac{\overline{Y} - \overline{X} - \delta}{\sigma\sqrt{1/n_X + 1/n_Y}} / \sqrt{s_p^2/\sigma^2}$,

(c) $\frac{\sum_{i=1}^{n_X}(X_i - \overline{X})^2}{\sigma^2} \sim \chi^2(n_X - 1)$, $\frac{\sum_{i=1}^{n_Y}(Y_i - \overline{Y})^2}{\sigma^2} \sim$?

(d) $\frac{\sum_{i=1}^{n_X}(X_i - \overline{X})^2}{\sigma^2} + \frac{\sum_{i=1}^{n_Y}(Y_i - \overline{Y})^2}{\sigma^2} \sim$ what distribution ?

The paired t-test: Under the paired random sample of size n from $N(\mu_Y, \sigma_Y^2)$ and $N(\mu_X, \sigma_X^2)$, then a common test is

$$\phi_p = \mathbf{1}(t > t_{\alpha, n-1}), \text{ where}$$

$$t = \frac{\overline{Y} - \overline{X} - \delta}{s\sqrt{1/n}} \text{ and } s^2 = \frac{1}{n-1}\sum_{i=1}^{n}(Y_i - X_i - \overline{Y - X})^2.$$

Importance of the independent normally distributed assumptions in both tests.

Chemical Example in Table 3.2. An experiment was performed on a factory by making in sequence 10 batches of chemical using a standard production method (A) followed by 10 batches of a chemical using a modified method (B). The data are

A: 89.7, 81.4, ..., 84.5
B: 84.7, 86.1, ..., 88.5

See Table 3.1 on page 69.

Summary:
$n_A = n_B = 10$,
$\overline{y}_A = 84.24$,
$\overline{y}_B = 85.54$,
$s_p^2 = 10.8727$,

H_o: $\mu_B - \mu_A = 0$, v.s. H_1: $\mu_B - \mu_A > 0$.
$\overline{y}_B - \overline{y}_A = 1.3$.
Is it significant ? **What does it mean ?**

We need to
(1) set α (= 0.05), and

(2) compute P($\overline{y}_B - \overline{y}_A \geq 1.3$) = ? **what is it called ?**
Then conclude that if P($\overline{y}_B - \overline{y}_A \geq 1.3$) $< \alpha$ ...

One often uses the two-sample t-test in Eq. (1), then the P-value is 19% here.
Is it significant ?
Do we reject H_o ?
Can we use paired t-test ?
Does the SD become larger or smaller if we use it ?

$$\sigma^2/(2n-2) \text{ v.s. } \sigma^2/(n-1).$$

$$s_p^2 = \frac{\sum_{i=1}^{n_X}(X_i-\overline{X})^2+\sum_{j=1}^{n_Y}(Y_j-\overline{Y})^2}{n_Y+n_X-2} \text{ v.s. } S^2_{Y_B-Y_A}$$

What is the conclusion if we use it ? P-value=P($T \geq \frac{\overline{y}_B-\overline{y}_A}{SE}$)
Introduce two alternative approaches next.
External Reference Distribution.
Old data. 210 batches of the chemical products recorded in time order before the 20 data:
x_1, ..., x_{210}
The old data (see p.120) provide an external reference distribution.
Under H_o, the 20 data can be viewed as a sample from the population of the 210 data.

Compute
$D_t = \sum_{i=t+10}^{t+19} x_i/10 - \sum_{i=t}^{t+9} x_i/10$, $t = 1$, ..., 191.
See the histogram Figure 3.3 on page 70.

$P(\overline{y}_B - \overline{y}_A \geq 1.3) = 9/191 \approx 0.047$. Is it significant ?
Recall that if one uses t-test, the P-value is 19%. **Anything wrong ?**

1. The lag-1 sample auto-correlation of the data is $r_1 = \hat{\rho}_1 = -0.29$.
   The data are not independent.
   If one pretends independence, it leads to incorrect conclusion.
2. Normal assumption may not be valid **(do we need to check it ?)**

Internal Reference distribution. Random sampling distribution.
A randomized design in the comparison of standard and modified fertilizer mixtures for tomato plants. 11 plants in a row. 5 with standard (A), 6 with modified (B). One way is to apply A to the first 5 and B to the next 6 in a row. There are correlation between locations and it is not a good idea without randomization.
Randomizing the order in the row (sample(1:11,5) = ?) resulting

location :	1	2	3	4	5	6	7	8	9	10	11
fertilizer :	*A*	*A*	*B*	*B*	*A*	*B*	*B*	*B*	*A*	*A*	*B*
yield :	29.2	11.4	26.6	23.7	25.3	28.5	14.2	17.9	16.5	21.1	24.3

(1)

Remark: Role of a statistician:
(1) randomization before an experiment (DOE);
(2) make inferences after the experiment.

```
> x=c(29.2,11.4,26.6,23.7,25.3,28.5,14.2,17.9,16.5,21.1, 24.3)
> z=c(3,4,6,7,8,11)
> mean(x[z])-mean(x[subset=−z])                    # results in $\overline{y}_B - \overline{y}_A \approx 1.69$.
```

To test H_o: $\mu_B - \mu_A = 0$ against H_1: $\mu_B - \mu_A > 0$.
Need to compute $P(\overline{y}_B - \overline{y}_A \geq 1.69) = ?$
Rather than using t-test, which needs normal assumption, and equal variance,
we make use of the
Permutation distribution.

Table (1) is one combination of selecting 5 out of 11.

1	2	3	4	5	6	7	8	9	10	11	
A	A	A	A	A	B	B	B	B	B	B	(2)
29.2	11.4	26.6	23.7	25.3	28.5	14.2	17.9	16.5	21.1	24.3	

is another combination under H_o: $\mu_B - \mu_A = 0$.

```
> mean(x[6:11])−mean(x[1:5])                    # results in −2.82
```

Eq.(2) yields $\overline{y}_B - \overline{y}_A \approx -2.82$; while
Eq.(1) yields $\overline{y}_B - \overline{y}_A \approx 1.69$.

There are $\binom{11}{5} = \frac{11!}{5!6!} = 11 \cdot 3 \cdot 2 \cdot 7 = 462$ such combinations.

```
> P=combn(1:11,6)
> P[,1:10]
```

```
      [,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8] [,9] [,10]
[1,]    1    1    1    1    1    1    1    1    1    1
[2,]    2    2    2    2    2    2    2    2    2    2
[3,]    3    3    3    3    3    3    3    3    3    3
[4,]    4    4    4    4    4    4    4    4    4    4
[5,]    5    5    5    5    5    5    6    6    6    6
[6,]    6    7    8    9   10   11    7    8    9   10
```

Thus these 462 combinations yield 462 $\overline{y}_B - \overline{y}_A$ values.
These 462 values form a (discrete) distribution called the **permutation distribution**.

```
    x=c(29.2,11.4,26.6,23.7,25.3,28.5,14.2,17.9,16.5,21.1, 24.3)
```

Either use loop

```
    N=choose(11,6)                  # =462
    y=1:N
    P=combn(1:11,6)                 # Can we use combn(1:11,5) ?
    for(i in 1:N)
        y[i]=mean(x[P[,i]])−mean(x[−P[,i]])
    length(y[y>=1.69])/N                     # result is 0.3203463
```

Or without loop:

```
    y=x[P]
    dim(y)=c(6,462)
    B=apply(y,2,sum)
    y=B/6−(sum(x)−B)/5
    length(y[y>=1.69])/N                     # result is 0.3203463
```

What is the conclusion of the test ?

```
    library(jmuOutlier)    (another codes)
    y=runif(16,0,1)
    x=runif(20,0,1)
    perm.test(y,x,alternative=c(”two.sided”, ”less”, ”greater”), mu=0, paired=FALSE,
all.perms=TRUE, plot=FALSE, stat=sum)
```

The permutation distribution can also be simulated by the R code as follows.

```
    x=c(29.2,11.4,26.6,23.7,25.3,28.5,14.2,17.9,16.5,21.1, 24.3)
    N=10000
    y=rep(0,N)
    for(i in 1:N){
        u=sample(x)
        y[i]=mean(u[1:6])-mean(u[7:11])
    }
    length(y[y>=1.69])/N # result is 0.3209
```

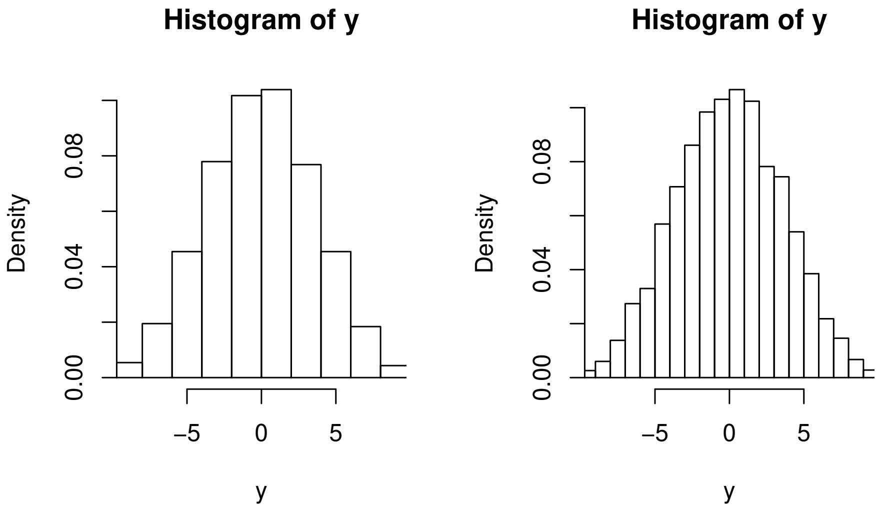

Figure 3.1. Histograms of permutation distribution v.s. simulation one

Should we use simulation here ?

Remark. The two-samples t-test $P(t_{n_A+n_B-2} > \frac{1.69}{s\sqrt{\frac{1}{n_A}+\frac{1}{n_B}}}) \approx 0.34)$ for the current data. If the normal assumption is not valid, the t-test is not applicable (though it happens to be close to 0.32

The permutation distribution is based on a different sample space from the sample space where the data come from. But if $n_A + n_B$ is large, the permutation distribution of $\overline{Y}_B - \overline{Y}_A$ is very close to $t_{n_A+n_B-2}$, whereas the two-sample t-test may not have the $t_{n_A+n_B-2}$ distribution (*e.g.* if the random variables satisfy $X_1 = \cdots = X_{n_A}$ and $Y_1 = \cdots = Y_{n_B}$), thus they are not independent).

Can we say $n_A + n_B$ is large here ?

Is it appropriate to apply randomization distribution in the chemical example ?

Remark. In the fertilizer example, the data are resulted from randomization, whereas in the previous chemical example, the data are in sequence.

A A A A A A A A A A B B B B B B B B B B

We use the External Reference distribution (old data) to get the P-value.

Can we use the permutation distribution to get the P-value in that example ?

No. If they had done

sample(1:20,10)

for the order of 10 batches of chemical using method A, then the permutation distribution would be valid.

3.2. Randomized paired comparison design: Boys shoes example. The shoe soles can be made of two different materials, A and B. To find out whether there is a difference between them, ten boys were chosen randomly to compare the shoe wear. Each boy wore a special pair of shoes. The decision as to whether the left or right sole was made with A or B was determined by

(1) convenience,

(2) by flipping a coin (or rbinom(n,1,0.5)).

Which result in a random sample ? (Took 2 steps in DOE. **Which 2 ?**)

The randomization results $\begin{pmatrix} boy: & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 \\ material\ A & L & L & R & L & R & L & L & L & R & L \end{pmatrix}$

The experiment results in

x=(0.8,0.6,0.3,-0.1,1.1,-0.2,0.3,0.5,0.5,0.3) $\# \ y_B - y_A$

Then 10 $y_B - y_A$'s yield

mean(x) # $\overline{y}_B - \overline{y}_A = 0.41$

Should we use two-sample t-test or paired t-test ?

What assumptions do we need in order to use one of them ?

Another way to compute P-value for $\overline{y}_B - \overline{y}_A \geq 0.41$ is the permutation distribution.
Under H_o: $\mu_B - \mu_A = 0$, a combination could be

(R L R L R L L L R L)

$$\begin{pmatrix} & R & L & R & L & R & L & L & L & R & L \\ real & L & L & R & L & R & L & L & L & R & L \end{pmatrix}$$

Then the data become

x=(-0.8,0.6,0.3,-0.1,1.1,-0.2,0.3,0.5,0.5,0.3)

Compare to the real data:

x=(0.8,0.6,0.3,-0.1,1.1,-0.2,0.3,0.5,0.5,0.3)

The randomized reference distribution under H_o: $\mu_A = \mu_B$ can be obtained as follows.

```
x=c(0.8,0.6,0.3,-0.1,1.1,-0.2,0.3,0.5,0.5,0.3)
sum(x) # result=4.1
y=1:1024 # initialize y
for(i1 in 0:1)
for(i2 in 0:1)
for(i3 in 0:1)
for(i4 in 0:1)
for(i5 in 0:1)
for(i6 in 0:1)
for(i7 in 0:1)
for(i8 in 0:1)
for(i9 in 0:1)
for(i10 in 0:1){
    i=c(i1,i2,i3,i4,i5,i6,i7,i8,i9,i10)
    h=0:9
    y[i%*%(2**h) +1]=sum(x*((-1)**i))
```

$$\# \; i1*2^0+i2*2^1+i3*2^2+\cdots+i10*2^9, \qquad (0,...,0)(2^0,2^1,...,2^9)'+1=1,$$

...

```
    # Examples:
```

$\#$ binary number $1110 = 1*2^3 + 1*2^2 + 1*2^1 + 0*2^0 = 14$

$\#$ ternary number $2101 = 2*3^3 + 1*3^2 + 0*3^1 + 1*3^0 = 64$

$\#$ decimal number $2101 = 2*10^3 + 1*10^2 + 0*10^1 + 1*10^0$

```
}
length(y[y>= 4.1])/1024                # result = 0.0068
hist(y); z=seq(-6,6,0.1);lines(z,dt(z,9))
```

The randomized reference distribution under H_o: $\mu_A = \mu_B$ can be approximated by simulation as follows.

```
N=10000
y=rep(0,N)
x=c(0.8,0.6,0.3,-0.1,1.1,-0.2,0.3,0.5,0.5,0.3)
for (i in 1:N) {
s=rbinom(10,1,0.5)
z=(-1)**s
y[i]=sum(x*z)
}
length(y[y>=4.1])/N              #0.0063
hist(y,xlim=c(-6,6), breaks=12, freq=F)
```

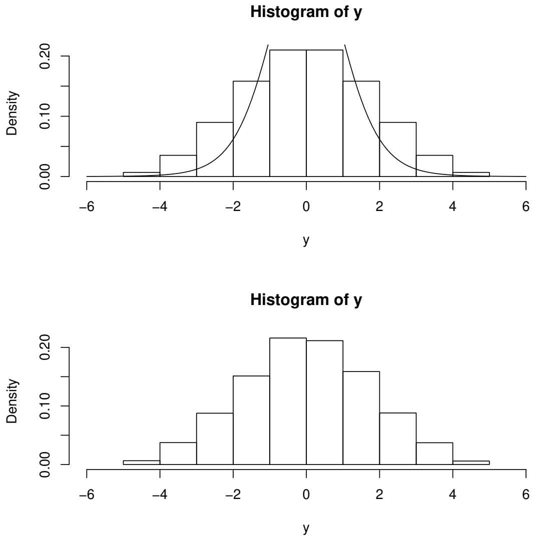

Figure 3.2. Histograms of permutation distribution v.s. simulation one

One can see from Figure 3.2 that the simulation distribution is very close to the true permutation distribution. The density of t_9 is displayed at the top of Fig. 3.2.

The P-value using the 1-sided paired t-test is 0.4%.

Any thing wrong with the solution 0.0068 or 0.4 ?

Is it one sided test or two-sided test ?

Can we mimic P=combn(1:10, ?) to write a code to replace the 1st one ?

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Chapter 10. Linear regression models.

10.1. Main assumption:

$Y = \beta_1 X_1 + \cdots + \beta_p X_p + \epsilon$, or

$E(Y|\mathbf{X}) = \beta_1 X_1 + \cdots + \beta_p X_p$, where

ϵ is unobservable random variable with $\underline{E(\epsilon|\mathbf{X}) = 0}$ (no assumption on $V(\epsilon|\mathbf{X})$ yet),

β_i's are parameters,

X_i's and Y are observable.

Given (independent) observations $(Y_i, x_{i1}, ..., x_{ip})$, $i = 1, ..., n$,

we shall make inference about β_i's.

Remark. A special case of the linear regression model is

$Y = \alpha + \beta X + \epsilon$.

Least squares estimator (LSE) minimizes

$S(\beta) = \sum_{i=1}^n (Y_i - \beta_1 x_{i1} - \cdots - \beta_p x_{ip})^2$ where $\beta = (\beta_1, ..., \beta_p)'$.

Notice that $S(\beta)$ can be written as a matrix form

$S(\beta) = (\mathbf{Y} - \mathbf{X}\beta)'(\mathbf{Y} - \mathbf{X}\beta)$

where $\mathbf{Y}' = (Y_1, ..., Y_n)$,

$$\mathbf{X} = (x_{ij})_{n\times p} = \begin{pmatrix} x_{11} & \cdots & x_{p1} \\ \vdots & \vdots & \vdots \\ x_{n1} & \cdots & x_{np} \end{pmatrix} \qquad\qquad \neq X$$

The LSE can be obtained by solving the normal equation

$\frac{\partial S}{\partial \beta} = \mathbf{0}$, a $p \times 1$ zero vector. $\qquad\qquad \frac{\partial S}{\partial \beta'} = ?$

That is,

$\mathbf{X}'(\mathbf{Y} - \mathbf{X}\beta) = \mathbf{0}$. $\qquad$ **(Why not $(\mathbf{Y} - \mathbf{X}\beta)'\mathbf{X} = \mathbf{0}$?)**

The LSE has the form

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

otherwise, the solution to LSE is not unique,

one often imposes further constraints to get a unique solution.

If ϵ is normal, then $\hat\beta$ is the MLE. Otherwise, it is a semi-parametric estimator.
Fitted value $\hat y_i = (x_{i1}, ..., x_{ip})\hat\beta$. $(= \hat E(Y|\mathbf{x}))$
Residuals $y_i - \hat y_i$, $i = 1, ..., n$.
If one further assumes that $V(\epsilon_i) = \sigma^2 \ \forall\ i$, then

$\hat\sigma^2 = \frac{1}{n-p}\sum_{i=1}^n (y_i - \hat y_i)^2$ is an unbiased estimator of σ^2,
and conditional on $\mathbf{X}$ (if one assumes $\mathbf{X}$ is random),
$V(\hat\beta) = \sigma^2(\mathbf{X}'\mathbf{X})^{-1}$ or $V(\hat\beta|\mathbf{X}) = \sigma^2(\mathbf{X}'\mathbf{X})^{-1}$ **(are they both correct ??)**
Is $V(\hat\beta)$ variance or covariance matrix ?

SE of $\hat\beta_j$ is $\sqrt{v}$, where v is obtained by the j-th diagonal element of $\hat\sigma^2(\mathbf{X}'\mathbf{X})^{-1}$
(why not $\sigma^2(\mathbf{X}'\mathbf{X})^{-1}$? SD = SE ? Are they r.v.'s ?)
Under NID a $(1-\alpha)100\%$ CI of β_j is $\hat\beta_j \pm t_{n-p,\alpha/2}SE$

Example 0: Suppose that $Y_i = \begin{cases} -\gamma + W_i & \text{if } i \in \{1, ..., n_-\} \\ \gamma + W_i & \text{if } i \in \{n_- + 1, ..., n,\} \end{cases}$ $n_- > 1$, and W_1, ..., W_n are i.i.d. from the exponential distribution and $E(W_1) = 1$. γ and W_i;s are unknown, though we know $W_i \sim Exp(1)$. Y_i's are observations. Derive the LSE and the MLE of γ based on these regression data.

Discussion. The typical linear regression model is
$Y_i = \beta_1 X_{i1} + \cdots + \beta_p X_{ip} + \epsilon_i = X_i'\beta + \epsilon_i$ with $E(\epsilon_i) = 0$.
$p = ?$
Do we observe Y_i ?
Do we observe $(X_{i1}, ..., X_{ip})$?
$W_i = \epsilon_i$?
Do we know β ? or $(\beta_1, ..., \beta_p)$?
If we rewrite th model as $Y_i = \alpha + \gamma X_i + \epsilon_i$, then $\alpha = ?$
Do we need to estimate α ?

Homework 10.1. Find the MLE and the LSE of β under the assumptions above.

Polynomial model: $Y_i = \beta_0 + \beta_1 x_i + \cdots + \beta_k x_i^k + \epsilon_i$, $i = 1, ..., n$.
k can be as large as $n-1$ if x_i's are all distinct.

Example 1. Data: (X_i, Y_i): (1,2), (3,4). The LSE $\hat\beta = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}$ under the models:
$Y = \beta_0 + \epsilon$, $\mathbf{X} = ?$
$Y = \beta_1 x + \epsilon$, $\mathbf{X} = ?$
$Y = \beta_0 + \beta_1 x + \epsilon$. $\mathbf{X} = ?$

If one fits model $Y = \beta_0 + \beta_1 x + \beta_2 x^2 + \epsilon$. Then $\mathbf{Y} = \begin{pmatrix} 2 \\ 4 \end{pmatrix}$, $\mathbf{X} = \begin{array}{c} \begin{array}{ccc} \beta_0 & \beta_1 & \beta_2 \end{array} \\ \begin{pmatrix} 1 & 1 & 1 \\ 1 & 3 & 9 \end{pmatrix} \end{array}$

rank of $\mathbf{X}'\mathbf{X}$ is 2. $\mathbf{X}'\mathbf{X}$ is not invertible. The LSE is not uniquely determined. We say that the parameter is not identifiable.

Possible modification: Add a constraint to β_i's, *e.g.* $\beta_0 = 0$ or $\beta_1 = \beta_2$, etc.:

models\X type :	*original*	*in model*	$\mathbf{X}$ *in LSE formula*	β
$Y = \beta_0 + \epsilon$	$1, 3$	$1, 1$	$(1, 1)'$	β_0
$Y = \beta_1 x + \epsilon$	$1, 3$	$1, 3$	$(1, 3)'$	β_1
$Y = \beta_0 + \beta_1 x + \epsilon$	$1, 3$	$(1, 1), (1, 3)$	$\begin{pmatrix} 1 & 1 \\ 1 & 3 \end{pmatrix}$	$(\beta_0, \beta_1)'$
$Y = \beta_0 + \beta_1 x + \beta_2 x^2 + \epsilon$	$1, 3$	$(1, 1, 1), (1, 3, 9)$	?	$(\beta_0, \beta_1, \beta_2)'$
$Y - 1 = \beta_1 x + \beta_2 x^2 + \epsilon$	$1, 3$	$(1, 1), (3, 9)$	?	$(\beta_1, \beta_2)'$
$Y = \beta_0 + \beta_1(x + x^2) + \epsilon$	$1, 3$	$(1, 2), (1, 12)$	?	$(\beta_0, \beta_1)'$

Example 2. One way anova table
$Y_{ij} = \mu + \alpha_j + \epsilon_{ij}$, $i = 1, ..., 4$, and $j = 1, 2, 3$.
Consider an example that there are three treatments A, B and C. There are I (=4) groups, each consists of 3 patients. Total of 12 patients. In each group, the 3 patients receive 3 different treatments separately. The result for the jth patient in the ith group is Y_{ij}.

Is it a linear regression model ?

$\beta =$?

LSE $= (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}$.

$\mathbf{X} =$? One possibility is based on $\mathbf{Y} = \mathbf{X}\beta + \mathbf{e}$,

$$\begin{pmatrix} Y_{11} \\ Y_{12} \\ Y_{13} \\ \vdots \\ Y_{41} \\ Y_{42} \\ Y_{43} \end{pmatrix} = \begin{pmatrix} Y_1 \\ Y_2 \\ Y_3 \\ \vdots \\ Y_{10} \\ Y_{11} \\ Y_{12} \end{pmatrix} = \begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ \vdots & & & \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \mu \\ \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{pmatrix} + \mathbf{e} \qquad\qquad Y_{ij} = \mu + \alpha_i + \epsilon_{ij}$$

$$= \begin{pmatrix} 1 & X_{11} & X_{12} & X_{13} \\ \vdots & & & \\ 1 & X_{n1} & X_{n2} & X_{n3} \end{pmatrix} \begin{pmatrix} \mu \\ \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{pmatrix} + \mathbf{e} = \mathbf{X}\beta + \mathbf{e}, \quad \mathbf{e} = (\epsilon_1, ..., \epsilon_{12})',$$

X_{i1}=$\mathbf{1}$(treatment=A for the $i-$th patient).

X_{i2}=$\mathbf{1}$(treatment=B for the $i-$th patient).

X_{i3}=$\mathbf{1}$(treatment=C for the $i-$th patient).

Notice that $X_{i1} + X_{i2} + X_{i3} = 1$.

$\mathbf{X}'\mathbf{X}$ is not invertible as

$\mathbf{X} = \begin{pmatrix} 1 & X_{11} & X_{12} & X_{13} \\ \vdots & \vdots & \vdots & \vdots \\ 1 & X_{n1} & X_{n2} & X_{n3} \end{pmatrix}$ is of rank at most 3, not 4,

as $\begin{pmatrix} X_{11} + X_{12} + X_{13} \\ \vdots \\ X_{n1} + X_{n2} + X_{n3} \end{pmatrix} = \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix}$ **why ?**

Thus the LSE for $Y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \beta_3 X_{i3} + \epsilon_i$ is not unique.

(We say that the parameters are not **identifiable**).

Three modifications:

M1. Revise the model. Let $Y_i = \beta_1 X_{i1} + \beta_2 X_{i2} + \beta_3 X_{i3} + \epsilon_i$ with $\mu = 0$,

$\beta = (\alpha_1, \alpha_2, \alpha_3)'$, $\mathbf{X} = \begin{pmatrix} X_{11} & X_{12} & X_{13} \\ \vdots & \vdots & \vdots \\ X_{n1} & X_{n2} & X_{n3} \end{pmatrix}$, $\hat\beta = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}$ works.

R codes: $lm(Y \sim X_1 + X_2 + X_3 - 1)$

Interpretation: β_i is the effect of treatment i (T_i).

M2. Impose a constraint $\alpha_1 = 0$ for the model

$Y_i = \mu + \alpha_1 X_{i1} + \alpha_2 X_{i2} + \alpha_3 X_{i3} + \epsilon_i$. $\qquad Y_i = (1, X_{i2}, X_{i3})(\mu, \alpha_2, \alpha_3)'$.

Let $(\beta_1, \beta_2, \beta_3)$ be as in M1.

Then $\beta_i = \mu + \alpha_i$, $i = 1$, 2, 3.

e.g., if $X_{i1} = 1$, then $Y_i = \beta_1 + \epsilon_i = \mu + \alpha_1 + \epsilon_i$, where $\alpha_1 = 0$, $\mu = \beta_1$, ...

i.e., μ is the effect of treatment 1, but α_i is the additional effect of T_i to T_1.

options(contrasts =c("contr.treatment", "contr.poly"))

$lm(Y \sim X_1 + X_2 + X_3)$.

M3. Impose another constraint $\sum_i \alpha_i = 0$ ($\alpha_3 = -\alpha_1 - \alpha_2$) for the model

$Y_i = \mu + \alpha_1 X_{i1} + \alpha_2 X_{i2} + \alpha_3 X_{i3} + \epsilon_i$

then $\mu + \alpha_i = \beta_i$, $i = 1, 2, 3$. $\qquad Y_i = (1, X_{i1} - X_{i3}, ????)(\mu, \alpha_1, \alpha_2)'$

i.e., μ is the average treatment effect, α_i is the additional effect of T_i.

options(contrasts =c("contr.sum", "contr.poly"))

$lm(Y \sim X_1 + X_2 + X_3)$

Example 3 (a simulation study on the Two way anova table).

$Y_{ij} = \mu + a_i + b_j + \epsilon_{ij}$, $i \in \{1, ..., 4\}$, $j \in \{1, ..., 6\}$

```
> y=rnorm(24)
> a=gl(4,6,24)
> b=gl(6,1,24)
> a
[1] 1 1 1 1 1 1 2 2 2 2 2 2 3 3 3 3 3 3 4 4 4 4 4 4 Levels: 1 2 3 4
> b
[1] 1 2 3 4 5 6 1 2 3 4 5 6 1 2 3 4 5 6 1 2 3 4 5 6 Levels: 1 2 3 4 5 6
> lm(y∼a+b−1) #1.
  a1      a2      a3      a4       b2       b3      b4      b5       b6
0.266   0.235   0.246  −0.379   −0.102   −0.319   0.913  −0.227   −0.125
```

$\hat{\mu}$ and $b1$= ? $(\mu, a_1, ..., a_4, b_1, ..., b_6) =$?

```
> lm(y∼a+b) #2
# or
# lm(y∼a+b, contrasts =c(”contr.treatment”, ”contr.poly”))
(Intercept)     a2       a3       a4       b2       b3      b4      b5       b6
   0.268      −0.031   −0.020   −0.645   −0.102   −0.319   0.913  −0.227   −0.125
```

$a1$,$b1$?

```
> options(contrasts =c(”contr.sum”, ”contr.poly”)) #3.
> lm(y∼a+b)
(Intercept)    a1      a2      a3      b1       b2       b3      b4      b5
   0.115      0.174   0.143   0.154  −0.023   −0.125   −0.342   0.890  −0.250
```

$a4$, $b6$?

Relation between these three ?

$\hat{E}(Y_{ij}) =$ intercept$+ai + bj =$ same ?

1.		$int. = 0$	$b1 = 0$							
int	$a1$	$a2$	$a3$	$a4$	$b1$	$b2$	$b3$	$b4$	$b5$	$b6$
0	0.27	0.24	0.25	−0.38	0	−0.10	−0.32	0.91	−0.23	−0.13
2.		$a1 = 0$	$b1 = 0$							
0.27	0	−0.03	−0.02	−0.65	0	−0.10	−0.32	0.91	−0.23	−0.13
3.		$a4 =?$	$b6 =?$							
0.12	0.17	0.14	0.15	−0.46	−0.02	−0.13	−0.34	0.89	−0.25	−0.15

$$\hat{E}(Y_{11}) = \begin{cases} 0 + 0.266 + 0 & \text{from \#1} \\ 0.268 + 0 + 0 & \text{from \#2} \quad \textbf{Are they the same ?} \\ 0.115 + 0.174 - 0.023 = 0.266 & \text{from \#3.} \end{cases}$$

What is X, β and $\hat{\beta}$ in the model $Y = X'\beta + \epsilon$ for lm($y \sim a + b$) in Ex. 3 ?

$$X = \begin{pmatrix} 1 \\ \mathbf{1}(a = 1) \\ \mathbf{1}(a = 2) \\ \mathbf{1}(a = 3) \\ \mathbf{1}(a = 4) \\ \mathbf{1}(b = 1) \\ \mathbf{1}(b = 2) \\ \mathbf{1}(b = 3) \\ \mathbf{1}(b = 4) \\ \mathbf{1}(b = 5) \\ \mathbf{1}(b = 6) \end{pmatrix} \text{ or } \begin{pmatrix} 1 \\ \mathbf{1}(a = 2) \\ \mathbf{1}(a = 3) \\ \mathbf{1}(a = 4) \\ \mathbf{1}(b = 2) \\ \mathbf{1}(b = 3) \\ \mathbf{1}(b = 4) \\ \mathbf{1}(b = 5) \\ \mathbf{1}(b = 6) \end{pmatrix} \text{ ? } \beta' = (\mu, a_2, ..., a_4, b_2, ..., b_6), \text{ and } \hat{\beta}' = \cdots \text{ ?}$$

The sample size is $n = 24$, $\hat{y} = X'\hat{\beta} = 0.27 + 0\mathbf{1}(a = 1) - 0.03\mathbf{1}(a = 2) -$
$0.02\mathbf{1}(a = 3) + \cdots + 0\mathbf{1}(b = 1) + \cdots - 0.23\mathbf{1}(b = 5) - 0.13\mathbf{1}(b = 6)$

What is β and $\mathbf{X}$ for $\hat{\beta} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}$?

$\beta = (\mu, a_2, a_3, a_4, b_2, ..., b_6)'$ and

$$\mathbf{X} = \begin{array}{c} \begin{array}{ccccccc} int & a2 & a3 & a4 & b2 & \cdots & b6 \end{array} \\ \left(\begin{array}{ccccccc} 1 & 0 & 0 & 0 & 0 & \cdots & 0 \\ 1 & 0 & 0 & 0 & 1 & \cdots & 0 \\ \vdots & & & & & & \\ 1 & 0 & 0 & 1 & 0 & \cdots & 1 \end{array}\right)_{n\times 9} \end{array} \qquad \textbf{Why ??}$$

```
a [1] 1 1 1 1 1 1 2 2 2 2 2 2 3 3 3 3 3 3 4 4 4 4 4 4
b [1] 1 2 3 4 5 6 1 2 3 4 5 6 1 2 3 4 5 6 1 2 3 4 5 6
```

Homework. 10.2. What is X and β for $\hat\beta = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}$ in $lm(y \sim a+b-1)$ in Example 3 ?

Example 3 (continued).

Another way to generate the same type of data:

```
> y=rnorm(24)
> a=rep(1,6)
> a=c(a,a+1,a+2,a+3)
> b=rep(1:6,4)
> lm(y~a+b) # #A
    (Output)
    (Intercept) a b
> a=factor(a)
> b=factor(b)
> lm(y~a+b) # #B
    (Output)
    (Intercept) a2 a3 a4 b2 b3 b4 b5 b6
```

What is X and β for $\hat\beta = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}$ in # A ?

What is X and β for $\hat\beta = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}$ in # B ?

What is the difference between outcomes # A and # B ?

```
    > lm(y~a+b−1) #1.
    > lm(y~a+b) #2
    > options(contrasts =c("contr.sum", "contr.poly")) #3.
    > lm(y~a+b)
```

Which is the way same as in Example 3 ? #A or #B ?

What do you expect the estimates $\underline{before}$ seeing output ?

```
> summary(lm(y~a+b))                    # justify the answer to the question
Coefficients:
    Estimate  Std. Error  t value  Pr(> |t|)
```

How to find the P-value to justify the answer to the previous question?
Is it Pr($>|t|$) ?

Homework 10.3.

1. Repeat Example 3 once yourself and answer the questions there.
2. Mimic Example 3 (continued) by inserting y=1+2*a+y right after b=rep(1:6,4) (not before each lm(y~a+b),as $2 * factor(a)$ does not work).

Then ask yourself relevant questions and answer them.

Hw due Wednesday before class. **Late hw -3, submit both .tex file and .pdf file !**

In regression analysis, there are several issues:

1. What is model for the data ? (LR, non-LR, Cox, Parametric) model ?
2. Can the model be simplifies ?
3. Does the model fit the data ?

Model checking

Question. Does a given set of data fits the given model (LR, non-LR, Cox, Lehmann, Parametric) ?

Ans. Various diagnostic plots, QQplots, residual plots, and model tests.
For example, for question about the LR model, test
H_0: $Y = \beta X + \epsilon$ v.s. H_1: $Y \neq \beta X + \epsilon$, $\quad X \in \mathcal{R}^p$.
Two common approaches.

1. A check of model fit. If there are replications in X_i's, that is, the model
$Y_i = \beta' X_i + \epsilon_i$, $i = 1, ..., n$,
can be written as
$Y_{ij} = \beta \mathbf{X}_{ij} + \epsilon_{ij}$, where
$j = 1, ..., J_i$,
$i = 1, ..., m$,
$X_{i1} = \cdots = X_{iJ_i}$, with $J_i > 1$ for some i,
and $X_{ij} \neq X_{kh}$ if $i \neq k$, $\quad$ *e.g*, $(X_1, ..., X_6) = (2, 2, 2, 1, 3, 3)$.
then a model lack-of-fit test of H_0^l: $\sigma_L = \sigma_E$ v.s. H_1^l: $\sigma_L \neq \sigma_E$
$\phi = \mathbf{1}(m_L/m_E > F_{df_L, df_E, \alpha})$, where
$m_E = \frac{1}{df_E} \sum_{i,j} (Y_{ij} - \overline{Y}_{i\cdot})^2$, (unbiased estimator of σ^2 under NID ($E(Y_{ij}) = \alpha_i$)
$m_L = \frac{1}{df_L} \sum_{i,j} (\overline{Y}_{i\cdot} - \hat{Y}_{ij})^2$, (unbiased estimator of σ^2 under NID and LR Model)
$df_E = \sum_i (J_i - 1)$ $(= n - m)$ and
$df_L = m - p$, df of residuals) $\quad = n - p - df_E = n - (p + df_E)$

Here, we make use of
$\sum_{i,j} Y_{ij}^2$
$= \sum_{i,j} (Y_{ij} - \overline{Y})^2 + \sum_{i,j} \overline{Y}^2 \quad = \sum_{i,j} Y_{ij}^2 - 2\overline{Y} \sum_{i,j} Y_{ij} + \sum_{i,j} (\overline{Y})^2 + \sum_{i,j} \overline{Y}^2$
$= \sum_{i,j} (Y_{ij} - \hat{Y}_{ij})^2 + \sum_{i,j} (\hat{Y}_{ij} - \overline{Y})^2 + \sum_{i,j} \overline{Y}^2$
$$= \underbrace{\sum_{i,j} (Y_{ij} - \overline{Y}_{i\cdot})^2}_{relate\ to\ m_E\ or\ m_L?} + \underbrace{\sum_{i,j} (\overline{Y}_{i\cdot} - \hat{Y}_{ij})^2}_{m_E\ or\ m_L?} + \sum_{i,j} (\hat{Y}_{ij} - \overline{Y})^2 + \sum_{i,j} \overline{Y}^2.$$
df: $(n - m)$ $\quad +(m - p)$ $\quad +(p - 1)+1$.

We also make use of NID.

Second way. If there is no replication, add another function to the model
$Y = \beta X + \epsilon$,
e.g., consider a new model
$Y = \beta X + \theta X^2 + \epsilon$ (or $Y = \beta X + \theta g(X) + \epsilon$, *e.g.*, $g(x) = (x^3, x^2)$),
and check whether $\theta = 0$, where $\theta \in \mathcal{R}$ (or $\mathcal{R}^q$ if $g(X) \in \mathcal{R}^q$).
That is, set
H_0^t: $\theta = 0$, v.s. H_1^t: $\theta \neq 0$.

(a) One test is t-test (if $q = 1$):
$\phi = \mathbf{1}(|\hat{\theta}|/\hat{\sigma}_{\hat{\theta}} > t_{n-p, \alpha/2})$.
If n is large and p is not so, the statistic does not rely on $\epsilon \sim N(\mu, \sigma^2)$.

(b) Another test is F-test:
Assuming $E(Y|X) = \beta' X + \theta' g(X)$, H_0: $\theta = 0$ v.s. H_1: $\theta \neq 0$.
Write $\mathbf{Y}_{n \times 1} = \mathbf{Z}_{n \times (p+q)} \gamma + \mathbf{e}$, where $\mathbf{Y} = (Y_1, ..., Y_n)'$,
$$\mathbf{Z} = \begin{pmatrix} X_1' & g(X_1)' \\ \cdots & \\ X_n' & g(X_n)' \end{pmatrix},$$
$$\mathbf{X} = \begin{pmatrix} X_1' \\ \cdots \\ X_n' \end{pmatrix},$$
$$\gamma = \begin{pmatrix} \beta \\ \theta \end{pmatrix}.$$
Let $\mathbf{C} = (\underbrace{\mathbf{0}}_{q \times p} \underbrace{I}_{q \times q})$, where I is an identity matrix.
The original H_0 becomes
H_0^f: $\mathbf{C}\gamma = \theta = 0$.
$\hat{\gamma} = (\mathbf{Z}'\mathbf{Z})^{-1}\mathbf{Z}'\mathbf{Y}$,
$\hat{\beta} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}$,

SSE= $\mathbf{Y}'\mathbf{Y} - \hat\gamma'\mathbf{Z}'\mathbf{Y}$ $(= ||\mathbf{Y} - \hat\gamma'\mathbf{Z}||^2)$, df= ?
SSW= $\mathbf{Y}'\mathbf{Y} - \hat\beta'\mathbf{X}'\mathbf{Y}$ $(= ||\mathbf{Y} - \hat\beta'\mathbf{X}||^2)$, df= ?

An F test is

$$\phi = \mathbf{1}\left(\frac{\frac{SSW-SSE}{q}}{\frac{SSE}{n-p-q}} > F_{q,n-p-q,\alpha}\right),$$

where q is the dimension of θ, which is 1 most of the time.
F-test relies on NID.

3 tests are introduced: (1) Lack of fit test if there are ties in X_i's, (2) t-test or F-test.

Q: 1. If there exist ties in X_i's, can we use all three approaches ?
2. If there do not exist ties in X_i's, can we use all three approaches ?

Impurity data. An experiment to determine how the initial rate of formation of an undesirable impurity (wu1dian3) Y depended on two factors:
(1) the concentration X_0 of monomer, (dan1ti3)
(2) the concentration X_1 of dimer. (shuang1ti3)
The relation is expected to be
$Y = \beta_0 X_0 + \beta_1 X_1 + \epsilon.$
The data are as follows.

order in experiment	X_0	X_1	Y	i	ij
3	0.34	0.73	5.75	1	11
6	0.34	0.73	4.79	2	12
2	0.58	0.69	5.44	3	21
4	1.26	0.97	9.09	4	31
1	1.26	0.97	8.59	5	32
5	1.82	0.46	5.09	6	41
why ordered ?					
define	$\mathbf{X}_0$	$\mathbf{X}_1$	$\mathbf{Y}$		

Can we use **all three approaches** for checking H_0: $E(Y|\mathbf{X}) = \beta_0 X_0 + \beta_1 X_1$?

Notice: $n = 6$, $i = 4$, $J_1 = J_3 = 2$ and $J_2 = J_4 = 1$.

$m_E = \frac{1}{df_E}\sum_{i,j}(Y_{ij} - \overline{Y}_{i\cdot})^2 = \frac{1}{2}(\frac{(5.75-4.79)^2}{2} + \frac{(9.09-8.59)^2}{2})$ **why ??**

```
((5.75-4.79)**2+ (9.09-8.59)**2)/4
[1] 0.2929
```

$m_L = \frac{1}{df_L}\sum_{i,j}(\overline{Y}_{i\cdot} - \hat Y_{ij})^2 = ?$

$\hat Y_{ij} = \hat\beta \mathbf{X}_{i,j}$= ?

$$\hat\beta = \begin{pmatrix} \mathbf{X}_0'\mathbf{X}_0 & \mathbf{X}_0'\mathbf{X}_1 \\ \mathbf{X}_0'\mathbf{X}_1 & \mathbf{X}_1'\mathbf{X}_1 \end{pmatrix}^{-1} \begin{pmatrix} \mathbf{X}_0'\mathbf{Y} \\ \mathbf{X}_1'\mathbf{Y} \end{pmatrix}$$

$$= \frac{1}{\mathbf{X}_0'\mathbf{X}_0\mathbf{X}_1'\mathbf{X}_1 - (\mathbf{X}_0'\mathbf{X}_1)^2} \begin{pmatrix} \mathbf{X}_1'\mathbf{X}_1 & -\mathbf{X}_0'\mathbf{X}_1 \\ -\mathbf{X}_0'\mathbf{X}_1 & \mathbf{X}_0'\mathbf{X}_0 \end{pmatrix} \begin{pmatrix} \mathbf{X}_0'\mathbf{Y} \\ \mathbf{X}_1'\mathbf{Y} \end{pmatrix}$$

Too tedious, thus use R

```
> x=c(0.34,0.73,5.75,
    0.34,0.73,4.79,
    0.58,0.69,5.44,
    1.26,0.97,9.09,
    1.26,0.97,8.59,
    1.82,0.46,5.09)
> dim(x)=c(3,6)
# y=lm(x[3,]~x[1,]+x[2,]−1)
> x=t(x)
> y=lm(x[,3]~x[,1]+x[,2]−1)
> y
    Coefficients:
```

```
x[,1]    x[,2]
1.207    7.123
```

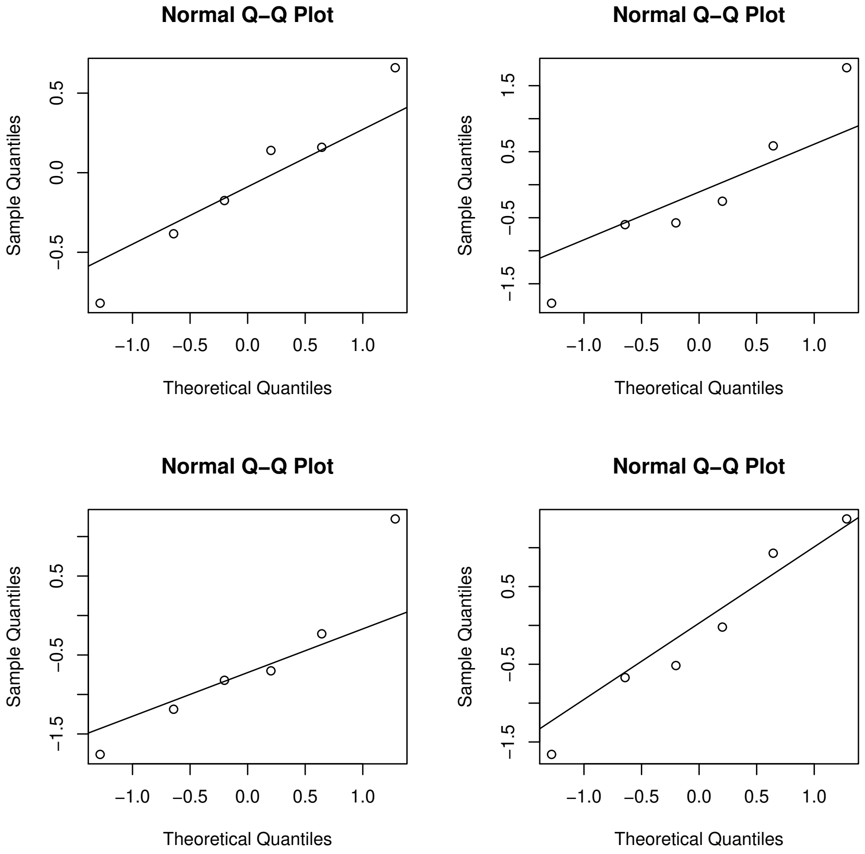


Fig. 10.1. QQ-plot data and rnorm(6) (3 times)   Why do this ?

```
par(mfrow=c(2,2))
qqnorm(y$resid)
qqline(y$resid)
z=rnorm(6)
qqnorm(z)
qqline(z)
......
```

```
> anova(y)
                 Df   Sum Sq   Mean Sq   F value   Pr(> F)
         x[,1]    1   207.693  207.693   624.29    1.523e − 05   ***
         x[,2]    1    58.901   58.901   177.05    0.0001844     ***
     Residuals    4     1.331    0.333
```

Lack of fit test $\phi = \mathbf{1}(F > F_{I-1,I(J-1),\alpha})$.

```
> z=c(1,1,2,3,3,4)
#z=factor(x[,1])
> Y=lm(x[,3]~x[,1]+x[,2]+factor(z)−1)
> anova(Y)
```

```
             Df   Sum Sq    Mean Sq        F value           Pr(> F)
    x[,1]     1   207.693   207.693        709.0903          0.001407        **
    x[,2]     1    58.901    58.901        201.0966          0.004936        **
factor(z)     2     0.745   m_L = 0.372    m_L/n_E = 1.2717  0.440202   p − value > 0.05?
Residuals     2     0.586   m_E = 0.293
```

f=1/1.27

```
1-pf(f,2,2)
```

Conclusion Do not reject the model,

and the data fit the linear regression model.

Are we done ?

The second way: H_o: $Y = \beta X + \epsilon$ v.s. H_1: $Y = \beta X + \theta g(X) + \epsilon$ with $\theta \neq 0$.

```
> z=lm(x[,3]~x[,1]+x[,2]+x[,1]*x[,2]−1)
> summary(z)
                 Estimate   Std. Error   t value   Pr(> |t|)
         x[, 1]    0.3844       0.5171     0.743     0.51120
         x[, 2]    6.4990       0.5226    12.437     0.00112           **
  x[, 1] : x[, 2]  1.6812       0.8668     1.939     0.14779   p − value > 0.05?
```

Conclusion ?

What else needs to be done ?

The third way:

```
> anova(z)
                 Df   Sum Sq   Mean Sq    F value     Pr(> F)
         x[, 1]   1  207.693   207.693  1055.2702  6.411e − 05              * * *
         x[, 2]   1   58.901    58.901   299.2726   0.0004209              * * *
  x[, 1] : x[, 2] 1    0.740     0.740     3.7615   0.1477919   p − value > 0.05?
      Residuals   3    0.590     0.197
```

Conclusion ?

Another code:

```
> anova(y,z)
    Model 1: x[, 3] ~ x[, 1] + x[, 2] - 1
    Model 2: x[, 3] ~ x[, 1] + x[, 2] + x[, 1] * x[, 2] - 1
        Res.Df     RSS      Df   Sum of Sq      F       Pr(> F)
    1      4      1.33075
    2      3      0.59044   1     0.74031     3.7615    0.1478
```

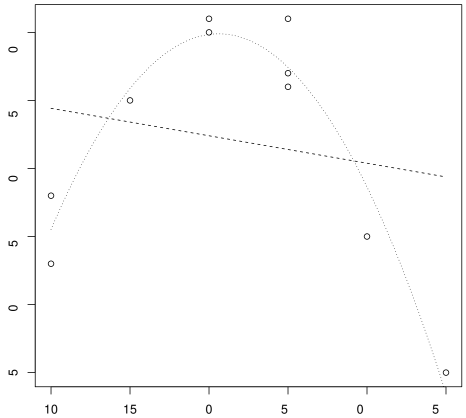
Example 4 (Growth rate data). The data in Table 10.7 is for the growth rate of rats (denoted by Y) fed various doses of a dietary supplement (denoted by X). From similar investigation, it was believed that the relation could be roughly linear. We shall test two models: a simple linear model and a quadratic model.

H_o: $E(Y|X) = \alpha + \beta X$ v.s. H_1: $E(Y|X) \neq \alpha + \beta X$.

```
y=c(73,78,85,90,91,87,86,91,75,65) # rate
x=c(10,10,15,20,20,25,25,25,30,35) # dose
a=factor(c(1,1,2,3,3,4,4,4,5,6))
#a=factor(x)
z=lm(y~x)
plot(x,y)
v=(100:350)/10
u=z$coef[1]+z$coef[2]*v
lines(v,u,lty=2)
z=lm(y~x+I(x^2))
z=z$coef
u=z[1]+z[2]*v+z[3]*v^2
lines(v,u,lty=3)
z=lm(y~x+a)
anova(z) # lack of fit test
```

```
                Df   Sum Sq   Mean Sq   F value   Pr(> F)
          x      1     24.5    24.502    3.6299   0.12946
          a      4    659.4   164.850   24.4222   0.00452   **
  Residuals      4     27.0     6.750
```

Conclusion: The linear regression model does not fit the data.



Now consider

H_o: $E(Y|X) = \beta_0 + \beta_1 X + \beta_2 X^2$ v.s. H_1: $E(Y|X) \neq \beta_0 + \beta_1 X + \beta_2 X^2$

First way, lack of fit.

z=lm(y∼x+I(xˆ 2)+a)
anova(z)

	Df	*Sum Sq*	*Mean Sq*	*F value*	*Pr(> F)*	
x	1	24.50	24.50	3.6299	0.1294567	
$I(x^2)$	1	641.20	641.20	94.9933	0.0006207	$***$
a	3	18.19	6.06	0.8985	0.5156739	
Residuals	4	27.00	6.75			

Conclusion: The quadratic regression model does fit the data.

Second way: H_o: $\beta_3 = 0$ v.s. H_1: $\beta_3 \neq 0$.

assuming $E(Y|X) = \beta_o + \beta_1 X + \beta_2 X^2 + \beta_3 X^3$.

z=lm(y∼x+I(xˆ 2)+I(xˆ 3))
summary(z)

	Estimate	*Std.Error*	*tvalue*	*Pr(> |t|)*	
(*Intercept*)	24.007599	19.712021	1.218	0.2690	
x	7.198068	3.179330	2.264	0.0642	.
$I(x^2)$	−0.222267	0.153348	−1.449	0.1974	
$I(x^3)$	0.001409	0.002276	0.619	0.5585	

Conclusion ?

Third way: H_o: $\beta_3 = 0$ v.s. H_1: $\beta_3 \neq 0$.

> anova(z)

	Df	*Sum Sq*	*Mean Sq*	*F value*	*Pr(> F)*
x	1	24.50	24.50	3.4608	0.1122
$I(x^2)$	1	641.20	641.20	90.5674	$7.677e-05$
$I(x^3)$	1	2.71	2.71	0.3834	0.5585
Residuals	6	42.48	7.08		

Conclusion ?

It seems that the data fit $Y \sim x^2$. How to check it ?

> Z=lm(y∼I(xˆ 2)+a)
> anova(Z)

	Df	*Sum Sq*	*Mean Sq*	*F value*	*Pr(> F)*
$I(x^2)$	1	91.42	91.421	13.544	0.021200
a	4	592.48	148.120	21.944	0.005533
Residuals	4	27.00	6.750		

Conclusion ?

Compare to z=lm(y∼x+I(xˆ 2)+a)

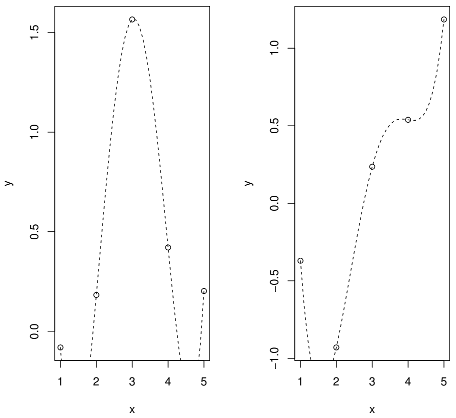
Q: Is it true that

the regression model fits the data if the regression curve fits the data well ? The answer can be found from the next example.

Example 5. Consider the model $logY \sim N(0,1)$.

```
x=1:5
y=exp(rnorm(5))
plot(x,y)
z=lm(y~x+I(x^ 2)+I(x^ 3)+I(x^ 4))
z=z$coef
v=(10:50)/10
u=z[1]+v*z[2]+z[3]*v^ 2+z[4]*v^ 3+z[5]*v^ 4
lines(v,u,lty=2)
```

Then $\hat{Y}_i = Y_i$ for all i. However, the data do not fit the polynomial regression model.
If we do it again the equation is totally different.



Model checking: Given a regression data set (X_i, Y_i)'s, to make statistical inferences on μ_Y, σ_Y, $Y = g(X) + \epsilon$ etc. we need to assume a certain model:
parametric models: normal ? exponential ? uniform ? etc.,
semi-parametric models: LR, NLR, Cox, Lehmann, among others.
which of them is appropriate ? Or none of them is ?
For example, if one choose LR model, say

$$Y_i = \beta X_i + \epsilon_i, \text{ and } \epsilon \sim N(0, \sigma^2), \tag{1}$$

and we can fit the data to the model and get the LSE of β, $F_{Y|X}$, SE of β, CI of β, and do testing about β and $F_{Y|X}$.
After these, we should ask
is the model in Eq. (1) appropriate for the data ?
is NID valid ? etc....
This is model checking. The tools are model diagnostic plots and model checking tests.
Example 6. Simulation studies on testing H_0: $Y = \beta X + W$ **(or with NID)** v.s. H_1: H_0 is not true (*i.e.* $Y \neq \beta X + W$ or NID is not true) with the R codes
(summary(y∼x+I(sin(x)))$coef[3,4]> 0.05)   # test $\phi = \mathbf{1}(p - value \leq 0.05)$ (1)
Ideally it tests H_0: $Y = \beta X + W$ **or with NID** v.s. H_1: $Y \neq \beta X + W$,
actually it tests H_0': $\theta = 0$ v.s. H_1': $\theta \neq 0$, under the assumption

$$Y = \beta X + \theta \sin X + W \textbf{ and NID}. \tag{6.1}$$

Simulation 1.

True model: $Y = X + \epsilon$, where $\epsilon \sim N(0,1)$ and $X \sim bin(3, 0.5)$.

Questions:

Is H_1' true ? How about H_1 ? Is H_0 true ? How about NID ?

What do you expect for the test ?

Sample size= 50, replication= 1000, $\beta = 1$, $\overline{\hat{\beta}}$= 0.996, sd= 0.17

Rate of accepting right H_0 is 0.952, $\hat{P}(H_1|H_0) = 0.048$, $\hat{P}(H_1'|H_0) = 0.048$, $P(H_1|H_0) =$?

Does the test work as expected ?

What do you expect if $n = 5000$?

$\hat{P}(H_0|H_1)$= 0.952 ? = ?

Simulation 2.

True model: $Y = \sin X + \epsilon$, where $X \sim bin(3, 0.5)$ and $\epsilon \sim N(0, 1)$.

H_0: $Y = \beta X + W$, H_1: $Y \neq \beta X + W$, H_1': $\theta \neq 0$ under assumption (6.1).

Questions: Is H_1' true ? How about H_1 ? Is H_0 true ? How about NID ?

What do you expect for the test ?

Sample size= 50, replication= 100, $\beta = 0$, $\overline{\hat{\beta}} = -0.003$, sd= 0.03

Rate of accepting wrong H_0 is 0.33. $\hat{P}(H_0|H_1) =$? $\hat{P}(H_0|H_1') =$?

$\hat{P}(H_1|H_0) = 1 - 0.33$?

Does the test work in this case ?

What do you expect if $n = 5000$ **?** $\hat{P}(H_0|H_1) \to 0$? $\hat{P}(H_0|H_1) \to 1$?

Simulation 3.

True model: $Y = X^{1/2} + \epsilon$, where $\epsilon \sim N(0,1)$ and $X \sim bin(3, 0.5)$.

H_0: $Y = \beta X + W$, H_1: $Y \neq \beta X + W$, H_1': $\theta \neq 0$ under assumption (6.1).

Questions: Is H_1' true ? How about H_1 ? Is H_0 true ? How about NID ?

What do you expect for the test ?

Sample size= 5000, replication= 100, β= 0, $\overline{\hat{\beta}}$= 0.5150, sd= 0.1761

Rate of accepting wrong H_0 is 0.00. $\hat{P}(H_0|H_1) = 0.00$ **??** $\hat{P}(H_0|H_1') = 0.00$ **??**

It says that H_1' is true, the model is $Y = \alpha + \beta X + \theta \sin X + \epsilon$.

Does the test work in this case ?

Both H_0 and H_1' are wrong, though H_1 is true. It happens to work.

Simulation 4.

True model $Y = X^{1/2} + \epsilon$, where $X \sim B * |W|$, $B \sim U(0, 3)$, $B \perp W$, and ϵ and $W \sim Cauchy$.

H_0: $Y = \beta X + W$, H_1: $Y \neq \beta X + W$, H_1': $Y = \beta X + \theta \sin X + W$, $\theta \neq 0$.

Questions: Is H_1' true ? How about H_1 ? Is H_0 true ? How about NID ?

What do you expect for the test ?

Sample size= 5000, replication= 100, $\beta = 0$, $\overline{\hat{\beta}}$= 0.0149, sd= 0.0141

rate of accepting wrong H_0 is 0.96. $\hat{P}(H_0|H_1) = 0.96$? $\hat{P}(H_0|H_1') = 0.96$?

Does the test work in this case ?

Remark. The homework solution is in my website. Quiz on 447 and 448 on Friday.

The codes for simulations 1-4 are as follows.

```
n=5000 # need to adjust for input sample
beta=1
NN=100 # No. of simulation replication
swb = 1 # switch for binomial covariant
swn = 0 # switch for normal error
sww = 1 # switch for wrong LR model
p=0 # No. of accepting H0
b=0 # LSE
s=0 # SD of LSE
for (N in 1:NN) {
    c=rbinom(n,3,0.5)
    if (swb == 0)
        c=abs(rcauchy(n))*c
    c=sort(c)
    e=rcauchy(n)
    if (swn == 1)
        e=rnorm(n)
    y=beta*c+e
    if (sww == 1)
        y=beta*sqrt(c)+e
    z=lm(y~c+I(sin(c)))
    b=b+z$co[2]
    s=s+z$co[2]*z$co[2]
    p=p+(summary(z)$coef[3,4]>0.05) }
(p=p/NN)
(b=b/NN)
(s=sqrt(s/NN-b*b))
summary(z)$coef
                Estimate   Std. Error    t value     Pr(> |t|)   (needs NID)
(Intercept)   -4.8670290    3.324966   -1.4637829   0.14331617
     c         2.8889273    1.472481    1.9619452   0.04982429
  I(sin(c))   -0.5723319    3.625139   -0.1578786   0.87455884
```

Example 7. Simulation on testing

H_0: $Y=\beta\sin X+W$ v.s. H_1: H_0 is false.

H_1': $Y=\beta\sin X+\theta X+W$, with $\theta\neq 0$, under NID.

The R codes

(summary(y~x+I(sin(x)))$coef[2,4]> 0.05)   # test $\phi=\mathbf{1}(p{-}value\leq 0.05)$

True model $Y=X+W$, where $X\sim bin(3,0.5)$ and $W\sim|Cauchy|$.

Questions:

Is H_1 true ?

Is H_1' true ?

Is H_0 true ?

What do you expect for the test ?

Sample size= 50, replication= 1000, $\theta=1$, $\hat\theta$= 2.324, sd= 47.06,

rate of accepting H_0 is 0.795. $\hat P(H_0|H_1)=0.795$? $\hat P(H_0|H_1')=0.795$? $\hat P(H_1|H_0)=1-0.795$?

Summary on the simulation studies.

There are many regression models:

the linear regression models,

the logistic regression models,

the generalized linear (regression) models,

the generalized additive models, etc..

Given a data set, one needs to check which model fits the data. This is to test

H_0: the data fits a given model, *e.g.*, $E(Y|X)=\beta'X$, v.s. H_1: H_0 is false.

To implement, people design H_1' instead. If H_0 and H_1' are not properly designed, then the previous 3 model checking tests can be misleading as in simulations 3 and 4 of Ex. 6.

The existing model checking tests are the tests of

H_0^t: $\xi(\cdot)=0$, v.s. H_1^t: $\xi(\cdot)\neq 0$, where $\xi(\mathbf{X})=E(Y|\mathbf{X})-\beta'\mathbf{X}$ has a certain form with NID.

e.g., $\xi=\theta g(\mathbf{X})$ in the 3 aforementioned model checking tests. In order to establish the distribution theories for the tests, each of these tests imposes certain regularity conditions on $F_{\mathbf{X},Y}$ such as NID, which specifies a parameter space for $F_{\mathbf{X},Y}$, say Θ_p, under which the test is valid. The Θ_p depends on the specific test and is a certain common regression model that contains Θ_0. For instance, in Example 6,

$$\Theta_p=\{F_{\mathbf{X},Y}:\ Y=\alpha+\beta X+\theta\sin X+\epsilon,\ \epsilon\sim N(0,\sigma^2),\ X\perp\epsilon\}.$$

Thus $\Theta_p\neq\Theta$, the family of all cdfs $F_{\mathbf{X},Y}$. If $F_{\mathbf{X},Y}\notin\Theta_p$, these tests are <u>*invalid*</u> in

the sense that the (asymptotic) distributions specified for these tests are false.
In simulation 1, H_0 is true and the model assumptions holds,

the test can either reject H_0 or do not reject. But $P(H_1|H_0) = 0.05$.

In simulation 2, H_1 is true, and the assumptions for the t-test hold.

The test rejects H_0 with probability $\to 1$ as $n \to \infty$
($P(H_0|H_1) \to 0$, $P(H_0|H_1') \to 0$, a consistent test). $P(H_1|H_0)$= ?

In simulations 3 and 4, both H_0 and H_1' are false, thus no $P(H_0|H_1')$.

The test can reject H_0 with probability 0 or 0.96, *i.e.*, $P(H_0|H_1)$ can be ≈ 0 or 0.96.

In Example 7, both H_0 and H_1' are false, as NID is false and $E(W|X)$ does not exist.

An estimate of $P(H_0|H_1)$ is ≈ 0.8.

Remark. Type I error, denoted by $H_1|H_0$, implies that H_0 is true. In Simulation 1 of Ex.6, it is true that $P(H_1|H_0) = 0.05$. It works as expected.
Type II error, denoted by $H_0|H_1$, implies that H_1 is true. In Simulation 2 of Ex.6, it is true that $P(H_0|H_1) \approx 0.33 \to 0$, as $n \to \infty$. It works as expected.
In Simulations 3 and 4 of Ex.6 and in Example 7, neither H_0 nor H_1' is true. Thus neither $P(H_1|H_0)$ nor $P(H_0|H_1')$ is a proper term. The test is based on invalid assumption in (6.1) Thus the test is not valid. Just like a random guess. $\hat{P}(H_0|H_1)$ can be ≈ 0, 0.8, 1.

Interpretation of one way anova $Y_{ij} = \mu + \alpha_i + \epsilon_{ij}$, $i = 1, 2, 3$; $j = 1, ..., 10$.
Another way:

$$E(Y_{ij}|X) = \mu + \sum_{i=1}^{3} \alpha_i \mathbf{1}(\text{Treatment= i for the } ij\text{−th person}) \qquad (1)$$

There are 3 treatments, each is applied to 10 people. α_i is the effect of treatment i.
From Eq. (1), there are 3 equations and 4 unknown variables (due to $i \in \{1, 2, 3\}$.

$E(Y_{1j}|X) = \mu + \alpha_1$,
$E(Y_{2j}|X) = \mu + \alpha_2$,
$E(Y_{3j}|X) = \mu + \alpha_3$, j=1,...,10.

(1) $\mu = 0$. α_i is the average effect of treatment i.

(2) $\alpha_1 = 0$. μ is the average effect of treatment 1. α_i is the deviation effect of treatment i from treatment 1. (Obviously $\alpha_1 = 0$).

(3) $\sum_{i=1}^{3} \alpha_i = 0$. μ is the average effect of the 3 treatments. α_i is the deviation effect of treatment i from the average.

```
x=1:3
x=rep(x,10)
y=4*x+rnorm(30)
lm(y∼x)
lm(y∼ factor(x)-1)
lm(y∼ factor(x))
options(contrasts =c(”contr.sum”, ”contr.poly”))
lm(y∼ factor(x))
```

$lm(y \sim x)$	$(Intercept)$	x		
$\hat{\beta}$	-0.5422	4.2430		
β	0	4		
$lm(y \sim factor(x) - 1)$		$factor(x)1$	$factor(x)2$	$factor(x)3$
$\hat{\beta}$		3.757	7.832	12.243
β		4	8	12
$lm(y \sim factor(x))$	$(Intercept)$		$factor(x)2$	$factor(x)3$
$\hat{\beta}$	3.757	$?$	4.075	8.486
β	4	0	4	8
$contr.sum$				
$lm(y \sim factor(x))$	$(Intercept)$	$factor(x)1$	$factor(x)2$	
$\hat{\beta}$	7.9439	-4.1871	-0.1119	$?$
β	8	-4	0	4

Remark.

Once contr.sum is applied, it remains there unless we apply options(contrasts =c(”contr.treatment”, ”contr.poly”))

Chapter 4. Comparing a number of entities

4.1. Analysis of Variance (ANOVA)

One-way ANOVA is to check the difference between several samples, in contrast to the t-test which is to check the difference between two samples.

Suppose that

$Y_{tj} = \tau_t + \epsilon_{tj}$, $t = 1, ..., I$ and $j = 1, ..., J$,

where $\epsilon_{tj} \sim N(0, \sigma^2)$, and τ_t is the averages of the $t-$th sample (a parameter).

H_o: $\tau_1 = \cdots = \tau_I$ v.s. H_1: at least one inequality.

If $I = 2$, we use $t-$ test.

Example 3. Let $I = 3$, $J = 2$, $\begin{pmatrix} Y_{11} & Y_{12} \\ Y_{21} & Y_{22} \\ Y_{31} & Y_{32} \end{pmatrix}$, then $n = 6$, $p = 3$,

$$\mathbf{Y} = \begin{pmatrix} Y_{11} \\ Y_{21} \\ Y_{31} \\ Y_{12} \\ Y_{22} \\ Y_{32} \end{pmatrix} = \mathbf{X}\beta + \mathbf{e},\ \mathbf{X} = ??\ \beta = ??$$

$X_{tj} = (X_{tj1}, X_{tj2}, X_{tj3})$, where $X_{tjk} = \mathbf{1}(t = k)$.

Remark. The model is $E(Y_{tj}) = \tau_t$, $t \in \{1, 2, 3\}$, $j \in \{1, 2\}$, which is often written as

$$E(Y_{tj}) = \tau_t = \eta + \alpha_t \tag{1}$$

$$E(Y_{tj}) = \tau_t = \eta + \alpha_t \text{ with } \alpha_1 = 0 \tag{2}$$

$$E(Y_{tj}) = \tau_t = \eta + \alpha_t \text{ with } \sum_{j=1}^{3} \alpha_j = 0 \tag{3}$$

$$E(Y_{tj}) = \tau_t = \alpha_t \ \text{ with } \eta = 0 \tag{4}$$

We say the parameters in Eq. (1) are not identifiable, as $\exists$ infinitely many solutions, *e.g.*,

$(\eta, \alpha_1, \alpha_2, \alpha_3) = (0, \tau_1, \tau_2, \tau_3)$,

$(\eta, \alpha_1, \alpha_2, \alpha_3) = (\tau_1, \tau_1 - \tau_1, \tau_2 - \tau_1, \tau_3 - \tau_1)$

$(\eta, \alpha_1, \alpha_2, \alpha_3) = (\overline{\tau}, \tau_1 - \overline{\tau}, \tau_2 - \overline{\tau}, \tau_3 - \overline{\tau})$ $\qquad (\overline{\tau} = \sum_{t=1}^{3} \tau_t / 3)$

are 3 solutions to Eq. (1).

Since the parameters in Eq. (1) are not identifiable, the LSE cannot be uniquely determined. Thus we either set $\eta = 0$, or $\alpha_1 = 0$ or $\sum_{t=1}^{I} \alpha_t = 0$.

For testing

H_o: $\tau_1 = \cdots = \tau_I$ v.s. H_1: H_o is false.

The test is $\phi = \mathbf{1}(F > F_{I-1,I(J-1),\alpha})$, where F is given in the ANOVA table.

Source of variation	*sum of squares*	*df*	*mean square*	F
Between treatments	$S_T = \sum_{t,j}(\overline{Y}_{t,\cdot} - \overline{Y})^2$	$\nu_T = I - 1$	$m_T = \frac{S_T}{\nu_T}$	
Within treatments	$S_R = \sum_{t,j}(Y_{tj} - \overline{Y}_{t,\cdot})^2$	$\nu_R = I(J-1)$	$m_R = \frac{S_R}{\nu_R}$	$\frac{m_T}{m_R}$
$(hint)$	$= \sum_i (Y_i - \hat{Y}_i)^2$	$= n - p$		
Total about $\overline{Y}$	$S_D = \sum_{i,j}(Y_{ij} - \overline{Y})^2$	$\nu_D = IJ - 1$		

due to NID and

$$\textstyle\sum_{t,j} Y_{tj}^2 = \underbrace{\sum_{t,j}(Y_{tj} - \overline{Y})^2}_{S_D} + \sum_{t,j}\overline{Y}^2 = \underbrace{\sum_{t,j}(\overline{Y}_{t\cdot} - \overline{Y})^2}_{?} + \underbrace{\sum_{t,j}(Y_{tj} - \overline{Y}_{t\cdot})^2}_{?} + \sum_{t,j}\overline{Y}^2.$$

Blood Coagulation Time Example.

Table 4.1 gives coagulation times for sample blood drawn from 24 animals receiving 4 different diets A, B, C and D.

Question: Is there evidence to indicate any real difference between the mean coagulation times for the four different diets ?

To randomized the outcomes, in addition to randomly select 24 animals,

one may randomly put them into four groups by (1) number them, and (2) use

```
> sample(1:24,replace=F)
    [1] 7 11 19 16 20 2 — 8 5 9 23 1 21 — 3 12 15 22 24 13 — 6 17 10 14 4 18
```

(What is the output in the following Table ?)

$$\text{The data are} \quad \begin{array}{cccc} A & B & C & D \\ 62^{(20)} & 63^{(12)} & 68^{(16)} & 56^{(23)} \\ 60^{(2)} & 67^{(9)} & 66^{(7)} & 62^{(3)} \\ 63^{(11)} & 71^{(15)} & 71^{(1)} & 60^{(6)} \\ 59^{(10)} & 64^{(14)} & 67^{(17)} & 61^{(18)} \\ 63^{(5)} & 65^{(4)} & 68^{(13)} & 63^{(22)} \\ 59^{(24)} & 66^{(8)} & 68^{(21)} & 64^{(19)} \end{array}, \ I = 4,\ J = 6,$$

Source of variation	*sum of squares*	*df*	*mean square*	F
Between treatments	$S_T = 228$	$\nu_T = 3$	$m_T = 76$	
Within treatments	$S_R = 112$	$\nu_R = 20$	$m_R = 5.6$	13.57
Between treatments	$S_T = \sum_{t,j}(\overline{Y}_{t,\cdot} - \overline{Y})^2$	$\nu_T = I - 1$	$m_T = \frac{S_T}{\nu_T}$	
Within treatments	$S_R = \sum_{t,j}(Y_{tj} - \overline{Y}_{t,\cdot})^2$	$\nu_R = I(J-1)$	$m_R = \frac{S_R}{\nu_R}$	$\frac{m_T}{m_R}$

```
> x=c( 62 , 63 , 68 , 56, 60 , 67 , 66 , 62, 63 , 71 , 71 , 60, 59 , 64 , 67 , 61, 63 , 65
, 68 , 63, 59 , 66 , 68 , 64)
> (treatment=gl(4,1,24))
    [1] 1 2 3 4 1 2 3 4 1 2 3 4 1 2 3 4 1 2 3 4 1 2 3 4
    Levels: 1 2 3 4
> (obj=lm(x~treatment))
```

$$\begin{array}{cccc} (Intercept) & treatment2 & treatment3 & treatment4 \\ 6.100e+01 & 5.000e+00 & 7.000e+00 & -9.999e-15 \\ \overline{Y}_{1\cdot} & \overline{Y}_{2\cdot} - \overline{Y}_{1\cdot} & \overline{Y}_{3\cdot} - \overline{Y}_{1\cdot} & \overline{Y}_{4\cdot} - \overline{Y}_{1\cdot} \end{array}$$

```
> anova(obj)
                Df   Sum Sq   Mean Sq   F value    Pr(> F)
    treatment    3     228      76.0     13.571   4.658e-05   ***
    Residuals   20     112       5.6
```

Summary:

H_o: $\tau_1 = \cdots = \tau_4$ v.s. H_1: at least one inequality.
Conclusion: Yes, reject H_o, as F is far away from 1 **(where do we know it ?)**

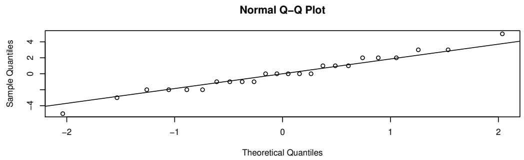
P-values is 0.00005.

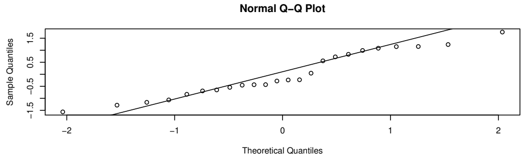
There is real difference between the mean coagulation times for the four different diets.

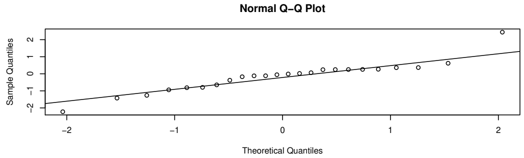
For one way anova (under control.sum):
$Y_{ij} = \eta + \alpha_i + \epsilon_{ij}$, $i \in \{1, ..., I\}$, $j \in \{1, ..., J\}$,
$\sum_i \alpha_i = 0$
=> $\overline{Y} = \eta + \overline{\epsilon}$,
$\overline{Y}_{i\cdot} = \eta + \alpha_i + \overline{\epsilon}_{i\cdot}$, $i \in \{1, ..., I\}$. One can also explain by
$(\hat{\eta}, \hat{\alpha}_1, ..., \hat{\alpha}_{I-1})' = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}$.

Blood Coagulation Time Example (continued).

```
> summary(lm(x~treatment-1))

                  Estimate   Std. Error   t value      Pr(> |t|)
      treatment1   61.0000      0.9661      63.14    < 2e − 16 ∗ ∗∗
      treatment2   66.0000      0.9661      68.32    < 2e − 16 ∗ ∗∗
      treatment3   68.0000      0.9661      70.39    < 2e − 16 ∗ ∗∗
      treatment4   61.0000      0.9661      63.14    < 2e − 16 ∗ ∗∗
> dim(x)=c(4,6); X=t(x)
> apply(X,2,mean)

    [1] 61 66 68 61

> summary(lm(x~treatment))

                     Estimate     Std. Error   t value      Pr(> |t|)
     (Intercept)    6.100e + 01   9.661e − 01   63.141    < 2e − 16 ∗ ∗∗
      treatment2    5.000e + 00   1.366e + 00    3.660      0.00156 ∗ ∗
      treatment3    7.000e + 00   1.366e + 00    5.123    5.18e − 05 ∗ ∗∗
      treatment4   −1.000e − 14   1.366e + 00    0.000        1.00000
> treat=rep(c(1,2,3,1),6)
    # what does 4→ 1 mean ? (see summary(lm(x~treatment-1)))
> a=lm(x~factor(treat))
> summary(a)

                    Estimate   Std. Error   t value      Pr(> |t|)
      (Intercept)    61.0000     0.6667      91.500    < 2e − 16 ∗ ∗∗
   factor(treat)2     5.0000     1.1547       4.330    0.000295 ∗ ∗∗
   factor(treat)3     7.0000     1.1547       6.062    5.14e − 06 ∗ ∗∗

> a=lm(x~factor(treat)-1)
> summary(a)   # compare "Estimate" in these two summaries.

                    Estimate   Std. Error   t value      Pr(> |t|)
   factor(treat)1    61.0000     0.6667      91.50     < 2e − 16 ∗ ∗∗
   factor(treat)2    66.0000     0.9428      70.00     < 2e − 16 ∗ ∗∗
   factor(treat)3    68.0000     0.9428      72.12     < 2e − 16 ∗ ∗∗
> anova(a) Analysis of Variance Table

                   Df   Sum Sq   Mean Sq   F value      Pr(> F)
   factor(treat)    3    98532     32844    6158.2   < 2.2e − 16 ∗ ∗∗
      Residuals    21      112         5

> qqnorm(a$resid)
> qqline(a$resid)
> b=rnorm(24)
> qqnorm(b)
> qqline(b) # repeat the last 3 lines one or two times why ?
```







Two-way ANOVA is to check the difference between several samples, and between blocks.

Suppose that

$$Y_{tj} = \eta + \tau_t + \beta_j + \epsilon_{tj},\ t = 1, ..., k \text{ and } j = 1, ..., n,$$

where $\epsilon_{tj} \sim N(0, \sigma^2)$, η, τ_t and β_j are parameters, subject to

$$\tau_1 = 0 = \beta_1 \text{ (or } \sum_t \tau_t = \sum_j \beta_j = 0).$$

We shall do three tests:

H_o^*: $\tau_1 = \cdots = \tau_k$ and $\beta_1 = \cdots = \beta_n$ v.s. H_1^*: at least one inequality.

H_o: $\tau_1 = \cdots = \tau_k$ v.s. H_1: at least one inequality.

H_o': $\beta_1 = \cdots = \beta_n$ v.s. H_1': at least one inequality.

Source of variation	*sum of squares*	*df*	*mean squares*	*F*
Between blocks	$S_B = \sum_{j=1}^n (\overline{Y}_{\cdot,j} - \overline{Y})^2$	$\nu_B = n - 1$	$m_B = \frac{S_B}{\nu_B}$	$\frac{m_B}{m_R}$
Between treatments	$S_T = \sum_{t=1}^k (\overline{Y}_{t,\cdot} - \overline{Y})^2$	$\nu_T = k - 1$	$m_T = \frac{S_T}{\nu_T}$	$\frac{m_T}{m_R}$
Within treatments and blocks	$S_R = \sum_{t,j}(Y_{t,j} - \overline{Y}_{t,\cdot} - \overline{Y}_{\cdot,j})^2$	$\nu_R = (k-1)(n-1)$	$m_R = \frac{S_R}{\nu_R}$	
Total about $\overline{Y}$	$S_D = \sum_{t,j}(Y_{tj} - \overline{Y})^2$	$\nu_D = kn - 1$		
H_0^*	$S_B + S_T$	$\nu_B + \nu_T$		$\frac{\frac{S_B+S_T}{\nu_B+\nu_T}}{m_R}$

$$\sum_{t,j} Y_{tj}^2 = S_D + \sum_{t,j} \overline{Y}^2 = S_B + S_T + S_R + \sum_{t,j} \overline{Y}^2.$$

Blood Coagulation Time Example (continued).

H_o^*: $\tau_1 = \cdots = \tau_k$, $\beta_1 = \cdots = \beta_n$ v.s. v.s. H_1^*: at least one inequality.

H_o: treatment effects: $\tau_1 = \cdots = \tau_k$ v.s. H_1: at least one inequality.

H_o': row effects $\beta_1 = \cdots = \beta_n$ v.s. H_1': at least one inequality.

```
> (row=gl(6,4,24))
    [1] 1 1 1 1 2 2 2 2 3 3 3 3 4 4 4 4 5 5 5 5 6 6 6 6
    Levels: 1 2 3 4 5 6
> (tr=lm(x∼treatment+row))
```

(Intercept)	*treatment*2	*treatment*3	*treatment*4	*row*2	*row*3
$5.925e+01$	$5.000e+00$	$7.000e+00$	$1.285e-14$	$1.500e+00$	$4.000e+00$
*row*4	*row*5	*row*6	↑		
$5.000e-01$	$2.500e+00$	$2.000e+00$	↓		

(Intercept)	*treatment*2	*treatment*3	*treatment*4	*row*2	*row*3
$\overline{Y}_{1\cdot} + \overline{Y}_{\cdot 1} - \overline{Y}$	$\overline{Y}_{2\cdot} - \overline{Y}_{1\cdot}$	$\overline{Y}_{3\cdot} - \overline{Y}_{1\cdot}$	$\overline{Y}_{4\cdot} - \overline{Y}_{1\cdot}$	$\overline{Y}_{\cdot 2} - \overline{Y}_{\cdot 1}$	$\overline{Y}_{\cdot 3} - \overline{Y}_{\cdot 1}$

$\hat{Y}_{11} = ?$

$\hat{Y}_{21} = ?$

$\overline{Y}_{2\cdot}+\overline{Y}_{\cdot 1}-\overline{Y}$

```
> summary(tr) Call: lm(formula = x ~ treatment + row)
                  Estimate    Std. Error   t value     Pr(> |t|)
 (Intercept)     5.925e+01    1.328e+00    44.630    < 2e-16 ***
  treatment2     5.000e+00    1.252e+00     3.995     0.00117 **
  treatment3     7.000e+00    1.252e+00     5.593    5.14e-05 ***
  treatment4    -1.088e-14    1.252e+00     0.000     1.00000
        row2     1.500e+00    1.533e+00     0.978     0.34335
        row3     4.000e+00    1.533e+00     2.609     0.01973*
        row4     5.000e-01    1.533e+00     0.326     0.74881
        row5     2.500e+00    1.533e+00     1.631     0.12374
        row6     2.000e+00    1.533e+00     1.305     0.21167
> u=lm(x~1)
```

> anova(u,tr) # **which null hypothesis does it test ?**

```
   Model 1: x ~ 1
   Model 2: x ~ treatment + row
      Res.Df    RSS    Df   Sum of Sq       F        Pr(> F)
   1    23     340.0
   2    15      70.5    8     269.5      7.1676   0.0005797   ***
> anova(tr)
                Df   Sum Sq   Mean Sq   F value    Pr(> F)
  treatment      3   228.0     76.0     16.170   5.745e-05
     row         5    41.5      8.3      1.766     0.1806      how many tests ?
  Residuals     15    70.5      4.7
```

$\frac{228+41.5}{3+5}/4.7 = 7.167553$ indent

```
> aov(x~treatment+row)
                         treatment    row    Residuals
  Sum of Squares           228.0     41.5      70.5       (see columns 1&2 of anova(tr))
  Deg. of Freedom            3         5        15
```

Residual standard error: 2.167948 ($=\sqrt{4.7}$).

Ans: Reject H_0^* and H_0, but not H_0', the row effect is not significant, the model should be $x \sim$ treatment

$x = 61$treatment[1 or 4] +66treatment[2]+ 68treatment[3]

($x = 61 \cdot \mathbf{1}$(treatment is type 1 or 4)+$66 \cdot \mathbf{1}$(treatment is type 2)+$68 \cdot \mathbf{1}$(treatment is type 3)

Derive the LSE directly for two way anova:

$Y_{ij} = \eta + \alpha_i + \gamma_j$, $i \in \{1, ..., I\}$, $j \in \{1, ..., J\}$,

$\sum_i \alpha_i = \sum_j \gamma_j = 0$ (contr.sum) (the simplest way).

$$=> \quad \sum_i \sum_j Y_{ij}/n = \sum_i \sum_j (\eta + \alpha_i + \gamma_j)/n = \eta + \sum_j \sum_i \alpha_i/n + \sum_i \sum_j \gamma_j/n.$$

$\overline{Y} = \eta$, $=> \hat{\eta} = \overline{Y}$; (due to MME).

$\overline{Y}_{i\cdot} = \eta + \alpha_i$, $i \in \{1, ..., I\}$, $=> \hat{\alpha}_i = \overline{Y}_{i\cdot} - \overline{Y}$;

$\overline{Y}_{\cdot j} = \eta + \gamma_j$, $j \in \{1, ..., J\}$, $=> \hat{\gamma}_j = \overline{Y}_{\cdot j} - \overline{Y}$;

$\hat{Y}_{ij} = \hat{\eta} + \hat{\alpha}_i + \hat{\gamma}_j = \overline{Y}_{i\cdot} + \overline{Y}_{\cdot j} - \overline{Y}$.

For instance, if $(I, J) = (3, 2)$, $\mathbf{Y} = \begin{pmatrix} Y_{11} \\ Y_{21} \\ Y_{31} \\ Y_{12} \\ Y_{22} \\ Y_{32} \end{pmatrix}$, $\beta = \begin{pmatrix} \eta \\ \alpha_1 \\ \alpha_2 \\ \gamma_1 \end{pmatrix}$, $\mathbf{X} = \begin{pmatrix} 1 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & -1 & -1 & 1 \\ 1 & 1 & 0 & -1 \\ 1 & 0 & 1 & -1 \\ 1 & -1 & -1 & -1 \end{pmatrix}$

$(\hat{\eta}, \hat{\alpha}_1, ..., \hat{\alpha}_{I-1}, \hat{\gamma}_1, ..., \hat{\gamma}_{J-1})' = (\mathbf{X'X})^{-1}\mathbf{X'Y}$ (contr.sum), $lm(y \sim row + col)$.

The LSE can also be derived by

$(\hat{\eta}, \hat{\alpha}_2, ..., \hat{\alpha}_I, \hat{\gamma}_2, ..., \hat{\gamma}_J)' = (\mathbf{X'X})^{-1}\mathbf{X'Y}$ (default), $lm(y \sim row + col)$.

If $(I,J)=(3,2)$, $\mathbf{Y}=\begin{pmatrix}Y_{11}\\Y_{21}\\Y_{31}\\Y_{12}\\Y_{22}\\Y_{32}\end{pmatrix}$, $\beta=\begin{pmatrix}\eta\\\alpha_2\\\alpha_3\\\gamma_2\end{pmatrix}$, $\mathbf{X}=\begin{pmatrix}1&0&0&0\\1&1&0&0\\1&0&1&0\\1&0&0&1\\1&1&0&1\\1&0&1&1\end{pmatrix}$

How about $(\hat\alpha_1,\hat\alpha_2,...,\hat\alpha_I,\hat\gamma_2,...,\hat\gamma_J)'=(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}$ (default) $(lm(y\sim row+col-1))$?

In two-way anova, $\hat Y_{ij}=\hat\eta+\hat\alpha_i+\hat\gamma_j=\overline{Y}_{i\cdot}+\overline{Y}_{\cdot j}-\overline{Y}$ is valid for the 3 models. It is easiest to derive the LSE through control.sum model, then to yield the other LSE's.

$lm(y\sim)$	$(Intercept)$	$r1$	$r2$	$r3$	$c1$	$c2$
$r+c$	$\overline{Y}_{1\cdot}+\overline{Y}_{\cdot1}-\overline{Y}$	0	$\overline{Y}_{2\cdot}-\overline{Y}_{1\cdot}$	$\overline{Y}_{3\cdot}-\overline{Y}_{1\cdot}$	0	$\overline{Y}_{\cdot2}-\overline{Y}_{\cdot1}$
sum	$\overline{Y}$	$\overline{Y}_{1\cdot}-\overline{Y}$	$\overline{Y}_{2\cdot}-\overline{Y}$	$\overline{Y}_{3\cdot}-\overline{Y}$	$\overline{Y}_{\cdot1}-\overline{Y}$	$\overline{Y}_{\cdot2}-\overline{Y}$
$r+c-1$	0	$\overline{Y}_{1\cdot}+\overline{Y}_{\cdot1}-\overline{Y}$	?	?	0	$\overline{Y}_{\cdot2}-\overline{Y}_{\cdot1}$

Key: $\hat Y_{ij}$ are the same in 3 forms. It is equivalent to the identifying the parameters in $E(Y_{ij})=\eta+\alpha_i+\gamma_j$:

	η	α_1	α_2	α_3	γ_1	γ_2
$i+j$	$E(Y_{1\cdot})+E(Y_{\cdot1})-E(Y_{\cdot\cdot})$	0	$E(Y_{2\cdot})-E(Y_{1\cdot})$	$E(Y_{3\cdot})-E(Y_{1\cdot})$	0	$E(Y_{\cdot2})-E(Y_{\cdot1})$
sum	$E(Y_{\cdot\cdot})$					
$i+j-1$	0					

A simulation for understanding the estimates.

```
> y=rnorm(6)
> (col=gl(2,3,6))
    [1] 1 1 1 2 2 2
> (row=gl(3,1,6))
    [1] 1 2 3 1 2 3
> x=y
> dim(x)=c(3,2)
> (a=mean(x))
    [1] -0.3406383
> mean(x[1,])-a
    [1] 0.6422441
> mean(x[2,])-a
    [1] -0.2224916
> mean(x[,1])-a
    [1] -0.07302435
> options(contrasts =c("contr.sum", "contr.poly"))
> lm(y~row)
```

$(Intercept)$	$row1$	$row2$
-0.3406	0.6422	-0.2225
$\overline{Y}$	$\overline{Y}_{1\cdot}-\overline{Y}$	$\overline{Y}_{2\cdot}-\overline{Y}$

```
> lm(y~col)
```

$(Intercept)$	$col1$
-0.34064	-0.07302
$\overline{Y}$	$\overline{Y}_{\cdot1}-\overline{Y}$

```
> lm(y~row+col)
```

$(Intercept)$	$row1$	$row2$	$col1$
-0.34064	0.64224	-0.22249	-0.07302
$\overline{Y}$	$\overline{Y}_{1\cdot}-\overline{Y}$	$\overline{Y}_{2\cdot}-\overline{Y}$	$\overline{Y}_{\cdot1}-\overline{Y}$

$>$ anova(lm(y$\sim$row+col)) #**What do you expect ?**

	Df	$Sum\ Sq$	$Mean\ Sq$	$F\ value$	$Pr(>F)$	$\hat\sigma$
row	2	0.63053	0.315267	1.2241	0.4496	0.561
col	1	0.07823	0.078233	0.3038	0.6369	0.279
$Residuals$	2	0.51508	0.257542			0.507
$row+col$	3	0.708	0.236	$\approx 1-$		0.486

What is (p, β, σ) in lm(y∼row+col) ?
What are the conclusions about H_0, H_0' and H_0^* ?
Are these null hypotheses really true ?

4.2. Randomized Block Designs

Penicillin Yield Example.
Yield due to 4 variants of the process A, B, C and D was obtained.
The raw experiment material (corn steep liquor) varied considerably.
Each blend of materials can make 4 runs.
So n=5 blends were prepared (ideally, randomly select 5 blends from possible more in storage), and $k = 4$ experiments were carried out for each blend.
First randomize the experiment by

```
      rep(sample(1:4,replace=F),5)
```

which is the order to use processes A, B, C and D for the 5 blends. The data are given as follows.

blends\treatments	*A*	*B*	*C*	*D*
1	$89^{(1)}$	$88^{(3)}$	$97^{(2)}$	$94^{(4)}$
2	$84^{(4)}$	$77^{(2)}$	$92^{(3)}$	$79^{(1)}$
3	$81^{?}$	$87^{?}$	$87^{?}$	$85^{?}$
4	$87^{?}$	$92^{?}$	$89^{?}$	$84^{?}$
5	$79^{?}$	$81^{?}$	$80^{?}$	$88^{?}$

```
      x=c(89,84,81,87,79, 88,77,87,92,81, 97,92,87,89,80, 94,79,85,84,88)
      dim(x)=c(5,4)
# x=matrix(c(89,84,81,87,79, 88,77,87,92,81, 97,92,87,89,80, 94,79,85,84,88),ncol=4)
      T = factor(as.vector(col(x))) # T=gl(4,5,20)
      B = factor(as.vector(row(x))) # B=gl(5,1,20)
      options(contrasts =c(”contr.sum”, ”contr.poly”))
      (obj=lm(as.vector(x)∼T+B))
      anova(obj)
```

Consider 3 hypotheses:

H_o: $\tau_A = \cdots = \tau_D$ v.s. H_1: at least one inequality.
H_o': $\gamma_1 = \cdots = \gamma_5$ v.s. H_1': at least one inequality.
H_o^*: $\tau_A = \cdots = \tau_D$ and $\gamma_1 = \cdots = \gamma_5$ v.s. H_1^*: at least one inequality.

	Df	*Sum Sq*	*Mean Sq*	*F value*	*Pr(> F)*	
T	3	70	23.333	1.2389	0.33866	
B	4	264	66.000	3.5044	0.04075	∗
Residuals	12	226	18.833			

$$F\ value = (70 + 264)/(3 + 4)/18.833 \approx 2.5 \text{ P-value ?}$$

```
> 1-pf(2.5,7,12)
      [1] 0.07821256
```

Conclusion How many statements ?

```
> summary(obj)
```

	Estimate	*Std. Error*	*t value*	*Pr(> |t|)*	
(Intercept)	86.0000	0.9704	88.624	$< 2e-16$	∗ ∗ ∗
T1	−2.0000	1.6808	−1.190	0.25708	
T2	−1.0000	1.6808	−0.595	0.56292	
T3	3.0000	1.6808	1.785	0.09956	.
B1	6.0000	1.9408	3.092	0.00934	∗∗
B2	−3.0000	1.9408	−1.546	0.14812	
B3	−1.0000	1.9408	−0.515	0.61573	
B4	2.0000	1.9408	1.031	0.32310	

Which constraint ?

The model can be simplified.

Should the model be $E(Y|X) = 86 + 6\mathbf{1}(B = 1)$? Or

```
> lm(x∼ factor(B==1))
    (Intercept)   factor(B == 1)1
       88.25          −3.75
```

$$\hat{E}(Y|X) = 88.25 - 3.75 \underbrace{\mathbf{1}(B \neq 1)}_{\textbf{why not } =??} .$$

4.3. is skipped.

4.4. Latin squares Latin squares deal with the case that there are 2 more equal-level factors with the same level as the treatment. (R, C, T) v.s. (R, T).

Car Emissions Data. 4 drivers using 4 different cars to test the feasibility of reducing air pollution by modifying a gas mixture with very small amounts of certain chemicals A, B, C and D. There are 4 cars and 4 drivers. For randomization, randomly select cars and drivers. Then there are several ways to carry out the experiments.

(1) Convenient way: $\begin{array}{ccccc} Drivers\backslash cars & 1 & 2 & 3 & 4 \\ I & A & B & C & D \\ II & A & B & C & D \\ III & A & B & C & D \\ IV & A & B & C & D \end{array}$ car and treatment effects are confounded

(2) Simple randomization: $\begin{array}{ccccc} Drivers\backslash cars & 1 & 2 & 3 & 4 \\ I & D & A & C & B \\ II & D & A & B & C \\ III & C & B & A & D \\ IV & A & C & D & B \end{array}$ based on R output below

```
> rep(sample(c("A","B","C","D")),4)
    [1] "D" "A" "C" "B" "D" "A" "B" "C" "C" "B" "A" "D" "A" "C" "D" "B"
```

(3) Latin Square: $\begin{array}{ccccc} Drivers\backslash cars & 1 & 2 & 3 & 4 \\ I & A & B & C & D \\ II & B & C & D & A \\ III & C & D & A & B \\ IV & D & A & B & C \end{array}$, which eliminates the block effects of cars and drivers, as each row and column has A, B, C, D

Compare $\begin{array}{ccccc} & 1 & 2 & 3 & 4 \\ I & A & B & C & D \\ II & D & A & B & C \\ III & B & C & D & A \\ IV & C & D & A & B \end{array}$, $\begin{array}{ccccc} & 1 & 2 & 3 & 4 \\ I & A & B & C & D \\ II & C & D & A & B \\ III & B & C & D & A \\ IV & D & A & B & C \end{array}$, $\begin{array}{ccccc} & 1 & 2 & 3 & 4 \\ I & A & B & C & D \\ II & C & D & A & B \\ III & D & A & B & C \\ IV & B & C & D & A \end{array}$

Relation between these 3 ?

The data are put in Table 2.

Drivers\cars	1	2	3	4
I	*A*	*B*	*D*	*C*
	19	24	23	26
II	*D*	*C*	*A*	*B*
	23	24	19	30
III	*B*	*D*	*C*	*A*
	15	14	15	16
IV	*C*	*A*	*B*	*D*
	19	18	19	16

which pattern of the above 3 ?

```
> y=c(19, 24, 23, 26, 23, 24, 19, 30, 15, 14, 15, 16, 19, 18, 19, 16)
> (col=gl(4,1,16))
    [1] 1 2 3 4 1 2 3 4 1 2 3 4 1 2 3 4
    Levels: 1 2 3 4
> (row=gl(4,4,16))
    [1] 1 1 1 1 2 2 2 2 3 3 3 3 4 4 4 4
    Levels: 1 2 3 4
> T=c(A,B,D,C,D,C,A,B,B,D,C,A,C,A,B,D) # Does it work ?
> T=c("A","B","D","C","D","C","A","B","B","D","C","A","C","A","B","D")
> T=c(1,2,4,3,4,3,1,2,2,4,3,1,3,1,2,4)
> T=factor(T)
> (obj=lm(y~col+row+T))
 (Intercept)      col2          col3          col4         row2         row3
  2.000e+01    1.000e+00   -1.088e-15    3.000e+00    1.000e+00   -8.000e+00
      row4         T2            T3           T4
 -5.000e+00   -4.000e-01    3.000e-01    1.000e+00
     > anova(obj)
              Df   Sum Sq   Mean Sq   F value   Pr(>F)
      T        3     40     13.333      2.5     0.156490          < 0.5
    col        3     24      8.000      1.5     0.307174           car
    row        3    216     72.000     13.5     0.004466   **    driver
 Residuals     6     32      5.333
> (40+24+216)/9/5.333
     [1] 5.8
> 1-pf(5.8,9,6) what does it mean ?
     [1] 0.023
> (ob=lm(y~T))
                         (Intercept)  T2  T3  T4
                             18        4   3   1

> anova(ob)

                 Df   Sum Sq   Mean Sq   F value   Pr(>F)
        T         3     40     13.333    0.5882    0.6343       > 0.5
    Residuals    12    272     22.667
```

H_o: $\tau_A=\tau_B=\tau_C=\tau_D$ v.s. H_1: H_o is false.

```
> summary(lm(y~row))
                  Estimate   Std. Error   t value    Pr(>|t|)
    (Intercept)    23.000      1.414       16.26     1.54e-09    ***
        row2        1.000      2.000        0.50     0.62612
        row3       -8.000      2.000       -4.00     0.00176      **
        row4       -5.000      2.000       -2.50     0.02792      *
```

Conclusion ? Based on anova(obj) or anova(ob) ?

Ans: Based on anova(obj). The P-value of T is smaller.

Also row effect is significant, the model can be simplified as

$\hat{E}(Y|X)=23-8\mathbf{1}(Drive_3)-5\mathbf{1}(Drive_4)$? $\mathbf{1}(Drive_3)=\mathbf{1}$(driver is #3)

```
> D=rep(1,4)
> D=c(D,D,D+2,D+3)
> D [1] 1 1 1 1 1 1 1 1 3 3 3 3 4 4 4 4
> summary(lm(y~factor(D)-1))
                  Estimate   Std. Error   t value    Pr(>|t|)
    (Intercept)    23.5000     0.9707     24.209    3.37e-12    ***
    factor(D)3     -8.5000     1.6813     -5.055     0.00022    ***
    factor(D)4     -5.5000     1.6813     -3.271     0.00608     **
```

The model is $\hat{E}(Y|X)=23.5-8.5\mathbf{1}(Drive_3)-5.5\mathbf{1}(Drive_4)$.

Graeco-Latin Squares deal with the case that
there are 3 block factors with levels equal the level of the treatment factor (3+1),
whereas Latin squares deal with the case that
there are 2 equal-level factors with the same level as the treatment (2+1).
One may try to superimpose two Latin Squares together.
Which of the following two can eliminate confounding effect ?

1	2	3	4	1	2	3	4	1	2	3	4	1	2	3	4	1	2	3	4
2	1	4	3	2	1	4	3	3	4	1	2	3	4	1	2	2	3	4	1
3	4	1	2	3	4	1	2	4	3	2	1	2	1	4	3	3	4	1	2
4	3	2	1	4	3	2	1	2	1	4	3	4	3	2	1	4	1	2	3

(1) latin sq., (2) replication, (3) permute 3 rows, (4) permute 2 rows, (5) different.

1−	−2			1−	−3			1−	−4			1−	−5		
11	22	33	44	11	22	33	44	11	22	33	44	11	22	33	44
22	11	44	33	23	14	41	32	23	14	41	32	22	13	44	31
33	44	11	22	34	43	12	21	32	41	14	23	33	44	11	22
44	33	22	11	42	31	24	13	44	33	22	11	44	31	22	13

Conclusion ?

1. Permute 3 rows of Latin square (1) works;

2. Permute 2 rows of Latin square or superimpose (5) does not work !

How to tell ?

No pair of numbers occurs twice.

Hyper-Graeco-Latin Squares deal with the case that there are 4 block factors with levels equal the level of the treatment factor (4+1).

A Hyper-Graeco-Latin Square used in a Martindale wear tester.

The martindale wear tester is a machine used for testing the wearing quality of types of cloth or other such materials.

* 4 pieces of cloth may be compared simultaneously in one machine cycle.

* The response is the weight loss in tenths of a milligram suffered by the test piece when it is rubbed again a standard grade of emory paper for 1000 revolutions of the machine.

* Specimens of the four different types of cloth (treatments) A, B, C, D whose wearing qualities are to be compared are mounted in 4 different specimen holders 1, 2, 3, 4.

* Each holder can be in any of the 4 positions P_1, P_2, P_3, P_4 on the machine.

* Each emory paper sheet α, β, γ, δ was cut into 4 quarters and each quarter used to complete a single cycle c_1, c_2, c_3 and c_4 of 1000 revolutions.

The object of the experiment:
(1) to make a more accurate comparison of the treatments
(2) to discover how much a total variability was contributed by the various factors:
holders, positions, emory paper and cycles.
One replication has 16 df.
Under control-sum, $1 + (4 + 1) \times (4 - 1) = 16$ dfs are needed, thus
two replications are needed **why ??**
Thus 4 additional cycles and 4 additional emory papers are needed.

So there are 32 experiments. It is important to consider randomizing the 32 experiments. In the first 16 runs, each run involves 5 conditions: (4+1) factors, each with 4 levels.
How to order them for randomization ?

In each circle, 4 experiments are carried out simultaneously, it needs 4 types of emory papers and 4 types of cloth. Each holder, position and circle are one unit, respectively. Each cloth and emory paper are cut to 4 pieces. If the qualify of cloth and emory papers are uniform, then no need to randomize (the textbook does not bother). Otherwise, in each replication of 16 experiments, we can randomize as follows.

for (i in 1:4) sample (1:4) (for 4 pieces of each emory paper in 4 circles),

for (i in 1:4) sample (1:4) (for 4 pieces of each type of cloth in 4 circles).
The data are as follows.

$cycles\backslash position$	P_1	P_2	P_3	P_4
c_1	$\alpha A1$	$\beta B2$	$\gamma C3$	$\delta D4$
	320	297	299	313
c_2	$\beta C4$	$\alpha D3$	$\delta A2$	$\gamma B1$
	266	227	260	240
c_3	$\gamma D2$	$\delta C1$	$\alpha B4$	$\beta A3$
	221	240	267	252
c_4	$\delta B3$	$\gamma A4$	$\beta D1$	$\alpha C2$
	301	238	243	290
c_5	$\epsilon A1$	$\xi B2$	$\theta C3$	$\kappa D4$
	285	280	331	311
c_6	$\xi C4$	$\epsilon D3$	$\kappa A2$	$\theta B1$
	268	233	291	280
c_7	$\theta D2$	$\kappa C1$	$\epsilon B4$	$\xi A3$
	265	273	234	243
c_8	$\kappa B3$	$\theta A4$	$\xi D1$	$\epsilon C2$
	306	271	270	272

replication I
Cycles: c_1, c_2, c_3, c_4
Treatments: A, B, C, D
Holders: 1, 2, 3, 4
Emory paper sheet: $\alpha,\ \beta,\ \gamma,\ \delta$

replication II
Cycles: c_5, c_6, c_7, c_8
Treatments: A, B, C, D
Holders: 1, 2, 3, 4
Emory paper sheet: $\epsilon,\ \xi,\ \theta,\ \kappa$

What is the property of the arrangement ?

Three Latin squares superimpose together twice.

$$\begin{array}{llll} \alpha A1 & & & \\ 111 & 222 & 333 & 444 \\ 234 & 143 & 412 & 321 \\ 342 & 431 & 124 & 213 \\ 423 & 314 & 241 & 132 \end{array} \qquad \begin{array}{l} pattern \\ 1 \\ 234 \\ 34 \\ 4 \end{array} \text{, but not } \begin{array}{llll} \alpha A1 & & & \\ 111 & 222 & 333 & 444 \\ 222 & 111 & 444 & 333 \\ 333 & 444 & 111 & 222 \\ 444 & 333 & 222 & 111 \end{array}$$

Notice:

1. (α, A), (α, 1), (A, 1), *etc.* will not occur twice.
2. Rows 2, 3, 4 belongs to $\{(2,1,4,3),\ (3,4,1,2),\ (4,3,2,1)\}$ in the order $\begin{array}{l} 111 \\ 234 \\ 34c \\ 4ab \end{array}$
3. The element (a,b,c) in the table is uniquely determined.

It is easier to set the Hyper-Graeco-Latin Square this way:

$$\begin{array}{llll} 1 & 2 & 3 & 4 \\ 2 & 1 & 4 & \\ 3 & 4 & 1 & \\ 4 & & & 1 \end{array} \rightarrow \text{LS=} \begin{array}{llll} 1 & 2 & 3 & 4 \\ 2 & 1 & 4 & 3 \\ 3 & 4 & 1 & 2 \\ 4 & 3 & 2 & 1 \end{array} \rightarrow \begin{array}{l} 1 \\ 234 \\ 34 \\ 4 \end{array} \rightarrow \begin{array}{l} 111 \\ 234 \\ 34 \\ 4\mathbf{?} \end{array} \rightarrow \begin{array}{l} 111 \\ 234 \\ 34? \\ 42 \end{array} \rightarrow \begin{array}{l} 111 \\ 234 \\ 342 \\ 42? \end{array} \rightarrow \begin{array}{l} 111 \\ 234 \\ 342 \\ 423 \end{array}$$

$$\text{What does it mean ?} \begin{array}{lcl} 111 & = & (1st, 1st, 1st)\ row\ of\ LSquare \\ 234 & = & \quad (2nd, 3rd, 4th)\ row\ of\ LS \\ 342 & = & \quad (3rd, 4th, 2nd)\ row\ of\ LS \\ 423 & = & \quad (4th, 2nd, 3rd)\ row\ of\ LS \end{array}$$

$$\rightarrow \begin{array}{llll} 111 & 2 & 3 & 4 \\ 234 & 1 & 4 & 3 \\ 342 & 4 & 1 & 2 \\ 423 & 3 & 2 & 1 \end{array} \rightarrow \begin{array}{llll} \alpha A1 & & & \\ 111 & 222 & 333 & 444 \\ 234 & 143 & 412 & 321 \\ 342 & 431 & 124 & 213 \\ 423 & 314 & 241 & 132 \end{array}$$

This may not work for other dimension, say 5.

Consider model

$Y \sim replication_1 + cycle_6 + position_3 + Emory_6 + holder_3 + treatment_3$, or

$Y = X\beta + \epsilon$, where Y is a 32×1 vector, β is a vector in $\mathcal{R}^{23}$ $(1+1+6+3+6+3+3 = 23)$, and X is a matrix of dimension 32×23.

```
> y=c(320, 297, 299, 313, 266, 227, 260, 240, 221, 240, 267, 252, 301, 238, 243,
290)
> z=c(y, 285, 280, 331, 311, 268, 233, 291, 280, 265, 273, 234, 243, 306, 271, 270,
272)
> options(contrasts =c("contr.sum", "contr.poly"))
> (P=gl(4,1,32))
```

```
      [1] 1 2 3 4 1 2 3 4 1 2 3 4 1 2 3 4 1 2 3 4 1 2 3 4 1 2 3 4 1 2 3 4
      Levels: 1 2 3 4
> r=gl(2,16,32) # replication index
> T=c(1,2,3,4,3,4,1,2,4,3,2,1,2,1,4,3)
> T=factor(c(T,T))
> H=c(1,2,3,4,4,3,2,1,2,1,4,3,3,4,1,2) # holder
> H=factor(c(H,H))
> (C1=c(rep(1,4),rep(0,8),rep(-1,4)))
      [1] 1 1 1 1 0 0 0 0 0 0 0 0 -1 -1 -1 -1 # why −1 ?
> (C2=c(rep(0,4),rep(1,4),rep(0,4),rep(-1,4)))
      [1] 0 0 0 0 1 1 1 1 0 0 0 0 -1 -1 -1 -1
> (C3=c(rep(0,8),rep(1,4),rep(-1,4)))
      [1] 0 0 0 0 0 0 0 0 1 1 1 1 -1 -1 -1 -1
> C5=c(rep(0,16),C1)
> C6=c(rep(0,16),C2)
> C7=c(rep(0,16),C3)
> C1=c(C1,rep(0,16)) # C1 is a factor or numerical variable ?
> C2=c(C2,rep(0,16))
> C3=c(C3,rep(0,16))
> E1=c(1,0,0,-1,0,1,-1,0,0,-1,1,0,-1,0,0,1) # emory
# α, β, γ, δ, β, α, δ, γ, γ, δ, α, β, δ, γ, β, α
> E2=c(0,1,0,-1,1,0,-1,0,0,-1,0,1,-1,0,1,0)
> E3=c(0,0,1,-1,0,0,-1,1,1,-1,0,0,-1,1,0,0)
> E5=c(rep(0,16),E1)
> E6=c(rep(0,16),E2)
> E7=c(rep(0,16),E3)
> E1=c(E1,rep(0,16))
> E2=c(E2,rep(0,16))
> E3=c(E3,rep(0,16))
> obj=lm(z ∼ T+H+P+C1+C2+C3 +C5+C6+C7 +E1+E2+E3+E5+E6+E7+r))█

> (ob=lm(z ∼ T))

      (Intercept)    T1       T2      T3
        271.469    −1.469   4.156   8.406
> obj
```

$$\begin{array}{cccccc}
(Intercept) & T1 & T2 & T3 & H1 & H2 \\
271.4688 & -1.4688 & 4.1563 & 8.4063 & -2.5938 & 0.5313 \\
H3 & P1 & P2 & P3 & C1 & C2 \\
2.5313 & 7.5312 & -14.0938 & 2.9063 & 40.1250 & -18.8750 \\
C3 & C5 & C6 & C7 & E1 & E2 \\
-22.1250 & 25.9375 & -7.8125 & -22.0625 & 8.8750 & -2.6250 \\
E3 & E5 & E6 & E7 & r1 & \\
-17.6250 & -19.8125 & -10.5625 & 10.9375 & -4.3438 &
\end{array} \tag{1}$$

Remark. LSE of treatment effects of two models are the same.

```
> C=c(C1,C2,C3,C5,C6,C7)
> dim(C)=c(32,6)
> E=c(E1,E2,E3,E5,E6,E7)
> dim(E)=c(32,6)
```

>lm(z∼T+H+P+C+E+r) difference between Eq.(1) and Eq.(2) ?

$$\begin{array}{cccccc} (Intercept) & T1 & T2 & T3 & H1 & H2 \\ 271.4688 & -1.4688 & 4.1563 & 8.4063 & -2.5938 & 0.5313 \\ H3 & P1 & P2 & P3 & C1 & C2 \\ 2.5313 & 7.5312 & -14.0937 & 2.9063 & 40.1250 & -18.8750 \\ C3 & C4 & C5 & C6 & E1 & E2 \\ -22.1250 & 25.9375 & -7.8125 & -22.0625 & 8.8750 & -2.6250 \\ E3 & E4 & E5 & E6 & r1 & \\ -17.6250 & -19.8125 & -10.5625 & 10.9375 & -4.3438 & \end{array} \tag{2}$$

Main concern: H_o: $\tau_A = \tau_B = \tau_C = \tau_D$ v.s. H_1: H_o fails.

```
> anova(lm(z∼T))
            Df   Sum Sq    Mean Sq   F value   Pr(> F)
     T       3   1705.3     568.45    0.6429    0.5939
Residuals   28  24758.6     884.24
```

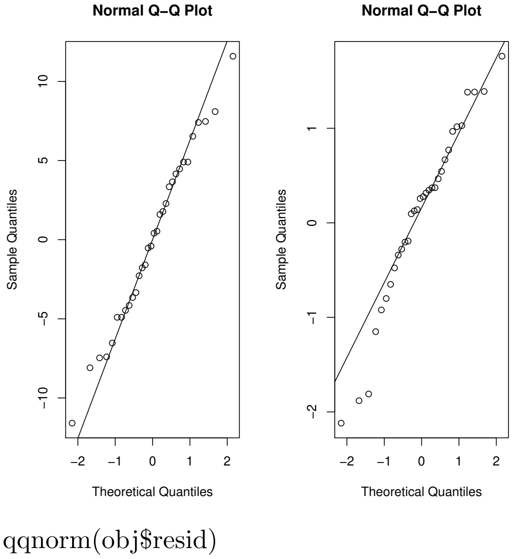
Conclusion ?

```
> anova(lm(z∼T+H+P+C+E+r))
            Df   Sum Sq    Mean Sq   F value   Pr(> F)
     T       3   1705.3     568.45    5.3908    0.021245
     H       3    109.1      36.36    0.3449    0.793790
     P       3   2217.3     739.11    7.0093    0.009925
     C       6  14770.4    2461.74   23.3455    5.273e-05
     E       6   6108.9    1018.16    9.6555    0.001698
     r       1    603.8     603.78    5.7259    0.040366
Residuals    9    949.0     105.45
```

Conclusion ?

```
> anova(lm(z∼T+P+C+E+r))
            Df   Sum Sq    Mean Sq   F value   Pr(> F)
     T       3   1705.3     568.45    6.4467    0.0075703    **
     P       3   2217.3     739.11    8.3822    0.0028332    **
     C       6  14770.4    2461.74   27.9181    2.221e-06   ***
     E       6   6108.9    1018.16   11.5467    0.0002213   ***
     r       1    603.8     603.78    6.8474    0.0225196    *
Residuals   12   1058.1      88.18
> anova(lm(y∼T+r))
            Df   Sum Sq    Mean Sq   F value   Pr(> F)
     T       3   1705.3     568.45    0.6354    0.5987
     r       1    603.8     603.78    0.6749    0.4185
Residuals   27  24154.8     894.62
```

Why different ?



qqnorm(obj$resid)

```
qqline(obj$resid)
z=rnorm(32)
qqnorm(z)
qqline(z)
```

Summary:

1. H_o^r: No difference in replication. ??
2. H_o^c: No difference in cycles. ??
3. H_o^H: No difference in specimen holder. P-value = 0.8 > 0.05.
4. H_o^P: No difference in positions. ??
5. H_o^e: No difference in emory papers. ??
6. H_o: $\tau_A = \tau_B = \tau_C = \tau_D$ v.s. H_1: H_o fails.
   Is the p-value for T 0.594, or 0.021 or 0.008, or 0.599 ?
   The difference is very significant.
   Reject H_o, and the treatment effect are not equal.
   Notice that without blocking factor P, C and E, the conclusion is different, even with replications.
   p-value for T is $0.59 > \alpha = 0.05$.
7. Preference of treatments (weight loss) $D > A > B > C$.

(Int)	$T1$	$T2$	$T3$
271	-1	4	8

There are several models:
(1) lm(y∼T)
(2) lm(y∼T+r)
(3) lm(y∼T+H+P+C+E+r)
(4) lm(y∼T+P+C+E+r)

Which of them is appropriate ?

What is the connection between the previous question and goodness-of-fit test ?
H_o: $E(Y|\mathbf{X}) = \beta'\mathbf{X}$ v.s. H_1: $E(Y|\mathbf{X}) = \beta'\mathbf{X} + \theta g(\mathbf{X})$.
Model (1) is a special case of Models (2), (3) and (4).
Does anova suggests that it can be simplified ?

Which of them is better ?

```
> anova(obj,ob)
    Model 1: z ∼ T + P + C+ E + r
    Model 2: z ∼ T
       Res.Df    RSS      Df    Sum of Sq     F        Pr(> F)
    1    12     1058.1
    2    28     24758.6   −16    −23700     16.799   8.058e − 06
> summary(obj)
                   Estimate   Std.Error   tvalue    Pr(> |t|)
    (Intercept)    271.4688    1.8153    149.546   < 2e − 16    ***
         T1        −1.4688     3.1442    −0.467    0.651505
         T2         4.1563     3.1442     1.322    0.218814
         T3         8.4063     3.1442     2.674    0.025471      *
         H1        −2.5938     3.1442    −0.825    0.430726
         H2         0.5313     3.1442     0.169    0.869561
         H3         2.5313     3.1442     0.805    0.441531
         P1         7.5312     3.1442     2.395    0.040206      *
         P2       −14.0937     3.1442    −4.483    0.001527      **
         P3         2.9063     3.1442     0.924    0.379429
         C1        40.1250     4.4465     9.024    8.35e − 06   ***
          ⋮
```

Q: Under model $lm(z \sim T)$ under control sum, if we write in the standard LR model form $Y_i = \beta X_i + \epsilon_i$, (Y_i, X_i, β)= ?
$Y = 271.5 - 1.5T1 + 4.2T2 + 8.4T3$?

β =(T1,T2,T3) ?
Or try

lm(formula = z ∼ T - 1)

$T1$	$T2$	$T3$	$T4$
270.0	275.6	279.9	260.4

$Y_i = z_i$,
$X_i' = (1, \mathbf{1}(T = 1), \mathbf{1}(T = 2), \mathbf{1}(T = 3), \mathbf{1}(T = 4))$, or more accurately,
$X_i' = (1, \mathbf{1}(T\ is\ cloth\ A), \mathbf{1}(T\ is\ cloth\ B), \mathbf{1}(T\ is\ cloth\ C), \mathbf{1}(T\ is\ cloth\ D))$,
$\beta' = (\beta_0, \beta_1, \beta_2, \beta_3, -\sum_{i=1}^3 \beta_i)$.
$\hat\beta' = (271.5, -1.5, 4.2, 8.4, -11.1)$.
Interpretation:

The mean wearing effect on the 4 cloths is 271.5 units,

effect on cloth A is 1.5 units lower,

effect on cloth B is 4.2 units higher,

effect on cloth C is 8.4 units higher,

effect on cloth D is 11.1 units lower.

Homework 4.1. 1. Suppose that each emory paper α, β, γ, δ can be cut into 8 pieces rather than 4 quaters and each piece is used to complete a single cicle c_1, ..., c_8 of 1000 revolutions. That is $(\epsilon, \xi, \theta, \kappa)$ are replaced by (α, β, γ, δ). Pretend the data remain the same. Revise the codes and do data analysis again.

4.5. Balanced incomplete block designs. The Martindale wear tester example is a complete block design. There are 4 treatment, and block size (Emory paper) is also 4.
If # of treatments > block size, then we have incomplete block designs, *e.g.*, if there are 4 treatment, and block size (Emory paper) is 3, then it is an incomplete block design.

A **balanced** incomplete block design:

		A	B	C	D
	1	α	β	γ	
circle of	2	β	γ		α
10^3 *revolutions*	3	γ		α	β
	4		α	β	γ

Its properties:
1. Within block of cycles, every pair of treatments appears twice. *e.g.* (A,B) occurs at blocks (circles) 1 and 2, and (A,D) occurs at blocks 2 and 3.
2. Every row contains each of α, β and γ.
3. Every column contains each of α, β and γ.
Thus each of α, β and γ block contains $\{A, B, C, D\}$ and circle $\{1, 2, 3, 4\}$.

Youden Squares: A second wear testing example. There are 7 treatment, and block size of emory paper is still 4, a balanced incomplete block design is as follows.

cycles\treatment	A	B	C	D	E	F	G	
1		α627		β248		γ563	δ252	DG
2	α344		β233			δ442	γ226	
3			α251	γ211	δ160		β297	DG
4	β337	δ537			γ195		α300	AB
5		γ520	δ278		β199	α595		
6	γ369			δ196	α185	β606		
7	δ396	β602	γ240	α273				AB

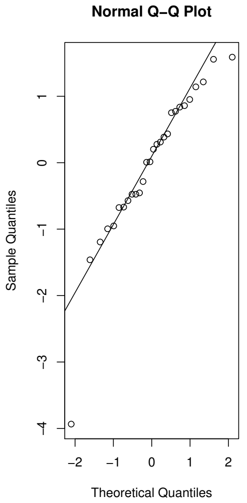
Within block of cycles, every pair of treatments appears twice.
e.g. In the block of cycles (A,B) occurs at blocks 4 and 7.
Each row and column contains α, β, γ, δ.

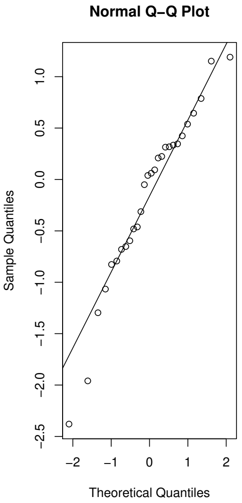
Does

cycles\treatment	A	B	C	D	E	F	G
1	α	β	γ	δ			
2	β	γ	δ				α
3	γ	δ				α	β
4	δ				α	β	γ
5				α	β	γ	δ
6			α	β	γ	δ	
7		α	β	γ	δ		

work ?

```
> y=c(627,248,563,252, 344,233,442,226, 251,211,160,297, 337,537,195,300,
    520,278,199,595, 369,196,185,606, 396,602,240,273)
> T=c(”B”,”D”,”F”,”G”, ”A”,”C”,”F”,”G”, ”C”,”D”,”E”,”G”, ”A”,”B”,”E”,”G”,
    ”B”,”C”,”E”,”F”, ”A”,”D”,”E”,”F”, ”A”,”B”,”C”,”D”)
> e=c(”a”,”b”,”r”,”d”, ”a”,”b”,”d”,”r”, ”a”,”r”,”d”,”b”, ”b”,”d”,”r”,”a”,
    ”r”,”d”,”b”,”a”, ”r”,”d”,”a”,”b”, ”d”,”b”,”r”,”a”)
> c= gl(7,4,28)
    [1] 1 1 1 1 2 2 2 2 3 3 3 3 4 4 4 4 5 5 5 5 6 6 6 6 7 7 7 7
> (z=lm(y~T)) # What is the LSE of TA ?
#                What is the LSE of wearing effect on cloth A ?
    (Intercept)    TB       TC        TD        TE       TF       TG
      361.50     210.00  −111.00   −129.50   −176.75   190.00   −92.75
> (x=lm(y~T+e+c))
    (Intercept)    TB        TC         TD         TE        TF
      408.429    191.357  −111.571   −147.643   −184.500   188.429
        TG         eb        ed         er         c2        c3
     −87.571     −7.571   −44.857    −35.857    −72.429   −23.786
        c4         c5        c6         c7
     −23.929     −9.286   −11.429     8.357
> anova(x)
                 Df   Sum q   Mean Sq   Fvalue     Pr(> F)
        T         6  589623    98271    96.4619   1.899e − 09   ∗ ∗ ∗
        e         3    9846     3282     3.2217    0.06125      .
        c         6   14570     2428     2.3837    0.09445      .
    Residuals    12   12225     1019
                                Can        we      simplify      ?
                                         Delete     e or c       ?

      e + c       9   24416    2712.9    2.6623     0.0583
                                                 pf(2.67, 9, 12)
> anova(x,z)
    Model 1: y ∼ T + e + c
    Model 2: y ∼ T
        Res.Df   RSS    Df   Sum of Sq    F      Pr(> F)
    1     12    12225
    2     21    36641   −9    −24416    2.663   0.05828   .
> summary(z)
                  Estimate   Std. Error   t value    Pr(> |t|)
    (Intercept)    361.50      20.89      17.309    6.61e − 14   ∗ ∗ ∗
        TB         210.00      29.54       7.110    5.17e − 07   ∗ ∗ ∗
        TC        −111.00      29.54      −3.758    0.001157      ∗∗
        TD        −129.50      29.54      −4.384    0.000259    ∗ ∗ ∗
        TE        −176.75      29.54      −5.984    6.13e − 06   ∗ ∗ ∗
        TF         190.00      29.54       6.433    2.24e − 06   ∗ ∗ ∗
        TG         −92.75      29.54      −3.140    0.004943      ∗∗

> qqnorm(studres(z))
> qqline(studres(z))
> u=rnorm(28)
> qqnorm(u)
```





```
> qqline(u)
```

Summary:

H_o: $\tau_A = \tau_B = \tau_C = \tau_D = \tau_E = \tau_F = \tau_G$ v.s. H_1: H_o fails.

p-value for T is $< 0.001 < \alpha = 0.05$.

The treatments are significantly different.

Reject H_o, and the treatment effect are not equal.

Which of the two model is appropriate ?

(1) $E(Y|\mathbf{X}) = \alpha + \beta_1' T$,

(2) $E(Y|\mathbf{X}) = \alpha + \beta_1' T + \beta_2' e + \beta_3' c$

Preference in treatments: $E > D > C > G > A > F > B$. **Why ?**

Interpretation of α under model (1) ?

The average effect of the 7 treatments ?

The average effect of Treatment A ?

Interpretation of β_i ?

Interpretation of α under model (2) ?

The average effect of the 7 treatments ?

The average effect of Treatment A ?

Interpretation of β_i ?

```
> names(summary(z))
    [1] ”call” ”terms” ”residuals” ”coefficients”
    [5] ”aliased” ”sigma” ”df” ”r.squared”
    [9] ”adj.r.squared” ”fstatistic” ”cov.unscaled”
> summary(lm(y∼T-1))$cov
          TA    TB    TC    TD    TE    TF    TG
    TA  0.25  0.00  0.00  0.00  0.00  0.00  0.00
    TB  0.00  0.25  0.00  0.00  0.00  0.00  0.00
    TC  0.00  0.00  0.25  0.00  0.00  0.00  0.00
    TD  0.00  0.00  0.00  0.25  0.00  0.00  0.00
    TE  0.00  0.00  0.00  0.00  0.25  0.00  0.00
    TF  0.00  0.00  0.00  0.00  0.00  0.25  0.00
    TG  0.00  0.00  0.00  0.00  0.00  0.00  0.25
    Residual standard error: 41.77 on 21 degrees of freedom
> (U=summary(lm(y∼T))$cov)
```

	(Intercept)	*TB*	*TC*	*TD*	*TE*	*TF*	*TG*
(Intercept)	0.25	−0.25	−0.25	−0.25	−0.25	−0.25	−0.25
TB	−0.25	0.50	0.25	0.25	0.25	0.25	0.25
TC	−0.25	0.25	0.50	0.25	0.25	0.25	0.25
TD	−0.25	0.25	0.25	0.50	0.25	0.25	0.25
TE	−0.25	0.25	0.25	0.25	0.50	0.25	0.25
TF	−0.25	0.25	0.25	0.25	0.25	0.50	0.25
TG	−0.25	0.25	0.25	0.25	0.25	0.25	0.50

Why is there such a big difference ?

Under the model $y \sim T - 1$,

$\hat\beta_A = \frac{\sum_{i=1}^n y_i \mathbf{1}(T_i=A)}{\sum_{i=1}^n \mathbf{1}(T_i=A)}$, where $n = ?$ 7 treatments and 4 blocks.

$\hat\beta_B = \frac{\sum_{i=1}^n y_i \mathbf{1}(T_i=B)}{\sum_{i=1}^n \mathbf{1}(T_i=B)}$, ...

$cov(\hat\beta_A, \hat\beta_B) = E(\hat\beta_A \cdot \hat\beta_B) - E(\hat\beta_A)E(\hat\beta_B)$.

Under the model $y \sim T$,

$\hat\beta_0 = \frac{\sum_{i=1}^n y_i \mathbf{1}(T_i=A)}{\sum_{i=1}^n \mathbf{1}(T_i=A)}$, $\hat\beta_A = 0$, $\hat\beta_B = \frac{\sum_{i=1}^n y_i \mathbf{1}(T_i=B)}{\sum_{i=1}^n \mathbf{1}(T_i=B)} - \hat\beta_0$, ...

```
> summary(lm(y~T-1))
          Estimate   Std. Error   t value    Pr(>|t|)
    TA     361.50      20.89       17.309   6.61e-14 ***
    TB     571.50      20.89       27.363   < 2e-16 ***
    TC     250.50      20.89       11.994   7.35e-11 ***
    TD     232.00      20.89       11.108   2.98e-10 ***
    TE     184.75      20.89        8.846   1.59e-08 ***
    TF     551.50      20.89       26.406   < 2e-16 ***
    TG     268.75      20.89       12.868   1.99e-11 ***
```

Is U really a covariance matrix ?

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

cov.unscaled=$(\mathbf{X}'\mathbf{X})^{-1}$.

```
> 0.25*41.77**2
[1] 436.1832
> 20.89**2
[1] 436.3921
```

Chapter 5. Factorial Designs at two levels

We shall look at 3 examples. Two are qualitative and one is quantitative.

5.2. Example 1: The effect of 3 factors on clarity of film.

An experiment to determine how the cloudiness of a floor wax is affected when certain changes are introduced into the formula for its preparation.

1 response: cloudiness of a floor.

3 factors each with two levels:

amount of emulsifier A (low, high) or (-,+),

amount of emulsifier B (low, high) or (-,+),

catalyst concentration C (low, high) or (-,+).

There are $2^3 = 8$ combinations and one needs 8 (random) runs of experiments. They are called 2^3 factorial designs.

run#	*A*	*B*	*C*	*results(N/Y)*	*or(−/+)*
1	−	−	−	*No*	−
2	+	−	−	*No*	−
3	−	+	−	*Yes*	+
4	+	+	−	*Yes*	+
5	−	−	+	*No*	−
6	+	−	+	*No*	−
7	−	+	+	*Yes*	+
8	+	+	+	*Yes*	+
compare					*same as B*

Results can also be given as **visual display** in Figure 5.1 (in the textbook). One can see from Figure 5.1 that cloudy is mainly due to high amount of emulsifier B. Factors A nd C are called **inert**.
Is the run number the order of experiments ? Then ?

5.3. The effects of 3 factors on 3 physical properties of a polymer solution.
In the previous example, there is just one response.
There are 3 responses in the current experiment
3 responses: Is the polymer solution
milky ? (y_1),
viscous ? (y_2),
yellow color ? (y_3).
3 factors each with two levels in the formulation of the solution:
amount of a reactive monomer (10,30)% or $(-,+)$,
the type of chain length regulator (A,B) or $(-,+)$,
amount of chain length regulator (1,3)% or $(-,+)$.

run#	1	2	3	*milky*?	*viscous*?	*yellow*?
1	$-$	$-$	$-$	$Y\ -$	$Y\ -$	$N\ -$
2	$+$	$-$	$-$	$N\ +$	$Y\ -$	$N\ -$
3	$-$	$+$	$-$	$Y\ -$	$Y\ -$	$N\ -$
4	$+$	$+$	$-$	$N\ +$	$Y\ -$	*Slightly* $++$
5	$-$	$-$	$+$	$Y\ -$	$N\ +$	$N\ -$
6	$+$	$-$	$+$	$N\ +$	$N\ +$	$N\ -$
7	$-$	$+$	$+$	$Y\ -$	$N\ +$	$N\ -$
8	$+$	$+$	$+$	$N\ +$	$N\ +$	*Slightly* $++$
compare to columns				1	3	Y if 1&2 both ++ *ow N*

See Figures 5.2 and 5.3 for visual display of the results.
Pay attention to the row of "compare columns" to the figures.

Notice that the response is qualitative in the previous two examples.
The factorial design can tell which factor do what to which response.

5.4. A pilot investigation.
1 response: yields of the experiment (numerical).
3 factors: temperature T (160, 180) or (−,+),
concentration C (20,40) or (−,+),
type of catalyst K (A,B) or (−,+).
There are duplicate runs (8+8=16).

run#	*T*	*C*	*K*	*average yields of* 2 *runs*	$y_{i1}^{(order)}$	$y_{i2}^{(order)}$
1	$-$	$-$	$-$	60	$59^{(6)}$	$61^{(13)}$
2	$+$	$-$	$-$	72	$74^{(2)}$	$70^{(4)}$
3	$-$	$+$	$-$	54	$50^{(1)}$	$58^{(16)}$
4	$+$	$+$	$-$	68	$69^{(5)}$	$67^{(10)}$
5	$-$	$-$	$+$	52	$50^{(8)}$	$54^{(12)}$
6	$+$	$-$	$+$	83	$81^{(9)}$	$85^{(14)}$
7	$-$	$+$	$+$	45	$46^{(3)}$	$44^{(11)}$
8	$+$	$+$	$+$	80	$79^{(7)}$	$81^{(15)}$

Table 5.3

Remark. Using average is only for the convenience of computing the main effects, not for anova.

5.5. Calculation of main effect.
Definition: Main effect of each factor $= \overline{y}_+ - \overline{y}_-$ (see the next tables).
Interpretation: the average difference between level 2 (+) of a factor and level 1 (-) (same as control.treatment)

Main effect of T: **Main effect of C:**

$run\#$	T	C	K	y_+		y_-	$yields$
1	$-$	$-$	$-$			60	
2	$+$	$-$	$-$	72			
3	$-$	$+$	$-$			54	
4	$+$	$+$	$-$	68			
5	$-$	$-$	$+$			52	
6	$+$	$-$	$+$	83			
7	$-$	$+$	$+$			45	
8	$+$	$+$	$+$	80			
				$\overline{y}_+$	$-$	$\overline{y}_-$	$=23$

$run\#$	T	C	K	y_+		y_-	$yields$
1		$-$	$-$			60	
2		$-$	$-$			72	
3		$+$	$-$	54			
4		$+$	$-$	68			
5		$-$	$+$			52	
6		$-$	$+$			83	
7		$+$	$+$	45			
8		$+$	$+$	80			
				$\overline{y}_+$	$-$	$\overline{y}_-$	$=-5$

Main effect of K:

$run\#$	T	C	K	y_+		y_-	$yields$
1			$-$			60	
2			$-$			72	
3			$-$			54	
4			$-$			68	
5			$+$	52			
6			$+$	83			
7			$+$	45			
8			$+$	80			
				$\overline{y}_+$	$-$	$\overline{y}_-$	$=1.5$

Four ways to compute with R-code:

```
> y=c(60,72,54,68,52,83,45,80)
> (a=rep(c(-1,1),4))
    [1] -1 1 -1 1 -1 1 -1 1
> (b=rep(c(-1,-1,1,1),2))
    [1] -1 -1 1 1 -1 -1 1 1
> c=rep(-1,4)
> (c=c(c,-c))
    [1] -1 -1 -1 -1 1 1 1 1
# First way to compute effects
> (v=c(y% *% a/4, y% *% b/4, y% *% c/4))
    [1] 23.0 −5.0 1.5 # main effects
# 2nd way to compute effects
> W=lm(y~a+b+c)
> W$coef[1:4]
    (Intercept)     a        b       c
       64.25      11.50   −2.50   0.75   # model 1: y = μ + β1 a + β2 b + β3 c + ε.
> c( 2*W$coef[2:4])
       a        b       c
     23.00   −5.00   1.50   # main effects
# 3rd way and the prefer way
> lm(y~factor(a)+factor(b)+factor(c) )$coef[1:4]
(Intercept)   factor(a)1   factor(b)1   factor(c)1
   54.5          23.0         −5.0          1.5      # main effects
    # factor(a)1 refers to 1(a=1)
#model 2: y = μ + β1 1(T = +) + β2 1(C = +) + β3 1(K = +) + ε.
> mean(y)
    [1] 64.25
The fourth way:
> options(contrasts =c(”contr.sum”, ”contr.poly”))
>U= lm(y~factor(a)+factor(b)+factor(c))$coef[1:4]
(Intercept)   factor(a)1   factor(b)1   factor(c)1
   64.25        −11.50        2.50        −0.75     factor(a)1 refers to 1(a=-1)
#model 3: y = μ + β1(1(T = −) − 1(T = +)) + β2(1(C = −) − 1(C = +))
      + β3(1(K = −) − 1(K = +)) + ε. (somewhat opposite to model 1).
> −2*U[2:4] # main effects
```

Remark. $\hat{\mathbf{Y}}$ remains unchanged in the last three ways.
Homework problem 5.5: Given the LSE by the fourth way, how to get the LSE under model 2 (the 3rd way) ?

5.6. Interaction.

Two-factor interaction for TC,

run#	T	C	K	y_+	y_-	*yields*
1	$-$	$-$		60		
2	$+$	$-$			72	
3	$-$	$+$			54	
4	$+$	$+$		68		
5	$-$	$-$		52		
6	$+$	$-$			83	
7	$-$	$+$			45	
8	$+$	$+$		80		
				$\overline{y}_+$	$-$ $\overline{y}_-$	$= 1.5$

Two-factor interaction for TK,

run#	T	C	K	y_+	y_-	*yields*
1	$-$		$-$	60		
2	$+$		$-$		72	
3	$-$		$-$	54		
4	$+$		$-$		68	
5	$-$		$+$		52	
6	$+$		$+$	83		
7	$-$		$+$		45	
8	$+$		$+$	80		
				$\overline{y}_+$	$-$ $\overline{y}_-$	$= 10$

Two-factor interaction for CK,

run#	T	C	K	y_+	y_-	*yields*
1		$-$	$-$	60		
2		$-$	$-$	72		
3		$+$	$-$		54	
4		$+$	$-$		68	
5		$-$	$+$		52	
6		$-$	$+$		83	
7		$+$	$+$	45		
8		$+$	$+$	80		
				$\overline{y}_+$	$-$ $\overline{y}_-$	$= 1.5$

Three-factor interaction

run#	T	C	K	y_+	y_-	*yields*
1	$-$	$-$	$-$		60	
2	$+$	$-$	$-$	72		
3	$-$	$+$	$-$	54		
4	$+$	$+$	$-$		68	
5	$-$	$-$	$+$	52		
6	$+$	$-$	$+$		83	
7	$-$	$+$	$+$		45	
8	$+$	$+$	$+$	80		
				$\overline{y}_+$	$-$ $\overline{y}_-$	$= 0$

R commands:

```
ab=a*b
ac=a*c
bc=b*c
abc=ab*c
a=factor(a)
b=factor(b)
c=factor(c)
ab=factor(ab) # why not ab=a*b ?
ac=factor(ac)
bc=factor(bc)
abc=factor(abc)
lm(y~a+b+c+ab+ac+bc+abc)
```

5.7. Estimation of variance of replicate runs.

(1) Under the i.i.d. N(μ, σ^2) assumption,

$\hat{\sigma}^2 = \frac{1}{df}\sum_{i=1}^{n}(Y_i - \hat{\beta}X_i)^2$ if df>0, where $\beta X \overset{def}{=} \beta' X$.

$\hat{\sigma}^2$ is the unbiased estimator using mean squared residuals, under the null hypothesis H_o: $E(Y|\mathbf{X}) = \beta\mathbf{X}$.

If there is no replicate runs ($r = 1$ under the full model), then

$\sum_{i=1}^{n}(Y_i - \hat{\beta}X_i)^2 = 0$, as there are 8 parameters and 8 observations y_{ij}'s.

Thus it is not a proper estimator in such case.

(2) If there are r replicate runs in a 2^3 factorial design, with responses

y_{ij}, $i = 1, ..., 8$ and $j = 1, ..., r$, let

$s_i^2 = \frac{1}{r-1}\sum_{j=1}^{r}(y_{ij} - \overline{y}_{i\cdot})^2$, $i = 1, ..., 8$.

If $r = 2$,

$s_i^2 = \frac{(y_{i1}-\overline{y}_{i\cdot})^2+(y_{i2}-\overline{y}_{i\cdot})^2}{2-1} = \frac{(y_{i1}-y_{i2})^2}{2}$, $i = 1, ..., 8$,

where $\overline{y}_{i\cdot} = \frac{y_{i1}+y_{i2}}{2}$.

$s^2 = \sum_{i=1}^{8} s_i^2/8$ is an (unbiased) estimator of σ^2.

$$s^2 = \hat{\sigma}^2?$$

Yes, if under the full model $y \sim a + b + c + ab + bc + ac + abc.$ $\quad (p = 8)$
No, if under the submodel, *e.g.* $y \sim I(a * b * c)$ $\quad (p = 2)$.
(3) Is the Mean Sq in each row of anova(), unbiased estimator of σ^2 ?
How about (Residual standard error)^2 in summary(lm()) ?
How about Residual Mean Sq in anova() ?

Simulation example 5.7.1

```
> a=rep(c(-1,1),4)
> b=rep(c(-1,-1,1,1),2)
> c=rep(-1,4)
> c=c(c,-c)
> a=c(a,a)
> b=c(b,b)
> c=c(c,c)
> ab=a*b
> ac=a*c
> bc=b*c
> e=rnorm(16)
> y=a+2*b−3*c+16*ab+bc+e
```

> (z=lm(y∼a+b+c+ab+bc)) $\begin{pmatrix} (Intercept) & a & b & c & ab & bc \\ -0.12 & 0.98 & 2.34 & -3.36 & 15.89 & 0.97 \end{pmatrix}$

Let $Y = \beta'\mathbf{X} + \epsilon$, where $\beta \in \mathcal{R}^p$. $p = ?$ $\beta = ?$ $\hat{\beta} = ?$

> anova(z) $\begin{pmatrix} & Df & Sum\ Sq & Mean\ Sq & F\ value & Pr(>F) & \\ a & 1 & 14.7 & 14.7 & 15.914 & 0.002562 & ** \\ b & 1 & 47.1 & 47.1 & 51.107 & 3.109e-05 & *** \\ c & 1 & 159.6 & 159.6 & 173.258 & 1.219e-07 & *** \\ ab & 1 & 3994.3 & 3994.3 & 4335.153 & 1.590e-14 & *** \\ bc & 1 & 39.7 & 39.7 & 43.034 & 6.391e-05 & *** \\ Residuals & 10 & 9.2 & 0.92 & & & \end{pmatrix}$

5 possible null hypotheses:
H_o^i: $\beta_i = 0$ for an $i \in \{1, ..., 5\}$.

Is H_o^i true ?
Is the model true (under the NID) ?
What can be said about the Mean Sq in anova table ??
Do they look like $\sigma^2 = 1$?

```
> z=lm(y∼a+b+c)
```

> anova(z) $\begin{pmatrix} & Df & Sum\ Sq & Mean\ Sq & F\ value & Pr(>F) \\ a & 1 & 14.7 & 14.66 & 0.0435 & 0.8383 \\ b & 1 & 47.1 & 47.09 & 0.1398 & 0.7150 \\ c & 1 & 159.6 & 159.63 & 0.4738 & 0.5043 \\ Residuals & 12 & 4043.2 & 336.93 & & \end{pmatrix}$

Three possible null hypotheses:
H_o^1: $\beta_1 = 0$.
H_o^2: $\beta_2 = 0$.
H_o^3: $\beta_3 = 0$.

Is H_o^i true ?
Is the model true (under the NID) ?
What can be said about the Mean Sq in anova table ??
Do they look like $\sigma^2 = 1$?

```
> mean((y[1:8]-y[9:16])**2/2)
    [1] 1.130107 # (= s^2 ≈ σ^2 ??)
```

Remark. If the model is wrong, s^2 is an unbiased estimators of σ^2, but not $\hat{\sigma}^2$ and other mean squares in anova.
If the model is correct, both $\hat{\sigma}^2$ and s^2 are unbiased.

Simulation example 5.7.2

> y=rnorm(16)
> z=lm(y∼a+b+c)

$$> \text{anova(z)} \begin{pmatrix} & Df & Sum\ Sq & Mean\ Sq & F\ value & Pr(>F) \\ a & 1 & 0.0212 & 0.02121 & 0.0282 & 0.869 \\ b & 1 & 0.8812 & 0.88119 & 1.1730 & 0.300 \\ c & 1 & 0.1444 & 0.14441 & 0.1922 & 0.668 \\ Residuals & 12 & 9.0148 & 0.75123 & & \end{pmatrix}$$

3 possible null hypotheses:
H_o^i: $\beta_i = 0$ for an $i \in \{1, ..., 3\}$.

Is H_o^i true ?
Is the model true (under the NID) ?
What can be said about the mean squares in anova table ??
Do they look like $\sigma^2 = 1$?

> z=lm(y∼a+b+c+ab+bc)
> anova(z)

$$\begin{pmatrix} & Df & Sum\ Sq & Mean\ Sq & F\ value & Pr(>F) \\ a & 1 & 0.0212 & 0.02121 & 0.0254 & 0.8765 \\ b & 1 & 0.8812 & 0.88119 & 1.0563 & 0.3283 \\ c & 1 & 0.1444 & 0.14441 & 0.1731 & 0.6861 \\ ab & 1 & 0.0176 & 0.01762 & 0.0211 & 0.8873 \\ bc & 1 & 0.6553 & 0.65531 & 0.7856 & 0.3963 \\ Residuals & 10 & 8.3419 & 0.83419 & & \end{pmatrix}$$

> mean((y[1:8]-y[9:16])**2/2)
[1] 0.986949

5 possible null hypotheses:
H_o^i: $\beta_i = 0$ for an $i \in \{1, ..., 5\}$.

Is H_o^i true ?
Is the model true (under the NID) ?
What can be said about the mean squares in anova table ??
Do they look like $\sigma^2 = 1$?

Remark. If the model is correct and H_o is correct, all mean squares are unbiased estimators of σ^2. But $\hat\sigma^2$ has smaller variance than the other Mean Sq., as its degree of freedom (Df) is larger. $\nu\hat\sigma^2/\sigma^2 \sim \chi^2(\nu)$ (with mean $= \frac{\nu}{2} \cdot 2$ $(= \alpha\beta)$, variance $= \alpha\beta^2 =$? Thus $E(\hat\sigma^2) = \sigma^2$ and $V(\hat\sigma^2) = 2\sigma^4/\nu$.

Simulation example 5.7.3

> n=100
> a=rexp(n)
> b=rbinom(n,5,0.5)
> a=c(a,a)
> b=c(b,b)
> e=rnorm(2*n)
> y=2+a+b+e
> z=lm(y∼a)
> anova(z)

$$\begin{pmatrix} & Df & Sum\ Sq & Mean\ Sq & F\ value & Pr(>F) \\ a & 1 & 215.36 & 215.365 & 111.09 & < 2.2e-16 *** \\ Residuals & 198 & 383.86 & 1.939 & & \\ & & & \boldsymbol{\sigma^2 = 1 \pm ??} & & \end{pmatrix}$$

Note: $SS/\sigma^2 \sim \chi^2(Df)$ with Var $2 * Df$. Thus $1 \pm 2\sqrt{2/Df} \approx 1 \pm 0.2$

> w=lm(y∼a+b)
> anova(w)

$$\begin{pmatrix} & Df & Sum\ Sq & Mean\ Sq & F\ value & Pr(>F) \\ a & 1 & 215.37 & 215.365 & 210.83 & <2.2e-16*** \\ b & 1 & 182.62 & 182.621 & 178.77 & <2.2e-16*** \\ Residuals & 197 & 201.24 & 1.022 & & \\ & & & \sigma^2\mathbf{=\ 1??} & & \end{pmatrix}$$

> mean((y[1:n]-y[(n+1):($2*n$)])$**$2/2)

[1] 0.9183548 # (= s^2)

σ^2 **= 1?**

Conclusion:

1. If the model is correct, $\frac{1}{n-p}\sum_i(Y_i-\hat{Y}_i)^2$ is an unbiased estimator of σ^2.
2. If the model is correct, $\beta_i=0$, the corresponding Mean Sq is unbiased.
3. If there are replications, s^2 is unbiased.

If the model is incorrect, $\frac{1}{n-p}\sum_i(Y_i-\hat{Y}_i)^2$ is not an unbiased estimator of σ^2. This can be proved by a counterexample as follows.

Counterexample : Let

$Y_{ij}=\beta_1X_i+\beta_2Z_i+\epsilon_{ij}$, $j=1$, 2, and $i=1$, ..., m,

where X_i, Z_i and ϵ_{ij} are independent $\sim N(0,\sigma^2)$.

$$s^2=\frac{1}{m}\sum_{i=1}^m\frac{(Y_{i1}-Y_{i2})^2}{2}$$
$$=\frac{1}{m}\sum_{i=1}^m\frac{(\epsilon_{i1}-\epsilon_{i2})^2}{2}$$
$$=\frac{1}{m}\sum_{i=1}^m(\frac{\epsilon_{i1}-\epsilon_{i2}}{\sqrt{2}\sigma})^2\sigma^2.$$

$\sum_{i=1}^m(\frac{\epsilon_{i1}-\epsilon_{i2}}{\sqrt{2}\sigma})^2\sim\chi^2(m)$.

=> $E(s^2)=\sigma^2$. (Abusing notation, treating s^2 as a r.v.).

Now if the model is chosen incorrectly, say, consider model,

$Y_{ij}=\beta_1X_i+W_{ij}$, where $W_{ij}=\beta_2Z_i+\epsilon_{ij}\sim N(0,(\beta_2^2+1)\sigma^2)$,

$\tilde{\sigma}^2=\frac{1}{n-p}\sum_{i=1}^m\sum_{j=1}^2(Y_{ij}-\hat{Y}_{ij})^2$ is an unbiased estimator of $(\beta_2^2+1)\sigma^2 \quad \neq\sigma^2$.

$n=?\ p=?$

$W_{i1}\perp W_{i2}$ **???**

$E(W_{11}W_{12})=E(\beta_2^2Z_1^2+\beta_2Z_1(\epsilon_{11}+\epsilon_{12})+\epsilon_{11}\epsilon_{12})=E(\beta_2^2Z_1^2)=\beta_2^2E(Z_1^2)$

$E(W_{11})E(W_{12})=\beta_2^2(E(Z_1))^2$. ...

Simulation example 5.7.4.

```
> a=rep(c(-1,1),4)
> b=rep(c(-1,-1,1,1),2)
> c=rep(-1,4)
> c=c(c,-c)
> n=80
> e=rnorm(n)
> a=rep(a,10)
> b=rep(b,10)
> c=rep(c,10)
> y=2*a−5*b+e
> a=factor(a)
> b=factor(b)
> c=factor(c)
> z=lm(y∼a+b+c)
> summary(z)
```

# Note that a, b and c are all factors.

Using Model: $Y_i=\beta_0+\beta_1X_{i1}+\beta_2X_{i2}+\cdots+\epsilon_i$

and under control treatment, X_{i1}**= ?**

What is β_0 **?**

What is β_1 **?**

Where to find $\hat{\beta}_j$**'s ?**

```
              Estimate   Std. Error   t value   Pr(> |t|)
(Intercept)   3.2353??     0.2014     16.064    < 2e − 16   ***
         a1    3.8619      0.2014     19.176    < 2e − 16   ***
         b1  −10.1350      0.2014    −50.323    < 2e − 16   ***
         c1   −0.2773      0.2014     −1.377      0.173
```

Residual standard error: 0.9007 on 76 degrees of freedom

$\hat{Y} \approx \beta_0 = -2 + 5 = 3$ if $a = -1 = b = c$ under control.treat.

$\hat{Y} \approx \beta_0 + \beta_1 + \beta_2 + \beta_3 = 3 + 4 - 10 + 0 = -3$ if $a = 1 = b = c$ under control.treat.

$\beta_0 \approx 0 \approx \overline{Y}$ under control.sum.

```
> anova(z)
             Df   Sum Sq    Mean Sq   F value     Pr(> F)
a             1   298.29    298.29    367.7073    < 2e − 16   ***
b             1   2054.37   2054.37   2532.4402   < 2e − 16   ***
c             1   1.54      1.54      1.8952      0.1727
Residuals    76   61.65     0.81
```

5.7.5. Homework. Carry out the simulations in §5.7 yourself with different parameters and $rnorm(n, 1, 2)$, then summarize the results and address the questions.

5.8. Interpretation of results.

Under NID assumption and 2^3 factorial designs,

$T_o = \frac{\overline{Y}-\beta_0}{\sqrt{s^2/n}} \sim t_{df}$, $\qquad (= N(0,1)/\sqrt{\chi^2(df)/df})$

$T = \frac{\hat{\beta}_j-\beta_j}{\sqrt{s^2(\frac{1}{4r}+\frac{1}{4r})}} \sim t_{df}$, where

$df = 2^k(r-1)$ for s^2 in 2^k factorial design with r replicates and under the full model. $\hat{\beta}_j$ refers to one of the 7 effects.

Remark. In the linear regression, if the model is correct, then we have

$T = \frac{\hat{\beta}_j-\beta_j}{\hat{\sigma}_j} \sim t_{n-p}$, where

$\hat{\sigma}_j^2$ is the $j-$th diagonal element of $\hat{\sigma}^2(\mathbf{X}'\mathbf{X})^{-1}$, and

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

Notice $n = 2^k r$ and $p = 2^k$ in the previous case.

Example of pilot study in §5.4.

The data presented in §5.4 are the 8 averages of 2 replications in a 2^3 factorial design. The 16 data rather than the averages are as follows.

```
> y=c(59,74,50,69,50,81,46,79, 61,70,58,67,54,85,44,81) # yield of experiments in
Table 5.3
> mean((y[1:8]-y[9:16])**2/2)
[1] 8
```

$= s^2$

$V(effect) = V(\overline{y}_+ - \overline{y}_-) = \sigma^2(\frac{1}{4r} + \frac{1}{4r})$

$SE = \sqrt{\frac{8}{4r} + \frac{8}{4r}} \approx 1.4.$

For the data in Table 5.3, df=8, $t_{8,0.025} \approx 2.3$, so a 95% confidence interval (CI) is

$\hat{\beta}_j \pm 2.3 \times 1.4$ (or $\hat{\beta}_j \pm 3.2$).

In practice, people prefer $\hat{\beta}_j \pm SE$, *i.e.*,

$\hat{\beta}_j \pm 1.4$, as it is more conservative (not relying on NID).

effects	70%*CI*		
T	23.0 ± 1.4		*temperature* (160, 180)
C	-5.0 ± 1.4		*concentration* (20, 40)
K		1.5 ± 1.4	*catalyst* (A, B)
TC		1.5 ± 1.4	
TK	10.0 ± 1.4		
CK		0.0 ± 1.4	
TCK		0.5 ± 1.4	
	important	*ignorable*	*if* $\lvert effect\rvert \leq s$ nearly or too small

```
> z=lm(y~a+b+c+ab+bc+ac+abc) #(a,b,c)=(T,C,K) (are factors)
> anova(z)
```

	Df	*Sum Sq*	*Mean Sq*	*F value*	*Pr*(> *F*)	
a	1	2116	2116	264.500	$2.055e-07$	$***$
b	1	100	100	12.500	0.007670	$**$
c	1	9	9	1.125	0.319813	
ab	1	9	9	1.125	0.319813	
bc	1	0	0	0.000	1.000000	
ac	1	400	400	50.000	0.000105	$***$
abc	1	1	1	0.125	0.732810	
Residuals	8	64	8	$(=\hat{\sigma}^2 = s^2)$		

Implication:

```
> w=lm(y~a+b+ac)
> anova(w,z)
    Model 1: y ~ a + b + ac
    Model 2: y ~ a + b + c + ab + bc + ac + abc
       Res.Df   RSS   Df Sum of Sq      F      Pr(> F)
    1     12     83
    2      8     64         419       0.5938    0.6772
> anova(w)
```

	Df	*Sum Sq*	*Mean Sq*	*F value*	*Pr*(> *F*)	
a	1	2116	2116.00	305.928	$6.631e-10$	$***$
b	1	100	100.00	14.458	0.002519	$**$
ac	1	400	400.00	57.831	$6.292e-06$	$***$
Residuals	12	83	6.92			

Estimator of σ^2 can be 6.92 rather than 8.

Summary. Recall that *a*, *b*, ..., *abc* are factors defined in §5.6.

What does the main effect mean ?

lm(y∼a+b+c+bc) <=>

$E(Y|\mathbf{X}) = \beta_0 + \beta_1\mathbf{1}(a=1) + \beta_2\mathbf{1}(b=1) + \beta_3\mathbf{1}(c=1) + \beta_4\mathbf{1}(bc=1)$,

where $\mathbf{X'} = (1, \mathbf{1}(a=1), \mathbf{1}(b=1), \mathbf{1}(c=1), \mathbf{1}(b=c\in\{-1,1\}))$ or

$E(Y|\mathbf{X}) = \beta_0 + \beta_{-1}\mathbf{1}(a=-1) + \beta_1\mathbf{1}(a=1) + \beta_{-2}\mathbf{1}(b=-1) + \beta_2\mathbf{1}(b=1) + \cdots$

$\mathbf{X'} = (1, \mathbf{1}(a=-1), \mathbf{1}(a=1), \mathbf{1}(b=-1), \mathbf{1}(b=1), ...)$ with $\beta_{-1} = 0 = \beta_{-2} = ...)$

lm(y∼a+b*c) <=>

$E(Y|\mathbf{X}) = \beta_0 + \beta_1\mathbf{1}(a=1) + \beta_2\mathbf{1}(b=1) + \beta_3\mathbf{1}(c=1) + \beta_4\mathbf{1}(b*c=1)$,

where $\mathbf{X'} = (1, \mathbf{1}(a=1), \mathbf{1}(b=1), \mathbf{1}(c=1), \mathbf{1}(b=c=1))$. (Compare to bc).

```
> lm(y~a+b*c)
    (Intercept)      a1          b1           c1         b1 : c1
    5.450e+01    2.300e+01   -5.000e+00   1.500e+00   3.553e-15

> lm(y~a+b+c+bc)
    (Intercept)      a1          b1           c1           bc
    5.450e+01    2.300e+01   -5.000e+00   1.500e+00   4.441e-16
```

Remark. It is easier to see the difference through the next model.

```
> lm(y~a+c+ac)
    (Intercept)    a1    c1    ac1
        47.0      23.0   1.5   10.0        # 1(ac = 1) = 1(a = c ∈ {−1, 1})
> (z=lm(y~a*c))
    (Intercept)    a1     c1     a1 : c1
        57.0      13.0   −8.5     20.0       # 1(a : c = 1) = 1(a = c = 1)
> predict(z,newdata=data.frame(a="-1",c="-1"))
```

$$57 \# = \underbrace{57+0+0+0}_{y\sim a*c} = \underbrace{47+0+0+10}_{y\sim a+c+ac}$$

```
> predict(z,newdata=data.frame(a="1",c="-1"))
    70 # = 57 + 13 + 0 + 0 = 47 + 23 + 0 + 0
> predict(z,newdata=data.frame(a="-1",c="1"))
    48.5 # = 57 + 0 − 8.5 + 0 = 47 + 0 + 1.5 + 0
> predict(z,newdata=data.frame(a="1",c="1"))
    81.5 # = 57 + 13 − 8.5 + 20 = 47 + 23 + 1.5 + 10
```

Observations:
(1) If one changes the model from $y \sim a+b+c+ab+ac+bc+abc)$ to $y \sim a+c+ac$,
the LSE of (β_a, β_c), remains the same,
due to the vectors in the table of contrast are orthogonal.
(2) If one changes the model from $y \sim a+b+c+ab+ac+bc+abc)$ to $y \sim a+c+a:c)$,
the LSE of (β_a, β_c) may not be the same,
as $(-1, 1, -1, 1, -1, 1, -1, 1)(-1, -1, -1, -1, -1, 1, -1, 1)' \neq 0 \quad (X_a' X_{a:c} \neq 0)$

$$\begin{pmatrix} a & = (& -1, & 1, & -1, & 1, & -1, & 1, & -1, & 1)' & \\ c & = (& -1, & -1, & -1, & -1, & 1, & 1, & 1, & 1)' & a'c = 0 \\ a:c & = (& -1, & -1, & -1, & -1, & -1, & 1, & -1, & 1)' & \\ a*(a:c) & = & 1 & -1 & 1 & -1 & 1 & 1 & 1 & 1 & = 4 \end{pmatrix}$$

(3) However, the prediction of Y remains the same.
Under control.treatment,
the intercept is the estimate of the mean response of Y at the low levels of factors.
The main effect is the est. of the change due to the factor changing from - to +.

The conclusion of the experiment: $Y \approx 47 + 23T - 8.5K + 20TK$.
To get high yields of the product, set

1. the temperature $T = 180$ (high);
2. the concentration at C=20 (low);
3. It was thought that the suppliers of catalyst K do not matter and they were supposed to produce the same type of catalyst. In fact c (or K) is not significant. However, they now notice that TK is significant. Further study of the data yields

run#	*T*	*C*	*K*	*outputs* :			
1	−		−		60		
2	+		−			72	
3	−		−		54		
4	+		−			68	
5	−		+	52			
6	+		+				83
7	−		+	45			
8	+		+				80
mean				48.5	57	70	81.5

They should select the better supplier (who supplies catalyst B (K+)).

Remark. A 2^2 factorial design $\begin{array}{ccc} - & - & y_1 \\ - & + & y_2 \\ + & - & y_3 \\ + & + & y_4 \end{array}$ can be viewed as an additive model for one-way ANOVA or two-way ANOVA.

For one-way anova: $Y_{ij} = \eta + \tau_i + \epsilon_{ij}$, $i, j \in \{1, 2\}$, where $(Y_{11}, Y_{12}, Y_{21}, Y_{22}) = (y_1, y_2, y_3, y_4)$.

For two-way anova: $Y_{ij} = \eta + \tau_i + \theta_j + \epsilon_{ij}$, $i, j \in \{1, 2\}$.
In particular, under two-way anova, one can write

$$Y_{ij} = \eta + \tau_i + \theta_j + \epsilon_{ij},\ i, j \in \{0, 1\}.$$

$$Y_{ij} = \eta + \tau_0 \mathbf{1}(i = 0) + \tau_1 \mathbf{1}(i = 1) + \theta_0 \mathbf{1}(j = 0) + \theta_1 \mathbf{1}(j = 1) + \epsilon_{ij},\ i, j \in \{0, 1\}.$$

$Y_{ij} = \eta + \tau_1 \mathbf{1}(i = 1) + \theta_1 \mathbf{1}(j = 1) + \epsilon_{ij}$, $i, j \in \{0, 1\}$, under control.treatment.
Q: $\tau_1 =$? if (1) under default; (2) under control.sum with H_0: $\tau_0 = \tau_1$.

5.9. Table of contrast.

Yates number	*mean*	*a*	*b*	*c*	*ab*	*ac*	*bc*	*abc*
1	1	−1	−1	−1	1	1	1	−1
2	1	1	−1	−1	−1	−1	1	1
3	1	−1	1	−1	−1	1	−1	1
4	1	1	1	−1	1	−1	−1	−1
5	1	−1	−1	1	1	−1	−1	1
6	1	1	−1	1	−1	1	−1	−1
7	1	−1	1	1	−1	−1	1	−1
8	1	1	1	1	1	1	1	1
df	8	4	4	4	4	4	4	4

Notice that $Y'(a, b, c, ab, ac, bc, abc)/4 =$(7 effects), where $Y' = (y_1, ..., y_8)$

5.10. Misuse of the ANOVA for 2^k factorial experiments.
If there is no replicate runs ($r = 1$), then ANOVA may not be very helpful (see explanation before Simulation example 5.7.1).
Skip the rest of the section.

5.11. Eyeing the data. In some special case, the interactions are negligible. Then the main factors are orthogonal, and one can do contour eyeballing.

Example of Testing worsted yarn. (jing fang mao xian) Table 5.6 shows part of the data from an investigation on the strength of the particular type of yarn under cycles of repeated loading. This is a 2^3 factorial design with 3 factors:
Length of specimen (A) ((250,350) mm),
amplitude of load cycle (B) ((8,10) mm),
load (C) ((40,50) g).

Yates #	*A*	*B*	*C*	*durance y*
1				28
2				36
3				22
4				31
5				25
6				33
7				19
8				26

Table 5.6

The effects are

mean	*A*	*B*	*C*	*AB*	*AC*	*BC*	*ABC*
27.5	8	−6	−3.5	0	−0.5	−0.5	−0.5

Notice the interaction effects are all negligible ($|-0.5| \leq |main\ effect|/7$).
$\vec{A}$, $\vec{B}$ and $\vec{C}$ are essentially orthogonal.
The direction of steepest ascent is then $(8, -6, -3.5)$.

The contour plane of a durance 25 is a hyperplane $25 = (8, -6, -3.5)\begin{pmatrix} A_o \\ B_o \\ C_o \end{pmatrix}$

where $A_o = (x_1-250)/(350-250)$, $B_o = (x_2-8)/(10-8)$, $C_o = (x_3-40)/(50-40)$, (see Figure 5.6). **Where are (250,350) come from ?**

The contour plane of a durance y is a hyperplane $y = (8, -6, -3.5)\begin{pmatrix} A_o \\ B_o \\ C_o \end{pmatrix} = f(\vec{x})$

5.12. Dealing with more than one response: A pet food experiment.
The manufacturer of pet food had received complaints that packages of food pellets received by the customers contained an unsatisfactorily large amount of powder.

The factory did a 2^3 factorial design to investigate it. All in two levels.

A. Conditioning Temperature: 80% at max, or max

B: Flow: 80% at max, or max

C: Compression zone: 2, or 2.5

Responses:

Y_1 – powder in product;

Y_2 – powder in plant;

Y_3 – a measure of yield;

Y_4 – energy consumed.

Y_1 was obtained after the same process as if a customer would eventually get it.
They tried to find out

the relation between Y_1 and Y_2, as well as

how to control the response Y_2 by adjusting the factors,

without losing too much in yield Y_3 and energy Y_4.

Responses in standard (Yates) order:

```
    y1=c(132,107,117,122,102,92,107,104)
    y2=c(166,162,193,185,173,192,196,164)
    y3=c(83, 85, 99, 102, 59, 75, 80,73)
    y4=c(235,224,255,250,233,223,250,249)
```

Rough estimates of errors are obtained through previous duplicated runs:

$\hat{\sigma}_1 = 5.6$ (for Y_1),

$\hat{\sigma}_{effect_1} = \hat{\sigma}_1\sqrt{\frac{1}{4}+\frac{1}{4}} = \hat{\sigma}_1/\sqrt{2} = 5.6/\sqrt{2} = 4.0,$

$\hat{\sigma}_2 = ...\ \hat{\sigma}_3 = ...\ \hat{\sigma}_4 = ...$

$$\hat{\sigma}_{effect_i} = \begin{cases} 4.0 & \text{if } i = 1 \text{ (for } Y_1) \\ 7.4 & \text{if } i = 2 \text{ (for } Y_2) \\ 4.9 & \text{if } i = 3 \text{ (for } Y_3) \\ 1.1 & \text{if } i = 4 \text{ (for } Y_4) \end{cases}$$

Finding:

There is no serious correlation between Y_1 and Y_2 by plotting (Y_1, Y_2) and

```
> cor(y1,y2)
    [1] -0.1686297
> summary(lm(y2~y1))
               Estimate   Std.Error   tvalue   Pr(> |t|)
(Intercept)    199.7701   50.1472     3.984    0.00725      => ŷ2 = 200 + 0 × y1
     y1        −0.1893    0.4518      −0.419   0.68976
```

		powder in product	*powder in plant*	*yield*	*energy*
		Y_1	Y_2	Y_3	Y_4
	$\hat{\sigma}_i$	4	7.4	4.9	1.1
	temp, A	−8.2	−6.3	3.5	−6.8∗
	flow, B	4.3	11.3	13∗	22.3∗
relate to	*zone, C*	−18.2∗	4.8	−20.5∗	−2.3
powder	*AB*	9.3∗	−13.7	−5.5	3.8∗
inert	*AC*	1.7	−0.3	1	1.3
inert	*BC*	4.3	−13.7	−3.5	−0.8
inert	*ABC*	−5.7	−11.7	−6	0.8

$$=> \text{adjustment should set} \begin{cases} \text{zone at + or 2.5, from row C,} \\ \text{temp*flow at −, from row AB.} \end{cases}$$

How to choose the levels from A and B ?

$(AB)-$	$energy(\hat{Y}_4)$	$\hat{Y}_1$	$yield(\hat{Y}_3)$
$(A+, B-)$	$-6.8 - 22.3$	$-8.2 - 4.3$	
$(A-, B+)$		$8.2 + 4.3$	$-3.5 + 13$

If energy saving is more important: $(A+, B-)$, which also decreases Y_1, otherwise $(A-, B+)$ $(\hat{Y}_3, \hat{Y}_1) = (-3.5 + 13, 8.2 + 4.3)$.

5.13. A 2^4 factorial design: Process development study

Often there are more factors to be investigated than can conventionally be accommodated within the time and budget available, but you will find that usually you can separate genuine effects from noise without replication. In a pilot study, if one plans 16 runs for a replicated 2^3 factorial design with 3 factors, it can be replaced by a 2^4 factorial design with 4 factors.

A process development study.

Factors:

1. (a). Catalyst charge (lb) (10,15) or (−,+), (yongliang)
2. (b). Temperature (^oC) (220,240) or (−,+),
3. (c). Pressure (psi) (50,80) or (−,+),
4. (d). Concentration (%) (10,12) or (−,+),

Table 5.10a. Data

Yates run #	1	2	3	4	*conversion*(%)	*random order*
1	−	−	−	−	70	8
2	+	−	−	−	60	2
3	−	+	−	−	89	10
4	+	+	−	−	81	4
5	−	−	+	−	69	15
6	+	−	+	−	62	9
7	−	+	+	−	88	1
8	+	+	+	−	81	13
9	−	−	−	+	60	16
10	+	−	−	+	49	5
11	−	+	−	+	88	11
12	+	+	−	+	82	14
13	−	−	+	+	60	3
14	+	−	+	+	52	12
15	−	+	+	+	86	6
16	+	+	+	+	79	7

```
x=c(70,60,89,81,69,62,88,81,60,
      49,88,82,60,52,86,79)
a=rep(c(-1,1),8)
b=rep(c(-1,-1,1,1),4)
c=rep(-1,4)
c=c(c,-c,c,-c)
d=c(rep(-1,8),rep(1,8))
ab=a*b
ac=a*c
ad=a*d
bc=b*c
bd=b*d
cd=c*d
abc=ab*c
abd=ab*d
acd=ac*d
bcd=bc*d
abcd=ab*cd
mean(x)
lm(x~factor(a))$coef[2]      # = ?
sum(x*a)/8                   # = ?
x%*%a/8                      # = ?
   round(lm(x~a*b*c*d)$coef[2:16],2)*2
```

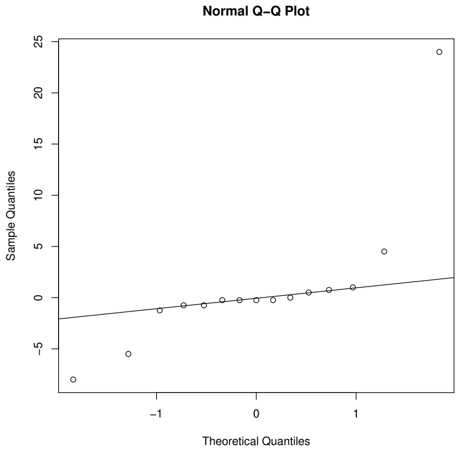


Figure 5.10

The average is 72.25.

The effects are

a	b	c	d	ab	ac	ad	bc	bd	cd
-8.00	24.00	-0.25	-5.50	1.00	0.75	0.00	-1.25	4.50	-0.25

abc	abd	acd	bcd	$abcd$
-0.75	0.50	-0.25	-0.75	-0.25

In a 2^3 factorial design with r replicates,
σ^2 is estimated by
$\tilde{\sigma}^2 = \frac{1}{2^3}\sum_{i=1}^{2^3} s_i^2$, where
$s_i^2 = \frac{1}{r-1}\sum_{h=1}^{r}(Y_{ih} - \overline{Y}_{i\cdot})^2$,
df of $\tilde{\sigma}^2$ is $2^3(r-1)$.
$V(effect) = \tilde{\sigma}^2(\frac{1}{4r} + \frac{1}{4r})$, as effect $= \overline{y}_+ - \overline{y}_-$.
A CI for effect is
effect $\pm t_{df,0.025}\sqrt{\tilde{\sigma}^2(\frac{1}{4r} + \frac{1}{4r})}$.

In this example, there is no replication (16 runs with 16 parameters).
The 5 3-factor and 4-factor interaction effects can be viewed as errors.
A conservative estimate of the SE of effect ($\sqrt{V(effect)}$ is
$\sqrt{\frac{\sum_{i=11}^{15} effect_i^2}{5}} \approx 0.55$ (treating each of the 5 effect$_i$'s as a variation of the **effect**).
The CI of effect is then
effect $\pm t_{5,0.025}0.55$ $(= 2.57 * 0.55)$.
It can be justified by qq-plot.
The significant effects can be found out:

a	b	c	d	ab	ac	ad	bc	bd	cd	
		-0.25		1.00	0.75	0.00	-1.25		-0.25	
-8.00	24.00		-5.50					4.50		$**$
abc	abd	acd	bcd	$abcd$						
	-0.75	0.50	-0.25	-0.75	-0.25					

Remark. Factor c and the interactions related to c are inert. It becomes a 2^3 factorial design, with replication $c = 2$. Thus we can use s^2 to estimate σ^2.

It is interesting to see from Figure 5.10 (see last page) that the significant effects can be detected by the qq-plot against normal distribution.

It is also interesting to see from the following stem-and-leaf plot that all but the 4 significant effects appear normal distribution.

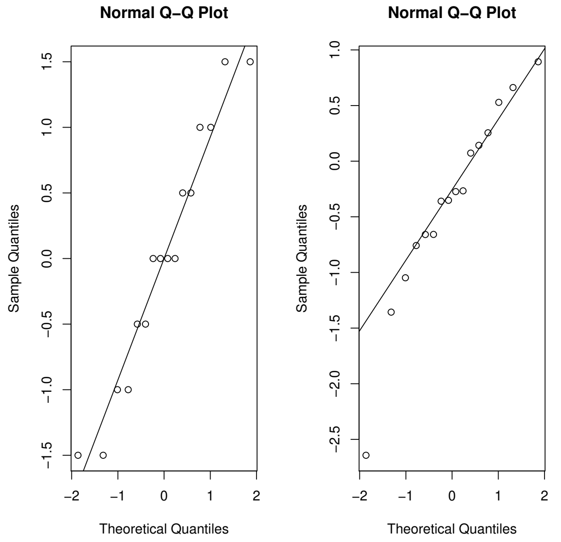
Thus one may use all but 4 effects to estimate V(effect)

```
u=c(-8.00,24.00,-0.25,-5.50 ,1.00 ,0.75, 0.00, -1.25, 4.50,-0.25,-0.75, 0.50,-0.25,-0.75,-0.25)
u=u[abs(u)<2]                    what is it ?
sort(u)

    [1] -1.25 -0.75 -0.75 -0.25 -0.25 -0.25 -0.25 0.00 0.50 0.75 1.00
stem(u)

    The decimal point is at the |
    -1 | 3
    -0 | 88
    -0 | 3333
     0 | 0
     0 | 58
     1 | 0
sqrt(mean(u*u))

    [1] 0.6571287                                        what is it ?
> summary(lm(x~a*b*d))
```

	Estimate	*Std. Error*	*t value*	$Pr(>\|t\|)$	
$(Intercept)$	$7.225e+01$	$3.307e-01$	218.463	$< 2e-16$	$***$
a	$-4.000e+00$	$3.307e-01$	-12.095	$2.02e-06$	$***$
b	$1.200e+01$	$3.307e-01$	36.285	$3.65e-10$	$***$
d	$-2.750e+00$	$3.307e-01$	-8.315	$3.30e-05$	$***$
$a:b$	$5.000e-01$	$3.307e-01$	1.512	0.169020	
$a:d$	$-3.955e-16$	$3.307e-01$	0.000	1.000000	
$b:d$	$2.250e+00$	$3.307e-01$	6.803	0.000137	$***$
$a:b:d$	$2.500e-01$	$3.307e-01$	0.756	0.471362	

Residual standard error: 1.323 on 8 degrees of freedom.

Remark. $s^2 = 1.323^2 = \hat{\sigma}^2$. The 3rd $\hat{\sigma}_{effect} = 1.332\sqrt{\frac{1}{4r} + \frac{1}{4r}}$ **What are the first two ?**



How to explain ties ?

Interpretation of the data.

1. Conversion changes -8% if catalyst charge switches from 10 to 15.
2. Pressure is inert.
3. To increase conversion set catalyst charge at 10 lb, temperature at 240^oC , concentration at 10%. It causes 33% increase.
4. Interaction between temperature and concentration can be seen from **Figure 5.11** in the textbook.
5. It reduces to a duplicated 2^3 FD.
6. $x = 72 - 4a + 12b - 2.75d + 2.25bd$. **Do we need to run lm() again for the LSE ?**

   (a). Catalyst charge (lb) (10,15) or $(-,+)$, (yongliang)

   (b). Temperature (^oC) (220,240) or $(-,+)$,

   (d). Concentration (%) (10,12) or $(-,+)$,

5.14. A first look at sequential assembly. The process of investigation includes interactive deduction and induction. Running an experiment can gain improvement on the production, but also indicates the possibility of even further advance and shows where additional runs needed to be made. It is called **sequential assembly**.

Experiment by Hill and Wiles (1975).

The object: to increase the disappointingly low yields of a chemical product.

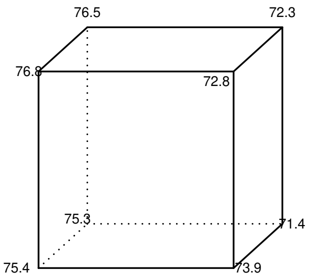
3 factorial designs were run in sequence but only the first will be described here.

In phase I, a 2^3 factorial design was run.

3 factors:
concentration C,
rate of reaction R,
temperature T.

run#	*C*	*R*	*T*	y_i (*yields*)
phase I				
1	$-$	$-$	$-$	
2	$+$	$-$	$-$	
3	$-$	$+$	$-$	
4	$+$	$+$	$-$	
5	$-$	$-$	$+$	
6	$+$	$-$	$+$	
7	$-$	$+$	$+$	
8	$+$	$+$	$+$	

```
> y=c(75.4,73.9,76.8,72.8,75.3,71.4,76.5,72.3)
```



Visual Display suggests that C is significant

```
> C=rep(c(-1,1),4), R=rep(c(-1,-1,1,1),2), c=rep(-1,4), T=c(c,-c)
> z=lm(y~ C*R*T)$coef
> c(z[1],2*z[2:8]) # (no need  to define factors) The effects are
```

$\overline{y}$	C	R	T	CR	CT	RT	CRT
74.3	-3.4	0.6	-0.85	-0.7	-0.65	0.45	0.55
intercept	*factors*						
76.3	??						
	significant						
	Why ?						

```
> H=lm(y~ factor(C))
```
Do we need to update the estimates ?

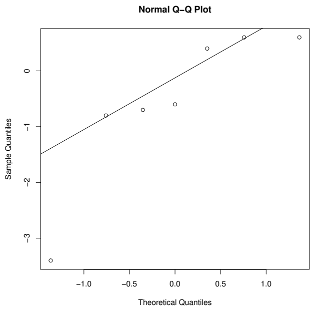


Fig. 1 QQplot

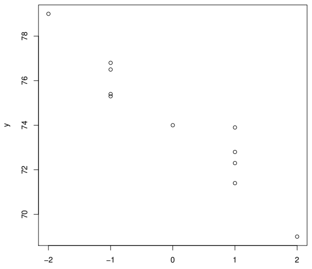


Fig. 2 (plot(a,y))

```
> qqnorm(z[2:8])
> qqline(z[2:8])
> sqrt(mean((2*z[3:8])**2)) [1] 0.6454972      # $\hat{\sigma} = 0.65$ or $\hat{\sigma}_{effect} = 0.65$ ?
> summary(H)$coef[2,2]                          [1] 0.6454972
> sqrt(anova(H)[2,3]/2) # $\sqrt{\sigma^2(\frac{1}{4}+\frac{1}{4})}$           [1] 0.6454972
```

Thus the model becomes $Y = \alpha + \beta\mathbf{1}(C = 1) + \epsilon$ or $\hat{Y} = 76.3 - 3.4\mathbf{1}(C = 1)$.
In phase II since C is significant, 3 runs were further made.
Purpose: To check whether the next new model is appropriate:

lm(y∼ C) # $\hat{y} = 74.3 - 1.7C$
Moreover, whether further improvement can be made.

run#	C	R	T	*phase II*
9	-2	0	0	
10	0	0	0	
11	2	0	0	

```
> y=c(y,79,74,69)
> a=c(C,-2,0,2)
> plot(a,y)                    # See above Fig. 2. What does it suggest ?
> (u=lm(y∼a))

    (Intercept) a

    74.22      -2.10
```

fitted equation: $\hat{Y}_u = 74.22 - 2.1a$.
Compare to the original simplified fitted equation:

$\hat{Y} = 76.0 - 3.4\mathbf{1}(C = 1)$ or $\hat{Y} = 74.3 - 1.7C$.

Can we further improve the yield by reducing the concentration C ?
Possible further experiment design ?

Remark. The difference between

$lm(y \sim a + b)$ and $lm(y \sim factor(a) + b)$, and 2^k factorial designs.

```
> n=20
> a=rbinom(n,3,0.5)
> b=rbinom(n,3,0.5)
> y=74−2*a+rnorm(n,0,2)
> x=factor(a)
> lm(y∼a)       # True model: $E(Y|X) = (\beta_0, \beta_1)(1, a)^t = 74 - 2a$
    (Intercept)       a
      74.011       −1.943
> lm(y∼x) # True model: $E(Y|X) = (\beta_1, ..., \beta_4)X$
                        $= 74 - 2\mathbf{1}(a = 1) - 4\mathbf{1}(a = 2) - 6\mathbf{1}(a = 3)$
    (Intercept)      x1          x2          x3
      73.764       −1.580     −3.824     −5.494
> lm(y∼x+b) # True model: $Y = (\beta_1, ..., \beta_5)(1, \mathbf{1}(a = 1), \mathbf{1}(a = 2), \mathbf{1}(a = 3), b)^t + \epsilon$
    $= 74 - 2\mathbf{1}(a = 1) - 4\mathbf{1}(a = 2) - 6\mathbf{1}(a = 3) + 0 \cdot b + \epsilon$
    (Intercept)      x1           x2           x3          b
     73.5866      −1.6907     −3.9429     −5.4584     0.1777
```

The LSE and prediction are all different now.

5.16. Blocking the 2^k factorial designs.

In a trial to be conducted using a 2^k factorial design, one either use 2^k different batches of raw materials or one batch of the same material. Otherwise, one may need blocking idea. Block sizes can be 2, 2^2, ..., 2^{k-1}. *e.g.*, for 2^3 FD, the block sizes are 2 and 4.

Block of size 4 for 2^3 FD. If one batch of raw material is only enough for 4 experiment, then partition according to 123 (or abc) = ±1.

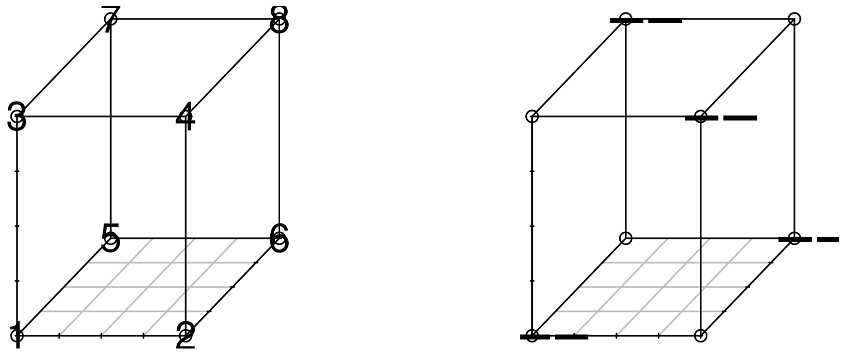
	mean	*a*	*b*	*c*	*ab*	*ac*	*bc*	*abc*
1	1	−1	−1	−1	1	1	1	−1
2	1	1	−1	−1	−1	−1	1	1
3	1	−1	1	−1	−1	1	−1	1
4	1	1	1	−1	1	−1	−1	−1
5	1	−1	−1	1	1	−1	−1	1
6	1	1	−1	1	−1	1	−1	−1
7	1	−1	1	1	−1	−1	1	−1
8	1	1	1	1	1	1	1	1
df	8	4	4	4	4	4	4	4

1	1	−1	−1	−1	1	1	1	−1	
4	1	1	1	−1	1	−1	−1	−1	
6	1	1	−1	1	−1	1	−1	−1	
7	1	−1	1	1	−1	−1	1	−1	*block* 1
2	1	1	−1	−1	−1	−1	1	1	*block* 2
3	1	−1	1	−1	−1	1	−1	1	
5	1	−1	−1	1	1	−1	−1	1	
8	1	1	1	1	1	1	1	1	

It leads to two sets of the run #:
$\{1, 4, 6, 7\}$ and $\{2, 3, 5, 8\}$

Drawback: It cannot estimate 3-factor interaction.
abc = block variable.

Advantage: See Figure 5.16
the batch I (1,4,6,7) and the batch II (2,3,5,8) are in 4 opposite vertices.



Remark. If we ignore the confounding effect, then what happans ? For example, in the previous case, suppose $Y = \beta_1 \mathbf{1}(a = 1) + \beta_2 \mathbf{1}(abc = 1) + \epsilon$, where β_2 is the confounding effect of different batch of raw materials and interaction abc. If we ignore confounding effects, and set $Y = \beta_1 \mathbf{1}(a = 1) + \epsilon_m$, then

$$\sigma^2_{\epsilon_m} = Var(\beta_2 \mathbf{1}(abc = 1) + \epsilon) = \beta_2^2 pq + \sigma^2 \qquad \textbf{Why ??}$$

Hence NID fails. If $\beta_2^2 + \sigma^2 > 2\beta_1$, then β_1 is likely to become insignificant.

Can we use ab, or ac, or bc ?

> Yes, but it is often that abc is inert. Moreover, it is not like abc which form 2 pair of opposite vertices. *e.g.* bc leads to (1,2,7,8), v.s. (3,4,5,6).

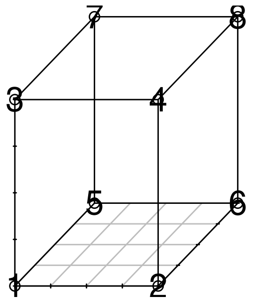
Can we use a or b or c as a partition factor ?

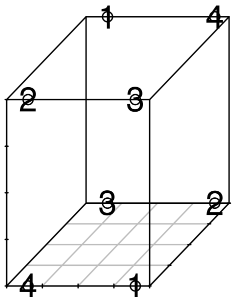
> No, we need to estimate the main effect, which is often more important than other effects, do not let it be confounded with the block factor.

Block of size 2 for 2^3 FD. If a batch of raw material can only be used in two experiments, partition according to (12,13) (or (ab,ac)).
It leads to 4 sets of the run due to $--$, $-+$, $+-$, $++$:

run #	**1**	**2**	**3**	$\mathbf{4 = 12}$	$\mathbf{5 = 13}$	*block#*	
1	−	−	−	+	+	*IV*	
2	+	−	−	−	−	*I*	
3	−	+	−	−	+	*II*	
4	+	+	−	+	−	*III*	
5	−	−	+	+	−	*III*	*Table* 1
6	+	−	+	−	+	*II*	
7	−	+	+	−	−	*I*	
8	+	+	+	+	+	*IV*	
2	+	−	−	−	−	*I*	
7	−	+	+	−	−	*I*	
3	−	+	−	−	+	*II*	
6	+	−	+	−	+	*II*	
4	+	+	−	+	−	*III*	*Table* 2
5	−	−	+	+	−	*III*	
1	−	−	−	+	+	*IV*	
8	+	+	+	+	+	*IV*	

The two block positions can be viewed as factors **4** and **5**, together with the original 3 factors **1**, **2**, and **3** (or a, b, c). Each pair is on the opposite vertex of the cube.





Thus there is no confounding (main) effects.

$$\begin{array}{cccc} & & \multicolumn{2}{c}{\textit{runs}} \\ \textit{variable } \mathbf{5} & + & (3,6) & (1,8) \\ & - & (2,7) & (4,5) \\ & & - & + \\ & & \multicolumn{2}{c}{\textit{variable } \mathbf{4}} \end{array}$$

The advantage of this approach is that the 3 factors a, b, c are all in different values (see Table 2).

How about let $(4,5) = (12,23)$? or (13,23) ?

Patterns not to partition. **(4,5)**= **(123,23)** (or (abc,bc)), due to $--, +-, -+, ++$.■

run #	**1**	**2**	**3**	**4 = 123**	**5 = 23**	*block#*
1	−	−	−	−	+	*III*
2	+	−	−	+	+	*IV*
3	−	+	−	+	−	*II*
4	+	+	−	−	−	*I*
5	−	−	+	+	−	*II*
6	+	−	+	−	−	*I*
7	−	+	+	−	+	*III*
8	+	+	+	+	+	*IV*

It leads to 4 sets of the run #:

	*			*		
4	+	+	−	−	−	*I*
6	+	−	+	−	−	*I*
3	−	+	−	+	−	*II*
5	−	−	+	+	−	*II*
1	−	−	−	−	+	*III*
7	−	+	+	−	+	*III*
2	+	−	−	+	+	*IV*
8	+	+	+	+	+	*IV*

The drawback of this approach is that factor a is the same in each block.

Not to partition according to (1,123) (or (a,abc), due to $--, +-, -+, ++$.

run #	**1**	**2**	**3**	**4 = 123**	*block#*
1	−	−	−	−	*I*
2	+	−	−	+	*IV*
3	−	+	−	+	*III*
4	+	+	−	−	*II*
5	−	−	+	+	*III*
6	+	−	+	−	*II*
7	−	+	+	−	*I*
8	+	+	+	+	*IV*

It leads to 4 sets of the run #:

	*			*	
1	−	−	−	−	*I*
7	−	+	+	−	*I*
4	+	+	−	−	*II*
6	+	−	+	−	*II*
3	−	+	−	+	*III*
5	−	−	+	+	*III*
2	+	−	−	+	*IV*
8	+	+	+	+	*IV*

The drawback of this approach is that factor a is the same in each block.

In the above two cases, the block factors confounded with a.

Generators and defining relations.

Recall the table of contrast:
$$\begin{array}{cccccccc}
I & a & b & c & ab & ac & bc & abc \\
\end{array}$$
$$\begin{pmatrix}
1 & -1 & -1 & -1 & 1 & 1 & 1 & -1 \\
1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 \\
1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 \\
1 & 1 & 1 & -1 & 1 & -1 & -1 & -1 \\
1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 \\
1 & 1 & -1 & 1 & -1 & 1 & -1 & -1 \\
1 & -1 & 1 & 1 & -1 & -1 & 1 & -1 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1
\end{pmatrix}.$$

It can be viewed as a 8×8 matrix, with each column being an 8×1 vector, say

(I **1** **2** **3** **12** **13** **23** **123**) or

$\big(I\quad \vec{a}\quad \vec{b}\quad \vec{c}\quad \vec{ab}\quad \vec{ac}\quad \vec{bc}\quad \vec{abc}\big)$.

Then I=**11**=**22**=**33**=**44**=**55**,

$\mathbf{1}I = \mathbf{1} = I\mathbf{1}$,

2I=**2**=I**2**, ... , as how we get ab, ac, ...

Recall in R, a*a=$(1, ..., 1)'$ and $a\% * \%a$ = ?

The defining relations **4**=**12** and **5**=**13** for two new factors in the previous cases are also called generators.

Then I=**2345** as **2345**= **231213**=I (=**124135**) and I=**124**=**135**

Namely, **45**=**23**, or **4** and **5** are confounded with **23**, **12**, **13**, **125**, **134** (none is a main effect), in the sense that each element in {**4**,**5**,**45**,**23**,**12**,**13**,**125**,**134**} is either **4** or **5** or **45**.

On the other hand, if we let **4**=**123** and **5**=**23**, and form 4 blocks (out of 8 runs) by $(\mathbf{4}, \mathbf{5})$, then I=**451** as I=**1234235**=**451**. Also I=**1234**=**235**.

That is, **45**=**1**, or **4** and **5** are confounded with **123**, **23**, **1**, **234**, etc. (with one main effect).

What happens to (**4**,**5**)=(**12**,**23**) or (**13**,**23**) ?

Finally, if we let **4**=**123** and form 4 blocks by $(\mathbf{1}, \mathbf{4})$,

Then **1** and **4** are clearly confounded with the block factor **1** (as well as, **4**, **123**, **23**, **14**). How about **4**=**13** and form 4 blocks by (**1**,**4**) ?

5.16.2. Homework. Answer the previous two question marks.

Connection between defining relations and blocking:

1. Use higher order interaction if possible.
2. The new defining factors have interaction of higher order.

For more details, see Table 5A.1 as follow.

Table 5A.1. Blocking Arrangements for 2^k FD.

k	block size	block generator	
3	4	123	*how about*
	2	12, 13	21, 23?
4	8	1234	
	4	124, 134	
	2	12, 23, 34	
5	16	12345	
	8	123, 345	
	4	125, 235, 345	
	2	12, 13, 34, 45	
6	32	123456	
	16	1236, 3456	
	8	135, 1256, 1234	
	4	126, 136, 346, 456	
	2	12, 23, 34, 45, 56	

Examples of 2^6 FD, with block size 8.

The first example (which is in the table).

Define B_1 = **135**, B_2=**1256** and B_3=**1234**. Then

B_1B_2=**1351256**=**236**,

B_1B_3=**1351234**=**245**,

B_3B_2=**12341256**=**3456**,

$B_1B_2B_3$=**13512561234**=**146** (no replication of numbers).

Thus B_1, B_2 and B_3 are confounded with **135**, **1256**, **1234**, **236**, **245**, **3456**, **146**.

Interpretation:

These effects **135**, **1256**, **1234**, **236**, **245**, **3456**, **146** cannot be estimated.

Their order (of interaction): 3+.

Another example (not in the table).

Define A_1=**12456**, B_2=**1256** and B_3=**1234**. Then

A_1B_2=**4**,

A_1B_3=**356**,

B_3B_2=**3456**,

$A_1B_2B_3$=**123**.

Interpretation:

These effects **12456**, **1256**, **1234**, **4**, **356**, **3456**, **123** cannot be estimated.

Their order: 1+

Is it appropriate ?

How about (**246**, **1236**, **2345**) ?

The third example. Define A_2=**1245**, B_2=**1256** and B_3=**1234**. Then

A_2B_2=**46**,

A_2B_3=**35**,

B_3B_2=**3456**,

$A_2B_2B_3$=**1236**.

Interpretation:

These effects **1245**, **1256 1234**, **46**, **35**, **3456**, **1236** cannot be estimated.

Their order: 2+.

Is it appropriate ?

Which is the best among these three ?

Capter 6 Fractional Factorial Designs

We shall introduce the concept through examples.

6.1. Experiment on effects of 5 factors on six properties of films in 8 runs.

Factors :		$-$	$+$	
A :	*catalyst*(%)	1	1.5	
B :	*additive*(%)	0.25	0.5	
C :	*emulsifier P* (%)	2	3	*ruhuaji*
D :	*emulsifier Q* (%)	1	2	
E :	*emulsifier R* (%)	1	2	
Response :	(*qualitative*)			
y_1 :	*hazy*?			
y_2 :	*adhere*?			
y_3 :	grease on top of film ?			
y_4 :	grease under film ?			
y_5 :	dull, adjusted pH			
y_6 :	dull, original pH			

A standard FD in such a case is 2^5 design with $n \geq 32$ experiments.

But it is done by a fractional factorial design in n=8 runs. The data are as follows.

run #	1	2	3	4 = 123	5 = 23	y_1	y_2	y_3	y_4	y_5	y_6
	A	B	C	E	D						
1	$-$	$-$	$-$	$-$	$+$	*no*	*no*	*yes*	*no*	*slightly*	*yes*
2	$+$	$-$	$-$	$+$	$+$	*no*	*yes*	*yes*	*yes*	*s*	*yes*
3	$-$	$+$	$-$	$+$	$-$	*no*	*no*	*no*	*yes*	*no*	*no*
4	$+$	$+$	$-$	$-$	$-$	*no*	*yes*	*no*	*no*	*no*	*no*
5	$-$	$-$	$+$	$+$	$-$	*yes*	*no*	*no*	*yes*	*no*	*s-no*
6	$+$	$-$	$+$	$-$	$-$	*yes*	*yes*	*no*	*no*	*no*	*no*
7	$-$	$+$	$+$	$-$	$+$	*yes*	*no*	*yes*	*no*	*s*	*yes*
8	$+$	$+$	$+$	$+$	$+$	*yes*	*yes*	*yes*	*yes*	*s*	*yes*
res	$y_2 \uparrow$		$y_1 \uparrow$	$y_4 \uparrow$	$y_3, y_5, y_6 \uparrow$	C	A	D	E	D	D

It is called a 2^{5-2} design, or a quarter fraction of the full 2^5 design.

The results in the last row in the table are the purpose of the experiment:

which level yields the desired result.

The set-ups of the two quantitative levels are based on the experience of engineers.

The values of the variables are not uniquely determined, at least in this experiment.
Notice: This is different from blocking, where (**12**,**13**) is used.
Justification: (High order) interactions are often negligible.
Can we choose **4=123** and **5=12** ?

Main difference between blocking factor and fractional FD:
The former tries to avoid confounding blocks with other effects.
The latter focuses on main effects assuming higher order interaction is insignificant.

Why FD and FFD ? There are two types of covariates: categorical and numerical.

Categorical variables are naturally factorial.

Numerical variable can also be specified as factor variables as in §6.1.
The purpose in FD is to find the tendency for desired results, not necessarily to find the linear relation. The FFD is try to use less experiments to find the tendency of more factors.

6.1.2. Homework. 1. Discuss a statistician what are the possible randomization steps for the experiment in §6.1 using the fractional FD. Notice that the raw materials include films, catalysts, additives, emulsifiers, among others.

6.2. Stability of new product, 4 factors in 8 runs (a half fractional FD).
A chemist in a lab was trying to formulate a household liquid product using a new process. The product had some nice properties but he had not found the value of factors to achieve the desired value y of stability at 25 or above.
So he carried out another experiment as follows.

$Factors:$		$-$	$+$
$A:$	*acid concentration*	20%	30%
$B:$	*catalyst concentration*	1%	2%
$C:$	*temperature*	100	150
$D:$	*monomer concentration* :	25%	50%

Let $D = 4 = 123$. The data according to Yates order are

```
y=c(20,14,17,10,19,13,14,10).
```

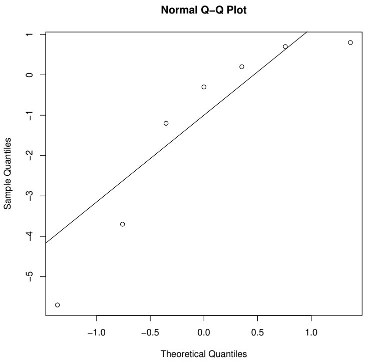
It was disappointed that the value $y \geq 25$ is not achieved in any of the cases. However, the experiment provided a trend for it.

	intercept	A	B	C	D			
The main effects:	19.25	−5.75	−3.75	−1.25	0.75	0.25	0.75	−0.25
	$\hat{\beta}_0$	$\hat{\beta}_A$	$\hat{\beta}_B$	$\hat{\beta}_C$	$\hat{\beta}_D$			

It occurs that the effect of D (or maybe C) is negligible,

```
> x=c(0.75,0.25,0.75,-0.25)                 (from the effects)
> round(2.33*sqrt(mean(x*x)),2)          normal scores: 1.64 1.96 2.33 2.58

[1] 1.30
```

or as displayed in the qqnorm() of the 7 effects.
It is simplified to $\hat{Y}_i = \hat{\beta}_o - 5.75\mathbf{1}(factor(A_i) = 1) - 3.75\mathbf{1}(factor(B_i) = 1)$ if $A_i \in \{20, 30\}$ & $B_i \in \{1, 2\}$.



run #	1	2	3	4 = 123	*y or R*
	A	*B*	*C*	*D*	
5	−	−	+	+	19
1	−	−	−	−	20
6	+	−	+	−	13
2	+	−	−	+	14
7	−	+	+	−	14
3	−	+	−	+	17
4	+	+	−	−	10
8	+	+	+	+	10

Ignoring columns C and D, the first two columns become a replicate 2^2 factorial design, as in Figure 6.1 (see Textbook p.238).
It seems from Figure 6.1 that one may simplify the relation as

$$y \approx \underbrace{\frac{20+19}{2}}_{how?} \underbrace{-5.75}_{where?} \underbrace{\frac{A-20}{10}}_{how?} -3.75(B-1) \text{ (in the unit of \%)} \qquad (1)$$

$$y \approx \overline{y} - \frac{5.75}{2}\frac{A-25}{5} - \frac{3.75}{2}\frac{B-1.5}{0.5} \text{ in control.sum with } \overline{y} = 14.625 \qquad (2)$$

Factors :		−	+
A :	*acid concentration*	20	30
B :	*catalyst concentration*	1	2

Eq. (1) is a <u>*guess*</u>, not from the LSE.
Roughly speaking, from Fig. 6.1,
if A=15 (%) and $B = 0.5$ (%), then Eq. (1) yields
$y = \frac{20+19}{2} - (5.75 + 3.75)(-0.5) = 24.25$.
Thus the stability value $y = 25$ can be reached if
acid concentration is set less than 15% and
catalyst concentration is set less than 0.5%.
The LSE:
> u=lm(y∼ a+b)$coef

(Intercept)	*a*1	*b*1
19.37	−5.75	−3.75
≠ 19.5	*(see Eq.*(1)	

> v=c(1, 0, −0.5, −0.6, −0.7)
> u[1]+v*(u[2]+u[3]) $\qquad 19.37 - 5.75\frac{A-20}{10} - 3.75(B-1) \geq 25?$

[1] 9.875 19.375 24.125 25.075 26.025

$\frac{A-20}{10} = -0.6$ => A=14

$B - 1 = -0.6$ => $B = 0.4$

The example illustrates:
1. How a fractional design was used for screening purposes to isolate 2 factors out of 4.
2. How a desirable direction in which to carry out further experiment was found.
6.2.2. Homework. What is the set up for the further experiment to serve the chemist's original plan ? How many experiments would you suggest ? Why ?

$Factors:$		$-$	$+$
$A:$	*acid concentration*	20%	30%
$B:$	*catalyst concentration*	1%	2%
$C:$	*temperature*	100	150
$D:$	*monomer concentration :*	25%	50%

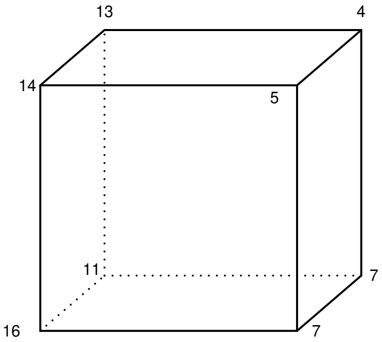
6.3. Another Half-fraction FD example. The modification of a bearing.
A manufacturer of bearing tries to improve their product of bearing.
A project team conjectured that they might need to modify
4 factors:
A: a particular characteristic of the manufacturing process for balls in the bearing,
B: the cage design,
C: the type of grease,
D: the amount of grease.
A 2^{4-1} half fractional FD was carried out with D corresponding to abc.

The results are

$Yates\ run\ \#$	1	2	3	4	5	6	7	8	
$failure\ rate\ y$	16	7	14	5	11	7	13	4	%

				abc			
R yields effects:	A	B	C	D	ab	ac	bc
	-7.7	-1.2	-1.7	-1.2	-1.3	1.2	0.7

The cube plots is



By experience, they suspected that interactions are inert (has little effect),
then it reduces to a 2^3 or duplicated 2^2 design (see Figure 6.2).
From this half fraction FD design experiment,
they found the major factors A and C to improve their bearing.

$y = 14.37 - 7.75 factor(a) - 1.75 factor(c)$

Both should be set at the "+" level (**why ?**)

6.4. The anatomy of the half fraction.
A complete 2^4 factorial design can estimate 16 independent quantities:
average, 4 main effects: A, B, C, D, and the interaction effects: AB, ..., ABCD.
A half fraction design using ABC to accommodate factor D.
Thus the main effect of D cannot distinguished from ABC interaction.
The main effect D is really

$l_D = \frac{1}{4}(-1, 1, 1, -1, 1, -1, -1, 1) \cdot (y_1, ..., y_8)$ (abc%*%y/4).

Thus l_D is really estimate the sum of the effects D and ABC, denoted by
$l_D \to D + ABC$.

The reason we said l_D is the main effect of D is that the 3-factor interactions are **often** negligible. For instance, in the example of §6.3, knowing ABC is inert by experience,

$effects$	$estimates$	effects assuming	3-factor interactions are inert
A	-7.7	A	
B	-1.2	B	
C	-1.7	C	
D	-1.2	$D(\&noise)$	(as ABCD=ABC(ABC)=I).
$AB+CD$	-1.3	AB	
$AC+BD$	1.2	AC	
$AD+BC$	0.7	BC	

The effects D and ABC are said to be **confounded**.
ABC is called an **alias** of D.
Under this design we also have

$l_A \to A+BCD$, $l_{AB} \to AB+CD$
$l_B \to B+ACD$, $l_{AC} \to AC+BD$
$l_C \to C+ABD$, $l_{BC} \to BC+AD$.

Table 1

Why ?

Recall AB represents interaction of A and B,
corresponding to their coordinates multiplying separately.
The AA corresponds to a vector with coordinates being all +1,
denoted by

I=AA=BB=CC=DD

Notice under the fractional factorial design

D=ABC (called the **generating relation**).

$$\text{I=DD=ABCD, } \overbrace{\text{A=BCD, B=ACD, C=ABD, AB=CD, AC=BD, AD=BC.}}^{combinations\ of\ ABCD\ in\ 2\ groups}$$

I=ABCD is also called the **generating relation** of the fractional FD.

The 2^{4-1} fractional factorial design used here is said to be of **resolution** 4, as the generating relation is

I=ABCD with 4 letters,

and no other products of less than **4 distinct** letters lead to I.
It is also denoted by 2^{4-1}_{IV} or "2 to the four minus 1, resolution four".
Remark. 2^{k-1} FFD may not be resolution k.
For instance, if the generating relation is

D=AB, (2^{4-1})

then

I=ABD.

$$\text{Also A=BD, B=AD, } \underbrace{\text{AC=BCD, BC=ACD, CD=ABC, I=ABD}}_{3\ letters\ on\ the\ right}\text{, C=}\underbrace{\text{ABCD}}_{4\ letters}\text{.}$$

No other products of less than 3 distinct letters lead to I.
The half fraction FD has a resolution 3, and is a 2^{4-1}_{III} (not 2^{4-1}_{IV}).
Thus 3-factor interaction may be confounded with 2-factor interaction. (AC=BCD)
If D=ABC, then 2-factor interaction is confounded with a 2-factor interaction (see Table 1 ↑).
Projectivity. Look at the next example of 4-run design in factors A, B, C:

	a	b	ab
$run\ \#$	A	B	C
1	$-$	$-$	$+$
2	$+$	$-$	$-$
3	$-$	$+$	$-$
4	$+$	$+$	$+$

a		ab
A	$run\ \#$	C
$-$	3	$-$
$+$	2	$-$
$-$	1	$+$
$+$	4	$+$
1		2

ab		b	
C	$run\ \#$	B	
$-$	2	$-$	
$+$	1	$-$	or (C,B) as (1,2).
$-$	3	$+$	
$+$	4	$+$	
1		2	

The design is a 2^{3-1}_{III}, as ABC=I.
If you drop one of the factor, you obtain a 2^2 FD in the remaining 2 factors.

It is said of projectivity P=2. The 2^2 FD in the next table can be viewed as 2^{3-1}_{III}:

Yates run #	*A*	*B*	*C*	
1	−	−	−	
4	+	+	−	(as $AB = -C$, see also Fig. 6.3 (p.244))
6	+	−	+	
7	−	+	+	

In general,

P=resolution of the design−1.

Denoted by

P=R−1.

Remark 6.3. See the previous example of 2^{4-1}_{IV} in Figure 6.2 with generating relation D=ABC. Then P=$4-1$=3. The geometric interpretation is clear from the figure, as well as the next table:

run #	1	2	3	$4 = 123$	*y or R*	*run #*	1	2	3	$4 = 123$	*y or R*	
	A	*B*	*C*	*D*			*A*	*B*	*C*	*D*		
	a	*b*	*c*				*a*	*b*		*c*		
1	−	−	−	−	20	1	−	−	−	−	20	*front*
2	+	−	−	+	14	6	+	−	+	−	13	
3	−	+	−	+	17	7	−	+	+	−	14	
4	+	+	−	−	10	4	+	+	−	−	10	
5	−	−	+	+	19	5	−	−	+	+	19	*back*
6	+	−	+	−	13	2	+	−	−	+	14	
7	−	+	+	−	14	3	−	+	−	+	17	
8	+	+	+	+	10	8	+	+	+	+	10	

run #	1	2	3	$4 = 123$	*y or R*		*run #*	1	2	3	$4 = 123$	*y or R*	
	A	*B*	*C*	*D*				*A*	*B*	*C*	*D*		
	a		*b*	*c*					*a*	*b*	*c*		
1	−	−	−	−	20	*bottom*	1	−	−	−	−	20	*L*
4	+	+	−	−	10		4	+	+	−	−	10	
7	−	+	+	−	14		6	+	−	+	−	13	
6	+	−	+	−	13		7	−	+	+	−	14	
3	−	+	−	+	17	*top*	2	+	−	−	+	14	*R*
2	+	−	−	+	14		3	−	+	−	+	17	
5	−	−	+	+	19		5	−	−	+	+	19	
8	+	+	+	+	10		8	+	+	+	+	10	

How to understand Figure 6.2 ? (see explanation figure on blackboard as well).

On the other hand, if the generating relation is D=AB, then P=3−1=2. Dropping one variable does not **always** reduce to a 2^3 FD (see Table 3 below).

run #	*a*	*b*	*c*	*ab*	*run #*	*a*	*b*	*c*	*ab*
	A	*B*	*C*	*D*		*A*	*B*	*C*	*D*
	1	2	3				1	2	3
1	−	−	−	+	2	+	−	−	−
2	+	−	−	−	3	−	+	−	−
3	−	+	−	−	6	+	−	+	−
4	+	+	−	+	7	−	+	+	−
5	−	−	+	+	1	−	−	−	+
6	+	−	+	−	4	+	+	−	+
7	−	+	+	−	5	−	−	+	+
8	+	+	+	+	8	+	+	+	+

Yes

run #	*a*	*b*	*ab*	
	A	*B*	*D*	
1	−	−	+	
2	+	−	−	
3	−	+	−	
4	+	+	+	??
5	−	−	+	
6	+	−	−	
7	−	+	−	
8	+	+	+	
?	−	−	−	

Dropping two variables *does* reduce to a (replicated) 2^2 FD (just need to consider 2 cases: (1) keep D, (2) otherwise.

(1) Keep D:

run #	*a*	*b*	*c*	*ab*	*run #*	*a*	*b*	*c*	*ab*	*run #*	*a*	*b*	*c*	*ab*
	A	*B*	*C*	*D*		*A*	*B*	*C*	*D*		*A*	*B*	*C*	*D*
	1			2			1		2				1	2
3	−	+	−	−	2	+	−	−	−	2	+	−	−	−
2	+	−	−	−	3	−	+	−	−	6	+	−	+	−
1	−	−	−	+	1	−	−	−	+	1	−	−	−	+
4	+	+	−	+	4	+	+	−	+	5	−	−	+	+
7	−	+	+	−	6	+	−	+	−	3	−	+	−	−
6	+	−	+	−	7	−	+	+	−	7	−	+	+	−
5	−	−	+	+	5	−	−	+	+	4	+	+	−	+
8	+	+	+	+	8	+	+	+	+	8	+	+	+	+

(2) Otherwise ?

6.5. The 2^{7-4}_{III} design: a bicycle example.

7 Factors:

A: seat (up,down),
B: dynamo (generator) (off, on),
C: handlebars (up, down),
D: gear (low, median),
E: raincoat (on, off),
F: breakfast (yes, no),
G: tires (hard, soft),

Response: y, climb hill in seconds.

run #	*a*	*b*	*c*	*ab*	*ac*	*bc*	*abc*	*y*
	A	*B*	*C*	*D*	*E*	*F*	*G*	
1	−	−	−	+	+	+	−	69
2	+	−	−	−	−	+	+	52
3	−	+	−	−	+	−	+	60
4	+	+	−	+	−	−	−	83
5	−	−	+	+	−	−	+	71
6	+	−	+	−	+	−	−	50
7	−	+	+	−	−	+	−	59
8	+	+	+	+	+	+	+	88

Table 6.4

Estimates of effects:

$l_A = 3.5$ seat (up,down),
$l_B = 12$ dynamo (generator) (off, on),
$l_C = 2.5$ handlebars (up, down), **typo in the textbook**
$l_D = 22.5$ gear (low, median),
$l_E = 1$ raincoat (on, off),
$l_F = 0.5$ breakfast (yes, no),
$l_G = 1.0$ tires (hard, soft),
Average=66.5

From previous experiments on the bicycle example, an estimate of the SD of repeated runs is 3. So the SE of the estimated effects is

$$\sqrt{\frac{3^2}{4} + \frac{3^2}{4}} = 2.1.$$

Thus there are only two factors which are distinguishable from noise. They are dynamo B and gear D. Or roughly, one can determine by

```
> z=c( 3.5, 12.0, 2.5, 22.5, 1.0, 0.5, 1.0)
> qqnorm(z)
> qqline(z)
    Or
> stem(z)
```

```
  The decimal point is 1 digit(s) to the right of the |
0 | 11134                    [0,5)
0 |                        [5,10)
1 | 2                      [10,15)
1 |                          [15,20)
2 | 2                      [20,25)
```

This fractional design can reduce the number of runs and present a replicated 2^2 FD for factors B and D, which is not very clear before the experiment.

Notice that (ignoring interactions of order 3+)

$l_I \to average.$

$l_A \to A + BD + CE + FG$

$l_B \to B + AD + CF + EG,$

$l_C \to C + AE + BF + DG,$

$l_D \to D + AB + EF + CG,$

$l_E \to E + AC + DF + BG,$

$l_F \to F + BC + DE + AG,$

$l_G \to G + CD + BE + AF,$

How are they obtained ?

The Defining Relations. The 4 generators

D=AB, E=AC, F=BC, G=ABC

yield 4 defining relations:

(1) $\binom{4}{1} = 4$ I=ABD=ACE=BCF=ABCG.

which lead to A=BD=CE=ABCF=BCG (not l_A).

To find all defining relations and to find all aliases, we need to add all words. There are $\sum_{i=1}^{4}\binom{4}{i} = 15$ defining relations: (from ABD=ACE=BCF=ABCG (=I)).

(1) $\binom{4}{1} = 4$: .....

(2) $\binom{4}{2} = 6$: (from ABD=ACE=BCF=ABCG (=I)),

I=(ABD)(ACE)=BCDE

I=(ABD)(BCF)=ACDF

I=(ABD)(ABCG)=CDG

I=(ACE)(BCF)=ABEF

I=(ACE)(ABCG)=BEG

I=(BCF)(ABCG)=AFG

(3) $\binom{4}{3} = 4$ from ABD=ACE=BCF=ABCG(=I),

I=DEF (=(ABD)(ACE)(BCF))

I=ADEG (=(ABD)(ACE)(ABCG))

I=BDFG (=(ABD)(BCF)(ABCG))

I=CEFG (=(ACE)(BCF)(ABCG))

(4) $\binom{4}{4} = 1$ from $\underbrace{ABD = ACE = BCF = ABCG}_{I=ABCDEFG}$(=I)

I=ABCDEFG

Remark. (1) In each of the 15 words, the letters are all distinct.

(2) Now it is clear why

$l_A \to A + BD + CE + FG$

due to I=ABD=ACE =AFG =ABCG=ACDF=ABEF =ADEG=ABCEDFG

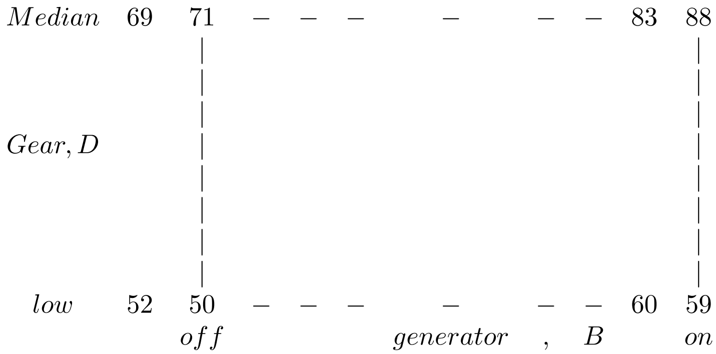
The shortest "word" in the 15 defining relations among (1) – (4) is 3.

It is called a 2^{7-4}_{III} FD.

Remark. This is different from the definition of resolution in half FD. But latter can be rephraced as this new one.

The 2^{7-4}_{III} can be viewed as a replicate 2^2 FD.

new run # in (D,B)	*a*	*b*	*c*	*ab*	*ac*	*bc*	*abc*	*y*
2	−	−	−	+	+	+	−	69
1	+	−	−	−	−	+	+	52
3	−	+	−	−	+	−	+	60
4	+	+	−	+	−	−	−	83
6	−	−	+	+	−	−	+	71
5	+	−	+	−	+	−	−	50
7	−	+	+	−	−	+	−	59
8	+	+	+	+	+	+	+	88



6.6. Eight-run designs Table 6.4 ignoring the response y can be used to produce the 2^3, the 2^{4-1}_{IV}, or the 2^{7-4}_{III} designs.

The latter two (not the first one) are called **nodal** designs, in the sense that for a given number of runs, the nodal design includes the largest number of factors at a given resolution.

The resolution R = the smallest # of distinct letters in the product.

There are

7 factors in 2^{7-4}_{III} design (where R=3).

4 factors in 2^{4-1}_{IV} design (where R=4).

There are 3 2^{4-1}_{III}:

a	*b*	*c*	*ab*	*ac*	*bc*	*abc*
A	*B*	*C*	*D*			
A	*B*	*C*		*E*		
A	*B*	*C*			*F*	

Remark. It won't matter whether one calls the factors A, B, C, D, or A, B, C, E. These 3 2^{4-1}_{III} generating relations are I=ABD, I=ACE and I=BCF, respectively.

R=3 **Why ?**

2^{4-1}_{IV}

a	*b*	*c*	*ab*	*ac*	*bc*	*abc*
A	*B*	*C*				*G*

The generating relation I=ABCG. R=4 **Why ?**

Between 2^{7-4}_{III} and 2^{4-1}_{IV}, we have 8-run 2^{5-2}_{III} and 2^{6-3}_{III} designs, but they are not nodal designs.

For example, if one considers a 5-factor design 2^{5-2}, there are 6 of them:

run #	*a*	*b*	*c*	*ab*	*ac*	*bc*	*abc*
	A	*B*	*C*	*D*	*E*		
	A	*B*	*C*	*D*		*F*	
	A	*B*	*C*		*E*	*F*	
	A	*B*	*C*	*D*			*G*
	A	*B*	*C*		*E*		*G*
	A	*B*	*C*			*F*	*G*
1	−	−	−	+	+	+	−
2	+	−	−	−	−	+	+
3	−	+	−	−	+	−	+
4	+	+	−	+	−	−	−
5	−	−	+	+	−	−	+
6	+	−	+	−	+	−	−
7	−	+	+	−	−	+	−
8	+	+	+	+	+	+	+

Table 6.6.

Note that I=ABCG=BCF in the last row of Table 6.6.

R=4 or R=3 in Table 6.6 ?

In Table 6.6, each of the 6 FD has either ABD=I, or I=ACE, or I=BCF and no product of two distinct letters = I, thus its resolution R=3.

Do we have 2^{8-5}_{II} design ?

run #	*a*	*b*	*c*	*ab*	*ac*	*bc*	*abc*	
	A	*B*	*C*	*D*	*E*	*F*	*G*	Then resolution = 3 or 2 ?
							H	

Comments:

The fractional FG is used to screen out significant factors from a larger group of factors.

It is hopeful to reduce to 2 factors by 2^{7-4}_{III}

It is hopeful to reduce to 3 factors by 2^{4-1}_{IV}

2^{8-5}_{II} can not even reduce to 1 factor, as G and H cannot be distinguished.

6.7. Using Table 6.6. An illustration.

$$\left(\begin{array}{cccccccccc} & a & b & c & ab & ac & bc & abc & Projectivity & P \\ 2^3 & A & B & C & & & & & & \\ 2^{4-1}_{IV} & A & B & C & & & & G & 3 & \\ 2^{7-4}_{III} & A & B & C & D & E & F & G & 2 & \end{array}\right)$$

For 2^{4-1}_{IV} design, ignoring 3-factor interaction,

$l_A \to A,$

$l_B \to B,$

$l_C \to C,$

$l_D \to AB + CG,$ (due to ABCG=I)

$l_E \to AC + BG,$

$l_F \to BC + AG,$

$l_G \to G.$

For 2^{7-4}_{III} design, ignoring 3-factor interaction,

$l_A \to A + BD + CE + FG,$

$l_B \to B + AD + CF + EG,$

$l_C \to C + AE + BF + DG,$

$l_D \to D + AB + EF + CG,$ (as discussed in §6.5)

$l_E \to E + AC + DF + BG,$

$l_F \to F + BC + DE + AG,$

$l_G \to G + CD + BE + AF.$

An Experiment. In the early stages of a lab experiment, 5 factors are given as follows.

$factors$		-1	$+1$	
$1:$	$concentration\ of\ \gamma$	94	96%	
$2:$	$proportion\ of\ \gamma\ to\ \alpha$	3.85	4.15	mol/mol
$3:$	$amount\ of\ solvent$	280	310	cm^3
$4:$	$proportion\ of\ \beta\ to\ \alpha$	3.5	5.5	mol/mol
$5:$	$reaction\ time$	2	4	hr

The best conditions known at that time were thought to be far from optimal and the main effects were believed to be dominant, but the interaction AC were thought to be active and needs to be avoid.
So the column corresponds to AC needs to be dropped in section column from Table 6.6.

One way is to select columns A, B, C, D, G: G should be selected as abc is of higher order of interaction. That is, the 5th factor is not denoted by E, but by G.

$run\ \#$	a	b	c	ab	ac	bc	abc	
	A	B	C	D			G	y
1	$-$	$-$	$-$	$+$	$+$	$+$	$-$	77.1
2	$+$	$-$	$-$	$-$	$-$	$+$	$+$	68.9
3	$-$	$+$	$-$	$-$	$+$	$-$	$+$	75.5
4	$+$	$+$	$-$	$+$	$-$	$-$	$-$	72.5
5	$-$	$-$	$+$	$+$	$-$	$-$	$+$	67.9
6	$+$	$-$	$+$	$-$	$+$	$-$	$-$	68.5
7	$-$	$+$	$+$	$-$	$-$	$+$	$-$	71.5
8	$+$	$+$	$+$	$+$	$+$	$+$	$+$	63.7

The estimates are

l_A	l_B	l_C	l_D	l_E	l_F	l_G	
-4.5	0.2	-5.6	-0.8	1.0	-0.8	-3.4	
s		s				s	$why?$

Do we have factors E and F ?

l_F can be viewed as a noise, then so does l_E in view of l_F.
The optimal yields might be obtained by moving in a direction such that the concentration of γ (A), the amount of solvent (C) and the reaction time (G) were all reduced. A serious of further experiments lead to a yield of 84% (v.s. 77.1%) for the chemical manufacturing process. **What experiments to be considered ?**

6.8. Sign switching, foldover and sequential assembly. Further runs may needed when fractional designs yield ambiguity, *i.e.*, confounding effects.

A strategy is **Foldover**:
A single column foldover:

multiply one selected column by -1, or switching sign of the column.
An example of Bicycle experiment, where B and D are significant effects.

run #	a	b	c	ab	ac	bc	abc	y
	A	B	C	D	E	F	G	
1	−	−	−	+	+	+	−	69
2	+	−	−	−	−	+	+	52
3	−	+	−	−	+	−	+	60
4	+	+	−	+	−	−	−	83
5	−	−	+	+	−	−	+	71
6	+	−	+	−	+	−	−	50
7	−	+	+	−	−	+	−	59
8	+	+	+	+	+	+	+	88
switch				$\times(-1)$				
9	−	−	−	−	+	+	−	47
10	+	−	−	+	−	+	+	74
11	−	+	−	+	+	−	+	84
12	+	+	−	−	−	−	−	62
13	−	−	+	−	−	−	+	53
14	+	−	+	+	+	−	−	78
15	−	+	+	+	−	+	−	87
16	+	+	+	−	+	+	+	60

Effect: These 16 runs provide unaliased estimates of the main effect D and all two-factor interactions involving D.

Reason:	$1st\ 2^3$:	l_A	l_B	l_C	l_D	l_E	l_F	l_G	l_I
		3.5	12	1	22.5	0.5	1.0	2.5	66.5
	$2nd\ 2^3$:	l'_A	l'_B	l'_C	l'_D	l'_E	l'_F	l'_G	l'_I
		0.7	10.2	2.7	25.2	1.7	2.2	−0.7	68.125

The first 8 runs yield (ignoring higher order interactions):

$l_A \to A + BD + CE + FG$,
$l_B \to B + AD + CF + EG$,
$l_C \to C + AE + BF + DG$,
$l_D \to D + AB + EF + CG$,
$l_E \to E + AC + DF + BG$,
$l_F \to F + BC + DE + AG$,
$l_G \to G + CD + BE + AF$,

The second 8 runs yield (ignoring higher order interactions):

$l'_A \to A - BD + CE + FG$,
$l'_B \to B - AD + CF + EG$,
$l'_C \to C + AE + BF - DG$,
$l'_D \to D - AB - EF - CG$,
$l'_E \to E + AC - DF + BG$,
$l'_F \to F + BC - DE + AG$,
$l'_G \to G - CD + BE + AF$,

Then ignoring three or high order interactions,

$0.5(l_A + l'_A) = 2.1 \to A + CE + FG$,
$0.5(l_B + l'_B) = 11.1 \to B + CF + EG$,
$0.5(l_C + l'_C) = 1.9 \to C + AE + BF$,
$0.5(l_D + l'_D) = 23.9 \to D$,
$0.5(l_E + l'_E) = -0.6 \to E + AC + BG$,
$0.5(l_F + l'_F) = 1.6 \to F + BC + AG$,
$0.5(l_G + l'_G) = 0.9 \to G + BE + AF$,

In fact, $0.5(l_A + l'_A) = 2.1 \to A + CE + FG + BCG + BEF$, as

$$\begin{aligned}0.5(l_A + l'_A) \to &[A + BD + CE + FG + BCG + BEF + CDF + DEG + BCDEFG\\ &+(A - BD + CE + FG + BCG + BEF - CDF - DEG - BCDEFG)]/2\\ &=A + CE + FG + BCG + BEF\end{aligned}$$

Recall for 2^{7-4}_{III} design, the 15 $(= \sum_{i=1}^{4} \binom{4}{i})$ defining relations are
I=ABD =CDG =DEF =ACE=BCF =BEG=AFG

=BCDE =ACDF =ADEG =BDFG   =ABCG =ABEF =CEFG
=ABCDEFG

Foldover yields

I=−ABD =−CDG =−DEF   =ACE=BCF =BEG=AFG
=−BCDE =−ACDF =−ADEG =−BDFG   =ABCG =ABEF =CEFG
=−ABCDEFG

Average them yields

I=ACE=BCF =BEG =AFG =ABCG =ABEF =CEFG   No D !

Moreover,

$0.5(l_A - l'_A) = 1.4 \to BD,$
$0.5(l_B - l'_B) = 0.9 \to AD,$
$0.5(l_C - l'_C) = -0.9 \to DG,$
$0.5(l_D - l'_D) = -1.4 \to AB + EF + CG,$
$0.5(l_E - l'_E) = 1.1 \to DF,$
$0.5(l_F - l'_F) = -0.6 \to DE,$
$0.5(l_G - l'_G) = 1.6 \to CD,$ **why ???**

$$\begin{aligned}
0.5(l_A - l'_A) \to &[A + BD + CE + FG + BCG + BEF + CDF + DEG + BCDEFG \\
&-(A - BD + CE + FG + BCG + BEF - CDF - DEG - BCDEFG)]/2 \\
&= BD + CDF + DEG + BCDEFG \\
(l_D - l'_D)/2 \to &[D + AB + EF + CG + BCE + ACF + AEG + BFG + ABCEFG \\
&+(-D + AB + EF + CG + BCE + ACF + AEG + BFG + ABCEFG)]/2 \\
&= [AB + EF + CG + BCE + ACF + AEG + BFG + ABCEFG \\
(l_D + l'_D)/2 \to &[D + AB + EF + CG + BCE + ACF + AEG + BFG + ABCEFG \\
&-(-D + AB + EF + CG + BCE + ACF + AEG + BFG + ABCEFG)]/2 \\
&= D
\end{aligned}$$

Notice that now D is not aliased with any 2 or 3-factor interaction ...
The column D foldover “de-alias” the main effect D and all its interaction with other effects.

So, $0.5(l_I + l'_I) = 67.3 \to$ average,
$0.5(l_I - l'_I) = -1.6 \to$ block effect (**which blocks ?**)

How to implement in R ?

```
> y=c(69, 52, 60, 83, 71, 50, 59, 88, 47, 74, 84, 62, 53, 78, 87, 60)
> a=rep(c(-1,1),4)
> b=rep(c(-1,-1,1,1),2)
> c=rep(-1,4)
> c=c(c,-c)
>z=lm(y[1:8]∼a*b*c)$coef
>(z=c(z[1],z[2:8]*2))
    66.5 3.5 12.0 1.0 22.5 0.5 1.0 2.5
> D=−a*b
> E=a*c
> F=b*c
> G=a*F
>x=lm(y[9:16]∼a+b+c+D+E+F+G)$coef
>(x=c(x[1],x[2:8]*2))
    68.125 0.750 10.250 2.750 25.250 −1.750 −2.250 −0.750
> (z+x)/2
    67.3125 2.1250 11.1250 1.8750 23.8750 −0.6250 −0.6250 0.8750                (1)■

> (z−x)/2
    1.375 0.875 −0.875 −1.375 1.125 1.625 1.625 −0.8125 1.375 0.875 −0.875 −1.375■
    1.125 1.625 1.625
> a=c(a,a)
> b=c(b,b)
> c=c(c,c)
> D=c(−D,D)                why not C(D,−D) ?                (see D=−a*b)
> E=c(E,E)
> F=c(F,F)
> G=c(G,G)
> lm(y∼a+b+c+D+E+F+G)$coef[2:8]*2
    2.125 11.125 1.875 23.875 −0.625 −0.625 0.875
lm(y∼factor(a)+factor(b)+factor(c)+factor(D)+factor(E)+factor(F)+factor(G))$coef[2:8]

    2.125 11.125 1.875 23.875 −0.625 −0.625 0.875
```

Can we apply it to other column ?

The foldover is part of sequential process of scientific learning,
in contrast to the "one-shot" experiment we have learned so far.
In the previous example, the first 8 run is the first shot.
If we stop, then it is a one-shot experiment.
In experimental design, we have initial informed guesses:

what factors to include ?
what response to measure ?
where to locate the experimental region ?
by how much to vary the factors ?
after the data are available, how to proceed ?

We do not expect to find answers to all the question in one-shot.
We can try smaller experiment to reduce the unknown possibilities gradually by making second guesses. Foldover is one of such strategy.

2^{7-4} FD → 16-run design.

Does the total of the 16 runs consist of a 2^{7-3} FD ? Where to find D ?

run #	*a*	*b*	*c*	*ab*	*ac*	*bc*	*abc*	*y*
	A	*B*	*C*	*D*	*E*	*F*	*G*	
1	−	−	−	+	+	+	−	69
2	+	−	−	−	−	+	+	52
3	−	+	−	−	+	−	+	60
4	+	+	−	+	−	−	−	83
5	−	−	+	+	−	−	+	71
6	+	−	+	−	+	−	−	50
7	−	+	+	−	−	+	−	59
8	+	+	+	+	+	+	+	88
switch				×(−1)				
9	−	−	−	−	+	+	−	47
10	+	−	−	+	−	+	+	74
11	−	+	−	+	+	−	+	84
12	+	+	−	−	−	−	−	62
13	−	−	+	−	−	−	+	53
14	+	−	+	+	+	−	−	78
15	−	+	+	+	−	+	−	87
16	+	+	+	−	+	+	+	60

16 runs FFD

run #	*a*	*b*	*c*	?	*ac*	*bc*	*abc*	*y*
	A	*B*	*C*	*D*	*E*	*F*	*G*	
9	−	−	−	−	+	+	−	47
2	+	−	−	−	−	+	+	52
3	−	+	−	−	+	−	+	60
12	+	+	−	−	−	−	−	62
13	−	−	+	−	−	−	+	53
6	+	−	+	−	+	−	−	50
7	−	+	+	−	−	+	−	59
16	+	+	+	−	+	+	+	60
1	−	−	−	+	+	+	−	69
10	+	−	−	+	−	+	+	74
11	−	+	−	+	+	−	+	84
4	+	+	−	+	−	−	−	83
5	−	−	+	+	−	−	+	71
14	+	−	+	+	+	−	−	78
15	−	+	+	+	−	+	−	87
8	+	+	+	+	+	+	+	88

2^{7-3} FFD

6.9. Multiple-column foldover. Its effect is that all main effects can be unaliased with two-factor interactions. (A single column (say D) foldover unaliases D with all interactions).

Chemical plants experiment. A number of similar chemical plants in different locations had been operated successfully for years. In a newly constructed plant certain filtration cycle took twice as long as the other plants. In order to find the reason, 7 factors are identified and a 2^{7-4}_{III} fractional design was carried out.

	$Factors$	$-$	$+$	
$A:$	$water\ supply$	$town\ reservoir$	$well$	
$B:$	$raw\ material$	$on\ site$	$other$	
$C:$	$temperature$	low	$high$	
$D:$	$recycle$	yes	no	
$E:$	$caustic\ soda$	$fast$	$slow$	$(kexingna)$
$F:$	$filter\ cloth$	new	old	
$G:$	$holdup\ time$	low	$high$	

	a	b	c	ab	ac	bc	abc	y
$run\ \#$	A	B	C	D	E	F	G	
1	$-$	$-$	$-$	$+$	$+$	$+$	$-$	68.4
2	$+$	$-$	$-$	$-$	$-$	$+$	$+$	77.7
3	$-$	$+$	$-$	$-$	$+$	$-$	$+$	66.4
4	$+$	$+$	$-$	$+$	$-$	$-$	$-$	81.0
5	$-$	$-$	$+$	$+$	$-$	$-$	$+$	78.6
6	$+$	$-$	$+$	$-$	$+$	$-$	$-$	41.2
7	$-$	$+$	$+$	$-$	$-$	$+$	$-$	68.7
8	$+$	$+$	$+$	$+$	$+$	$+$	$+$	38.7

foldover	$-a$	$-b$	$-c$	$-ab$	$-ac$	$-bc$	$-abc$	y
$run\ \#$	A	B	C	D	E	F	G	
9	$+$	$+$	$+$	$-$	$-$	$-$	$+$	66.7
10	$-$	$+$	$+$	$+$	$+$	$-$	$-$	65.0
11	$+$	$-$	$+$	$+$	$-$	$+$	$-$	86.4
12	$-$	$-$	$+$	$-$	$+$	$+$	$+$	61.9
13	$+$	$+$	$-$	$-$	$+$	$+$	$-$	47.8
14	$-$	$+$	$-$	$+$	$-$	$+$	$+$	59.0
15	$+$	$-$	$-$	$+$	$+$	$-$	$+$	42.6
16	$-$	$-$	$-$	$-$	$-$	$-$	$-$	67.6

For the 2^{7-4}_{III} design, the defining relations:
I= ABD=ACE=BCF =CDG =BEG=AFG =DEF
=ABEF =ABCG=BCDE=ACDF =ADEG=BDFG=CEFG= ABCDEFG.

Estimates:

$l_A = \underline{-10.9} \to A + BD + CE + FG$,
due to I=ABD=ACE =AFG,
and ignoring high order interactions: +BCG +CDF +BEF +DEG +BCDEFG.

$l_B = -2.8 \to B + AD + CF + EG$,
due to I=ABD=BCF =BEG

$l_C = \underline{-16.6} \to C + AE + BF + DG$,
due to I=ACE=BCF =CDG

$l_D = 3.2 \to D + AB + EF + CG$,
due to I=ABD =CDG=DEF

$l_E = \underline{-22.8} \to E + AC + DF + BG$,
due to I=ACE =BEG=DEF

$l_F = -3.4 \to F + BC + DE + AG$,
due to I=BCF =AFG=DEF

$l_G = 0.5 \to G + CD + BE + AF$,
due to I=CDG=BEG=AFG.

The estimates and summary(y∼a*b+b*c+a*c) (why ignore ℓ_G ?) suggest that the causes are factors A, C and E. To further investigate, another 8 runs were made.

The defining relation for the foldover is
I= −ABD=−ACE=−BCF =−CDG =−BEG=−AFG=−DEF = −ABCDEFG
=ABCG=BCDE=ACDF =ABEF =ADEG=BDFG=CEFG

$l'_A \to A - BD - CE - FG$,

due to I=−ABD=−ACE =−AFG,

and ignoring high order interactions: BCG+CDF+BEF+DEG−BCDEFG

$l'_B \to B - AD - CF - EG$,
$l'_C \to C - AE - BF - DG$,
$l'_D \to D - AB - EF - CG$,
$l'_E \to E - AC - DF - BG$,
$l'_F \to F - BC - DE - AG$,
$l'_G \to G - CD - BE - AF$.

Then

$0.5(l_A + l'_A) = \underline{-6.7} \to A$, ignoring BCG+CDF+BEF+DEG,
$0.5(l_B + l'_B) = -3.9 \to B$,
$0.5(l_C + l'_C) = -0.4 \to C$,
$0.5(l_D + l'_D) = 2.7 \to D$,
$0.5(l_E + l'_E) = \underline{-19.2} \to E$,
$0.5(l_F + l'_F) = -0.1 \to F$,
$0.5(l_G + l'_G) = -4.3 \to G$,
$0.5(l_I + l'_I) = 63.6$.
$0.5(l_A - l'_A) = -4.2 \to BD + CE + FG$,
$0.5(l_B - l'_B) = 1.1 \to AD + CF + EG$,
$0.5(l_C - l'_C) = \underline{-16.2} \to AE + BF + DG$,
$0.5(l_D - l'_D) = 0.5 \to AB + EF + CG$ (no high order interaction, except ABCEFG)
$0.5(l_E - l'_E) = -3.6 \to AC + DF + BG$,
$0.5(l_F - l'_F) = -3.4 \to BC + DE + AG$,
$0.5(l_G - l'_G) = 4.8 \to CD + BE + AF$,
$0.5(l_I - l'_I) = 3.0$.

```
x=c(-6.7,-3.9,-0.4,2.7,-19.2,-0.1,-4.3,0.5,-3.6,1.1,-16.2, 4.8,-3.4,-4.2,3)
round(x,0)
    [1] -7 -4 0 3 -19 0 -4 0 -4 1 -16 5 -3 -4 3
sort(x)
    [1] -19.2 -16.2 -6.7 -4.3 -4.2 -3.9 -3.6 -3.4 -0.4 -0.1 0.5 1.1 2.7 3.0 4.8
stem(x)
    −1 | 96
    −1 |
    −0 | 7
    −0 | 4444300
    +0 | 1133
    +0 | 5
```

Thus it suggests that rather than A, C and E in the first 2^{7-4}_{III} FD, the multiple foldover finds that the main causes are A, E and AE **(why not BF+DG ?)**, C is a noise.

On one hand, the stem and leaf plot suggests that
the main causes are E and AE, but A is also a noise.

On the other hand, the Analysis of Variance Table suggests that A is marginally significant.

```
     Model 1: y ∼ E + I(A * E)
     Model 2: y ∼ A + E + I(A * E)
   Res.Df    RSS    Df   Sum of Sq      F       Pr(> F)
1      13     645.94
2      12     467.05    1       178.89      4.5962    0.05322    .
```

$y = 63.6 - 9.6E - 8.1AE + \epsilon$ (or $\hat{y} = 63.6 - 9.6E - 8.1AE$, where $\overline{y} = 63.6$) ?

$y = 63.6 - 19.2\mathbf{1}(E = 1) - 16.2\mathbf{1}(AE = 1) + \epsilon$?

Improvement can be obtained by E=+1 (caustic soda slow) and A=+1 (well water).

An economic alternative to total foldover.

The foldover took 8 runs to find out the previous conclusion,

but there were simpler ways to do it.
Since the 8-run 2_{III}^{7-4} experiment indicates that A, C and E are **possibly** not inert, we can consider 2^3 FD with factor A, C and E.

	A	C	E
1	$-$	$-$	$+$
2	$+$	$-$	$-$
3	$-$	$-$	$+$
4	$+$	$-$	$-$
5	$-$	$+$	$-$
6	$+$	$+$	$+$
7	$-$	$+$	$-$
8	$+$	$+$	$+$

run #	*a*	*b*	*c*	*ab*	*ac*	*bc*	*abc*	*y*
	A		*C*		*E*			
2	$+$		$-$		$-$			77.7
4	$+$		$-$		$-$			81.0
5	$-$		$+$		$-$			78.6
7	$-$		$+$		$-$			68.7
1	$-$		$-$		$+$			68.4
3	$-$		$-$		$+$			66.4
6	$+$		$+$		$+$			41.2
8	$+$		$+$		$+$			38.7

	1	2	3
?	$-$	$-$	$-$
2, 4	$+$	$-$	$-$
5, 7	$-$	$+$	$-$
?	$+$	$+$	$-$
1, 3	$-$	$-$	$+$
?	$+$	$-$	$+$
?	$-$	$+$	$+$
6, 8	$+$	$+$	$+$

Then runs 1-8 can be treated as 4 pairs of replicates, leading to estimate of SD

$$s^2 = \frac{\sum_{i=1}^4 d_i^2/2}{4} = 14.9 \text{ with df } 4. \ (= \hat{V}(\epsilon) \ ? \text{ or } \hat{V}(effect) \ ? \ d_i = ?) \qquad (1)$$

Reason: Recall under model $Y = \beta' X + \epsilon$ with $\beta \in \mathcal{R}^p$,
$\frac{1}{n-p}\sum_{j=1}^n (Y_j - \hat{\beta}' X_j)^2$ has df $n-p$.
$d_i^2/2 = \frac{1}{n-p}\sum_{j=1}^n (Y_j - \hat{\beta}' X_j)^2$, under model $Y_j = \mu + \epsilon$, $n = 2$ and $p = ?$
Thus it has df =1.
Add 4 more runs (instead of 8) yields

run #	*a*	*b*	*c*	*ab*	*ac*	*bc*	*abc*	*y*	
	A		*C*		*E*				
16	$-$		$-$		$-$			67.6	
2, 4	$+$		$-$		$-$			77.7	81.0
5, 7	$-$		$+$		$-$			78.6	68.7
11	$+$		$+$		$-$			86.4	
1, 3	$-$		$-$		$+$			68.4	66.4
13	$+$		$-$		$+$			47.8	
10	$-$		$+$		$+$			65.0	
6, 8	$+$		$+$		$+$			41.2	38.7

The 12 runs lead to estimates (through $lm(y \sim a*c + a*e + c*e)\$coef[2:7]*2$)

l_A	l_C	l_E	l_{AC}	l_{AE}	l_{CE}
-5.0	0.7	-21.7	-1.1	-17.3	-5.8
		s		s	?

with $\hat{\sigma}_{effect} = s\sqrt{\frac{1}{6}+\frac{1}{6}} = 2.23$ (why /6 ?) and $t_{0.025,4} \approx 2.8$. s is as in Eq.(1).
$2.8 \times 2.23 \approx 6.24$.
The effect is not significant if $|effect| < 6.24$. (P-value =0.06).
Thus, the main causes are E and AE, same as the 16-run results. Moreover, A, C and CE are not significant.
Remark. Notice that under the economic alternative design with 12 runs, l_A *etc.* are derived from $lm(y \sim \cdots)$, not from $\overline{y}_+ - \overline{y}_-$, as can be seen from the table.

```
> mean(y[c(2,4,11,13,6,8)])-mean(y[c(16,5,7,1,3,10)])
    [1] -6.983333
```

	l_a	l_c	l_e	l_{ac}	l_{ae}	l_{ce}
$\overline{y}_+ - \overline{y}_-$	-6.98	-5.05	-22.08	-8.35	-17.05	-7.52
$lm(y \sim \cdot)\$coef[\text{-}1]*2$	-5.04	-0.71	-21.71	-1.11	-17.29	-5.83
foldover	-6.7	-0.4	-19.2	-3.6	-16.2	-4.2
	$l_A - l'_A$	$l_C - l'_C$	$l_E - l'_E$	$l_E + l'_E$	$l_C + l'_C$	$l_A + l'_A$

Thus $\overline{y}_+ - \overline{y}_-$ is not applicable in foldover. Moreover, unlike the 2^k FD, given lm(y∼a*c*e) the final model needs to be estimated again. See the next R outputs.

```
> lm(y~factor(a) + factor(c) + factor(e) + factor(a*e)+factor(c*e))$coef
(Intercept)   factor(a)1   factor(c)1   factor(e)1   factor(c*e)1   factor(a*e)1
  90.39167     -5.03750      0.71250    -22.08333     -5.83750      -17.28750

> x=lm(y~a*c+a*e+c*e)$coef
> c(x[1],x[-1]*2)
(Intercept)       a          c          e          a:c         a:e         c:e
  65.89375    -5.03750   0.71250   -21.71250   -1.11250   -17.28750   -5.83750
```

It turns out to be different from $\overline{y}_+ - \overline{y}_-$.

```
> w=lm(y~e+I(a*e)+I(c*e))$coef
> c(w[1],w[-1]*2)
      (Intercept)          e           I(a*e)        I(c*e)
       65.625000     -22.083333   -17.050000    -7.516667
> V=lm(y~e +I(a*e))$coef
> c(V[1],V[2:3]*2)
      (Intercept)          e           I(a*e)
        65.62500      -22.08333    -17.05000
```

It turns out to be the same as $\overline{y}_+ - \overline{y}_-$.

```
> anova(h,z)
      Analysis of Variance Table
      Model 1: y ~ e + I(a * e)
      Model 2: y ~ e + I(a * e) + I(c * e)
           Res.Df   RSS    Df   Sum of Sq      F       Pr(> F)
      1       9     308.3
      2       8     138.8   1       169.5      9.7672   0.01412    *
```

Thus the model is $\hat{y} = 65.6 - 22.1e - 17.1a * e - 7.5c * e$.

R program for computing effects.

```
y1=c(68.4, 77.7, 66.4, 81.0, 78.6, 41.2, 68.7, 38.7)
a=rep(c(-1,1),4)
b=rep(c(-1,-1,1,1),2)
c=rep(-1,4)
c=c(c,-c)
z=lm(y1~a*b*c)$coef
summary(lm(y1~a*b+a*c+b*c))
                     Estimate   Std.Error    tvalue     Pr(> |t|)
      (Intercept)    65.0875     0.2625     247.952     0.00257    **
           a         -5.4375     0.2625     -20.714     0.03071    *
           b         -1.3875     0.2625      -5.286     0.11903
           c         -8.2875     0.2625     -31.571     0.02016    *
         a:b          1.5875     0.2625       6.048     0.10432
         a:c        -11.4125     0.2625     -43.476     0.01464    *
         b:c         -1.7125     0.2625      -6.524     0.09683    .
Analysis of Variance Table
      Model 1: y1 ~ a * b + a * c + b * c
      Model 2: y1 ~ a + c + I(a * c)
           Res.Df    RSS     Df   Sum of Sq       F       Pr(> F)
      1       1      0.551
      2       4     59.575   -3    -59.024     35.691     0.1223

A=a
B=b
C=c
ab=a*b
ac=a*c
bc=b*c
abc=ab*c
a=-a
```

```
b=−b
c=−c
ab=−ab
ac=−ac
bc=−bc
abc=−abc
y2=c(66.7, 65.0, 86.4, 61.9, 47.8, 59.0, 42.6, 67.6)
(x=lm(y2∼a+b+c+ab+ac+bc+abc)$coef)
    (Intercept)      a        b       c      ab       ac
      62.125     −1.250   −2.500  7.875   1.125   −7.800
        bc         abc
       1.650     −4.575
(x=lm(y2∼a*b*c)$coef) #Does it work ?
    (Intercept)      a        b       c      a : b    a : c
      62.125     −1.250   −2.500  7.875   −1.125   7.800
       b : c      a : b : c
      −1.650     −4.575
lm(y2∼ −A*B*C) #Does it work ?
u=round(z+x,1) # $l_A$, $l_B$, $l_C$, $l_D$, $l_E$, $l_F$, ......
v=round(z-x,1)
sort(c(v,u[1]/2,u[-1]))
                            a : c      c            a          a : b : c      a      b
                            −19.2      −16.2        −6.7       −4.3           −4.2   −3.9
                            a : c      b : c        c          b : c          a : b  b
                            −3.6       −3.4         −0.4       −0.1           0.5    1.1
                            a : b      (Intercept)  a : b : c  (Intercept)
                            2.7        3.0          4.8        63.6
x=lm(y2∼a*b*c)$coef
u=round(z+x,1)
v=round(z-x,1)
sort(c(v,u[1]/2,u[-1]))
                            a : c      c            a          a : b : c      a      b
                            −19.2      −16.2        −6.7       −4.3           −4.2   −3.9
                            a : c      b : c        c          b : c          a : b  b
                            −3.6       −3.4         −0.4       −0.1           0.5    1.1
                            a : b      (Intercept)  a : b : c  (Intercept)
                            2.7        3.0          4.8        63.6
d=c(1,2,16)
(s=sqrt(mean(x[-d]**2))) # treating the other estimates as noises.
    [1] 3.526929
s*qt(0.975,13)
    [1] 7.619468 # cut point for significance, which suggests that a= −6.7 is not
significant.
```

```
    # Another way:
a=c(A,a)
c=c(C,c)
b=c(B,b)
ab=c(A*B,ab)
ac=c(A*C,ac)
bc=c(B*C,bc)
abc=c(A*B*C,abc)
y=c(y1,y2)


AA=c(A,A)
BB=c(B,B)
CC=c(C,C)
EE=AA*CC
sort(round(lm(y∼a+b+c+ab+ac+bc+abc +AA*BB*CC)$coef[-1]*2,1)) # effects
```

after foldover

```
    E       AE        A
   ac       CC        a       abc    AA         b          AA:CC   BB:CC
 -19.2    -16.2     -6.7     -4.3   -4.2      -3.9          -3.6    -3.4
    c       bc     AA:BB      BB     ab    AA:BB:CC
  -0.4     -0.1      0.5      1.1    2.7       4.8
```

round((lm(y~ AA*BB*CC)$coef*2),1) # effects unchanged

```
(Intercept)    AA    BB     CC    AA:BB    AA:CC    BB:CC    AA:BB:CC
   127.2      -4.2   1.1  -16.2     0.5     -3.6     -3.4       4.8
```

(lm(y~ e+a:e)$coef*2)

```
  (Intercept)        e          e:a
   127.2125     -19.2125   -16.1625
```

(lm(y~ a+e+a:e)$coef*2)

```
  (Intercept)        a           e           a:e
   127.2125     -6.6875    -19.2125    -16.1625
```

(lm(y~a+c+e+AA+CC+EE)$coef*2)

```
  (Intercept)        a          c           e          AA          CC          EE
   127.2125     -6.6875    -0.4125   -19.2125    -4.1875    -16.1625    -3.6125
Analysis of Variance Table
    Model 1: y ~ a + c + e + AA + CC + EE
    Model 2: y ~ e + CC
       Res.Df    RSS    Df   Sum of Sq      F       Pr(> F)
    1     9     344.03
    2    13     645.94  -4    -301.91     1.9745    0.1822
Analysis of Variance Table
    Model 1: y ~ a + c + e + AA + CC + EE
    Model 2: y ~ a + e + CC
       Res.Df    RSS    Df   Sum of Sq      F       Pr(> F)
    1     9     344.03
    2    12     467.05  -3    -123.02     1.0728    0.4083
Analysis of Variance Table
    Model 1: y ~ e + CC
    Model 2: y ~ a + e + CC
       Res.Df    RSS    Df   Sum of Sq      F       Pr(> F)
    1    13     645.94
    2    12     467.05   1     178.89     4.5962    0.05322   .
```

An economic alternative:

```
d=c(16,11,13,10)
a=c(A,a[d])
c=c(C,c[d])
e=c(A*C,ac[d])
d=c(8,3,5,2)          # d+8=c(16,11,13,10)
y=c(y1,y2[d])
x=lm(y~a*c*e)
summary(x)
d=c(16,11,13,10)-8
a=c(A,-A[d])
c=c(C,-C[d])
e=c(A*C,-A[d]*C[d])
y=c(y1,y2[d])
x=lm(y~a*c*e)
x=lm(y~a*c*e)
summary(x)
```

	Estimate	*Std Error*	*t value*	*Pr*(> |*t*|)	
(*Intercept*)	65.8938	1.1816	55.764	$6.19e-07$	$***$
a	-2.5188	1.1816	-2.132	0.10003	
c	0.3562	1.1816	0.301	0.77807	
e	-10.8562	1.1816	-9.187	0.00078	$***$
$a:c$	-0.5562	1.1816	-0.471	0.66235	
$a:e$	-8.6438	1.1816	-7.315	0.00186	$**$
$c:e$	-2.9188	1.1816	-2.470	0.06894	.
$a:c:e$	-0.8062	1.1816	-0.682	0.53251	

Residual standard error: 3.859 on 4 degrees of freedom

$s=\sqrt{14.9}=3.86$ computed by replications s^2, and matching summary().

```
u=lm(y∼a*c+e*c+a*e)
summary(u)
anova(u,x)
```

	Estimate	*Std Error*	*t value*	*Pr*(> |*t*|)	
(*Intercept*)	65.6250	1.0528	62.331	$2.01e-08$	$***$
a	-2.5188	1.1167	-2.256	0.073765	.
c	0.3562	1.1167	0.319	0.762610	
e	-10.8562	1.1167	-9.722	0.000196	$***$
$a:c$	-0.5562	1.1167	-0.498	0.639536	
$c:e$	-2.9188	1.1167	-2.614	0.047457	$*$
$a:e$	-8.6438	1.1167	-7.740	0.000575	$***$

Residual standard error: 3.647 on 5 degrees of freedom

If ignoring ace, $\hat\sigma=\sqrt{\frac{1}{n-p}\sum_{i=1}^{12}(Y_i-\hat Y_i)^2}=3.65$ with df 5.

Analysis of Variance Table

Model 1: y ∼ a * c + e * c + a * e

Model 2: y ∼ e + I(a * e)

	Res.Df	*RSS*	*Df*	*Sum of Sq*	*F*	*Pr*(> *F*)	
1	5	66.509					
2	9	308.334	-4	-241.82	4.545	0.06398	.

Analysis of Variance Table

Model 1: y ∼ a * c + e * c + a * e

Model 2: y ∼ e + I(a * e) + I(c * e)

	Res.Df	*RSS*	*Df*	*Sum of Sq*	*F*	*Pr*(> *F*)
1	5	66.509				
2	8	138.833	-3	-72.325	1.8124	0.2617

Analysis of Variance Table

Model 1: y ∼ e + I(a * e)

Model 2: y ∼ e + I(a * e) + I(c * e)

	Res.Df	*RSS*	*Df*	*Sum of Sq*	*F*	*Pr*(> *F*)		
1	9	308.33						
2	8	138.83	1	169.5	9.7672	0.01412	$*$	**conclusion**?

Conclusion: AE and E are significant and CE is significant.

Remark: There are three conclusion based on whether CE is significant:

(1) In last ANOVA (economic alternative), AE, E and CE are all significant.

(2) In full foldover, CE is on the boundary (p-value=0.053) (in contrast to the conclusion in (1).

(3) In the ecomonic alternative, recall

l_A	l_C	l_E	l_{AC}	l_{AE}	l_{CE}
-5.0	0.7	-21.7	-1.1	-17.3	-5.8
		s		s	$p-value=0.06$ *using replications*

The last conclusion (0.06 based on $\hat\sigma_{effect}=2.23$) might be more reliable, as it

relies on replications and does not rely on N(.,.).
Of course, if NID is true, statement (2) is more reliable, as it sample size is larger.

Estimation of SD of effects.

```
y1=c(68.4, 77.7, 66.4, 81.0, 78.6, 41.2, 68.7, 38.7)
a=rep(c(-1,1),4)
b=rep(c(-1,-1,1,1),2)
c=rep(-1,4)
c=c(c,-c)
(z=lm(y1~a*b*c)$coef[-1]*2)
        a          b          c        a:b        a:c        b:c      a:b:c
  -10.875     -2.775    -16.575      3.175    -22.825     -3.425      0.525
        s                     s                     s
x=z$coef[c(2,4,6,7)]
sqrt(mean(x**2)) # SD of effects
    [1] 2.733587
x=lm(y1~a*c)
summary(x)
                    Estimate   Std.Error    tvalue    Pr(> |t|)
    (Intercept)       65.087       1.364    47.702    1.16e-06    ***
              a       -5.437       1.364    -3.985     0.01633      *
              c       -8.287       1.364    -6.074     0.00371     **
         I(a*c)      -11.412       1.364    -8.364     0.00112     **
    2 × effects      -10.8         2.734
                     -16.57        2.734
                     -22.82        2.734
                                SD_effects
Residual standard error: 3.859 on 4 degrees of freedom
```

$3.859\sqrt{\frac{1}{4}+\frac{1}{4}} = 2.734$

```
sqrt(2*mean(x**2)) # compare to Residual standard error in summary
    [1] 3.865876 # SD of errors.
```

Effect $=\overline{y}_{+}-\overline{y}_{-}$.

$Var(effect) = \sigma_\epsilon^2(\frac{1}{4}+\frac{1}{4})$.

Recall that runs 1-8 can be treated as 4 pairs of replicates corresponding to factors a and c, leading to estimate of SD

$\hat{S}_\epsilon^2 = s^2 = \frac{\sum_{i=1}^4 d_i^2/2}{4} = 14.9$ with df 4 and $\sqrt{14.9} = 3.86$.

Remark related to homework 6.2.2. EQ.(2) is the equation for the contour plane.

$$y \approx 14.63 - \frac{5.75}{2}\frac{A-25}{5} - \frac{3.75}{2}\frac{B-1.5}{0.5} \qquad \text{in control.sum} \tag{2}$$

$(A, B) = (14, 0.4)$ is a point on the contour plane

$$25.075 = 14.625 - \frac{5.75}{2}\frac{A-25}{5} - \frac{3.75}{2}\frac{B-1.5}{0.5}$$

It is a straght line on the AB plane (with A-axis and B-axis). $(A, B) = (20, 1.5)$ is a point on the contour plane $0 = \frac{5.75}{2}\frac{A-25}{5} + \frac{3.75}{2}\frac{B-1.5}{0.5}$ or $B = 1.5 - \frac{5.75}{3.75}\frac{A-25}{10}$ (from

$$14.625 = 14.625 - \frac{5.75}{2}\frac{A-25}{5} - \frac{3.75}{2}\frac{B-1.5}{0.5}).$$

It is another straght line on the AB plane.

6.10. Increasing design resolution from III to IV by foldover.

The foldover in §6.9 increases the resolution from III to IV.
Before multiple column foldover, there are 15 defining relations:

I=ABD =ACE=BCF =CDG =DEF =BEG=AFG =ABCDEFG
=ABCG =BCDE =ACDF =ADEG =BDFG =ABEF =CEFG

Adding the foldover, only 4-letter defining relations remain and the resolution becomes 4.

I= ABCG=BCDE=ACDF =ABEF =ADEG=BDFG=CEFG (total of 7).

If we choose 3 letters from ABCG (=I), we can form a replicated 2^3 FD, based on I=ABCG. *i.e.,* (A,B,C), (A,B,G), (A,C,G), (B,C,G)

So total of $4 \times 7 = 28$ combinations,
out of total of $\binom{7}{3} = 35$.

This is the advantage of such an approach.

Notice that a single column foldover yield defining relation

I=ACE=BCF =BEG =ABCG =ABEF =CEFG

The resolution is ?

Recall that the single column foldover results in a 2^{7-3}_{III} design.

Look at the previous 16-run experiment. Is it a 2^{7-3} design ? If so, it is a 2^{7-3}_{IV} design.

	run #	*a*	*b*	*c*	*ab*	*ac*	*bc*	*abc*	*y*	(*table of contrast*)
		A	*B*	*C*	*D*	*E*	*F*	*G*		(*defining factors*)
	1	−	−	−	+	+	+	−	68.4	
	2	+	−	−	−	−	+	+	77.7	
	3	−	+	−	−	+	−	+	66.4	
	4	+	+	−	+	−	−	−	81.0	
	5	−	−	+	+	−	−	+	78.6	
	6	+	−	+	−	+	−	−	41.2	
	7	−	+	+	−	−	+	−	68.7	
Original order	8	+	+	+	+	+	+	+	38.7	
	run #	$-a$	$-b$	$-c$	$-ab$	$-ac$	$-bc$	$-abc$	*y*	
	9	+	+	+	−	−	−	+	66.7	
	10	−	+	+	+	+	−	−	65.0	
	11	+	−	+	+	−	+	−	86.4	
	12	−	−	+	−	+	+	+	61.9	
	13	+	+	−	−	+	+	−	47.8	
	14	−	+	−	+	−	+	+	59.0	
	15	+	−	−	+	+	−	+	42.6	
	16	−	−	−	−	−	−	−	67.6	

		a	*b*	*c*	$-ab$	$-ac$	$-bc$	*abc*	
	16	−	−	−	−	−	−	−	67.6
	15	+	−	−	+	+	−	+	42.6
	14	−	+	−	+	−	+	+	59.0
Reverse the last 8	13	+	+	−	−	+	+	−	47.8
	12	−	−	+	−	+	+	+	61.9
	11	+	−	+	+	−	+	−	86.4
	10	−	+	+	+	+	−	−	65.0
	9	+	+	+	−	−	−	+	66.7

Columns A B C G form a replicated 2^3 FD, (see a, b, c, abc cloumns), not a 2^4 FD.

The main component of 2^4 (or 2^{7-3}) FD: a,b,c,d columns.

Replacing G by other 3 choices from I=ABCG: A B C D, A B C E and A B C F.

Is A B C D 2^4 FD ? Try order 16,2,3,13,12,6,7,9, 1,15,14,4,5,11,10,8.

Are A B C E and A B C F 2^4 FD ? Note these 3 are related to ABCG=I

run #	*a*	*b*	*c*	*ab*	*ac*	*bc*	*abc*	*y*	(*table of contrast*)
	A	*B*	*C*	*D*	*E*	*F*	*G*		(*defining factors*)

Are these 2^4 FD ?

	A	B	C	E
16	−	−	−	−
2	+	−	−	−
14	−	+	−	−
4	+	+	−	−
5	−	−	+	−
11	+	−	+	−
7	−	+	+	−
9	+	+	+	−
1	−	−	−	+
15	+	−	−	+
3	−	+	−	+
13	+	+	−	+
12	−	−	+	+
6	+	−	+	+
10	−	+	+	+
8	+	+	+	+

	A	B	C	F
16	−	−	−	−
15	+	−	−	−
3	−	+	−	−
4	+	+	−	−
5	−	−	+	−
6	+	−	+	−
10	−	+	+	−
9	+	+	+	−
1	−	−	−	+
2	+	−	−	+
14	−	+	−	+
13	+	+	−	+
12	−	−	+	+
11	+	−	+	+
7	−	+	+	+
8	+	+	+	+

I=ABCG

What are the FD patterns for the cases by replacing one letter from

ABCG=BCDE=ACDF =ABEF =ADEG=BDFG=CEFG (=I) ?

Like ABCG, they are not 2^4 FD, but replicated 2^{4-1} fractional FD:

I=ABCG

	A	B	C	G
16	−	−	−	−
15	+	−	−	+
14	−	+	−	+
13	+	+	−	−
12	−	−	+	+
11	+	−	+	−
10	−	+	+	−
9	+	+	+	+
1	−	−	−	−
2	+	−	−	+
3	−	+	−	+
4	+	+	−	−
5	−	−	+	+
6	+	−	+	−
7	−	+	+	−
8	+	+	+	+

	1	2	123	3
	A	B	C	G
16	−	−	−	−
11	+	−	+	−
10	−	+	+	−
13	+	+	−	−
12	−	−	+	+
15	+	−	−	+
14	−	+	−	+
9	+	+	+	+
1	−	−	−	−
6	+	−	+	−
7	−	+	+	−
4	+	+	−	−
5	−	−	+	+
2	+	−	−	+
3	−	+	−	+
8	+	+	+	+

$(A,C,G)=(1,2,3)$
$(B,C,G)=(1,2,3)$?

I=ABEF

run #	1 *A*	2 *B*	*C*	*D*	123 *E*	3 *F*
16	$-$	$-$				$-$
15	$+$	$-$				$-$
10	$-$	$+$				$-$
9	$+$	$+$				$-$
12	$-$	$-$				$+$
11	$+$	$-$				$+$
14	$-$	$+$				$+$
13	$+$	$+$				$+$
5	$-$	$-$				$-$
6	$+$	$-$				$-$
3	$-$	$+$				$-$
4	$+$	$+$				$-$
1	$-$	$-$				$+$
2	$+$	$-$				$+$
7	$-$	$+$				$+$
8	$+$	$+$				$+$

I=ADEG

run #	1 *A*	2 *D*	3 *E*	*F*	123 *G*
16	$-$	$-$	$-$		$-$
9	$+$	$-$	$-$		$+$
14	$-$	$+$	$-$		$+$
11	$+$	$+$	$-$		$-$
12	$-$	$-$	$+$		$+$
13	$+$	$-$	$+$		$-$
10	$-$	$+$	$+$		$-$
15	$+$	$+$	$+$		$+$
7	$-$	$-$	$-$		$-$
2	$+$	$-$	$-$		$+$
5	$-$	$+$	$-$		$+$
4	$+$	$+$	$-$		$-$
3	$-$	$-$	$+$		$+$
6	$+$	$-$	$+$		$-$
1	$-$	$+$	$+$		$-$
8	$+$	$+$	$+$		$+$

or I=BCDE=ACDF =BDFG=CEFG

This is a 2^{7-3}_{IV} design. It can scan 3 out of 7 factors to form a replicated 2^3 FD for all $\binom{7}{3} = 35$ patterns, though $7 \times 4 = 28$ of them cannot form 2^4 FD.

6.10.1. Homework. Are A D E F, B D E F, C D E F 2^4 FDs ? Prove or disprove it.

6.10.2. Homework. Prove or disprove it. Can (B, D, F) be chosen as (a,b,c) ? How about (A, B, D) ?

6.11. 16-run design.

For computation purpose, instead define the orthogonal array in Table 6.14a, one can use

```
z=lm(y∼ a*b*c*d)

2*z$coef[2:16]
```

where y is the response variable and a, b, c, d are variables defined as follows.

```
a=c(−1, 1, −1, 1, −1, 1, −1, 1, −1, 1, −1, 1, −1, 1, −1, 1)

b=c(−1, −1, 1, 1, −1, −1, 1, 1, −1, −1, 1, 1, −1, −1, 1, 1)

c=c(−1, −1, −1, −1, 1, 1, 1, 1, −1, −1, −1, −1, 1, 1, 1, 1)

d=c(−1, −1, −1, −1, −1, −1, −1, −1, 1, 1, 1, 1, 1, 1, 1, 1)
```

nodal *designs*	*a*	*b*	*c*	*d*	*ab*	*ac*	*ad*	*bc*	*bd*	*cd*	*abc*	*abd*	*acd*	*bcd*	*abcd*
2^4	*A*	*B*	*C*	*D*											
2^{5-1}_V	*A*	*B*	*C*	*D*											*P*
2^{8-4}_{IV}	*A*	*B*	*C*	*D*							*L*	*M*	*N*	*O*	
2^{15-11}_{III}	*A*	*B*	*C*	*D*	*E*	*F*	*G*	*H*	*J*	*K*	*L*	*M*	*N*	*O*	*P*

2^4 is not a nodal design. Neither is the 2^{7-3}_{IV} in §6.10. Note that for convenience, in 2^{5-1}_V design, the 5-th factors are denoted by P, instead of by E.
I is not used as it denote columns with all +'s.

The alias structure for 16-run nodal designs are given in Table 6.14c.

Table 6.14c. Alias Structure for Sixteen Run Nodal Designs

$$\left(\begin{array}{cccc}
 & 2^{5-1}_{V} & 2^{8-4}_{IV} & 2^{15-11}_{III} \\
a & A & A & A+BE+\cdots \\
b & B & B & B+AE+\cdots \\
c & C & C & C+AF+\cdots \\
d & D & D & D+AG+\cdots \\
ab & AB & AB+CL+DM+NO & E+AB+\cdots \\
ac & AC & AC+BL+DN+MO & F+AC+\cdots \\
ad & AD & AD+BM+CN+LO & G+AD+\cdots \\
bc & BC & AL+BC+DO+MN & H+AL+\cdots \\
bd & BD & AM+BD+CO+LN & J+AM+\cdots \\
cd & CD & AN+BO+CD+LM & K+AN+\cdots \\
abc & DP & L & L+AH+\cdots \\
abd & CP & M & M+AJ+\cdots \\
acd & BP & N & N+AK+\cdots \\
bcd & AP & O & O+AP+\cdots \\
abcd & P & AO+BN+CM+DL & P+AO+\cdots
\end{array}\right)$$

Notice that the higher order interactions are ignored in the table.
It is due to the defining relation:

2^{5-1}_{V}: I=ABCDP,

2^{8-4}_{IV}: I=$\underbrace{\text{ABCL=ABDM=ACDN=BCDO}}_{\binom{4}{1}}=\underbrace{...=ADLO}_{\binom{4}{2}}=\underbrace{ALMN=...=DMNO}_{\binom{4}{3}}$

$=\underbrace{ABCDLMNO}_{\binom{4}{4}}$, total of $2^4-1=15$.

2^{15-11}_{IV}: I=ABE=..., total of $\binom{11}{1}+\binom{11}{2}+\cdots+\binom{11}{11}=2^{11}-1$

6.12. The nodal half replicate of 2^5 FD.

Reactor example. Table 6.15 shows the data and estimates from a complete 2^5 factorial design in factor A, B, C, D, E.

factor		−	+	
$A:$	*feed rate* (L/min)	10	15	
$B:$	*catalyst*(%)	1	2	
$C:$	*agitation*(rpm)	100	120	*jiaodong*
$D:$	*temperature*(^oC)	140	180	
$E:$	*concentration*	3	4	

```
a=c(a,a)
b=c(b,b)
c=c(c,c)
d=c(d,d)
e=rep(-1,16)
e=c(e,-e)
y=c(61, 53, 63, 61, 53, 56, 54, 61, 69, 61, 94, 93, 66, 60, 95, 98,
    56, 63, 70, 65, 59, 55, 67, 65, 44, 45, 78, 77, 49, 42, 81, 82)
(x=sort(round(lm(y~a*b*c*d*e)$coef[2:32]*2,1)))
    d:e           e       a:c:e      a:b:e          a        a:d     a:c:d    b:c:d:e
 −11.00       −6.25       −2.50      −1.87      −1.37      −0.88     −0.75      −0.63
      c   a:b:c:d:e       b:d:e    a:b:c:d        a:e      b:c:e     c:d:e    a:b:d:e
  −0.62       −0.50       −0.25       0.00       0.12       0.13      0.13       0.62
  a:d:e         a:c         b:c        c:e    a:c:d:e      b:c:d       a:b      a:b:d
   0.63        0.75        0.87       0.87       1.00       1.13      1.37       1.38
  a:b:c     a:b:c:e         b:e        c:d          d        b:d         b
   1.50        1.50        2.00       2.12      10.75      13.25     19.50
stem(x)
−1 || 1
−0 || 6
```

```
−0 || 321111110
+0 || 00001111111112222
+0 ||
+1 || 13
+1 ||
+2 || 0
```

The stem and leaf plot or the normal plot (Fig.6.7a) of the 31 LSEs indicates that over the ranges studied, only the estimates of the main effects B, D and E, and the interactions BD and DE are distinguishable from the noise.

summary(lm(y∼b*d*e))

	Estimate	*Std. Error*	*t value*	$Pr(>\|t\|)$	
$(Intercept)$	65.5000	0.5774	113.449	$< 2e-16$	$***$
b	9.7500	0.5774	16.887	$8.00e-15$	$***$
d	5.3750	0.5774	9.310	$1.95e-09$	$***$
e	-3.1250	0.5774	-5.413	$1.47e-05$	$***$
$b:d$	6.6250	0.5774	11.475	$3.14e-11$	$***$
$b:e$	1.0000	0.5774	1.732	0.0961	.
$d:e$	-5.5000	0.5774	-9.526	$1.26e-09$	$***$
$b:d:e$	-0.1250	0.5774	-0.217	0.8304	

z=lm(y∼b*d*e)
w=lm(y∼b*d+d*e)
anova(w,z) Analysis of Variance Table

Model 1: y ∼ b * d + d * e

Model 2: y ∼ b * d * e

	Res.Df	*RSS*	*Df*	*Sum of Sq*	*F*	$Pr(>F)$
1	26	288.5				
2	24	256.0	2	32.5	1.5234	0.2383

Final Model: $E(Y|X) = 65.5 + 9.8b + 5.4d - 3.1e + 6.6b * d - 5.5d * e$; or
$E(Y|X)$ =**??**+19.6I(b=1)+10.8I(d=1)-6.2I(e=1)+13.2I(b*d=1)-11.0I(d*e=1).

Thus the experiment screens out 3 factors from 5. It turns out that one can use 2^{5-1} nodal design to surve the purpose.

run #	*A*	*B*	*C*	*D*	*E*			
1	−	−	−	−	−	1	17*	+
2*	+	−	−	−	−			−
3*	−	+	−	−	−			−
4	+	+	−	−	−	4	20*	+
5*	−	−	+	−	−			−
6	+	−	+	−	−	6	22*	+
7	−	+	+	−	−	7	23*	+
8*	+	+	+	−	−			−
9*	−	−	−	+	−			−
10	+	−	−	+	−	10	26*	+
11	−	+	−	+	−	11	27*	+
12*	+	+	−	+	−			−
13	−	−	+	+	−	13	29*	+
14*	+	−	+	+	−			−
15*	−	+	+	+	−			−
16	+	+	+	+	−	16	32*	+
17*	−	−	−	−	+		17	+
18	+	−	−	−	+			−
19	−	+	−	−	+			−
20*	+	+	−	−	+		20	+
21	−	−	+	−	+			−
22*	+	−	+	−	+		22	+
23*	−	+	+	−	+		23	+
24	+	+	+	−	+			−
25	−	−	−	+	+			−
26*	+	−	−	+	+		26	+
27*	−	+	−	+	+		27	+
28	+	+	−	+	+			−
29*	−	−	+	+	+		29	+
30	+	−	+	+	+			−
31	−	+	+	+	+			−
32*	+	+	+	+	+		32	+
new design of 2_V^{5-1}	*a*	*b*	*c*	*d*		*replace E*	*by*	$e = abcd$

Table 6.15

The full 2^5 requires 32 runs. If the experimenter had chosen instead to just make the 16 runs marked with asterisks in Table, 6.15, then only the data of the next Table would have been available.

$y_1 \sim y_{16}$	53	63	53	61	69	93	60	95
runs	2	3	5	8	9	12	14	15
$y_{17} \sim y_{32}$	56	65	55	67	45	78	49	82
runs	17	20	22	23	26	27	29	32

The generating relation is E=ABCD. The defining relation is I=ABCDE.

```
s=c(2,3,5,8,9,12,14,15,17,20,22,23,26,27,29,32)
(x=round(lm(y[s]~a[s]*b[s]*c[s]*d[s])$coef[2:16]*2,1))
    a         b         c         d       a:b   a:c   b:c   a:d       b:d      c:d
  -2.0      20.5       0.0      12.2      1.5   0.5   1.5   -0.7      10.8     0.3
             B                   D                                   BD
a:b:c     a:b:d     a:c:d     b:c:d                            a:b:c:d
  -9.5       2.2       1.2       1.2                              -6.2
  DE                                                               E
```

Note that the main effects and 2-factor interaction effects are not very different from those from the full 2^5 design.

	a	b	c	d	$a:b$	$a:c$	$b:c$	$a:d$	$b:d$	$c:d$
2^5 :	-1.4	19.5	-0.6	10.8	1.4	0.7	0.9	-0.9	13.2	2.1
2^{5-1} :	-2.0	20.5	0.0	12.2	1.5	0.5	1.5	-0.7	10.8	0.3
		B		D					BD	
	$d:e$		$a:b:c$	$a:b:d$	$a:c:d$	$b:c:d$		e	$\cdots$	
2^5 :	$(-11$	$+$	$1.5)$	1.4	-0.7	1.1		-6.2	$\cdots$	
2^{5-1} :	$(=)$	-9.5		2.2	1.2	1.2		-6.2	?	
		DE						$ABCD$		

ABC is aliased with DE due to I=ABCDE.
Moreover, the normal plot shows the similar pattern.
stem(x,3)

```
-0 | 06
-0 | 21
 0 | 00111222
 0 |
 1 | 12
 1 |
 2 | 1
```

sort(x)

DE	E								
$a:b:c$	$a:b:c:d$	a	$a:d$	c	$c:d$	$a:c$	$a:c:d$	$b:c:d$	$a:b$
-9.5	-6.2	-2.0	-0.7	0.0	0.2	0.5	1.3	1.3	1.5
$b:c$	$a:b:d$	$b:d$	d	b					
1.5	2.2	10.7	12.2	20.5					

(u=summary(lm(y1∼b*d+e+a*b*c)))   # redefine y1, a, b, c, d
# summary(lm(y1∼b*d+e+I(a*b*c)))

	Estimate	*Std. Error*	*t value*	$Pr(>\|t\|)$	
(*Intercept*)	$6.525e+01$	$6.638e-01$	98.298	$2.07e-09$	$***$
b	$1.025e+01$	$6.638e-01$	15.441	$2.07e-05$	$***$
d	$6.125e+00$	$6.638e-01$	9.227	0.000251	$***$
e	$-3.125e+00$	$6.638e-01$	-4.708	0.005300	$**$
a	$-1.000e+00$	$6.638e-01$	-1.506	0.192295	
c	$5.412e-16$	$6.638e-01$	0.000	1.000000	
$b:d$	$5.375e+00$	$6.638e-01$	8.097	0.000466	$***$
$b:a$	$7.500e-01$	$6.638e-01$	1.130	0.309803	
$a:c$	$2.500e-01$	$6.638e-01$	0.377	0.721908	
$b:c$	$7.500e-01$	$6.638e-01$	1.130	0.309803	
$b:a:c$	$-4.750e+00$	$6.638e-01$	-7.156	0.000828	$***$

Residual standard error: 2.655 on 5 degrees of freedom
Multiple R-squared: 0.9894, Adjusted R-squared: 0.9683
F-statistic: 46.75 on 10 and 5 DF, p-value: 0.0002622

v=summary(lm(y1∼b*d+e+I(a*b*c)))
anova(u,v)

The 2_V^{5-1} can be used as a factor screen. In this example, factors A and C are inert. They can be checked from the half fraction factorial design. It is called a factor screen of order [16,5,4] (16 runs, 5 factors and projectivity 4). If one wants the full design, it can be obtained by foldover (on which factors ?)

6.13. The 2_{IV}^{8-4} nodal 16th fraction of a 2^8 factorial. This design is useful to screen 3 out of 8 factors in this 16-run design. A $[16, 8, 3]$ factor screen for 16 runs, 8 factors at projectivity 3. There are $\binom{8}{3} = 56$ ways.

nodal															
designs	a	b	c	d	ab	ac	ad	bc	bd	cd	abc	abd	acd	bcd	$abcd$
2_{IV}^{8-4}	A	B	C	D							L	M	N	O	
	A	B	C	D							E	F	G	H	??

There are $(\binom{4}{1}+\binom{4}{2}+\binom{4}{3}+\binom{4}{4}=15)$ defining relations:

$$\begin{aligned} I &= \underbrace{ABCL = ABDM = ACDN = BCDO}_{\binom{4}{1}} \\ &= \underbrace{CDLM = BDLN = ADLO = BCMN = ACMO = ABNO}_{\binom{4}{2}} \\ &= \underbrace{ALMN = BLMO = CLNO = DMNO}_{\binom{4}{3}} = ABCDLMNO \end{aligned}$$

A Paint trial. In developing a paint for certain vehicles a customer required that the paint have high glossiness (y_1 on a scale 1 to 100) (guang-ze-du) and acceptable abrasion resistance (y_2 on a scale of 1 to 10) (nai-mo-xing). They believe that there are two main factors, say A and B. However, the factors A and B

either produce high glossiness but low abrasion,

or produce low glossiness but acceptable abrasion,

For instance,

A	$-$	$+$	$-$	$+$	$-$	$+$	$-$	$+$	
B	$-$	$-$	$+$	$+$	$-$	$-$	$+$	$+$	*ideal*
y_1 :	53	78	48	78	68	61	70	65	≥ 65
y_2 :	6.3	2.1	6.9	2.5	3.1	4.3	3.4	3.0	≥ 5

According to the paint technologist, there are 6 more factors, C, D, E, F, G, H. They want to find out how to select the factors to obtain high glossiness and high abrasion, The experiments results in data as follows.

y_1 = c(53,60,68,78,48,67,55,78,49,68,61,81,52,70,65,82)

y_2 = c(6.3,6.1,5.5,2.1,6.9,5.1,6.4,2.5,8.2,3.1,4.3,3.2,7.1,3.4,3.0,2.8)

lm(y_1 ~ a*b*c*d)$coef[2:16]*2

Effects are

	A	B	C	D	E	F	G	H							
y_1	**16.6**	**12.6**	-0.1	2.6	-0.1	-0.9	-3.6	1.9	0.9	2.6	1.9	-1.9	-0.1	2.6	-0.4
y_2	**-2.4**	**-2.0**	-0.2	-0.7	0.1	**1.6**	0.6	-0.3	0.3	0.0	-0.1	0.1	-0.1	-0.4	-0.2

Sorting the effects of y_1:

```
-3.6 -1.9 -0.9 -0.4 -0.1 -0.1 -0.1 0.9 1.9 1.9 2.6 2.6 2.6 12.6 16.6;
-0 | 4210000
 0 | 122333
 0 |
 1 | 3
 1 | 7
```

Sorting the effects of y_2:

```
-2.4 -2.0 -0.7 -0.4 -0.3 -0.2 -0.2 -0.1 -0.1 0.0 0.1 0.1 0.3 0.6 1.6
-2 | 40
-1 |
-1 |
-0 | 7
-0 | 432211
 0 | 0113
 0 | 6
 1 |
 1 | 6
```

Analysis of Variance Table

Model 1: y[1,] ~ a + b + I(a * b * d)

Model 2: y[1,] ~ a * b * d

	Res.Df	*RSS*	*Df*	*Sum of Sq*	*F*	*Pr(> F)*
1	12	181.25				
2	8	136.50	4	44.75	0.6557	0.6394

The ANOVA and stem-and-leaf plot suggest that

effects on y_1 are not significant different from error if $y_1 \in (-3.6, 2.6)$,

effects on y_2 are not significantly different from error if $y_2 \in (-0.7, 0.6)$.

Thus in addition to factors A and B, factor F is also an important factor.

Hence we screen 3 factors out of 8.

x=lm(y[1,]∼a+b+I(a*b*d))

		Estimate	*Std Error*	*t value*	*Pr(> |t|)*	
	(*Intercept*)	64.6875	0.9413	68.719	$< 2e-16$	$***$
summary(x)	a	8.3125	0.9413	8.831	$7.46e-07$	$***$
	b	6.3125	0.9413	6.706	$1.46e-05$	$***$
	$I(a*b*d)$	-0.4375	0.9716	-0.450	0.661	

$Y_1 = 64.7 + 8.3a + 6.3b + \epsilon.$

$Y_1 = 50.1 + 16.6 \times \mathbf{1}(a = 1) + 12.6 \times \mathbf{1}(b = 1) + \epsilon$ **how**?

x=lm(y[2,]∼a+b+I(a*b*d))

		Estimate	*Std Error*	*t value*	*Pr(> |t|)*	
	(*Intercept*)	4.7500	0.1647	28.842	$1.88e-12$	$***$
summary(x)	a	-1.2125	0.1647	-7.362	$8.71e-06$	$***$
	b	-1.0250	0.1647	-6.224	$4.42e-05$	$***$
	$I(a*b*d)$	0.8000	0.1647	4.858	0.000393	$***$

$Y_2 = 4.8 - 1.2a - 1.0b + 0.8a * b * d + \epsilon.$

$Y_2 = 6.2 - 2.4 \times \mathbf{1}(a = 1) - 2.1 \times \mathbf{1}(b = 1) + 1.6 \times \mathbf{1}(a * b * d = 1) + \epsilon.$

How to obtain high y_1 (≥ 65) and acceptable y_2 (≥ 5) if A and B can be numerical?
The contour plots (based on Eq.s (1) and (2)) in Figure 6.9 (in the textbook) suggest
that at + level of A, at − level of B and + level of F (*i.e.* - level of d)
would make possible of substantial improvement in (high) glossiness y_1 (≥ 65) while maintaining an acceptable level of abrasion resistance y_2 (≥ 5).

$Y_1 = 64.7 + 8.3a + 6.3b + \epsilon.$ $\qquad Y_1(1, -1, 1) = 66.7$

$Y_2 = 4.8 - 1.2a - 1.0b + 0.8a * b * d + \epsilon.$ $\qquad Y_2(1, -1, 1) = 5.4.$

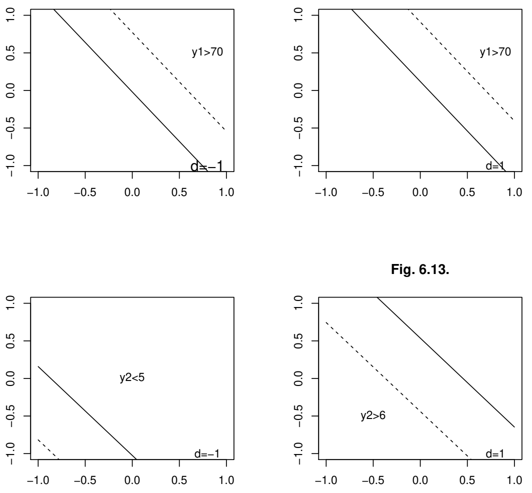


Fig. 6.13.

a,b-axis, (F=abd= ±1)

```
A=c(-1,1)
x=lm(y[1,]∼a+b+I(a*b*d))$coef
B=(65-x[1]-x[2]*A+x[4])/x[3] # (65=x[1]+x[2]*A +x[3]*B -x[4])
plot(A,B, ylim=c(-1,1), type=”l”, lty=1)
B=(70-x[1]-x[2]*A+x[4])/x[3]
lines(A,B, type=”l”, lty=2)
text(0.8,-1,”(F=-1)”) # (a,b,d)∈ {(1,−1,−1),(−1,1,−1)}
text(0.8,0.5,”y1>70”)
B=(65-x[1]-x[2]*A-x[4])/x[3] #+level
plot(A,B, ylim=c(-1,1), type=”l”, lty=1)
B=(70-x[1]-x[2]*A-x[4])/x[3]
```

```
lines(A,B, type=”l”, lty=2)
text(0.8,-1,”(F=1)”) # (a,b,d)∈ {(1, −1, 1), (−1, 1, 1)}
text(0.8,0.5,”y1>70”)
x=lm(y[2,]∼a+b+I(a*b*d))$coef
B=(5-x[1]-x[2]*A+x[4])/x[3]
plot(A,B, ylim=c(-1,1), type=”l”, lty=1)
B=(6-x[1]-x[2]*A+x[4])/x[3]
lines(A,B, type=”l”, lty=2)
text(0.8,-1,”(F=-1)”)
text(0.0,0.0,”y2<5”)
B=(5-x[1]-x[2]*A-x[4])/x[3] #+level
plot(A,B, ylim=c(-1,1), type=”l”, lty=1)
B=(6-x[1]-x[2]*A-x[4])/x[3]
lines(A,B, type=”l”, lty=2)
text(0.8,-1,”(F=1)”)
text(-0.5,-0.5,”y2>6”)
```

6.13.2. Homework. Draw the contour plots for the region in (A,B) with $F = +1$ such that both y_1 and y_2 acceptable.

6.14. 2^{15-11}_{III} **design**. It can be used to screen for two factors amount 15 factors.
A speedometer casing example. Postextrusion shrinkage of a speedometer casing had produced undesirable noise. The objective of the experiment was to find a way to reduce the shrinkage.
A considerable length (in > 300 meters) of product was made during each run and measurements were made at 4 equally spaced points, the responses are

the averages and log variances of the 4 measurements.

```
y=c(48.5,57.5,8.8,17.5,18.5,14.5,22.5,17.5,12.5,12,45.5,53.5,17,27.5,34.2,58.2) #mean

s=c(-0.8,-0.8,0.4,0.3,-0.2,0.1,-0.3,1.1,-0.1,-0.2,0.7,-0.9,0.7,-0.9,0.1,0.7,0.6) #run log variance
```

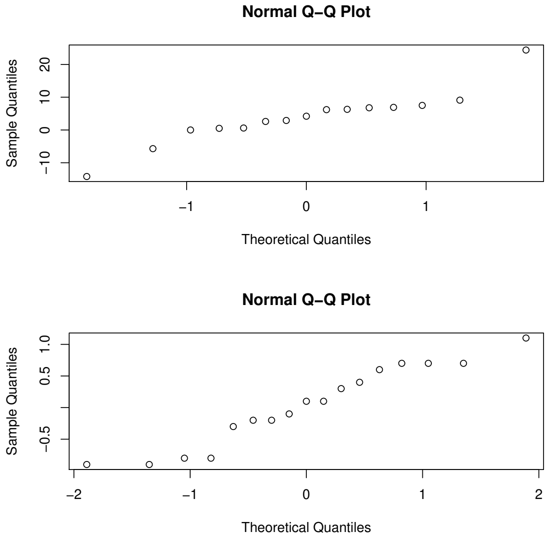
The 15 factors are

A: liner tension, (chen ban zhangli)
B: liner line speed, (ban lun xian speed)
C: liner die, (ban lun mo ju)
D: liner outsider diameter, (chen guan outsider diameter)
E: melt temperature,
F: coating material,
G: liner temperature,
H: braid tension, (bian zhi tension)
J: wire braid type, (xian bian zhi lei xing)
K: liner material,
L: cooling method,
M: screen pack,
N: coating die type, (tu cheng mo ju lei xing)
O: wire diameter,
P: line speed.

```
x=lm(y∼a*b*c*d)$coef[2:16]*2
```

a	b	c	d	$a:b$	$a:c$	$b:c$	$a:d$	$b:d$	$c:d$
6.3	6.2	-5.7	6.9	2.6	0.0	7.5	4.2	$\underline{24.4}$	9.1
A	B	C	D	E	F	G	H	**J**	K

$a:b:c$	$a:b:d$	$a:c:d$	$b:c:d$	$a:b:c:d$
0.5	2.9	6.7	$\underline{-14.2}$	0.7
L	M	N	**O**	P



Normal plot of mean and log variance of the measurements

The second normal plot about s did not reveal any important factors.
The 1st normal plot and stem-and-leaf plot of y reveals important factors.

```
−1| 4
−0| 6
−0|
+0| 011334
+0| 667789
+1|
+1|
+2| 4
```

It turns out from the normal plot of the effects due to averages that the factors O, J and C are important factors.

nodal			*c*						*bd*					*bcd*	
designs	*a*	*b*	*c*	*d*	*ab*	*ac*	*ad*	*bc*	*bd*	*cd*	*abc*	*abd*	*acd*	*bcd*	*abcd*
2^{15-11}_{III}	*A*	*B*	*C*	*D*	*E*	*F*	*G*	*H*	*J*	*K*	*L*	*M*	*N*	*O*	*P*

```
> J=b*d
> O=J*c
> x=lm(y∼factor(c)+factor(J)+factor(O))
> summary(x)
                Estimate   Std.Error   tvalue    Pr(> |t|)
(Intercept)      26.863      5.351      5.020    0.000299   ***
factor(c)1       −5.737      5.351     −1.072    0.304693           O ∗ J      (1)
factor(J)1       24.388      5.351      4.558    0.000657   ***     b ∗ d
factor(O)1      −14.163      5.351     −2.647    0.021305   ∗       J ∗ c
    Residual standard error: 10.7 on 12 degrees of freedom
    Multiple R-squared: 0.7068, Adjusted R-squared: 0.6335
    F-statistic: 9.643 on 3 and 12 DF, p-value: 0.001612
anova(u,w)
    Model 1: y ∼ J*O
    Model 2: y ∼ J + O
      Res.Df    RSS     Df   Sum of Sq      F       Pr(> F)
    1   12     1374.3
    2   13     1506.0   −1    −131.68     1.1497    0.3047
```

Notice that C is alias with the interaction of OJ, *i.e.*, I=OJC, as O=bcd and J=bd.
Conclusion: The model is

$y = 26.87 + 24.38 \times \mathbf{1}(J = 1) - 14.16 \times \mathbf{1}(O = 1)$ (see (1) above) ? Or

$$y = \overbrace{23.99}^{26.87-5.74/2=} +24.38 \times \mathbf{1}(J=1) - 14.16 \times \mathbf{1}(O=1), \text{ or}$$
$$y = \underbrace{29.11}_{=23.99+12.19-7.08} +12.19 \times J - 7.08 \times O,\ J,O = \pm 1.$$

In order to reduce the shrinkage, set factors J and O at levels -1 and +1, respectively.

Remark. The results using summary(lm(y ∼ factor(c) + factor(J) + factor(O))) can be derived directly as follows. The 2^{15-11}_{III} design can be viewed as a 4 replicated 2^2 factorial design with $(\mathbf{1},\mathbf{2}) = (J,O)$, $\begin{array}{ccccc} j & - & + & - & + \\ o & - & - & + & + \\ type\ \# & 1 & 2 & 3 & 4 \end{array}$ with their average of y_i's.

From the table of contract of 2^{15-11}_{III}, we have

J	+	+	−	−	+	+	−	−	−	−	+	+	−	−	+	+
O	−	−	+	+	+	+	−	−	+	+	−	−	−	−	+	+
types	2	2	3	3	4	4	1	1	3	3	2	2	1	1	4	4
run #	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16

```
> s=c(7,8,13,14,1,2,11,12,3,4,9,10,5,6,15,16) # where are they come from ?
> mean(y[s[1:4]]) # 21.1
> mean(y[s[5:8]]) # 51.3
> mean(y[s[9:12]]) # 12.7
> mean(y[s[13:16]]) # 31.4
> mean(y)
    [1] 29.10625
```

The results lead to $\begin{array}{ccc} O+ & 12.7 & 31.4 \\ O- & 21.1 & 51.3 \\ & J- & J+ \end{array}$

$$=> \begin{array}{cccc} \hat\beta_J = 24.45 & \overline{y}_{j-} & \overline{y}_{j+} & \\ O+ & 12.7 & 31.4 & \overline{y}_{o+} \\ O- & 21.1 & 51.3 & \overline{y}_{o-} \\ & J- & J+ & -14.15 = \hat\beta_O \end{array}$$

```
> sqrt((var(y[s[1:4]])+var(y[s[5:8]])+var(y[s[9:12]])+var(y[s[13:16]]))/4)
    [1] 10.70166 # estimating residual SD directly, same as in summary(x)
> y=c(21.1,51.3,12.7,31.4)
> v=lm(y∼J+O)$coef
> c(v[1],2*v[2:3])
       (ȳ)          J           O
    29.10625   24.38750   −14.16250
```

So the 2^{15-11}_{III} fractional FD successfully screens 2 factors from 15 factors.

6.15. Constructing other two-level fractions. Adding a factor to a nodal design. Recall Table 6.14b for 16-run nodal designs. **How many ?** Consider for example, 2^{8-4}_{IV}. One can choose a factor which is most likely to be inert and it is likely to be factor P.

nodal *designs*	*a*	*b*	*c*	*d*	*ab*	*ac*	*ad*	*bc*	*bd*	*cd*	*abc*	*abd*	*acd*	*bcd*	*abcd*
2^4	*A*	*B*	*C*	*D*											
2^{5-1}_V	*A*	*B*	*C*	*D*											*P*
2^{8-4}_{IV}	*A*	*B*	*C*	*D*							*L*	*M*	*N*	*O*	
2^{15-11}_{III}	*A*	*B*	*C*	*D*	*E*	*F*	*G*	*H*	*J*	*K*	*L*	*M*	*N*	*O*	*P*
non − nodal															
2^{9-5}_{III}	*A*	*B*	*C*	*D*							*L*	*M*	*N*	*O*	*P*

The alias structure :

	2_{IV}^{8-4}	$1st\ 2_{III}^{9-5}$
a	A	$A+OP$
b	B	$B+NP$
c	C	$C+MP$
d	D	$D+LP$
ab	$AB+CL+DM+NO$	
ac	$AC+BL+DN+MO$	
ad	$AD+BM+CN+LO$	*same*
bc	$AL+BC+DO+MN$	*as*
bd	$AM+BD+CO+LN$	2_{IV}^{8-4}
cd	$AN+BO+CD+LM$	
abc	L	$L+DP$
abd	M	$M+CP$
acd	N	$N+BP$
bcd	O	$O+AP$
$abcd$	$AO+BN+CM+DL$	$P+AO+BN+CM+DL$

6.15.2. Remark. The previous non-nodal 2^{9-5} design is of resolution III. The reason is as follows.

The generating relation is I=ABCDP, together with 4 generating relations from 2_{IV}^{8-4} FFD. There are $2^5-1=31$ defining relations. 15 of them are the same as the 2_{IV}^{8-4} FFD, which has either 4 letters or 8 letters.

2_{IV}^{8-4}: $\text{I}=\underbrace{\text{ABCL=ABDM=ACDN=BCDO}}_{\binom{4}{1}}=\underbrace{...=ADLO}_{\binom{4}{2}}=\underbrace{ALMN=...=DMNO}_{\binom{4}{3}}$

$=\underbrace{ABCDLMNO}_{\binom{4}{4}}$, total of $2^4-1=15$.

Another 15 are due to ABCDP times each of the previous 15. Since each of these 4-letter words does not contain all of ABCD, their products with ABCDP have lengths ≥ 3. *e.g.*, The 1st one is ABCL. ABCDP(ABCL)=DLP. Moreover, ABCDP(ABCDLMNO)=LMNOP.

Are there other non-nodal 2^{9-5} design of resolution III ? Consider the next example.

(1) I =ABCL=ABDM=ACDN=BCDO =ABE (E=AB replacing P=ABCD).

It's resolution is III, the reason is as follows.

There are 31 defining relations, which consists of original 15 from the 2_{IV}^{8-4} FFD + ABE, and ABE times each of the original 14 4-letter words, which do not contain E. Thus, the shortest one of the latter 15 products is ABE(ABXY)=EXY. Moreover,

ABCDLMNO(ABE)=DELMNO.

6.16. Elimination of block effects. Fractional designs may be run in blocks with suitable contrast used as "block variable". A design in $\underline{2^q}$ blocks is defined by q independent contrast. All effects (including aliases) associated with these chosen contrasts and all their interactions are confounded with blocks. Consider the 2_V^{5-1}

design as follows.

run #	*a*	*b*	*c*	*d*	*e* = *abcd*	*ab*	*ac*	*ad*	*bc*	*abc*
1	−	−	−	−	+	+	+	+	+	−
2	+	−	−	−	−	−	−	−	+	+
3	−	+	−	−	−	−	+	+	−	+
4	+	+	−	−	+	+	−	−	−	−
5	−	−	+	−	−	+	−	+	−	+
6	+	−	+	−	+	−	+	−	−	−
7	−	+	+	−	+	−	−	+	+	−
8	+	+	+	−	−	+	+	−	+	+
9	−	−	−	+	−	+	+	−	+	−
10	+	−	−	+	+	−	−	+	+	+
11	−	+	−	+	+	−	+	−	−	+
12	+	+	−	+	−	+	−	+	−	−
13	−	−	+	+	+	+	−	−	−	+
14	+	−	+	+	−	−	+	+	−	−
15	−	+	+	+	−	−	−	−	+	−
16	+	+	+	+	+	+	+	+	+	+

$q = 1$. A 2_V^{5-1} in two blocks of either runs. (*e.g.* male or female patients). If one believes that AC is most likely to be negligible, then 2^1 blocks can be decided as follows.
1. the 8 runs 2, 4, 5, ..., 15, having − in the AC column;
2. the other 8 runs having + in the AC column.
The block contrast is AC. AC is confounded with the block factor, say **6**, with 2 levels.

$q = 2$. A 2_V^{5-1} design in 4 blocks of 4 runs. (*e.g.* a pack of raw material enough for 4 runs). If one uses AC and BC to define blocks, then the sign (- -), (- +), (+ -) and (+ +) can be the 4 blocks.
(−−): runs 4, 5, 12, 13;
(−+): runs 2, 7, 11, 15;
......
In this case, AC and BC are confound with the block factor **6** with 4 levels (or 2 new block factors F=AC and G=BC.

run #	*a*	*b*	*c*	*d*	*abcd*	*ab*	*ac*	*ad*	*bc*	*abc*
8	+	+	+	−	−	+	+		+	+
9	−	−	−	+	−	+	+		+	−
16	+	+	+	+	+	+	+		+	+
1	−	−	−	−	+	+	+		+	−
2	+	−	−	−	−	−	−		+	+
15	−	+	+	+	−	−	−		+	−
7	−	+	+	−	+	−	−		+	−
10	+	−	−	+	+	−	−		+	+
14	+	−	+	+	−	−	+		−	−
3	−	+	−	−	−	−	+		−	+
6	+	−	+	−	+	−	+		−	−
11	−	+	−	+	+	−	+		−	+
12	+	+	−	+	−	+	−		−	−
13	−	−	+	+	+	+	−		−	+
4	+	+	−	−	+	+	−		−	−
5	−	−	+	−	−	+	−		−	+

$q = 3$. Is it possible to use ab, ac, bc for the case of $q = 3$?
How about other combinations ?
Ans. (ab, ac, ad) works; and (ab, ac, abc) works.

Minimum-Aberration 2^{k-p} designs. Before given its definition, consider first the three 2_{IV}^{7-2} designs in the following table.

Table 6.21. 3 choices for a 2_{IV}^{7-2} fractional FD

	design(a) *share* 2 #	*design(b)* *share* 1 #	*design(c)* *share* 3 #
2 *generators*	$6 = 123,\ 7 = 234$	$6 = 123,\ 7 = 145$	$6 = 1234,\ 7 = 1235$
3 *defining*	$I = 1236 = 2347 = 1467$	$I = 1236 = 1457$	$I = 4567$
relations		$= 234567$	$= 12346 = 12357$
$\binom{4}{2}$ *alliases from* 1*st*	$12 + 36$	$12 + 36$	$45 + 67$
(*with* 2 *letters*)	$13 + 26$	$13 + 26$	$46 + 57$
	$16 + 23$	$16 + 23$	$47 + 56$
$\binom{4}{2}$ *alliases from* 2*nd*	$23 + 47$	$14 + 57$	
(*with* 2 *letters*)	$24 + 37$	$15 + 47$	
	$27 + 34$	$17 + 45$	
$\binom{4}{2}$ *alliases from* 3*rd*	$14 + 67$		
(*with* 2 *letters*)	$16 + 47$		
	$17 + 46$		
distinct patterns	$12 + 36$	$12 + 36$	$45 + 67$
	$13 + 26$	$13 + 26$	$46 + 57$
	$16 + 23 + 47$	$16 + 23$	$47 + 56$
		$14 + 57$	
	$24 + 37$	$15 + 47$	
	$27 + 34$	$17 + 45$	
	$14 + 67$		
	$17 + 46$		
total # words:	15	12	6

How about 6=12345 and ($\underbrace{7 = 12}_{R<IV}$ or $\underbrace{7 = 123}_{R=IV}$ or $\underbrace{7 = 1234}_{R<IV}$) ? (Resolution)

The 4-th and the 6-the have resolution <IV, which is not desirable, and
the 5-th: 6=12345 and 7=123 => I=123456=1237=4567 is similar to design (b).
Which pattern has the least # of shortest words among defining relations ?

Definition. The minimum-aberration design is the one that minimizes the number of words in the defining relation having minimum length with the largest resolution.

Note: 123456, 1237, 4567 are all called words.

See for examples, 2_V^{7-2}, 2_{VI}^{6-1} and 2^5 designs as follows.

2_{IV}^{7-2} **fractional FD design**: There are several types of them. In each type, Factors 1, 2, 3, 4, 5 (as well as 6, 7) are aliased with 3-factor or high order interactions, Table 6.21 above gives an example of each of three types, where 2-factor interactions which are aliased with (only) 2-factor interactions are given there.

Which design is better ?

Design 4 or 6 is not of resolution IV, and is out of consideration.

Design (b) or (a) has 2 or 3 words of length 4.

Design (c), as it has the least number of 2 factor interactions.

Design (c) is the minimum-aberration 2_{IV}^{7-2} design, with 1 word of length 4.

Is it the unique minimum-aberration 2_{IV}^{7-2} design ?

Remark. 2^{7-2} minimum-aberration design is not defined for 2_{III}^{7-2}, as it is not as good as 2_{IV}^{7-2} design.

2^5 **FD.** $\nexists$ defining generator. So it is also a minimum-aberration 2^5 design.

2_V^{6-1} **fractional FD designs:** There is just one (a nodal design), with a unique defining generator $6 = 12345$. So it is the minimum-aberration 2_{VI}^{6-1} design.

There are also 2_V^{7-2}, ..., $2_{??}^{31-16}$ designs.

Table 6.22 is for general 2^{k-p} FD with Table 6.21 as the special case.

Explain it via the next table.

	# of variables k (or factors)	
# of runs	5	6
4		
8	$\frac{1}{4}$ *Fractional FD of* 2^5	$\frac{1}{8}$ *Fractional FD of* 2^6
16	$\frac{1}{2}$ *Fractional FD of* 2^5	$\frac{1}{4}$ *Fractional FD of* 2^6
32	1 *FD of* 2^5	$\frac{1}{2}$ *Fractional FD of* 2^6
64	2 *replicated FD of* 2^5	1 *FD of* 2^6
128	4 *replicated FD of* 2^5	2 *replicated FD of* 2^6

$123456789\overline{10} = ABCDEFGHJK$

What are the nodal designs in row 1 ?

What are the nodal designs in row 2 ?

What are the nodal designs in row 3 ?

Chapter 7. Additional Fractionals and Analysis

7.1. Plackett and Burman designs. For screening a large number of factors, one can use 2^k factorial designs. The number of runs are

n= 4, 8, 16, 32, 64, 128, 256, ...

The gaps are getting wider fast.

The Plackett and Burman (PB) designs has the advantage that it slows down the pace.

n=12, (2^4), 20, 24, 28, (2^5), ..., a multiple of 4 (skipped 2^k).

If $n = 2^k$, it is just FD. Otherwise, it is generated by the first row. For example, **a 12-run PB design (PB$_{12}$)** is constructed as follows.

$$\underbrace{+-+---+++}_{**}\underbrace{-}_{*}+$$

$$+\underbrace{+-+---+++}_{**}\underbrace{-}_{*}$$

$$\underbrace{-}_{*}+\underbrace{+-+---+++}_{**}$$

$+-++-+---++$

$++-++-+---+$

$+++-++-+---$

$-+++-++-+--$

$--+++-++-+-$

$---+++-++-+$

$+---+++-++-$

$-+---+++-++$

$-----------$

A B C D E F G H J K L

Table 7.1

Thus the PB design is determined by the first row (except 2^k FD).

This can be done in R as follows.

```
> x=rep(0,132)
> dim(x)=c(12,11)
> x[1,]=c(1,-1,1,-1,-1,-1,1,1,1,-1,1) # (the first row of PB design)
> for(i in 1:10)
> x[i+1,]=c(x[i,11],x[i,1:10])
> x[12,]=rep(-1,11)
```

a b c d e f g h j k l

$+-+---+++-+$

$++-+---+++-$

$-++-+---+++$

$+-++-+---++$

$++-++-+---+$

$+++-++-+---$

$-+++-++-+--$

$- - + + + - + + - + -$
$- - - + + + - + + - +$
$+ - - - + + + - + + -$
$- + - - - + + + - + +$
$- - - - - - - - - - -$

Notice that

neither of f,g,h,j,k,l are two-factor products of a, b, c, d, e,
no vector is of the pattern $- + - + - + -+$...
but these 11 vectors together with I form a basis of the space.
$t(x[, 1 : 11])\% * \%x[, 1 : 11]$ is a 11×11 diagonal matrix $(12)\mathbf{I}$.

```
> y1=c(56,93,67,60,77,65,95,49,44,63,63,61)
> a=c(1,2,4,5,6,10) # from the first column of the PB12 design matrix (with +).
> 0.5*(mean(y1[a])-mean(y1[-a]))
> lm(y1~x[,1:3]) # lm(y1~x[,1]+x[,2]+x[,3])
> lm(y1~x[,1]*x[,2]*x[,3])
(ȳ+ − ȳ−)/2   2.916667
(Intercept)   x[,1:3]1   x[,1:3]2   x[,1:3]3
  66.083        2.917     10.583     −0.750
(Intercept)    x[,1]      x[,2]      x[,3]    x[,1]:x[,2]   x[,1]:x[,3]   x[,2]:x[,3]   x[,1]:x[,2]:x[,3]
  64.5625     3.1875     8.9375    −1.3125     −1.6875       −4.9375        0.8125          −4.5625
```

Notice that the first 3 effects are all different in the models y1~x[,1]*x[,2]*x[,3]) and y1~x[,1:3]) and they do not differ from the main effects by a factor of 2.

Advantage of PB design.

PB_{12} is a [12, 11, 3] screen, producing $1\frac{1}{2}$ replicated 2^3 factorial design (for its meaning, see Figure 7.1 below) for any of $\binom{11}{3} = 165$ choices.

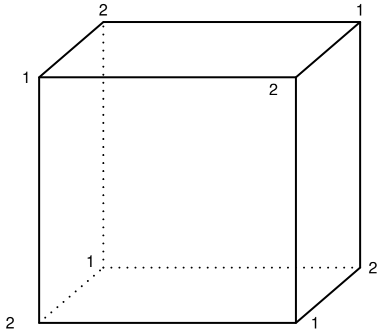


Fig. 1

For instance, choose C, E, F again.

run #		*C*		*EF*			*run #*	*CEF*	
1	$+-$	$+$	$-$	$--$	$+++-+$		2	$---$	1
2	$++$	$-$	$+$	$--$	$-+++-$		12	$---$	$*$
3	$-+$	$+$	$-$	$+-$	$--+++$		1	$+--$	2
4	$+-$	$+$	$+$	$-+$	$---++$		5	$-+-$	3
5	$++$	$-$	$+$	$+-$	$+---+$		3	$++-$	4
6	$++$	$+$	$-$	$++$	$-+---$	shuffled as	8	$++-$	$*$
7	$-+$	$+$	$+$	$-+$	$+-+--$		11	$--+$	5
8	$--$	$+$	$+$	$+-$	$++-+-$		7	$+-+$	6
9	$--$	$-$	$+$	$++$	$-++-+$		4	$+-+$	$*$
10	$+-$	$-$	$-$	$++$	$+-++-$		9	$-++$	7
11	$-+$	$-$	$-$	$-+$	$++-++$		10	$-++$	$*$
12	$--$	$-$	$-$	$--$	$-----$		6	$+++$	8

Now compare PB_{12} to a 2^{8-4}_{IV} (nodal) design. 2^{8-4}_{IV} design is a [16,8,3] screen, that is, it projects a duplicated 2^3 factorial for any one of the $\binom{8}{3} = 56$ choices.

For instance, pick C, E, F factors from 2^{8-4}_{IV} fractional design. By rearrangement, it becomes clear that it is a duplicated 2^3 FD.

2^{8-4}_{IV}			C		F				E	
run #	a	b	c	d	abd	ab	ac	bc	abc	
1	−	−	−	−	−	+	+	+	−	1
2	+	−	−	−	+	−	−	+	+	7
3	−	+	−	−	+	−	+	−	+	7
4	+	+	−	−	−	+	−	−	−	1
5	−	−	+	−	−	+	−	−	+	4
6	+	−	+	−	+	−	+	−	−	6
7	−	+	+	−	+	−	−	+	−	6
8	+	+	+	−	−	+	+	+	+	4
9	−	−	−	+	+	+	+	+	−	5
10	+	−	−	+	−	−	−	+	+	3
11	−	+	−	+	−	−	+	−	+	3
12	+	+	−	+	+	+	−	−	−	5
13	−	−	+	+	+	+	−	−	+	8
14	+	−	+	+	−	−	+	−	−	2
15	−	+	+	+	−	−	−	+	−	2
16	+	+	+	+	+	+	+	+	+	8

shuffled as

run #	C	E	F	
1	−	−	−	1
4	−	−	−	
14	+	−	−	2
15	+	−	−	
10	−	+	−	3
11	−	+	−	
5	+	+	−	4
8	+	+	−	
9	−	−	+	5
12	−	−	+	
6	+	−	+	6
7	+	−	+	
2	−	+	+	7
3	−	+	+	
13	+	+	+	8
16	+	+	+	

The PB_{12} is a [12,11,3] screen. The PB_{16} is the same as 2^4 FD. Among PB_{16},
the 2^{8-4}_{IV} (nodal design) is a [16,8,3] screen,
the 2^{15-11}_{III} (nodal design) is a [16,15,2] screen.

Is something strange ?

12-run PB_{12} is a [12,11,3] screen. $\binom{11}{3} = 165$.

16-run 2^{8-4}_{IV} is a [16,8,3] screen. $\binom{8}{3} = 56$. $(8 < 11)$

16-run 2^{11-7}_{III} is a [16,11,2] screen. $(2 < 3)$

16-run 2^{15-11}_{III} is a [16,15,2] screen.

Should we have **more choices** for screening 3 factors in PB_{16} than in PB_{12} ?

Ans. Yes, as explained as follows. $PB_{16} = 2^4$ FD and
2^{8-4}_{IV} design, 2^{11-7}_{III} design and 2^{15-11}_{III} design are special cases of PB_{16} design.

nodal *designs*	a	b	c	d	ab	ac	ad	bc	bd	cd	abc	abd	acd	bcd	$abcd$
2^{5-1}_{V}	A	B	C	D											P
2^{8-4}_{IV}	A	B	C	D							L	M	N	O	
2^{15-11}_{III}	A	B	C	D	E	F	G	H	J	K	L	M	N	O	P

2^{15-11}_{III} FD:

a. (1, 2, (12)) (or (a,b,ab)) is 4-duplicated tetrahedral design (see 1 in Fig. 1) ($\binom{15}{2} = 105$ of them). That is, choose 2 from 15 factors, and the third one is uniquely determined by the first two, *e.g.*, (1234), (12), (34) (or P, E, K, and PEK=I) (see the next Table).

b. (1,2,(13)) (or (a,b,ac)) is a duplicated 2^3 FD ($\binom{4}{2}\binom{5}{1} = 30$ many of them and $(1)(2)(13)\neq$I, *i.e.*, choose 2 from (a,b,c,d) (say a, b), choose 1 from 5
(the possible remainings from (ab, ac, ad, bc, bd, cd) \ ab) (see the next Table).

c. Choose 3 from $1, 2, 3, 4,$ (123), (124), (134), (234) form the 2^{8-4}_{IV} design.
($\binom{8}{3} = 56$ of them).

d. The other combinations (not in cases (a), (b) and (c)) of selecting 3 out the 15 factors can also be screened out, as there is no more cases that I=3-letter product as in (a).

Totally, it can screen $\binom{15}{3} - \binom{15}{2} = 350$ ($>$ 165 screened by PB_{12}).

What is the difference between case b and case a ?

12(12) =I (or $xy(xy)$ =I), but 12(13) $\neq$I.

run#	*a*	*b*	*ab*	*vertex*	2^4				2^4				
1	−	−	+	5	*run#*	*a*	*b*	*ac*	*run#*	*a*	*b*	*ac*	
5	−	−	+	5	1	−	−	+	13	−	−	−	1
2	+	−	−	2	2	+	−	−	5	−	−	−	
6	+	−	−	2	3	−	+	+	2	+	−	−	2
3	−	+	−	3	4	+	+	−	10	+	−	−	
7	−	+	−	3	5	−	−	−	7	−	+	−	3
4	+	+	+	8	6	+	−	+	15	−	+	−	
8	+	+	+	8	7	−	+	−	4	+	+	−	4
					8	+	+	+	12	+	+	−	
9	−	−	+	5	9	−	−	+	1	−	−	+	5
13	−	−	+	5	10	+	−	−	9	−	−	+	
10	+	−	−	2	11	−	+	+	14	+	−	+	6
14	+	−	−	2	12	+	+	−	6	+	−	+	
11	−	+	−	3	13	−	−	−	3	−	+	+	7
15	−	+	−	3	14	+	−	+	11	−	+	+	
12	+	+	+	8	15	−	+	−	8	+	+	+	8
16	+	+	+	8	16	+	+	+	16	+	+	+	

Should PB_{16} have more choices for screening 3 factors than PB$_{12}$?
Ans. It indeed screens more combinations of 3 factors (350 of them) than PB$_{12}$ (which has $\binom{11}{3} = 165$ of them),

but not all $\binom{15}{3}$ (= 455).

However, PB_{12} screens all $\binom{11}{3}$.

Generator rows for constructing PB design.

PB$_{12}$ $++-+++---+-$, a [12,11,3] screen.

PB$_{20}$ $++--++++-+-+----++-$, a [20,19,3] screen.

PB$_{24}$ $+++++-+-++--++--+-+----$, a [24,23,3] screen.

Table 7.2

Remark. The PB$_{20}$ and PG$_{24}$ can be generated as PB$_{12}$, with all −'s in the last row.

Remark. The PB$_{12}$ in Table 7.2 is different from the one in Table 7.1.

$+-+---+++-+$, (the old one)

$++-+++---+-$ (the new one).

$-+-+++---+-$ old $\times(-1) \neq$ new.

The projective properties of the PB$_{20}$ design. (Plackett and Burman)
Table 7.3 displays a PB$_{20}$ design, where for convenience,
row and column operations are made, as well as products of columns, so that
the variables A and B are renamed to reproduce a 2^2 factorial replicated 5 times,
the last 5 columns are replaced by products of the original columns.

Thus its first and last rows are not the same as in Table 7.2.
and none of its row are all −'s.

Attach Table 7.3 AB CDEF GHJK LMNO PQRS T

There are two cases in PB$_{20}$.
If one chooses A, B together with any column except T, say C (see the next table),

it is a duplicated 2^3 FD with a tetrahedral design.

	run																				
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	
A	+	+	+	+	+	+	+	+	+	+	−	−	−	−	−	−	−	−	−	−	*c*
B	+	+	+	+	+	−	−	−	−	−	+	+	+	+	+	−	−	−	−	−	*b*
C	+	−	−	−	+	+	−	+	−	+	−	−	+	+	+	−	−	+	+	−	*a*
2^3	8	7				6	5				3			4		1			2		
2^3			7		8			6	5			3	4				1	2			
te				7						6					4					1	

It is easy to see the 2 2^3 FD from the next table:

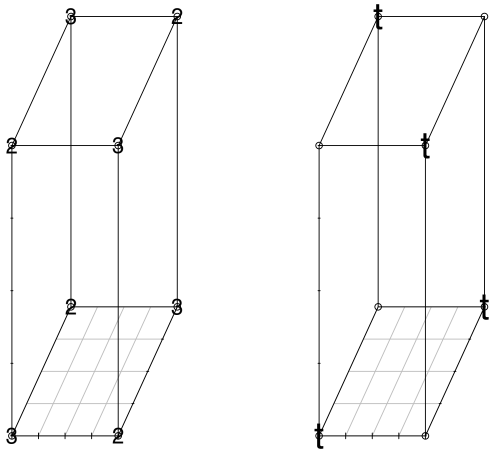
1sr 2^3				*2nd* 2^3	*tetrahedral*
run#	*C*	*B*	*A*	*run#*	*run#*
16	−	−	−	17	20
19	+	−	−	18	
11	−	+	−	12	
14	+	+	−	13	15
7	−	−	+	9	
6	+	−	+	8	10
2	−	+	+	3	4
1	+	+	+	5	

Two 2^3 factorial designs above and one with * tetrahedral design.
Otherwise,, it is one 2^3 FD plus a 2_{III}^{3-1} design replicated 3 times. The next table shows that the transpose of the first 3 columns of Table 7.3 or A, B, T.

						run															
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	
A	+	+	+	+	+	+	+	+	+	+	−	−	−	−	−	−	−	−	−	−	*c*
B	+	+	+	+	+	−	−	−	−	−	+	+	+	+	+	−	−	−	−	−	*b*
T	−	−	−	−	+	+	+	+	+	−	+	+	+	+	−	−	−	−	−	+	*a*
2^3				7	8				6	5				4	3				1	2	
3 *te*	7	7	7			6	6	6			4	4	4			1	1	1			

One 2^3 factorial designs and the tetrahedral design replicates 3 times.
It turns out among $\binom{19}{3} = 969$ choices of choosing 3 factors out of 19,
only 57 (19 × 3) produce the latter patterns, the rest are all $2\frac{1}{2}$ replicates.
Since each pattern contains at least one 2^3 FD, it can screen 3 factors.

Fig. 7.2.



Analysis of PB$_{12}$ design with 5 factors. For 2^k designs, every main effect and 2-factor interaction only occur once. For the case for PB designs, the 2-factor interactions occur more than once. Using Table 7.1 (the standard table for PB$_{12}$ design, then the alias structure is given in Table 7.4. In particular,

$l_A \to A + \frac{1}{3}(-BC + BD + BE - CD - CE - DE)$,
$l_B \to B + \frac{1}{3}(-AC + AD + AE - CD + CE - DE)$,
$l_C \to C + \frac{1}{3}(-AB - AD - AE - BD + BE - DE)$,
$l_D \to D + \frac{1}{3}(+AB - AC - AE - BC - BE - CE)$,

$$l_E \to E + \tfrac{1}{3}(+AB - AC - AD + BC - BD - CD),$$

$$l_F \to \tfrac{1}{3}(-AB + AC - AD + AE + BC - BD - BE + CD - CE - DE),$$

$$l_G \to \tfrac{1}{3}(-AB - AC - AD + AE - BC + BD - BE + CD - CE + DE),$$

$$l_H \to \tfrac{1}{3}(+AB + AC - AD - AE - BC - BD - BE - CD + CE + DE),$$

$$l_J \to \tfrac{1}{3}(-AB - AC - AD - AE + BC + BD - BE - CD - CE - DE),$$

$$l_K \to \tfrac{1}{3}(-AB - AC + AD - AE - BC - BD - BE + CD + CE - DE),$$

$$l_L \to \tfrac{1}{3}(-AB + AC + AD - AE - BC - BD + BE - CD - CE + DE).$$

Table 7.4

$$\mathrm{ABC} = (-1,-1,-1,-1,-1,1,-1,1,-1,1,1,-1)^t = \begin{pmatrix} -1\\ -1\\ -1\\ -1\\ -1\\ 1\\ -1\\ 1\\ -1\\ 1\\ 1\\ -1 \end{pmatrix}. \qquad \mathrm{BC} = \begin{pmatrix} -1\\ -1\\ -1\\ -1\\ -1\\ 1\\ -1\\ 1\\ -1\\ 1\\ 1\\ -1 \end{pmatrix} \mathrm{A}.$$

ABC here is a vector of ±1 with 1/3 being +1. ($\to$A+$\frac{-1}{3}$BC).

Recall I=ABC yields $A = BC$ ($\ell_A \to$ A+BC $\cdots$).

```
> x[,1]*x[,2]*x[,3]                    # ABC
[1] -1 -1 -1 -1 -1 1 -1 1 -1 1 1 -1
> x[,1]*x[,2]*x[,4]            # ABD
[1] 1 1 1 -1 1 -1 -1 1 1 1 1 -1
```

ABD here is a vector of ±1 with 1/3 being −1. (A+$\frac{1}{3}$BD).

Revisit Reactor Example in Table 6.15 in §6.12. Table 6.15 is a 2^5 factorial design in 5 factors, A, B, C, D, E.

$factor$		$-$	$+$	
$A:$	$feed\ rate\ (L/min)$	10	15	
$B:$	$catalyst(\%)$	1	2	
$C:$	$agitation(rpm)$	100	120	$jiaodong$
$D:$	$temperature(^oC)$	140	180	
$E:$	$concentration$	3	4	

The analysis for the full 32-run design led to the conclusion that

the effects B, D, BD, E and DE are likely significant.

Later it was shown that the 16-run 2^{5-1}_V design led to the same conclusion.
Question: Can it be done by PB$_8$?

PB_n starts with n=12, (16), 20, ... Moreover, it is $(2^k, 2^k-1, 2)$ screen design
Question: Can it be done by PB$_{12}$?

We rewrite Table 7.5 as follows.

$run\ \#\ in\ PB_{12}$	1	2	3	4	5	6	7	8	9	10	11	12
$run\ \#\ in\ 2^5$	6	12	23	14	28	24	15	29	25	18	3	1

by comparing the designs about A, B, C, D, E.

run	A	B	C	D	E	a	b	c	d	e	f	g	h	j	k	l
6	1	−1	1	−1	−1	+	−	+	−	−	−	+	+	+	−	+
12	1	1	−1	1	−1	+	+	−	+	−	−	−	+	+	+	−
23	−1	1	1	−1	1	−	+	+	−	+	−	−	−	+	+	+
14	1	−1	1	1	−1	+	−	+	+	−	+	−	−	−	+	+
28	1	1	−1	1	1	+	+	−	+	+	−	+	−	−	−	+
24	1	1	1	−1	1	+	+	+	−	+	+	−	+	−	−	−
15	−1	1	1	1	−1	−	+	+	+	−	+	+	−	+	−	−
29	−1	−1	1	1	1	−	−	+	+	+	−	+	+	−	+	−
25	−1	−1	−1	1	1	−	−	−	+	+	+	−	+	+	−	+
18	1	−1	−1	−1	1	+	−	−	−	+	+	+	−	+	+	−
3	−1	1	−1	−1	−1	−	+	−	−	−	+	+	+	−	+	+
1	−1	−1	−1	−1	−1	−	−	−	−	−	−	−	−	−	−	−

They yield (ordered) effects in Table 7.0 below:

	e	l	h	f	c	k	g	a	d	j	b
PD_{12} :	−10.5	−9.8	−8.8	−2.2	−1.5	−0.5	2.2	5.8	7.2	7.2	21.2
2^5 *or* 2^{5-1}_V :	E								D		B

```
stem(x,3)
  -1 | 10
  -0 | 9
  -0 | 221
   0 | 2
   0 | 677
   1 |
   1 |
   2 | 1
```

The plot suggests that effects B and E, or maybe D, J and L or H are real, (versus B, E, D, BD and DE in 2^5 FD). **What is the reason for the difference ?**

	PB_{12}	2^5
$l_B \to B + \frac{1}{3}(-AC + AD + AE - CD + CE - DE)$	21.2	19.5
$l_D \to D + \frac{1}{3}(+AB - AC - AE - BC - BE - CE)$	7.2	10.8
$l_E \to E + \frac{1}{3}(+AB - AC - AD + BC - \underline{BD} - CD)$	−10.5	−6.3
$l_H \to \frac{1}{3}(+AB + AC - AD - AE - BC - BD - BE - CD + CE + \underline{DE})$	−8.8	
$l_J \to \frac{1}{3}(-AB - AC - AD - AE + BC + \underline{BD} - BE - CD - CE - DE)$	7.2	
$l_L \to \frac{1}{3}(-AB + AC + AD - AE - BC - BD + BE - CD - CE + \underline{DE})$	−9.8	

Part of Table 7.4

From design 2^5, BD= 13.25 and DE=−11.0 are significant.
One way to modify is to notice from Table 7.4 that

the first 5 effects are single factor effects, and the others are 2-factor effects.

Among the 5 factors, B, D, E are indeed larger than the other two.

So try the model $summary(lm(y \sim b*d*e+h+j+l))$ $(11-1$ parameters).

	$Estimate$	$Std.Error$	$tvalue$	$Pr(>\|t\|)$	
$(Intercept)$	66.0833	0.4488	147.256	$4.61e-05$	$***$
b	9.4583	0.5262	17.974	0.00308	$**$
d	3.4583	0.5017	6.893	0.02041	$*$
e	−3.3333	0.5262	−6.334	0.02403	$*$
h	−1.5000	0.6346	−2.364	0.14188	
j	0.4167	0.7773	0.536	0.64556	
l	−1.7500	0.7773	−2.251	0.15320	
$b:d$	5.7500	0.8244	6.975	0.01994	$*$
$b:e$	−0.3750	0.6731	−0.557	0.63349	
$d:e$	−3.3750	0.8244	−4.094	0.05481	.
$b:d:e$	NA	NA	NA	NA	

And try the model $lm(y \sim b*d*e+j+l)$

	Estimate	*Std.Error*	*tvalue*	*Pr*(> |*t*|)			
(*Intercept*)	66.0833	0.7136	92.602	$2.78e-06$	***		
b	9.0833	0.7979	11.385	0.00145	**		
d	3.4583	0.7979	4.335	0.02265	*		
e	−2.9583	0.7979	−3.708	0.03409	*		
j	−0.3333	1.1283	−0.295	0.78694		*see* PB_{12}	7.2
l	−1.0000	1.1283	−0.886	0.44075		*see* PB_{12}	−9.8
$b:d$	6.8750	1.0704	6.423	0.00765	**	(Table 7.0	*above*)
$b:e$	−0.3750	1.0704	−0.350	0.74925			
$d:e$	−4.5000	1.0704	−4.204	0.02457	*		
$b:d:e$	*NA*	*NA*	*NA*	*NA*			

It seems that the model can be simplified by lm(y1~b*d+d*e)

	Estimate	*Std.Error*	*tvalue*	*Pr*(> |*t*|)	
(*Intercept*)	66.0833	0.6855	96.402	$8.4e-11$	***
b	9.0000	0.7271	12.378	$1.7e-05$	***
d	3.5833	0.6855	5.227	0.001962	**
e	−2.8750	0.7271	−3.954	0.007502	**
$b:d$	7.1250	0.7271	9.799	$6.5e-05$	***
$d:e$	−4.7500	0.7271	−6.533	0.000614	***

Analysis of Variance Table

Model 1: y ~ b * d * e + h + j + l

Model 2: y ~ b * d + d * e

	Res.Df	*RSS*	*Df*	*Sum of Sq*	*F*	*Pr*(> *F*)
1	2	4.833				
2	6	33.833	−4	−29	3	0.2653

The analysis suggests that the effect B, E, D BD and DE are significant, which is consistent with the previous 2_V^{5-1} conclusion.

$$y = 66.083 + 9b + 3.583d - 2.875e + 7.125bd - 4.750de$$

$$y = 66.341 + 9b + 3.841d - 3.068e + 7.318bd - 4.750de + 0.773bac$$

Note that the estimates are not exact the same under a different model, even it implies the final model.

	Estimate	*Std.Error*	*tvalue*	*Pr*(> |*t*|)	
(*Intercept*)	66.3409	0.7617	87.097	$3.78e-09$	***
d	3.8409	0.7617	5.043	0.003958	**
e	−3.0682	0.7762	−3.953	0.010820	*
b	9.0000	0.7432	12.111	$6.78e-05$	***
$d:e$	−4.7500	0.7432	−6.392	0.001389	**
$d:b$	7.3182	0.7762	9.428	0.000227	***
$I(b*a*c)$	0.7727	0.8963	0.862	0.428006	

Chapter 8. Factorial designs and data transformation.

In a 2^k factorial design, we have k factors and each has two levels. In contrast to 2-level factorial designs, there are multi-level factorial designs, namely, the level of some factor can be 3 or more, such as Latin Squares.

8.1. A two-way (factorial) design.

Taxic agents. Data: Survival time (in 10 hrs) of animals, which is randomly allocated to each of 12 combinations of 3 poisons (I, II III), and 4 treatments (A, B, C, D). Each combination has 4 replications. Thus we have two factors here: poison and treatment, with 3 and 4 levels, respectively. The data are as follows.

	treatment	*A*	*B*	*C*	*D*
poison	*I*	0.31	0.82	0.43	0.45
	I	0.45	1.10	0.45	0.71
	I	0.46	0.88	0.63	0.66
	I	0.43	0.72	0.76	0.62
	II	0.36	0.92	0.44	0.56
	II	0.29	0.61	0.35	1.02
	II	0.40	0.49	0.31	0.71
	II	0.23	1.24	0.40	0.38
	III	0.22	0.30	0.23	0.30
	III	0.21	0.37	0.25	0.36
	III	0.18	0.38	0.24	0.31
	III	0.23	0.29	0.22	0.33

or

$P\backslash T$	1	2	3	4
1	0.31	$\cdots$		
1				
$\vdots$				
$\vdots$				
$\vdots$				
$\vdots$				
$\vdots$				
$\vdots$				
$\vdots$				
$\vdots$				
$\vdots$				
$\vdots$				

This is formulated by the two-way anova model
$Y_{tij} = \eta + \tau_t + \pi_i + \omega_{ti} + \epsilon_{tij}$, $t = 1, ..., \mathrm{N}$, $i = 1, ..., k$, $j = 1, ..., m$. (N,k,m)= ?
Or $\mathbf{Y} = \mathbf{X}\beta$ (*i.e.*, $Y_h = \beta' X_h + \epsilon_h$, $h = 1, ...,$ n (=?))

What are the parameters ? degree of freedom =? observations ?

(X_h, Y_h) **?** $\beta =$**?** Is X_h numerical or a factor ? How about T_h or P_h ?

$$Y_h = \eta + \sum_{t=1}^{N} \tau_t \mathbf{1}(T_h = t) + \sum_{i=1}^{k} \pi_i \mathbf{1}(P_h = i) + \sum_{i=1}^{k}\sum_{t=1}^{N} \omega_{ti} \mathbf{1}(T_h = t)\mathbf{1}(P_h = i) + \epsilon_h,$$

Which of the next 2 commands is convenient ?

```
lm(Y∼X)
lm(Y∼T*P)
```

In the R codes in §8.1, $lm(x \sim t * p)$.
Analysis of Variance Table (ANOVA).
$\overline{y}_{ti\cdot} - \overline{y} = (\overline{y}_{\cdot i\cdot} - \overline{y}) + (\overline{y}_{t\cdot\cdot} - \overline{y}) + (\overline{y}_{ti\cdot} - \overline{y}_{t\cdot\cdot} - \overline{y}_{\cdot i\cdot} + \overline{y})$,
where $\overline{y} = \frac{1}{mkN}\sum_{t,i,j} Y_{tij}$, ...

source of variation	*sum of squares*	*df*	*mean sq.*
poisons	$\sum_{t,i,j}(\overline{y}_{\cdot i\cdot} - \overline{y})^2$	$k-1$	
treatments	$\sum_{t,i,j}(\overline{y}_{t\cdot\cdot} - \overline{y})^2$	$N-1$	
interactions	$\sum_{t,i,j}(\overline{y}_{ti\cdot} - \overline{y}_{t\cdot\cdot} - \overline{y}_{\cdot i\cdot} + \overline{y})^2$	$(k-1)(N-1)$	
between group	$\sum_{t,i,j}(\overline{y}_{ti\cdot} - \overline{y})^2$	$kN-1$	
within group	$\sum_{t,i,j}(y_{tij} - \overline{y}_{ti\cdot})^2$	$(m-1)\times k \times N$	

$\sum_{t,i,j}(Y_{tij} - \overline{y})^2$
$= \sum_{t,i,j}(Y_{tij} - \overline{y}_{ti\cdot} + \overline{y}_{ti\cdot} - \overline{y})^2$
$= \sum_{t,i,j}](Y_{tij} - \overline{y}_{ti\cdot})^2 + (\overline{y}_{ti\cdot} - \overline{y})^2]$
$= \sum_{t,i,j}[(Y_{tij} - \overline{y}_{ti\cdot})^2 + (\overline{y}_{ti\cdot} - \overline{y}_{t\cdot\cdot} - \overline{y}_{\cdot i\cdot} + \overline{y} + \overline{y}_{t\cdot\cdot} - \overline{y} + \overline{y}_{\cdot i\cdot} - \overline{y})^2]$
$= \sum_{t,i,j}[(Y_{tij} - \overline{y}_{ti\cdot})^2 + (\overline{y}_{ti\cdot} - \overline{y}_{t\cdot\cdot} - \overline{y}_{\cdot i\cdot} + \overline{y})^2 + (\overline{y}_{t\cdot\cdot} - \overline{y})^2 + (\overline{y}_{\cdot i\cdot} - \overline{y})^2]$

```
> (x=read.table(”toxic.txt”))
> x=unlist(x)
> (t=gl(4,12,48)) # treatment
    [1] 1 1 1 1 1 1 1 1 1 1 1 1 2 2 2 2 2 2 2 2 2 2 2 2 3 3 3 3 3 3 3 3 3 3 3 3 4 4
    [39] 4 4 4 4 4 4 4 4 4 4
    Levels: 1 2 3 4
> (p=rep(gl(3,4,12),4)) #poison
    [1] 1 1 1 1 2 2 2 2 3 3 3 3 1 1 1 1 2 2 2 2 3 3 3 3 1 1 1 1 2 2 2 2 3 3 3 3 1 1
    [39] 1 1 2 2 2 2 3 3 3 3
    Levels: 1 2 3
> (z=lm(x∼t*p))
```

$Y_{tij} = \eta_{ti} = \eta + \tau_t + \pi_i + \omega_{ti} + \epsilon_{tij}$,

$$Y_h = \eta + \sum_{t=1}^{N} \tau_t \mathbf{1}(T_h = t) + \sum_{i=1}^{k} \pi_i \mathbf{1}(P_h = i) + \sum_{i=1}^{k}\sum_{t=1}^{N} \omega_{ti} \mathbf{1}(T_h = t, P_h = i) + \epsilon_h,$$

$h = 1, ..., N * k * m$. **Notice that the parameters in the above equation are not uniquely determined**, *i.e.*, not identifiable.

$Y_h = \beta' X_h + \epsilon_h$, $\epsilon \perp X$.

```
> summary(z)
                Estimate   Std. Error   t value    Pr(> |t|)
  (Intercept)    0.41250    0.07457      5.532    2.94e − 06   ***
          t2     0.46750    0.10546      4.433    8.37e − 05   ***
          t3     0.15500    0.10546      1.470     0.1503
          t4     0.19750    0.10546      1.873     0.0692        .
          p2    −0.09250    0.10546     −0.877     0.3862
          p3    −0.20250    0.10546     −1.920     0.0628        .
       t2 : p2   0.02750    0.14914      0.184     0.8547
       t3 : p2  −0.10000    0.14914     −0.671     0.5068
       t4 : p2   0.15000    0.14914      1.006     0.3212
       t2 : p3  −0.34250    0.14914     −2.297     0.0276        *
       t3 : p3  −0.13000    0.14914     −0.872     0.3892
       t4 : p3  −0.08250    0.14914     −0.553     0.5836
```

Understanding the model and the summary(z):

$\tau_1 =$?

$\pi_1 =$?

$w_{t1} =$?

$w_{1i} =$?

$E(Y_h|X_h) = \hat{\beta}' X_h$?

$\hat{E}(Y_h|X_h) =$? (numerically) if $h = 1$ ((t, p) =(1,1))

$\hat{E}(Y_h|X_h) =$? (numerically) if h =39 ((t, p) =(4,1))

$\hat{E}(Y_h|X_h) =$? (numerically) if $h = 36$. (($t = p$ =3).

```
> v=lm(x∼I(t==2)*I(p==3))
> anova(v,z)
   Model 1: x ∼ I(t == 2) * I(p == 3)
   Model 2: x ∼ t * p
      Res.Df    RSS     Df   Sum of Sq      F       Pr(> F)
   1    44     1.23851
   2    36     0.80072   8    0.43779     2.4603    0.0308    *
> anova(z)
            Df   Sum Sq    Mean Sq   F value     Pr(> F)
       t     3   0.92121   0.30707   13.8056   3.777e − 06   ***
       p     2   1.03301   0.51651   23.2217   3.331e − 07   ***
     t : p   6   0.25014   0.04169    1.8743     0.1123
> w=lm(x∼t+p)
> summary(w)
                Estimate   Std. Error   t value    Pr(> |t|)
  (Intercept)    0.45229    0.05592      8.088    4.22e − 10   ***
          t2     0.36250    0.06458      5.614    1.43e − 06   ***
          t3     0.07833    0.06458      1.213     0.23189
          t4     0.22000    0.06458      3.407     0.00146      **
          p2    −0.07313    0.05592     −1.308     0.19813
          p3    −0.34125    0.05592     −6.102    2.83e − 07   ***
> anova(w,z)
   Model 1: x ∼ t + p
   Model 2: x ∼ t * p
      Res.Df    RSS     Df   Sum of Sq      F       Pr(> F)
   1    42     1.05086
   2    36     0.80072   6    0.25014     1.8743    0.1123
> s=lm(x∼I(t==2)+I(t==4)+I(p==3))
> anova(s,z)
```

```
    Res.Df     RSS     Df   Sum of Sq       F       Pr(> F)
  1    44    1.13046
  2    36    0.80072    8     0.32973    1.8531    0.09888   .
> summary(s)
                         Estimate   Std. Error   t value    Pr(> |t|)
     (Intercept)          0.45490    0.03658      12.435    5.34e − 16   ***
  I(t == 2)TRUE           0.32333    0.05667       5.706    9.13e − 07   ***
  I(t == 4)TRUE           0.18083    0.05667       3.191     0.00262     **
  I(p == 3)TRUE          −0.30469    0.04908      −6.208    1.67e − 07   ***
```

Are these effects ?

So the final model is

$Y = 0.45 + 0.32\mathbf{1}(T = 2) + 0.18\mathbf{1}(T = 4) - 0.3\mathbf{1}(P = 3) + \epsilon.$

Or $Y = 0.45 + 0.32\mathbf{1}(T = B) + 0.18\mathbf{1}(T = C) - 0.3\mathbf{1}(P = 3) + \epsilon.$

8.2. Simplification and increased sensitivity from transformation. The analysis in §8.1 is based on the assumption that $Y = \beta'\mathbf{X}+\epsilon$, where $\epsilon \sim N(0, \sigma^2)$ and $\mathbf{X} \perp \epsilon$. The residual plot $(\overline{y}_{ti\cdot}, y_{tij} - \overline{y}_{ti\cdot})$'s in Fig. 8.1 (see panel (1,1)) has a funnel shape. If $\sigma_{Y|\mathbf{X}}$ is a function of $\eta = E(Y|\mathbf{X})$ $(Y > 0)$, say $\sigma_{Y|\mathbf{X}} \propto \eta^{\alpha}$ (or $\ln\sigma_{Y|\mathbf{X}} \approx c + \alpha\ln\eta$), then $g(Y) = \begin{cases} Y^{\lambda} & \text{if } \lambda = 1 - \alpha \neq 0 \\ logY & \text{if } \lambda = 1 - \alpha = 0 \end{cases}$ is the variance stabilizing transformation. α can be estimated by the slope of the regression line lm$(\ln\hat{\sigma}_Y \sim \ln\hat{\mu}_Y)$, where $\hat{\mu}_Y$ and $\hat{\sigma}_Y$ are estimates, which are available if there are replications such as in the Taxic agents data (see Fig. 8.1), with $(u, v) = (\hat{\mu}, \hat{\sigma}_Y) = (\overline{y}_{ti}, s_{y_{ti}})$ (the mean and SD of the 4 (t, i) replicates).

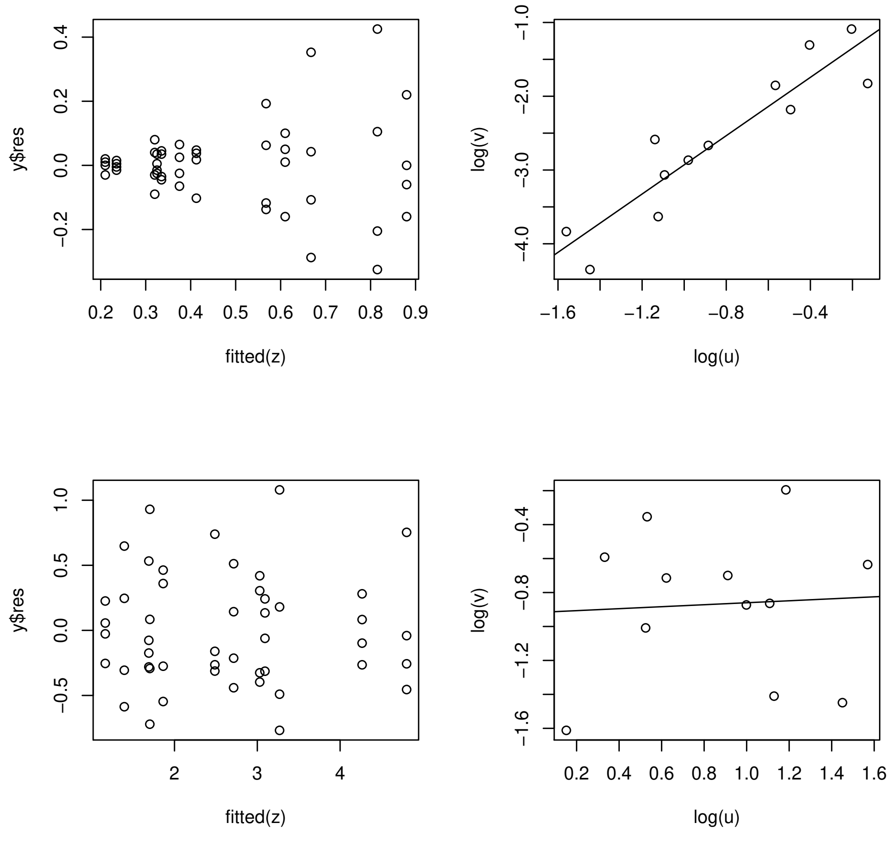


Fig. 8.1. ((y, z, u, v) is given in the R codes)

For the Taxic agents data, the top two panels in Fig. 8.1 are plots (fitted, residuals) and $(\overline{y}_{ti\cdot}, s_{ti\cdot})$. From panel (1,2) in Fig. 8.1, $(-1.5, -0.4)$ and $(0, -1)$ leads to the

slope $\hat{\alpha} \approx \frac{-1-(-4)}{0.0-(-1.5)} = 2$ and $\hat{\lambda} = -1$. Thus it is appropriate to let the variance stabilizing transformation be $g(Y) = 1/Y$. The bottom two panels of Fig. 8.1 are plots (fitted, residuals) and $(\overline{1/y_{ti\cdot}}, s_{ti\cdot})$ after y is replaced by y^{-1}. The slope ≈ 0.
Variance stabilizing transformations when $\sigma_{Y|\mathbf{X}} \propto \eta^{\alpha}$, where $\eta = E(Y|\mathbf{X})$.

dependency			*variance*	
of			*stabilizing*	
on η	α	$\lambda = 1-\alpha$	*transformation*	*example*
$\sigma \propto \eta^2$	2	-1	*reciprocal*	
$\sigma \propto \eta^{3/2}$	3/2	$-1/2$	*reciprocal square root*	
$\sigma \propto \eta$	1	0	*log*	
$\sigma \propto \eta^{1/2}$	1/2	1/2	*square root*	*poisson frequency*
$\sigma \propto const$	0	1	*no transformation*	

The codes to produce Fig. 8.1 are given below.

```
func1= function(x) {
    z=lm(x~t*p) plot(fitted(z),resid(z))
    y=x
    dim(y)=c(4,12)
    u=apply(y,2,mean)
    v=apply(y,2,sd)
    z=lm(log(v)~log(u))
    plot(log(u),log(v))
    abline(z)
}
par(mfrow=c(2,2))
func1(x)
x=1/x
func1(x)
w=lm(x~t*p)
summary(w)
              Estimate   Std. Error   t value    Pr(>|t|)
(Intercept)    2.48688    0.24499     10.151    4.16e-12   ***
     t2       -1.32342    0.34647     -3.820    0.000508   ***
     t3       -0.62416    0.34647     -1.801    0.080010    .
     t4       -0.79720    0.34647     -2.301    0.027297    *
     p2        0.78159    0.34647      2.256    0.030252    *
     p3        2.31580    0.34647      6.684    8.56e-08   ***
   t2:p2      -0.55166    0.48999     -1.126    0.267669
   t3:p2       0.06961    0.48999      0.142    0.887826
   t4:p2      -0.76974    0.48999     -1.571    0.124946
   t2:p3      -0.45030    0.48999     -0.919    0.364213
   t3:p3       0.08646    0.48999      0.176    0.860928
   t4:p3      -0.91368    0.48999     -1.865    0.070391    .
anova(w)
```

```
              Df   Sum Sq   Mean Sq   F value     Pr(>F)
       t       3   20.414    6.8048   28.3431   1.376e-09   ***
       p       2   34.877   17.4386   72.6347   2.310e-13   ***
      t:p      6    1.571    0.2618    1.0904     0.3867
  Residuals   36    8.643    0.2401
```

The analysis is more sensitive than the one gets from §8.1.

```
> u=lm(x~t+p)
> summary(u)
```

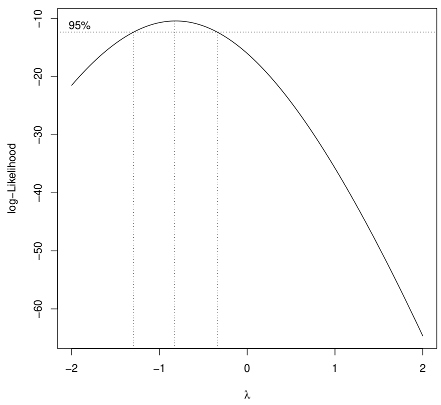
	$Estimate$	$Std.\ Error$	$t\ value$	$Pr(>\|t\|)$	
$(Intercept)$	2.6977	0.1744	15.473	$< 2e-16$	$***$
$t2$	-1.6574	0.2013	-8.233	$2.66e-10$	$***$
$t3$	-0.5721	0.2013	-2.842	0.00689	$**$
$t4$	-1.3583	0.2013	-6.747	$3.35e-08$	$***$
$p2$	0.4686	0.1744	2.688	0.01026	$*$
$p3$	1.9964	0.1744	11.451	$1.69e-14$	$***$

So the final model is
$1/y = 2.7-1.7\mathbf{1}(T=2)-0.6\mathbf{1}(T=3)-1.4\mathbf{1}(T=4)+0.5\mathbf{1}(P=2)+2.0\mathbf{1}(P=3)+\epsilon$
v.s. $Y = 0.45+0.32\mathbf{1}(T=B)+0.18\mathbf{1}(T=C)-0.3\mathbf{1}(P=3)+\epsilon$ from the end of §8.1:

		Df	$Sum\ Sq$	$Mean\ Sq$	$F\ value$	$Pr(>F)$	
anova(w)	t	3	0.92121	0.30707	13.8056	$3.777e-06$	$***$
	p	2	1.03301	0.51651	23.2217	$3.331e-07$	$***$
	$t:p$	6	0.25014	0.04169	1.8743	0.1123	$v.s.$ 0.3867

Remark. The variance stabilizing transformation is actually the boxcox method.

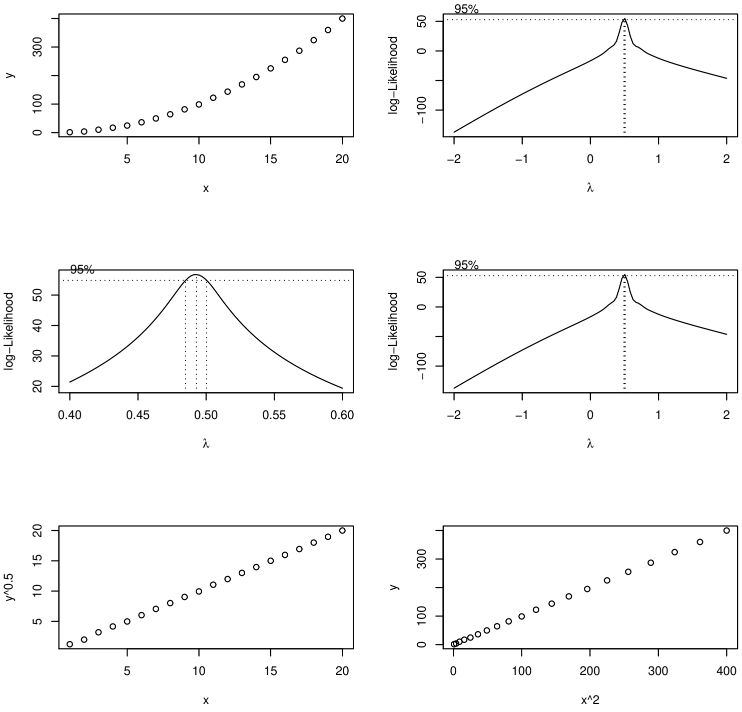
```
 library(MASS)
 boxcox(x~t*p)
  b=boxcox(x~t*p)
  I=which(b$x==max(b$x))
  b$x[I]
 [1] 2
```
$(=\alpha = 1-\lambda)$



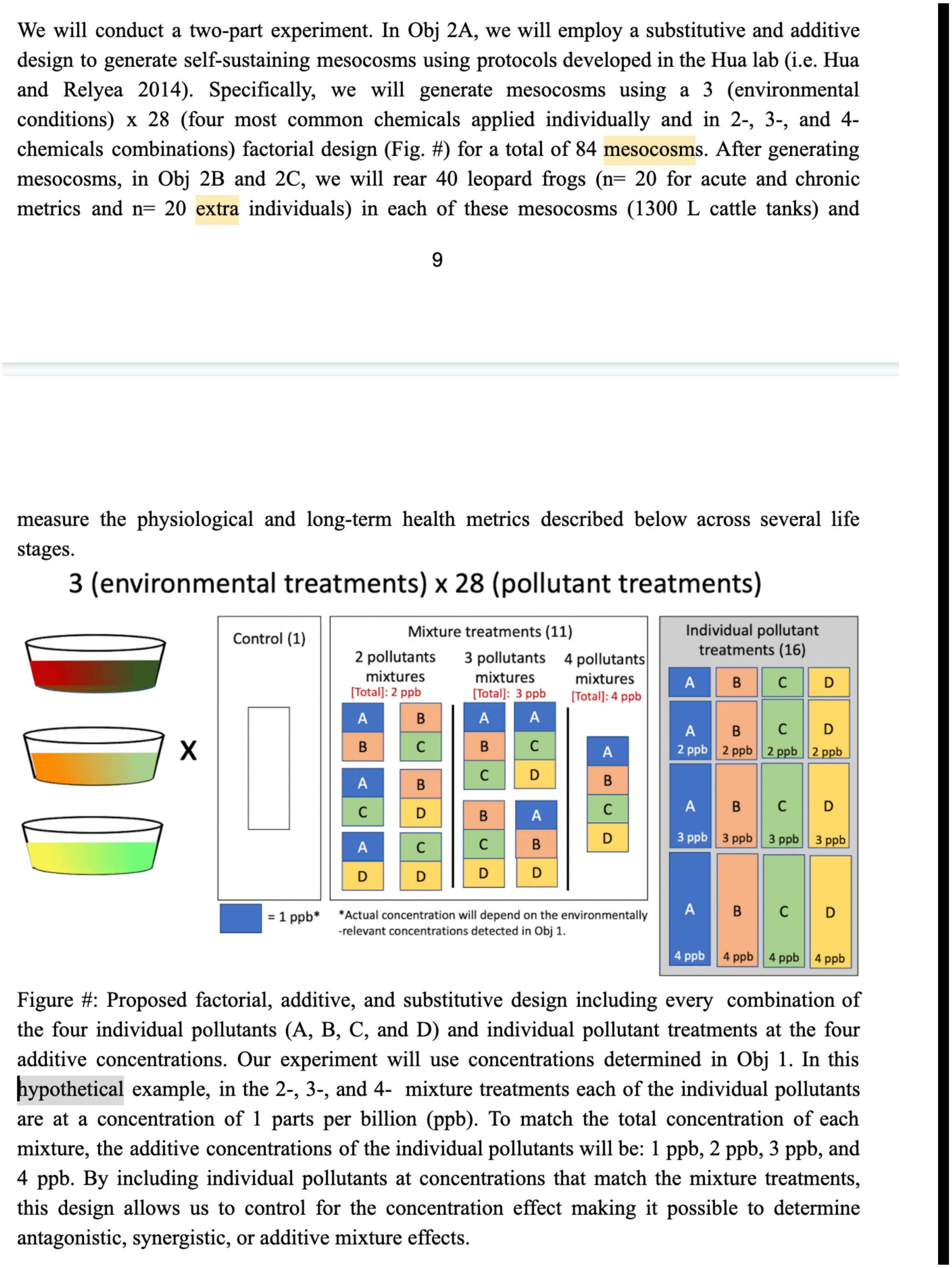
It suggests that $\lambda = 1-\alpha \approx -1$ too.

Another simulation example.

```
library(MASS)
n=20
x=1:20
y=x**2+rnorm(n)
W=lm(y~ x)
# y^{1/2} = x + e
par(mfrow=c(3,2))
plot(x,y)
boxcox(W,plotit=T)
boxcox(W,plotit=T,lambda=
   seq(0.4,0.6,by=0.01))
b=boxcox(y~ x)
I=which(b$y==max(b$y))
b$x[I]
[1] 0.5050505      (= α)
plot(x,y**0.5)
plot(x**2,y)
```



A consultant problem (see the attached fd.pdf).



We will conduct a two-part experiment. In Obj 2A, we will employ a substitutive and additive design to generate self-sustaining mesocosms using protocols developed in the Hua lab (i.e. Hua and Relyea 2014). Specifically, we will generate mesocosms using a 3 (environmental conditions) x 28 (four most common chemicals applied individually and in 2-, 3-, and 4-chemicals combinations) factorial design (Fig. #) for a total of 84 mesocosms. After generating mesocosms, in Obj 2B and 2C, we will rear 40 leopard frogs (n= 20 for acute and chronic metrics and n= 20 extra individuals) in each of these mesocosms (1300 L cattle tanks) and

measure the physiological and long-term health metrics described below across several life stages.

Figure #: Proposed factorial, additive, and substitutive design including every combination of the four individual pollutants (A, B, C, and D) and individual pollutant treatments at the four additive concentrations. Our experiment will use concentrations determined in Obj 1. In this hypothetical example, in the 2-, 3-, and 4- mixture treatments each of the individual pollutants are at a concentration of 1 parts per billion (ppb). To match the total concentration of each mixture, the additive concentrations of the individual pollutants will be: 1 ppb, 2 ppb, 3 ppb, and 4 ppb. By including individual pollutants at concentrations that match the mixture treatments, this design allows us to control for the concentration effect making it possible to determine antagonistic, synergistic, or additive mixture effects.

Comment: There are two types of set-up: 1. Numerical: The box on the right represents numerical in 1, 2, 3, 4 ppb. 2. Factor: The rest are factors.

Q: 1. How many factor variables ? 2 or else ?

2. What are the levels of each variable ?

If the 4 variables are treated as linear variables, then the inputs for the right group

is ...
Otherwise, one may check whether it is quadratic relation.
$i*$(1,0,0,0 ...), $i \in \{1,2,3,4\}$ $i*$(0,1,0,0,0 ...), $i \in \{1,2,3,4\}$
$i*$(0,0,1,0,0 ...), $i \in \{1,2,3,4\}$ $i*$(0,0,0,1,0 ...), $i \in \{1,2,3,4\}$

For measurement 1 ppb, there are 4 pollutants factors: A, B, C, D, each having 2 levels $(-,+)$ or (control, 1 ppb). The standard table of contrast is

a	b	c	d	ab	ac	ad	bc	bd	cd	abc	abd	acd	bcd	$abcd$
$-$	$-$	$-$	$-$											
$+$	$-$	$-$	$-$											
$-$	$+$	$-$	$-$											
$+$	$+$	$-$	$-$											
$-$	$-$	$+$	$-$											
$+$	$-$	$+$	$-$											
$-$	$+$	$+$	$-$											
$+$	$+$	$+$	$-$											
$-$	$-$	$-$	$+$											
$+$	$-$	$-$	$+$											
$-$	$+$	$-$	$+$											
$+$	$+$	$-$	$+$											
$-$	$-$	$+$	$+$											
$+$	$-$	$+$	$+$											
$-$	$+$	$+$	$+$											
$+$	$+$	$+$	$+$											

Use factor(), it becomes $-1 \to 0$, $+1 \to 1$, thus the table becomes

a	b	c	d	ab	ac	ad	bc	bd	cd	abc	abd	acd	bcd	$abcd$
0	0	0	0											
1	0	0	0											
0	1	0	0											
1	1	0	0											
0	0	1	0											
1	0	1	0											
0	1	1	0											
1	1	1	0											
0	0	0	1											
1	0	0	1											
0	1	0	1											
1	1	0	1											
0	0	1	1											
1	0	1	1											
0	1	1	1											
1	1	1	1											

Note $(-1)(-1) = +1$ but factor(-1)*factor(-1)=0. There are 4+6+4+1 df, together with average effect, total of 16 df.

The enviromental variable is a 3-level factor, say take values E1, E2 and E3, total of 2 df. Now together with the 4 pollutant factors,

there are 4+2 main effects,

2×4 2-factors interactions,

2×6 3-factors interactions,

2×4 4-factors interactions,

2×1 5-factors interactions,

1 intercept parameter.

The total df is 6+8+12+8+2+1=37. Let e and f denote the 2nd and 3rd enviromental treatments.

run	e	f	a	b	c	d

The model is $\mathbf{Y} = \mathbf{X}\beta$, where $n = 48$ $(= 2^4 \times 3)$, β is a 37×1 vector, $\mathbf{X}$ is a 48×37 matrix with the coordinate of the first column always being 1.

$ea \quad eb \quad ec \quad ed \quad eab \quad eac \quad ead \quad ebc \quad ebd \quad ecd \quad eabc \quad eabd \quad eacd \quad ebcd \quad eabcd$

$fa \quad fb \quad fc \quad fd \quad fab \quad fac \quad fad \quad fbc \quad fbd \quad fcd \quad fabc \quad fabd \quad facd \quad fbcd \quad fabcd$

X without the 1st column is

run	*e*	*f*	*a*	*b*	*c*	*d*	*ea*	*eb*	*ec*	*ed*	*eab*	*eac*	*ead*	*ebc*	⋯	*eabcd*	*fa*	*fb*	⋯	*fabcd*
1	0	0	0	0	0	0														
2	0	0	1	0	0	0														
3	0	0	0	1	0	0														
4	0	0	1	1	0	0														
5	0	0	0	0	1	0														
6	0	0	1	0	1	0														
7	0	0	0	1	1	0														
8	0	0	1	1	1	0														
9	0	0	0	0	0	1														
10	0	0	1	0	0	1														
11	0	0	0	1	0	1														
12	0	0	1	1	0	1														
13	0	0	0	0	1	1														
14	0	0	1	0	1	1														
15	0	0	0	1	1	1														
16	0	0	1	1	1	1														
17	1	0	0	0	0	0														
⋮																				
32	1	0	1	1	1	1														
33	0	1	0	0	0	0														
	⋮																			
48	0	1	1	1	1	1														

Chapter 12. Some Application of Response Surface Methods

Response surface methodology (RSM) is a collection of mathematical and statistical techniques for empirical model building. By careful design of experiments, the objective is to optimize a response (output variable) which is influenced by several independent variables (input variables).

12.1. Iterative experimentation to improve a product design.

An experiment is a series of tests, called runs, in which changes are made in the input variables in order to identify the reasons for changes in the output response. In an experiment, choices of

different factors,
different ranges for the factors,
different qualitative and blocking factors,
transformations for the factors,
responses and their metrics,
models,

will make a difference in the conclusions.
However, in an iterative sequence of experiments, they may nevertheless arrive at a similar or equally satisfactory solutions.

A paper helicopter design experiment.
Initial experiment.

Factor			-1	$+1$		
$P:$	*paper type*	x_1	*regular*	*bound*		
$l:$	*wing length*	x_2	$3in$	4.75	$x_2 = (l - 3.875)/0.875 = \pm 1$	
$L:$	*body length*	x_3	$3in$	4.75	$x_3 = (L - 3.875)/0.875 = \pm 1$	
$W:$	*body width*	x_4	$1.25in$	$2in$	$x_4 = (W - 1.625)/0.375 = \pm 1$	(1)
$F:$	*fold*	x_5	*No*	*Yes*		
$T:$	*taped body*	x_6	*No*	*Yes*	*no need to adjust*	
$C:$	*paper clip*	x_7	*No*	*Yes*		
$M:$	*taped wing*	x_8	*No*	*Yes*		

Let $\overline{y}_i$ and s_i be the data from repeated flight times of the 16 helicopters made according to the 2^{8-4}_{IV} design **(what are the generating relations ?)**

```
y=c(236,185,259,318,180,195,246,229,196,203,230,261,168,197,220,241) # (ȳi)
s=c(2.1,4.7,2.7,5.3,7.7,7.7,9,3.2,11.5,10.1,2.9,15.3,11.3,11.7,16,6.8)
a=rep(c(-1,1),8)
b=rep(c(-1,-1,1,1),4)
c=rep(c(rep(-1,4),rep(1,4)),2)
d=c(rep(-1,8),rep(1,8))
```

Q: Are a, b, c and d factors ?

P	l	L	W	F	T	C	M
5.87	27.75	-13.25	-8.25	3.75	1.37	-10.88	-3.88

$\sigma_{effect} \approx 4.5$.

From the output and statistics analysis (try yourself), l, L, W and C are real.
Since C, the paper clip factor, reduces the flight time,
any further experiment does not add paper clip.
Then the model is simplified as

$y = 223 + 28x_2 - 13x_3 - 8x_4$ # from lm(y∼ x2+x3+x4)

Another 5 helicopters were made roughly according to the steepest ascent direction.
= ?

	helicopter	1	2	3	4	5	
$l:$	*wing length*	4	4.75	5.5	6.25	7	
$L:$	*body length*	3.82	3.46	3.10	2.75	2.39	(the optimal value $y \approx 347$).
$W:$	*body width*	1.61	1.52	1.42	1.33	1.24	
	$\overline{y}$	275	304	$\underline{347}$	275	227	
	s	9.4	13.5	20	57.3	38.9	

Note that l increases by 0.75 each time,
L decreases by 0.36, 0.36, 0.35, 0.36,
W decreases by 0.1 roughly each time.
Why this way ?

```
a=c(28,-13,-8)                  (see l, L, W)
b=c(4,3.82,1.61)                  (see 1st column of above table)
d=c(4.75,3.46,1.52)                  (see 2nd column ...)
e=c(3.875,3.875,1.625)                  (see Eq. (1) above)
r=c(0.875,0.875,0.375)                  (see Eq. (1) above)
x=a/sum(a)
y=(b-e)/r
x/y
    [1] 28.00000 29.54545 28.57143
y=(d-e)/r
x/y
    [2] 4.000000 3.915663 4.081633
```

What is in common in [1] and [2] ?

The engineers suggest that the wing area (lw) and the wing length ratio (l/w) may be factors that has impact on the flight time. So another set of 18 experiments were run.

Factor		-1	0	$+1$
A :	*wing area (lw)*	11.8	12.4	13
R :	*wing length ratio*	2.25	2.52	2.78
W :	*body width*	1	1.25	1.5
L :	*body length*	1.5	2	2.5

Note. The estimates are based on numerical covariates, but not factors.

To allow for the fitting of a second-order model, 2+12 additional runs were added. Now total of $2^4 + 2 + 12 = 30$ runs.

```
> lm(y∼a+b+c+d+I(a*a)+I(b*b)+I(c*c)+I(d*d)+I(a*b)+I(a*c)
    +I(a*d)+I(b*c)+I(b*d)+I(c*d))
```

$$\begin{aligned}\hat{y} =&370.83\\ &-0.08x_1+5.08x_2+0.25x_3-6.08x_4\\ &-1.79x_1^2-1.42x_2^2-2.29x_3^2-0.08x_4^2\\ &-2.88x_1x_2-3.75x_1x_3+4.38x_1x_4\\ &+4.63x_2x_3-1.50x_2x_4-2.13x_3x_4\end{aligned}\tag{12.2}$$

By eliminating the inert effects, the equation can be simplified as

$$\begin{aligned}\hat{y} =&370.83\\ &5.08x_2-6.08x_4\\ &-1.79x_1^2-2.29x_3^2\\ &-2.88x_1x_2-3.75x_1x_3+4.38x_1x_4\\ &+4.63x_2x_3-2.13x_3x_4\end{aligned}\tag{12.3}$$

Note: The fitted equation (12.3) is not the same as the output from R program, unless adjust the values of intercept and squared terms. See codes below.

```
> lm(y∼b+d+I(a*a)+I(c*c)+I(a*b)+I(a*c) +I(a*d)+I(b*c)+I(c*d))
```

$$\begin{aligned}\hat{y} =&369.5\\ &+5.08x_2-6.08x_4\\ &-1.66x_2^2-2.13x_3^2\\ &-2.88x_1x_2-3.75x_1x_3+4.38x_1x_4\\ &+4.63x_2x_3-2.13x_3x_4\end{aligned}$$

```
> w=lm(y b+d+I(a*a)+I(c*c)+I(a*b)+I(a*c)+I(a*d)+I(b*c)+I(c*d))
> anova(z,w)
Model 1: y   a + b + c + d + I(a * a) + I(b * b) + I(c * c) + I(d * d)
    + I(a * b) + I(a * c) + I(a * d) + I(b * c) + I(b * d) + I(c * d)
Model 2: y   b + d + I(a * a) + I(c * c) + I(a * b) + I(a * c)
    + I(a * d) + I(b * c) + I(c * d)
      Res.Df    RSS     Df   SumofSq      F       Pr(> F)
  1     15     194.17
  2     20     289.17   −5     −95      1.4678    0.2579
```

Based on Eq.(12.2), we can have canonical form

$$\hat{y} = 371.4 - 4.66X_1^2 - 3.81X_2^2 - 3.27X_3^2 - 1.2X_4^2 \tag{12.4}$$

where $X_1 = (0.39, -0.45, 0.8, -0.07)(x_1, x_2, x_3, x_4)'$,
$X_2 = (-0.76, -0.5, 0.12, 0.39)(x_1, x_2, x_3, x_4)'$,
$X_3 = (0.52, -0.45, -0.45, 0.57)(x_1, x_2, x_3, x_4)'$,
$X_4 = (-0.04, -0.58, -0.37, -0.72)(x_1, x_2, x_3, x_4)'$.

Appendix. The marginal distribution (MD) approach. The MD approach consists a speical type of graphing and tests for model checking. Notice that existing model checking tests for testing

$$H_0\colon Y = \beta X + W \text{ and } X \perp W \text{ v.s. } H_1\colon H_0 \text{ is false.} \qquad (1.1)$$

like the F-test and t-test tests are valid if

(1) $Y = \beta X + \theta g(X) + \epsilon$ is true, (it changes H_1 to H_1^o: $\theta \neq 0$).

(2) $X \perp \epsilon$,

(3) $\epsilon \sim N(0, \sigma^2)$.

If (1) or (3) fails, the existing tests are not valid, and can be worse than random guessing, let alone being consistent. Of course, if no better choice, something is better than no choice.

We shall introduce a new approach for model checking. It can be applied to various models, including the LR models. It is always consistent for testing H_0: $Y = \beta X + W$ and $X \perp W$ v.s. H_1: H_0 is false.

A.1. Preliminary. We assume that

$(\mathbf{X}_1, Y_1)$, ..., $(\mathbf{X}_n, Y_n)$ are i.i.d. observations from $F_{\mathbf{X},Y}$, with density function $f_{\mathbf{X},Y}$, where $\mathbf{X}$ is a p-dimensional random vector and Y is a response variable.

Let $F_{Y|\mathbf{X}}$ be the conditional cdf with density function $f_{Y|\mathbf{X}}$.

Denote $F_o = F_{Y|\mathbf{X}}(\cdot|\mathbf{0})$, which is called the baseline cdf of $F_{Y|\mathbf{X}}$.

The LR model is often formulated by

$$Y = \alpha + \beta'\mathbf{X} + \epsilon, \text{ where } E(\epsilon|\mathbf{X}) = 0. \qquad (1.2)$$

If the conditional variance $Var(W|\mathbf{X})$ does not depend on $\mathbf{X}$, it is called an ordinary linear regression (OLR) model, otherwise, it is called a weighted linear regression (WLR) model. **Q:** Does WLR model satisfy H_0 in (1.1) ?

Remark 1. Advantages that the LR model is specified by Eq. (1.1) rather than (1.2) are as follow:

(1) Eq. (1.2) but not (1.1) requires that $E(Y|\mathbf{X})$ exists;

(2) In general, β but not α is identifiable under censorship models;

(3) It is often less important to estimate α than β, the effect of $\mathbf{X}$ on Y.

Under the OLR model, there are several consistent estimators of β if $F_{\mathbf{X},Y} \in \Theta_{lse}$,

$$where \;\; \Theta_{lse} = \{F_{\mathbf{X},Y}\colon \Sigma_{\mathbf{X}} \text{ is non-singular and } Cov(\mathbf{X}, Y) \text{ exists}\}, \qquad (1.3)$$

and $\Sigma_{\mathbf{X}}$ is the $p \times p$ covariance matrix of $\mathbf{X}$. They include

the semi-parametric MLE (SMLE) Y&W (2003) (if F_o is discontinuous),

the modified SMLE (MSMLE) (see Y&W (2002)), $(L = \prod_i f(Y_i - \beta X_i))$

the least squares estimator (LSE) and

the quantile or median regression estimator.

Yu and Wong (2002) show that

the MSMLE is still consistent if $E(\ln f_W(W))$ exists, and

the MSMLE (or SMLE) $\tilde\beta$ satisfy $P(\tilde\beta \neq \beta$ infinitely often$) = 0$ if F_W isn't cts.

However, the LSE is inconsistent if $E(|Y||\mathbf{X}) = \infty$.

Given $F_{\mathbf{X},Y} \in \Theta$ (the family of all joint cdf of $(\mathbf{X}, Y)$), $F_o = F_{Y|\mathbf{X}}(\cdot|\mathbf{0})$ is well defined, even if $(\mathbf{X}, Y)$ does not satisfy the linear regression model in H_0: $Y = \beta'\mathbf{X} + W$, where $E(W)$ may not exist. Let

$$\Theta_0 = \{F_{\mathbf{X},Y}:\; Y = \beta'\mathbf{X} + W, \text{ where } W \perp \mathbf{X}, \beta \text{ and } F_W \text{ are unknown}\} \qquad (2.1)$$

$(F_W = F_o)$. Then Eq. (1.1) can be specified as H_0: $F_{\mathbf{X},Y} \in \Theta_0$. The next lemma characterizes various LR models and motivating the MD approach for the LR model.

Lemma 1. *$F_{Y|\mathbf{X}}$ is a function of (F_o, β) and $F_Y(t) = E(F_{Y|\mathbf{X}}(t|\mathbf{X}))$. Moreover, if $F_{\mathbf{X},Y} \in \Theta_0$, then $F_{Y|\mathbf{X}}(t|x) = F_o(t - \beta'x)$.*

For convenience, we write $F_Y(t) = F_Y(t;\beta)$, as F_Y is a function of the parameter β if $F_{\mathbf{X},Y} \in \Theta_o$. Given β and $F_{\mathbf{X},Y}$, which may or may not belong to the LR model, define another r.v..

$$Y^* = \beta'\mathbf{X} + W^*, \text{ where } F_{W^*}(\cdot) = F_{Y|\mathbf{X}}(\cdot|\mathbf{0}) \text{ and } \mathbf{X} \perp W^*. \tag{2.2}$$

By Lemma 1, the cdf of Y^* is

$$F_{Y^*}(t) \ = E(F_o(t - \beta'\mathbf{X})) \text{ (denoted also by } F_{Y^*}(t;\beta)). \tag{2.3}$$

Q: Is F_{Y^*} related to $F_{\mathbf{X},Y}$?

Theorem 1. *If $F_{\mathbf{X},Y} \in \Theta_0$ (see Eq. (2.1)), then*

(a) $F_o(\cdot) = F_{Y|\mathbf{X}}(\cdot|\mathbf{0}) = \mathbf{F}_{\mathbf{Y}^*|\mathbf{X}}(\cdot|\mathbf{0})$,

(b) $F_{Y|\mathbf{X}} = F_{Y^*|\mathbf{X}}$, and

(c) $F_Y = F_{Y^*}$.

If $F_{\mathbf{X},Y} \in \Theta \setminus \Theta_0$, then

(e) $F_o(\cdot) = F_{Y|\mathbf{X}}(\cdot|\mathbf{0}) = \mathbf{F}_{\mathbf{Y}^*|\mathbf{X}}(\cdot|\mathbf{0})$, and

(d) $F_{Y|\mathbf{X}} \neq F_{Y^*|\mathbf{X}}$.

Notice that if $F_{\mathbf{X},Y} \in \Theta_0$ as in (2.1), $E(Y|\mathbf{X})$ may not exist.

Corollary 1. (1) $F_{\mathbf{X},Y} \in \Theta_0$ iff $F_{Y|\mathbf{X}} = F_{Y^*|\mathbf{X}}$;

(2) $F_{\mathbf{X},Y} \in \Theta_0 => F_Y = F_{Y^*}$.

Corollary 1 motivates the MD plot and the MD test. Given data $(\mathbf{X}_i, Y_i)$'s from $F_{\mathbf{X},Y}$, if $F_{\mathbf{X},Y} \in \Theta_0$ in (2.1), then β in $F_{Y^*}(t;\beta)$ is uniquely determined by $F_{\mathbf{X},Y}$. It is often that β in $F_{Y^*}(t;\beta)$ can also be uniquely determined by $F_{\mathbf{X},Y}$ even if $F_{\mathbf{X},Y} \notin \Theta_0$, such as in the case that $F_{\mathbf{X},Y} \in \Theta_{lse}$ (see (1.3)). One estimates β by the LSE if one feels confident that $\Theta_p = \Theta_{lse}$, or by the modified semi-parametric MLE (MSMLE) otherwise. In this course, we only use the LSE for illustration.

A.2. The MD plot. The edf of $F_Y(t)$ is $\hat{F}_Y(t) = \frac{1}{n}\sum_{i=1}^n \mathbf{1}(Y_i \le t)$. We call the 95% pointwise confidence interval of $F_Y(t)$, *i.e.*, $\hat{F}_Y(t) \pm 1.96\sqrt{\hat{F}_Y(t)(1-\hat{F}_Y(t))/n}$, the confidence band (CB) of F_Y. The MD plot is

to plot $y = \hat{F}_{Y^*}(t)$ and $y = \hat{F}_Y(t)$, or together with the 95% CB of F_Y,
or to plot $y = \hat{S}_{Y^*}(t)$ and $y = \hat{S}_Y(t)$, or the CB of S_Y,
where $S_Y = 1 - F_Y$, $\hat{S}_Y = 1 - \hat{F}_Y(t)$, etc.

$\hat{F}_{Y^*}(t) = \frac{1}{n}\sum_{i=1}^n \hat{F}_o(t - \hat{\beta}X_i)$,
$\hat{\beta}$ is a consistent estimator of β,
$\hat{F}_o(t) \to F_o(t)$ a.s.

If the two curves are close, *e.g*, the curve of $y = \hat{F}_{Y^*}(t)$ lies within the CB of F_Y,
then it suggests that the model does fit the data.
If most of the curve of $y = \hat{F}_{Y^*}(t)$ lies outside the CB of F_Y,
then it suggests that the model does not fit the data.

The key of our new approach is to construct an estimator of the baseline cdf F_o, say $\hat{F}_o$, which satisfies that for each t, $\hat{F}_o(t) \xrightarrow{P} F_o(t)$ $\forall$ $F_{\mathbf{X},Y} \in \Theta$.

We now explain how to construct the estimators $\hat{F}_o$ and $\hat{F}_{Y^*}$.

For simplicity, we first explain in the case that

$$X \in \mathcal{R} \text{ and } Y = \beta X + W, \text{ where } f_X(0) > 0. \tag{2.4}$$

Then, there are observations X_1, ..., X_m satisfying $|X_i| < \delta_n$ for some $\delta_n = cn^{-1/3}$. If $n \approx 100$ then ideally choose c so that $m \ge 20$.

$$\hat{F}_o(t) = \frac{1}{m}\sum_{i=1}^m \mathbf{1}(Y_i \le t) \to F_o(t) \ (= F_{Y|X}(t|0)) \text{ if } n \to \infty \tag{2.5}$$

$$\begin{aligned} \hat{F}_{Y^*}(t) =& \frac{1}{n}\sum_{i=1}^n \hat{F}_o(t - \hat{\beta}X_i) = \frac{1}{mn}\sum_{i=1}^n\sum_{j=1}^m \mathbf{1}(Y_j + \hat{\beta}X_i \le t) \\ =& \frac{1}{mn}\sum_{i=1}^n\sum_{j=1}^m \mathbf{1}(W_j^* + \hat{\beta}X_i \le t), \end{aligned}$$

where $\hat\beta$ is a consistent estimator of β *e.g.* the LSE based on (X_i, Y_i)'s. One can replace $\hat F_{Y^*}$ by $\tilde F_{Y^*}$, the edf based on n "observations" $Y_i^* = \hat\beta X_i + W_i^*$, $i = 1$, ..., n, W_i^*'s are n samples with replacement from $\{Y_1, ..., Y_m\}$ (where $X_i \approx 0$ and $W_i^* \perp X$). If (2.4) fails ($f_X(0) \neq 0$), then $\exists$ a mode of f_X, denoted by a. Since

$$\beta'\mathbf{X} + W = \underbrace{\beta'(\mathbf{X} - a)}_{=\check X} + \underbrace{\beta' a + W}_{=\check W}, \text{ and } W \perp \mathbf{X} \text{ iff } W - \beta' a \perp (\mathbf{X} - a), \qquad (2.6)$$

we can replace X_i by $\check X_i = X_i - a$, $i = 1$, ..., n.
Eq. (2.5) remains the same, treating $\check X_i$ as X_i, where $|\check X_i| < \delta_n$ for $i = 1$, ..., m.
Remark 3. In application, a can be the center of an interval where X_i's are most concentrated.

Without loss of generality (WLOG), we shall assume hereafter that the zero vector satisfies

$$f_{\mathbf{X}}(\mathbf{0}) > \mathbf{0} \text{ and } Y_1, ..., Y_m \text{ are the } Y_i\text{'s where } ||\mathbf{X}_i|| \le \delta_n,\ \delta_n \to 0\ (e.g.,\ \delta_n = cn^{\frac{-1}{3p}} \qquad (2.7)$$

$c = r/2$ and $r = \max_{i,j} ||\mathbf{X}_i - \mathbf{X}_j||$) and $||\cdot||$ is a norm.
Remark 4. *One may wonder whether a naive estimator of F_o is the edf $\check F_o$ based on $\hat W_i$'s ($= Y_i - \hat\beta'\mathbf{X}_i$). This $\check F_o$ is a consistent estimator of F_o if H_0 in Eq. (2.1) is true. The drawback of this naive approach is that if H_0 in Eq. (2.1) is false then $\check F_o$ is not consistent. We shall present 2 examples that $\check F_{Y^*}$ based on such $\check F_o$ suggests that the data fit the incorrect models Θ_0. Thus it does not serve our purpose of a diagnostic tool.*

If the curve of $\hat F_{Y^*}(t)$ lies either entirely outside or entirely inside the confidence band of $\hat F_Y(t)$, then the indication is quite clear. Otherwise, it is quite subjective to say whether the two curves are close. Thus it is desirable to derive certain statistical tests.
A.3. The MD test The MD plotting method leads to a class of tests of H_0: $F_{\mathbf{X},Y} \in \Theta_0$, as follows.

$$T_1 = \int |\hat F_Y(t) - \hat F_{Y^*}(t)| d\hat F_Y(t) = \sum_t |\hat F_Y(t) - \hat F_{Y^*}(t)| \hat f_Y(t), \qquad (2.8)$$

or $T_2 = \sup_t |\hat F_Y(t) - \hat F_{Y^*}(t)|$,
$T_3 = \int \mathcal{W}(t)(\hat F_Y(t) - \hat F_{Y^*}(t)) dG(t)$,
or $T_4 = \int \mathcal{W}(t)|\hat F_Y(t) - \hat F_{Y^*}(t)|^k dG(t)$, where $k \ge 1$, $\mathcal{W}(\cdot)$ is a weight function, and dG is a measure, *e.g.*, dt, $d\hat F_o$, $d\hat F_Y$ and $d\hat F_{Y^*}(t)$. These tests are really testing

$$H_0^{MD}\text{: } F_Y = F_{Y^*}, \text{ v.s. } H_1^{MD}\text{: } F_Y \neq F_{Y^*}, \text{ where } Y^* \text{ is defined in Eq. (2.2).}$$

Recall H_0: $Y = \beta X + W$ and $X \perp W$ v.s. H_1: H_0 is not true.
Or v.s. H_1^o: $Y = \beta X + \theta G(x) + \epsilon$, $\theta \neq 0$ and under NID.
Definition. The tests T_1, ..., T_4 in Eq. (2.8) are called the MD tests.

The percentiles of these T_j's can be estimated by resampling as follows.

- b1. In view of Remark 3 and Eq. (2.6), WLOG, we can assume that (2.7) holds. OW, let $\check X_i = X_i - a$, where a is specified in Remark 3.
- b2. Obtain $\hat\beta$, an estimator of β based on $(\mathbf{X}_i, Y_i)$'s under H_0, such as the LSE if it is sure that $F_{\mathbf{X},Y} \in \Theta_{lse}$, or the SMLE if there exist ties in the data, otherwise, the MSMLE.
- b3. Take a random sample of size m from the $\mathbf{X}_i$'s in a neighborhood of $\mathbf{0}$, say $Neib(\mathbf{0}, \delta_\mathbf{n})$, where m and δ_n are as in (2.7), and take another random sample of size $n - m$ from the $\mathbf{X}_i$'s outside $Neib(\mathbf{0}, \delta_\mathbf{n})$. It yields a sample of $\mathbf{X}_i$'s, say $\mathbf{X}_1^{(1)}$, ..., $\mathbf{X}_n^{(1)}$.
- b4. Generate a random sample of size n from $\hat F_o$, say, $W_1^{(1)}$, ..., $W_n^{(1)}$.

b5. Let $Y_i^{(1)} = \hat\beta'\mathbf{X}_i^{(1)} + W_i^{(1)}$, $i = 1, ..., n$.

b6. Now, obtain a value of T_1, say $T_1^{(1)}$, based on $(X_i^{(1)}, Y_i^{(1)})$'s and Eq. (2.8).

b7. Repeat the steps b3, ..., b6 a large number of times, say 100 times, obtain $T_1^{(j)}$ for $j = 2$, ..., 100. Thus the desired percentile can be estimated by the edf of these $T^{(j)}$'s.

Remark 5. The MD tests are valid tests of
H_0^{MD}: $F_Y = F_{Y^*}$ against H_1^{MD}: $F_Y \neq F_{Y^*}$.
It is worth mentioning that even when H_0 in Eq. (2.1) fails and $E(|Y||\mathbf{X}) = \infty$,
the asymptotic distribution of the MD test still holds.
In particular, if H_0 is not true but $F_{Y^*} = F_Y$,
the MD test would make type I error for testing H_o^{MD} with probability (w.p.) p_o and type II error for testing H_0: $Y = \beta X + W$ in (2.1) w.p.$(1 - p_o)$, where p_o is the size of the MD test. This is not the case for all existing tests.

For instance, the goodness-of-fit test tests H_0: $\sigma_L = \sigma_E$ under NID.

The t-test tests H_o: $\theta = 0$ with $Y = \beta X + \theta g(X) + \epsilon$ under NID.

If the assumption fails, the type II error depends on the real model and $\neq 1-\alpha$.

Remark 6. A valid test for H_0: $Y = \beta X + W$ v.s. H_1: $Y \neq \beta'\mathbf{X} + W$ is based on $\hat F_{\mathbf{X},Y} - \hat F_{\mathbf{X},Y^*}$, where $F_{\mathbf{Y},Y*}$ is the joint distribution function, Y^* is defined as in (2.2), and $\hat F_{\mathbf{X},Y^*}$ is its edf. However, it is more convenient to use the MD approach, as it has a diagnostic plot and most of the time $F_Y \neq F_{Y^*}$ if H_1 is true.

Example 2.1. We generated data (X_i, Y_i), $i = 1, ..., n$ from the Cox model $h_{T|X}(t|x) = h_o(t)\exp(x)$, where $h_o = 1(t \geq 0)$, *i.e.*, $S_{T|X}(t|x) = e^{-te^x\mathbf{1}(t>0)}$, $Y = T - E(T|X)$, $X \sim U(-4/k, 4)$, $k \approx n^{0.7}$, and n is between 60 and 300.

```
n=100
k=n**0.7
x=runif(n,-4/k,4)
y=rexp(n,exp(x))-exp(-x)    #so that E(Y|X)=0
```

We fitted the data to the OLR (or WLR model), that is,
H_0: $Y = \beta X + W$ (& $X \perp W$).

The Cox model does not belong to any LR model. We compare the MD test to two existing tests in the literature: gam test and SS-test.
The gam test is invalid, as $X \not\perp Y - \beta X - E(Y|X)$, violating its required assumption.
The t-test and the goodness-of-fit test are also invalid, as no NID.
The SS-test is valid under the assumption in this example (it only requires finite $E(Y|\mathbf{x})$).

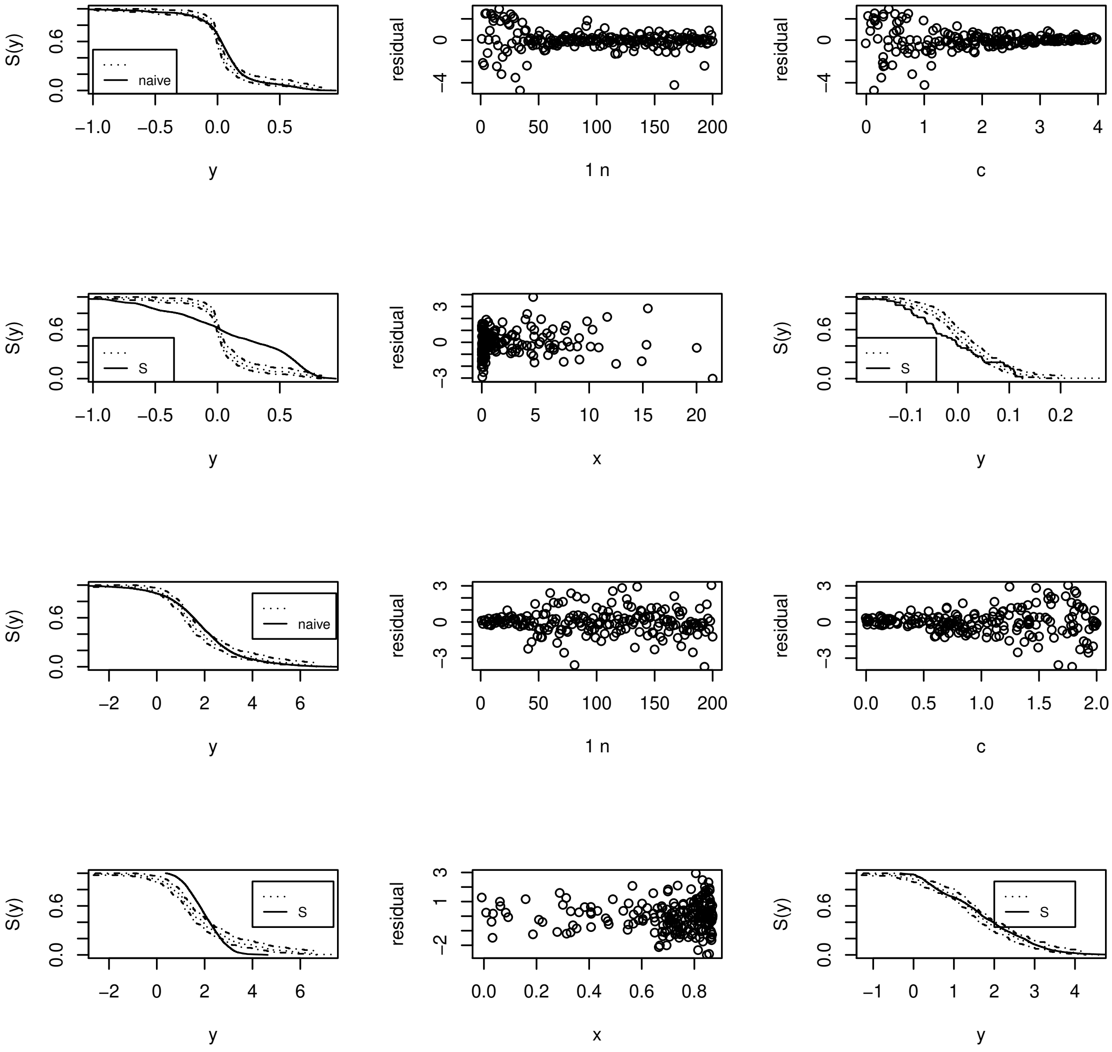
For such data with a sample size $n = 200$, the residual plots (see panels (1,2) and (1,3) in Figure 1) and the MD plot (see panel (2,1)) suggest that the OLR model may not fit the data, but the residual plot in panel (2,2) suggests that a WLR model with a weight function $\sqrt{|(X-4)^3\mathbf{1}(X < 3.7) + (X - 4.5)^3\mathbf{1}(X \geq 3.7)|}$ might work. However, the MD plot (see panel (2,3)) suggests that the WLR model does not fit the data neither. Thus the MD plots are better.

The simulation results suggest that the MD test T_1 performs very well for testing the incorrect OLR model, even when $n = 60$. The MD test can detect that the data do not fit the WLR model for large sample sizes such as $n \geq 200$.

For comparison sake, we also generated random samples from another WLR model:

$Y = X + W$, where $W = 1 + \epsilon\sqrt{X + 0.3}$, $\epsilon \perp X$, $\epsilon \sim N(0, 1)$, $X \sim U(0, 2)$,
Under this model, we carried out two sets of simulation studies. We first fitted the data to the OLR model $Y = \beta X + W$, where $W \perp X$. The residual plots (see panels (3,2) and (3,3)) and the MD plot (see panel (4,1)) of Figure 1 suggest that the OLR model does not fit the data, but a WLR model might work (see panels (4,2) and (4,3)).

The naive estimator $\check{S}^*$ ($= 1 - \check{F}_{Y^*}$ see Remark 4) suggests that the data from the Cox model and from the WLR model all fit the OLR model (see panels (1,1) and (3,1)). Thus it is useless. We also applied the same three tests to the WLR model. Since the data were from the WLR model, thus we estimated $P(H_0|H_1)$ for fitting the OLR model and $P(H_1|H_0)$ for fitting the WLR model, where H_0^2: the model is the WLR model v.s. H_1^2: H_0^2 is not true. The simulation results are presented in the bottom half of Table 1.



Cox data	naive $\check{S}^*$ for OLR	(i, residual)	(X_i,residual) for OLR
	MD plot for OLR	(X_i,residual) for WLR	MD plot for WLR
WLR data	naive $\check{S}^*$ for OLR	(i, residual)	(X_i,residual) for OLR
	MD plot for OLR	(X_i,residual) for WLR	MD plot for WLR

Figure 1. Residuals and MD plots under the Cox Model or the WLR model

Model:		OLR			WLR		
Data	Test:	T_1	SS	gam	T_1	SS	gam
	n	$\hat{p}_{0\mid 1}$	$\hat{p}_{0\mid 1}$	$\hat{p}_{0\mid 1}$	$\hat{p}_{0\mid 1}$	$\hat{p}_{0\mid 1}$	$\hat{p}_{0\mid 1}$
Cox	60	0.01	0.06	1.00	0.78	0.96	1.00
	200	0.00	0.00	1.00	0.19	0.95	1.00
	300	0.00	0.00	1.00	0.02	0.94	1.00
		$\hat{p}_{0\mid 1}$	$\hat{p}_{0\mid 1}$	$\hat{p}_{0\mid 1}$	$\hat{p}_{1\mid 0}$	$\hat{p}_{1\mid 0}$	$\hat{p}_{1\mid 0}$
WLR	60	0.03	0.00	0.59	0.04	0.05	0.08
	120	0.00	0.00	0.60	0.04	0.05	0.07

$\hat{p}_{0|1}$ is the estimate of $P(H_0|H_1)$ and $\hat{p}_{1|0}$ is the estimate of $P(H_1|H_0)$

Table 1. Simulation Results in Example 2.1

Homework. 1. Write the R codes to recover panels in Figure 1, except [2,3] and [4,3].

2. Write the R codes to recover the first column of Table 1, the results on MD test based on T_1 statistic. Then make comparison to the $t-test$ for those 5 cases. You should use the same data to do the two tests.

In the original MD method, $\hat{F}(t)$ is a smooth version of the edf. So we discuss as follows.

Remark. The idea for generating random numbers for a continuous distribution F_X: $F_X(X) \sim U(0,1)$. Let $Y \sim U(0,1)$, $F_X^{-1}(Y) \sim F_X$.

Example 8. Suppose that F is a piecewise uniform distribution on $(0,1)$ and $(3,4)$ with weights 1/4 and 3/4. A pseudo random number of $n = 10$ can be generated as follows.

```
> n=10
> x=runif(n)
> m=length(x[x<0.25])
> y=runif(m)
> z=runif(n-m)+3
> y [1] 0.08246115 0.76996953
> z [1] 3.848005 3.442600 3.142384 3.670791 3.537500 3.897043 3.558773 3.388922
```

Example 9. Suppose that F is piecewise uniform on $(0,0.5)$ and $(3,6)$ with weights 1/5 and 3/5 and $F(x) = 1-0.2e^{-x+7}$ if $x > 7$. That is $F(x) = \begin{cases} 0 & \text{if } x < 0 \\ 0.4x & \text{if } x \in [0,0.5] \\ 0.2 & \text{if } x \in (0.5,3) \\ 0.2+0.2(x-3) & \text{if } x \in [3,6] \\ 0.8 & \text{if } x \in (6,7) \\ 1-0.2e^{-x+7} & \text{if } x > 7 \end{cases}$

Thus $F^{-1}(t) = \begin{cases} t/0.4 & \text{if } t \in [0,0.2] \\ \frac{t-0.2}{0.2}+3 & \text{if } t \in (0.2,0.8] \\ 7-\ln\frac{1-t}{0.2} & \text{if } t \in (0.8,1] \end{cases}$

9 pseudo random numbers can be generated as follows.

```
> (x=sort(runif(9)))
    [1] 0.01509044 0.03312090 0.19840396 0.28440890 0.33304866 0.35577466 0.48100012
    [8] 0.59806993 0.85603151
> y=x
> (k=ceiling(x*5)) # Why ×5 ?
    [1] 1 1 1 2 2 2 3 3 5
> (u=x[k==1]*2.5)
    [1] 0.03772610 0.08280224 0.49600990
> (v=7-log(5*(1-x[k==5])))
    [1] 7.328723
> (x=x[k>1&k<5])
    [1] 0.2844089 0.3330487 0.3557747 0.4810001 0.5980699
> round(c(u,(x-0.2)*5+3,v),2)
    [1] 0.04 0.08 0.50 3.42 3.67 3.78 4.41 4.99 7.33
> y=c(y[k==1]*2.5, 5*(y[k>1&k<5]-0.2)+3, 7-log(5*(1-y[k==5])))
> round(y,2)
    [1] 0.04 0.08 0.50 3.42 3.67 3.78 4.41 4.99 7.33
```

Remark. Given a n distinct Y_i, their edf is $\hat{F}(t) = \frac{1}{m}\sum_{i=1}^m \mathbf{1}(Y_i \leq t)$. WLOG, assume that $Y_1 < \cdots < Y_m$. A linear interpolation to the discrete $\hat{F}$ is

$$\begin{aligned}\tilde{F}(t) =& \frac{1}{m}\sum_{i=1}^m [\frac{t-(Y_i-\epsilon)}{\epsilon}\mathbf{1}(t \in (Y_i-\epsilon, Y_i)) + \mathbf{1}(Y_i \leq t)] \\ =& \begin{cases} \frac{j-1}{m} + \frac{t-Y_j+\epsilon}{m\epsilon} & \text{if } t \in (Y_j-\epsilon, Y_j],\ j \in \{1,...,m\} \\ \cdots & \text{if } \cdots, \end{cases}\end{aligned}$$

where $\epsilon = \min_{i<j\leq m}|Y_i - Y_j|$,