Chapter 8

Orthogonal Designs

Orthogonal designs for factors with two levels can be fit using least squares. The orthogonality of the contrasts allows each coefficient to be estimated independently of the other variables in the model.

This chapter covers 2^k factorial designs, 2_R^{k-f} fractional factorial designs and Plackett Burman PB(n) designs. The entries in the design matrix $\boldsymbol{X}$ are either -1 or 1. The columns of the design matrix $\boldsymbol{X}$ are orthogonal: $\boldsymbol{c}_i^T \boldsymbol{c}_j = 0$ for $i \neq j$ where $\boldsymbol{c}_i$ is the ith column of $\boldsymbol{X}$. Also $\boldsymbol{c}_i^T \boldsymbol{c}_i = n$, and the absolute values of the column entries sum to n.

The first column of $\boldsymbol{X}$ is $\mathbf{1}$, the vector of ones, but the remaining columns of $\boldsymbol{X}$ are the coefficients of a contrast. Hence the ith column $\boldsymbol{c}_i$ has entries that are -1 or 1, and the entries of the ith column $\boldsymbol{c}_i$ sum to 0 for $i > 1$.

8.1 Factorial Designs

Factorial designs are a special case of the k way Anova designs of Chapter 6, and these designs use **factorial crossing** to compare the effects (main effects, pairwise interactions, ..., k-fold interaction) of the k factors. If $A_1, ..., A_k$ are the factors with l_i levels for $i = 1, ..., k$; then there are $l_1 l_2 \cdots l_k$ treatments where each treatment uses exactly one level from each factor. The sample size $n = m \prod_{i=1}^k l_i \geq m\ 2^k$. Hence the sample size grows exponentially fast with k. Often the number of replications $m = 1$.

Definition 8.1. An experiment has n runs where a **run** is used to measure a response. A run is a treatment = a combination of k levels. So each run uses exactly one level from each of the k factors.

Often each run is expensive, for example, in industry and medicine. A goal is to improve the product in terms of higher quality or lower cost. Often the subject matter experts can think of many factors that might improve the product. The number of runs n is minimized by taking $l_i = 2$ for $i = 1, ..., k$.

Definition 8.2. A 2^k *factorial design* is a k way Anova design where each factor has two levels: low $= -1$ and high $= 1$. The design uses $n = m2^k$ runs. Often the number of replications $m = 1$. Then the sample size $n = 2^k$.

A 2^k factorial design is used to screen potentially useful factors. Usually at least $k = 3$ factors are used, and then $2^3 = 8$ runs are needed. Often the units are time slots, and each time slot is randomly assigned to a run = treatment. The subject matter experts should choose the two levels. For example, a quantitative variable such as temperature might be set at 80^oF coded as -1 and 100^oF coded as 1, while a qualitative variable such at type of catalyst might have catalyst A coded as -1 and catalyst B coded as 1.

Improving a process is a sequential, iterative process. Often high values of the response are desirable (eg yield), but often low values of the response are desirable (eg number of defects). Industrial experiments have a budget. The initial experiment may suggest additional factors that were omitted, suggest new sets of two levels, and suggest that many initial factors were not important or that the factor is important, but the level of the factor is not.

Suppose $k = 5$ and A, B, C, D and E are factors. Assume high response is desired and high levels of A and C correspond to high response where A is qualitative (eg 2 brands) and C is quantitative but set at two levels (eg temperature at 80 and 100^oF). Then the next stage may use an experiment with factor A at its high level and at a new level (eg a new brand) and C at the highest level from the previous experiment and at a higher level determined by subject matter experts (eg at 100 and 120^oF).

Rule of thumb 8.1. Do not spend more than 25% of the budget on the initial experiment. It may be a good idea to plan for four experiments, each taking 25% of the budget.

Definition 8.3. Recall that a **contrast** $C = \sum_{i=1}^p d_i \mu_i$ where $\sum_{i=1}^p d_i = 0$, and the estimated contrast is $\hat{C} = \sum_{i=1}^p d_i \overline{Y}_{i0}$ where μ_i and $\overline{Y}_{i0}$ are appropriate population and sample means. In a **table of contrasts**, the coefficients d_i of the contrast are given where a $-$ corresponds to -1 and a $+$ corresponds to 1. Sometimes a column I corresponding to the overall mean is given where each entry is a $+$. The column corresponding to I is not a contrast.

To make a table of contrasts there is a rule for main effects and a rule for interactions.

a) In a table of contrasts, the column for A starts with a $-$ then a $+$ and the pattern repeats. The column for B starts with 2 $-$'s and then 2 $+$'s and the pattern repeats. The column for C starts with 4 $-$'s and then 4 $+$'s and the pattern repeats. The column for the ith main effects factor starts with 2^{i-1} $-$'s and 2^{i-1} $+$'s and the pattern repeats where $i = 1, ..., k$.

b) In a table of contrasts, a column for an interaction containing several factors is obtained by multiplying the columns for each factor where $+ = 1$ and $- = -1$. So the column for ABC is obtained by multiplying the column for A, the column for B and the column for C.

A table of contrasts for a 2^3 design is shown below. The first column is for the mean and is not a contrast. The last column corresponds to the cell means. Note that $\overline{y}_{1110} = y_{111}$ if $m = 1$. So $\overline{\boldsymbol{y}}$ might be replaced by $\boldsymbol{y}$ if $m = 1$. Each row corresponds to a run. Only the levels of the main effects A, B and C are needed to specify each run. The first row of the table corresponds to the low levels of A, B and C. Note that the divisors are 2^{k-1} except for the divisor of I which is 2^k where $k = 3$.

	I	A	B	C	AB	AC	BC	ABC	$\overline{\boldsymbol{y}}$
	+	−	−	−	+	+	+	−	$\overline{y}_{1110}$
	+	+	−	−	−	−	+	+	$\overline{y}_{2110}$
	+	−	+	−	−	+	−	+	$\overline{y}_{1210}$
	+	+	+	−	+	−	−	−	$\overline{y}_{2210}$
	+	−	−	+	+	−	−	+	$\overline{y}_{1120}$
	+	+	−	+	−	+	−	−	$\overline{y}_{2120}$
	+	−	+	+	−	−	+	−	$\overline{y}_{1220}$
	+	+	+	+	+	+	+	+	$\overline{y}_{2220}$
divisor	8	4	4	4	4	4	4	4	

The table of contrasts for a 2^4 design is below. The column of ones corresponding to I was omitted. Again rows correspond to runs and the levels of the main effects A, B, C and D completely specify the run. The first row of the table corresponds to the low levels of A, B, C and D. In the second row, the level of A is high while B, C and D are low. Note that the interactions are obtained by multiplying the component columns where $+ = 1$ and $- = -1$. Hence the first row of the column corresponding to the ABC entry is $(-)(-)(-) = -$.

run	A	B	C	D	AB	AC	AD	BC	BD	CD	ABC	ABD	ACD	BCD	ABCD
1	−	−	−	−	+	+	+	+	+	+	−	−	−	−	+
2	+	−	−	−	−	−	−	+	+	+	+	+	+	−	−
3	−	+	−	−	−	+	+	−	−	+	+	+	−	+	−
4	+	+	−	−	+	−	−	−	−	+	−	−	+	+	+
5	−	−	+	−	+	−	+	−	+	−	+	−	+	+	−
6	+	−	+	−	−	+	−	−	+	−	−	+	−	+	+
7	−	+	+	−	−	−	+	+	−	−	−	+	+	−	+
8	+	+	+	−	+	+	−	+	−	−	+	−	−	−	−
9	−	−	−	+	+	+	−	+	−	−	−	+	+	+	−
10	+	−	−	+	−	−	+	+	−	−	+	−	−	+	+
11	−	+	−	+	−	+	−	−	+	−	+	−	+	−	+
12	+	+	−	+	+	−	+	−	+	−	−	+	−	−	−
13	−	−	+	+	+	−	−	−	−	+	+	+	−	−	+
14	+	−	+	+	−	+	+	−	−	+	−	−	+	−	−
15	−	+	+	+	−	−	−	+	+	+	−	−	−	+	−
16	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+

Randomization for a 2^k design: The runs are determined by the levels of the k main effects in the table of contrasts. So a 2^3 design is determined by the levels of A, B and C. Similarly, a 2^4 design is determined by the levels of A, B, C and D. Randomly assign units to the $m2^k$ runs. Often the units are time slots. If possible, perform the $m2^k$ runs in random order.

Genuine run replicates need to be used. A common error is to take m measurements per run, and act as if the m measurements are from m runs. If as a data analyst you encounter this error, average the m measurements into a single value of the response.

Definition 8.4. If the response depends on the two levels of the factor, then the factor is called **active**. If the response does not depend on the two levels of the factor, then the factor is called **inert**.

Active factors appear to change the mean response as the level of the factor changes from -1 to 1. Inert factors do not appear to change the response as the level of the factor changes from -1 to 1. An inert factor could be needed but the level low or high is not important, or the inert factor may not be needed and so can be omitted from future studies. Often subject matter experts can tell whether the inert factor is needed or not.

The 2^k designs are used for **exploratory data analysis**: they provide answers to the following questions.

i) Which combinations of levels are best?

ii) Which factors are active and which are inert? That is, use the 2^k design to screen for factors where the response depends on whether the level is high or low.

iii) How should the levels be modified to improve the response?

If all 2^k runs give roughly the same response, then choose the levels that are cheapest to increase profit. Also the system is robust to changes in the factor space so managers do not need to worry about the exact values of the levels of the factors.

In an experiment, there will be an interaction between management, subject matter experts (often engineers) and the data analyst (statistician).

Remark 8.1. If $m = 1$, then there is one response per run but k main effects, $\binom{k}{2}$ 2 factor interactions, $\binom{k}{j}$ j factor interactions, and 1 k way interaction. Then the MSE df $= 0$ unless at least one high order interaction is assumed to be zero. A full model that includes all k main effects and all $\binom{k}{2}$ two way interactions is a useful starting point for response, residual and transformation plots. The higher order interactions can be treated as potential terms and checked for significance. As a rule of thumb, significant interactions tend to involve significant main effects.

Definition 8.5. An **outlier** corresponds to a case that is far from the bulk of the data.

Rule of thumb 8.2. Mentally add 2 lines parallel to the identity line and 2 lines parallel to the $r = 0$ line that cover most of the cases. Then a case is an outlier if it is well beyond these 2 lines. This rule often fails for large outliers since often the identity line goes through or near a large outlier so its residual is near zero. A response that is far from the bulk of the data in the response plot is a "large outlier" (large in magnitude).

Rule of thumb 8.3. Often an outlier is very good, but more often an outlier is due to a measurement error and is very bad.

Definition 8.6. A **critical mix** is a single combination of levels, out of 2^k, that gives good results. Hence a critical mix is a good outlier.

Be able to pick out active and inert factors and good (or the best) combinations of factors (cells or runs) from the table of contrasts = table of runs. Often the table will only contain the contrasts for the main effects. If high values of the response are desirable, look for high values of $\overline{y}$ for $m > 1$. If $m = 1$, then $\overline{y} = y$. The following two examples help illustrate the process.

O	H	C	y
$-$	$-$	$-$	5.9
$+$	$-$	$-$	4.0
$-$	$+$	$-$	3.9
$+$	$+$	$-$	1.2
$-$	$-$	$+$	5.3
$+$	$-$	$+$	4.8
$-$	$+$	$+$	6.3
$+$	$+$	$+$	0.8

Example 8.1. Box, Hunter and Hunter (2005, p. 209-210) describes a 2^3 experiment with the goal of reducing the wear rate of deep groove bearings. Here $m = 1$ so $n = 8$ runs were used. The 2^3 design employed two levels of osculation (O), two levels of heat treatment (H), and two different cage designs (C). The response Y is the bearing failure rate and low values of the observed response y are better than high values.

a) Which two combinations of levels are the best?

b) If two factors are active, which factor is inert?

Solution: a) The two lowest values of y are 0.8 and 1.2 which correspond to $+++$ and $++-$. (Note that if the 1.2 was 4.2, then $+++$ corresponding to 0.8 would be a critical mix.)

b) C would be inert since O and H should be at their high + levels.

run	R	T	C	D	y
1	−	−	−	−	14
2	+	−	−	−	16
3	−	+	−	−	8
4	+	+	−	−	22
5	−	−	+	−	19
6	+	−	+	−	37
7	−	+	+	−	20
8	+	+	+	−	38
9	−	−	−	+	1
10	+	−	−	+	8
11	−	+	−	+	4
12	+	+	−	+	10
13	−	−	+	+	12
14	+	−	+	+	30
15	−	+	+	+	13
16	+	+	+	+	30

Example 8.2. Ledolter and Swersey (2007, p. 80) describes a 2^4 experiment for a company that manufactures clay plots to hold plants. For one of the company's newest products, there had been an unacceptably high number of cracked pots. The production engineers believed that the following factors are important: R = rate of cooling (slow or fast), T = kiln temperature (2000^{o}F or 2060^{o}F), C = coefficient of expansion of the clay (low or high), and D = type of conveyor belt (metal or rubberized) used to allow employees to handle the pots. The response y is the percentage of cracked pots per run (so small y is good).

a) For fixed levels of R, T and C, is the $D+$ level or $D-$ level of D better (compare run 1 with run 9, 2 with 10, ..., 8 with 16).

b) Fix D at the better level. Is the $C-$ or $C+$ level better?

c) Fix C and D at the levels found in a) and b). Is the $R-$ or $R+$ level better?

d) Which factor seems to be inert?

Solution: a) $D+$ since for fixed levels of R, T and C, the number of cracks is lower if $D = +$ than if $D = -$.

b) $C-$

c) $R-$ d) T.

A 2^k design can be fit with least squares. In the table of contrasts let a "+ = 1" and a "− = −1." Need a row for each response: can't use the mean response for each fixed combination of levels. Let $\boldsymbol{x}_0$ correspond to I, the column of 1s. Let $\boldsymbol{x}_i$ correspond to the ith main effect for $i = 1, ..., k$. Let $\boldsymbol{x}_{ij}$ correspond to 2 factor interactions, and let $\boldsymbol{x}_{i_1,...,i_G}$ correspond to G way interactions for $G = 2, ..., k$. Let the design matrix $\boldsymbol{X}$ have columns corresponding to the $\boldsymbol{x}$. Then $\boldsymbol{X}$ will have $n = m2^k$ rows. Let $\boldsymbol{y}$ be the vector of responses.

The table below relates the quantities in the 2^3 table of contrasts with the quantities used in least squares. The design matrix

$$\boldsymbol{X} = [\boldsymbol{x}_0, \boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3, \boldsymbol{x}_{12}, \boldsymbol{x}_{13}, \boldsymbol{x}_{23}, \boldsymbol{x}_{123}].$$

Software often does not need the column of ones $\boldsymbol{x}_0$.

$\boldsymbol{x}_0$	$\boldsymbol{x}_1$	$\boldsymbol{x}_2$	$\boldsymbol{x}_3$	$\boldsymbol{x}_{12}$	$\boldsymbol{x}_{13}$	$\boldsymbol{x}_{23}$	$\boldsymbol{x}_{123}$	$\boldsymbol{y}$
I	A	B	C	AB	AC	BC	ABC	$\boldsymbol{y}$

The table below relates quantities in the 2^4 table of contrasts with the quantities used in least squares. Again $\boldsymbol{x}_0$ corresponds to I, the column of ones, while $\boldsymbol{y}$ is the vector of responses.

$\boldsymbol{x}_1$	$\boldsymbol{x}_2$	$\boldsymbol{x}_3$	$\boldsymbol{x}_4$	$\boldsymbol{x}_{12}$	$\boldsymbol{x}_{13}$	$\boldsymbol{x}_{14}$	$\boldsymbol{x}_{23}$	$\boldsymbol{x}_{24}$	$\boldsymbol{x}_{34}$	$\boldsymbol{x}_{123}$	$\boldsymbol{x}_{124}$	$\boldsymbol{x}_{134}$	$\boldsymbol{x}_{234}$	$\boldsymbol{x}_{1234}$
A	B	C	D	AB	AC	AD	BC	BD	CD	ABC	ABD	ACD	BCD	ABCD

Definition 8.7. The **least squares model** for a 2^k design contains a least squares population coefficient β for each x in the model. The model can be written as $Y = \boldsymbol{x}^T\boldsymbol{\beta} + e$ with least squares fitted values $\hat{Y} = \boldsymbol{x}^T\hat{\boldsymbol{\beta}}$. In matrix form the model is $\boldsymbol{Y} = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{e}$ and the vector of fitted values is $\hat{\boldsymbol{Y}} = \boldsymbol{X}\hat{\boldsymbol{\beta}}$. The *biggest possible model* contains all of the terms. The **second order model** contains β_0, all main effects and all second order interactions, and is recommended as the initial full model for $k \geq 4$. The **main effects model** removes all interactions. If a model contains an interaction, then the model should also contain all of the corresponding main effects. Hence if a model contains x_{123}, the model should contain x_1, x_2 and x_3.

Definition 8.8. The coefficient β_0 corresponding to I is equal to the population "I effect" of x_0, and the (sample) I effect $= \hat{\beta}_0$. For an x other than x_0, the **population effect** for x is 2β, the change in Y as x changes two units from −1 to 1, and the (sample) **effect** is $2\hat{\beta}$. The (sample) coefficient $\hat{\beta}$ estimates the population coefficient β.

Suppose the model using all of the columns of $\boldsymbol{X}$ is used. If some columns are removed (eg those corresponding to the insignificant effects), then for 2^k designs the following quantities remain unchanged for the terms that were not deleted: the effects, the coefficients, SS(effect) = MS(effect). The MSE, SE(effect), F and t statistics, pvalues, fitted values and residuals do change.

The regression equation corresponding to the significant effects (eg found with a QQ plot of Definition 8.9) can be used to form a reduced model. For example, suppose the full (least squares) fitted model is $\hat{Y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_{i1} + \hat{\beta}_2 x_{i2} + \hat{\beta}_3 x_{i3} + \hat{\beta}_{12} x_{i12} + \hat{\beta}_{13} x_{i13} + \hat{\beta}_{23} x_{i23} + \hat{\beta}_{123} x_{i123}$. Suppose the A, B and AB effects are significant. Then the reduced (least squares) fitted model is $\hat{Y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_{i1} + \hat{\beta}_2 x_{i2} + \hat{\beta}_{12} x_{i12}$ where the coefficients ($\hat{\beta}$'s) for the reduced model can be taken from the full model since the 2^k design is orthogonal.

The coefficient $\hat{\beta}_0$ corresponding to I is equal to the I effect, but the coefficient of a factor x corresponding to an *effect* is $\hat{\beta} = 0.5$ *effect*. Consider significant effects and assume interactions can be ignored.

i) If a large response Y is desired and $\hat{\beta} > 0$, use $x = 1$. If $\hat{\beta} < 0$, use $x = -1$.

ii) If a small response Y is desired and $\hat{\beta} > 0$, use $x = -1$. If $\hat{\beta} < 0$, use $x = 1$.

Rule of thumb 8.4. To predict Y with $\hat{Y}$, the number of coefficients = the number of $\hat{\beta}$'s in the model should be $\leq n/2$, where the sample size n = number of runs. Otherwise the model is overfitting.

From the regression equation $\hat{Y} = \boldsymbol{x}^T \hat{\boldsymbol{\beta}}$, be able to predict Y given $\boldsymbol{x}$. Be able to tell whether $x = 1$ or $x = -1$ should be used. Given the x values of the main effects, get the x values of the interactions by multiplying the columns corresponding to the main effects.

Least squares output in symbols is shown on the following page. Often "Estimate" is replaced by "Coef" or "Coefficient". Often "Intercept" is replaced by "Constant". The t statistic and pvalue are for whether the term or effect is significant. So t_{12} and p_{12} are for testing whether the x_{12} term or AB effect is significant.

The least squares coefficient = 0.5 (effect). The sum of squares for an x corresponding to an effect is equal to SS(effect). SE(coef) = SE($\hat{\beta}$) = 0.5 SE(effect) = $\sqrt{MSE/n}$. Also SE($\hat{\beta}_0$) = $\sqrt{MSE/n}$.

	Coef or Est.	Std.Err	t	pvalue
Intercept or constant	$\hat{\beta}_0$	SE(coef)	t_0	p_0
x_1	$\hat{\beta}_1$	SE(coef)	t_1	p_1
x_2	$\hat{\beta}_2$	SE(coef)	t_2	p_2
x_3	$\hat{\beta}_3$	SE(coef)	t_3	p_3
x_{12}	$\hat{\beta}_{12}$	SE(coef)	t_{12}	p_{12}
x_{13}	$\hat{\beta}_{13}$	SE(coef)	t_{13}	p_{13}
x_{23}	$\hat{\beta}_{23}$	SE(coef)	t_{23}	p_{23}
x_{123}	$\hat{\beta}_{123}$	SE(coef)	t_{123}	p_{123}

Example 8.3. a) The biggest possible model for the 2^3 design is $Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{12} x_{12} + \beta_{13} x_{13} + \beta_{23} x_{23} + \beta_{123} x_{123} + e$ with least squares fitted or predicted values given by $\hat{Y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_{i1} + \hat{\beta}_2 x_{i2} + \hat{\beta}_3 x_{i3} + \hat{\beta}_{12} x_{i12} + \hat{\beta}_{13} x_{i13} + \hat{\beta}_{23} x_{i23} + \hat{\beta}_{123} x_{i123}$.

The second order model is $Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{12} x_{12} + \beta_{13} x_{13} + \beta_{23} x_{23} + e$. The main effects model is $Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + e$.

b) A typical least squares output for the 2^3 design is shown below. Often "Estimate" is replaced by "Coef".

```
Residual Standard Error=2.8284 = sqrt(MSE)
R-Square=0.9763 F-statistic (df=7, 8)=47.0536 p-value=0

          Estimate Std.Err t-value Pr(>|t|)
Intercept    64.25  0.7071 90.8632   0.0000
x1           11.50  0.7071 16.2635   0.0000
x2           -2.50  0.7071 -3.5355   0.0077
x3            0.75  0.7071  1.0607   0.3198
x12           0.75  0.7071  1.0607   0.3198
x13           5.00  0.7071  7.0711   0.0001
x23           0.00  0.7071  0.0000   1.0000
x123          0.25  0.7071  0.3536   0.7328
```

c) i) The least squares coefficient or "estimate" = effect/2. So in the above table, the A effect = 2(11.5) = 23. If $\boldsymbol{x}$ corresponds to the least squares coefficient, then the coefficient = $(\boldsymbol{x}^T \boldsymbol{y})/(\boldsymbol{x}^T \boldsymbol{x})$.

ii) The sum of squares = means square corresponding to an x is equal to the sum of squares = mean square of the corresponding effect. If $\boldsymbol{x}$ corresponds to the least squares coefficient, then the SS = MS = $(\boldsymbol{x}^T\boldsymbol{y})^2/(\boldsymbol{x}^T\boldsymbol{x})$.

iii) Suppose $m \geq 2$. Then SE(coef) = SE(effect)/2 = $0.5\sqrt{MSE/(m2^{k-2})}$. Hence in the above table, SE(effect) = 2(.7071) = 1.412.

iv) The t statistic t_0 = coef/SE(coef), and $t_0^2 = F_0$ where $t_0 \approx t_{df_e}$ and $F_0 \approx F_{1,df_e}$ where $df_e = (m-1)2^k$ is the MSE df. Hence the pvalues for least squares and the 2^k software are the same. For example, the pvalue for testing the significance of x_1 = pvalue for testing significance of A effect = 0.000 in the above table. Also $t_A = 16.2635$ and $t_A^2 = F_A = 264.501$.

v) The MSE, fitted values and residuals are the same for the least squares output and the 2^k software.

Suppose the two levels of the quantitative variable are $a < b$ and x is the actual value used. Then code x as $c \equiv c_x = \dfrac{2x-(a+b)}{b-a}$. Note that the code gives $c = -1$ for $x = a$ and $c = 1$ for $x = b$. Thus if the 2 levels are $a = 100$ and $b = 200$ but $x = 187$ is observed, then code x as $c = [2(187) - (100+200)]/[200-100] = 0.74$.

There are several advantages to least squares over 2^k software. The disadvantage of the following four points is that the design will no longer be orthogonal: the estimated coefficients $\hat{\beta}$ and hence the estimated effects will depend on the terms in the model. i) If there are several missing values or outliers, delete the corresponding rows from the design matrix $\boldsymbol{X}$ and the vector of responses $\boldsymbol{y}$ as long as the number of rows of the design matrix $\geq$ the number of columns. ii) If the exact quantitative levels are not observed, replace them by the observed levels c_x in the design matrix. iii) If the wrong levels are used in a run, replace the corresponding row in the design matrix by a row corresponding to the levels actually used. iv) The number of replications per run i can be m_i, that is, do not need $m_i \equiv m$.

Definition 8.9. A *normal QQ plot* is a plot of the effects versus standard normal percentiles. There are $L = 2^k - 1$ effects for a 2^k design.

Rule of thumb 8.5. The nonsignificant effects tend to follow a line closely in the middle of the plot while the significant effects do not follow the line closely. Significant effects will be the most negative or the most positive effects.

Know how to find the effect, the standard error of the effect, the sum of squares for an effect and a confidence interval for the effect from a table of contrasts using the following rules.

Let $\boldsymbol{c}$ be a column from the table of contrasts where $+ = 1$ and $- = -1$. Let $\overline{\boldsymbol{y}}$ be the column of cell means. Then the effect corresponding to $\boldsymbol{c}$ is

$$effect = \frac{\boldsymbol{c}^T \overline{\boldsymbol{y}}}{2^{k-1}}. \tag{8.1}$$

If the number of replications $m \geq 2$, then the standard error for the effect is

$$SE(effect) = \sqrt{\frac{MSE}{m2^{k-2}}}. \tag{8.2}$$

Sometimes MSE is replaced by $\hat{\sigma}^2$.

$$SE(mean) = \sqrt{\frac{MSE}{m2^k}} \tag{8.3}$$

where $m2^k = n$, $m \geq 2$ and sometimes MSE is replaced by $\hat{\sigma}^2$.

The sum of squares for an effect is also the mean square for the effect since $df = 1$.

$$MS(effect) = SS(effect) = m2^{k-2}(effect)^2 \tag{8.4}$$

for $m \geq 1$.

A 95% confidence interval (CI) for an effect is

$$effect \pm t_{df_e, 0.975}\ SE(\text{effect}) \tag{8.5}$$

where df_e is the MSE degrees of freedom. Use $t_{df_e, 0.975} \approx z_{0.975} = 1.96$ if $df_e > 30$. The effect is significant if the CI does not contain 0, while the effect is not significant if the CI contains 0.

Rule of thumb 8.6. Suppose there is no replication so $m = 1$. Find J interaction mean squares that are small compared to the bulk of the mean squares. Add them up to make MSE with $df_e = J$. So

$$MSE = \frac{\text{sum of small MS's}}{J}.$$

This method uses data snooping and MSE tends to underestimate σ^2. So the F test statistics are too large and the pvalues too small. *Use this method for exploratory data analysis, not for inference based on the F distribution.*

Rule of thumb 8.7. MS(effect) = SS(effect) $\approx \sigma^2 \chi^2_1 \approx MSE\chi^2_1$ if the effect is not significant. $MSE \approx \sigma^2 \chi^2_{df_e}/df_e$ if the model holds. A rule of thumb is that an effect is significant if MS $> 5MSE$. The rule comes from the fact that $\chi^2_{1,0.975} \approx 5$.

Below is the Anova table for a 2^3 design. Suppose $m = 1$. For A, use $H_0 : \mu_{100} = \mu_{200}$. For B, use $H_0 : \mu_{010} = \mu_{020}$. For C, use $H_0 : \mu_{001} = \mu_{002}$. For interaction, use H_0 : no interaction. If $m > 1$, the subscripts need an additional 0, eg $H_0 : \mu_{1000} = \mu_{2000}$.

Source	df	SS	MS	F	p-value
A	1	SSA	MSA	F_A	p_A
B	1	SSB	MSB	F_B	p_B
C	1	SSC	MSC	F_C	p_C
AB	1	SSAB	MSAB	F_{AB}	p_{AB}
AC	1	SSAC	MSAC	F_{AC}	p_{AC}
BC	1	SSBC	MSBC	F_{BC}	p_{BC}
ABC	1	SSABC	MSA	F_{ABC}	p_{ABC}
Error	$(m-1)2^k$	SSE	MSE		

Following Rule of thumb 8.6, if $m = 1$, pool J interaction mean squares that are small compared to the bulk of the data into an MSE with $df_e = J$. Such tests are for exploratory purposes only: the MSE underestimates σ^2, so the F test statistics are too large and the pvalues = $P(F_{1,J} > F_0)$ are too small. For example $F_0 = F_A = MSA/MSE$. As a convention for using an F table, use the denominator df closest to $df_e = J$, but if $df_e = J > 30$ use denominator df = ∞.

Below is the Anova table for a 2^k design. For A, use $H_0 : \mu_{10\cdots0} = \mu_{20\cdots0}$. The other main effect have similar null hypotheses. For interaction, use H_0 : no interaction. If $m = 1$ use a procedure similar to Rule of Thumb 8.6 for exploratory purposes.

One can use t statistics for effects with $t_0 = \dfrac{\text{effect}}{SE(effect)} \approx t_{df_e}$ where df_e is the MSE df. Then $t_0^2 = MS(effect)/MSE = F_0 \approx F_{1,df_e}$.

Source	df	SS MS	F	p-value
k main effects	1	eg SSA = MSA	F_A	p_A
$\binom{k}{2}$ 2 factor interactions	1	eg SSAB = MSAB	F_{AB}	p_{AB}
$\binom{k}{3}$ 3 factor interactions	1	eg SSABC = MSABC	F_{ABC}	p_{ABC}
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
$\binom{k}{k-1}$ $k-1$ factor interactions				
the k factor interaction	1	SSA$\cdots$L = MSA$\cdots$L	$F_{A\cdots L}$	$p_{A\cdots L}$
Error	$(m-1)2^k$	SSE MSE		

	I	A	B	C	AB	AC	BC	ABC	$\overline{\boldsymbol{y}}$
	+	−	−	−	+	+	+	−	6.333
	+	+	−	−	−	−	+	+	4.667
	+	−	+	−	−	+	−	+	9.0
	+	+	+	−	+	−	−	−	6.667
	+	−	−	+	+	−	−	+	4.333
	+	+	−	+	−	+	−	−	2.333
	+	−	+	+	−	−	+	−	7.333
	+	+	+	+	+	+	+	+	4.667
divisor	8	4	4	4	4	4	4	4	

Example 8.4. Box, Hunter and Hunter (2005, p. 189) describes a 2^3 experiment designed to investigate the effects of planting depth (0.5 or 1.4 in.), watering (once or twice daily) and type of lima bean (baby or large) on yield. The table of contrasts is shown above. The number of replications $m = 3$.

a) Find the A effect.
b) Find the AB effect.
c) Find SSA = MSA.
d) Find SSAB = MSAB.
e) If MSE = 0.54, find SE(effect).

Solution: a) The A effect =

$$\frac{-6.333 + 4.667 - 9 + 6.667 - 4.333 + 2.333 - 7.333 + 4.667}{4} = -8.665/4$$

$= -2.16625$. Note that the appropriate + and − signs are obtained from the A column.

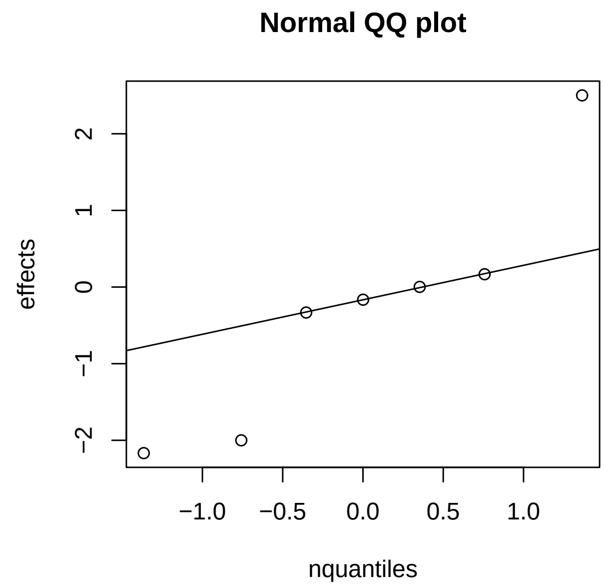

Figure 8.1: QQ plot for Example 8.4

b) The AB effect =

$$\frac{6.333 - 4.667 - 9 + 6.667 + 4.333 - 2.333 - 7.333 + 4.667}{4} = -1.333/4$$

$= -0.33325.$

c) $SSA = m2^{k-2}(effect)^2 = 3(2)(-2.16625)^2 = 28.1558.$

d) $SSAB = 6(effect)^2 = 6(-0.33325)^2 = 0.6663.$

e)

$$SE(effect) = \sqrt{\frac{MSE}{m2^{k-2}}} = \sqrt{\frac{0.54}{3(2)}} = \sqrt{0.09} = 0.3.$$

The `regpack` functions `twocub` and `twofourth` can be used to find the effects, SE(effect), and QQ plots for 2^3 and 2^4 designs. The `twofourth` function also makes the response and residual plots based on the second order model for 2^4 designs.

For the data in Example 8.4, the output on the following page shows that the A and C effects have values -2.166 and -2.000 while the B effect is

2.500. These are the three significant effects shown in the QQ plot in Figure 8.1. The two commands below produced the output.

```
z<-c(6.333,4.667,9,6.667,4.333,2.333,7.333,4.667)
twocub(z,m=3,MSE=0.54)

$Aeff
[1] -2.16625
$Beff
[1] 2.50025
$Ceff
[1] -2.00025
$ABeff
[1] -0.33325
$ACeff
[1] -0.16675
$BCeff
[1] 0.16675
$ABCeff
[1] 0.00025
$MSA
[1] 28.15583
$MSB
[1] 37.5075
$MSC
[1] 24.006
$MSAB
[1] 0.6663334
$MSAC
[1] 0.1668334
$MSABC
[1] 3.75e-07
$MSE
[1] 0.54
$SEeff
[1] 0.3
```

8.2 Fractional Factorial Designs

Definition 8.10. A 2_R^{k-f} **fractional factorial design** has k factors and takes $m2^{k-f}$ runs where the number of replications m is usually 1. The design is an orthogonal design and each factor has two levels low $= -1$ and high $= 1$. R is the **resolution** of the design.

Definition 8.11. A main effect or q factor interaction is **confounded** or **aliased** with another effect if it is not possible to distinguish between the two effects.

Remark 8.2. A 2_R^{k-f} design has no q factor interaction (or main effect for $q = 1$) confounded with any other effect consisting of less than $R - q$ factors. So a 2_{III}^{k-f} design has $R = 3$ and main effects are confounded with 2 factor interactions. In a 2_{IV}^{k-f} design, $R = 4$ and main effects are not confounded with 2 factor interactions but 2 factor interactions are confounded with other 2 factor interactions. In a 2_V^{k-f} design, $R = 5$ and main effects and 2 factor interactions are only confounded with 4 and 3 way or higher interactions respectively. The R = 4 and R = 5 designs are good because the 3 way and higher interactions are rarely significant, but these designs are more expensive than the R = 3 designs.

In a 2_R^{k-f} design, each effect is confounded or aliased with 2^{f-1} other effects. Thus the Mth main effect is really an estimate of the Mth main effect plus 2^{f-1} other effects. If $R \geq 3$ and none of the two factor interactions are significant, then the Mth main effect is typically a useful estimator of the population Mth main effect.

Rule of thumb 8.8. Main effects tend to be larger than q factor interaction effects, and the lower order interaction effects tend to be larger than the higher order interaction effects. So two way interaction effects tend to be larger than three way interaction effects.

Rule of thumb 8.9. Significant interactions tend to have significant component main effects. Hence if A, B, C and D are factors, B and D are inert and A and C are active, then the AC effect is the two factor interaction most likely to be active. If only A was active, then the two factor interactions containing A (AB, AC, and AD) are the ones most likely to be active.

Suppose each run costs \$1000 and $m = 1$. The 2^k factorial designs need 2^k runs while fractional factorial designs need 2^{k-f} runs. These designs use the fact that three way and higher interactions tend to be inert for experiments.

Remark 8.3. Let $k_o = k - f$. Some good fractional factorial designs for $k_o = 3$ are shown below. The designs shown use the same table of contrasts as the 2^3 design and can be fit with 2^3 software.

2^3	A	B	C	AB	AC	BC	ABC
2_{IV}^{4-1}	A	B	C	AB+	AC+	BC+	D
2_{III}^{5-2}	A	B	C	D	E	BC+	BE+
2_{III}^{6-3}	A	B	C	D	E	F	AF+
2_{III}^{7-4}	A	B	C	D	E	F	G

Consider the 2_{IV}^{4-1} design. It has 4 factors A, B, C and D. The D main effect is confounded with the ABC three way interaction, which is likely to be inert. The "D effect" is the D effect plus the ABC effect. But if the ABC effect is not significant, then the "D effect" is a good estimator of the population D effect. Confounding = aliasing is the price to pay for using fractional factorial desings instead of the more expensive factorial designs.

If $m = 1$, the 2_{IV}^{4-1}design uses 8 runs while a 2^4 factorial design uses 16 runs. The runs for the 2_{IV}^{4-1} are defined by the 4 main effects: use the first 3 columns and the last column of the table of contrasts for the 2^3 design to define the runs. Randomly assign the units (often time slots) to the runs.

Remark 8.4. Some good fractional factorial designs for $k_o = k - f = 4$ are shown below. The designs shown use the same table of contrasts as the 2^4 design and can be fit with 2^4 software. Here the designs are i) 2^4, and the fractional factorial designs ii) 2_V^{5-1}, iii) 2_{IV}^{6-2}, iv) 2_{IV}^{7-3}, v) 2_{IV}^{8-4}, vi) 2_{III}^{9-5} and vii) 2_{III}^{15-11}.

```
design
i)   A  B  C D  AB  AC  AD  BC  BD  CD  ABC  ABD  ACD  BCD ABCD
ii)  A  B  C D  AB  AC  AD  BC  BD  CD   DE   CE   BE   AE   E
iii) A  B  C D  AB+ AC+ AD+ BC+ BD+ CD+   E  3int 3int   F  AF+
iv)  A  B  C D  AB+ AC+ AD+ BC+ BD+ CD+   E  3int   F    G  AG+
v)   A  B  C D  AB+ AC+ AD+ BC+ BD+ CD+   E    F    G    H  AH+
vi)  A  B  C D  AB+ AC+ AD+ BC+ BD+ CD+   E    F    G    H   J
vii) A  B  C D   E   F   G   H   J   K    L    M    N    O   P
```

Remark 8.5. Let $k_o = k - f$ for a 2^{k-f}_R design. The QQ plot for 2^{k-f}_R designs is used in a manner similar to that of 2^k designs where $k = k_o$. The formulas for effects and mean squares are like the formulas for a 2^{k_o} design. Let $\boldsymbol{c}$ be a column from the table of contrasts where $+ = 1$ and $- = -1$. Let $\overline{\boldsymbol{y}}$ be the column of cell means. Need $MSE = \hat{\sigma}^2$ to be given or estimated by setting high order interactions to 0 for $m = 1$. Typically $m = 1$ for fractional factorial designs. The following formulas ignore the "I effect."

a) The effect corresponding to $\boldsymbol{c}$ is $effect = \dfrac{\boldsymbol{c}^T \overline{\boldsymbol{y}}}{2^{k_o-1}}$.

b) The standard error for the effect is $SE(effect) = \sqrt{\dfrac{MSE}{m2^{k_o-2}}}$.

c) $SE(mean) = \sqrt{\dfrac{MSE}{m2^{k_o}}}$ where $m2^{k_o} = n$.

d) The sum of squares and mean square for an effect are $MS(effect) = SS(effect) = m2^{k_o-2}(effect)^2$.

Consider the designs given in Remarks 8.3 and 8.4. Least squares estimates for the 2^{k-f}_R designs with $k_o = 3$ use the design matrix corresponding to a 2^3 design while the designs with $k_o = 4$ use the design matrix corresponding to the 2^4 design given in Section 8.1.

Randomly assign units to runs. Do runs in random order if possible. In industry, units are often time slots (periods of time), so randomization consists of randomly assigning time slots to units, which is equivalent to doing the runs in random order. For the above 2^{k-f}_R designs, fix the main effects using the corresponding columns in the two tables of contrasts given in Section 8.1 to determine the levels needed in the $m2^{k-f}$ runs.

The fractional factorial designs can be fit with least squares, and the model can be written as $Y = \boldsymbol{x}^T\boldsymbol{\beta} + e$ with least squares fitted values $\hat{Y} = \boldsymbol{x}^T\hat{\boldsymbol{\beta}}$. In matrix form the model is $\boldsymbol{Y} = \boldsymbol{X\beta} + \boldsymbol{e}$ and the vector of fitted values is $\hat{\boldsymbol{Y}} = \boldsymbol{X}\hat{\boldsymbol{\beta}}$.

The biggest possible model for a 2^{k-f}_R design where $k - f = 3$ is $Y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \beta_3 x_{i3} + \beta_{12} x_{i12} + \beta_{13} x_{i13} + \beta_{23} x_{i23} + \beta_{123} x_{i123} + e_i$ with least squares fitted or predicted values given by $\hat{Y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_{i1} + \hat{\beta}_2 x_{i2} + \hat{\beta}_3 x_{i3} + \hat{\beta}_{12} x_{i12} + \hat{\beta}_{13} x_{i13} + \hat{\beta}_{23} x_{i23} + \hat{\beta}_{123} x_{i123}$.

The regression equation corresponding to the significant effects (eg found with a QQ plot) can be used to form a reduced model. For example, suppose the full (least squares) fitted model is $\hat{Y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_{i1} + \hat{\beta}_2 x_{i2} + \hat{\beta}_3 x_{i3} + \hat{\beta}_{12} x_{i12} +$

$\hat{\beta}_{13} x_{i13} + \hat{\beta}_{23} x_{i23} + \hat{\beta}_{123} x_{i123}$. Suppose the A, B and AB effects are significant. Then the reduced (least squares) fitted model is $\hat{Y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_{i1} + \hat{\beta}_2 x_{i2} + \hat{\beta}_{12} x_{i12}$ where the coefficients ($\hat{\beta}$'s) for the reduced model can be taken from the full model since fractional factorial designs are orthogonal.

For the fractional factorial designs, the coefficient $\hat{\beta}_0$ corresponding to I is equal to the I effect, but the coefficient of a factor x corresponding to an *effect* is $\hat{\beta} = 0.5$ *effect*. Consider significant effects and assume interactions can be ignored.

i) If a large response Y is desired and $\hat{\beta} > 0$, use $x = 1$. If $\hat{\beta} < 0$, use $x = -1$.

ii) If a small response Y is desired and $\hat{\beta} > 0$, use $x = -1$. If $\hat{\beta} < 0$, use $x = 1$.

From the regression equation $\hat{Y} = \boldsymbol{x}^T \hat{\boldsymbol{\beta}}$, be able to predict Y given $\boldsymbol{x}$. Be able to tell whether $x = 1$ or $x = -1$ should be used. Given the x values of the main effects, get the x values of the interactions by multiplying the columns corresponding to the main effects in the interaction. Least squares output is similar to that in Section 8.1. The least squares coefficient = 0.5 (effect). The sum of squares for an x corresponding to an effect is equal to SS(effect). SE(coef) = SE($\hat{\beta}$) = 0.5 SE(effect) = $\sqrt{MSE/n}$. Also SE($\hat{\beta}_0$) = $\sqrt{MSE/n}$.

Assume none of the interactions are significant. Then the 2^{7-4}_{III} fractional factorial design allows estimation of 7 main effects in $2^3 = 8$ runs. The 2^{15-11}_{III} fractional factorial design allows estimation of 15 main effects in $2^4 = 16$ runs. The 2^{31-26}_{III} fractional factorial design allows estimation of 31 main effects in $2^5 = 32$ runs.

Fractional factorial designs with $k - f = k_o$ can be fit with software meant for 2^{k_o} designs. Hence the `regpack` functions `twocub` and `twofourth` can be used for the $k_o = 3$ and $k_o = 4$ designs that use the standard table of contrasts. The response and residual plots given by `twofourth` are not appropriate, but the QQ plot and the remaining output is relevant. Some of the interactions will correspond to main effects for the fractional factorial design.

For example, if the Example 8.4 data was from a 2^{4-1}_{IV} design, then the A, B and C effects would be the same, but the D effect is the effect labelled ABC. So the D effect ≈ 0.

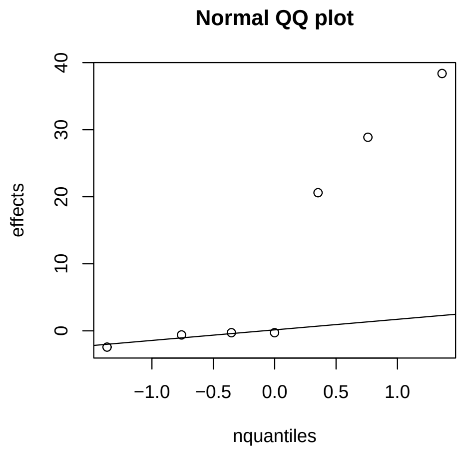

Figure 8.2: QQ plot for Example 8.5

```
Aeff   Beff   Ceff   ABeff  ACeff  BCeff  ABCeff
20.625 38.375 -0.275 28.875 -0.275 -0.625 -2.425
```

Example 8.5. Montgomery (1984, p 344-346) gives data from a 2^{7-4}_{III} design with the QQ plot shown in Figure 8.2. The goal was to study eye focus time with factors A = sharpness of vision, B = distance of target from eye, C = target shape, D = illumination level, E = target size, F = target density and G = subject. The R function `twocub` gave the effects above.

a) What is the D effect?

b) What effects are significant?

Solution: By the last line in the table given in Remark 8.3, note that for this design, A, B, C, AB, AC, BC, ABC correspond to A, B, C, D, E, F, G. So the AB effect from the output is the D effect.

a) 28.875, since the D effect is the AB effect.

b) A, B and D since these are the effects that do not follow the line in the QQ plot shown in Figure 8.2.

I	A	B	C	AB	AC	BC	ABC	y
+	−	−	−	+	+	+	−	86.8
+	+	−	−	−	−	+	+	85.9
+	−	+	−	−	+	−	+	79.4
+	+	+	−	+	−	−	−	60.0
+	−	−	+	+	−	−	+	94.6
+	+	−	+	−	+	−	−	85.4
+	−	+	+	−	−	+	−	84.5
+	+	+	+	+	+	+	+	80.3

Example 8.6. The above table of 2^3 contrasts is for 2^{5-2}_{III} data.
a) Estimate the B effect.
b) Estimate the D effect.
Solution: a)

$$\frac{-86.8 - 85.9 + 79.4 + 60 - 94.6 - 85.4 + 84.5 + 80.3}{4}$$

$= -48.5/4 = -12.125.$

b) Use Remark 8.3 to see that the D effect corresponds to the ABC column. So the D effect =

$$\frac{86.8 - 85.9 - 79.4 + 60 + 94.6 - 85.4 - 84.5 + 80.3}{4}$$

$= -13.5/4 = -3.375.$

8.3 Plackett Burman Designs

Definition 8.12. The *Plackett Burman PB(n) designs* have k factors where $2 \leq k \leq n-1$. The factors have 2 levels and orthogonal contrasts like the 2^k and 2^{k-f}_R designs. The PB(n) designs are resolution 3 designs, but the confounding of main effects with 2 factor interactions is complex. The PB(n) designs use n runs where n is a multiple of 4. The values $n = 12, 20, 24, 28$ and 36 are especially common.

Fractional factorial designs need at least 2^{k_o} runs. Hence if there are 17 main effects, 32 runs are needed for a 2^{17-12}_{III} design while a PB(20) design only needs 20 runs. The price to pay is that the confounding pattern of the main effects with the two way interactions is complex. Thus the PB(n) designs are usually used with main effects, and it is assumed that all interactions are insignificant. So the Plackett Burman designs are main effects designs used to screen k main effects when the number of runs n is small. Often $k = n - 4, n - 3, n - 2$ or $n - 1$ is used. We will assume that the number of replications $m = 1$.

A contrast matrix for the PB(12) design is shown below. Again the column of plusses corresponding to I is omitted. If $k = 8$ then effects A to H are used but effects J, K and L are "empty." As a convention the mean square and sum of squares for factor E will be denoted as MSe and SSe while MSE $= \hat{\sigma}^2$.

run	A	B	C	D	E	F	G	H	J	K	L
1	+	−	+	−	−	−	+	+	+	−	+
2	+	+	−	+	−	−	−	+	+	+	−
3	−	+	+	−	+	−	−	−	+	+	+
4	+	−	+	+	−	+	−	−	−	+	+
5	+	+	−	+	+	−	+	−	−	−	+
6	+	+	+	−	+	+	−	+	−	−	−
7	−	+	+	+	−	+	+	−	+	−	−
8	−	−	+	+	+	−	+	+	−	+	−
9	−	−	−	+	+	+	−	+	+	−	+
10	+	−	−	−	+	+	+	−	+	+	−
11	−	+	−	−	−	+	+	+	−	+	+
12	−	−	−	−	−	−	−	−	−	−	−

The PB(n) designs are k factor 2 level orthogonal designs. So finding effects, MS, SS, least squares estimates et cetera for PB(n) designs is similar to finding the corresponding quantities for the 2^k and 2_R^{k-f} designs. Randomize units (often time slots) to runs and least squares can be used.

Remark 8.6. For the PB(n) design, let $\boldsymbol{c}$ be a column from the table of contrasts where $+ = 1$ and $- = -1$. Let $\boldsymbol{y}$ be the column of responses since $m = 1$. If $k < n - 1$, pool the last $J = n - 1 - k$ "empty" effects into the MSE with $df = J$ as the full model. This procedure is done before looking at the data, so is not data snooping. The MSE can also be given or found by pooling insignificant MS's into the MSE, but the latter method uses data snooping. This pooling needs to be done if $k = n - 1$ since then there is no df for MSE. The following formulas ignore the I effect.

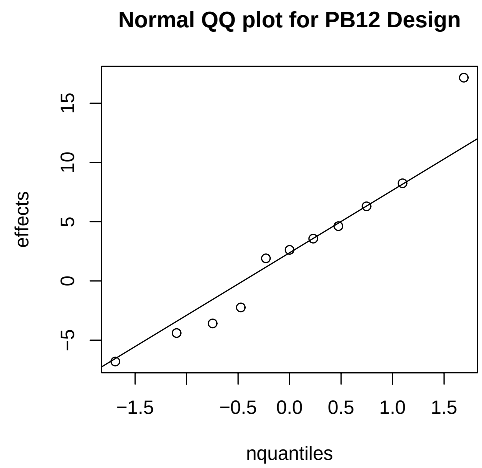

Figure 8.3: QQ Plot for Example 8.7

a) The effect corresponding to $\boldsymbol{c}$ is $effect = \dfrac{\boldsymbol{c}^T\boldsymbol{y}}{n/2} = \dfrac{2\boldsymbol{c}^T\boldsymbol{y}}{n}$.

b) The standard error for the effect is $SE(effect) = \sqrt{\dfrac{MSE}{n/4}} = \sqrt{\dfrac{4MSE}{n}}$.

c) $SE(mean) = \sqrt{\dfrac{MSE}{n}}$.

d) The sum of squares and mean sum of squares for an effect is $MS(effect) = SS(effect) = \dfrac{n}{4}(effect)^2$.

For the PB(n) design, the least squares coefficient = 0.5 (effect). The sum of squares for an x corresponding to an effect is equal to SS(effect). SE(coef) = SE($\hat{\beta}$) = 0.5 SE(effect) = $\sqrt{MSE/n}$. Also SE($\hat{\beta}_0$) = $\sqrt{MSE/n}$.

Example 8.7. On the following page is least squares output using PB(12) data from Ledolter and Swersey (2007, p. 244-256). There were $k = 10$ factors so the MSE has 1 df and there are too many terms in the model. In this case the QQ plot shown in Figure 8.7 is more reliable for finding significant effects.

a) Which effects, if any, appear to be significant from the QQ plot?

b) Let the reduced model $\hat{Y} = \hat{\beta}_0 + \hat{\beta}_{r1}x_{r1} + \cdots + \hat{\beta}_{rj}x_{rj}$ where j is the number of significant terms found in a). Write down the reduced model.

c) Want large Y. Using the model in b), choose the x values that will give large Y, and predict Y.

```
          Estimate Std.Err t-value Pr(>|t|)
Intercept   6.7042  2.2042  3.0416   0.2022
c1          8.5792  2.2042  3.8922   0.1601
c2         -1.7958  2.2042 -0.8147   0.5648
c3          2.3125  2.2042  1.0491   0.4847
c4          4.1208  2.2042  1.8696   0.3127
c5          3.1542  2.2042  1.4310   0.3883
c6         -3.3958  2.2042 -1.5406   0.3665
c7          0.9542  2.2042  0.4329   0.7399
c8         -1.1208  2.2042 -0.5085   0.7005
c9          1.3125  2.2042  0.5955   0.6581
c10         1.7875  2.2042  0.8110   0.5662
```

Solution: a) The most significant effects are either in the top right or bottom left corner. Although the points do not all scatter closely about the line, the point in the bottom left is not significant. So none of the effects corresponding to the bottom left of the plot are significant. A is the significant effect with value $2(8.5792) = 17.1584$. See the top right point of Figure 8.7.

b) $\hat{Y} = 6.7042 + 8.5792x_1$.

c) $\hat{Y} = 6.7042 + 8.5792(1) = 15.2834$.

The `regpack` function `pb12` can be used to to find effects and MS(effect) for PB(12) data. Least squares output and a QQ plot are also given.

8.4 Summary

1) In a table of contrasts, the contrast for A starts with a $-$ then a $+$ and the pattern repeats. The contrast for B starts with 2 $-$'s and then 2 $+$'s and the pattern repeats. The contrast for C starts with 4 $-$'s and then 4$+$'s and the pattern repeats. The contrast for the ith main effects factor starts with 2^{i-1} $-$'s and 2^{i-1} $+$'s and the pattern repeats for $i = 1, ..., k$.

2) In a table of contrasts, a column for an interaction containing several factors is obtained by multiplying the columns for each factor where $+ = 1$

and $- = -1$. So the column for ABC is obtained by multiplying the column for A, the column for B and the column for C.

3) Let $\boldsymbol{c}$ be a column from the table of contrasts where $+ = 1$ and $- = -1$. Let $\overline{\boldsymbol{y}}$ be the column of cell means. Then the effect corresponding to $\boldsymbol{c}$ is $effect = \dfrac{\boldsymbol{c}^T\overline{\boldsymbol{y}}}{2^{k-1}}$.

4) If the number of replications $m \geq 2$, then the standard error for the effect is

$$SE(effect) = \sqrt{\frac{MSE}{m2^{k-2}}}.$$

Sometimes MSE is replaced by $\hat{\sigma}^2$.

5)

$$SE(mean) = \sqrt{\frac{MSE}{m2^k}}$$

where $m2^k = n$, $m \geq 2$ and sometimes MSE is replaced by $\hat{\sigma}^2$.

6) Since $df = 1$, the sum of squares and mean square for an effect is

$$MS(effect) = SS(effect) = m2^{k-2}(effect)^2$$

for $m \geq 1$.

7) If a single run out of 2^k cells gives good values for the response, then that run is called a critical mix.

8) A factor is active if the response depends on the two levels of the factor, and is inert, otherwise.

9) Randomization for a 2^k design: randomly assign units to the $m2^k$ runs. The runs are determined by the levels of the k main effects in the table of contrasts. So a 2^3 design is determined by the levels of A, B and C. Similarly, a 2^4 design is determined by the levels of A, B, C and D. Perform the $m2^k$ runs in random order if possible.

10) A table of contrasts for a 2^3 design is shown on the following page. The first column is for the mean and is not a contrast. The last column corresponds to the cell means. Note that $\overline{y}_{1110} = y_{111}$ if $m = 1$. So $\overline{\boldsymbol{y}}$ might be replaced by $\boldsymbol{y}$ if $m = 1$.

	I	A	B	C	AB	AC	BC	ABC	$\overline{\boldsymbol{y}}$
	+	−	−	−	+	+	+	−	$\overline{y}_{1110}$
	+	+	−	−	−	−	+	+	$\overline{y}_{2110}$
	+	−	+	−	−	+	−	+	$\overline{y}_{1210}$
	+	+	+	−	+	−	−	−	$\overline{y}_{2210}$
	+	−	−	+	+	−	−	+	$\overline{y}_{1120}$
	+	+	−	+	−	+	−	−	$\overline{y}_{2120}$
	+	−	+	+	−	−	+	−	$\overline{y}_{1220}$
	+	+	+	+	+	+	+	+	$\overline{y}_{2220}$
divisor	8	4	4	4	4	4	4	4	

11) Be able to pick out active and inert factors and good (or the best) combinations of factors (cells or runs) from the table of contrasts = table of runs.

12) Plotted points far away from the identity line and $r = 0$ line are potential outliers, but often the identity line goes through or near an outlier that is large in magnitude. Then the case has a small residual.

13) A 95% confidence interval (CI) for an effect is

$$\text{effect} \pm \text{t}_{\text{df}_\text{e},0.975}\text{SE(effect)}$$

where df_e is the MSE degrees of freedom. Use $t_{df_e,0.975} \approx z_{0.975} = 1.96$ if $df_e > 30$. The effect is significant if the CI does not contain 0, while the effect is not significant if the CI contains 0.

14) Suppose there is no replication so $m = 1$. Find J interaction mean squares that are small compared to the bulk of the mean squares. Add them up to make MSE with $df_e = J$. So

$$MSE = \frac{\text{sum of small MS's}}{J}.$$

This method uses data snooping and MSE tends to underestimate σ^2. So the F test statistics are too large and the pvalues too small. *Use this method for exploratory data analysis, not for inference based on the F distribution.*

15) MS = SS $\approx \sigma^2\chi^2_1 \approx MSE\chi^2_1$ if the effect is not significant. $MSE \approx \sigma^2\chi^2_{df_e}/df_e$ if the model holds. A rule of thumb is that an effect is significant if MS $> 5MSE$. The rule comes from the fact that $\chi^2_{1,.975} \approx 5$.

16) The table of contrasts for a 2^4 design is below. The column of ones corresponding to I was omitted.

run	A	B	C	D	AB	AC	AD	BC	BD	CD	ABC	ABD	ACD	BCD	ABCD
1	−	−	−	−	+	+	+	+	+	+	−	−	−	−	+
2	+	−	−	−	−	−	−	+	+	+	+	+	+	−	−
3	−	+	−	−	−	+	+	−	−	+	+	+	−	+	−
4	+	+	−	−	+	−	−	−	−	+	−	−	+	+	+
5	−	−	+	−	+	−	+	−	+	−	+	−	+	+	−
6	+	−	+	−	−	+	−	−	+	−	−	+	−	+	+
7	−	+	+	−	−	−	+	+	−	−	−	+	+	−	+
8	+	+	+	−	+	+	−	+	−	−	+	−	−	−	−
9	−	−	−	+	+	+	−	+	−	−	−	+	+	+	−
10	+	−	−	+	−	−	+	+	−	−	+	−	−	+	+
11	−	+	−	+	−	+	−	−	+	−	+	−	+	−	+
12	+	+	−	+	+	−	+	−	+	−	−	+	−	−	−
13	−	−	+	+	+	−	−	−	−	+	+	+	−	−	+
14	+	−	+	+	−	+	+	−	−	+	−	−	+	−	−
15	−	+	+	+	−	−	−	+	+	+	−	−	−	+	−
16	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+

17) Below is the Anova table for a 2^3 design. Let $m = 1$. For A, use $H_0 : \mu_{100} = \mu_{200}$. For B, use $H_0 : \mu_{010} = \mu_{020}$. For C, use $H_0 : \mu_{001} = \mu_{002}$. For interaction, use H_0 : no interaction.

Source	df	SS	MS	F	p-value
A	1	SSA	MSA	F_A	p_A
B	1	SSB	MSB	F_B	p_B
C	1	SSC	MSC	F_C	p_C
AB	1	SSAB	MSAB	F_{AB}	p_{AB}
AC	1	SSAC	MSAC	F_{AC}	p_{AC}
BC	1	SSBC	MSBC	F_{BC}	p_{BC}
ABC	1	SSABC	MSA	F_{ABC}	p_{ABC}
Error	$(m-1)2^k$	SSE	MSE		

18) If $m = 1$, pool J interaction mean squares that are small compared to the bulk of the data into an MSE with $df_e = J$. Such tests are for exploratory purposes only: the MSE underestimates σ^2, so the F test statistics are too large and the pvalues $= P(F_{1,J} > F_0)$ are too small. For example $F_0 = F_A =$

MSA/MSE. As a convention for using an F table, use the denominator df closest to $df_e = J$, but if $df_e = J > 30$ use denominator df $= \infty$.

19) Below is the Anova table for a 2^k design. For A, use $H_0 : \mu_{10\cdots 0} = \mu_{20\cdots 0}$. The other main effect have similar null hypotheses. For interaction, use H_0 : no interaction. If $m = 1$ use a procedure similar to point 18) for exploratory purposes.

Source	df	SS MS	F p-value
k main effects	1	eg SSA = MSA	F_A p_A
$\binom{k}{2}$ 2 factor interactions	1	eg SSAB = MSAB	F_{AB} p_{AB}
$\binom{k}{3}$ 3 factor interactions	1	eg SSABC = MSABC	F_{ABC} p_{ABC}
⋮	⋮	⋮	⋮ ⋮
$\binom{k}{k-1}$ $k-1$ factor interactions			
the k factor interaction	1	SSA$\cdots$L = MSA$\cdots$L	$F_{A\cdots L}$ $p_{A\cdots L}$
Error	$(m-1)2^k$	SSE MSE	

20) Genuine run replicates need to be used. A common error is to take m measurements per run, and act as if the m measurements are from m runs. If as a data analyst you encounter this error, average the m measurements into a single value of the response.

21) One can use t statistics for effects with $t_0 = \dfrac{\text{effect}}{SE(effect)} \approx t_{df_e}$ where df_e is the MSE df. Then $t_0^2 = MS(effect)/MSE = F_0 \approx F_{1,df_e}$.

22) A 2^k design can be fit with least squares. In the table of contrasts let a "+ = 1" and a "$-$ = $-$1." Need a row for each response: can't use the mean response for each fixed combination of levels. Let $\boldsymbol{x}_0$ correspond to I, the column of 1s. Let $\boldsymbol{x}_i$ correspond to the ith main effect for $i = 1, ..., k$. Let $\boldsymbol{x}_{ij}$ correspond to 2 factor interactions, and let $\boldsymbol{x}_{i_1,...,i_G}$ correspond to G way interactions for $G = 2, ..., k$. Let the design matrix X have columns corresponding to the $\boldsymbol{x}$. Let $\boldsymbol{y}$ be the vector of responses.

23) The table below relates the quantities in the 2^3 table of contrasts with the quantities used in least squares. The design matrix

$$\boldsymbol{X} = [\boldsymbol{x}_0, \boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3, \boldsymbol{x}_{12}, \boldsymbol{x}_{13}, \boldsymbol{x}_{23}, \boldsymbol{x}_{123}].$$

Software often does not need the column of ones $\boldsymbol{x}_0$.

$\boldsymbol{x}_0$	$\boldsymbol{x}_1$	$\boldsymbol{x}_2$	$\boldsymbol{x}_3$	$\boldsymbol{x}_{12}$	$\boldsymbol{x}_{13}$	$\boldsymbol{x}_{23}$	$\boldsymbol{x}_{123}$	$\boldsymbol{y}$
I	A	B	C	AB	AC	BC	ABC	$\boldsymbol{y}$

24) The table below relates quantities in the 2^4 table of contrasts with the quantities used in least squares. Again $\boldsymbol{x}_0$ corresponds to I, the column of ones, while $\boldsymbol{y}$ is the vector of responses.

$\boldsymbol{x}_1$	$\boldsymbol{x}_2$	$\boldsymbol{x}_3$	$\boldsymbol{x}_4$	$\boldsymbol{x}_{12}$	$\boldsymbol{x}_{13}$	$\boldsymbol{x}_{14}$	$\boldsymbol{x}_{23}$	$\boldsymbol{x}_{24}$	$\boldsymbol{x}_{34}$	$\boldsymbol{x}_{123}$	$\boldsymbol{x}_{124}$	$\boldsymbol{x}_{134}$	$\boldsymbol{x}_{234}$	$\boldsymbol{x}_{1234}$
A	B	C	D	AB	AC	AD	BC	BD	CD	ABC	ABD	ACD	BCD	ABCD

25) A typical least squares output for the 2^3 design is shown below. Often "Estimate" is replaced by "Coef".

```
          Estimate Std.Err t-value Pr(>|t|)
Intercept    64.25  0.7071 90.8632   0.0000
x1           11.50  0.7071 16.2635   0.0000
x2           -2.50  0.7071 -3.5355   0.0077
x3            0.75  0.7071  1.0607   0.3198
x12           0.75  0.7071  1.0607   0.3198
x13           5.00  0.7071  7.0711   0.0001
x23           0.00  0.7071  0.0000   1.0000
x123          0.25  0.7071  0.3536   0.7328
```

26) i) The least squares coefficient or "estimate" = effect/2. So in the above table, the A effect = 2(11.5) = 23. If $\boldsymbol{x}$ corresponds to the least squares coefficient, then the coefficient = $(\boldsymbol{x}^T\boldsymbol{y})/(\boldsymbol{x}^T\boldsymbol{x})$.

ii) The sum of squares = means square corresponding to an $x_{i\cdots}$ is equal to the sum of squares = mean square of the corresponding effect. If $\boldsymbol{x}$ corresponds to the least squares coefficient, then the SS = MS = $(\boldsymbol{x}^T\boldsymbol{y})^2/(\boldsymbol{x}^T\boldsymbol{x})$.

iii) Suppose $m \geq 2$. Then SE(coef) = SE(effect)/2 = $0.5\sqrt{MSE/(m2^{k-2})}$. Hence in the above table, SE(effect) = 2(.7071) = 1.412.

iv) The t statistic t_0 = coef/SE(coef), and $t_0^2 = F_0$ where $t_0 \approx t_{df_e}$ and $F_0 \approx F_{1,df_e}$ where $df_e = (m-1)2^k$ is the MSE df. Hence the pvalues for least squares and the 2^k software are the same. For example, the pvalue for testing the significance of x_1 = pvalue for testing significance of A effect = 0.000 in the above table. Also $t_A = 16.2635$ and $t_A^2 = F_A = 264.501$.

v) The MSE, fitted values and residuals are the same for the least squares output and the 2^k software.

27) There are several advantages to least squares over 2^k software. i) If there are several missing values or outliers, delete the corresponding rows from the design matrix $\boldsymbol{X}$ and the vector of responses $\boldsymbol{y}$ as long as the number of rows of the design matrix $\geq$ the number of columns. ii) If the exact quantitative levels are not observed, replace them by the observed levels in

the design matrix. See point 28). iii) If the wrong levels are used in a run, replace the corresponding row in the design matrix by a row corresponding to the levels actually used.

28) Suppose the two levels of the quantitative variable are $a < b$ and x is the actual value used. Then code x as $c = \dfrac{2x - (a+b)}{b-a}$. Note that the code gives $c = -1$ for $x = a$ and $c = 1$ for $x = b$.

29) A normal QQ plot is a plot of the effects versus standard normal percentiles. There are $L = 2^k - 1$ effects for a 2^k design. A rule of thumb is that nonsignificant effects tend to follow a line closely in the middle of the plot while the significant effects do not follow the line closely. Significant effects will be the most negative or the most positive effects.

30) A 2_R^{k-f} *fractional factorial design* has k factors and takes $m2^{k-f}$ runs where the number of replications m is usually 1.

31) Let $k_o = k - f$. Some good fractional factorial designs for $k_o = 3$ are shown below. The designs shown use the same table of contrasts as the 2^3 design given in point 10), and can be fit with 2^3 software.

2^3	A	B	C	AB	AC	BC	ABC
2_{IV}^{4-1}	A	B	C	AB+	AC+	BC+	D
2_{III}^{5-2}	A	B	C	D	E	BC+	BE+
2_{III}^{6-3}	A	B	C	D	E	F	AF+
2_{III}^{7-4}	A	B	C	D	E	F	G

32) Some good fractional factorial designs for $k_o = k - f = 4$ are shown below. The designs shown use the same table of contrasts as the 2^4 design given in point 16), and can be fit with 2^4 software. Here the designs are i) 2^4, and the fractional factorial designs ii) 2_V^{5-1}, iii) 2_{IV}^{6-2}, iv) 2_{IV}^{7-3}, v) 2_{IV}^{8-4}, vi) 2_{III}^{9-5} and vii) 2_{III}^{15-11}.

```
design
i)    A  B  C D  AB  AC  AD  BC  BD  CD  ABC  ABD  ACD  BCD ABCD
ii)   A  B  C D  AB  AC  AD  BC  BD  CD   DE   CE   BE   AE   E
iii)  A  B  C D  AB+ AC+ AD+ BC+ BD+ CD+   E  3int 3int   F  AF+
iv)   A  B  C D  AB+ AC+ AD+ BC+ BD+ CD+   E  3int   F    G  AG+
v)    A  B  C D  AB+ AC+ AD+ BC+ BD+ CD+   E    F    G    H  AH+
vi)   A  B  C D  AB+ AC+ AD+ BC+ BD+ CD+   E    F    G    H   J
vii)  A  B  C D   E   F   G   H   J   K    L    M    N    O   P
```

33) Let $k_o = k - f$ for a 2_R^{k-f} design. Then the formulas for effects and mean squares are like the formulas for a 2^{k_o} design. Let $\boldsymbol{c}$ be a column from the table of contrasts where $+ = 1$ and $- = -1$. Let $\overline{\boldsymbol{y}}$ be the column of cell means. Need $MSE = \hat{\sigma}^2$ to be given or estimated by setting high order interactions to 0 for $m = 1$. Typically $m = 1$ for fractional factorial designs.

a) The effect corresponding to $\boldsymbol{c}$ is $effect = \dfrac{\boldsymbol{c}^T \overline{\boldsymbol{y}}}{2^{k_o-1}}$.

b) The standard error for the effect is $SE(effect) = \sqrt{\dfrac{MSE}{m2^{k_o-2}}}$.

c) $SE(mean) = \sqrt{\dfrac{MSE}{m2^{k_o}}}$ where $m2^{k_o} = n$.

d) The mean square and sum of squares for an effect are
$MS(effect) = SS(effect) = m2^{k_o-2}(effect)^2$.

34) Least squares estimates for the 2_R^{k-f} designs in points 31) and 32) are obtained by using the design matrix corresponding to the table of contrasts in point 10) for $k_o = 3$ and point 16) for $k_o = 4$.

35) The QQ plot for 2_R^{k-f} designs is used in a manner similar to point 29).

36) Randomly assign units to runs. Do runs in random order if possible. In industry, units are often time slots (periods of time), so randomization consists of randomly assigning time slots to units, which is equivalent to doing the runs in random order. For the 2_R^{k-f} designs in points 31) and 32), fix the main effects using the corresponding columns of contrasts given in points 10) and 16) to determine the levels needed in the $m2^{k-f}$ runs.

37) Active factors appear to change the mean response as the level of the factor changes from -1 to 1. Inert factors do not appear to change the response as the level of the factor changes from -1 to 1. An inert factor could be needed but the level low or high is not important, or the inert factor may not be needed and so can be omitted from future studies. Often subject matter experts can tell whether the inert factor is needed or not.

38) A 2_R^{k-f} design has no q factor interaction (or main effect for $q = 1$) confounded with any other effect consisting of less than $R - q$ factors. So a 2_{III}^{k-f} design has $R = 3$ and main effects are confounded with 2 factor interactions. In a 2_{IV}^{k-f} design, $R = 4$ and main effects are not confounded with 2 factor interactions but 2 factor interactions are confounded with other 2 factor interactions. In a 2_V^{k-f} design, $R = 5$ and main effects and 2 factor

interactions are only confounded with 4 and 3 way or higher interactions respectively.

39) In a 2_R^{k-f} design, each effect is confounded or aliased with 2^{f-1} other effects. Thus the Mth main effect is really an estimate of the Mth main effect plus 2^{f-1} other effects. If $R \geq 3$ and none of the two factor interactions are significant, then the Mth main effect is typically a useful estimator of the population Mth main effect.

40) The R = 4 and R = 5 designs are good because the 3 way and higher interactions are rarely significant, but these designs are more expensive than the R = 3 designs.

41) In this text, most of the DOE models can be fit with least squares, and the model can be written as $Y = \boldsymbol{x}^T\boldsymbol{\beta} + e$ with least squares fitted values $\hat{Y} = \boldsymbol{x}^T\hat{\boldsymbol{\beta}}$. In matrix form the model is $\boldsymbol{Y} = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{e}$ and the vector of fitted values is $\hat{\boldsymbol{Y}} = \boldsymbol{X}\hat{\boldsymbol{\beta}}$.

42) The full model for a 2^3 or 2_R^{k-f} design where $k - f = 3$ is
$Y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \beta_3 x_{i3} + \beta_{12} x_{i12} + \beta_{13} x_{i13} + \beta_{23} x_{i23} + \beta_{123} x_{i123} + e_i$
with least squares fitted or predicted values given by
$\hat{Y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_{i1} + \hat{\beta}_2 x_{i2} + \hat{\beta}_3 x_{i3} + \hat{\beta}_{12} x_{i12} + \hat{\beta}_{13} x_{i13} + \hat{\beta}_{23} x_{i23} + \hat{\beta}_{123} x_{i123}$.

43) An interaction such as x_{i123} satisfies $x_{i123} = (x_{i1})(x_{i2})(x_{i3})$.

44) For orthogonal designs like 2^k, 2_R^{k-f} or PB(n) (described in point 52)), the x value of an effect takes on values -1 or 1. The columns of the design matrix $\boldsymbol{X}$ are orthogonal: $\boldsymbol{c}_i^T\boldsymbol{c}_j = 0$ for $i \neq j$ where $\boldsymbol{c}_i$ is the ith column of $\boldsymbol{X}$.

45) Suppose the full model using all of the columns of $\boldsymbol{X}$ is used. If the some columns are removed (eg those corresponding to the insignificant effects), then for orthogonal designs in point 44) the following quantities remain unchanged for the terms that were not deleted: the effects, the coefficients, SS(effect) = MS(effect). The MSE, SE(effect), F and t statistics, pvalues, fitted values and residuals do change.

46) The regression equation corresponding to the significant effects (eg found with a QQ plot) can be used to form a reduced model. For example, suppose the full (least squares) fitted model is $\hat{Y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_{i1} + \hat{\beta}_2 x_{i2} + \hat{\beta}_3 x_{i3} + \hat{\beta}_{12} x_{i12} + \hat{\beta}_{13} x_{i13} + \hat{\beta}_{23} x_{i23} + \hat{\beta}_{123} x_{i123}$. Suppose the A, B and AB effects are significant. Then the reduced (least squares) fitted model is $\hat{Y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_{i1} + \hat{\beta}_2 x_{i2} + \hat{\beta}_{12} x_{i12}$ where the coefficients ($\hat{\beta}$'s) for the reduced model are taken from the full model.

47) For the designs in 44), the coefficient $\hat{\beta}_0$ corresponding to I is equal to the I effect, but the coefficient of a factor x corresponding to an *effect* is $\hat{\beta} = 0.5$ *effect*. Consider significant effects and assume interactions can be ignored.

i) If a large response Y is desired and $\hat{\beta} > 0$, use $x = 1$. If $\hat{\beta} < 0$, use $x = -1$.

ii) If a small response Y is desired and $\hat{\beta} > 0$, use $x = -1$. If $\hat{\beta} < 0$, use $x = 1$.

48) Rule of thumb: to predict Y with $\hat{Y}$, the number of coefficients = the number of $\hat{\beta}$'s in the model should be $\leq n/2$, where the sample size n = number of runs.

49) From the regression equation $\hat{Y} = \boldsymbol{x}^T \hat{\boldsymbol{\beta}}$, be able to predict Y given $\boldsymbol{x}$. Be able to tell whether $x = 1$ or $x = -1$ should be used. Given the x values of the main effects, get the x values of the interactions using 43).

50) Least squares output for an example and in symbols are shown below and on the following page for the designs in 44). Often "Estimate" is replaced by "Coef" or "Coefficient". Often "Intercept" is replaced by "Constant". The t statistic and pvalue are for whether the term or effect is significant. So t_{12} and p_{12} are for testing whether the x_{12} term or AB effect is significant.

```
Residual Standard Error=2.8284 = sqrt(MSE)
R-Square=0.9763 F-statistic (df=7, 8)=47.0536 p-value=0

          Estimate Std.Err t-value Pr(>|t|)
Intercept    64.25  0.7071 90.8632   0.0000
x1           11.50  0.7071 16.2635   0.0000
x2           -2.50  0.7071 -3.5355   0.0077
x3            0.75  0.7071  1.0607   0.3198
x12           0.75  0.7071  1.0607   0.3198
x13           5.00  0.7071  7.0711   0.0001
x23           0.00  0.7071  0.0000   1.0000
x123          0.25  0.7071  0.3536   0.7328
```

	Coef or Est.	Std.Err	t	pvalue
Intercept or constant	$\hat{\beta}_0$	SE(coef)	t_0	p_0
x1	$\hat{\beta}_1$	SE(coef)	t_1	p_1
x2	$\hat{\beta}_2$	SE(coef)	t_2	p_2
x3	$\hat{\beta}_3$	SE(coef)	t_3	p_3
x12	$\hat{\beta}_{12}$	SE(coef)	t_{12}	p_{12}
x13	$\hat{\beta}_{13}$	SE(coef)	t_{13}	p_{13}
x23	$\hat{\beta}_{23}$	SE(coef)	t_{23}	p_{23}
x123	$\hat{\beta}_{123}$	SE(coef)	t_{123}	p_{123}

51) The least squares coefficient = 0.5 (effect). The sum of squares for an x corresponding to an effect is equal to SS(effect). SE(coef) = SE($\hat{\beta}$) = 0.5 SE(effect) = $\sqrt{MSE/n}$. Also SE($\hat{\beta}_0$) = $\sqrt{MSE/n}$.

52) The Plackett Burman PB(n) designs have k factors where $2 \leq k \leq n-1$. The factors have 2 levels and orthogonal contrasts like the 2^k and 2_R^{k-f} designs. The PB(n) designs are resolution 3 designs, but the confounding of main effects with 2 factor interactions is complex. The PB(n) designs use n runs where n is a multiple of 4. The values $n = 12, 20, 24, 28$ and 36 are especially common.

53) The PB(n) designs are usually used with main effects so assume that all interactions are insignificant. So they are main effects designs used to screen k main effects when the number of runs n is small. Often $k = n-4, n-3, n-2$ or $n-1$ is used. We will assume that the number of replications $m = 1$.

54) If $k = n-1$ there is no df for MSE. If $k < n-1$, pool the last $J = n-1-k$ "empty" effects into the MSE with $df = J$ as the full model. This procedure is done before looking at the data, so is not data snooping.

55) The contrast matrix for the PB(12) design is shown on the following page. Again the column of plusses corresponding to I is omitted. If $k = 8$ then effects A to H are used but effects J, K and L are "empty." As a convention the mean square and sum of squares for factor E will be denoted as MSe and SSe while MSE = $\hat{\sigma}^2$.

run	A	B	C	D	E	F	G	H	J	K	L
1	+	-	+	-	-	-	+	+	+	-	+
2	+	+	-	+	-	-	-	+	+	+	-
3	-	+	+	-	+	-	-	-	+	+	+
4	+	-	+	+	-	+	-	-	-	+	+
5	+	+	-	+	+	-	+	-	-	-	+
6	+	+	+	-	+	+	-	+	-	-	-
7	-	+	+	+	-	+	+	-	+	-	-
8	-	-	+	+	+	-	+	+	-	+	-
9	-	-	-	+	+	+	-	+	+	-	+
10	+	-	-	-	+	+	+	-	+	+	-
11	-	+	-	-	-	+	+	+	-	+	+
12	-	-	-	-	-	-	-	-	-	-	-

56) The PB(n) designs are k factor 2 level orthogonal designs. So finding effects, MS, SS, least squares estimates et cetera for PB(n) designs is similar to finding the corresponding quantities for the 2^k and 2_R^{k-f} designs.

57) For the PB(n) design, let $\boldsymbol{c}$ be a column from the table of contrasts where $+ = 1$ and $- = -1$. Let $\boldsymbol{y}$ be the column of responses since $m = 1$. For $k < n-1$, MSE can be found for the full model as in 54). MSE can also be given or found by pooling insignificant MS's into the MSE, but the latter method uses data snooping.

a) The effect corresponding to $\boldsymbol{c}$ is $effect = \dfrac{\boldsymbol{c}^T\boldsymbol{y}}{n/2} = \dfrac{2\boldsymbol{c}^T\boldsymbol{y}}{n}$.

b) The standard error for the effect is $SE(effect) = \sqrt{\dfrac{MSE}{n/4}} = \sqrt{\dfrac{4MSE}{n}}$.

c) $SE(mean) = \sqrt{\dfrac{MSE}{n}}$.

d) The sum of squares and mean square for an effect is
$MS(effect) = SS(effect) = \dfrac{n}{4}(effect)^2$.

58) For the PB(n) design, the least squares coefficient = 0.5 (effect). The sum of squares for an x corresponding to an effect is equal to SS(effect). SE(coef) = SE($\hat{\beta}$) = 0.5 SE(effect) = $\sqrt{MSE/n}$. Also SE($\hat{\beta}_0$) = $\sqrt{MSE/n}$.

8.5 Complements

Box, Hunter and Hunter (2005) and Ledolter and Swersey (2007) are excellent references for k factor 2 level orthogonal designs.

Suppose it is desired to increase the response Y and that $A, B, C, ...$ are the k factors. The main effects for $A, B, ...$ measure

$$\frac{\partial Y}{\partial A}, \frac{\partial Y}{\partial B},$$

et cetera. The interaction effect AB measures

$$\frac{\partial Y}{\partial A \partial B}.$$

Hence

$$\frac{\partial Y}{\partial A} \approx 0, \frac{\partial Y}{\partial B} \approx 0 \text{ and } \frac{\partial \text{Y}}{\partial \text{A} \partial \text{B}} \text{ large}$$

implies that the design is in the neighborhood of a maximum of a response that looks like a ridge.

An estimated contrast is $\hat{C} = \sum_{i=1}^{p} d_i \overline{Y}_{i0}$, and

$$SE(\hat{C}) = \sqrt{MSE \sum_{i=1}^{p} \frac{d_i^2}{n_i}}.$$

If $d_i = \pm 1$, $p = 2^k$ and $n_i = m$, then $SE(\hat{C}) = \sqrt{MSE \;\; 2^k/m}$. For a 2^k design, an effect can be written as a contrast with $d_i = \pm 1/2^{k-1}$, $p = 2^k$ and $n_i = m$. Thus

$$SE(effect) = \sqrt{MSE \sum_{i=1}^{2^k} \frac{1}{m} \frac{1}{2^{2k-2}}} = \sqrt{\frac{MSE}{m 2^{k-2}}}.$$

There is an " algebra" for computing confounding patterns for fractional factorial designs. Let M be any single letter effect (A, B, C et cetera), and let I be the identity element. Then i) $IM = M$, ii) $MM = I$ and iii) multiplication is commutative: $LM = ML$.

For a 2_R^{k-1} design, set one main effect equal to an interaction, eg $D = ABC$. The equation $D = ABC$ is called a "generator." Note that $DD = I = DABC = ABCD$. The equation $I = ABCD$ is the generating relationship.

Then $MI = M = ABCDM$, so M is confounded or aliased with $ABCDM$. So $A = AI = AABCD = BCD$ and A is confounded with BCD. Similarly, $BD = BDI = BDABCD = AC$, so BD is confounded with AC.

For a 2_R^{k-2} design, 2 main effects L and M are set equal to an interaction. Thus $L^2 = I$ and $M^2 = I$, but it is also true that $L^2M^2 = I$. As an illustration, consider the 2_{IV}^{6-2} design with $E = ABC$ and $F = BCD$. So $E^2 = I = ABCE$, $F^2 = I = BCDF$ and $F^2E^2 = I = ABCEBCDF = ADEF$. Hence the generating relationship $I = ABCE = BCDF = ADEF$ has 3 "words," and each effect is confounded with 3 other effects. For example, $AI = AABCE = ABCDF = AADEF$ or $A = BCE = ABCDF = DEF$.

For a 2_R^{k-f} design, f main effects $L_1, ..., L_F$ are set equal to interactions. There are $\binom{f}{1}$ equations of the form $L_i^2 = I$, $\binom{f}{2}$ equations of the form $L_i^2 L_j^2 = I$, $\binom{f}{3}$ equations of the form $L_{i1}^2 L_{i2}^2 L_{i3}^2 = I$, ..., $\binom{f}{f}$ equations of the form $L_1^2 L_2^2 \cdots L_f^2 = I$. These equations give a generating relationship with $2^f - 1$ "words," so each effect is confounded with $2^f - 1$ other effects.

If the generating relationship is $I = W_1 = W_2 = \cdots = W_{2^f-1}$, then the resolution R is equal to the length of the smallest word. So $I = ABC$ and $I = ABCE = ABC = ADEF$ both have $R = 3$.

The convention is to ignore 3 way or higher order interactions. So the alias patterns for the k main effects and the $\binom{k}{2}$ 2 way interactions with other main effects and 2 way interactions is of interest.

8.6 Problems

Problems with an asterisk * are especially important.

```
Output for 8.1: Residual Standard Error=2.8284 R-Square=0.9763
F-statistic (df=7, 8)=47.0536 p-value=0
           Estimate Std.Err t-value Pr(>|t|)
Intercept     64.25  0.7071 90.8632   0.0000
x1            11.50  0.7071 16.2635   0.0000
x2            -2.50  0.7071 -3.5355   0.0077
x3             0.75  0.7071  1.0607   0.3198
x12            0.75  0.7071  1.0607   0.3198
x13            5.00  0.7071  7.0711   0.0001
x23            0.00  0.7071  0.0000   1.0000
x123           0.25  0.7071  0.3536   0.7328
```

8.1. From the least squares output on the previous page, what is the AB effect?

I	A	B	C	AB	AC	BC	ABC	Y
+	−	−	−	+	+	+	−	3.81
+	+	−	−	−	−	+	+	4.28
+	−	+	−	−	+	−	+	3.74
+	+	+	−	+	−	−	−	4.10
+	−	−	+	+	−	−	+	3.75
+	+	−	+	−	+	−	−	3.66
+	−	+	+	−	−	+	−	3.82
+	+	+	+	+	+	+	+	3.68

8.2. Ledolter and Swersey (2007, p. 108 - 109) describes a 2^3 experiment designed to increase subscriptions of the magazine *Ladies' Home Journal.* The 2005 campaign made 8 brochures containing an order card. Each brochure was mailed to 15042 households, and the response Y was the percentage of orders. Factor A was *front side of order card* with (−1) highlighting "Double our Best Offer" and (+1) highlighting "We never had a bigger sale." Factor B was *back side of order card* with (−1) emphasizing "Two extra years free," while (+1) featured magazine covers of a previous issue. Factor C was *brochure cover* with (−1) featuring Kelly Ripa and (+1) Dr. Phil. Assume $m = 1$.

a) Find the A effect.

b) Find the C effect.

c) Find SSC = MSC.

d) If two of the three factors A, B and C are active, which is inactive?

I	A	B	C	AB	AC	BC	ABC	y
+	−	−	−	+	+	+	−	86.8
+	+	−	−	−	−	+	+	85.9
+	−	+	−	−	+	−	+	79.4
+	+	+	−	+	−	−	−	60.0
+	−	−	+	+	−	−	+	94.6
+	+	−	+	−	+	−	−	85.4
+	−	+	+	−	−	+	−	84.5
+	+	+	+	+	+	+	+	80.3

8.3. The table of 2^3 contrasts on the previous page is for 2^{5-2}_{III} data.

a) Estimate the B effect.

b) Estimate the D effect.

8.4. Suppose that for 2^3 data with $m = 2$, the MSE = 407.5625. Find SE(effect).

	I	A	B	C	AB	AC	BC	ABC	y
	+	−	−	−	+	+	+	−	63.6
	+	+	−	−	−	−	+	+	76.8
	+	−	+	−	−	+	−	+	60.3
	+	+	+	−	+	−	−	−	80.3
	+	−	−	+	+	−	−	+	67.2
	+	+	−	+	−	+	−	−	71.3
	+	−	+	+	−	−	+	−	68.3
	+	+	+	+	+	+	+	+	74.3
divisor	8	4	4	4	4	4	4	4	

8.5. Ledolter and Swersey (2007, p. 131) describe a 2^{7-4}_{III} data set shown with the table of 2^3 contrasts above. Estimate the D effect.

	I	A	B	C	AB	AC	BC	ABC	$\overline{y}$
	+	−	−	−	+	+	+	−	32
	+	+	−	−	−	−	+	+	35
	+	−	+	−	−	+	−	+	28
	+	+	+	−	+	−	−	−	31
	+	−	−	+	+	−	−	+	48
	+	+	−	+	−	+	−	−	39
	+	−	+	+	−	−	+	−	28
	+	+	+	+	+	+	+	+	29
divisor	8	4	4	4	4	4	4	4	

8.6. Kuehl (1994, p. 361-366) describes a 2^3 experiment designed to investigate the effects of furnace temperature (1840 or 1880^{o}F), heating time (23 or 25 sec) and transfer time (10 or 12 sec) on the quality of a leaf spring used for trucks. (The response Y was a measure of the quality.) The table of contrasts is shown above.

a) Find the A effect.
b) Find the B effect.
c) Find the AB effect.
d) If $m = 1$, find SSA.
e) If $m = 1$, find SSB.
f) If $m = 1$, find SSAB.
g) If $m = 2$ and MSE = 9, find SE(effect).
(The SE is the same regardless of the effect.)

h) Suppose high $Y = y$ is desirable. If two of the factors A, B and C are inert and one is active, then which is active and which are inert. (Hint: look at the 4 highest values of $\overline{y}$. Is there a pattern?)

i) If one of the factors has an interaction with the active factor, what is the interaction (eg AB, AC or BC)?

8.7. Suppose the B *effect* = −5, $SE(effect) = \sqrt{2}$ and $df_e = 8$.
i) Find a 95% confidence interval for the B *effect.*
ii) Is the B *effect* significant? Explain briefly.

8.8. Copy the Box, Hunter and Hunter (2005, p. 199) product development data from (www.math.siu.edu/olive/regdata.txt) into *R*.

Then type the following commands.

```
out <- aov(conversion~K*Te*P*C,devel)
summary(out)
```

a) Include the output in *Word.*
b) What are the five effects with the biggest mean squares?
Note: an AB interaction is denoted by A:B in *R*.

8.9. Get the SAS program from (www.math.siu.edu/olive/reghw.txt) for this problem. The data is the pilot plant example from Box, Hunter and Hunter (2005, p. 177-186). The response varible is Y=yield, while the three predictors (T = temp, C = concentration, K = catalyst) are at two levels.
a) Print out the output but do not turn in the first page.
b) Do the residual and response plots look ok?

8.10. Get the data from (www.math.siu.edu/olive/reghw.txt) for this problem. The data is the pilot plant example from Box, Hunter and Hunter (2005, p. 177-186) examined in Problem 8.9. Minitab needs the levels for the factors and the interactions.

Highlight the data and use the menu commands "Edit>Copy." In Minitab, use the menu command "Edit>PasteCells." After a window appears, click on ok.

Below C1 type "A", below C2 type "B", below C3 type "C" and below C8 type "yield."

a) Use the menu command "STAT>ANOVA>Balanced Anova" put "yield" in the responses box and

A|B|C

in the Model box. Click on "Storage." When a window appears, click on "Fits" and "Residuals." Then click on "OK". This window will disappear. Click on "OK."

b) Next highlight the bottom 8 lines and use the menu commands "Edit>Delete Cells". Then the data set does not have replication. Use the menu command "STAT>ANOVA>Balanced Anova" put "yield" in the responses box and

A B C A*C

in the Model box. Click on "Storage." When a window appears, click on "Fits" and "Residuals." Then click on "OK". This window will disappear. Click on "OK."

(The model A|B|C would have resulted in an error message, not enough data.)

c) Print the output by clicking on the top window and then clicking on the printer icon.

d) Make a response plot with the menu commands "Graph>Plot" with *yield* in the *Y box* and *FIT2* in the *X box*. Print by clicking on the printer icon.

e) Make a residual plot with the menu commands "Graph>Plot" with *RESI2* in the *Y box* and *FIT2* in the *X box*. Print by clicking on the printer icon.

f) Do the plots look ok?

8.11. Get the *R* code and data for this problem from (www.math.siu.edu/olive/reghw.txt). The data is the pilot plant example from Box, Hunter and Hunter (2005, p. 177-186) examined in Problems 8.9 and 8.10.

a) Copy and paste the code into *R*. Then copy and paste the output into *Notepad*. Print out the page of output.

b) The least squares estimate = coefficient for x_1 is half the A effect. So what is the A effect?

8.12. a) Obtain and the *R* program `twocub` from (www.math.siu.edu/olive/regpack.txt). To get the effects, mean squares and SE(effect) for the Box, Hunter and Hunter (2005, p. 177) pilot plant data, type the following commands and include the output in *Word*.

```
mns <- c(60,72,54,68,52,83,45,80)
twocub(mns,m=2,MSE=8)
```

b) Which effects appear to be significant from the QQ plot? (Match the effects on the plot with the output on the screen.)

8.13. Box, Hunter and Hunter (2005, p. 237) describe a 2_{IV}^{4-1} fractional factorial design. Assuming that you downloaded the `twocub` function in the previous problem, type the following commands.

```
mns <- c(20,14,17,10,19,13,14,10)
twocub(mns,m=1)
```

a) Include the output in *Word*, print out the output and label the effects on the output with the corresponding effects from a 2_{IV}^{4-1} fractional factorial design.

b) Include the QQ plot in *Word*. Print out the plot. Which effects (from the fractional factorial design) seem to be significant?

8.14. a) Download (www.math.siu.edu/olive/regpack.txt) into *R*, and type the following commands.

```
mns <- c(14,16,8,22,19,37,20,38,1,8,4,10,12,30,13,30)
twofourth(mns)
```

This is the Ledolter and Swersey (2007, p. 80) cracked pots 2^4 data and the response and residual plots are from the model without 3 and 4 factor interactions.

b) Copy the plots into *Word* and print the plots. Do the response and residual plots look ok?

8.15. Download (www.math.siu.edu/olive/regpack.txt) into *R*. The data is the PB(12) example from Box, Hunter and Hunter (2005, p. 287).

a) Type the following commands. Copy and paste the QQ plot into *Word* and print the plot.

```
resp <- c(56,93,67,60,77,65,95,49,44,63,63,61)
pb12(resp,k=5)
```

b) Copy and paste the output into *Notepad* and print the output.

c) As a 2^5 design, the effects B, D, BD, E and DE were thought to be real. The PB(12) design works best when none of the interactions is significant. From the QQ plot and the output for the PB(12) design, which factors, if any, appear to be significant?

d) The output gives the A, B, C, D and E effects along with the corresponding least squares coefficients $\hat{\beta}_1$, ..., $\hat{\beta}_5$. What is the relationship between the coefficients and the effects?

For parts e) to g), act as if the PB(12) design with 5 factors is appropriate.

e) The full model has $\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2 + \hat{\beta}_3 x_3 + \hat{\beta}_4 x_4 + \hat{\beta}_5 x_5$. The reduced model is $\hat{Y} = \hat{\beta}_0 + \hat{\beta}_j x_j$ where x_j is the significant term found in c). Give the numerical formula for the reduced model.

f) Compute $\hat{Y}$ using the full model if $x_i = 1$ for $i = 1, ..., 5$. Then compute $\hat{Y}$ using the reduced model if $x_j = 1$.

g) If the goal of the experiment is to produce large values of Y, should $x_j = 1$ or $x_j = -1$ in the reduced model? Explain briefly.