Experimental Design and Biostatistics (TAMS38)
Lecture 8 – Fractional factorial design of type 2^{k-p}

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Example 1 – Glazing ceramic

When glazing ceramic one uses three color pigments A, B, C.

To find a good combination, one design a 2^3 experiment where each pigment occur in low or high dose.

The glazing result are then being scored. Hence, the collected data y is the score for the different level combinations and only one observation for each combination.

If we use notation from Lecture 7 then we have:

2^3-factorial design

$$\underbrace{\begin{pmatrix} y_{(1)} \\ y_a \\ y_b \\ y_{ab} \\ y_c \\ y_{ac} \\ y_{bc} \\ y_{abc} \end{pmatrix}}_{=\boldsymbol{y}} \quad \text{with} \quad \begin{array}{c} \begin{array}{cccccccc} I & A & B & AB & C & AC & BC & ABC \end{array} \\ \underbrace{\begin{pmatrix} 1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 \\ 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 \\ 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 \\ 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 \\ 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{pmatrix}}_{=\boldsymbol{F}} \end{array}$$

and the parameter vector (in complete three factor model) $\boldsymbol{\xi} = \begin{pmatrix} \mu \\ \tau_1 \\ \beta_1 \\ (\tau\beta)_{11} \\ \gamma_1 \\ (\tau\gamma)_{11} \\ (\beta\gamma)_{11} \\ (\tau\beta\gamma)_{111} \end{pmatrix}$

As we see, we keep as before only parameters with the positive indices, but of course do we also have the others, i.e., $\tau_{-1} = -\tau_1$.

When we have only one observation of each level combination (one observation per cell) we use the following equation to estimate all mean parameters (see Lecture 7)

$$\boldsymbol{y} = \mathbf{F}\hat{\boldsymbol{\xi}},$$

which can also be written as

$$\begin{pmatrix} y_{(1)} \\ y_a \\ \vdots \\ y_{abc} \end{pmatrix} = \hat{\mu} \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} + \hat{\tau}_1 \begin{array}{c} A \\ \begin{pmatrix} -1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} \end{array} + \cdots + \widehat{(\tau\beta\gamma)}_{111} \begin{array}{c} ABC \\ \begin{pmatrix} -1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} \end{array} \tag{1}$$

Example 1, cont.

The planning is complicated due to the oven, where the glazing will take place, since it only can manage four objects at a time.

Suppose that we take two batches

$$(i)\left\{\begin{array}{ccccl} (1) & b & c & bc & \text{first batch (block } l=-1) \\ a & ab & ac & abc & \text{second batch (block } l=1) \end{array}\right.$$

Hence, we will have a model with a block effect

$$\begin{aligned} y_{ijk(l)} = \mu + \tau_i + \beta_j + (\tau\beta)_{ij} + \gamma_k + (\tau\gamma)_{ik} + (\beta\gamma)_{jk} \\ + (\tau\beta\gamma)_{ijk} + q_l + \varepsilon_{ijk(l)} \end{aligned}$$

with all restrictions and $\sum_l q_l = 0$, i.e., also $q_{-1} = -q_1$.

The right hand side of (**??**) will have one more term for (i) above:

$$\hat{q}_1 \cdot \begin{pmatrix} -1 \\ 1 \\ -1 \\ 1 \\ -1 \\ 1 \\ -1 \\ 1 \end{pmatrix} \qquad \text{level combination:} \qquad \begin{array}{cl} (1) & l = -1 \\ a & l = 1 \\ b & l = -1 \\ ab & l = 1 \\ c & l = -1 \\ ac & l = 1 \\ bc & l = -1 \\ abc & l = 1 \end{array}$$

But, this is the same as the A-vector, i.e.,

$$\begin{pmatrix} y_{(1)} \\ \vdots \\ y_{abc} \end{pmatrix} = \hat{\mu} \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix} + (\hat{\tau}_1 + \hat{q}_1) \begin{pmatrix} -1 \\ \vdots \\ 1 \end{pmatrix} + \cdots + \widehat{(\tau\beta\gamma)}_{111} \begin{pmatrix} -1 \\ \vdots \\ 1 \end{pmatrix},$$

which means that we can just estimate the sum $(\hat{\tau}_1 + \hat{q}_1)$ and not the parameters separately.

This is of course not good and we must do in some other way...

Let I be the same as the ones in ABC-vector, i.e., let

$$(ii) \begin{cases} (1) \quad ab \quad ac \quad bc & \text{first batch (block } I=-1) \\ a \quad b \quad c \quad abc & \text{second batch (block } I=1) \end{cases}$$

with the parameter equations:

$$\begin{pmatrix} y_{(1)} \\ \vdots \\ y_{abc} \end{pmatrix} = \hat{\mu} \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix} + \hat{\tau}_1 \begin{pmatrix} -1 \\ \vdots \\ 1 \end{pmatrix} + \cdots + \left(\widehat{(\tau\beta\gamma)}_{111} + \hat{q}_1 \right) \begin{pmatrix} -1 \\ \vdots \\ 1 \end{pmatrix}$$

Hence, the block effect and the ABC-effect can not be separated.

We must be careful when considering $\left(\widehat{(\tau\beta\gamma)}_{111} + \hat{q}_1 \right)$.

Now, we solve the equations as above with the matrix $\boldsymbol{F}$.

Example 2 – Chemical process

For a chemical process one have measured the level of contamination in the final product, when each of the four factors A, B, C and D has been varied on two levels.

The experiment was conducted in two blocks, where the division between the blocks were done following the rule

$$H = ABCD.$$

Resultat:

(1)	1.43	c	1.53	d	1.54	cd	1.84
a	1.35	ac	1.61	ad	1.67	acd	1.70
b	1.22	bc	1.35	bd	1.48	bcd	1.48
ab	1.35	abc	1.27	abd	1.45	$abcd$	1.59

Observations should be analyzed with the 2^4-factorial design with factors A, B, C and D and then using the reduced model, see Minitab output below.

a) Which observations are included in each block?
b) What are the most important parameters? Is there a difference between the blocks?
c) Estimating, for the reduced model, the expected value of the level combination that looks to be the best.

a)

	H		H
(1)	$(-1)^4 = 1$	d	-1
a	$1 \cdot (-1)^3 = -1$	ad	1
b	$1 \cdot (-1)^3 = -1$	bd	1
ab	$1^2 \cdot (-1)^2 = 1$	abd	-1
c	$1 \cdot (-1)^3 = -1$	cd	1
ac	1	acd	-1
bc	1	bcd	-1
abc	-1	$abcd$	1

Block $H = -1: \quad a, b, c, abc, d, abd, acd, bcd$
Block $H = \ 1: \quad (1), ab, ac, bc, ad, bd, cd, abcd$

Analyze the data like if there were no block with the model

Model 1 Complete model is given by

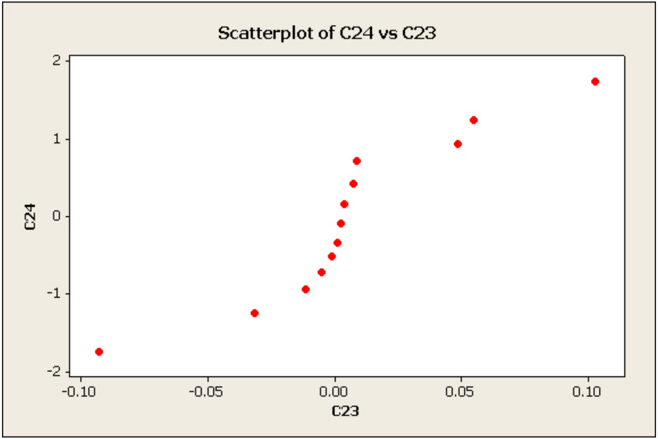
$$\begin{aligned} Y_{ijkl(\nu)} = \mu &+ \tau_i + \beta_j + (\tau\beta)_{ij} + \gamma_k + (\tau\gamma)_{ik} \\ &+ (\beta\gamma)_{jk} + (\tau\beta\gamma)_{ijk} + \delta_l + (\tau\delta)_{il} + \cdots \\ &+ (\tau\beta\gamma\delta)_{ijkl} + \kappa_\nu + \varepsilon'_{ijkl(\nu)}. \end{aligned}$$

When we interpret the results, we must remember that the block parameter can not be separated from $(\tau\beta\gamma\delta)_{1111}$ that is parameter 16 in the parameter vector.

```
MTB > let c17=c17/100
MTB > copy c17 m2
MTB > copy c1-c16 m1
MTB > trans m1 m3
MTB > mult m3 m2 m4
MTB > copy m4 c18
MTB > let c19=c18/16
MTB > set c20
DATA> 1:16
DATA> end
MTB > sort c19 c20 c21 c22
MTB > print c21-c22
```

Data Display

Row	C21	C22
1	-0.09250	3
2	-0.03125	7
3	-0.01125	6
4	-0.00500	14
5	-0.00125	11
6	0.00125	10
7	0.00250	8
8	0.00250	12
9	0.00375	13
10	0.00750	15
11	0.00750	2
12	0.00875	4
13	0.04875	16
14	0.05500	5
15	0.10250	9
16	1.49125	1




```
MTB > copy c21 c23;
SUBC> omit 16.
MTB > nscores c23 c24
MTB > plot c24*c23
```

b) In the plot we see that the important effects are number 3, 7, 9, 5, 16, i.e., B, BC, D, C and $(ABCD + H)$.

We assume that it is the block effect which differ from zero in $(ABCD + H)$.

Now, we do analysis using the reduced model.

Model 2 B-level j, C-level k, D-level l and H-level ν give

$$\begin{aligned} Y_{jkl\nu} &= \mu + \beta_j + \gamma_k + (\beta\gamma)_{jk} + \delta_l + \kappa_\nu + \varepsilon_{jkl\nu} \\ &= m_{jk} + \delta_l + \kappa_\nu + \varepsilon_{jkl\nu}. \end{aligned}$$

```
MTB > ANOVA 'Y' = B|C D H;
SUBC>   Means B|C D H.
```

ANOVA: Y versus B, C, D, H

```
Analysis of Variance for Y

Source  DF        SS        MS       F      P
B        1  0.136900  0.136900  231.05  0.000
C        1  0.048400  0.048400   81.69  0.000
B*C      1  0.015625  0.015625   26.37  0.000
D        1  0.168100  0.168100  283.71  0.000
H        1  0.038025  0.038025   64.18  0.000
Error   10  0.005925  0.000593
Total   15  0.412975

S = 0.0243413   R-Sq = 98.57%   R-Sq(adj) = 97.85%
```

Means

B	N	Y
-1	8	1.5838
1	8	1.3987

C	N	Y
-1	8	1.4363
1	8	1.5463

B	C	N	Y
-1	-1	4	1.4975
-1	1	4	1.6700
1	-1	4	1.3750
1	1	4	1.4225

D	N	Y
-1	8	1.3887
1	8	1.5938

H	N	Y
-1	8	1.4425
1	8	1.5400

Construct confidence interval for $\kappa_1 - \kappa_{-1}$.

$$\hat{\kappa}_1 - \hat{\kappa}_{-1} = \bar{y}_{...1} - \bar{y}_{....} - (\bar{y}_{...-1} - \bar{y}_{....}) = \bar{y}_{...1} - \bar{y}_{...-1}$$

$$\text{var}\left(\overline{y}_{...1} - \overline{y}_{...-1}\right) = \frac{\sigma^2}{8} + \frac{\sigma^2}{8}.$$

Furthermore, the estimator of σ^2 is $s^2 = \frac{SS_E}{10} = 0.000592$, $s = 0.02433$; $df = 10$; $t(10)$-table give $t = 2.23$. Hence,

$$I_{\kappa_1 - \kappa_{-1}} = \left(0.0975 \mp 2.23 \cdot s\sqrt{\frac{1}{8} + \frac{1}{8}}\right) \approx (0.070, 0.125)$$

There is significant difference between the blocks.

c) We want low values for y.

We see that $\widehat{m}_{jk}$ has the smallest value for $j = 1$, $k = -1$, i.e., $\widehat{m}_{1,-1} = 1.3750$;

$\hat{\delta}_1 = 0.10250$; choose $l = -1$; $\hat{\kappa}_1 = 0.04875$; choose $\nu = -1$.

B-level 1, C-level -1, D-level -1, block -1 give

$$\widehat{E(Y_{1,-1,-1,-1})} = 1.3750 - 0.10250 - 0.04875 \approx 1.224$$

The general 2^{k-p} fractional factorial design

Since experiments can be expensive, both in time and money, fractional factorial designs has been popular.

1. One often finds the main effects and interaction effects of low order.
2. If some factors do **not** effect the response, then the design can be reduced to a complete design for the remaining significant factors.
3. One can do the runs sequentially, i.e., add more observations so one can do a complete design.

2^{4-1} fractional factorial design

Suppose we want a 2^4 factorial design with the factors A, B, C, D,, but we can just take 8 observations.

We can do a complete 2^3 design for A, B, C.

If we want to add the factor D we have to ignore some interaction effects.

With 8 observations we can estimate 8 mean parameters, while the complete 2^4 design has 16 parameters.

We have to design our experiment in a smart way!

For the complete 2^3 design with the factors A, B, C and only one observation per combination we have

$$\underbrace{\begin{pmatrix} y_{(1)} \\ y_a \\ y_b \\ y_{ab} \\ y_c \\ y_{ac} \\ y_{bc} \\ y_{abc} \end{pmatrix}}_{=\boldsymbol{y}} \text{ with } \begin{array}{c} \begin{array}{cccccccc} I & A & B & AB & C & AC & BC & ABC \end{array} \\ \underbrace{\begin{pmatrix} 1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 \\ 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 \\ 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 \\ 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 \\ 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{pmatrix}}_{=\boldsymbol{F}} \end{array}$$

and the parameter vector (in complete three factor model)
$$\boldsymbol{\xi} = \begin{pmatrix} \mu \\ \tau_1 \\ \beta_1 \\ (\tau\beta)_{11} \\ \gamma_1 \\ (\tau\gamma)_{11} \\ (\beta\gamma)_{11} \\ (\tau\beta\gamma)_{111} \end{pmatrix}$$

For 2^{4-1}-fractional factorial design with A, B, C, D all the levels of D-factor should also vary, but we can only take 8 observations.

Let the D-vector, which gives the levels for the D-factor, be given by the formula

$$D = ABC,$$

where ABC is the column vector in $\boldsymbol{F}$ for the coefficient $(\tau\beta\gamma)_{111}$.

Hence, we will have the design

Obs. for 2^3 design	A	B	C	$D = ABC$	Obs. for 2^{4-1} design
$y_{(1)}$	-1	-1	-1	-1	$y_{(1)}$
y_a	1	-1	-1	1	y_{ad}
y_b	-1	1	-1	1	y_{bd}
y_{ab}	1	1	-1	-1	y_{ab}
y_c	-1	-1	1	1	y_{cd}
y_{ac}	1	-1	1	-1	y_{ac}
y_{bc}	-1	1	1	-1	y_{bc}
y_{abc}	1	1	1	1	y_{abcd}

Of course it will be different if we choose $D = -ABC$ instead, or something else.

We analyze the design above with all 16 parameters, but condition $D = ABC$ gives that the parameters $(\tau\beta\gamma)_{111}$ and δ_1 will have the same coefficient vector and we can just estimate the sum $(\tau\beta\gamma)_{111} + \delta_1$.

We say that effect D and effect ABC are **aliases**.

Aliases means that two or more parameters can not be separated as they get exactly the same coefficient vector in the equations that provide parameter estimates.

There are more aliases!

On aliases in the fractional factorial design

In the design matrix $\boldsymbol{F}$ for the complete model there are columns I, A, B, AB, C, $\ldots$ with coefficients of μ, τ_1, β_1, $(\tau\beta)_{11}$, γ_1, $\ldots$, where for example τ_1 is the parameter that describes the main effect of A and $(\tau\beta)_{11}$ is the parameter that describes interaction between A and B.

If we have a fractional factorial design these columns corresponds to the coefficient vectors for additional parameters, which means that certain parameters can not be separated.

One can only estimate their sum, i.e., those effect are **aliases**.

Let I, A, B, AB, ... be the column vectors in the matrix $\boldsymbol{F}$. We know that $AB = A \cdot B$ if the multiplication is elementwise.

Further, $BC = B \cdot C$ and $A^2 = I$, $B^2 = I$ etc.

Hence,

$$D = ABC \iff D^2 = DABC \iff I = ABCD$$

Generator.

$I = ABCD$ is called the **generator** for the design.

With the generator $I = ABCD$ we also have more aliases.

$$\begin{aligned}
A &= A^2BCD = BCD;\\
B &= AB^2CD = ACD;\\
AB &= A^2B^2CD = CD;\\
C &= ABD;\\
AC &= BD;\\
BC &= AD;\\
ABC &= D;\\
I &= ABCD.
\end{aligned}$$

We analyze 2^3-factorial design, but we have the other parameter vector $\boldsymbol{\xi_{mod}}$. Equation

$$\boldsymbol{y} = \boldsymbol{F}\hat{\boldsymbol{\xi}}_{\boldsymbol{mod}}$$

gives estimators of the parameter vector (see Lecture 7).

Hence, we have

$$\frac{1}{8}\boldsymbol{F}' \begin{pmatrix} y_{(1)} \\ y_{ad} \\ y_{bd} \\ y_{ab} \\ y_{cd} \\ y_{ac} \\ y_{bc} \\ y_{abcd} \end{pmatrix} \text{ for the parameter vector } \begin{pmatrix} \mu + (\tau\beta\gamma\delta)_{1111} \\ \tau_1 + (\beta\gamma\delta)_{111} \\ \beta_1 + (\tau\gamma\delta)_{111} \\ (\tau\beta)_{11} + (\gamma\delta)_{11} \\ \gamma_1 + (\tau\beta\delta)_{111} \\ (\tau\gamma)_{11} + (\beta\delta)_{11} \\ (\beta\gamma)_{11} + (\tau\delta)_{11} \\ (\tau\beta\gamma)_{111} + \delta_1 \end{pmatrix} = \boldsymbol{\xi}_{mod}$$

Note that the observations are sorted as in a 2^3 design for the factors A, B, C.

From the normal probability plot we find the interesting effects, but there are now aliases as given above.

If $A, B, AB, \ldots$ denotes the main effects of A resp. B, interaction effect between A and B etc. and I denotes "base effect" that is given by parameter μ, then we have our estimated parameter vector that corresponds to the effects

$$I + ABCD,\ A + BCD,\ B + ACD,\ AB + CD,\\ C + ABD,\ AC + BD,\ BC + AD,\ ABC + D$$

Problem?

The interpretation of the effects must be handled with caution, see for example Example 8.1 in the course book.

No way to estimate the variance σ^2.

For this kind of design it is often appropriate to ignore one or more factors to obtain a reduces design for the most interesting factors.

Resolution

Definition. A design is of **resolution** R if no p-factor effect is aliased with another effect containing less than $R - p$ factors.

The design above has resolution IV.

Resolution IV designs are the designs in which no main effects aliased with any other main effect or with any two-factor interaction, but two-factor interactions are aliased with each other.

Design of type 2^{k-2}

Assume that we want to study k factors, but we want to do only 2^{k-2} measurements.

2^{k-2}**-fractional factorial design:** Construct the complete model for $k-2$ factors for example the first ones. Then, "sacrifice" two appropriate interaction effects and apply the remaining factors of this coefficient columns for the "sacrificed" effects.

Consider which effects can not be separated.

Sometimes one needs to split up experiment to blocks, and then you have to sacrifice further interaction effects.

Example 3

We want to do a 2^{7-3} design with the factors A, B, C, D, E, F, G and one observation per combination, i.e.,16 observations.

Start with a complete design for A, B, C, D, i.e., 16 level combinations with observations

$$(1), a, b, ab, c, ac, bc, abc, d, ad, \ldots, abcd.$$

For the three factors E, F, G we use the rules

$$E = ABC, \quad F = BCD, \quad G = ABD \tag{2}$$

which give the combinations

$$(1), aeg, befg, \ldots, cef, \ldots, abcdefg$$

i.e., the observations that we should take in experiment.

Observations are still sorted as for 2^4-factorial design and we calculated the estimates of parameters in the same way as for 2^4-factorial design.

We treat the parameter vector as the one for 2^4-factorial design but must note that each estimate of parameter in 2^4 design is actually a sum of the estimates of parameters that have the same coefficient vector.

Hence, to interpret the results, we need to find out which parameters have the same coefficient vectors.

We have three generators given by (**??**) above. Making all possible products of them ($\binom{3}{2} + \binom{3}{3} = 4$ products) we obtain all possible generators in chosen design.

The new generators are

$$EF = AD,\ EG = CD,\ FG = AC,\ EFG = B$$

So we can put them all together as

$$I = ABCE,\ I = BCDF,\ I = ABDG,\ I = ADEF,$$
$$I = CDEG,\ I = ACFG,\ I = BEFG.$$

To obtain aliases for, for example, A and BC we multiply each generator with A or BC, respectively. We obtain

$$\begin{aligned} &A + BCE + ABCDF + BDG + DEF \\ &\quad + ACDEG + CFG + ABEFG \end{aligned}$$

and

$$\begin{aligned} &BC + AE + DF + ACDG + ABCDEF \\ &\quad + BDEG + ABFG + CEFG, \end{aligned}$$

respectively.

Each parameter estimation becomes a sum of eight estimated parameters that can not be separated.

This design has resolution IV.

Example 4 (Ex. 3 Lecture 1) – 2^{7-4}

One wants to study how seven factors effect the growth of a special bacteria. Each factor has two levels.

If one want to find the best combination of all levels, the one which gives the best growth, one have to do $2^7 = 128$ studies, which sometimes can be to many.

With a reduced *(fractional) factorial design* it can be enough to do $2^3 = 8$ studies if we choose them smart, to analyze the main effects.

$$
\underbrace{\begin{pmatrix} y_{(1)(def)} \\ y_{a(fg)} \\ y_{b(eg)} \\ y_{ab(d)} \\ y_{c(dg)} \\ y_{ac(e)} \\ y_{bc(f)} \\ y_{abc(defg)} \end{pmatrix}}_{=\boldsymbol{y}}
\text{ with }
\begin{array}{c}
\begin{array}{cccccccc} & & & D= & & E= & F= & G= \\ I & A & B & AB & C & AC & BC & ABC \end{array} \\
\underbrace{\begin{pmatrix}
1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 \\
1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 \\
1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 \\
1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 \\
1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 \\
1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 \\
1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1
\end{pmatrix}}_{=\boldsymbol{F}}
\end{array}
$$

and a parameter vector, if we skip all the interaction effects.
$\boldsymbol{F}$ is the design matrix for the complete 2^3 design.

$$
\boldsymbol{\xi_{mod}} = \begin{pmatrix} \mu \\ \tau_1 \\ \beta_1 \\ \delta_1 \\ \gamma_1 \\ e_1 \\ f_1 \\ g_1 \end{pmatrix}
\begin{array}{l} \\ \\ \\ \leftarrow \text{param. for effect D aliased AB} \\ \\ \leftarrow \text{param. for effect E aliased AC} \\ \leftarrow \text{param. for effect F aliased BC} \\ \leftarrow \text{param. for effect G aliased ABC} \end{array}
$$

The estimators for the parameters are the solution to the equation

$$
\boldsymbol{y} = \boldsymbol{F}\hat{\boldsymbol{\xi}}_{\boldsymbol{mod}}.
$$

One can analyses the problem with a few numbers of observations, but then with a very limited model / design.

Conclusion

Try to **avoid** designs like this.

Always verify your results with extra observations.

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