01NEX - Lecture 07 2^k Factorial Design (2) Center point, Blocking, Confounding

Jiri Franc

Czech Technical University
Faculty of Nuclear Sciences and Physical Engineering
Department of Mathematics

Last Lesson - A single Replicate 2^k **Designs**

- 2^k factorial design is a design with one observation at each corner of the "cube" and sometimes is called single replicated design.
- Very widely used type of design, especially in first planning and testing.
- If the factors are spaced too closely, it increases the chances that the noise will overwhelm the signal in the data.
- More aggressive spacing is usually best.
- Lack of replication causes potential problems in statistical testing:
 - With no replication, fitting the full model results in zero degrees of freedom for error.
 - Omit higher-order interactions and estimate error.
 - Normal probability plotting of effects (Daniels,1959).
 - Lenth's method Pareto plot (Lenth, 1989).
- Create contour plots and find optimal settings for numerical variables.

2^k Designs are Optimal Designs

Two-level factorial designs have many interesting properties. One of the most useful is that 2^k designs minimize the variance of the model regression coefficients.

Consider a simple case the 2² design with one replicate and coded variables.

The regression model fitted to the data is

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \varepsilon.$$

Four runs in this design in terms of the regression model are

(1) =
$$\beta_0 + \beta_1(-1) + \beta_2(-1) + \beta_{12}(-1)(-1) + \varepsilon_1$$

 $a = \beta_0 + \beta_1(1) + \beta_2(-1) + \beta_{12}(1)(-1) + \varepsilon_2$
 $b = \beta_0 + \beta_1(-1) + \beta_2(1) + \beta_{12}(-1)(1) + \varepsilon_3$
 $ab = \beta_0 + \beta_1(1) + \beta_2(1) + \beta_{12}(1)(1) + \varepsilon_4$

In matrix form

$$\mathbf{v} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}.$$

2^k Designs are Optimal Designs (2)

Regression coefficients β 's are estimated by the Ordinary Least Squares (OLS)

$$\hat{\boldsymbol{\beta}}^{(OLS)} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}.$$

where

The $\mathbf{X}'\mathbf{X}$ matrix is diagonal because the 2^k designs are orthogonal.

2^k Designs are Optimal Designs (3)

In 2^2 example the regression coefficients β 's are

$$\hat{\beta}^{(OLS)} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y} = \begin{pmatrix} \frac{(1)+a+b+ab}{-(1)+a-b+ab} \\ \frac{-(1)-a+b+ab}{4} \\ \frac{-(1)-a+b+ab}{4} \\ \frac{(1)-a-b+ab}{4} \end{pmatrix}$$

The least squares estimates of the model regression coefficients are exactly equal to one-half of the usual effect estimates!

It turns out that the variance of any model regression coefficient is easy to find

$$Var(\hat{\beta}) = \frac{\sigma^2}{\text{diagonal elements of } \mathbf{X}'\mathbf{X}} = \frac{\sigma^2}{n2^k} = \frac{\sigma^2}{N}.$$

All model regression coefficients have the same variance and this is the minimum possible variance for the regression coefficient.

2^k Designs are Optimal Designs (3)

For fitting the first-order model or the first-order model with interaction, the 2^k design is (equations for 2^2 design)

- D-optimal: design minimizes the variance of the model regression coefficients.
- G-optimal: the model that we fit to the data from the experiment minimizes the maximum prediction variance over the design region.

$$Var(\hat{y}(x_1, x_2)) = Var(\hat{\beta}_0 + \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2 + \hat{\beta}_{12} x_1 x_2)$$
$$= \frac{\sigma^2}{4} (1 + x_1 + x_2 + x_1 x_2)$$

▶ I-optimal: the smallest possible value of the average prediction variance that can be obtained from a k-run design.

$$I = \frac{1}{A} \int_{-1}^{1} \int_{-1}^{1} Var(\hat{y}(x_1, x_2)) dx_1 dx_2$$

=
$$\frac{1}{4} \int_{-1}^{1} \int_{-1}^{1} \frac{\sigma^2}{4} (1 + x_1 + x_2 + x_1 x_2) dx_1 dx_2 = \frac{4\sigma^2}{9},$$

where A is the volume of the design space.

Addition of Center Points to a 2^k Designs

In two level factorial design we assume linearity in the factor effects. If the interaction is presented in the model, the curvature in the response function can be modeled by different ways.

First-order model (interaction)

$$y = \beta_0 + \sum_{j=1}^k \beta_j x_j + \sum_{i < j} \beta_{ij} x_i x_j + \epsilon$$

Second-order response surface model

$$y = \beta_0 + \sum_{j=1}^{k} \beta_j x_j + \sum_{i < j} \beta_{ij} x_i x_j + \sum_{j=1}^{k} \beta_{jj} x_j^2 + \epsilon$$

Addition of Center Points

- Based on the idea of replicating some of the runs in a factorial design.
- Runs at the center provide an estimate of error and allow the experimenter to distinguish between models.

The method is based on replicating certain point in a 2^k factorial that will provide protection against curvature from the second order effects as well as allow an independent estimate of error to be obtained.

- ▶ Center point consists of n_C replicates run in $x_1 = x_2 = ... = x_k = 0$.
- k factors have to be quantitative.
- Center points do not affects the usual estimates in 2^k design.

Addition of Center Points to a 2^k Designs

Compute

- $ightharpoonup ar{y}_F$ the average of all runs at the all factorial points
- $ightharpoonup \bar{y}_C$ the average of the n_C runs at the center point
- $ightharpoonup ar{y}_F ar{y}_C$ the difference between two averages

If the difference $\bar{y}_F - \bar{y}_C$ is small, then the center point lie on or near the hyperplane passing through the factorial points.

If the difference $\bar{y}_F - \bar{y}_C$ is large, then the quadratic curvature is present.

A single-degree-of-freedom sum of squares for pure quadratic curvature

$$SS_{Pure\ quadratic} = \frac{n_F n_C (\bar{y}_F - \bar{y}_C)^2}{n_F + n_C}$$

SS can be incorporated into ANOVA and run hypothesis testing

$$H_0: \sum_{j=1}^k \beta_{jj} = 0 \quad H_1: \sum_{j=1}^k \beta_{jj} \neq 0.$$

Instead of ANOVA we can use a t-test to test for curvature (in estimation of regression coefficients in a linear model with).

Example from the last lesson - Unreplicated 2^k **Factorial Designs**

The 2⁴ factorial design was used to investigate the effects of four factors on the filtration rate of a resin for a chemical process plant. The factors are:

A: temperature,

B: pressure,

C: concentration of chemical formaldehyde,

D: stirring rate.

Run	01	Fa	ctor			Filtration Rate
Number	A	В	С	D	Run Label	(gal/h)
1	-	-	-	-	(1)	45
2	+	-	-	-	а	71
3	-	+	-	= .	ь	48
4	+	+	-	(-	ab	65
5	_	-	+	=	c	68
6	+	_	+	_	ac	60
7	2	+	+	43	bc	80
8	+	+	+	-	abc	65
9	-	-	-	+	d	43
10	+	-	-	+	ad	100
11	7	+	-	+	bd	45
12	+	+		+	abd	104
13	-	-	+	+	cd	75
14	+	-	+	+	acd	86
15	_	+	+	+	bcd	70
16	+	+	+	+	abcd	96

Unreplicated 2^k **Factorial Designs**

Pilot Plant Filtration Rate Experiment - FrF2 package

```
Factor settings: Responses:
A B C D
                [1] Filtration
1 -1 -1 -1 -1
2 1 1 1 1
The design itself:
A B C D Filtration A B C D Filtration
1 -1 -1 -1 -1
                    45 -1 -1 -1 1
                                         43
2 1 -1 -1 -1
                   71 \quad 1 \quad -1 \quad -1 \quad 1
                                         100
3 -1 1 -1 -1
                    48 -1 1 -1 1
                                         45
4 1 1 -1 -1
                    65 1 1 -1 1
                                         104
5 -1 -1 1 -1
                    68 \quad -1 \quad -1 \quad 1 \quad 1
                                         75
6 1 -1 1 -1
                   60 1 -1 1 1
                                         86
                   80 -1 1 1 1
7 -1 1 1 -1
                                         70
 1 1 1 -1
                    65 1 1 1 1
                                         96
```

Pilot Plant Filtration Rate Experiment

Box plot

boxplot(Filtration ~ A , main = "Factor A - Temperature")

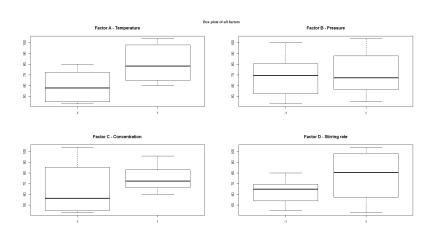


Illustration of center points adding in Pilot Plant Filtration Rate Experiment

Suppose that four center points are added to this experiment, and at the points $x_1 = x_2 = x_3 = x_4 = 0$ the four observed filtration rates were 73, 75, 66, 69.

The average of four center points is $\bar{y}_C = 70.75$, and the average of the 16 factorial runs is $\bar{y}_F = 70.06$. Since are very similar, we suspect that there is no strong curvature present.

$$MS_{E} = \frac{SS_{E}}{n_{C} - 1} = \frac{\sum_{Center\ points} (y_{i} - \bar{y})}{n_{C} - 1} = \frac{\sum_{i=1}^{4} (y_{i} - 70.75)^{2}}{4 - 1} = 16.25$$

$$SS_{Pure\ quadratic} = \frac{n_{F}n_{C}(\bar{y}_{F} - \bar{y}_{C})^{2}}{n_{F} + n_{C}} = \frac{(16)(4)(-0.69)^{2}}{16 + 4} = 1.51$$

Pure Error has 3 DF and Curvature has only 1 DF. The F-statistic is 0.093 and the P-value of the test is 0.780924.

We cannot reject the null hypothesis!

Addition of Center Points to a 2^k Designs

Anova tables for design with center points.

```
> rate3$E <- c(rep(0,times=16),rep(1,times=4))</pre>
> aov model2= aov(Rate~A*B*C*D+E, data=rate3)
> summary(aov_model2)
Df Sum Sq Mean Sq F value Pr(>F)
           1 1870.6 1870.6 115.112 0.00173 **
Α
В
           1 39.1 39.1 2.404 0.21882
           1 390.1 390.1 24.004 0.01627 *
С
D
           1 855.6 855.6 52.650 0.00540 **
F.
           1 1.5 1.5 0.093 0.78024
A:B
           1 0.1 0.1 0.004 0.95445
    1 1314.1 1314.1 80.865 0.00290 **
A:C
B:C
           1 22.6 22.6 1.388 0.32362
A:D
           1 1105.6
                   1105.6 68.035 0.00373 **
           1 0.6 0.6 0.035 0.86427
B:D
C:D
           1 5.1 5.1 0.312 0.61569
A:B:C
           1 14.1 14.1 0.865 0.42086
           1 68.1 68.1 4.188 0.13320
A:B:D
A:C:D
           1 10.6 10.6 0.650 0.47910
           1 27.6 27.6 1.696 0.28376
B:C:D
A:B:C:D
          1 7.6 7.6 0.465 0.54407
Residuals 3 48.8 16.2
```

 $SS_{Purequadratic} = 1.51$ and $SS_{Pureerror} = 48.75$

Anova tables for original design and for design with center points.

```
> anova(aov(Filtration2~A*C+A*D, data=rate2))
Response: Filtration2
         Df Sum Sq Mean Sq F value Pr(>F)
Α
          1 1870.56 1870.56 95.865 1.928e-06 ***
          1 390.06 390.06 19.990 0.001195 **
С
          1 855.56 855.56 43.847 5.915e-05 ***
D
   1 1314.06 1314.06 67.345 9.414e-06 ***
A:C
   1 1105.56 1105.56 56.659 1.999e-05 ***
A:D
Residuals 10 195.13 19.51
> anova(aov(Filtration4~A*C+A*D, data=rate4))
Response: Filtration4
         Df Sum Sq Mean Sq F value Pr(>F)
          1 1870.56 1870.56 106.721 6.235e-08 ***
Α
С
          1 390.06 390.06 22.254 0.0003301 ***
D
          1 855.56 855.56 48.812 6.382e-06 ***
A:C
   1 1314.06 1314.06 74.971 5.389e-07 ***
       1 1105.56 1105.56 63.075 1.490e-06 ***
A:D
Residuals 14 245.39 17.53
```

Is a quadratic effect needed (is the cube indificator significant)?

Coefficients:

```
Estimate Std. Error t value Pr(>|t|)
                70.7500
                           2.1656 32.670 7.27e-14 ***
(Intercept)
                10.8125
                           1.0828 9.986 1.83e-07 ***
Α
                4.9375
                           1.0828 4.560 0.000535 ***
C
                7.3125
                           1.0828 6.753 1.36e-05 ***
iscube(rate4)TRUE -0.6875 2.4212 -0.284 0.780924
              -9.0625
                           1.0828 -8.369 1.36e-06 ***
A:C
               8.3125
                           1.0828 7.677 3.50e-06 ***
A:D
```

Residual standard error: 4.331 on 13 degrees of freedom Multiple R-squared: 0.9578, Adjusted R-squared: 0.9383 F-statistic: 49.2 on 6 and 13 DF, p-value: 3.424e-08

The null hypothesis cannot be rejected.

Function iscube produce factor variable, generally we can add any quadratic variable by $\mathbb{I}(\mathbb{A}^2)$:

```
lm.default(formula = Filtr \sim A + C + D + A:C + A:D + I(A^2),
data = rate num2)
Residuals:
Min 1Q Median 3Q Max
-6.3750 -1.8750 0.0625 2.9062 5.7500
Coefficients:
Estimate Std. Error t value Pr(>|t|)
(Intercept) 70.7500 2.1656 32.670 7.27e-14 ***
A
           10.8125 1.0828 9.986 1.83e-07 ***
C
          4.9375 1.0828 4.560 0.000535 ***
          7.3125 1.0828 6.753 1.36e-05 ***
D
I(A^2) -0.6875 2.4212 -0.284 0.780924
A:C -9.0625 1.0828 -8.369 1.36e-06 ***
         8.3125 1.0828 7.677 3.50e-06 ***
A : D
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 '' 1
Residual standard error: 4.331 on 13 degrees of freedom
Multiple R-squared: 0.9578, Adjusted R-squared: 0.9383
F-statistic: 49.2 on 6 and 13 DF, p-value: 3.424e-08
```

Blocking in the 2^k Factorial Design

Sometimes, it is not feasible or practical to run completely randomized experiment.

- Blocking is a technique for dealing with controllable nuisance variables (design factors that probably have an effect on the response, but we are not interested in that effect)
- ► Two cases are considered (Replicated designs x Unreplicated designs)
- If there are *n* replicates of the design, then each replicate is a block
- Each replicate is run in one of the blocks (time periods, batches of raw material, etc.)
- Runs within the block are randomized

Simple Blocking Example

Chemical Process Example

A - reactant concentration, B - catalyst amount, y - recovery Nuisance Variable - Raw Materials. Only four trials per batch.

	Factor A B		Factor Treatment		Replicate		
			Combination	I	П	Ш	Total
(1)	_	_	A low, B low	28	25	27	80
a	+	-	A high, B low	36	32	32	100
b		: +:	A low, B high	18	19	23	60
ab	+	+	A high, B high	31	30	29	90

Simple Blocking Example

2 factors, 3 replicates (blocks)

	Block 1	Block 2	Block 3
	(1) = 28	(1) = 25 $a = 32$	(1) = 27
	(1) = 28 $a = 36$	a = 32	(1) = 27 $a = 32$
	b = 18	b = 19	b = 23
	ab = 31	ab = 30	ab = 29
Block totals:	$B_1 = 113$	$B_2 = 106$	$B_3 = 111$

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0	P-Value
Blocks	6.50	2	3.25		
A (concentration)	208.33	1	208.33	50.32	0.0004
B (catalyst)	75.00	1	75.00	18.12	0.0053
AB	8.33	1	8.33	2.01	0.2060
Error	24.84	6	4.14		
Total	323.00	11			

Confounding in the 2^k Factorial Design

What do we do if the block size is smaller than the number of treatment combinations in one replicate?

- Consider the 2⁵ case. May be impossible to replicate all in one block.
- Information about higher order interactions become confounded with the blocks.

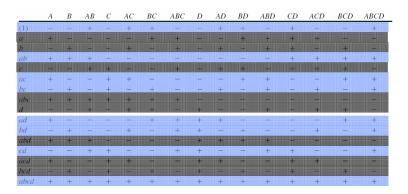
How do we confound into two blocks?

- Choose highest order interaction.
- ightharpoonup For this contrast, assign all + to one block, and all to the other block.
- Randomize the order in which the experiments are run within the block.

Number	A	B	C	D	Run Label	(gal/h)
1	_	-	-	-	(1)	45
2	+	-	-	-	а	71
3	_	+	-	-	b	48
4	+	+	_	_	ab	65
5	_	-	+	-	С	68
6	+	-	+	-	ac	60
7	_	+	+	-	bc	80
8	+	+	+	-	abc	65
9	_	-	-	+	d	43
10	+	-	-	+	ad	100
11	_	+	-	+	bd	45
12	+	+	-	+	abd	104
13	_	-	+	+	cd	75
14	+	_	+	+	acd	86
15	_	+	+	+	bcd	70
16	+	+	+	+	abcd	96

Suppose only 8 runs can be made from one batch of raw material.

Suppose only 8 runs can be made from one batch of raw material



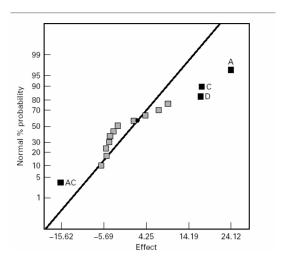
Example of confounding with ABCD interaction.

The ABCD interaction (or the block effect) will not considered as part of the error term.

The result of the analysis will be unchanged from mentioned example.

Let the first eight runs (in run order) have filtration rate reduced by 20 units. This is the simulated "block effect".

Run Order	Std. Order	Factor A: Temperature	Factor B: Pressure	Factor <i>C</i> : Concentration	Factor D: Stirring Rate	Response Filtration Rate
8	1	-1	-1	-1	-1	25
11	2	1	-1	-1	-1	71
1	3	-1	1	-1	-1	28
3	4	1	1	-1	-1	45
9	5	-1	-1	1	-1	68
12	6	1	-1	1	-1	60
2	7	-1	1	1	-1	60
13	8	1	1	1	-1	65
7	9	-1	-1	-1	1	23
6	10	1	-1	-1	1	80
16	11	-1	1	-1	1	45
5	12	1	1	-1	1	84
14	13	-1	-1	1	1	75
15	14	1	-1	1	1	86
10	15	-1	1	1	1	70
4	16	1	1	1	1	76



From the previous case one important interaction is not identified (AD).

Failing to block when we should have causes problems in interpretation the result of an experiment and can mask the presence of real factor effects.

Suggested Blocking Arrangements for the 2^k Factorial Design

Number of Factors, k	Number of Blocks, 2 ^p	Block Size, 2 ^{k-p}	Effects Chosen to Generate the Blocks	Interactions Confounded with Blocks
3	2	4	ABC	ABC
	4	2	AB, AC	AB, AC , BC
4	2	8	ABCD	ABCD
	4	4	ABC, ACD	ABC, ACD, BD
	8	2	AB, BC, CD	AB, BC, CD, AC, BD, AD, ABCD
5	2	16	ABCDE	ABCDE
	4	8	ABC, CDE	ABC, CDE, ABDE
	8	4	ABE, BCE, CDE	ABE, BCE, CDE, AC, ABCD, BD, ADE
	16	2	AB, AC, CD, DE	All two- and four-factor interactions (15 effects)
6	2	32	ABCDEF	ABCDEF
	4	16	ABCF, CDEF	ABCF, CDEF, ABDE
	8	8	ABEF, ABCD, ACE	ABEF, ABCD, ACE, BCF, BDE, CDEF, ADF
	16	4	ABF, ACF, BDF, DEF	ABF, ACF, BDF, DEF, BC, ABCD, ABDE, AD, ACDE, CE, CDF, BCDEF, ABCEF, AEF, BE
	32	2	AB, BC, CD, DE, EF	All two-, four-, and six-factor interactions (31 effects)
7	2	64	ABCDEFG	ABCDEFG
	4	32	ABCFG, CDEFG	ABCFG, CDEFG, ABDE
	8	16	ABCD, CDEF, ADFG	ABC, DEF, AFG, ABCDEF, BCFG, ADEG, BCDEG
	16	8	ABCD, EFG, CDE, ADG	ABCD, EFG, CDE, ADG, ABCDEFG, ABE, BCG, CDFG, ADEF, ACEG, ABFG, BCEF, BDEG, ACF, BDF

Blocking with more than two block

- ▶ The two level factorial can be confounded in 2, 4, 8, ... (2p, p > 1) blocks.
- For four blocks, select two effects to confound, automatically confounding a third effect.
- Choice of confounding schemes non trivial see enclosed paper.

Blocking - summary, again

- Block when you can and randomize what you cannot.
- When in doubt, block.
- Block out the nuisance variables you know about, randomize as much as possible and rely on randomization to help balance out unknown nuisance effects.

Exercises

Exercise:

Finish problems 6.31 and 6.32 from the last lecture.

Exercise:

Solve problems 6.26, 6.27 following by 7.7 and 7.8. described below (from C. Montgomery DAoE - 8. edition).

An experiment was run in a semiconductor fabrication plant in an effort to increase yield. Five factors, each at two levels, were studied. The factors (and levels) were A = aperture setting (small, large), B = exposure time (20% below nominal, 20% above nominal), C = development time (30 and 45 s), D = mask dimension (small, large), and E = etch time (14.5 and 15.5 min). The unreplicated 2^5 design was run.

(1) = 7	d = 8	e = 8	de = 6
a = 9	ad = 10	ae = 12	ade = 10
b = 34	bd = 32	be = 35	bde = 30
ab = 55	abd = 50	abe = 52	abde = 53
c = 16	cd = 18	ce = 15	cde = 15
ac = 20	acd = 21	ace = 22	acde = 20
bc = 40	bcd = 44	bce = 45	bcde = 41
abc = 60	abcd = 61	abce = 65	abcde = 63

Exercises

- Construct a normal probability plot of the effect estimates. Which effects appear to be large?
- 2. Conduct an analysis of variance to confirm your findings for part (1).
- Write down the regression model relating yield to the significant process variables.
- 4. Plot the residuals on normal probability paper. Is the plot satisfactory?
- Plot the residuals versus the predicted yields and versus each of the five factors. Comment on the plots.
- 6. Interpret any significant interactions.
- 7. What are your recommendations regarding process operating conditions?
- 8. Project the 2⁵ design in this problem into a 2^k design in the important factors. Sketch the design and show the average and range of yields at each run. Does this sketch aid in interpreting the results of this experiment?

Exercises

- 9. Suppose that the experimenter had run four center points in addition to the 32 trials in the original experiment. The yields obtained at the center point runs were 68, 74, 76, and 70. Reanalyze the experiment, including a test for pure quadratic curvature. Discuss what your next step would be.
- Construct and analyze a design in two blocks with ABCDE confounded with blocks.
- Construct and analyze a design in four blocks. Suggest a reasonable confounding scheme.