01NAEX - Lecture 05
Introduction to 2^k Factorial Design

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Introduction to 2^k Factorial Design

By a factorial design, we mean that in each complete replication of the experiment all possible combinations of the levels of the factors are investigated.

- 2^k Factorial Design is special case of the general factorial design with k factors, all at 2 levels.
- The two levels are usually called low (-) and high (+).
- 2^k Factorial Design is widely used in industrial experimentation, especially in the early stages of experimental work, when many factors are likely to be investigated.

Factors could be

- **quantitative**
  (such as two values of temperature, pressure, time, ...)
- **qualitative**
  (two operators, male and female, presence and absence)

It is assumed that **response is approximately linear over the range chosen.**

We assume that

- factors are fixed,
- the design is completely randomized,
- the usual normality assumptions are satisfied.

The analysis procedure for a Factorial Design includes:

- Select factors and their range.
- Design formulation.
- Estimation of factor effects.
- Model formulation.
- Statistical testing (ANOVA).
- Refine the model.
- Analyze residuals (graphical).
- Interpret results.

The 2^2 Design - Chemical process example

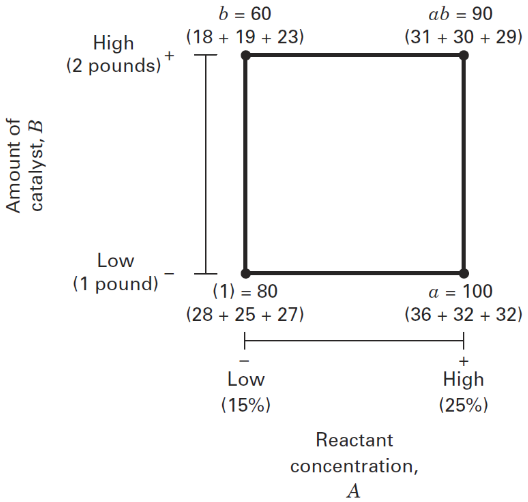
The 2^2 Design is the simplest case. In this example we consider an investigation into the effect of the concentration of the reactant and the amount of the catalyst on converision in a chemical process.

	Factor A	Factor B	Treatment Combination	Replicate I	Replicate II	Replicate III	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

- factor A - reactant concentration
- factor B - catalyst amount
- response y - recovery

The goal is to determine if adjustments to these factors would increase yield.

Treatment combinations in the Chemical process example of 2^2 design



- Low (-) and high (+) levels of a factor are arbitrary terms.
- The high level of any factor in the treatment combination is denoted by the corresponding lowercase letter.
- (1) is used to denote both factors at the low level.

The 2^2 Design - Estimation of factor effects

The symbols (1), *a, b, and ab represents the total of all n replicates taken at the treatment combinations.*

$$
\begin{array}{lll}
\textbf{\textit{main effect of A:}} & A & = \frac{1}{2n}(ab + a - b - (1)) = \bar{y}_{A^+} - \bar{y}_{A^-} \\
\textbf{\textit{main effect of B:}} & B & = \frac{1}{2n}(ab - a + b - (1)) = \bar{y}_{B^+} - \bar{y}_{B^-} \\
\textbf{\textit{interaction effect of AB:}} & AB & = \frac{1}{2n}(ab - a - b + (1))
\end{array}
$$

*Where the **interaction effect AB** is defined as the average difference between the effect of A at high level of B and the effect of A at the low level of B.*

The 2^2 Design - Chemical process example

The estimation of average effects in chemical process example is:

$$
\begin{array}{llcl}
\textbf{main effect of A} & A & = & \frac{1}{2\times 3}(90+100-60-80) = 8.33 \\
\textbf{main effect of B} & B & = & \frac{1}{2\times 3}(90+60-100-80) = 5.00 \\
\textbf{interaction effect of AB} & AB & = & \frac{1}{2\times 3}(90+80-100-60) = 1.67
\end{array}
$$

Faster manually calculating of sum of squares: $SS_A = \frac{[Contrast_A^2]}{N}$.

$$
\begin{aligned}
SS_A &= \tfrac{1}{12}(90+100-60-80)^2 = 208.33 \\
SS_B &= \tfrac{1}{12}(90+60-100-80)^2 = 75.00 \\
SS_{AB} &= \tfrac{1}{12}(90+80-100-60)^2 = 8.33 \\
SS_T &= \sum_{i=1}^{2}\sum_{j=1}^{2}\sum_{k=1}^{n} y_{ijk}^2 - \frac{y_{...}^2}{N} = 323.00 \\
SS_E &= SS_T - SS_A - SS_B - SS_{AB} = 31.33
\end{aligned}
$$

The 2^2 Design - Chemical process example

The Analysis of Variance for the Chemical process example, model with interaction effect:

```
> summary(yield.aov1 <- aov(yield~reactant*catalyst))
                  Df  Sum Sq Mean Sq F value   Pr(>F)
reactant           1  208.33  208.33  53.191 8.44e-05 ***
catalyst           1   75.00   75.00  19.149  0.00236 **
reactant:catalyst  1    8.33    8.33   2.128  0.18278
Residuals          8   31.33    3.92
---------
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1
```

Recap: Notation in R and Python statsmodels.formula.api:

- $Y \sim X$ response variable Y is is modeled as a function of predictor X.
- $+X$ add (include) another explanatory variable X.
- $-X$ delete (exclude) variable X.
- $X : Z$ include the interaction between explanatory variables X and Z.
- $*$ include the explanatory variables X, Z, and the interactions between them.

The 2^2 Design - Chemical process example

The Analysis of Variance for the Chemical process example, model without interaction effect:

```
> summary(yield.aov2 <- aov(yield~reactant+catalyst))
            Df Sum Sq Mean Sq F value   Pr(>F)
reactant     1 208.33  208.33   47.27 7.27e-05 ***
catalyst     1  75.00   75.00   17.02  0.00258 **
Residuals    9  39.67    4.41


> anova(yield.aov2,yield.aov1)
Analysis of Variance Table

Model 1: yield ~ reactant + catalyst
Model 2: yield ~ reactant * catalyst
  Res.Df    RSS Df Sum of Sq      F Pr(>F)
1      9 39.667
2      8 31.333  1    8.3333 2.1277 0.1828

---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1
```

The 2^2 Design - Chemical process example

The summary of linear regression model with coded variables $x_i = \pm 1$.

In our example $x_1 = +1$, if concentration is at the high level and -1 if concentration is at the low level. Other variables in the same way.

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3$$

```
Call:    lm(formula = yield ~ reactant.num * catalyst.num)
Coefficients:
                         Estimate Std.Error t value Pr(>|t|)
(Intercept)              27.5000  0.5713   48.135  3.84e-11***
reactant.num              4.1667  0.5713    7.293  8.44e-05***
catalyst.num             -2.5000  0.5713   -4.376  0.00236 **
reactant.num:catalyst.num 0.8333  0.5713    1.459  0.18278

Residual standard error: 1.979 on 8 degrees of freedom
Multiple R-squared: 0.903,     Adjusted R-squared: 0.8666
F-statistic: 24.82 on 3 and 8 DF,  p-value: 0.0002093
```

$$y = 27.5 + 4.2x_1 - 2.5x_2 + 0.8x_3$$

Note: $x_3 = x_1 \cdot x_2$.

The 2^2 Design - Chemical process example

Since the influence of the interaction effect is not significance, we remove it from the model:

```
Call:   lm(formula = yield ~ reactant.num + catalyst.num)
Coefficients:
                Estimate Std. Error t value Pr(>|t|)
(Intercept)      27.500      0.606  45.377 6.13e-12 ***
reactant.num      4.167      0.606   6.875 7.27e-05 ***
catalyst.num     -2.500      0.606  -4.125  0.00258 **

Residual standard error: 2.099 on 9 degrees of freedom
Multiple R-squared: 0.8772,     Adjusted R-squared: 0.8499
F-statistic: 32.14 on 2 and 9 DF,  p-value: 7.971e-05

> anova(yield.lm_coded2,yield.lm_coded1)
Analysis of Variance Table
Model 1: yield ~ reactant.num + catalyst.num
Model 2: yield ~ reactant.num * catalyst.num
  Res.Df    RSS Df Sum of Sq      F Pr(>F)
1      9 39.667
2      8 31.333  1    8.3333 2.1277 0.1828
```

The 2^2 Design - Chemical process example

The linear regression model in natural factors levels:

```
Call: lm(formula = yield ~ reactant.num + catalyst.num)
Coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept)   18.3333     3.0902   5.933  0.00022 ***
reactant.num   0.8333     0.1212   6.875 7.27e-05 ***
catalyst.num  -5.0000     1.2121  -4.125  0.00258 **

Residual standard error: 2.099 on 9 degrees of freedom
Multiple R-squared: 0.8772,     Adjusted R-squared: 0.8499
F-statistic: 32.14 on 2 and 9 DF,  p-value: 7.971e-05
```

Conversion between Coded and Natural Variables:

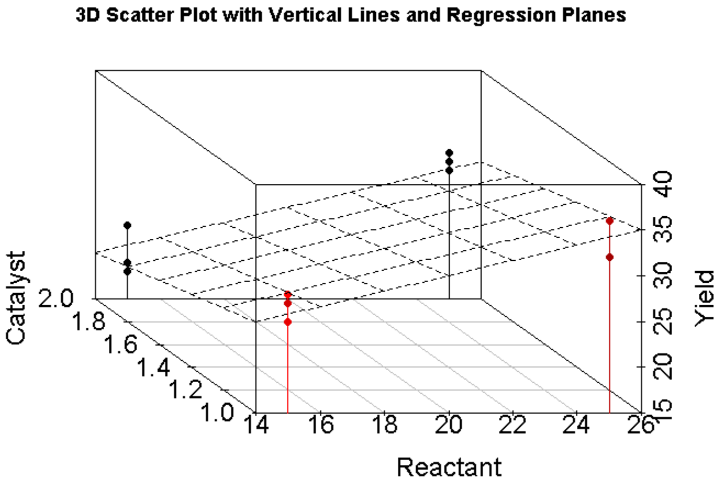
$$\begin{aligned}\hat{y} &= 27.5 + 4.2\left(\frac{Con - (Con_l + Con_h)/2}{(Con_h - Con_l)/2}\right) - 2.5\left(\frac{Cat - (Cat_l + Cat_h)/2}{(Cat_h - Cat_l)/2}\right)\\ &= 18.3 + 0.83 \cdot Concentration - 5.00 \cdot Catalyst\end{aligned}$$

Concentration: Low = 15 and High = 25

Catalyst: Low = 1 and High = 2

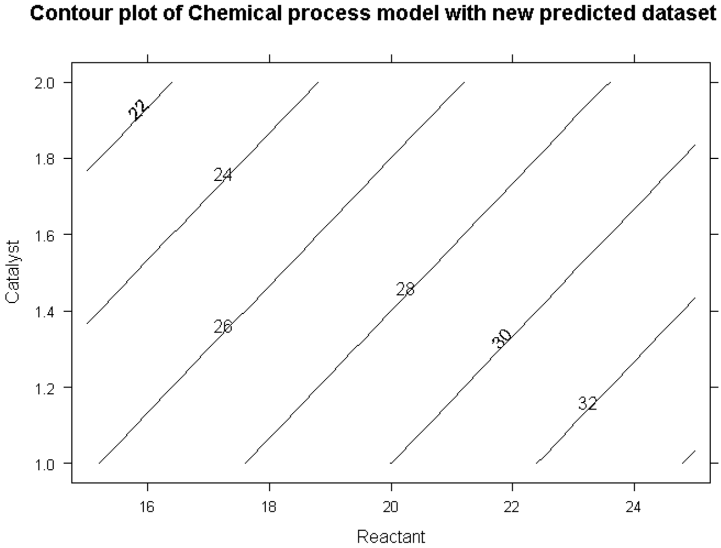
The 2^2 Design - Chemical process example

The linear regression model in natural factors levels can be used to generate response surface plots.



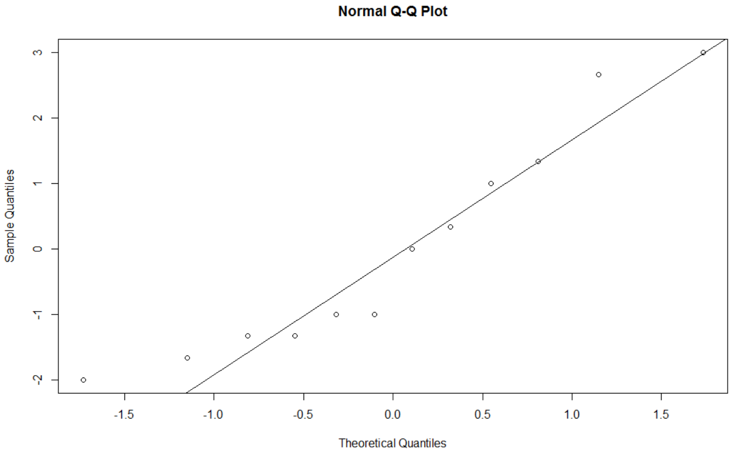
The 2^2 Design - Chemical process example

The linear regression model in natural factors levels can be used to generate response contour plots.



The 2^2 Design - Chemical process example

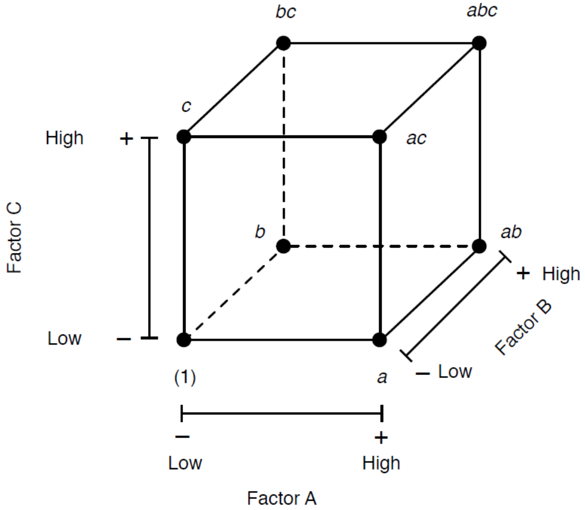
The model adequacy checking - normal plot of residuals.



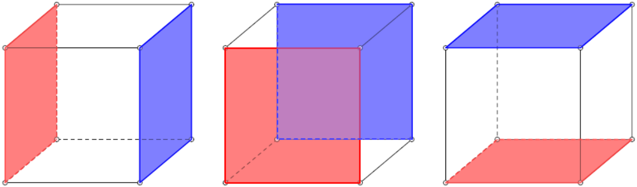
+ perform all normality and homoscedasticity tests.

The 2^3 Design

If we now consider three factors, A, B, and C, we obtain a 2^3 factorial design with eight treatment combinations that can be displayed as a cube.

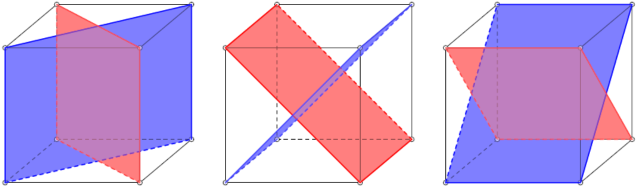


Geometric presentation of contrast corresponding to the main effects and interactions in the 2^3 factorial design.



A B C

(a) Main effects

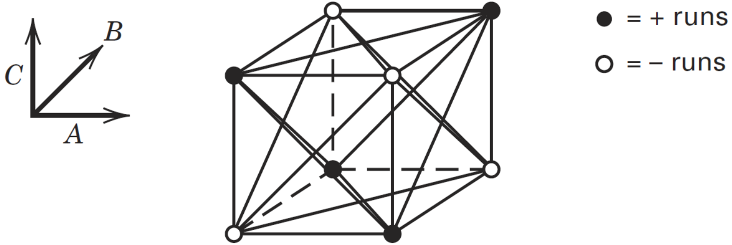


AB AC BC

(b) Two-factor interaction

The 2^3 Design

Geometric presentation of contrast corresponding to the main effects and interactions in the 2^3 factorial design.



ABC

The 2^3 Design

Three different notations used for the runs in the 2^k design:

Run	A	B	C	Labels	A	B	C
1	-	-	-	(1)	0	0	0
2	+	-	-	a	1	0	0
3	-	+	-	b	0	1	0
4	+	+	-	ab	1	1	0
5	-	-	+	c	0	0	1
6	+	-	+	ac	1	0	1
7	-	+	+	bc	0	1	1
8	+	+	+	abc	1	1	1

- $\pm$ notation is called Yates's order.
- Lowercase letter label to identify the treatment combinations.
- 1 and 0 denote high and low factor levels.

The 2^3 Design

Algebraic Signs for Calculating Effects in the 2^3 Design:

Treatment Combination	Factorial Effect							
	I	A	B	AB	C	AC	BC	ABC
(1)	+	−	−	+	−	+	+	−
a	+	+	−	−	−	−	+	+
b	+	−	+	−	−	+	−	+
ab	+	+	+	+	−	−	−	−
c	+	−	−	+	+	−	−	+
ac	+	+	−	−	+	+	−	−
bc	+	−	+	−	+	−	+	−
abc	+	+	+	+	+	+	+	+

Note that except for column I, every column has an equal number of $+$ and $-$ signs.
The product of any two columns yields a column in the table (i.e. $A \times B = AB$, $AB \times BC = AB^2C = AC$).
Orthogonality is an important property shared by all factorial designs.

The estimation of average effects:

$$\begin{aligned}
&\textbf{main effect of A:} & A &= \bar{y}_{A^+} - \bar{y}_{A^-} \\
& & &= \tfrac{1}{4n}\,(a + ab + ac + abc - (1) - b - c - bc) \\
&\textbf{main effect of B:} & B &= \bar{y}_{B^+} - \bar{y}_{B^-} \\
& & &= \tfrac{1}{4n}\,(b + ab + bc + abc - (1) - a - c - ac) \\
&\textbf{main effect of C:} & C &= \bar{y}_{C^+} - \bar{y}_{C^-} \\
& & &= \tfrac{1}{4n}\,(c + ac + bc + abc - (1) - a - b - ab) \\
&\textbf{interaction of AB:} & AB &= \tfrac{1}{4n}\,(abc + ab + c + (1) - a - b - ac - bc) \\
&\textbf{interaction of AC:} & AC &= \tfrac{1}{4n}\,(abc + ac + b + (1) - a - c - ab - bc) \\
&\textbf{interaction of BC:} & BC &= \tfrac{1}{4n}\,(abc + bc + a + (1) - b - b - ab - ac) \\
&\textbf{interaction of ABC:} & ABC &= \tfrac{1}{4n}\,(abc + a + b + c - ab - ac - bc - (1))
\end{aligned}$$

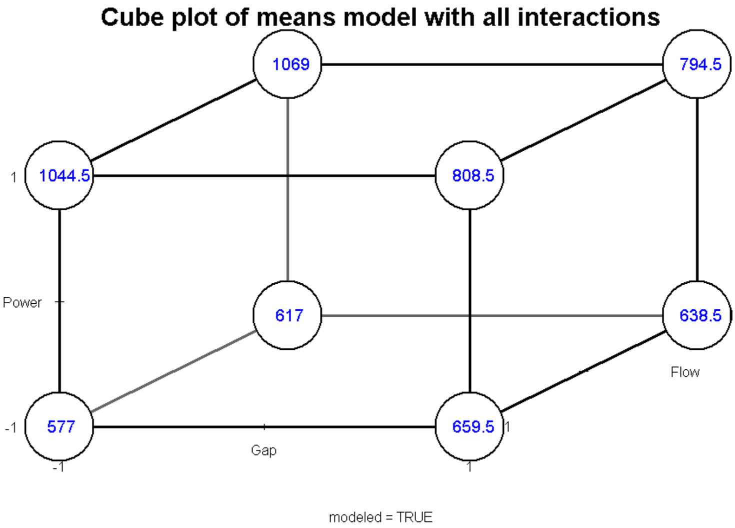
The 2^3 Design - The Etch Plasma Experiment

The design factors are

- A: gap between electrodes in cm
  Low (-1) 0.8 and High (+1) 1.2
- B: gas C_2F_6 flow in SCCM
  Low (-1) 125 and High (+1) 200
- C: RF power applied to the cathode in W
  Low (-1) 275 and High (+1) 325

	Coded Factors			Etch Rate		
Run	A	B	C	Replicate 1	Replicate 2	Total
1	-1	-1	-1	550	604	$(1) = 1154$
2	1	-1	-1	669	650	$a = 1319$
3	-1	1	-1	633	601	$b = 1234$
4	1	1	-1	642	635	$ab = 1277$
5	-1	-1	1	1037	1052	$c = 2089$
6	1	-1	1	749	868	$ac = 1617$
7	-1	1	1	1075	1063	$bc = 2178$
8	1	1	1	729	860	$abc = 1589$

The 2^3 Design - The Etch Plasma Experiment



The 2^3 Design - The Etch Plasma Experiment

Analysis of Variance results:

```
> summary(aov(etch~A*B*C))
Df  Sum Sq  Mean Sq  F value    Pr(>F)
A            1   41311    41311  18.339 0.002679 **
B            1     218      218   0.097 0.763911
C            1  374850   374850 166.411 1.23e-06 **
A:B          1    2475     2475   1.099 0.325168
A:C          1   94403    94403  41.909 0.000193 **
B:C          1      18       18   0.008 0.930849
A:B:C        1     127      127   0.056 0.818586
Residuals    8   18020     2253
```

Gap (A), Power (C) and its interaction are highly significant.
We remove other variables and compare new reduced model with this one.

The 2^3 Design - The Etch Plasma Experiment

Analysis of Variance results of reduced model and computed Lack of fit.

```
> summary(etch~A*C)
            Df Sum Sq Mean Sq F value    Pr(>F)
A            1  41311   41311   23.77 0.000382 ***
C            1 374850  374850  215.66 4.95e-09 ***
A:C          1  94403   94403   54.31 8.62e-06 ***
Residuals   12  20858    1738

Analysis of Variance Table
Model 1: etch ~ A * C
Model 2: etch ~ A * B * C
  Res.Df   RSS Df Sum of Sq      F Pr(>F)
1     12 20858
2      8 18021  4    2837.2 0.3149 0.8604
```

Lack of fit is the difference between Residuals in reduced models and pure error (residuals) in old model with all variables and interactions.

The 2^3 Design - The Etch Plasma Experiment

Linear regression model results for coded (± 1) variables.

Estimated effects are double of mentioned values.

```
Call: lm(formula = etch ~ A.num * B.num * C.num)

Coefficients:
Estimate Std. Error t value Pr(>|t|)
(Intercept)         776.062     11.865  65.406 3.32e-12 ***
A.num               -50.812     11.865  -4.282 0.002679 **
B.num                 3.688     11.865   0.311 0.763911
C.num               153.062     11.865  12.900 1.23e-06 ***
A.num:B.num         -12.437     11.865  -1.048 0.325168
A.num:C.num         -76.812     11.865  -6.474 0.000193 ***
B.num:C.num          -1.062     11.865  -0.090 0.930849
A.num:B.num:C.num     2.813     11.865   0.237 0.818586

Residual standard error: 47.46 on 8 degrees of freedom
Multiple R-squared: 0.9661,     Adjusted R-squared: 0.9364
F-statistic: 32.56 on 7 and 8 DF,  p-value: 2.896e-05
```

The 2^3 Design - The Etch Plasma Experiment

Linear regression results for reduced model with coded (± 1) variables.

```
Call: lm(formula = etch ~ A.num * C.num)
Coefficients:
              Estimate Std. Error t value Pr(>|t|)
(Intercept)    776.06      10.42  74.458  < 2e-16 ***
A.num          -50.81      10.42  -4.875 0.000382 ***
C.num          153.06      10.42  14.685 4.95e-09 ***
A.num:C.num    -76.81      10.42  -7.370 8.62e-06 ***

Residual standard error: 41.69 on 12 degrees of freedom
Multiple R-squared: 0.9608,     Adjusted R-squared: 0.9509
F-statistic: 97.91 on 3 and 12 DF,  p-value: 1.054e-08
```

The proportion of total variability in etch rate that is explained by this reduced model is

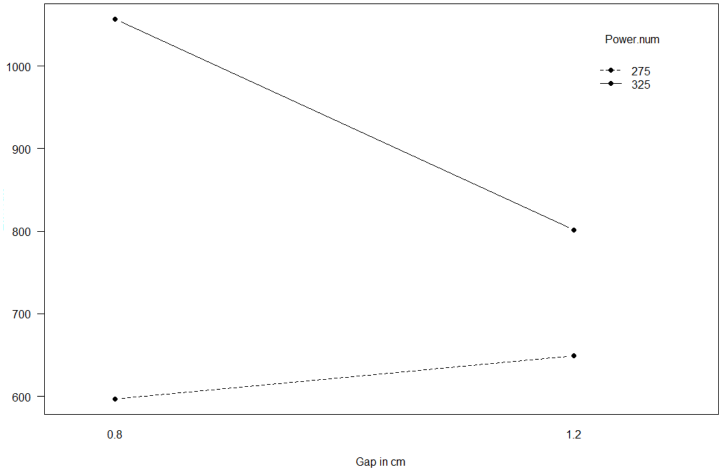
$$R^2 = 1 - \frac{SS_{Res}}{SS_{Total}} = \frac{SS_{Model}}{SS_{Total}} = \frac{SS_A + SS_C + SS_{AC}}{SS_{Total}} = \frac{510564}{531422} = 0.961$$

It is smaller than for the full model, but the removing of the nonsignificant terms from the full model is good for reducing the length of confidence intervals and for predicting.

The 2^3 Design - Plasma Etch Rate Experiment

The interaction plot.

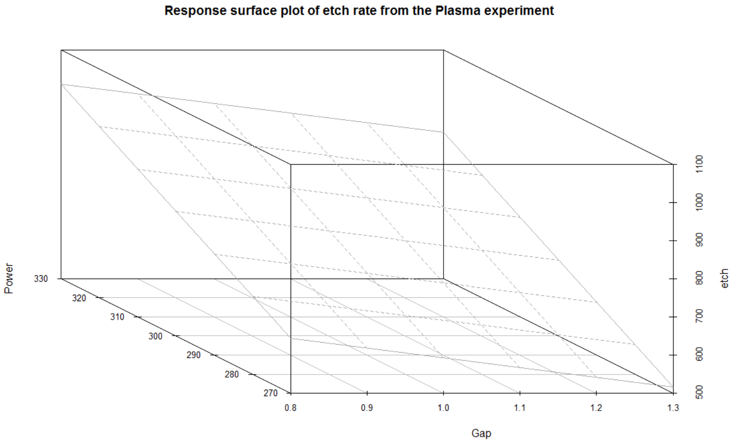
```
interaction.plot(Gap.num,Power.num,etch,type="b",pch=19,
                 fixed=T,xlab="Gap in cm",ylab="Etch rate")
```



The 2^3 Design - Plasma Etch Rate Experiment

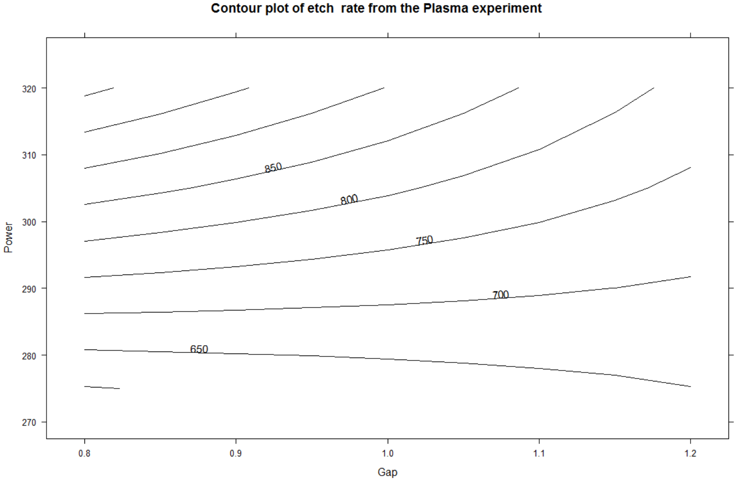
The linear regression model in natural factors levels can be used to generate response surface plots.

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \hat{\beta}_3 x_3 + \hat{\beta}_{13} x_1 x_3 = 776.06 - 50.81 x_1 + 153.06 x_3 - 76.81 x_1 x_3$$



The 2^3 Design - Plasma Etch Rate Experiment

The linear regression model in natural factors levels can be used to generate response contour plots.



Model Summary Statistics:

Standard error of model coefficients:

$$se(\hat{\beta}) = \sqrt{\frac{\sigma^2}{2n^k}} = \sqrt{\frac{MS_E}{2n^k}} = \sqrt{\frac{1738}{16}} = \frac{41.69}{4} = 10.42.$$

The standard errors of all model coefficients are equal because the design is orthogonal.

Confidence interval on model coefficients:

$$\hat{\beta} - t_{\alpha/2,df_E} se(\hat{\beta}) \leq \beta \leq \hat{\beta} + t_{\alpha/2,df_E} se(\hat{\beta}),$$

where $df_E = N - p = 12$ stands for the number of degrees of freedom for error, N is the total number of runs in the experiment and p is the number of parameters in the regression model.

In a general 2^k Factorial Design will be

- k main effects
- $\binom{k}{2}$ two-factor interactions
- $\binom{k}{3}$ three-factor interactions
- $\vdots$
- 1 k-factor interaction

The General 2^k Factorial Design

```
> k=3
> plan2a <-  FrF2(2^k, k, replications = 2, randomize = FALSE,
                 factor.names = c("A", "B", "C"))
> plan2a
run.no  run.no.  std.rp  A  B  C
1       1           1.1 -1 -1 -1
2       2           2.1  1 -1 -1
3       3           3.1 -1  1 -1
4       4           4.1  1  1 -1
5       5           5.1 -1 -1  1
6       6           6.1  1 -1  1
7       7           7.1 -1  1  1
8       8           8.1  1  1  1
9       9           1.2 -1 -1 -1
10      10          2.2  1 -1 -1
11      11          3.2 -1  1 -1
12      12          4.2  1  1 -1
13      13          5.2 -1 -1  1
14      14          6.2  1 -1  1
15      15          7.2 -1  1  1
16      16          8.2  1  1  1
class=design, type= full factorial
NOTE: columns run.no and run.no.std.rp are annotation, not part of the
result <-  rnorm(16)
plan2a <-  add.response(plan2a,result)
```

Unreplicated 2^k Factorial Design

- These are 2^k factorial designs 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.
  - Pooling high-order interactions to estimate error.
  - Normal probability plotting of effects (Daniels, 1959).

Examples and further discussion in the next lesson.

Today Exercise

Solve problems 6.1, 6.2.
(from D. C. Montgomery DAoE ed.8 - chapter 6)

6.1. An engineer is interested in the effects of cutting speed (A), tool geometry (B), and cutting angle (C) on the life (in hours) of a machine tool. Two levels of each factor are chosen, and three replicates of a 2^3 factorial design are run. The results are as follows:

			Treatment	Replicate		
A	*B*	*C*	**Combination**	**I**	**II**	**III**
−	−	−	(1)	22	31	25
+	−	−	*a*	32	43	29
−	+	−	*b*	35	34	50
+	+	−	*ab*	55	47	46
−	−	+	*c*	44	45	38
+	−	+	*ac*	40	37	36
−	+	+	*bc*	60	50	54
+	+	+	*abc*	39	41	47

(a) Estimate the factor effects. Which effects appear to be large?

(b) Use the analysis of variance to confirm your conclusions for part (a).

(c) Write down a regression model for predicting tool life (in hours) based on the results of this experiment.

(d) Analyze the residuals. Are there any obvious problems?

(e) On the basis of an analysis of main effect and interaction plots, what coded factor levels of A, B, and C would you recommend using?

6.2. Reconsider part (c) of Problem 6.1. Use the regression model to generate response surface and contour plots of the tool life response. Interpret these plots. Do they provide insight regarding the desirable operating conditions for this process?