Topic 14: 2^K factorial design (II)

Montgomery: chapter 6

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Outline

- General 2^k factorial design
- Unreplicated factorial design

General 2^k Design

- k factors: A, B, . . ., K each with 2 levels $(+,-)$
- consists of all possible level combinations (2^k treatments) each with n replicates
- Classify factorial effects:

type of effect	label	the number of effects
main effects (of order 1)	$A, B, C, \ldots, K$	k
2-factor interactions (of order 2)	$AB, AC, \ldots, JK$	$\binom{k}{2}$
3-factor interactions (of order 3)	$ABC, ABD, \ldots, IJK$	$\binom{k}{3}$
$\ldots$	$\ldots$	$\ldots$
k-factor interaction (of order k)	$ABC \cdots K$	$\binom{k}{k}$

- In total, how many effects?
- Each effect (main or interaction) has 1 degree of freedom

  full model (i.e. model consisting of all the effects) has $2^k - 1$ degrees of freedom.
- Error component has $2^k(n-1)$ degrees of freedom (why?).
- One-to-one correspondence between effects and contrasts:
  - For main effect: convert the level column of a factor using $- \Rightarrow -1$ and $+ \Rightarrow 1$
  - For interactions: multiply the contrasts of the main effects of the involved factors, componentwisely.

General 2^k Design: Analysis

- Estimates:

$$\text{grand mean}: \frac{\sum \bar{y}_{i.}}{2^k}$$

For effect with contrast $C = (c_1, c_2, \ldots, c_{2^k})$, its estimate is

$$\text{effect} = \frac{\sum c_i \bar{y}_i}{2^{(k-1)}}$$

- Variance

$$\text{Var(effect)} = \frac{\sigma^2}{n2^{k-2}}$$

what is the standard error of the effect?

- t-test for H_0: effect=0. Using the confidence interval approach,

$$\text{effect} \pm t_{\alpha/2, 2^k(n-1)} \text{S.E.(effect)}$$

Using ANOVA model:

- Sum of Squares due to an effect, using its contrast,

$$\text{SS}_{\text{effect}} = \frac{\left(\sum c_i \bar{y}_{i.}\right)^2}{2^k/n} = n2^{k-2}(\text{effect})^2$$

- SS_T and SS_E can be calculated as before and a ANOVA table including SS due to the effects and SS_E can be constructed and the effects can be tested by F-tests.

Using regression:

- Introducing variables x_1, . . ., x_k for main effects, their products are used for interactions, the following regression model can be fitted

$$y = \beta_0 + \beta_1 x_1 + \ldots + \beta_k x_k + \ldots + \beta_{12\ldots k} x_1 x_2 \cdots x_k + \epsilon$$

The coefficients are estimated by half of effects they represent, that is,

$$\hat{\beta} = \frac{\text{effect}}{2}$$

Unreplicated 2^k Design -- Filtration Rate Experiment

factor				
A	B	C	D	filtration
$-$	$-$	$-$	$-$	45
$+$	$-$	$-$	$-$	71
$-$	$+$	$-$	$-$	48
$+$	$+$	$-$	$-$	65
$-$	$-$	$+$	$-$	68
$+$	$-$	$+$	$-$	60
$-$	$+$	$+$	$-$	80
$+$	$+$	$+$	$-$	65
$-$	$-$	$-$	$+$	43
$+$	$-$	$-$	$+$	100
$-$	$+$	$-$	$+$	45
$+$	$+$	$-$	$+$	104
$-$	$-$	$+$	$+$	75
$+$	$-$	$+$	$+$	86
$-$	$+$	$+$	$+$	70
$+$	$+$	$+$	$+$	96

Unreplicated 2^k Design

- No degree of freedom left for error component if full model is fitted.
- Formulas used for estimates and contrast sum of squares are given in Slides 5-6 with n=1
- No error sum of squares available, cannot estimate σ^2 and test effects in both the ANOVA and Regression approaches.
- **Approach 1**: pooling high-order interactions
  - Often assume 3 or higher interactions do not occur
  - Pool estimates together for error
  - Warning: may pool significant interaction

Unreplicated 2^k Design

- Approach 2: Using the normal probability plot (QQ plot) to identify significant effects.
  - Recall
    $$\text{Var}(\text{effect}) = \frac{\sigma^2}{2^{(k-2)}}$$
    If the effect is not significant (=0), then the effect estimate follows $N(0, \frac{\sigma^2}{2^{(k-2)}})$
  - Assume all effects not significant, their estimates can be considered as a random sample from $N(0, \frac{\sigma^2}{2^{(k-2)}})$
  - QQ plot of the estimates is expected to be a linear line
  - Deviation from a linear line indicates significant effects

Using SAS to generate QQ plot for effects - data

```
data filter;
 do D = -1 to 1 by 2;do C = -1 to 1 by 2;
 do B = -1 to 1 by 2;do A = -1 to 1 by 2;
 input y @@;  output;
 end; end; end; end;
datalines;
45 71 48 65 68 60 80 65 43 100 45 104 75 86 70 96
;
proc print data=filter;
run;


data inter;       /* Define Interaction Terms */
 set filter;
 AB=A*B; AC=A*C; AD=A*D; BC=B*C; BD=B*D; CD=C*D; ABC=AB*C; ABD=AB*D;
 ACD=AC*D; BCD=BC*D; ABCD=ABC*D;
 run;
proc print data=inter;
run;
```

Obs	**D**	**C**	**B**	**A**	**y**	**AB**	**AC**	**AD**	**BC**	**BD**	**CD**	**ABC**	**ABD**	**ACD**	**BCD**	**ABCD**
1	-1	-1	-1	-1	45	1	1	1	1	1	1	-1	-1	-1	-1	1
2	-1	-1	-1	1	71	-1	-1	-1	1	1	1	1	1	1	-1	-1
3	-1	-1	1	-1	48	-1	1	1	-1	-1	1	1	1	-1	1	-1
4	-1	-1	1	1	65	1	-1	-1	-1	-1	1	-1	-1	1	1	1
5	-1	1	-1	-1	68	1	-1	1	-1	1	-1	1	-1	1	1	-1
6	-1	1	-1	1	60	-1	1	-1	-1	1	-1	-1	1	-1	1	1
7	-1	1	1	-1	80	-1	-1	1	1	-1	-1	-1	1	1	-1	1
8	-1	1	1	1	65	1	1	-1	1	-1	-1	1	-1	-1	-1	-1
9	1	-1	-1	-1	43	1	1	-1	1	-1	-1	-1	1	1	1	-1
10	1	-1	-1	1	100	-1	-1	1	1	-1	-1	1	-1	-1	1	1
11	1	-1	1	-1	45	-1	1	-1	-1	1	-1	1	-1	1	-1	1
12	1	-1	1	1	104	1	-1	1	-1	1	-1	-1	1	-1	-1	-1
13	1	1	-1	-1	75	1	-1	-1	-1	-1	1	1	1	-1	-1	1
14	1	1	-1	1	86	-1	1	1	-1	-1	1	-1	-1	1	-1	-1
15	1	1	1	-1	70	-1	-1	-1	1	1	1	-1	-1	-1	1	-1
16	1	1	1	1	96	1	1	1	1	1	1	1	1	1	1	1

```
proc glm data=inter;  /* GLM Proc to Obtain
Effects */
 class A B C D AB AC AD BC BD CD ABC ABD ACD BCD
ABCD;
 model y=A B C D AB AC AD BC BD CD ABC ABD ACD
BCD ABCD;
 estimate 'A' A -1 1; estimate 'AC' AC -1 1;
 run;


proc reg outest=effects data=inter;    /* REG
Proc to Obtain Effects */
 model y=A B C D AB AC AD BC BD CD ABC ABD ACD
BCD ABCD;
 run;
```

Source	DF	Sum of Squares	Mean Square	F Value	Pr > F
Model	15	5730.937500	382.062500	.	.
Error	0				
Corrected Total	15				

Source	DF	Type III SS	Mean Square	F Value	Pr > F
A	1	1870.562500	1870.562500	.	.
B	1	39.062500	39.062500	.	.
C	1	390.062500	390.062500	.	.
D	1	855.562500	855.562500	.	.
AB	1	0.062500	0.062500	.	.
AC	1	1314.062500	1314.062500	.	.
AD	1	1105.562500	1105.562500	.	.
BC	1	22.562500	22.562500	.	.
BD	1	0.562500	0.562500	.	.
CD	1	5.062500	5.062500	.	.
ABC	1	14.062500	14.062500	.	.
ABD	1	68.062500	68.062500	.	.
ACD	1	10.562500	10.562500		

Parameter	Estimate	Standard Error	t Value	Pr > |t|
A	21.6250000	.	.	.
AC	-18.1250000	.	.	.

Output (Proc reg)

Parameter Estimates					
Variable	DF	Parameter Estimate	Standard Error	t Value	Pr > |t|
Intercept	1	70.06250	.	.	.
A	1	10.81250	.	.	.
B	1	1.56250	.	.	.
C	1	4.93750	.	.	.
D	1	7.31250	.	.	.
AB	1	0.06250	.	.	.
AC	1	-9.06250	.	.	.
AD	1	8.31250	.	.	.
BC	1	1.18750	.	.	.
BD	1	-0.18750	.	.	.
CD	1	-0.56250	.	.	.
ABC	1	0.93750	.	.	.
ABD	1	2.06250	.	.	.
ACD	1	-0.81250	.	.	.
BCD	1	-1.31250	.	.	.
ABCD	1	0.68750	.	.	.

```
data effect2; set effects;
 drop y intercept _RMSE_;
 run;

proc transpose data=effect2 out=effect3;
run;

data effect4; set effect3; effect=col1*2;
run;

proc sort data=effect4; by effect;
run;

proc print data=effect4;
run;
```

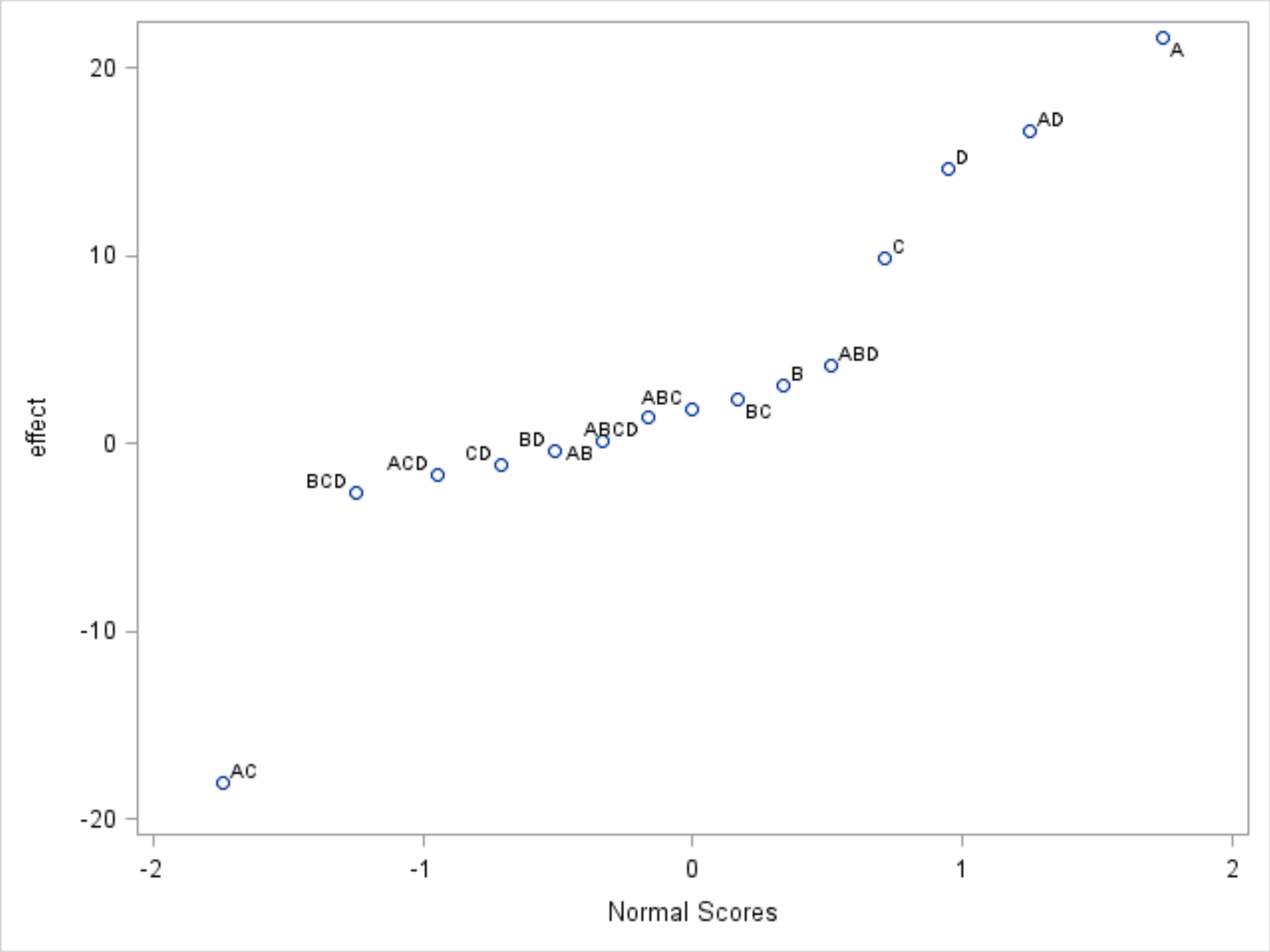
Obs	_NAME_	COL1	effect
1	AC	-9.0625	-18.125
2	BCD	-1.3125	-2.625
3	ACD	-0.8125	-1.625
4	CD	-0.5625	-1.125
5	BD	-0.1875	-0.375
6	AB	0.0625	0.125
7	ABCD	0.6875	1.375
8	ABC	0.9375	1.875
9	BC	1.1875	2.375
10	B	1.5625	3.125
11	ABD	2.0625	4.125
12	C	4.9375	9.875
13	D	7.3125	14.625
14	AD	8.3125	16.625
15	A	10.8125	21.625

```
proc rank data=effect4 out=effect5
normal=blom;
 var effect; ranks neff;
 run;

proc print data=effect5;
run;


proc sgplot data=effect5;
scatter x=neff y=effect/datalabel=_NAME_;
xaxis label='Normal Scores';
run;
```

Ranked effects

Obs	_NAME_	COL1	effect	neff
1	AC	-9.0625	-18.125	-1.73938
2	BCD	-1.3125	-2.625	-1.24505
3	ACD	-0.8125	-1.625	-0.94578
4	CD	-0.5625	-1.125	-0.71370
5	BD	-0.1875	-0.375	-0.51499
6	AB	0.0625	0.125	-0.33489
7	ABCD	0.6875	1.375	-0.16512
8	ABC	0.9375	1.875	0.00000
9	BC	1.1875	2.375	0.16512
10	B	1.5625	3.125	0.33489
11	ABD	2.0625	4.125	0.51499
12	C	4.9375	9.875	0.71370
13	D	7.3125	14.625	0.94578
14	AD	8.3125	16.625	1.24505
15	A	10.8125	21.625	1.73938

Proc sgplot



A
AD
D
C
ABD
B
ABC
BC
ABCD
BD
AB
CD
ACD
BCD
AC
20
10
0
-10
-20
effect
-2
-1
0
1
2
Normal Scores

Filtration Experiment Analysis

Fit a linear line based on small effects, identify the effects which are potentially significant, then use ANOVA or regression fit a sub-model with those effects.

1. Potentially significant effects: A, AD, C, D, AC.

2. Use main effect plot and interaction plot

3. ANOVA model involving only A, C, D and their interactions (projecting the original unreplicated 2^4 experiment onto a replicated 2^3 experiment)

4. regression model only involving A, C, D, AC and AD.

5. Diagnostics using residuals.

ANOVA with A, C and D and their interactions

```
proc glm data=filter;
class A C D;
model y=A|C|D;
====================================
Source          DF     Sum  Squares      Mean Square     F Value    Pr > F
Model            7     5551.437500      793.062500       35.35     <.0001
Error            8      179.500000       22.437500
Cor Total       15     5730.937500

Source          DF        Type I SS      Mean Square     F Value    Pr > F
A                1     1870.562500     1870.562500       83.37     <.0001
C                1      390.062500      390.062500       17.38     0.0031
A*C              1     1314.062500     1314.062500       58.57     <.0001
D                1      855.562500      855.562500       38.13     0.0003
A*D              1     1105.562500     1105.562500       49.27     0.0001
C*D              1        5.062500        5.062500        0.23     0.6475
A*C*D            1       10.562500       10.562500        0.47     0.5120
*ANOVA confirms that A, C, D, AC and AD are significant effects
```

Regression Model

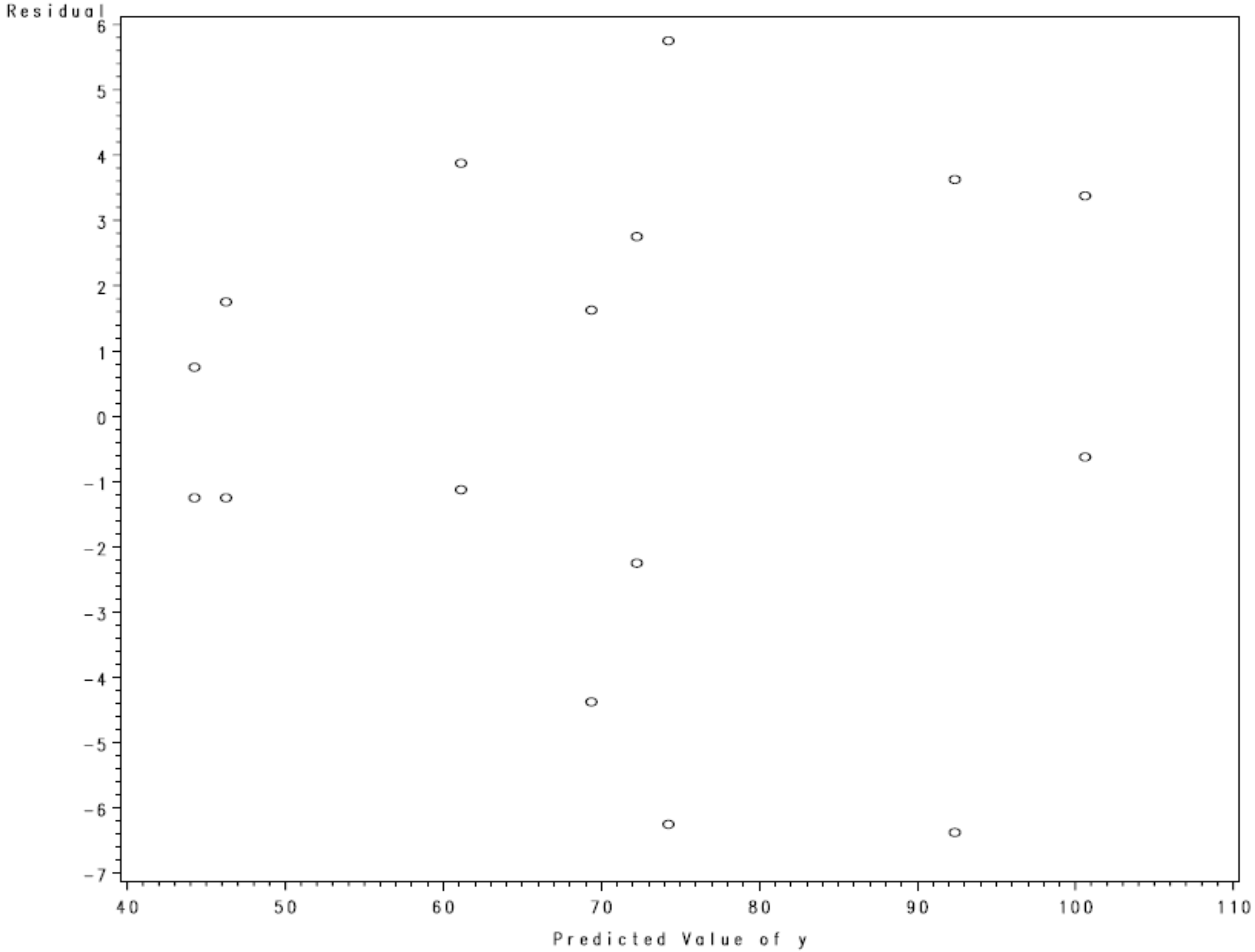
```
* the same date step

data inter; set filter; AC=A*C; AD=A*D;

proc reg data=inter; model y=A C D AC AD;
output out=outres r=res p=pred;

proc gplot data=outres; plot res*pred; run;

===========================
Dependent Variable: y
                    Analysis of Variance
                          Sum of           Mean
Source           DF      Squares         Square    F Value    Pr > F
Model             5   5535.81250     1107.16250      56.74    <.0001
Error            10    195.12500       19.51250
Corrected Total  15   5730.93750

Root MSE              4.41730    R-Square     0.9660
```

Dependent Mean	70.06250	Adj R-Sq	0.9489
Coeff Var	6.30479		

Parameter Estimates

Variable	DF	Parameter Estimate	Standard Error	t Value	Pr > |t|
Intercept	1	70.06250	1.10432	63.44	<.0001
A	1	10.81250	1.10432	9.79	<.0001
C	1	4.93750	1.10432	4.47	0.0012
D	1	7.31250	1.10432	6.62	<.0001
AC	1	-9.06250	1.10432	-8.21	<.0001
AD	1	8.31250	1.10432	7.53	<.0001

Residual plot



Response Optimization / Best Setting Selection

Use x_1, x_3, x_4 for A, C, D; and x_1x_3, x_1x_4 for AC,AD respectively. The regression model gives the following function for the response (filtration rate):

$$y = 70.06 + 10.81x_1 + 4.94x_3 + 7.31x_4 - 9.06x_1x_3 + 8.31x_1x_4$$

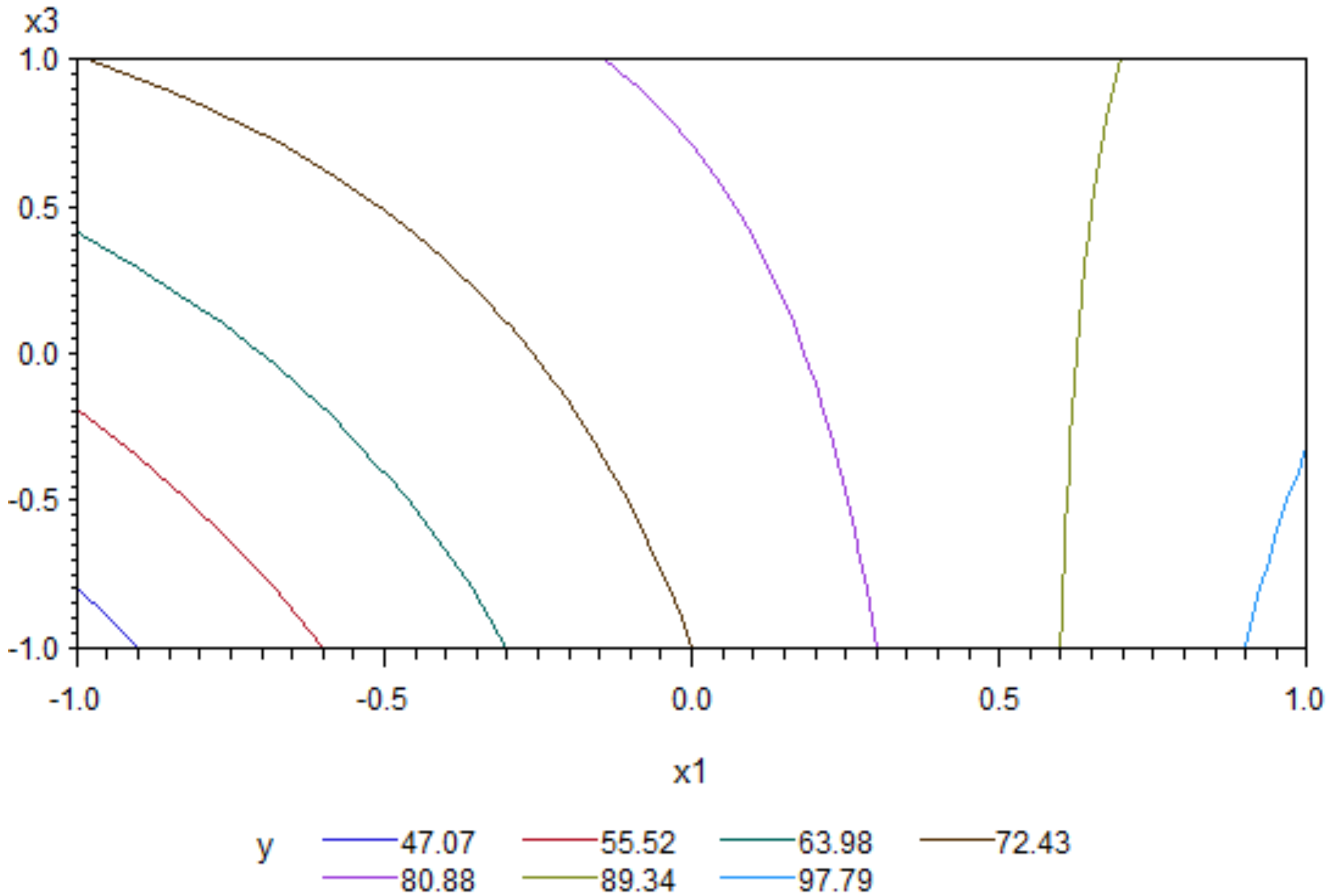
Want to maximize the response. Let D be set at high level ($x_4 = 1$)

$$y = 77.37 + 19.12x_1 + 4.94x_3 - 9.06x_1x_3$$

Contour plot

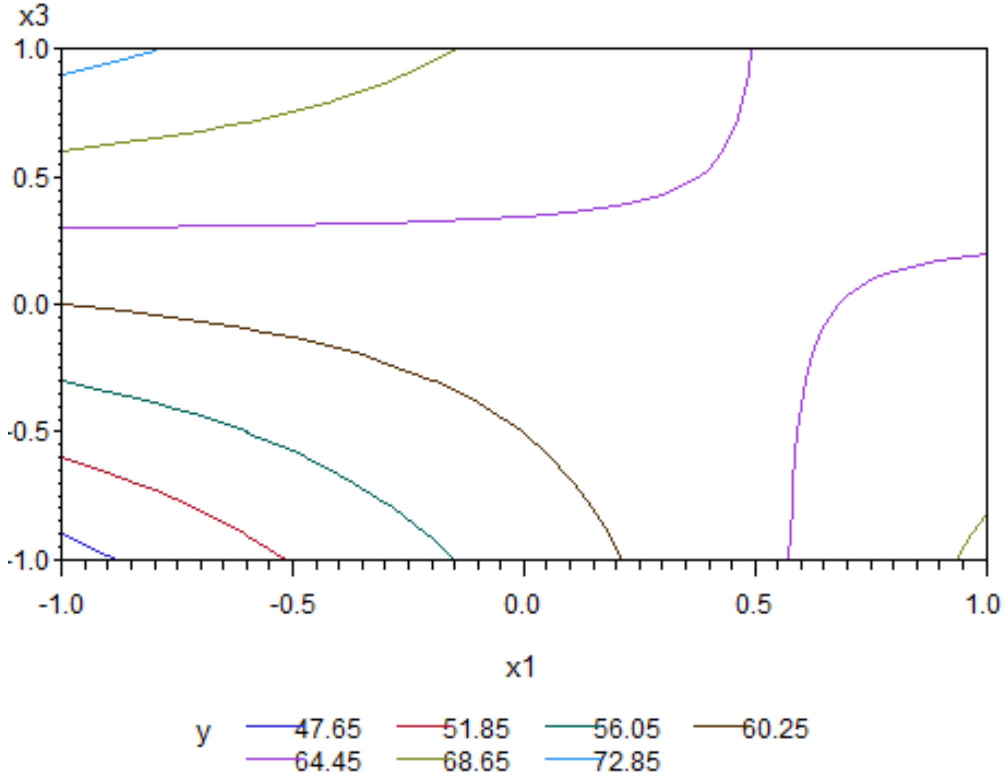
```
goption colors=(none);
data one;
do x1 = -1 to 1 by .1;
  do x3 = -1 to 1 by .1;
   y=77.37+19.12*x1 +4.94*x3 -9.06*x1*x3 ; output;
   end; end;
proc gcontour data=one; plot x3*x1=y;
run; quit;
```

Contour Plot for Response Given *D* (= +1)



D= -1

```
data one;
do x1 = -1 to 1 by .1;
do x3 = -1 to 1 by .1;
y=62.75+2.5*x1 +4.94*x3 -9.06*x1*x3 ; output;
end; end;
proc gcontour data=one; plot x3*x1=y;
run;
```



Last slide

- Read Sections: 6.4-6.5