Response surface example

We wish to maximize the variable called "Yield".

There are 2 factors: Time, Temperature

Guess: Time = 35

Temp = 155

We construct a 2^2 design with 5 center points

(9 runs altogether)

H_0: no curvature

H_1: curvature

p-value = .814

So we fail to reject the hypothesis of no Curvature

(we couldn't detect curvature)

Now, fit a linear model:

$$\hat{y} = 40.4444 + .775(\text{time}) + .325(\text{temp})$$

Our gradient vector is $\begin{bmatrix} .775 \\ .325 \end{bmatrix}$ or $\begin{bmatrix} 1 \\ .4 \end{bmatrix}$ (3)

Arbitrarily decide that 1 step in the "time" direction is 5 sec. Simultaneously, take 4/10 of a step in the "temperature" direction.

So add 5 seconds to the time & 2 seconds to the temperature.

Keep doing this process until you see an apparent maximum. This occurs at (85, 175)

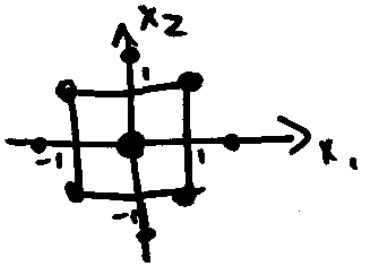
(4)

We now construct a new 2^2 design with center points at this value.

The test for curvature now has a p-value of .003, so we reject the null hypothesis of "no curvature".

We set up a Central Composite design:

4 corner points
5 center points
4 star points



(5)

Now, fit a full quadratic model:

$$\hat{y} = 79.940 + .995(\text{time}) + .5152(\text{temp}) - 1.376(\text{time}^2) - 1.001(\text{temp}^2) + .250(\text{time} * \text{temp})$$

$$\vec{b} = \begin{bmatrix} .995 \\ .5152 \end{bmatrix}, \quad B = \begin{bmatrix} -1.376 & .125 \\ .125 & -1.001 \end{bmatrix}$$

(6)

$$\hat{x}_M = -\frac{1}{2} B^{-1} \vec{b} = \begin{bmatrix} .389 \\ .306 \end{bmatrix} \begin{matrix} = x_1 \\ = x_2 \end{matrix}$$

optimal time = $85 + .389(5) = 86.945$

optimal temp = $175 + .306(5) = 176.53$

Final step: find the eigenvalues of B
* verify that they are both negative

HW #6 * 11.1, 11.8

Time	Temp	x1	x2	Yield
30	150	-1	-1	39.3
30	160	-1	1	40
40	150	1	-1	40.9
40	160	1	1	41.5
35	155	0	0	40.3
35	155	0	0	40.5
35	155	0	0	40.7
35	155	0	0	40.2
35	155	0	0	40.6

Step	x1	x2	Time	Temp	Yield
Home	0	0	35	155	
Delta	1	0.4	5	2	
1	1	0.4	40	157	41
2	2	0.8	45	159	42.9
3	3	1.2	50	161	47.1
4	4	1.6	55	163	49.7
5	5	2	60	165	53.8
6	6	2.4	65	167	59.9
7	7	2.8	70	169	65
8	8	3.2	75	171	70.4
9	9	3.6	80	173	77.6
10	10	4	85	175	80.3
11	11	4.4	90	177	76.2
12	12	4.8	95	179	75.1

Time	Temp	x1	x2	Yield
80	170	-1	-1	76.5
80	180	-1	1	77
90	170	1	-1	78
90	180	1	1	79.5
85	175	0	0	79.9
85	175	0	0	80.3
85	175	0	0	80
85	175	0	0	79.7
85	175	0	0	79.8

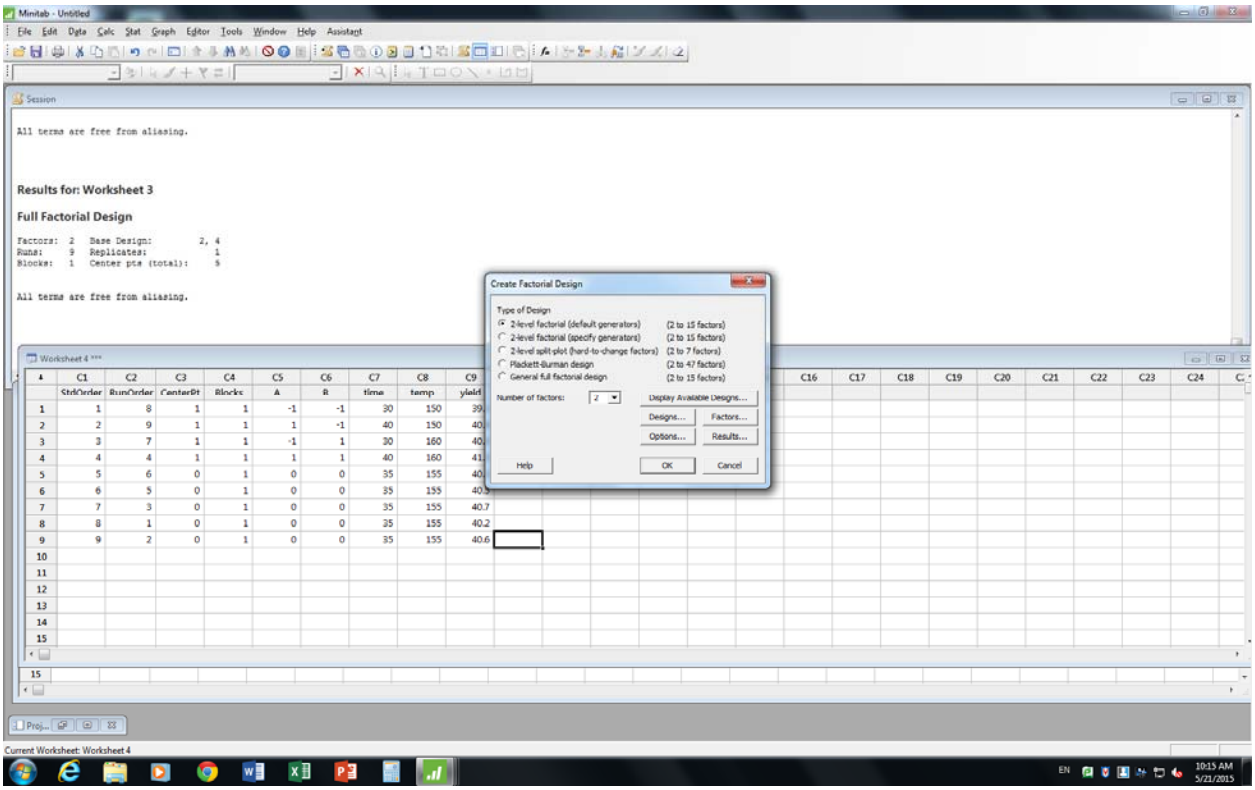
Time	Temp	x1	x2	Yield
80	170	-1	-1	76.5
80	180	-1	1	77
90	170	1	-1	78
90	180	1	1	79.5
85	175	0	0	79.9
85	175	0	0	80.3
85	175	0	0	80
85	175	0	0	79.7
85	175	0	0	79.8
92.07	175	1.414	0	78.4
77.93	175	-1.414	0	75.6
85	182.07	0	1.414	78.5
85	167.93	0	-1.414	77

STEP 1

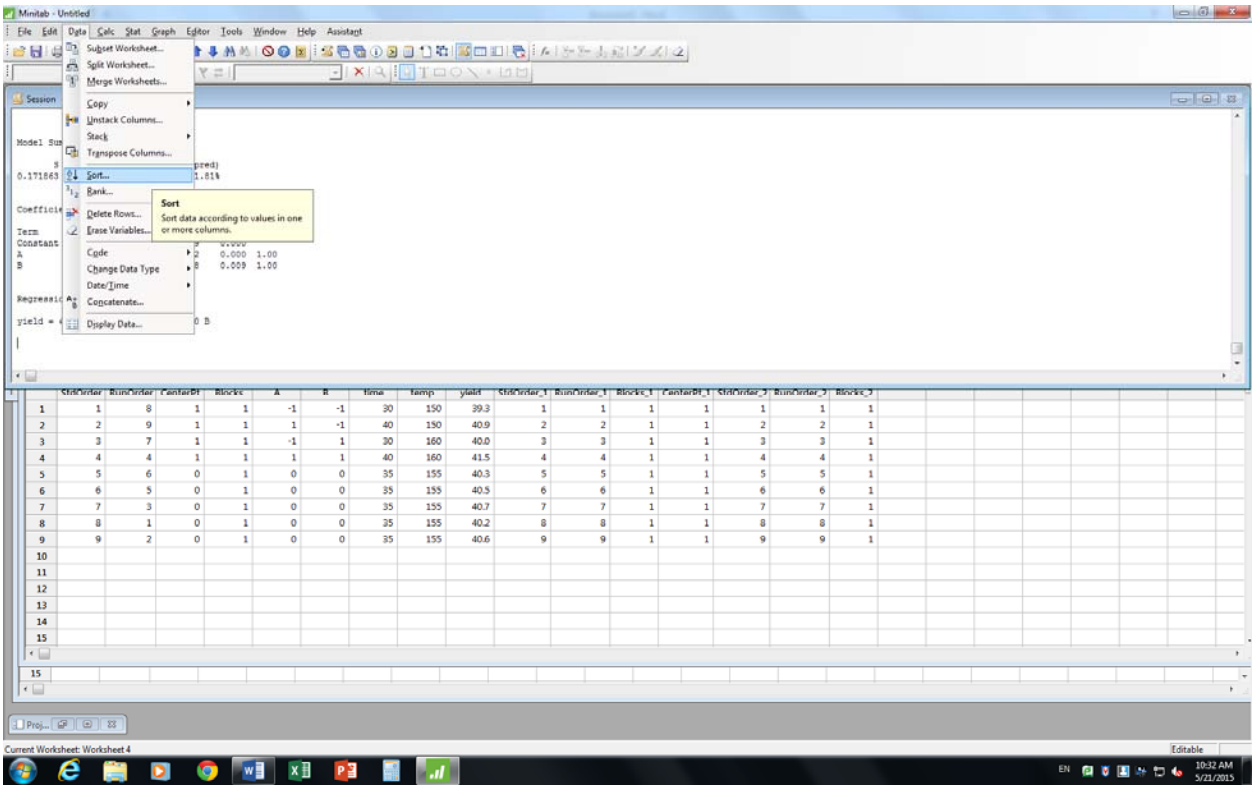
2^2 design with center points (5 center points)

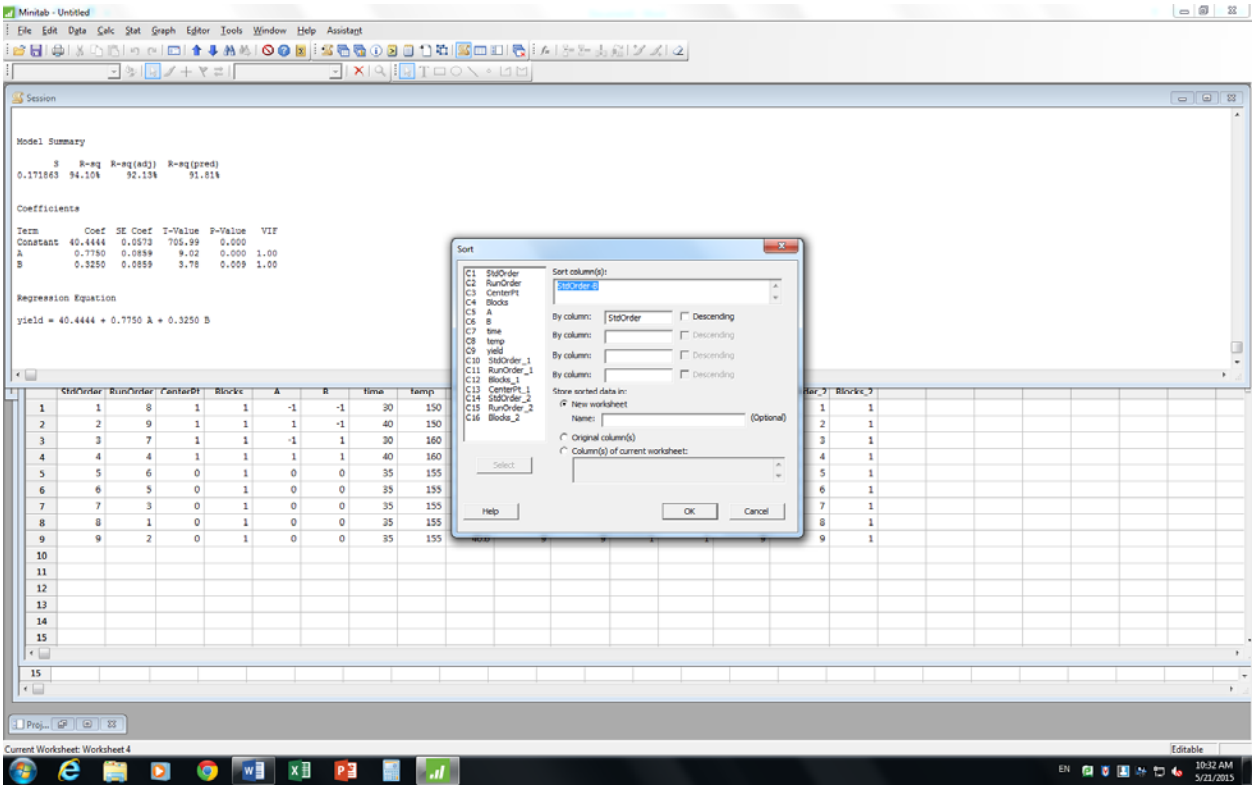
Stat →DOE→Factorial→create factorial design

(choose 2 factors)

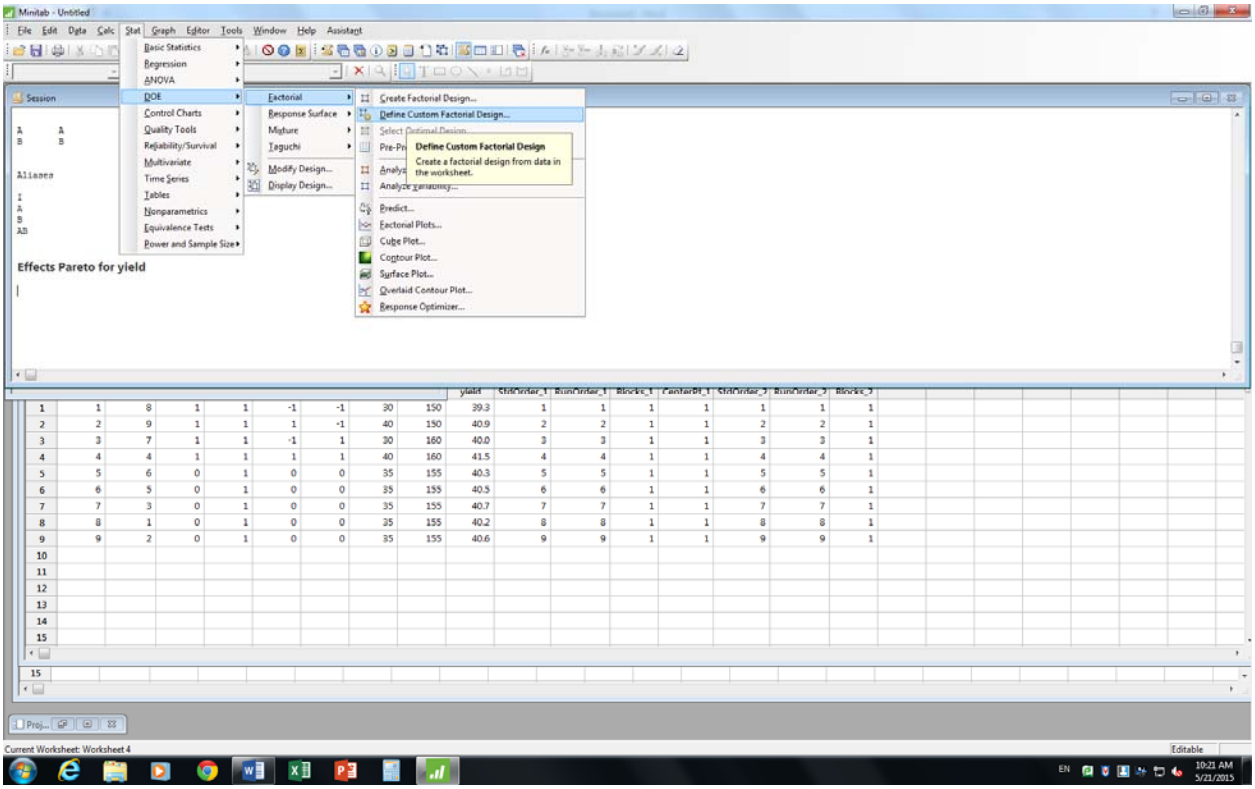


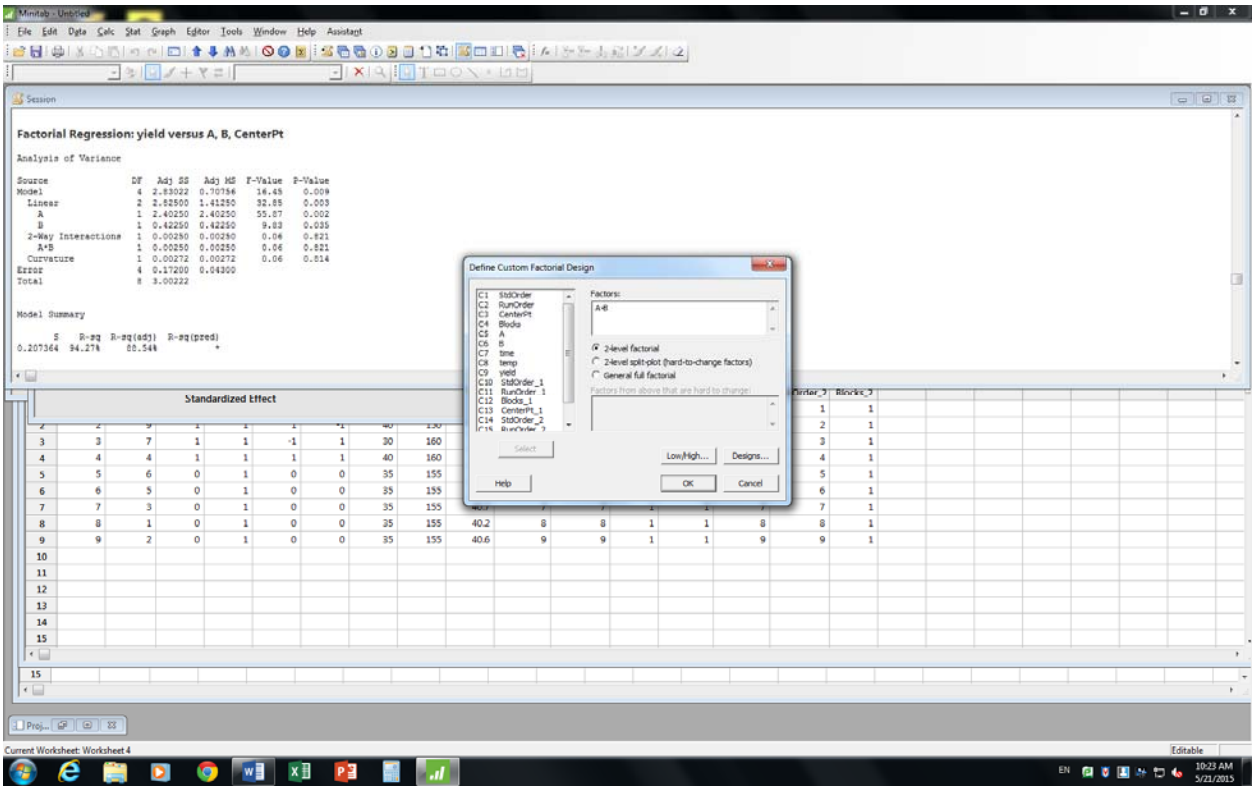
Sort it by standard order

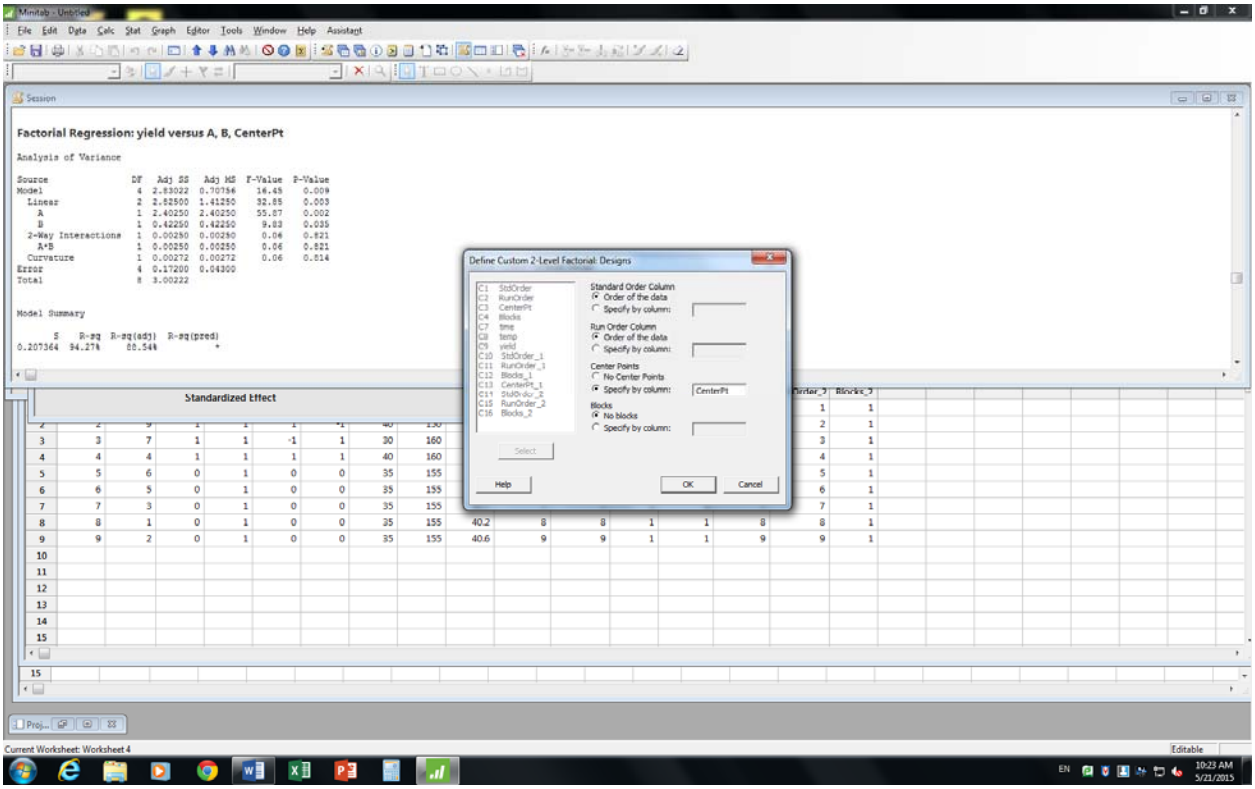

Minitab - Untitled
File Edit Data Calc Stat Graph Editor Tools Window Help Assistant
Subset Worksheet...
Split Worksheet...
Merge Worksheets...
Copy
Unstack Columns...
Stack
Transpose Columns...
Sort...
Rank...
Delete Rows...
Erase Variables...
Code
Change Data Type
Date/Time
Concatenate...
Display Data...
Sort
Sort data according to values in one or more columns.
Session
Current Worksheet: Worksheet 4
Editable

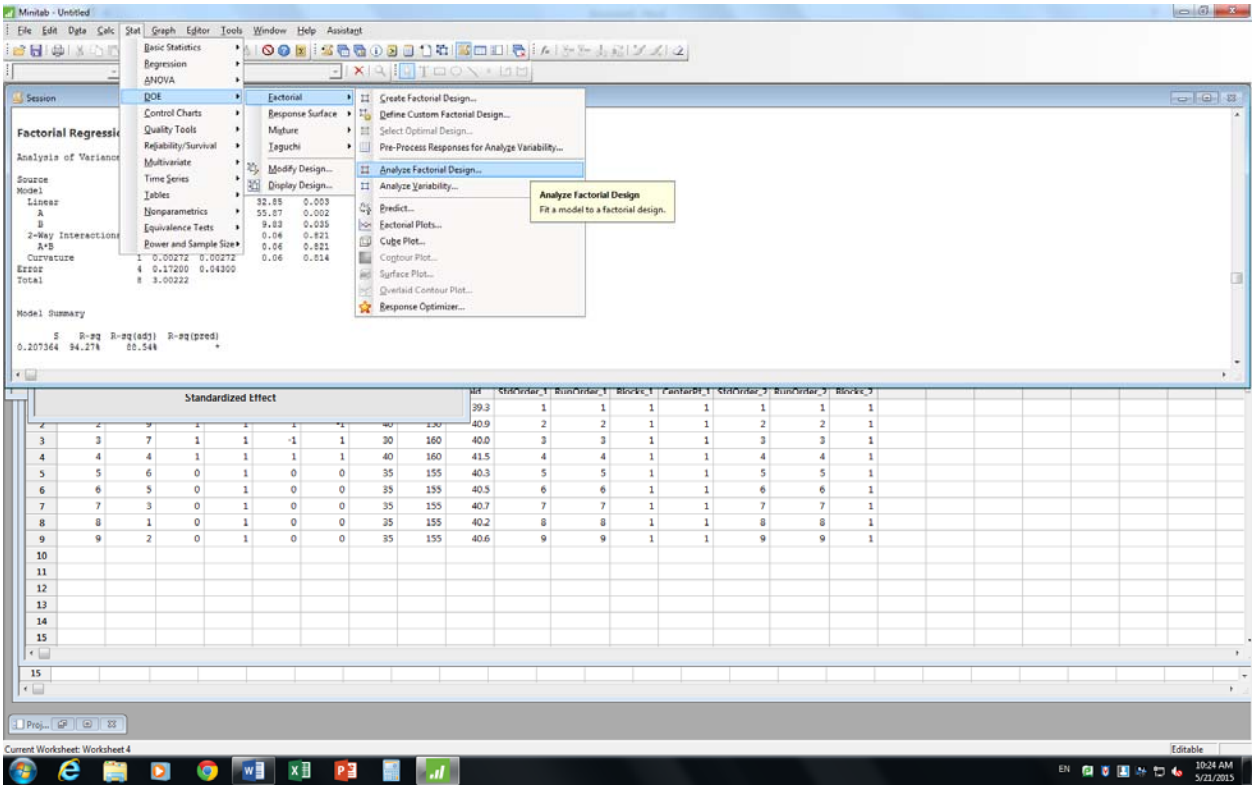

Minitab - Untitled
Session
Model Summary
S R-sq R-sq(adj) R-sq(pred)
0.171863 94.10% 92.13% 91.81%
Coefficients
Term Coef SE Coef T-Value P-Value VIF
Constant 40.4444 0.0573 705.99 0.000
A 0.7750 0.0859 9.02 0.000 1.00
B 0.3250 0.0859 3.78 0.009 1.00
Regression Equation
yield = 40.4444 + 0.7750 A + 0.3250 B
Sort
Sort column(s):
By column:
Descending
Store sorted data in:
New worksheet
Name:
(Optional)
Original column(s)
Column(s) of current worksheet:
Select
Help
OK
Cancel
Current Worksheet: Worksheet 4
Editable

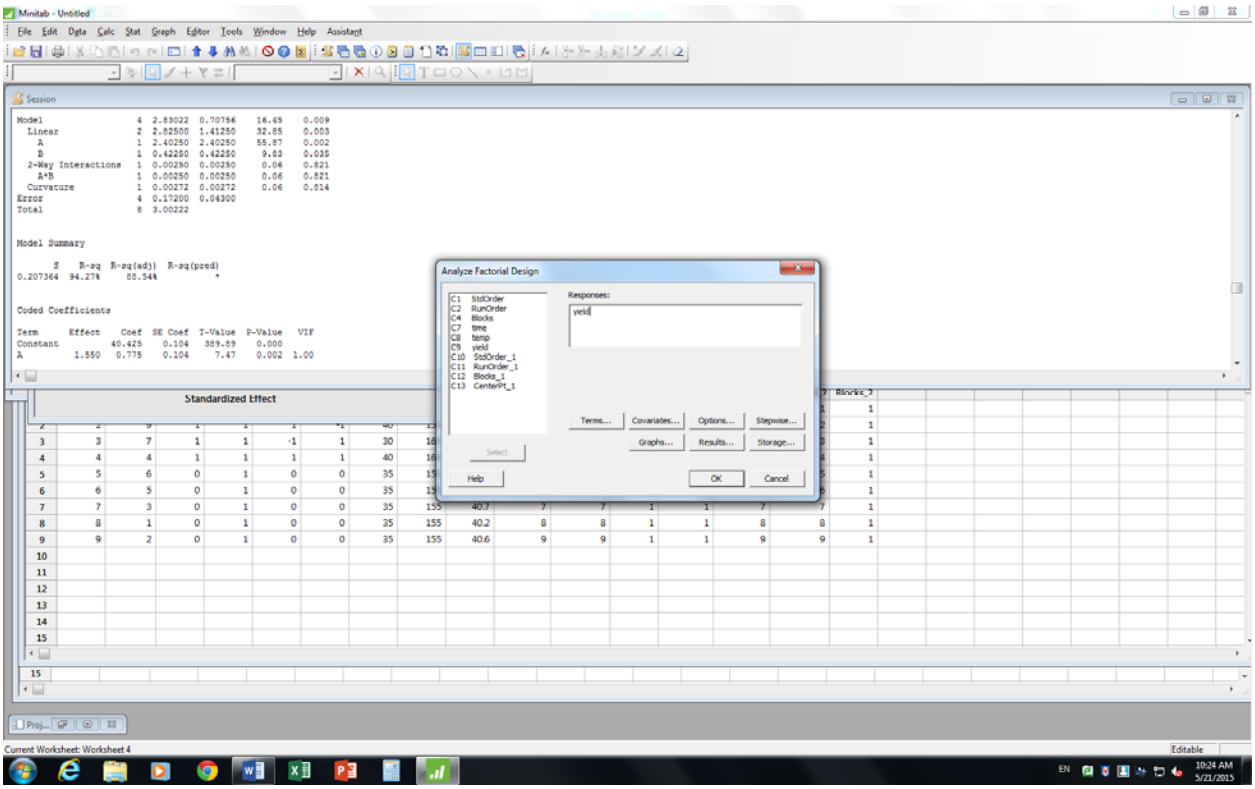
Now analyze the data



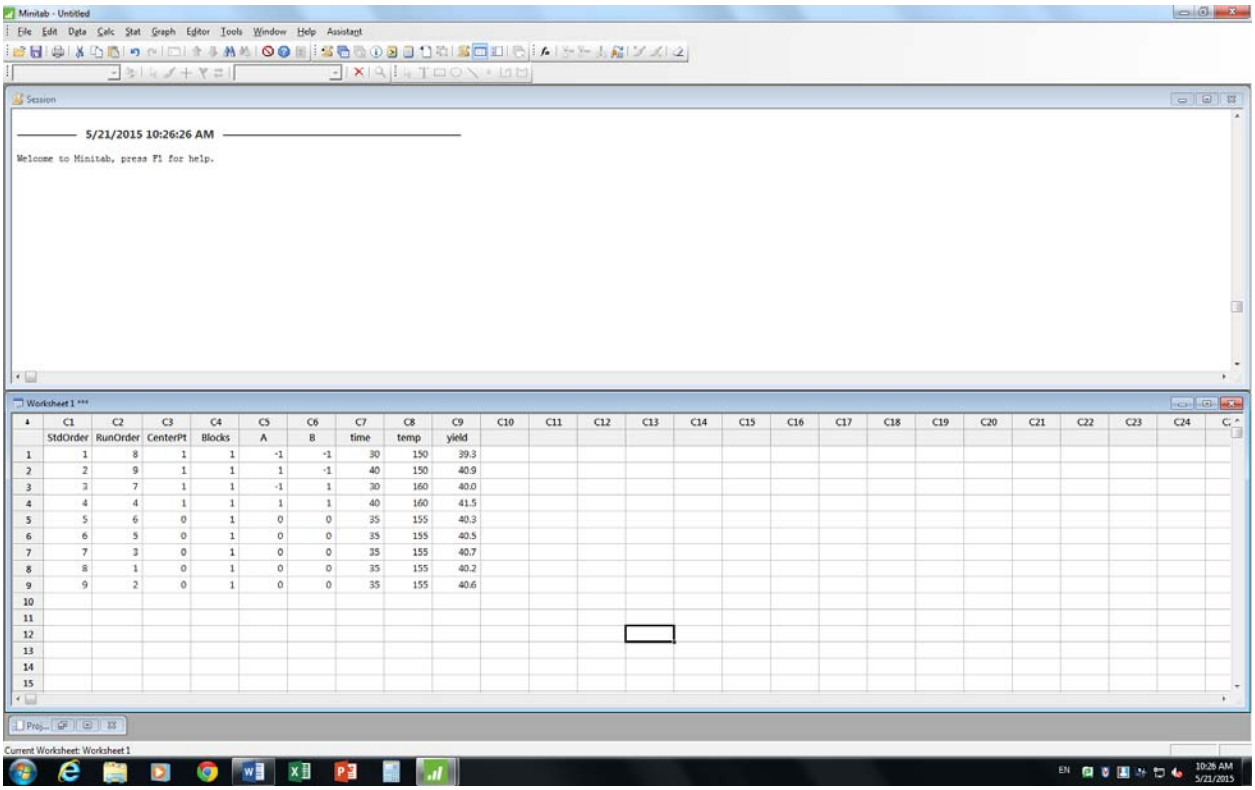



Factorial Regression: yield versus A, B, CenterPt
Analysis of Variance
Model Summary
Define Custom 2-Level Factorial Designs
Standardized Effect


Stat
DOE
Factorial
Create Factorial Design...
Define Custom Factorial Design...
Analyze Factorial Design...
Analyze Factorial Design
Fit a model to a factorial design.
Response Optimizer...
Standardized Effect


Minitab - Untitled
Session
Model 4 2.83022 0.70756 16.45 0.009
Linear 2 2.82500 1.41250 32.85 0.003
A 1 2.40250 2.40250 55.87 0.002
B 1 0.42250 0.42250 9.83 0.035
2-Way Interactions 1 0.00250 0.00250 0.06 0.821
A*B 1 0.00250 0.00250 0.06 0.821
Curvature 1 0.00272 0.00272 0.06 0.814
Error 4 0.17200 0.04300
Total 8 3.00222
Model Summary
S R-sq R-sq(adj) R-sq(pred)
0.207364 94.27% 88.54% *
Coded Coefficients
Term Effect Coef SE Coef T-Value P-Value VIF
Constant 40.425 0.104 389.59 0.000
A 1.550 0.775 0.104 7.47 0.002 1.00
Standardized Effect
Analyze Factorial Design
C1 StdOrder
C2 RunOrder
C4 Blocks
C7 time
C8 temp
C9 yield
C10 StdOrder_1
C11 RunOrder_1
C12 Blocks_1
C13 CenterPt_1
Responses:
yield
Terms...
Covariates...
Options...
Stepwise...
Graphs...
Results...
Storage...
Select
Help
OK
Cancel
Current Worksheet: Worksheet 4
Editable

DATA


Minitab - Untitled
Session
5/21/2015 10:26:26 AM
Welcome to Minitab, press F1 for help.
Worksheet 1 ***
C1 StdOrder
C2 RunOrder
C3 CenterPt
C4 Blocks
C5 A
C6 B
C7 time
C8 temp
C9 yield
1 1 8 1 1 -1 -1 30 150 39.3
2 2 9 1 1 1 -1 40 150 40.9
3 3 7 1 1 -1 1 30 160 40.0
4 4 4 1 1 1 1 40 160 41.5
5 5 6 0 1 0 0 35 155 40.3
6 6 5 0 1 0 0 35 155 40.5
7 7 3 0 1 0 0 35 155 40.7
8 8 1 0 1 0 0 35 155 40.2
9 9 2 0 1 0 0 35 155 40.6
Current Worksheet: Worksheet 1

OUTPUT:

Factorial Regression: yield versus A, B, CenterPt

Analysis of Variance

Source	DF	Adj SS	Adj MS	F-Value	P-Value
Model	4	2.83022	0.70756	16.45	0.009
Linear	2	2.82500	1.41250	32.85	0.003
A	1	2.40250	2.40250	55.87	0.002
B	1	0.42250	0.42250	9.83	0.035
2-Way Interactions	1	0.00250	0.00250	0.06	0.821
A*B	1	0.00250	0.00250	0.06	0.821
Curvature	1	0.00272	0.00272	0.06	0.814
Error	4	0.17200	0.04300		
Total	8	3.00222			

Model Summary

S	R-sq	R-sq(adj)	R-sq(pred)
0.207364	94.27%	88.54%	*

Coded Coefficients

Term	Effect	Coef	SE Coef	T-Value	P-Value	VIF
Constant		40.425	0.104	389.89	0.000	
A	1.550	0.775	0.104	7.47	0.002	1.00
B	0.650	0.325	0.104	3.13	0.035	1.00
A*B	-0.050	-0.025	0.104	-0.24	0.821	1.00
Ct Pt		0.035	0.139	0.25	0.814	1.00

Regression Equation in Uncoded Units

yield = 40.425 + 0.775 A + 0.325 B - 0.025 A*B + 0.035 Ct Pt

Alias Structure

Factor	Name
A	A
B	B

Aliases

I
A
B
AB

Fits and Diagnostics for Unusual Observations

Obs	yield	Fit	Resid	Std Resid	
1	39.300	39.300	0.000	*	X
2	40.900	40.900	0.000	*	X

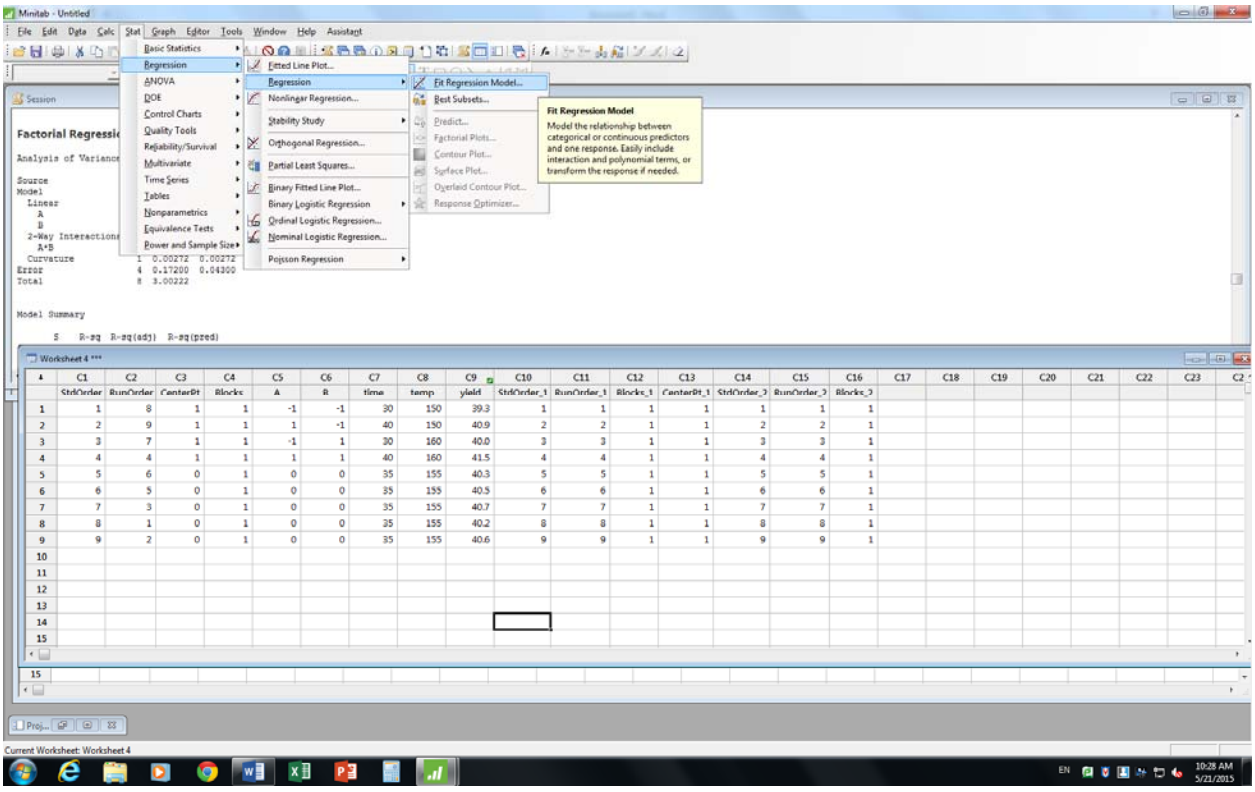
```
  3  40.000  40.000  0.000       *  X
  4  41.500  41.500  0.000       *  X

X  Unusual X
```

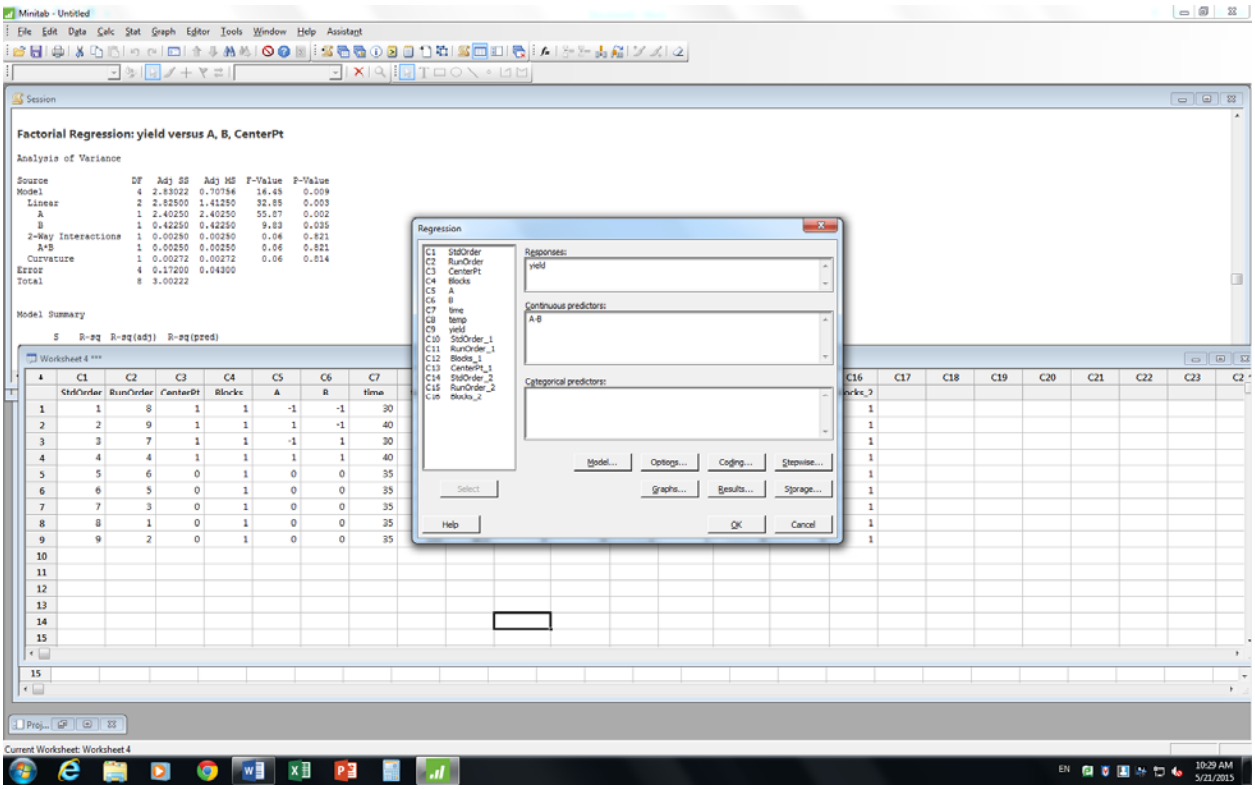
$$H_0: no\ curvature$$

$$H_1: there\ is\ curvature$$

STEP 2:

Fit a regression line





OUTPUT

Regression Analysis: yield versus A, B

Analysis of Variance

Source	DF	Adj SS	Adj MS	F-Value	P-Value
Regression	2	2.82500	1.41250	47.82	0.000
A	1	2.40250	2.40250	81.34	0.000
B	1	0.42250	0.42250	14.30	0.009
Error	6	0.17722	0.02954		
Lack-of-Fit	2	0.00522	0.00261	0.06	0.942
Pure Error	4	0.17200	0.04300		
Total	8	3.00222			

Model Summary

S	R-sq	R-sq(adj)	R-sq(pred)
0.171863	94.10%	92.13%	91.81%

Coefficients

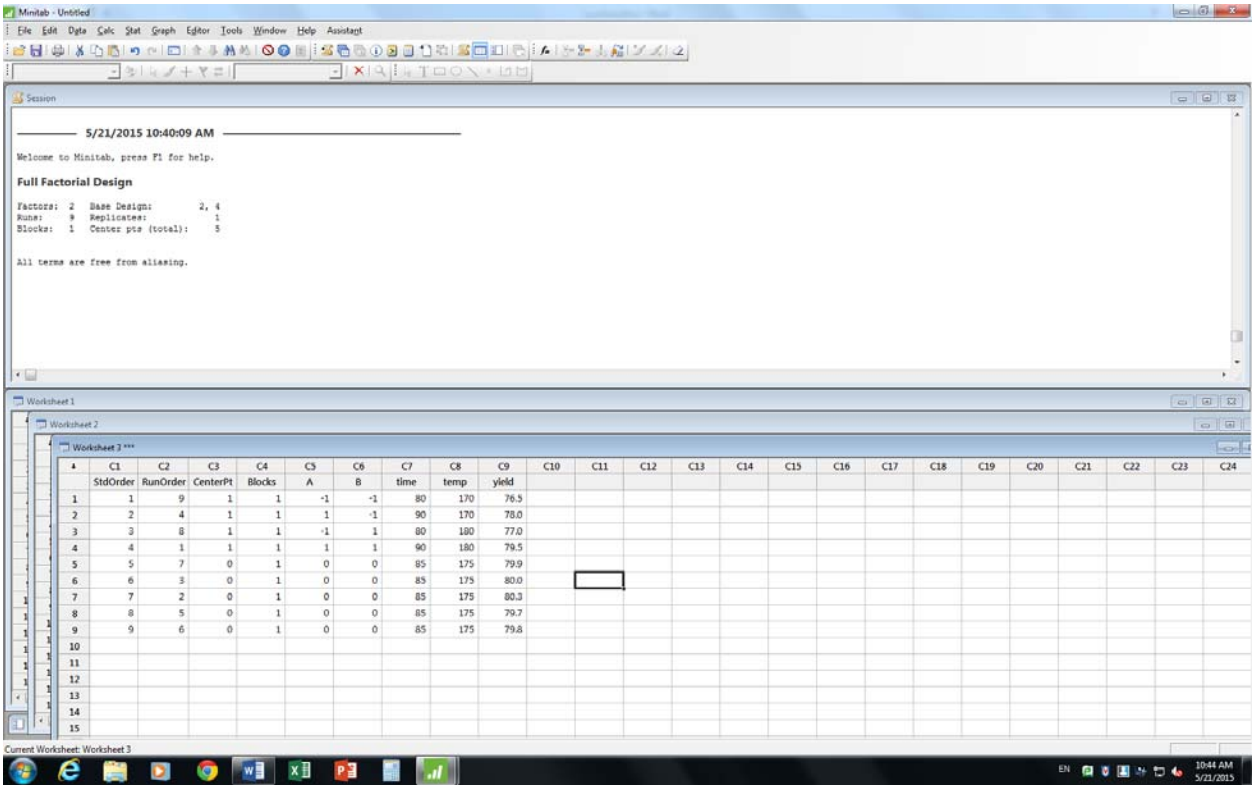
Term	Coef	SE Coef	T-Value	P-Value	VIF
Constant	40.4444	0.0573	705.99	0.000	
A	0.7750	0.0859	9.02	0.000	1.00

Response surfaces

```
B          0.3250   0.0859     3.78    0.009  1.00
```

```
Regression Equation

yield = 40.4444 + 0.7750 A + 0.3250 B
```

NEW DATA



	C1	C2	C3	C4	C5	C6	C7	C8	C9
	StdOrder	RunOrder	CenterPt	Blocks	A	B	time	temp	yield
1	1	9	1	1	-1	-1	80	170	76.5
2	2	4	1	1	1	-1	90	170	78.0
3	3	8	1	1	-1	1	80	180	77.0
4	4	1	1	1	1	1	90	180	79.5
5	5	7	0	1	0	0	85	175	79.9
6	6	3	0	1	0	0	85	175	80.0
7	7	2	0	1	0	0	85	175	80.3
8	8	5	0	1	0	0	85	175	79.7
9	9	6	0	1	0	0	85	175	79.8
10									
11									
12									
13									
14									
15									

Step 1 output for new data

Factorial Regression: yield versus A, B, CenterPt

Analysis of Variance

Source	DF	Adj SS	Adj MS	F-Value	P-Value
Model	4	15.9080	3.9770	75.04	0.001
Linear	2	5.0000	2.5000	47.17	0.002
A	1	4.0000	4.0000	75.47	0.001
B	1	1.0000	1.0000	18.87	0.012
2-Way Interactions	1	0.2500	0.2500	4.72	0.096
A*B	1	0.2500	0.2500	4.72	0.096
Curvature	1	10.6580	10.6580	201.09	0.000
Error	4	0.2120	0.0530		
Total	8	16.1200			

Model Summary

S	R-sq	R-sq(adj)	R-sq(pred)
0.230217	98.68%	97.37%	*

Coded Coefficients

Term	Effect	Coef	SE Coef	T-Value	P-Value	VIF
Constant		77.750	0.115	675.45	0.000	
A	2.000	1.000	0.115	8.69	0.001	1.00
B	1.000	0.500	0.115	4.34	0.012	1.00
A*B	0.500	0.250	0.115	2.17	0.096	1.00
Ct Pt		2.190	0.154	14.18	0.000	1.00

Regression Equation in Uncoded Units

yield = 77.750 + 1.000 A + 0.500 B + 0.250 A*B + 2.190 Ct Pt

Alias Structure

Factor	Name
A	A
B	B

Aliases

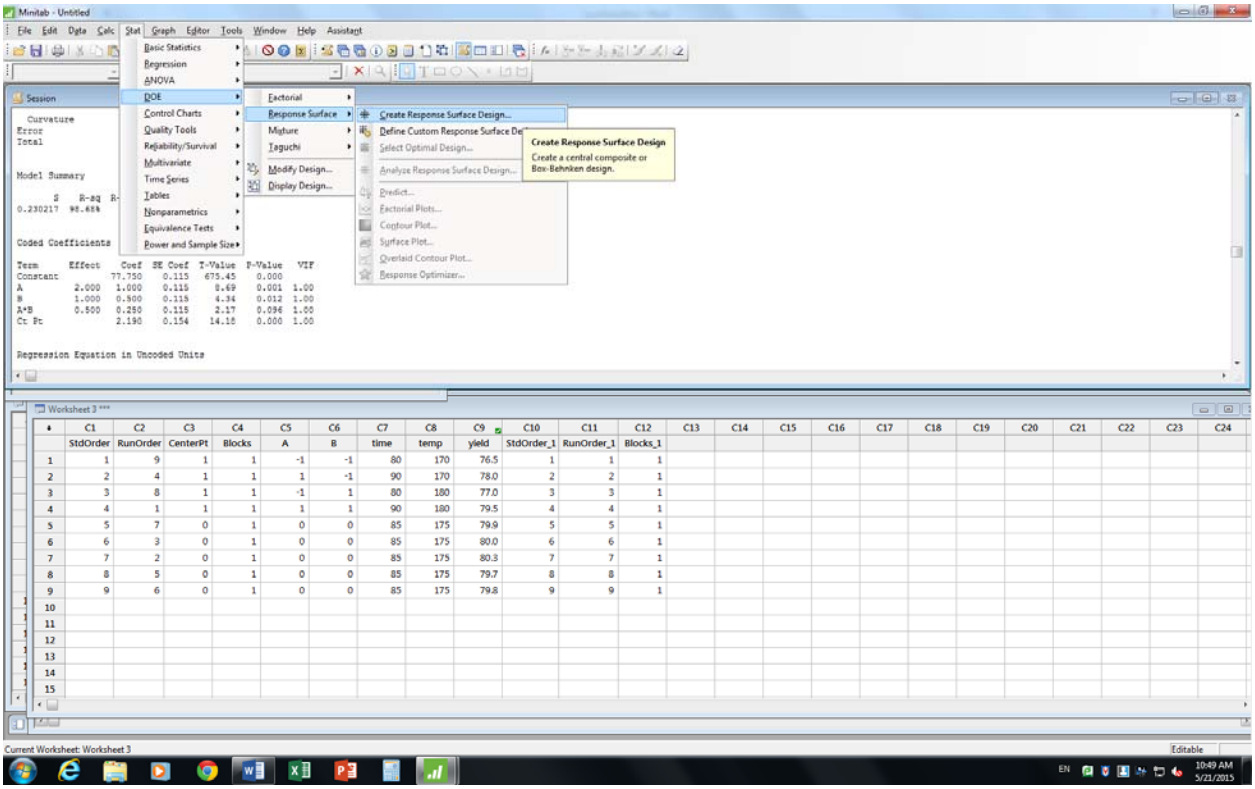
I
A
B
AB

Fits and Diagnostics for Unusual Observations

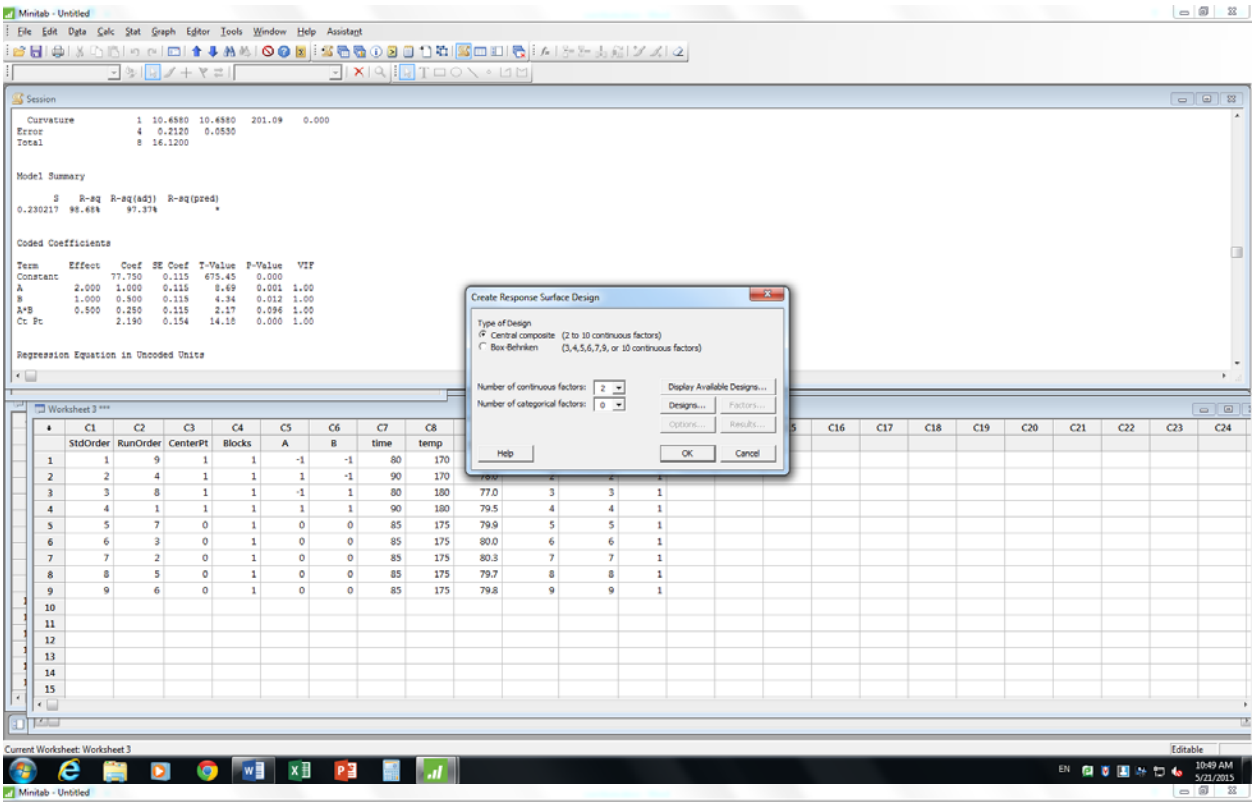
Obs	yield	Fit	Resid	Std Resid	
1	76.500	76.500	0.000	*	X
2	78.000	78.000	0.000	*	X

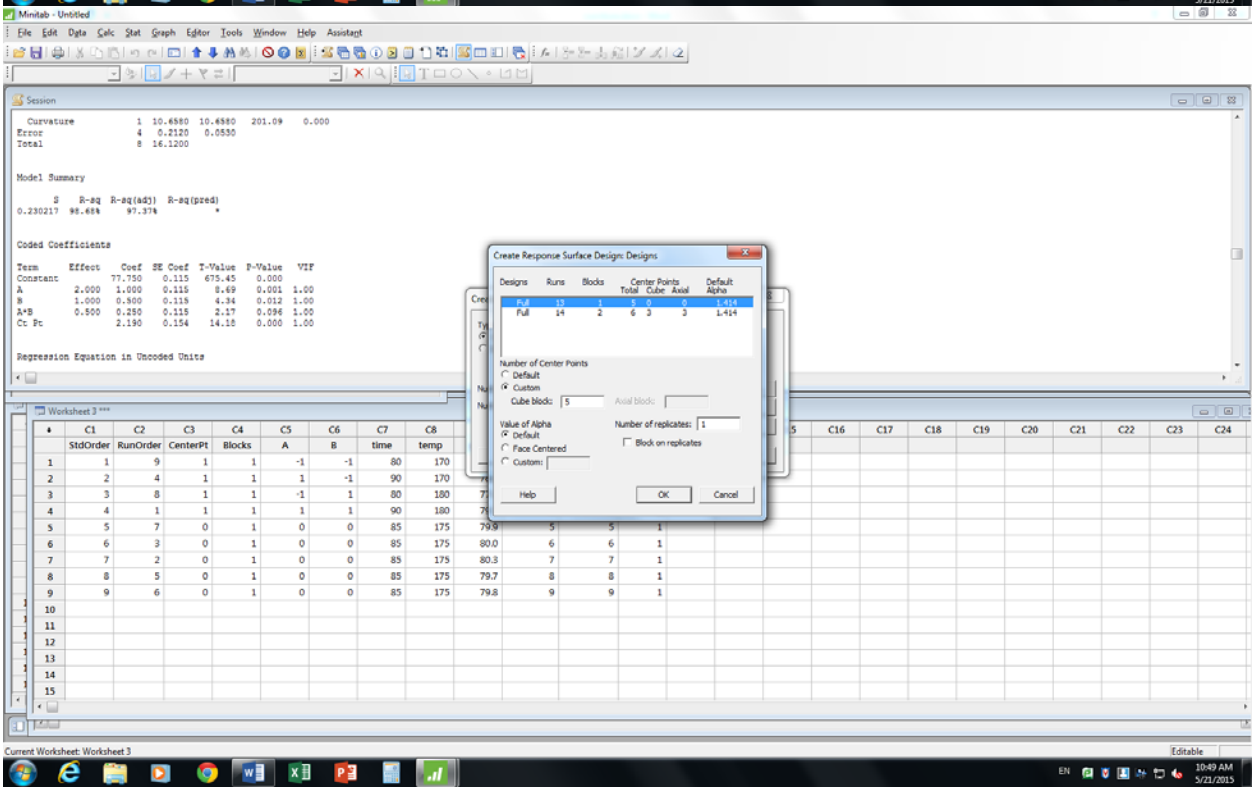
```
  3  77.000  77.000  0.000       *  X
  4  79.500  79.500  0.000       *  X

X  Unusual X
```

After this, since p-value<0.05 we will do the following:

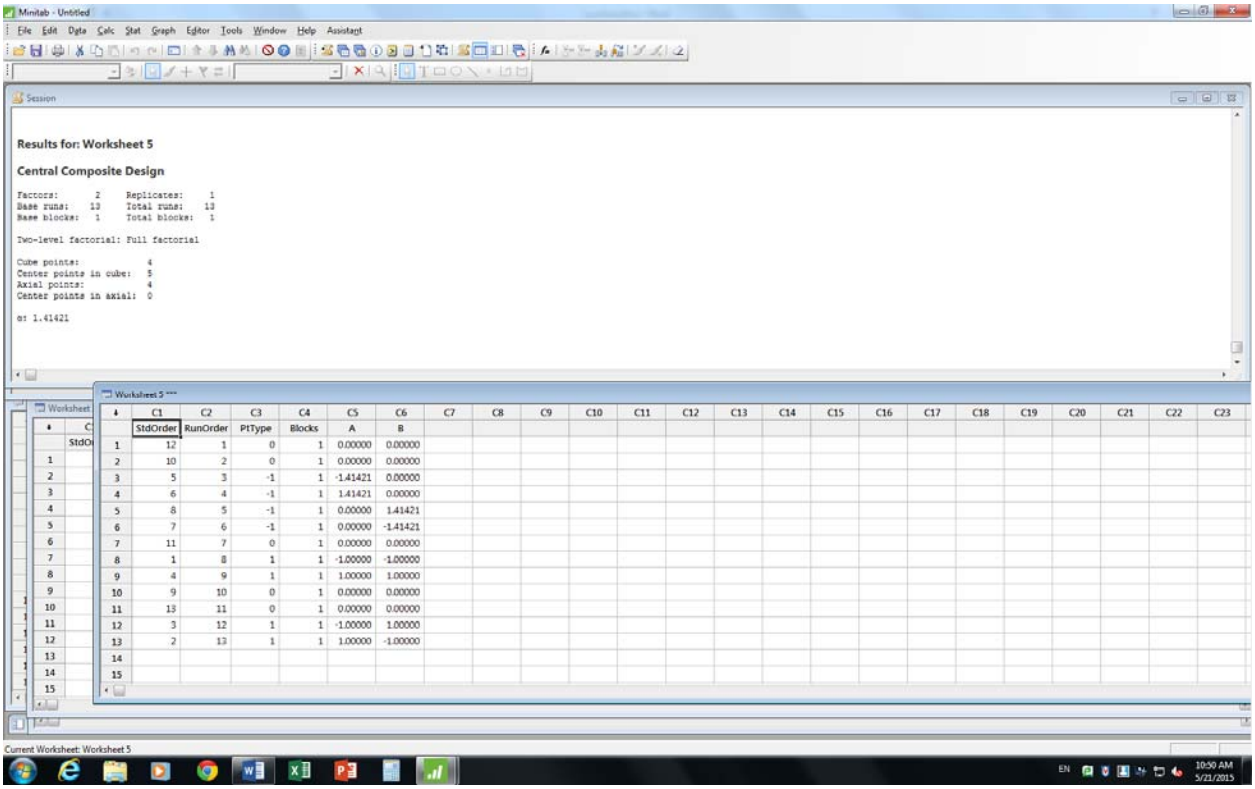


Response surfaces

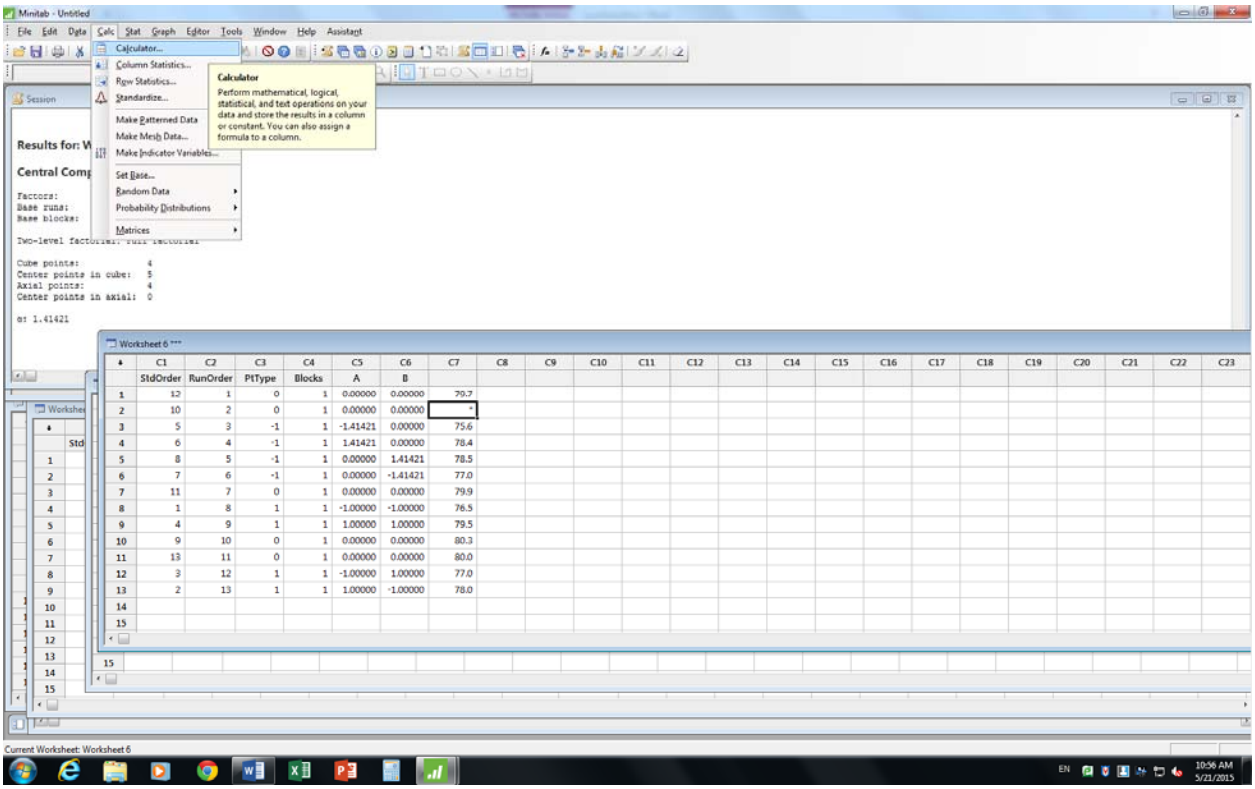


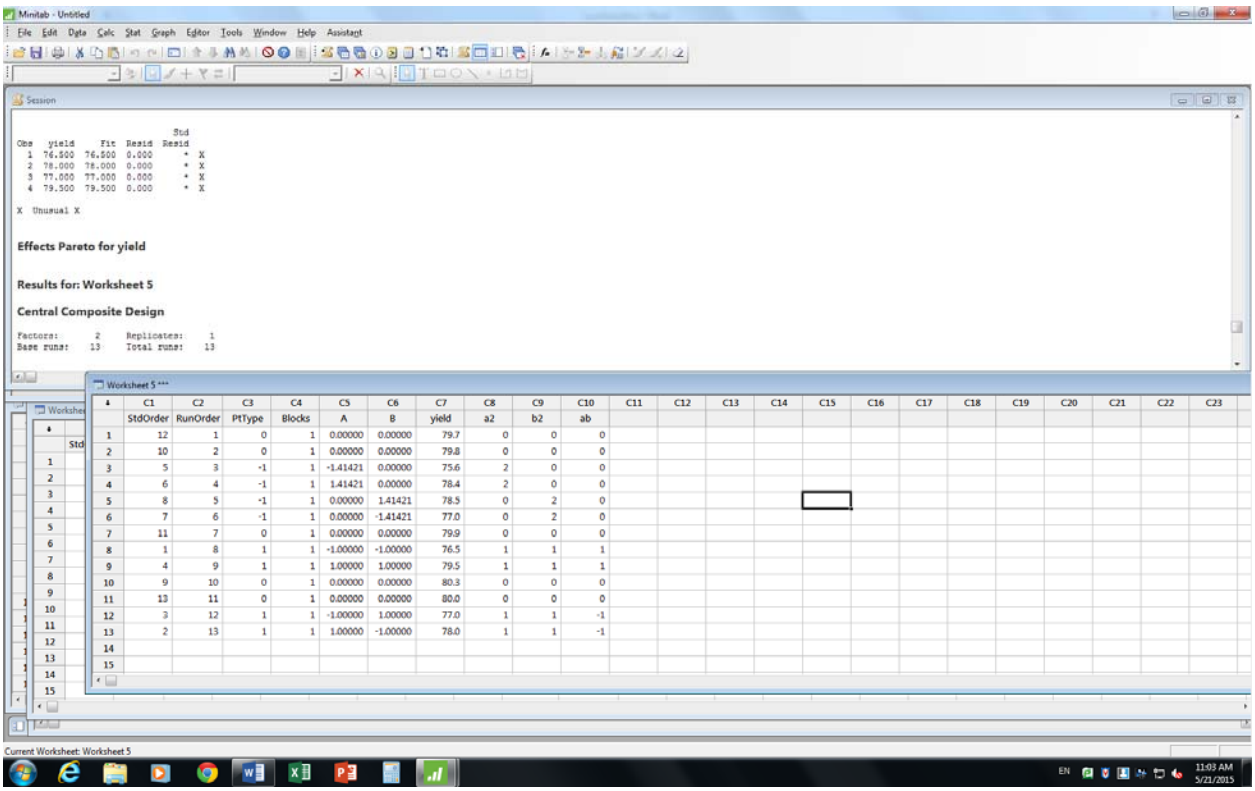


It gives us



Find A^2, B^2 and A*B


Minitab - Untitled
File Edit Data Calc Stat Graph Editor Tools Window Help Assistant
Calculator...
Column Statistics...
Row Statistics...
Standardize...
Make Patterned Data
Make Mesh Data...
Make Indicator Variables...
Set Base...
Random Data
Probability Distributions
Matrices
Calculator
Perform mathematical, logical, statistical, and text operations on your data and store the results in a column or constant. You can also assign a formula to a column.
Session
Results for: W
Central Comp
Factors:
Base runs:
Base blocks:
Cube points: 4
Center points in cube: 5
Axial points: 4
Center points in axial: 0
α: 1.41421
Worksheet 6 ***
C1 StdOrder C2 RunOrder C3 PtType C4 Blocks C5 A C6 B C7
1 12 1 0 1 0.00000 0.00000 79.7
2 10 2 0 1 0.00000 0.00000
3 5 3 -1 1 -1.41421 0.00000 75.6
4 6 4 -1 1 1.41421 0.00000 78.4
5 8 5 -1 1 0.00000 1.41421 78.5
6 7 6 -1 1 0.00000 -1.41421 77.0
7 11 7 0 1 0.00000 0.00000 79.9
8 1 8 1 1 -1.00000 -1.00000 76.5
9 4 9 1 1 1.00000 1.00000 79.5
10 9 10 0 1 0.00000 0.00000 80.3
11 13 11 0 1 0.00000 0.00000 80.0
12 3 12 1 1 -1.00000 1.00000 77.0
13 2 13 1 1 1.00000 -1.00000 78.0
Current Worksheet: Worksheet 6
10:56 AM
5/21/2015


Minitab - Untitled
File Edit Data Calc Stat Graph Editor Tools Window Help Assistant
Session
Obs yield Fit Resid Std Resid
1 76.500 76.500 0.000 * X
2 78.000 78.000 0.000 * X
3 77.000 77.000 0.000 * X
4 79.500 79.500 0.000 * X
X Unusual X
Effects Pareto for yield
Results for: Worksheet 5
Central Composite Design
Factors: 2 Replicates: 1
Base runs: 13 Total runs: 13
Worksheet 5 ***
C1 StdOrder C2 RunOrder C3 PtType C4 Blocks C5 A C6 B C7 yield C8 a2 C9 b2 C10 ab
1 12 1 0 1 0.00000 0.00000 79.7 0 0 0
2 10 2 0 1 0.00000 0.00000 79.8 0 0 0
3 5 3 -1 1 -1.41421 0.00000 75.6 2 0 0
4 6 4 -1 1 1.41421 0.00000 78.4 2 0 0
5 8 5 -1 1 0.00000 1.41421 78.5 0 2 0
6 7 6 -1 1 0.00000 -1.41421 77.0 0 2 0
7 11 7 0 1 0.00000 0.00000 79.9 0 0 0
8 1 8 1 1 -1.00000 -1.00000 76.5 1 1 1
9 4 9 1 1 1.00000 1.00000 79.5 1 1 1
10 9 10 0 1 0.00000 0.00000 80.3 0 0 0
11 13 11 0 1 0.00000 0.00000 80.0 0 0 0
12 3 12 1 1 -1.00000 1.00000 77.0 1 1 -1
13 2 13 1 1 1.00000 -1.00000 78.0 1 1 -1
Current Worksheet: Worksheet 5
11:03 AM
5/21/2015

Now run regression with all the quadratic forms that was created in last step.

Regression Analysis: yield versus A, B, a2, b2, ab

Analysis of Variance

Source	DF	Adj SS	Adj MS	F-Value	P-Value
Regression	5	28.2478	5.6496	79.85	0.000
A	1	7.9198	7.9198	111.93	0.000
B	1	2.1232	2.1232	30.01	0.001
a2	1	13.1761	13.1761	186.22	0.000
b2	1	6.9739	6.9739	98.56	0.000
ab	1	0.2500	0.2500	3.53	0.102
Error	7	0.4953	0.0708		
Lack-of-Fit	3	0.2833	0.0944	1.78	0.290
Pure Error	4	0.2120	0.0530		
Total	12	28.7431			

Model Summary

S	R-sq	R-sq(adj)	R-sq(pred)
0.266000	98.28%	97.05%	91.84%

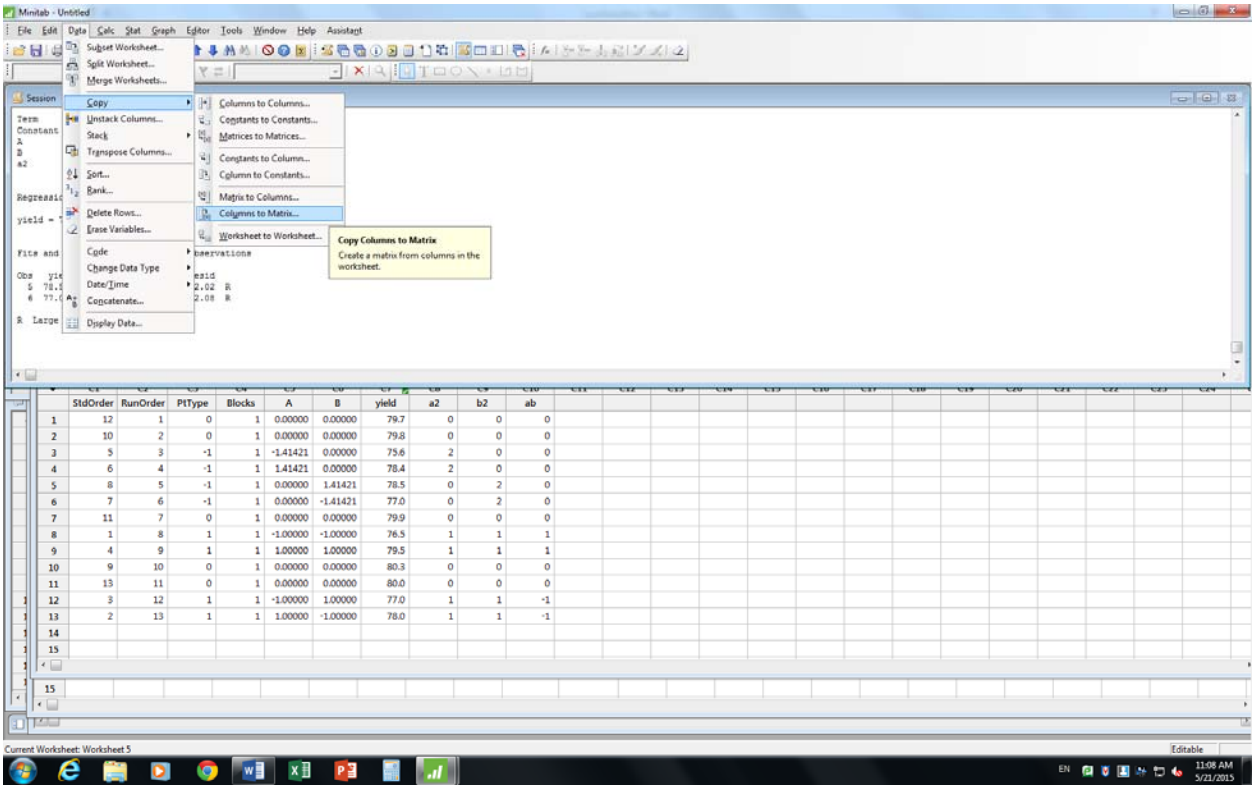
Coefficients

Term	Coef	SE Coef	T-Value	P-Value	VIF
Constant	79.940	0.119	672.00	0.000	
A	0.9950	0.0940	10.58	0.000	1.00
B	0.5152	0.0940	5.48	0.001	1.00
a2	-1.376	0.101	-13.65	0.000	1.02
b2	-1.001	0.101	-9.93	0.000	1.02
ab	0.250	0.133	1.88	0.102	1.00

Regression Equation

yield = 79.940 + 0.9950 A + 0.5152 B - 1.376 a2 - 1.001 b2 + 0.250 ab

NEW STEP


Minitab - Untitled
File Edit Data Calc Stat Graph Editor Tools Window Help Assistant
Subset Worksheet...
Split Worksheet...
Merge Worksheets...
Copy
Unstack Columns...
Stack
Transpose Columns...
Sort...
Rank...
Delete Rows...
Erase Variables...
Code
Change Data Type
Date/Time
Concatenate...
Display Data...
Columns to Columns...
Constants to Constants...
Matrices to Matrices...
Constants to Column...
Column to Constants...
Matrix to Columns...
Columns to Matrix...
Worksheet to Worksheet...
Copy Columns to Matrix
Create a matrix from columns in the worksheet.
StdOrder RunOrder PtType Blocks A B yield a2 b2 ab
1 12 1 0 1 0.00000 0.00000 79.7 0 0 0
2 10 2 0 1 0.00000 0.00000 79.8 0 0 0
3 5 3 -1 1 -1.41421 0.00000 75.6 2 0 0
4 6 4 -1 1 1.41421 0.00000 78.4 2 0 0
5 8 5 -1 1 0.00000 1.41421 78.5 0 2 0
6 7 6 -1 1 0.00000 -1.41421 77.0 0 2 0
7 11 7 0 1 0.00000 0.00000 79.9 0 0 0
8 1 8 1 1 -1.00000 -1.00000 76.5 1 1 1
9 4 9 1 1 1.00000 1.00000 79.5 1 1 1
10 9 10 0 1 0.00000 0.00000 80.3 0 0 0
11 13 11 0 1 0.00000 0.00000 80.0 0 0 0
12 3 12 1 1 -1.00000 1.00000 77.0 1 1 -1
13 2 13 1 1 1.00000 -1.00000 78.0 1 1 -1
Current Worksheet: Worksheet 5
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5/21/2015

11.1. A chemical plant produces oxygen by liquifying air and separating it into its component gases by fractional distillation. The purity of the oxygen is a function of the main condenser temperature and the pressure ratio between the upper and lower columns. Current operating conditions are temperature (ξ_1) = −220°C and pressure ratio (ξ_2) = 1.2. Using the following data, find the path of steepest ascent:

Temperature (ξ_1)	Pressure Ratio (ξ_2)	Purity
−225	1.1	82.8
−225	1.3	83.5
−215	1.1	84.7
−215	1.3	85.0
−220	1.2	84.1
−220	1.2	84.5
−220	1.2	83.9
−220	1.2	84.3

11.8. The data shown in the Table P11.2 were collected in an experiment to optimize crystal growth as a function of three variables x_1, x_2, and x_3. Large values of y (yield in grams) are desirable. Fit a second-order model and analyze the fitted surface. Under what set of conditions is maximum growth achieved?

■ TABLE P11.2

The Crystal Growth Experiment, Problem 11.8

x_1	x_2	x_3	y
−1	−1	−1	66
−1	−1	1	70
−1	1	−1	78
−1	1	1	60
1	−1	−1	80
1	−1	1	70
1	1	−1	100
1	1	1	75
−1.682	0	0	100
1.682	0	0	80
0	−1.682	0	68
0	1.682	0	63
0	0	−1.682	65
0	0	1.682	82
0	0	0	113
0	0	0	100
0	0	0	118
0	0	0	88
0	0	0	100
0	0	0	85