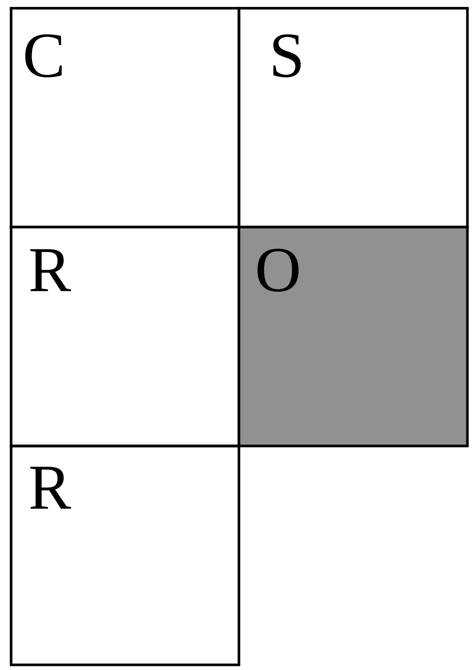
Chapter 10

Optimization Designs

Optimization Designs



Focus: A Few Continuous Factors

Output: Best Settings

Reference: Box, Hunter & Hunter
Chapter 15

Optimization Designs

C	S
R	O 2^k with Center Points Central Composite Des. Box-Behnken Des.
R	

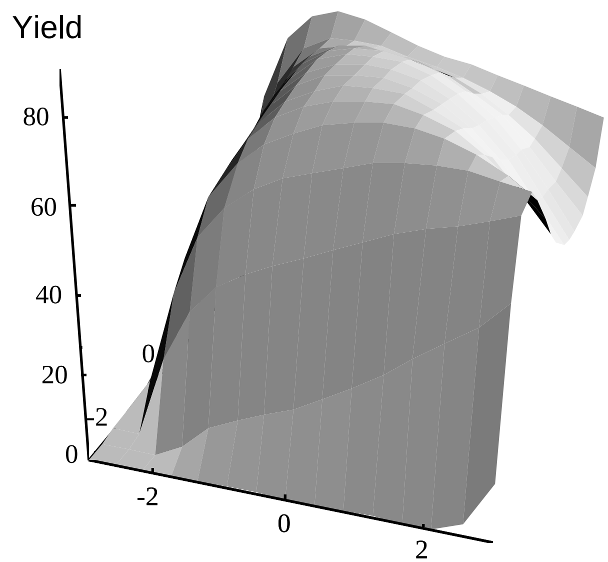
Response Surface Methodology

A Strategy of Experimental Design for finding optimum setting for factors. (Box and Wilson, 1951)

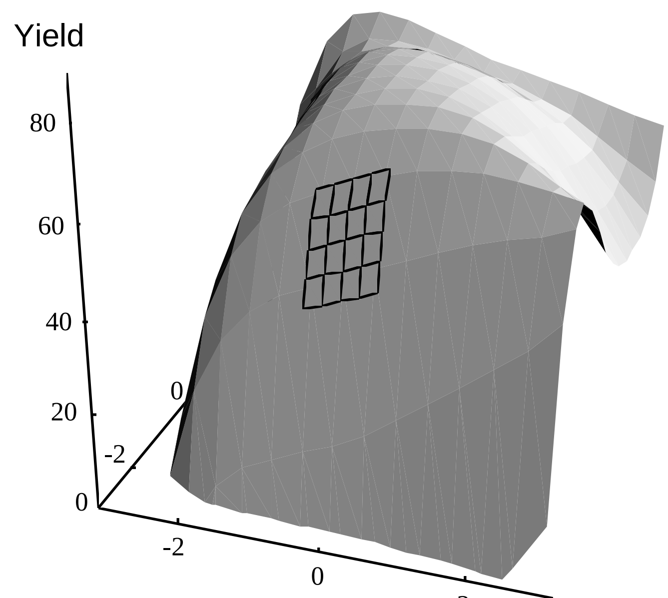
Response Surface Methodology

- **When you are a long way from the top of the mountain, a slope may be a good approximation**
- **You can probably use first–order designs that fit a linear approximation**
- **When you are close to an optimum you need quadratic models and second–order designs to model curvature**

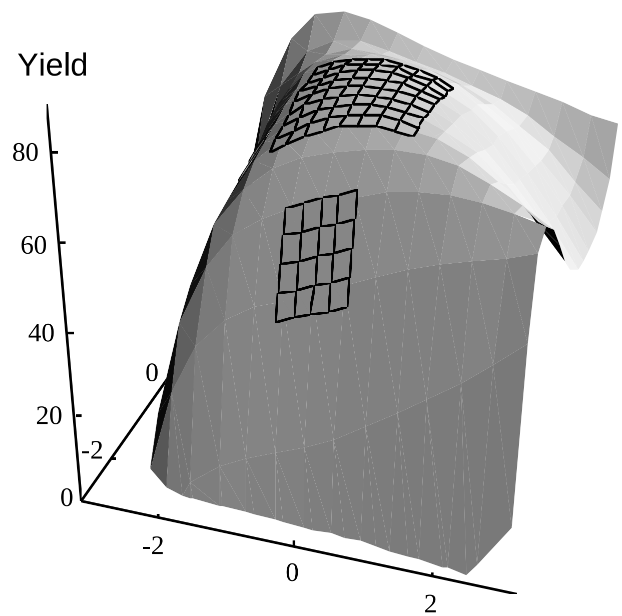
Response Surface



First Order Strategy

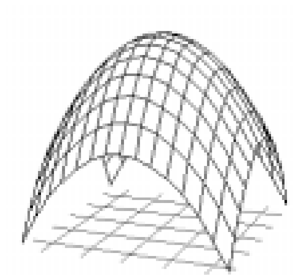


Second Order Strategy

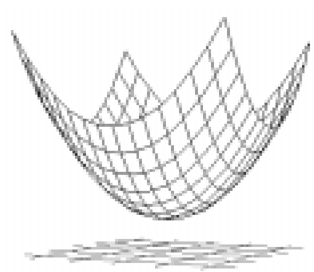


Quadratic Models can only take certain forms

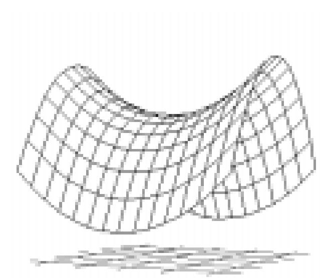
Maximum



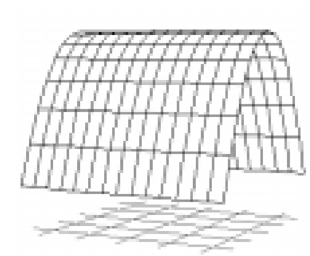
Minimum



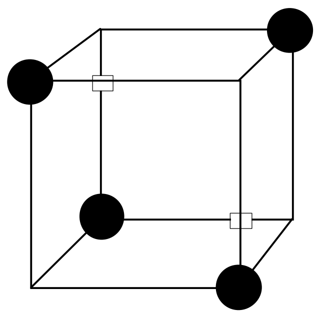
Saddle Point



Stationary Ridge

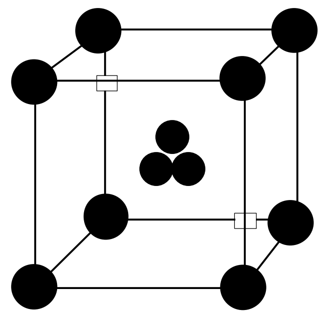


Sequential Assembly of Experimental Designs as Needed



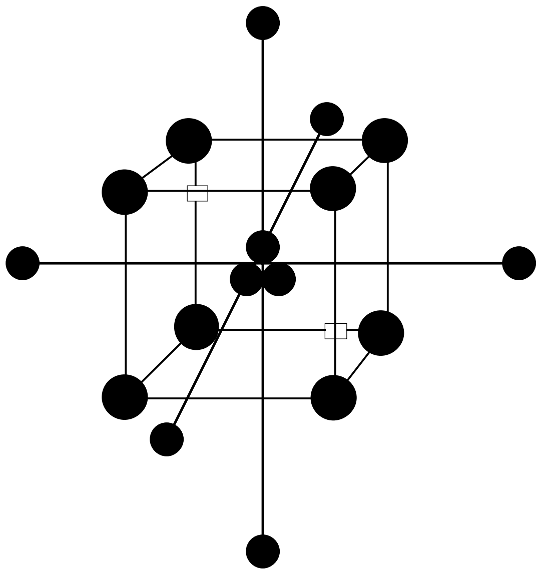
Fractional Factorial

•Linear model



Full Factorial w/Center points

•Main effects
•Interactions
•Curvature check



Central Composite Design

•Full quadratic model

Example: Improving Yield of a Chemical Process

	Levels		
Factor	–	0	+
Time (min)	70	75	80
Temperature (°C)	127.5	130	132.5

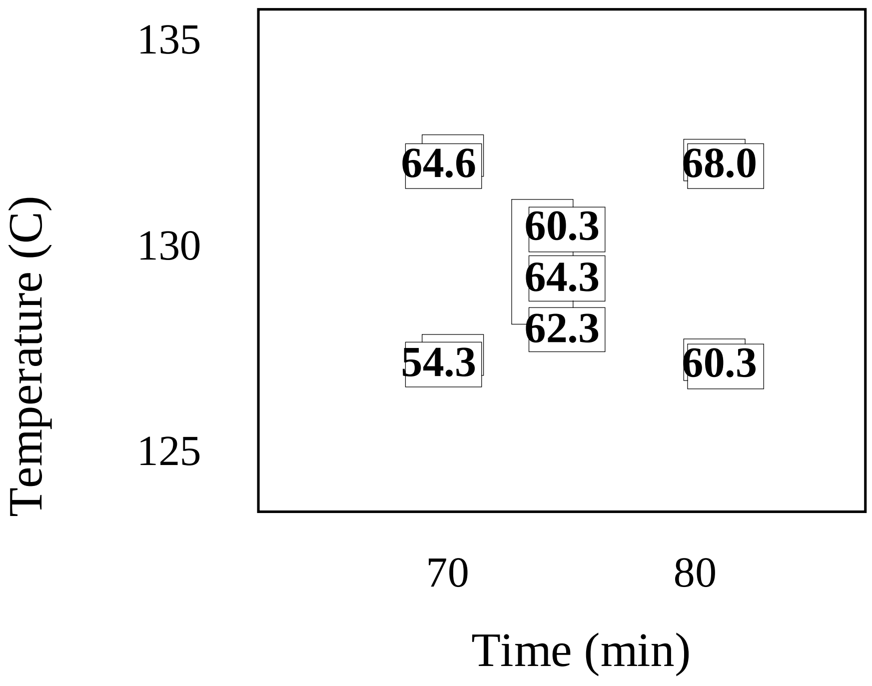
Strategy

- **Fit a first order model**
- **Do a curvature check to determine next step**

Use a 2^2 Factorial Design With Center Points

	x_1	x_2
1	–	–
2	+	–
3	–	+
4	+	+
5	0	0
6	0	0
7	0	0

Plot the Data



Scaling Equations

$$x_i = \frac{\text{(Original Units)} - \text{(Average of Original Units)}}{\tfrac{1}{2}\text{(Range of Original Units)}}$$

$$x_1 = \frac{\text{time} - 75 \text{ minutes}}{5 \text{ minutes}} \qquad x_2 = \frac{\text{temperature} - 130°\text{C}}{2.5°\text{C}}$$

Results From First Factorial Design

Run	*Factors in original units*		*Factors in coded units*		*Response*
	Time (min.)	Temp. (°C)			Yield (gms)
	x_1	x_2	x_1	x_2	y
1	70	127.5	–	–	54.3
2	80	127.5	+	–	60.3
3	70	132.5	–	+	64.6
4	80	132.5	+	+	68.0
5	75	130.0	0	0	60.3
6	75	130.0	0	0	64.3
7	75	130.0	0	0	62.3

Curvature Check by Interactions

- **Are there any large two factor interactions? If not, then there is probably not significant curvature.**
- **If there are many large interaction effects then we should not follow a path of steepest ascent because there is curvature.**

Here, ℓ_{time}=4.7, ℓ_{temp} =9.0, and $\ell_{\text{time*temp}}$=-1.3, so the main effects are larger and thus there is little curvature.

Curvature Check with Center Points

- **Compare the average of the factorial points, $\bar{y}_f$, with the average of the center points, $\bar{y}_c$. If they are close then there is probably no curvature?**

Statistical Test: $n_f = \#$ of points in factorial

$n_c = \#$ of points in center

$s_c =$ Standard deviation of points in center

$$\bar{y}_f - \bar{y}_c \pm t_{\alpha/2, n_c - 1} s_c \sqrt{\frac{1}{n_f} + \frac{1}{n_c}}$$

If zero is in the confidence interval then there is no evidence of curvature.

Curvature Check with Center Points

$$61.8 - 62.3 \pm 4.303\,(2)\sqrt{\frac{1}{4} + \frac{1}{3}}$$

$$-0.5 \pm 6.57$$

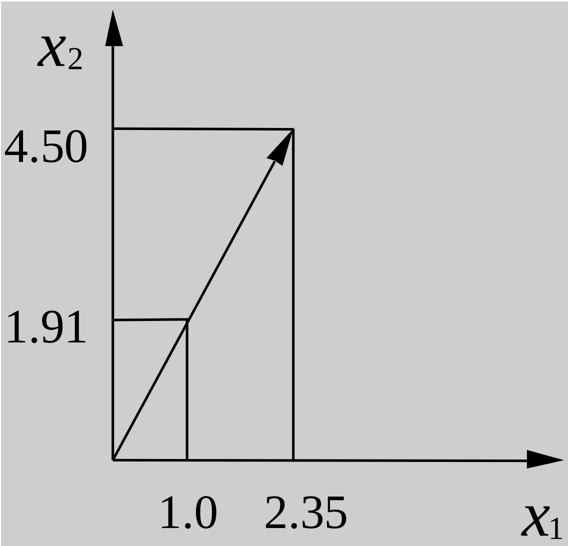
No Evidence of Curvature!!

Fit the First Order Model

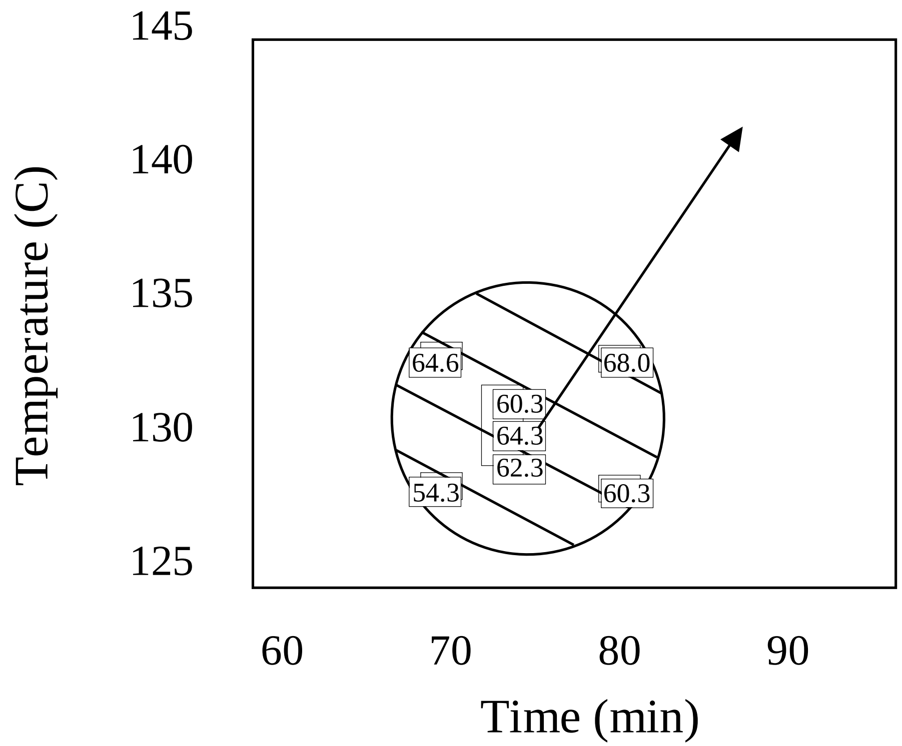
$$\hat{y} = 62.0 + 2.35x_1 + 4.5x_2$$

Path of Steepest Ascent: Move 4.50 Units in x_2 for Every 2.35 Units in x_1

Equivalently, for every one unit in x_1 we move 4.50/2.35=1.91 units in x_2



The Path in the Original Factors



Scaling Equations

$$x_1 = \frac{\text{time} - 75 \text{ minutes}}{5 \text{ minutes}} \qquad x_2 = \frac{\text{temperature} - 130^\circ\text{C}}{2.5^\circ\text{C}}$$

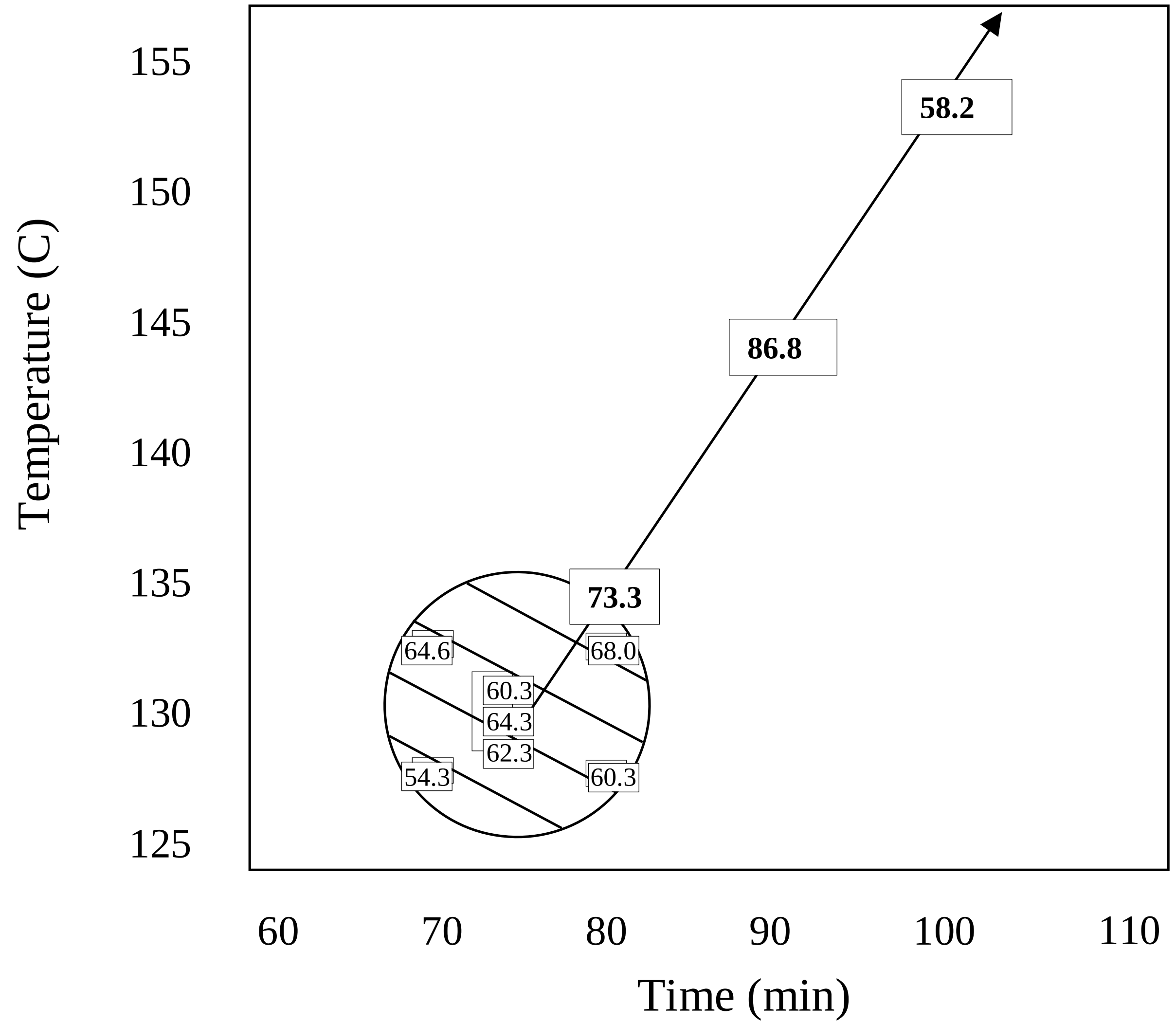
$$\text{time} = 5x_1 + 75 \quad \text{minutes}$$

$$\text{temperature} = 2.5x_2 + 130\ ^\circ\text{C}$$

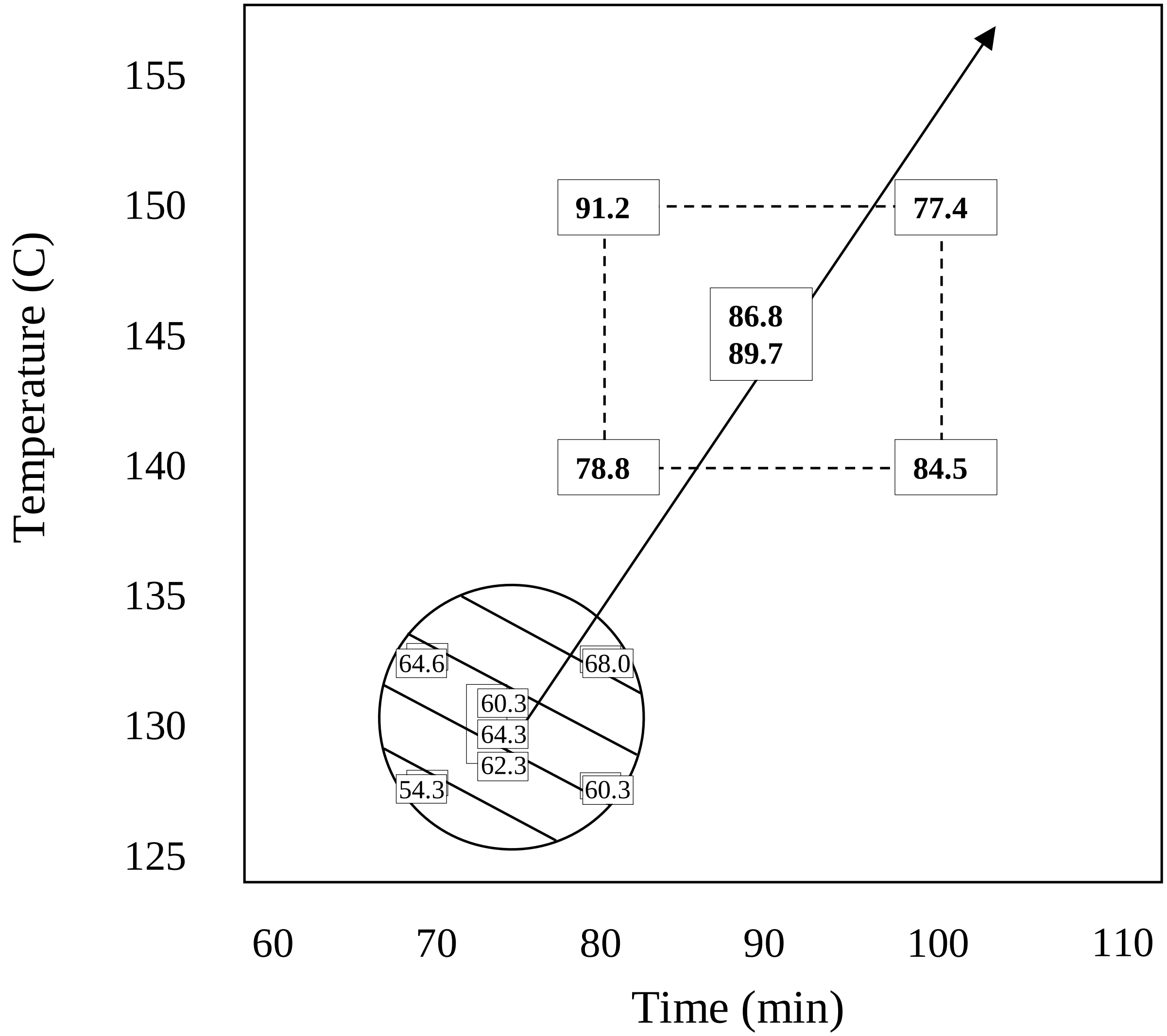
Points on the Path of Steepest Ascent

	Factors in coded units		Factors in original units		Run	Response
			Time (min.)	Temp. (°C)		Yield (gms)
	x_1	x_2	x_1	x_2		y
center conditions	0	0	75	130.0	5,6,7	62.3
path of steepest ascent	1	1.91	80	134.8	8	73.3
	2	3.83	85	139.6		
	3	5.74	90	144.4	10	86.8
	4	7.66	95	149.1		
	5	9.57	100	153.9	9	58.2

Exploring the Path of Steepest Ascent



A Second Factorial



Results of Second Factorial Design

Run	*Factors in original units*		*Factors in coded units*		*Response*
	Time (min.)	Temp. (°C)			Yield (gms)
	x_1	x_2	x_1	x_2	y
11	80	140	–	–	78.8
12	100	140	+	–	84.5
13	80	150	–	+	91.2
14	100	150	+	+	77.4
15	90	145	0	0	89.7
16	90	145	0	0	86.8

Curvature Check by Interactions

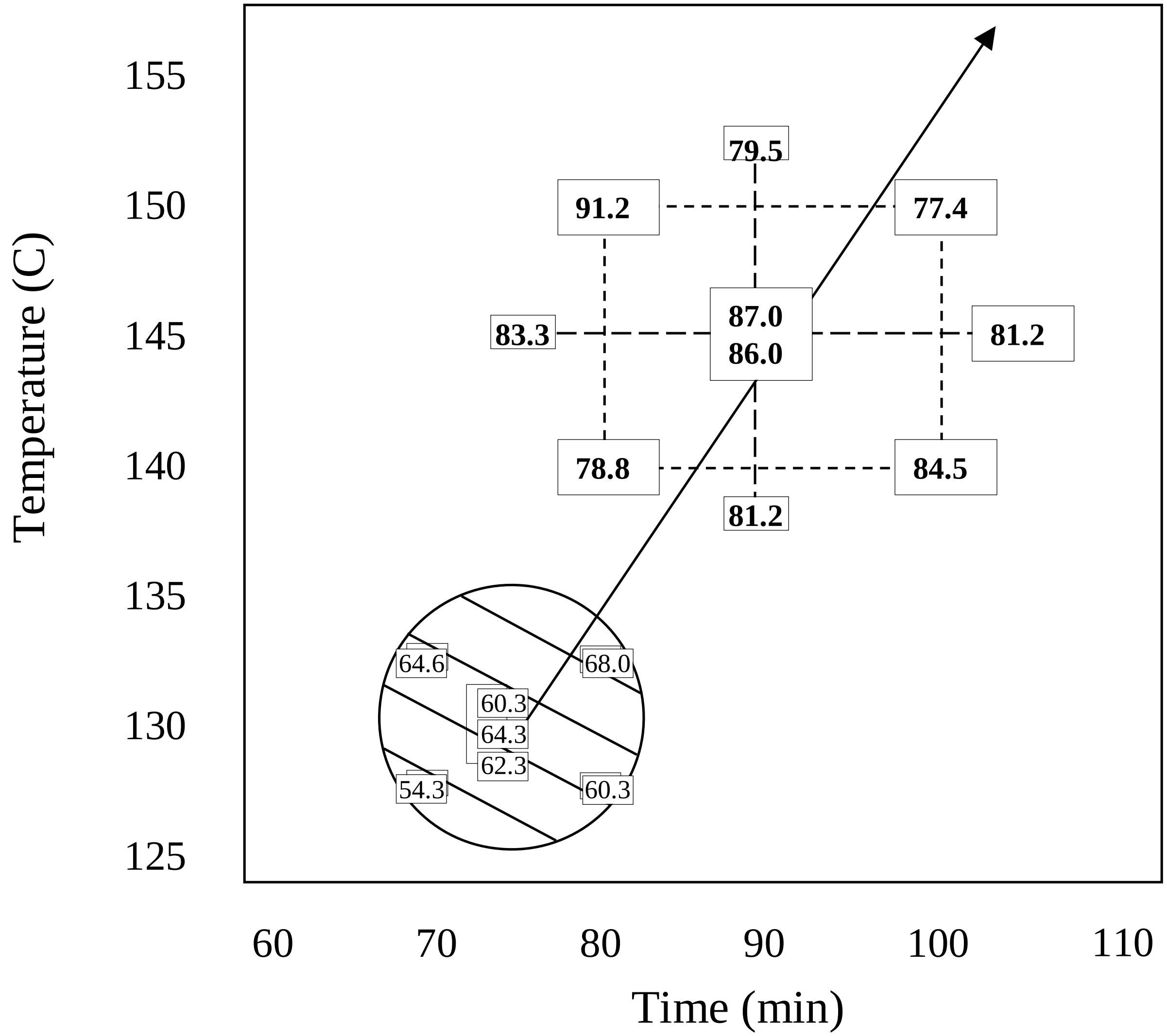
Here, ℓ_{time}=-4.05, ℓ_{temp}=2.65, and $\ell_{time*temp}$=-9.75, so the interaction term is the largest, so there appears to be curvature.

New Scaling Equations

$$x_1 = \frac{\text{time} - 90 \text{ minutes}}{10 \text{ minutes}}$$

$$x_2 = \frac{\text{temperature} - 145^\circ\text{C}}{5^\circ\text{C}}$$

A Central Composite Design



The Central Composite Design and Results

Run	*Variables in original units*		*Variables in coded units*		*Response*
	Time (min.)	Temp. (°C)			Yield (gms)
	x_1	x_2	x_1	x_2	y
	second first-order design				
11	80	140	–	–	78.8
12	100	140	+	–	84.5
13	80	150	–	+	91.2
14	100	150	+	+	77.4
15	90	145	0	0	89.7
16	90	145	0	0	86.8
	runs added to form a composite design				
17	76	145	$-\sqrt{2}$	0	83.3
18	104	145	$+\sqrt{2}$	0	81.2
19	90	138	0	$-\sqrt{2}$	81.2
20	90	152	0	$+\sqrt{2}$	79.5
21	90	145	0	0	87.0
22	90	145	0	0	86.0

Must Use Regression to find the Predictive Equation

The Quadratic Model in Coded units

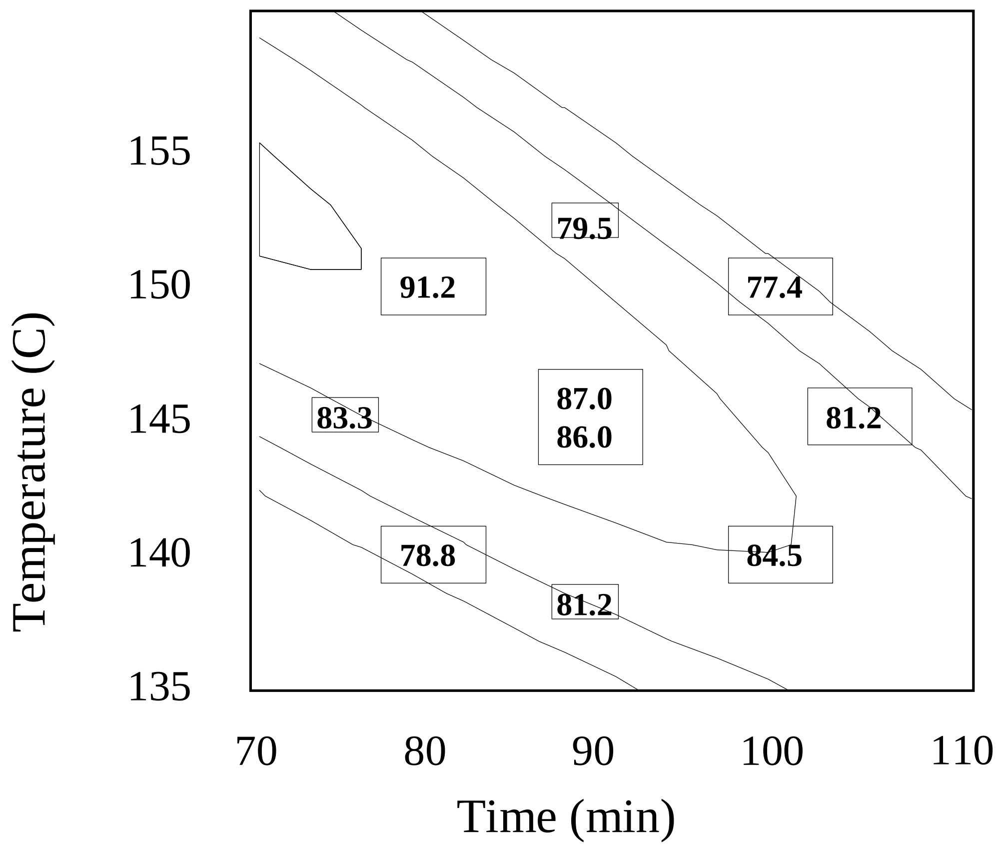
$$\hat{y} = 87.38 - 1.38x_1 + 0.36x_2$$
$$-2.14x_1^2 - 3.09x_2^2 - 4.88x_1x_2$$

Must Use Regression to find the Predictive Equation

The Quadratic Model in Original units

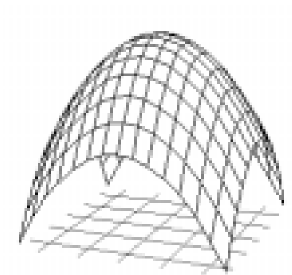
$$\hat{y} = -3977 + 17.86 * time + 45.00 * temp$$
$$-0.0975 * time * temp - 0.0215 * time^2 - 0.1247 * temp^2$$

The Fitted Surface in the Region of Interest

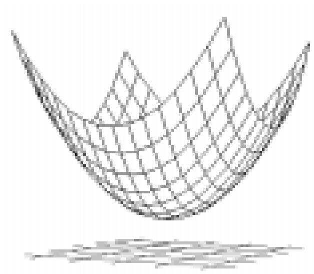


Quadratic Models can only take certain forms

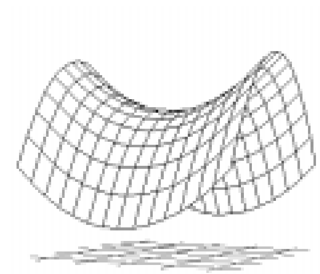
Maximum



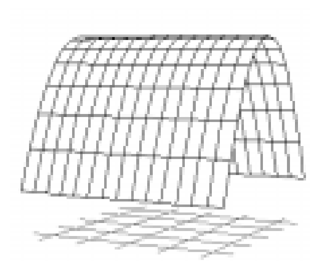
Minimum



Saddle Point



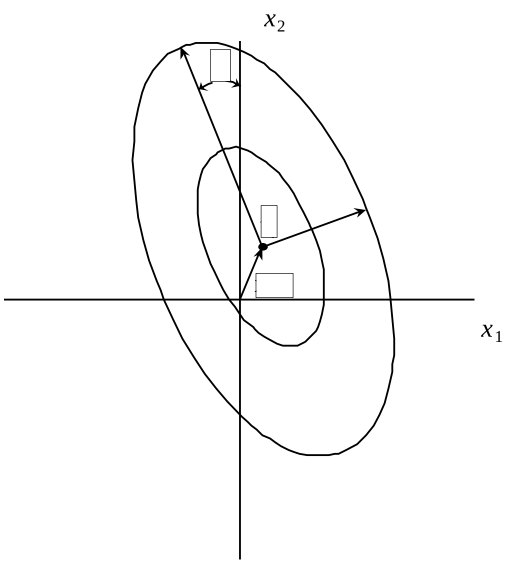
Stationary Ridge

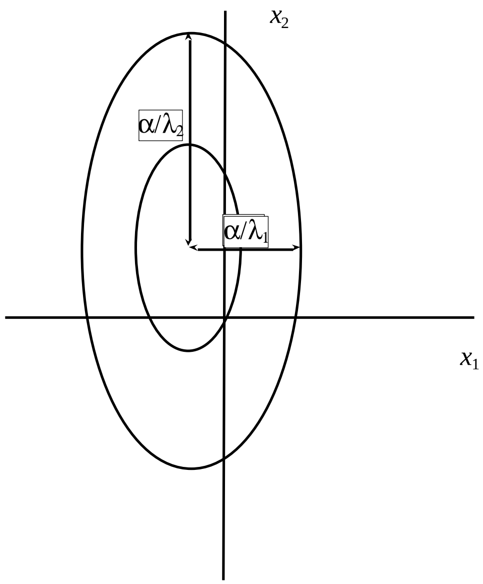


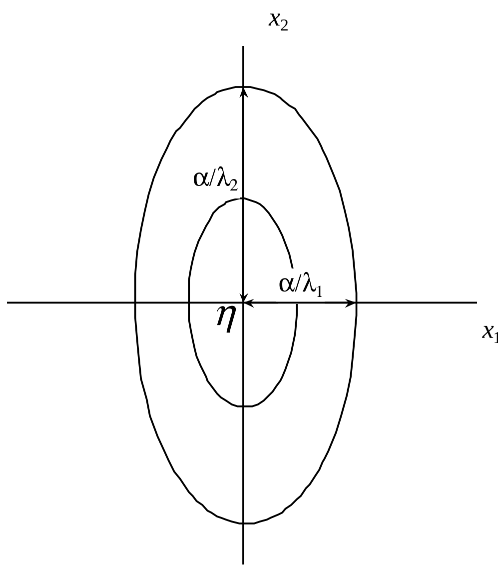
Canonical Analysis

Enables us to analyze systems of maxima and minima in many dimensions and, in particular to identify complicated ridge systems, where direct geometric representation is not possible.

Two Dimensional Example







$$\hat{y} = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2$$

$$\hat{y} = \beta_0 + \phi_1 x_1 + \phi_2 x_2 + \lambda_1 x_1^2 + \lambda_2 x_2^2$$

$$\hat{y} = \eta + \lambda_1 x_1^2 + \lambda_2 x_2^2$$

α is a constant

Quadratic Response Surfaces

- **Any two quadratic surfaces with the same eigenvalues (λ's) are just shifted and rotated versions of each other.**
- **The version which is located at the origin and oriented along the axes is easy to interpret without plots.**

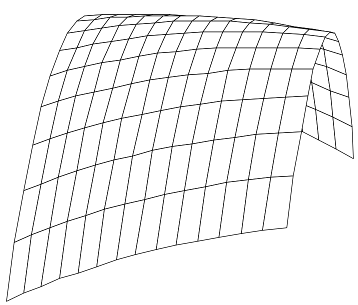
The Importance of the Eigenvalues

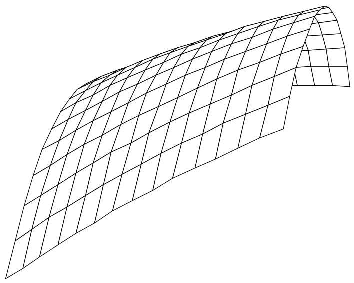
- **The shape of the surface is determined by the signs and magnitudes of the eigenvalues.**

Type of Surface	Eigenvalues
Minimum	All eigenvalues positive
Saddle Point	Some eigenvalues positive and some negative
Maximum	All eigenvalues negative
Ridge	At least one eigenvalue zero

Stationary Ridges in a Response Surface

- **The existence of stationary ridges can often be exploited to maintain high quality while reducing cost or complexity.**





Response Surface Methodology

Goals	Tools
Select Factors and Levels and Responses	Brainstorming
Eliminate Inactive Factors	Fractional Factorials (Res III)
Find Path of Steepest Ascent	Fractional Factorials (Higher Resolution from projection or additional runs)
Follow Path	Single Experiments until Improvement stops
Find Curvature	Center Points (Curvature Check) Fractional Factorials (Res > III) (Interactions > Main Effects)
Model Curvature	Central Composite Designs Fit Full Quadratic Model

Continued on Next Page

Goals

Understand the shape of the surface

Find out what the optimum looks like Point, Line, Plane, etc.

If there is a rising ridge, then follow it.

If there is a stationary ridge, then find the cheapest place that is optimal.

Tools

Canonical Analysis
- A-Form if Stationary Point is outside Experimental Region
- B-Form if Stationary Point is inside Experimental Region

Reduce the Canonical Form with the DLR Method

Translate the reduced model back and optimum formula back to original coordinates

Translate the reduced model back and optimum formula back to original coordinates