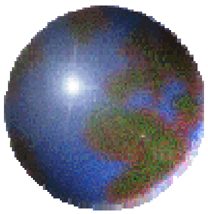
Response Surface Methodology: 50 Years Later



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05 July, 2005

Response Surface Methodology

Box and Wilson (1951)

"On the Experimental Attainment of Optimum Condition," *JRSS-B*, **13**, 1-45.

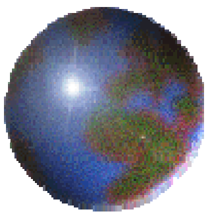
Box and Hunter (1957)

"Multi-Factor Experimental Designs for Exploring Response Surface," *Annals of Mathematical Statistics*, **28**, 195-241.

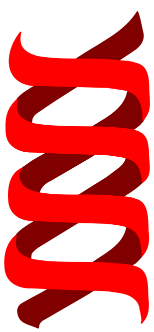
Ambitious Goal

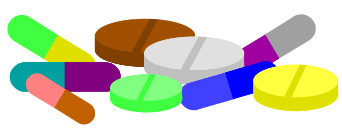
- What is Response Surface Methodology?
- What type of problems they had in mind back to 1950?
- What was available in 1950?
- What type of problems today
  (50 years later)?
- What is available today?
- Can we do something significantly different?

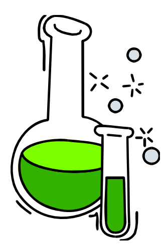
What is RSM All About?

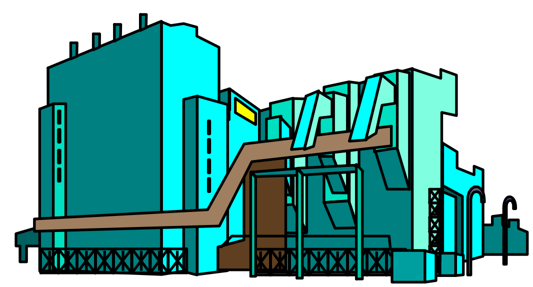


The Experimenter is like a person attempting to map the depth of the sea by making soundings at a limited number of places









- 給我
  一把槌子，
  全世界的問題都像
  一根釘子

Basic Approach

- If we are far away from the top, all we need is to find the direction for improvement...in this case, a first-order approximation may be sufficient.
- If we are close to the top, all we need is to find the exact location of the top...in this case, a more complicated model (such as a second-order model) is needed.

Illustrative Example (BH^2)

- Response (y): Yield
- Input Variable (x_1): time
- Input Variable (x_2): temperature

$$y = f(x_1, x_2) + \varepsilon$$

run*	variables in original units		variables in coded units		response: yield (grams)
	time (min)	temperature (°C)	x_1	x_2	y
1	70	127.5	−1	−1	54.3
2	80	127.5	+1	−1	60.3
3	70	132.5	−1	+1	64.6
4	80	132.5	+1	+1	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

Least Square Fitting:

$y = 62.01 + 2.35x_1 + 4.50x_2 + \varepsilon$

$b_{12} = -0.65\ (\pm 0.75)$

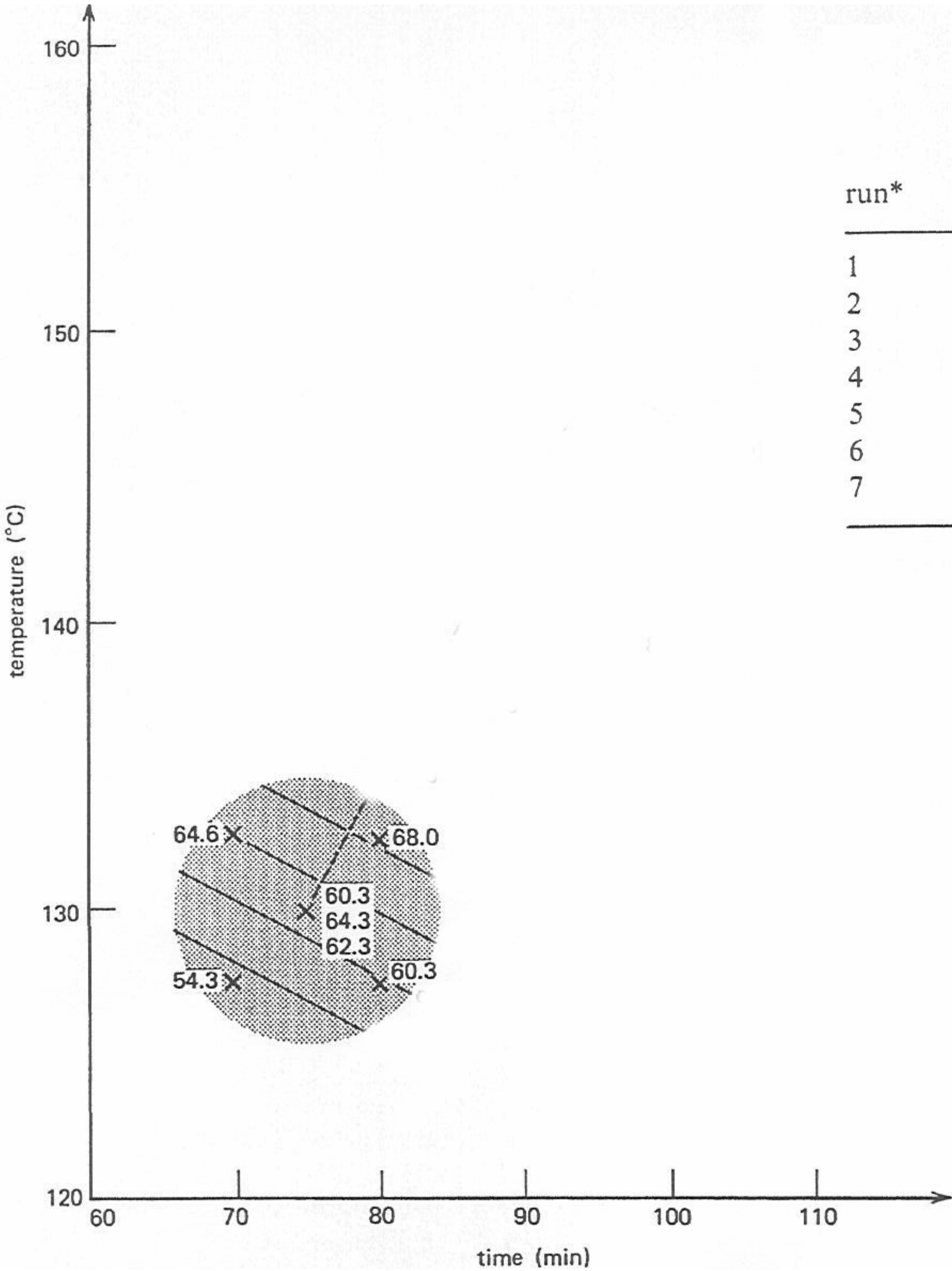
$b_{11} + b_{22} = -0.50\ (\pm 1.15)$

Conclusion:

First-order model is adequate.

Action Taken:

Steepest Ascent
—direction for improvement
— 2.35:4.50 (or 1:1.91)



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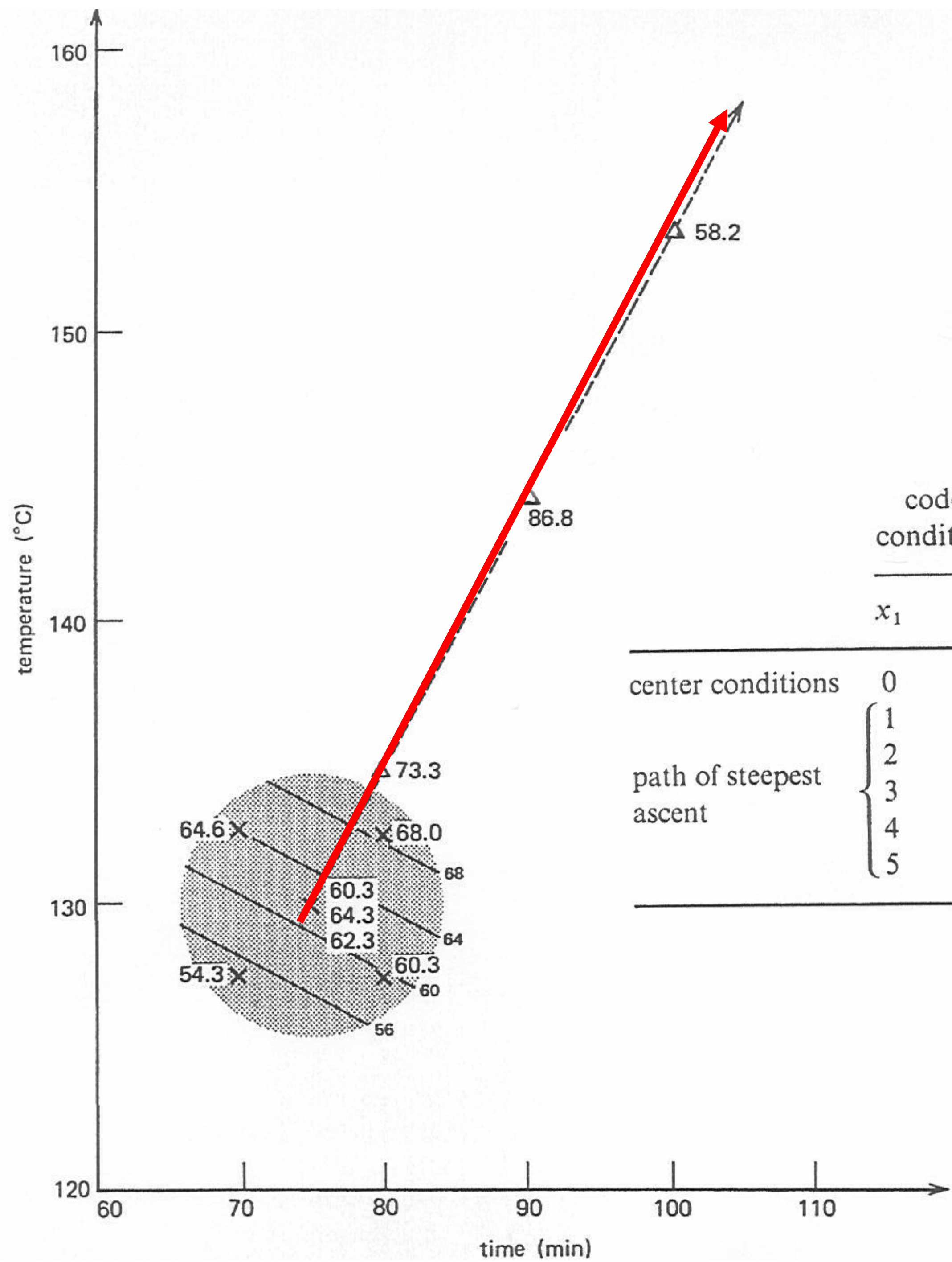
Run more experiments…

…following the direction of 1:1.91 (= 2.35 : 4.50)

	coded conditions x_1	coded conditions x_2	time (min) t	temperature (°C) T	run	observed yield
center conditions	0	0	75	130.0	5, 6, 7	62.3 (average)
path of steepest ascent	1	1.91	80	134.8	8	73.3
path of steepest ascent	2	3.83	85	139.6		
path of steepest ascent	3	5.74	90	144.4	10	86.8
path of steepest ascent	4	7.66	95	149.1		
path of steepest ascent	5	9.57	100	153.9	9	58.2



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Conclusion:
Use Point #10 as the new center point and start all over again!!

run*	variables in original units: time (min)	temperature (°C)	variables in coded units: x_1	x_2	response: yield (grams)
11	80	140	−1	−1	78.8
12	100	140	+1	−1	84.5
13	80	150	−1	+1	91.2
14	100	150	+1	+1	77.4
15	90	145	0	0	89.7
16	90	145	0	0	86.8

Least Square Fitting:

$y = 84.73 - 2.025x_1 + 1.325x_2 + \varepsilon$

$b_{12} = -4.88\ (\pm 0.75)$

$b_{11} + b_{22} = -5.28\ (\pm 1.15)$

Conclusion:

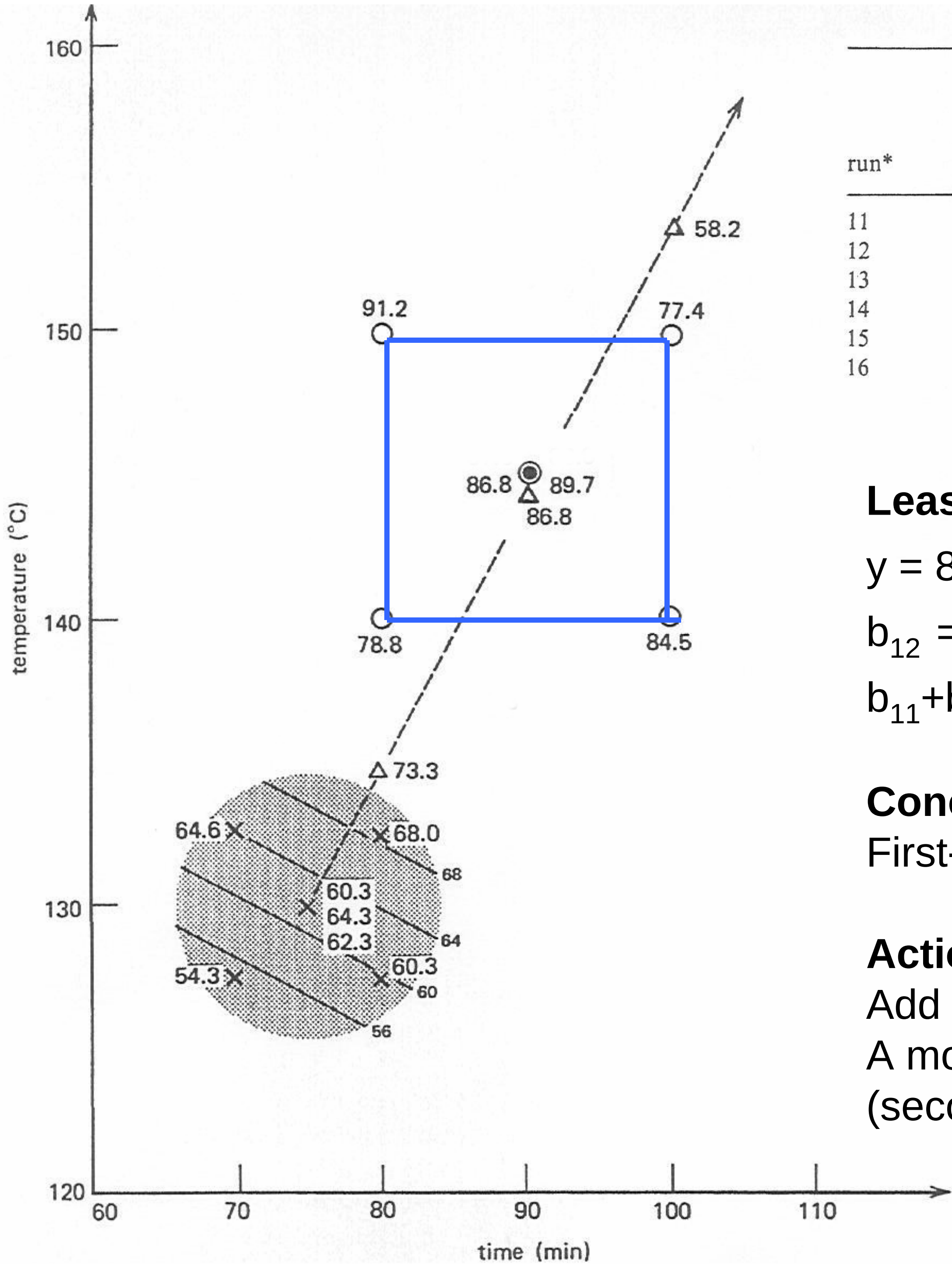
First-Order Model is inadequate!

Action Taken:

Add few more points for fitting

A more complicated

(second-order) model.



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Add few more points for fitting a second-order model.

run*	variables in original units: time (min)	temperature (°C)	variables in coded units: x_1	x_2	response: yield (grams)	
11	80	140	-1	-1	78.8	second first-orde design
12	100	140	$+1$	-1	84.5	
13	80	150	-1	$+1$	91.2	
14	100	150	$+1$	$+1$	77.4	
15	90	145	0	0	89.7	
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17	76	145	$-\sqrt{2}$	0	83.3	runs added to form a composit design
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	
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Least Square Fitting:

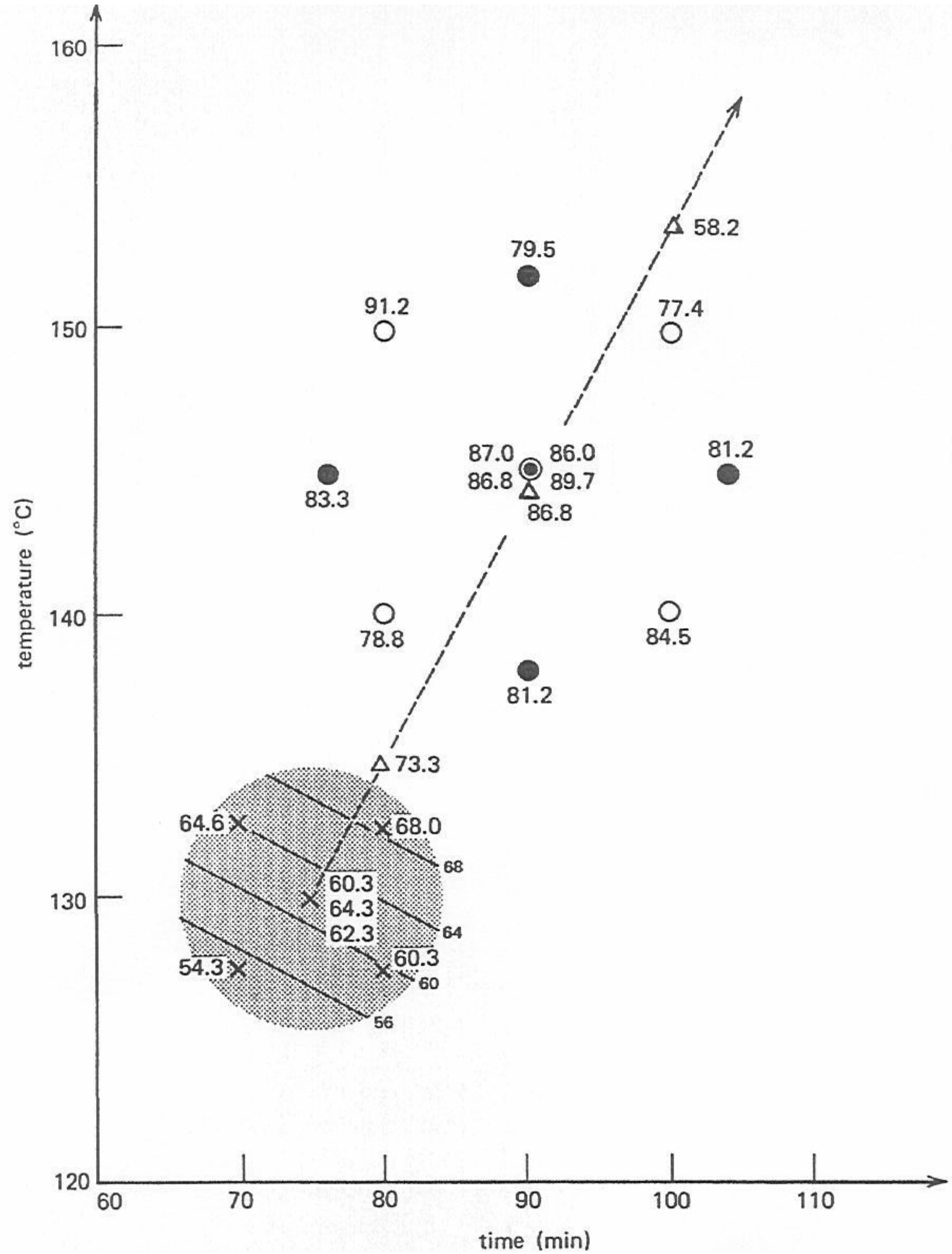
$$y = 87.36 - 1.39x_1 + 0.37x_2 + 2.15\,x_1^2 - 3.12\,x_2^2 - 4.88\,x_1\,x_2 + \varepsilon$$

Conclusion:

Second-Order model is adequate!

Action Taken:

Finding Optimal Setting!



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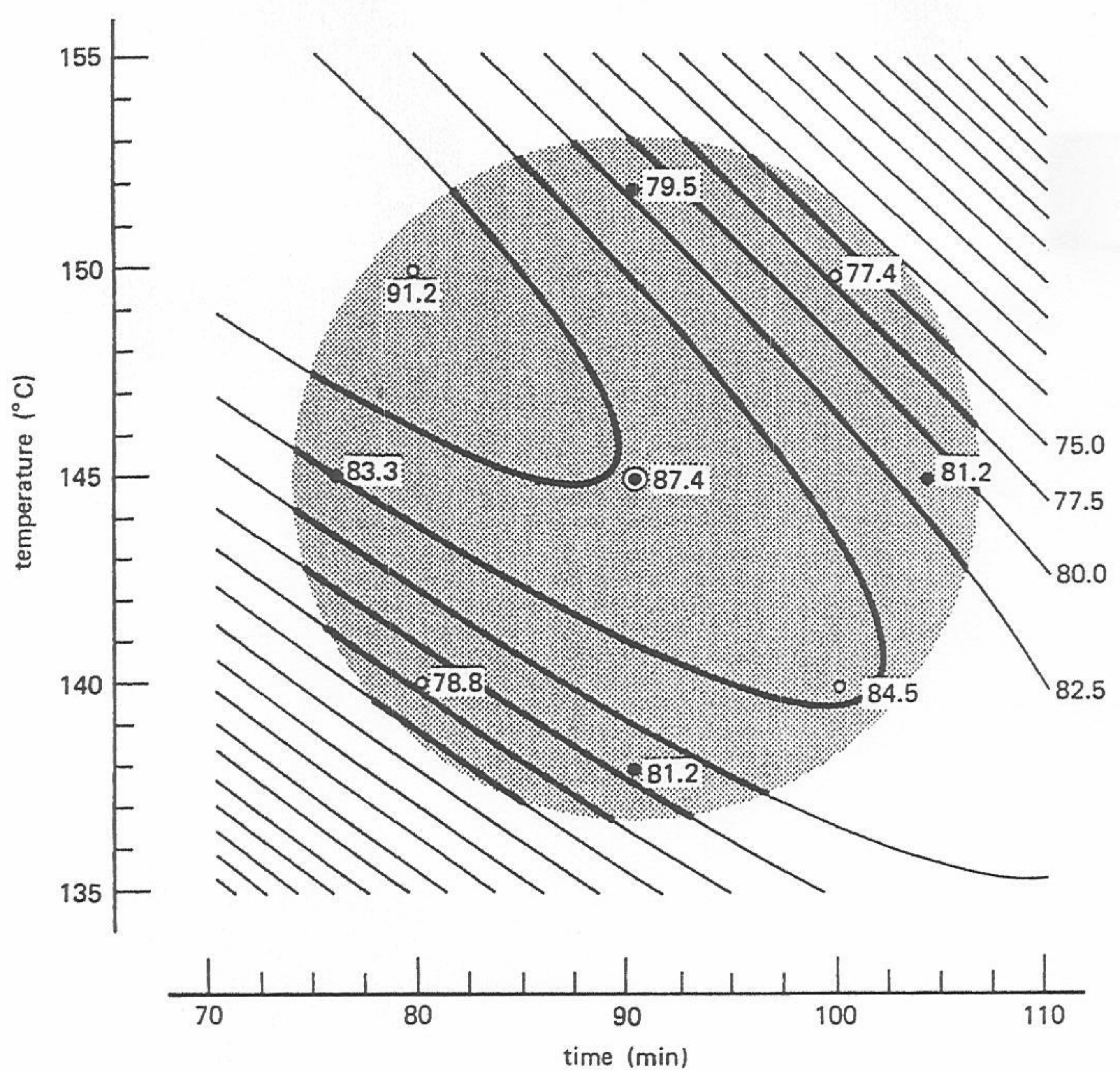

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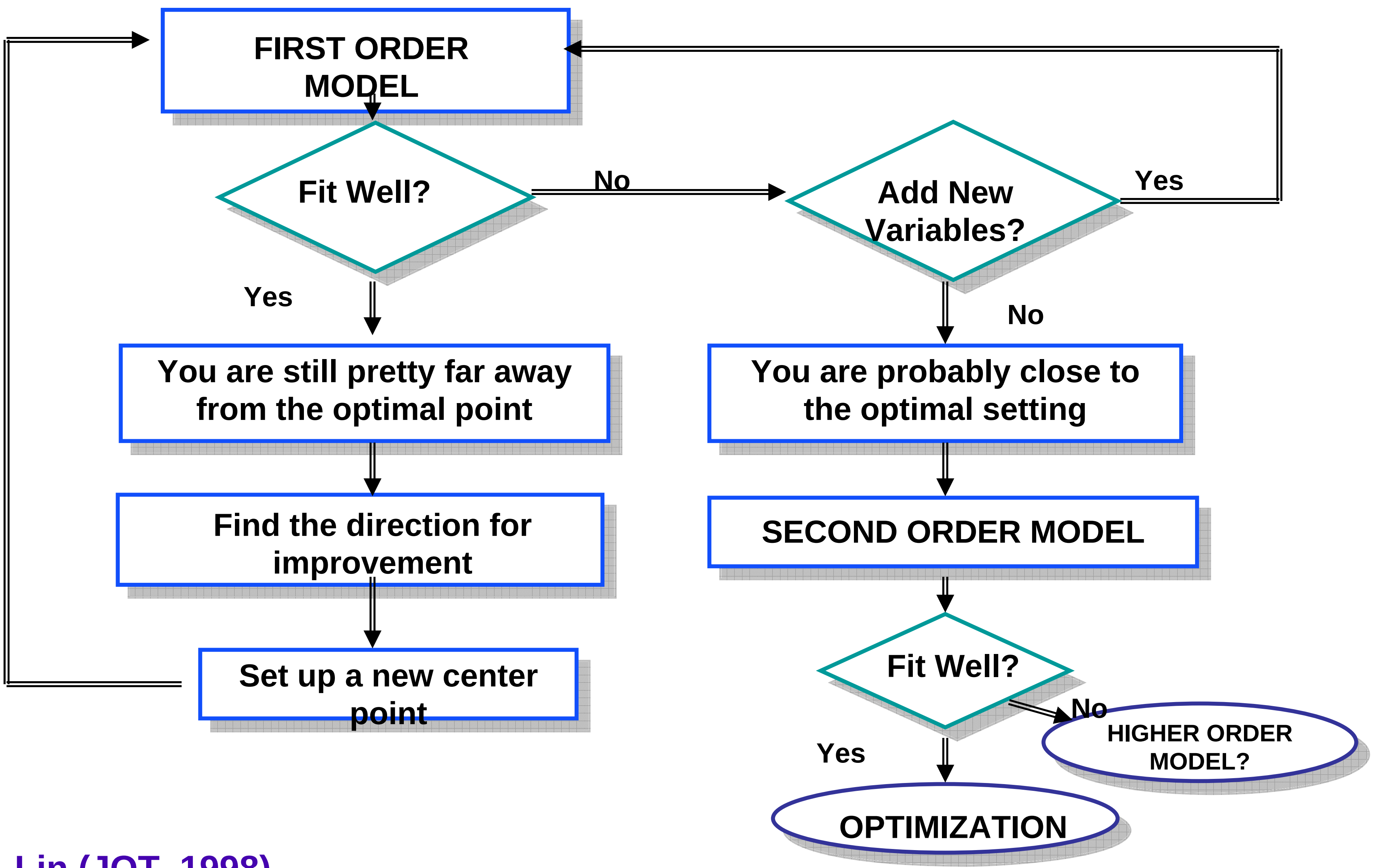
Final Remarks

- The global optimum turns out to be
  x_1=80 minutes
  x_2=150 ^oC
  E(y)=91.2
  (as oppose to 62.5 at the beginning)

- Is such an optimal setting *feasible*?


FIRST ORDER MODEL
Fit Well?
No
Add New Variables?
Yes
Yes
No
You are still pretty far away from the optimal point
You are probably close to the optimal setting
Find the direction for improvement
SECOND ORDER MODEL
Set up a new center point
Fit Well?
No
HIGHER ORDER MODEL?
Yes
OPTIMIZATION

Lin (JQT, 1998)

Response Surface Methodology
(Box and Draper, 1987)

- WHICH (Screening)
- HOW (Empirical Model Building)
- WHY (Mechanistic Model Building)

What are the issues?

- Data Collection:
  - What will be a good design? For what purpose?
- Data Analysis:
  - What will be a good model?
- Optimization:
  - Objective function?
- Confirmation

Response Surface Methodology Theoretical Formulation

$$y = f(x, \theta) + \varepsilon$$

$$x \in \Omega$$

- Objective
  - Find

    $x = x^*$ such that y is optimized.
- Basic Assumption/Belief
  - Life is Good

    — y is a smooth function of x

Data Structure & Coding

#	X_1	X_2	….	X_k	Resp
1					y_1
2					y_2
.		Design			.
.		Matrix			.
.					.
n					y_n

We have "control" on the design matrix!!!

$$y = f(x, \theta) + \varepsilon \qquad x \in \Omega$$

Issues to be Addressed

- $\boldsymbol{x}$: variable selection
  - Screening Input variables $x_1, x_2, \ldots, x_k$
- $\boldsymbol{f}$: model selection
- $\boldsymbol{\Theta}$: parameter estimation
- ε: error properties (stochastic)
- Ω: Experimental Region

Special Case-I

- $\boldsymbol{x}$: known
  - Input variables $x_1, x_2, \ldots, x_k$
- $\boldsymbol{f}$: model selection
  - First-Order Polynomial $y=\beta_0+\Sigma\beta_i x_i+\varepsilon$
- Θ: parameter estimation
  - Least square fitting
- ε: error properties
  - i.i.d. $N(0,\sigma^2)$
- Ω: Experimental Region
  - Correctly identified.

A (Typical) Special Case

- $\boldsymbol{x}$: known
  - Input variables $x_1, x_2, \ldots, x_k$
- $\boldsymbol{f}$: model selection
  - Second-Order Polynomial $y = \beta_0 + \Sigma\beta_i x_i + \Sigma\beta_{ij} x_i x_j + \varepsilon$
- Θ: parameter estimation
  - Least square fitting
- ε: error properties
  - i.i.d. $N(0,\sigma^2)$
- Ω: Experimental Region
  - Correctly identified.

RSM: General Steps

- Define
- Design
- Modeling
- Estimation
- Optimization
- Forecasting
- Confirmation

Design of Screening Experiments

- Two-Level Fractional Factorials
- Plackett & Burman Design (Hadamard Matrix)
- Two-Level Orthogonal Arrays
- Regular Simplex & T-optimal
- p-efficient Designs
- Supersaturated Designs

Lin(2003)

MODEL

$$Y = \underset{\sim}{1} \cdot \mu + X \underset{\sim}{\beta} + \underset{\sim}{\varepsilon}$$

$Y_{n\times 1}$: observable data

$X_{n\times k}$: design matrix

$\beta_{k\times 1}$: parameter vector

$\varepsilon_{n\times 1}$: noise

$N = \{i_1, i_2, \ldots, i_p\}$ inert factor

$A = \{i_{p+1}, i_{p+2}, \ldots, i_k\}$ active factor

$N \cup A = \{1, 2, \ldots, k\}$

Goal

Test $H_j : \beta_j = 0$ vs. $H_j^c : \beta_j \neq 0$

$$\begin{cases} H_j \text{ is true if } j \in N \\ H_j^c \text{ is true if } j \in A \end{cases}$$

Examples

- ANONA Approach:
  - Orthogonal Array (n=4t)
- First-Order Model:
  - Minimal-Point Design (n=k+1)
- Significant Test Approach
  - Good estimate of σ!
- Others?

About Model Building

- Smoothing assumption in *f*.
- Typically polynomial model is assumed, as the empirical model building.
- Spline Fitting
- Artificial Neural Network
- Radial Basis Function
- Non- (Semi-) Parametric Fitting
- Optimality versus Robustness

Designs for Model Building

- Central Composite Design (CCD)
- Small Composite Design
- Box and Behnken Design
- Three-Level Design
- Uniform Design
- Others

$$y = \beta_0 + \sum \beta_i x_i + \sum \beta_{ij} x_i x_j + \sum \beta_{ii} x_i^2 + \varepsilon$$

Parameter Estimation

- Least Square Estimate
- Likelihood approach (with proper assumption on the distribution)
- Bayesian approach, when appropriate
- Black-Box approach, such as Artificial Neural Network

Assumption on Noise

- i.i.d. $N(0, \sigma^2)$ Assumption
- Generalized Least square
- Generalized Linear model

- Bayesian Approach

- Confidence Interval & significant test

Objectives

- Overall Surface structure
- Optimal value of y
- Corresponding setup x*
- Future exploration

How About

- Goodness/Badness of fit
- Optimal y outside the current domain
- Confidence Region of y*
- Confidence Region of x*

Second-Order Polynomial Model

- Estimation: β vs $\hat{\beta}$
- Bias: f vs $\hat{f}$
- Prediction: y_{max} vs $\hat{y}_{\max}$
- Prediction: x^* vs $\hat{x}^*$
- Point Estimate & Confidence Region (Sweet Spot)
- General f?

Assignment #1

- Suppose that
  $y_1=\alpha_0+\alpha_1 x+\alpha_{11}x^2+\varepsilon_1$ and
  $y_2=\beta_0+\beta_1 x+\beta_{11}x^2+\varepsilon_2$
  Find $x=x^*$ such that both Y_i's are maximized.

- Suppose that
  $y_1=f_1(x,\theta_1)+\varepsilon_1$ and $y_2=f_2(x,\theta_2)+\varepsilon_2$
  Find $x=x^*$ such that both Y_i's are maximized.
  What will you do?

Assignment #2

- In general, suppose that

$y_1 = f_1(x, \theta_1) + \varepsilon_1$,

$y_2 = f_2(x, \theta_2) + \varepsilon_2$,

...

$y_p = f_p(x, \theta_p) + \varepsilon_p$.

Find $x = x^*$ such that all y_i's are maximized.

Assignment #3

An expensive experiment has five (5) experimental variables ($x_1, \ldots, x_5$) each at two levels. Provide a design for such a study, under the scenarios

(a) the budget is unlimited and

(b) the budget is very tight. For each design you provide, explain what can be estimated and why your design is a good one.