Design and Analysis of Computer Experiments with Branching and Nested Factors

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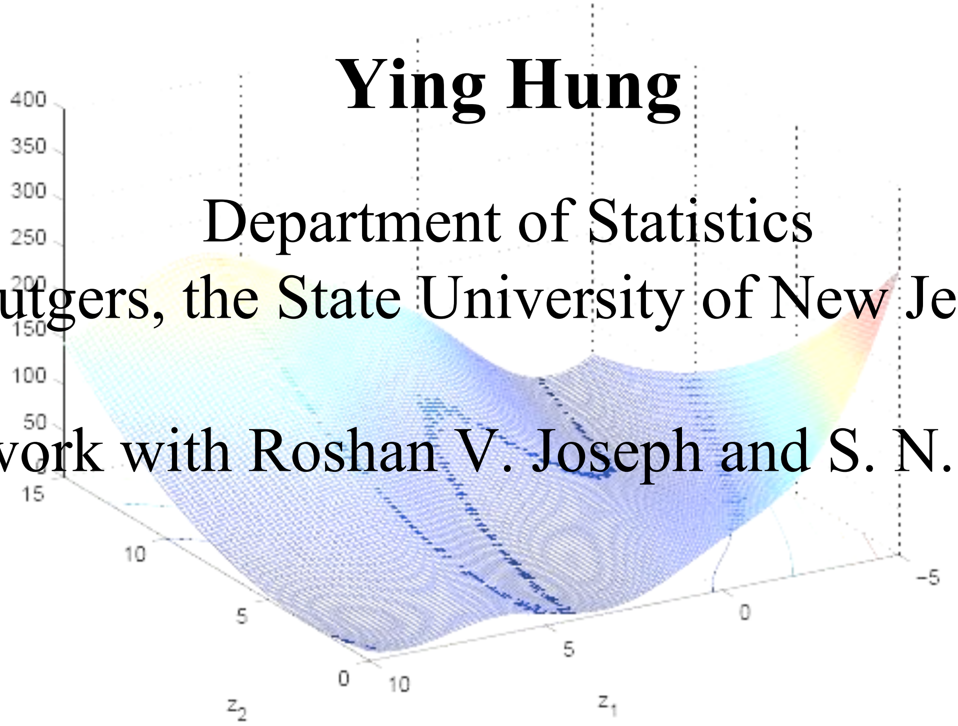
Joint work with Roshan V. Joseph and S. N. Melkote



Overview

- What is computer experiment?
- Computer experiments with branching and nested factors.
    - ✓ New class of designs.
    - ✓ Optimality criteria.
    - ✓ New metamodel.

Introduction to Computer Experiments

- First computer experiments were conducted at Los Alamos National Laboratory to study the behavior of nuclear weapons.

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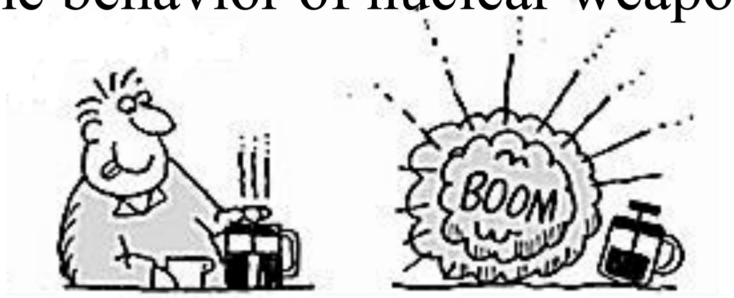

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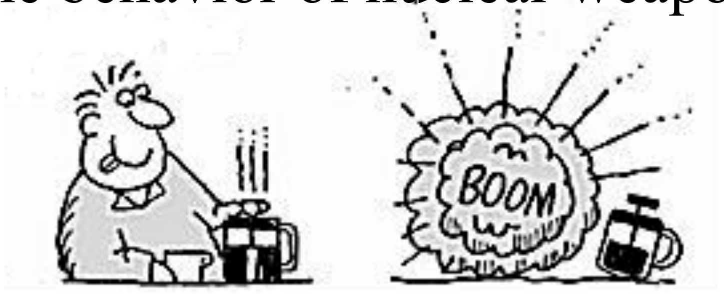
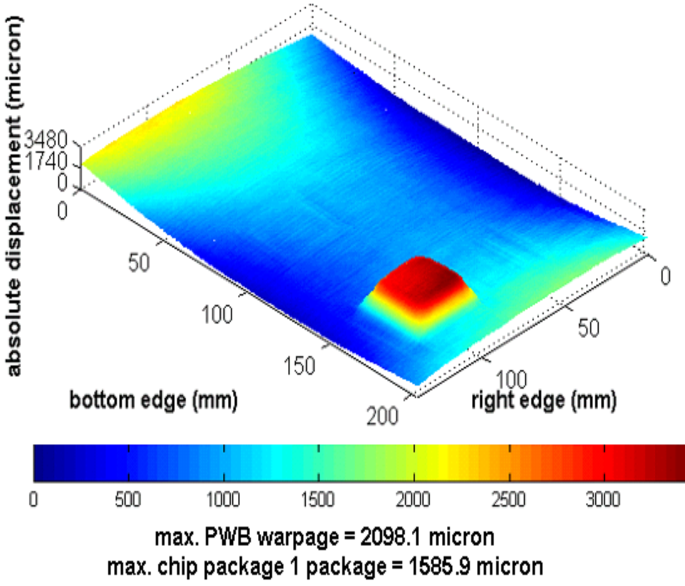
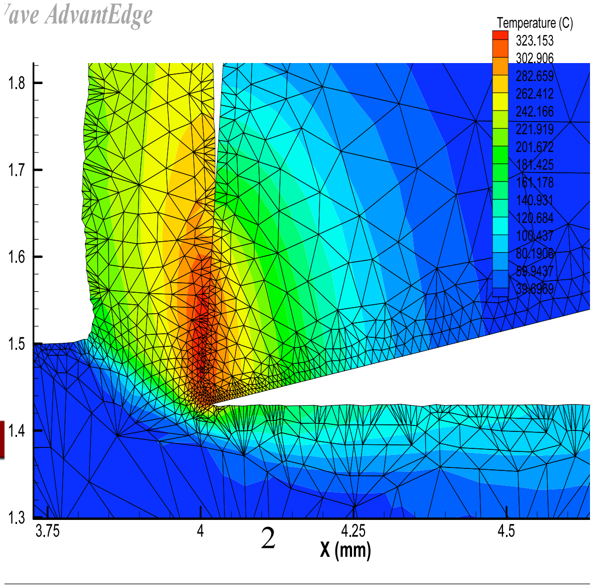
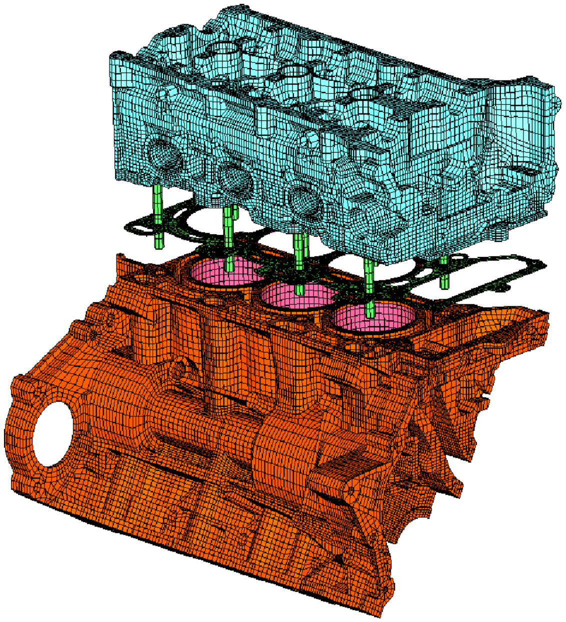


- Applications: biology, environmental science and engineering etc.







Introduction to Computer Experiments

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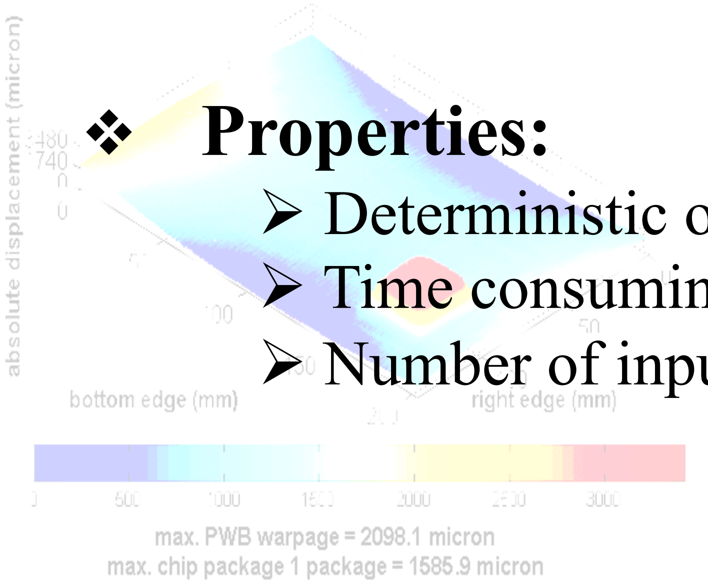
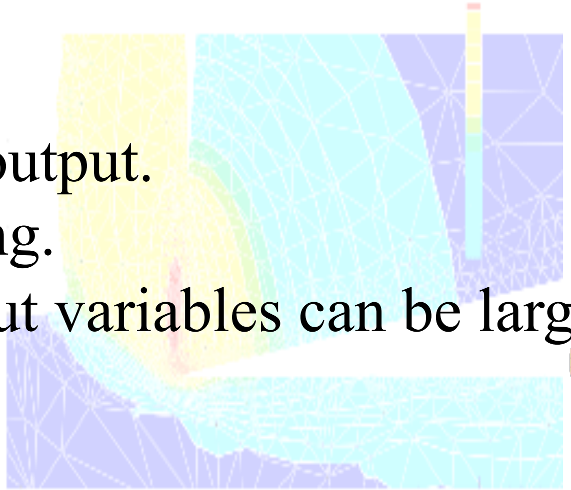
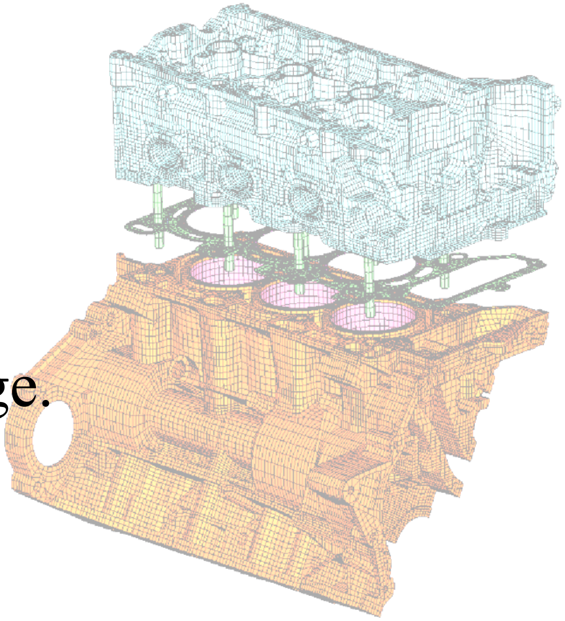
- ❖ Computer experiments are becoming popular because many physical experiments are difficult or impossible to perform.

- ❖ Applications: biology, environmental science and engineering etc.

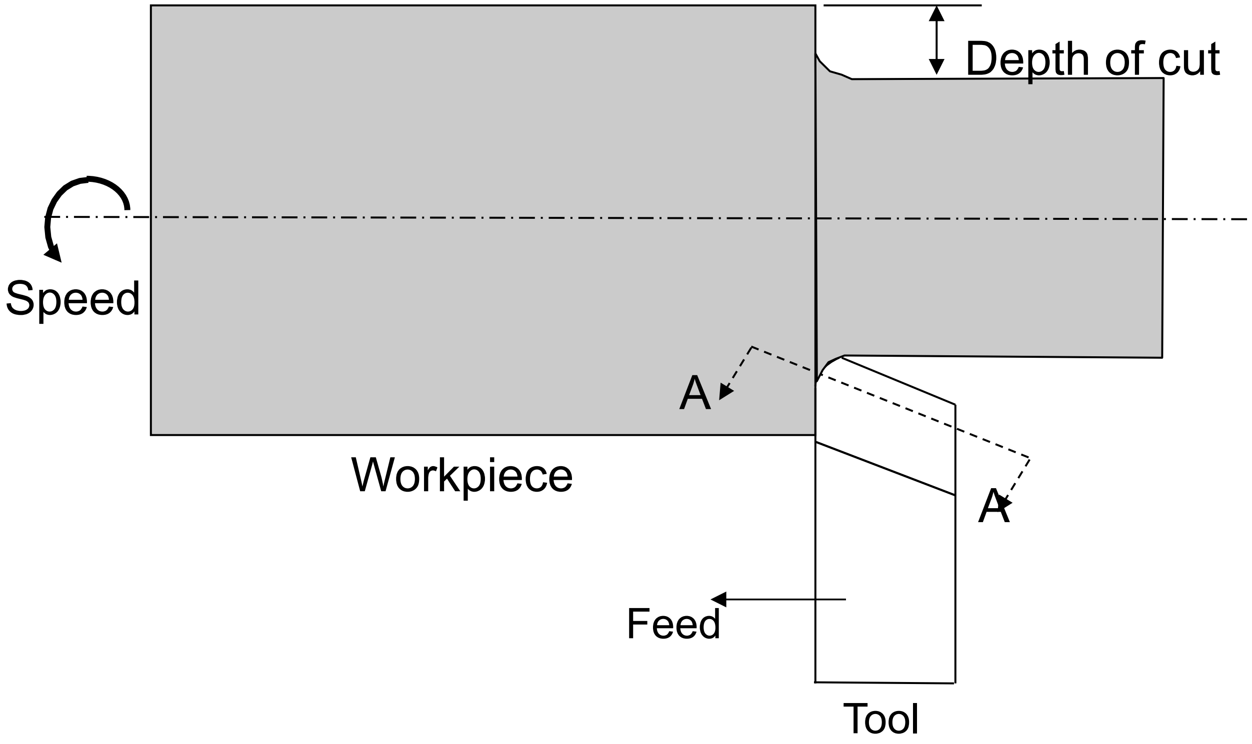
- ❖ **Properties:**
  - ➢ Deterministic output.
  - ➢ Time consuming.
  - ➢ Number of input variables can be large.





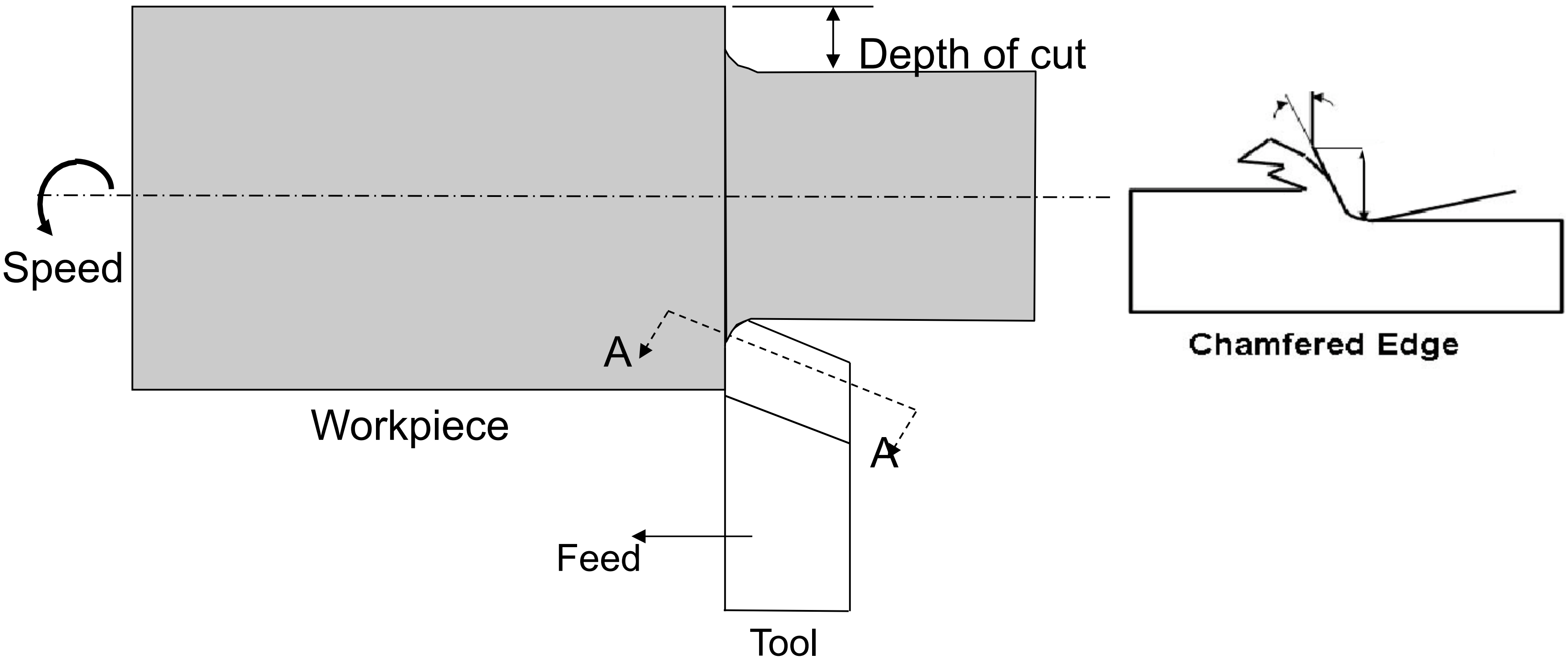


Motivating Example: Hard Turning



- Objective: minimize cutting force

Motivating Example: Hard Turning



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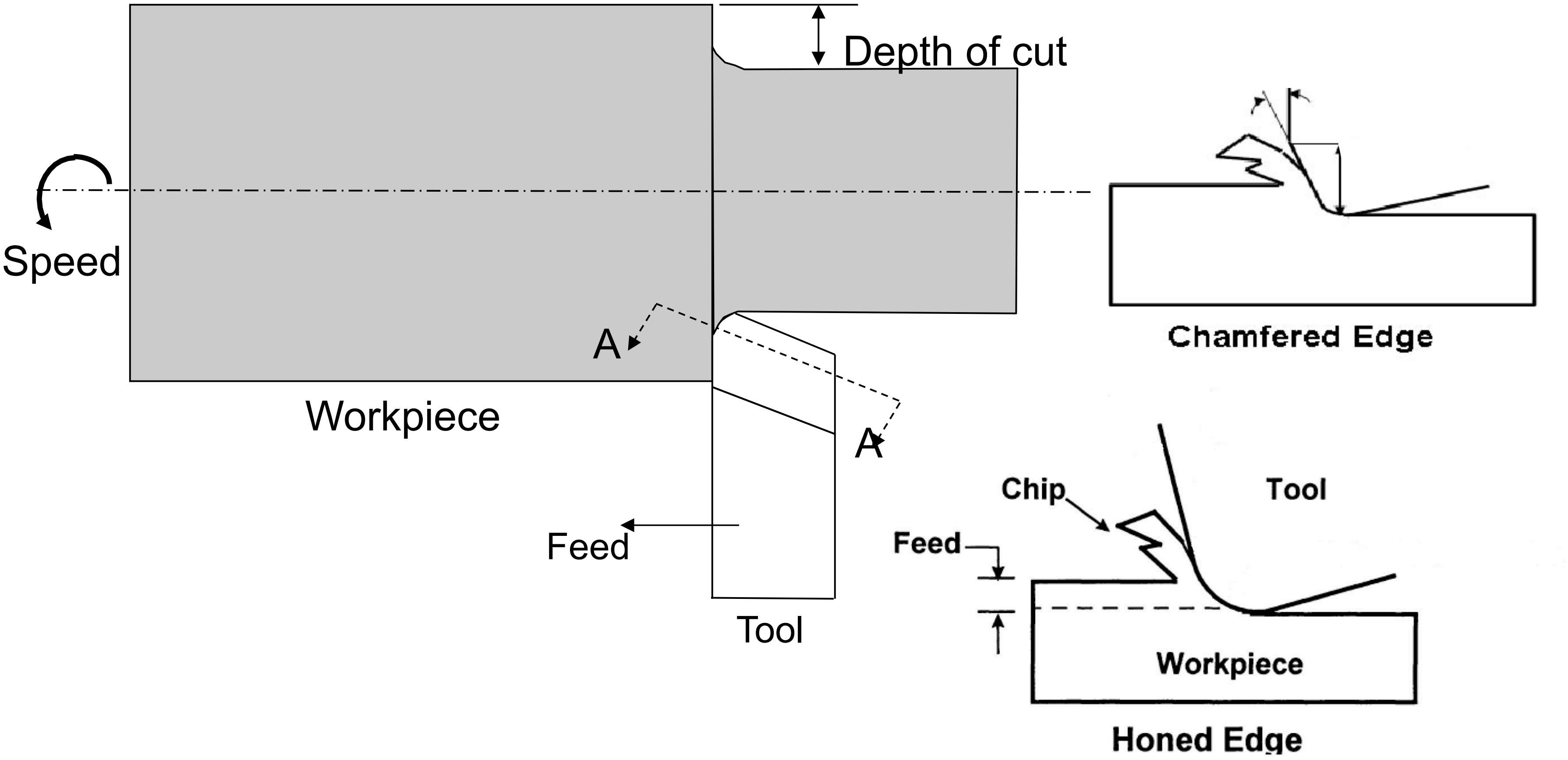

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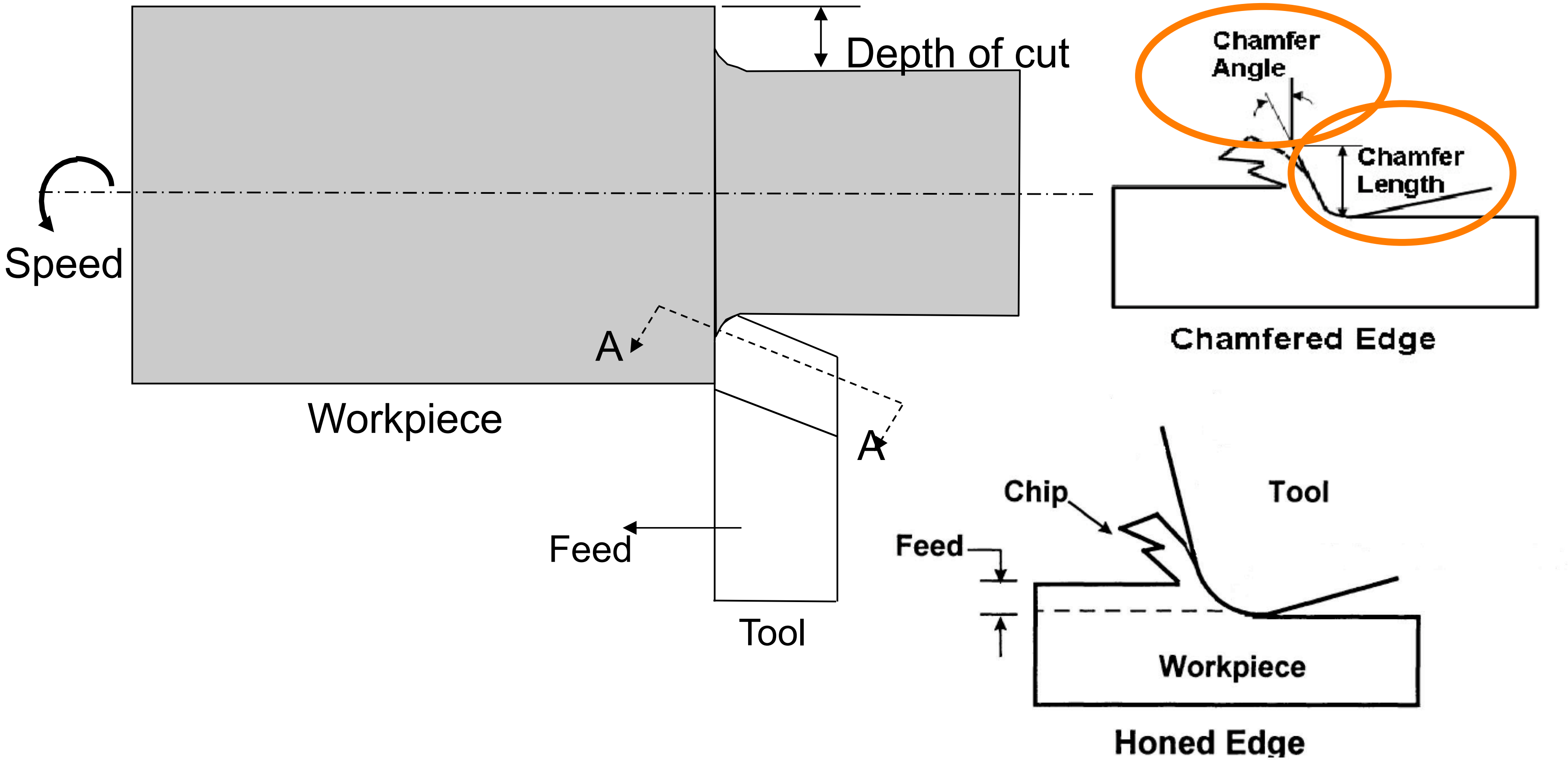
Motivating Example: Hard Turning



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Branching and Nested Factors

- Nested factor: A factor that can change with respect to the level of another factor.
- Branching factor: A factor within which other factors are nested.

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Hard turning experiment

Branching factor	z_1	Tool

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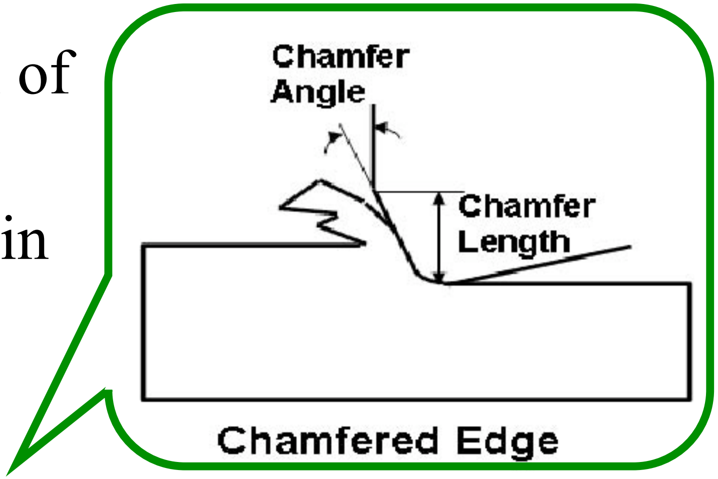
Hard turning experiment

Branching factor	z_1	Tool (chamfer)



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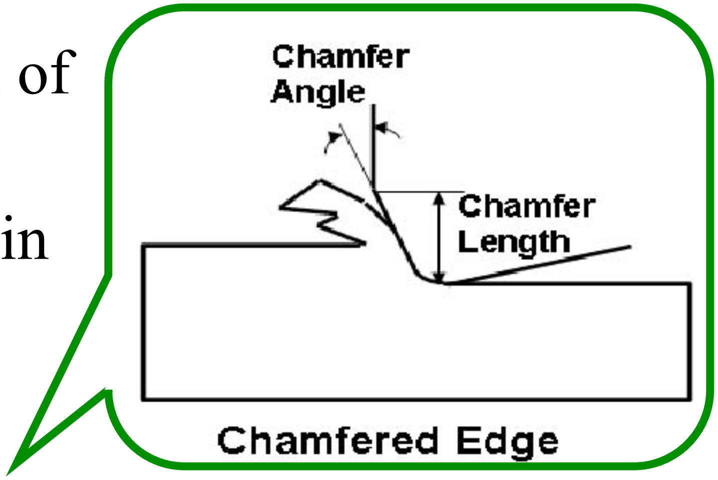

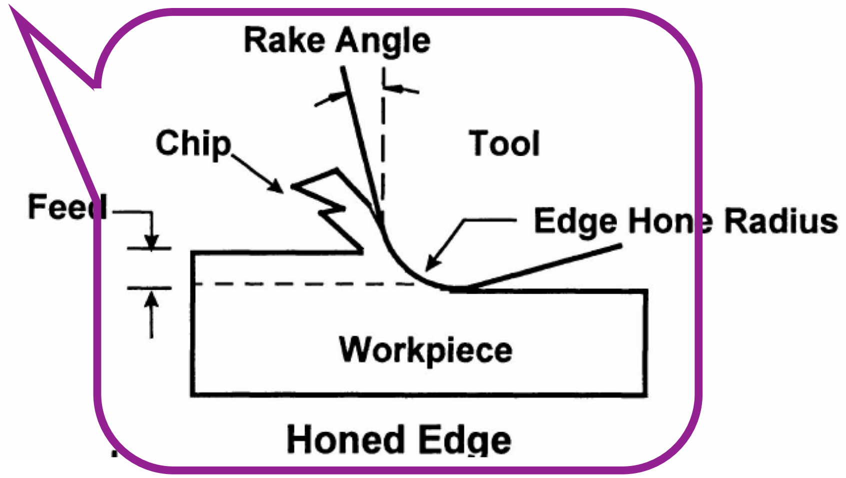

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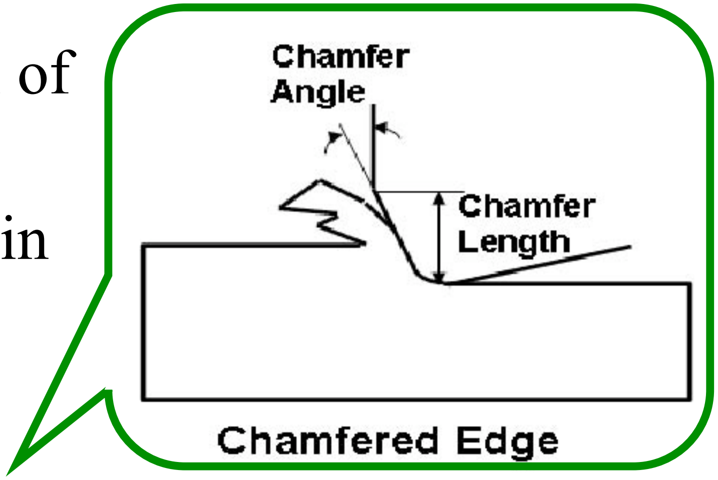

Hard turning experiment

Branching factor	z_1	Tool (chamfer & hone)
Nested factors	**$v_1 \| z_1$=chamfer** **$v_2 \| z_1$=chamfer**	**Angle** **Length**

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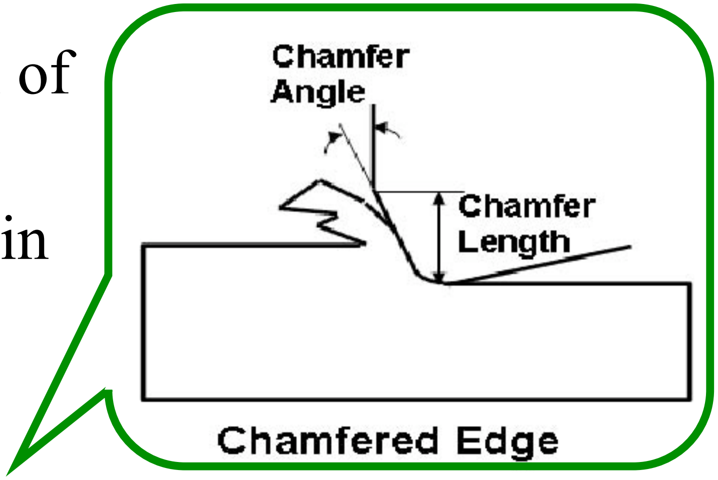
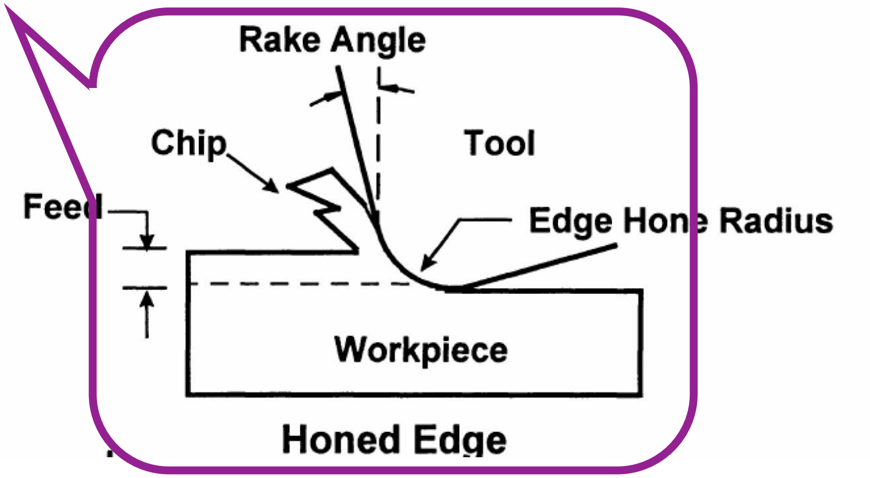
Hard turning experiment

Branching factor	z_1	Tool (chamfer & hone)
Nested factors	**$v_1\|z_1=$chamfer** **$v_2\|z_1=$chamfer** **$v_1\|z_1=$hone** **$v_2\|z_1=$hone**	**Angle** **Length** **None** **None**



Chamfered Edge



Honed Edge

Computer Experiments in Machining

Type of Factor	Notation	Factor	Ranges
Branching factors	z_1	**Tool** (Cutting edge shape)	chamfer & hone
Nested factors	$\mathbf{v_1 \| z_1}$**=chamfer**	**Angle**	17~ 20
	$\mathbf{v_2 \| z_1}$**=chamfer**	**Length**	115~140
	$\mathbf{v_1 \| z_1}$**=hone**	**None**	None
	$\mathbf{v_2 \| z_1}$**=hone**	**None**	None
Shared factors	$\mathbf{x_1}$	Cutting edge radius	5~25
	$\mathbf{x_2}$	Rake angle	-15 ~ -5
	$\mathbf{x_3}$	Tool nose radius	0.4 ~ 1.6
	$\mathbf{x_4}$	Cutting speed	120 ~ 240
	$\mathbf{x_5}$	Feed	0.05 ~ 0.15
	$\mathbf{x_6}$	Depth of cut	0.1 ~ 0.25

Design with Branching and Nested Factors

- Properties

➢ Branching factors are qualitative, which cannot be divided into intervals.

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- ➢ Branching-by-nested *interaction* can be significant.

Design with Branching and Nested Factors

Printed circuit board (PCB) manufacturing

- Properties

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Design with Branching and Nested Factors

Printed circuit board (PCB) manufacturing

Two surface preparation methods

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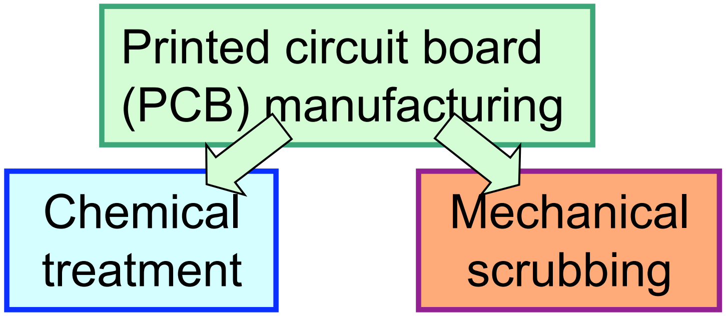
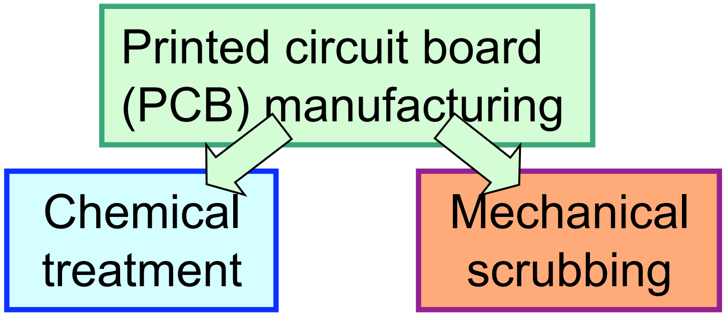


Design with Branching and Nested Factors

- Properties

Branching factor



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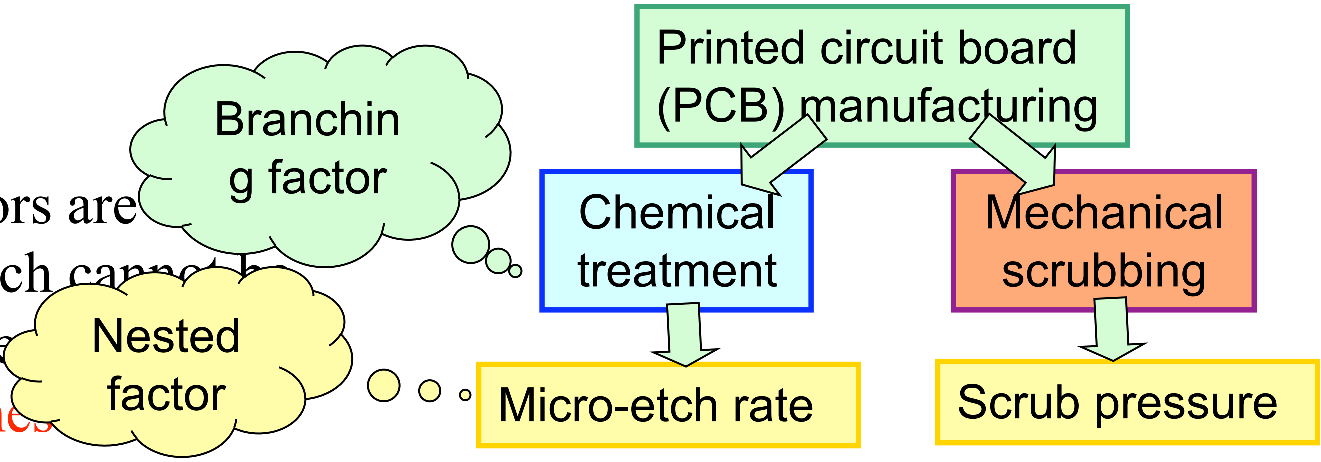

Branchin g factor

Nested factor

Printed circuit board (PCB) manufacturing

Chemical treatment

Mechanical scrubbing

Micro-etch rate

Scrub pressure

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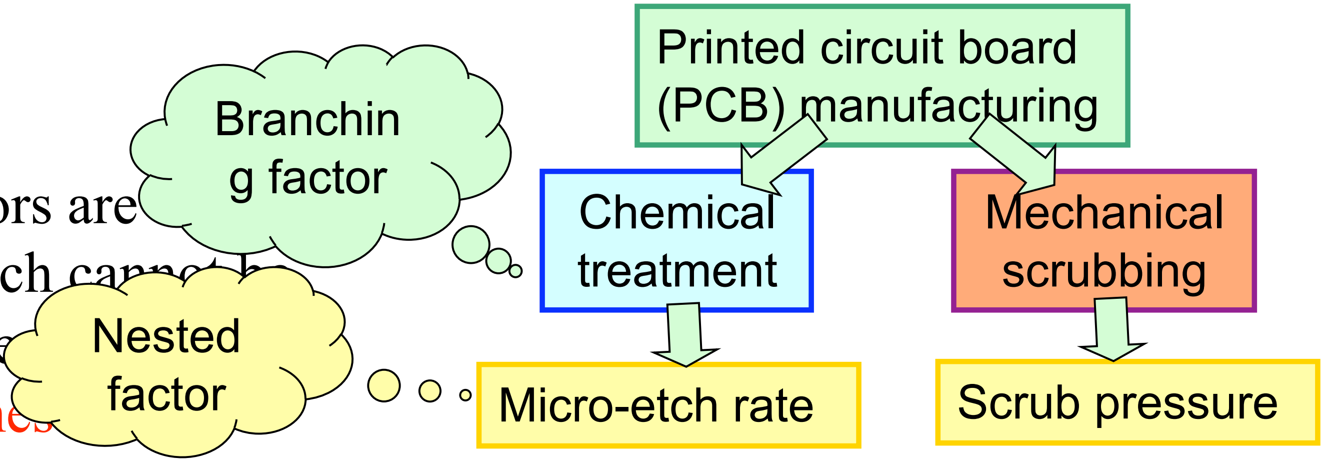

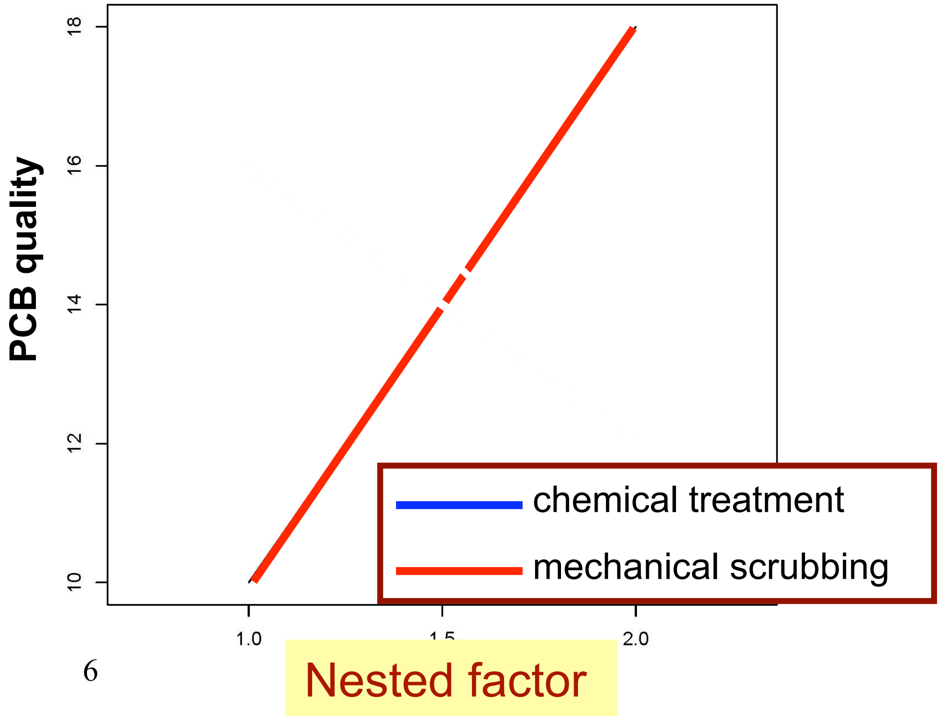

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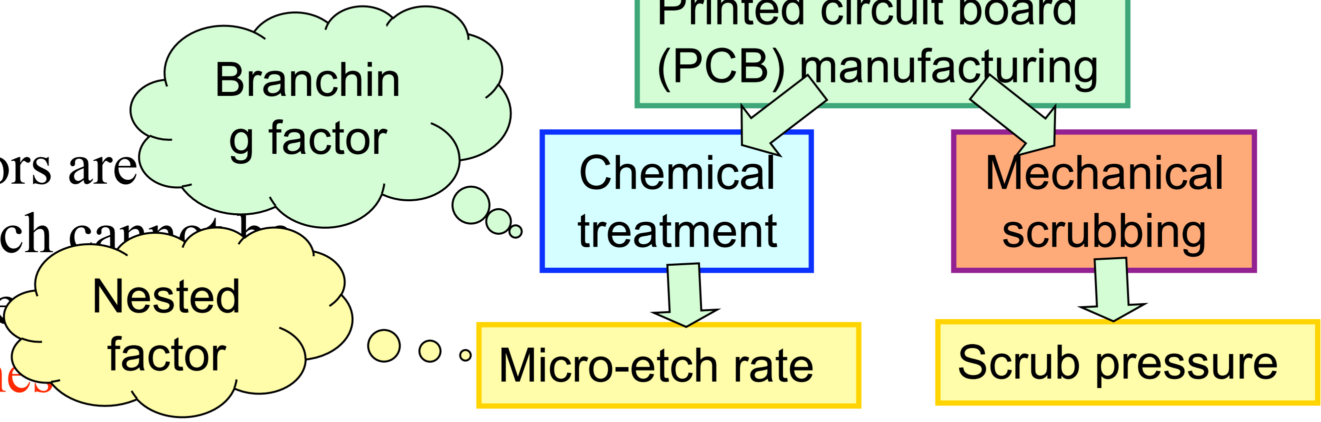

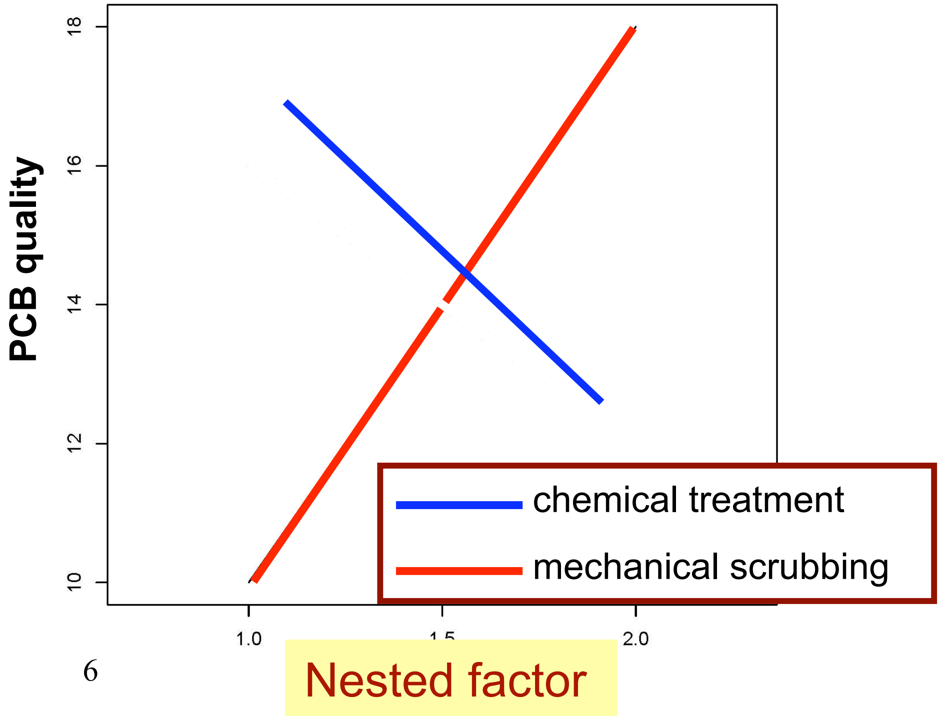

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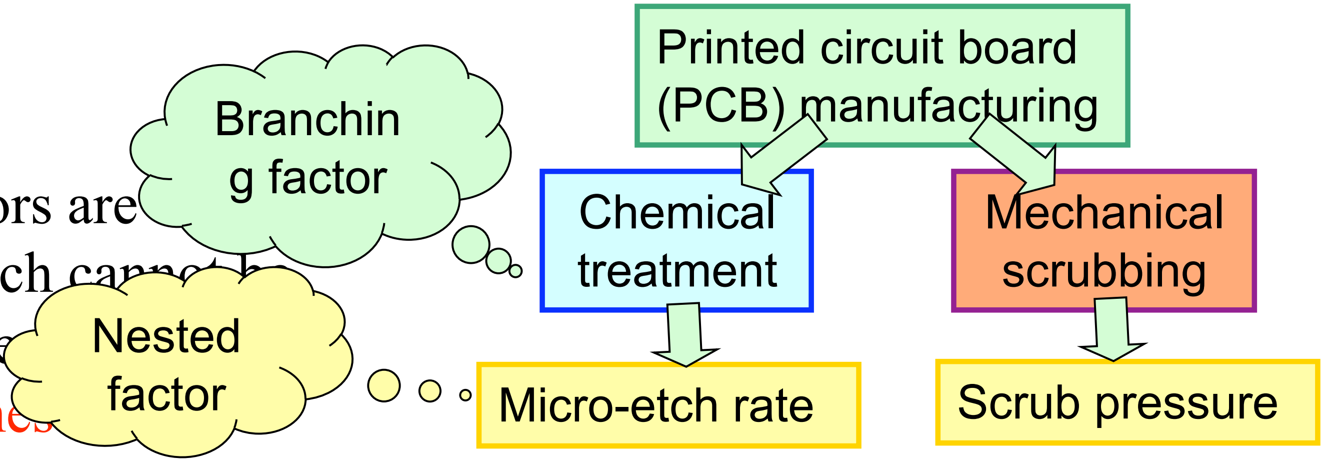

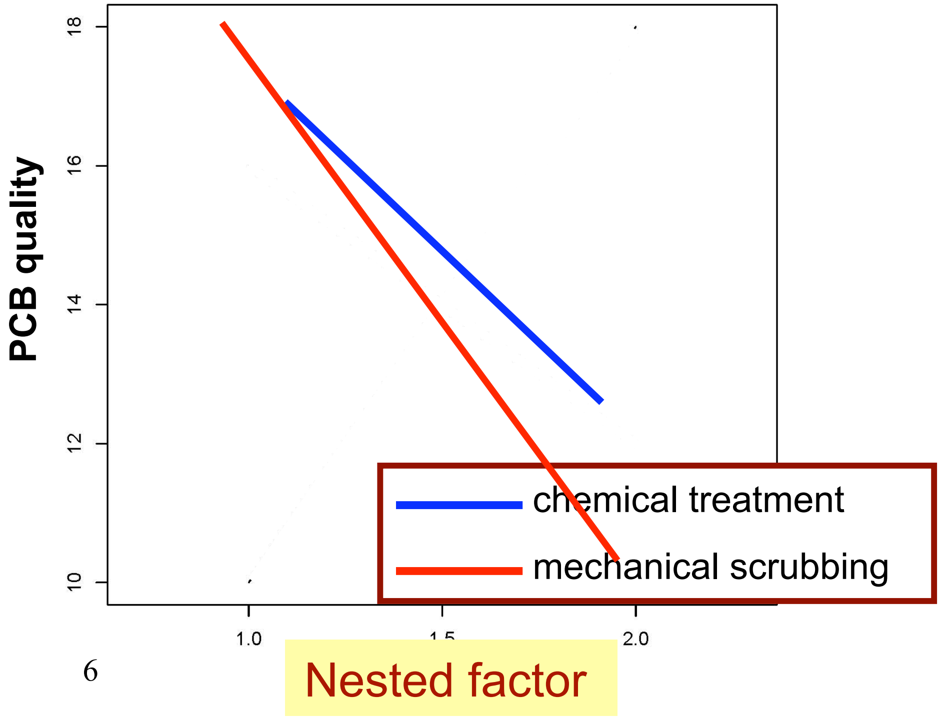

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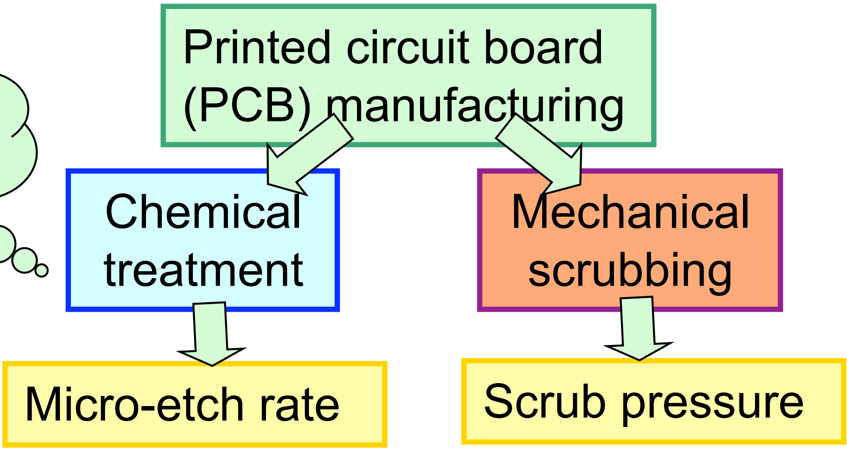


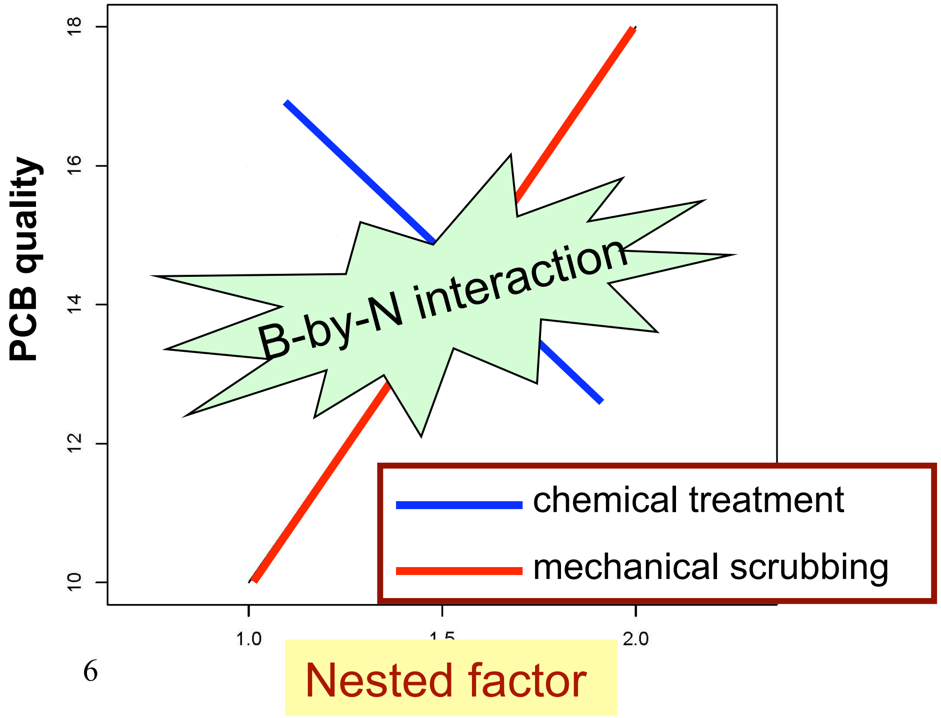
Printed circuit board (PCB) manufacturing

Chemical treatment

Mechanical scrubbing

Micro-etch rate

Scrub pressure



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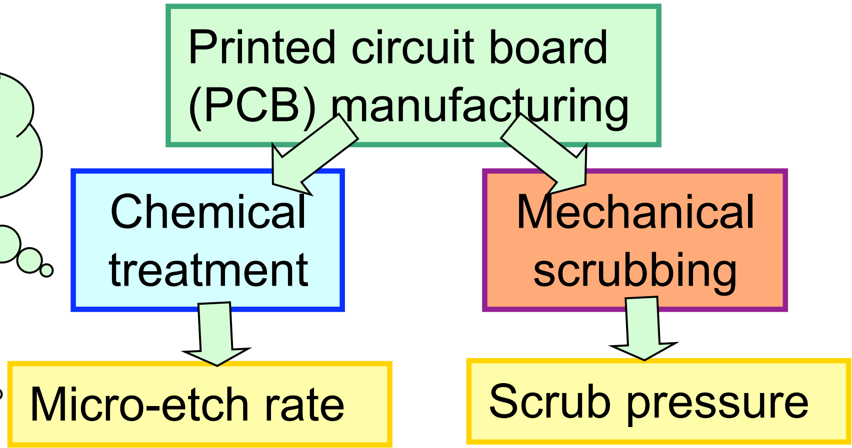
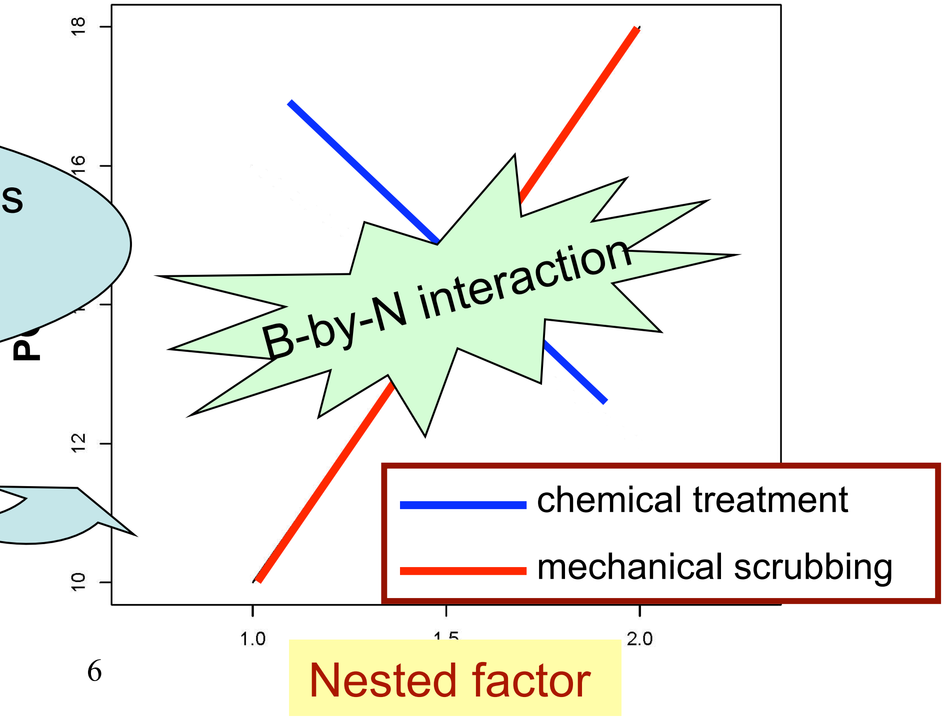


Any main effect correlated with this B-by-N interaction will be misspecified.



Computer Experiments with Branching and Nested Factors

- Branching and nested factors (Phadke, 1989; Taguchi, 1987).
- Challenges in design:
  - Involve both quantitative and qualitative factors.
  - Some two-factor interactions are important.
- Challenges in modeling:
  - No correlation function defined for nested factors.
- First work on design and analysis of computer experiments with branching and nested factors.

Computer Experiments with Branching and Nested Factors

- Branching and nested factors (Phadke, 1989; Taguchi, 1987).
- Challenges in design:

No existing design can be applied directly.

- Challenges in modeling:

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Computer Experiments with Branching and Nested Factors

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- Challenges in design:

No existing design can be applied directly.

- Challenges in modeling:

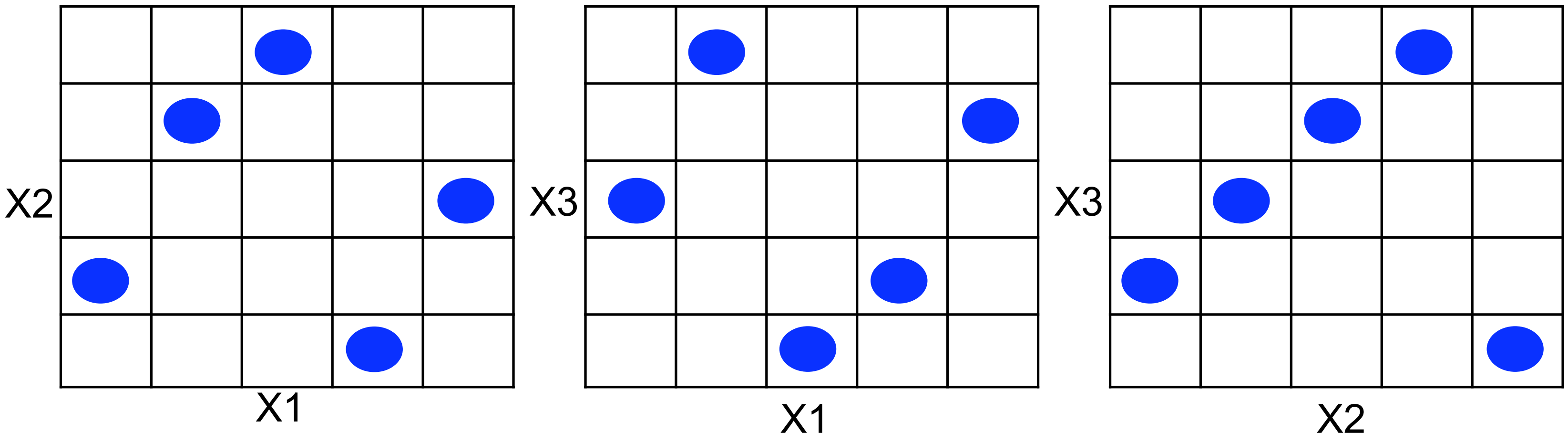
No suitable model available.

- First work on design and analysis of computer experiments with branching and nested factors.

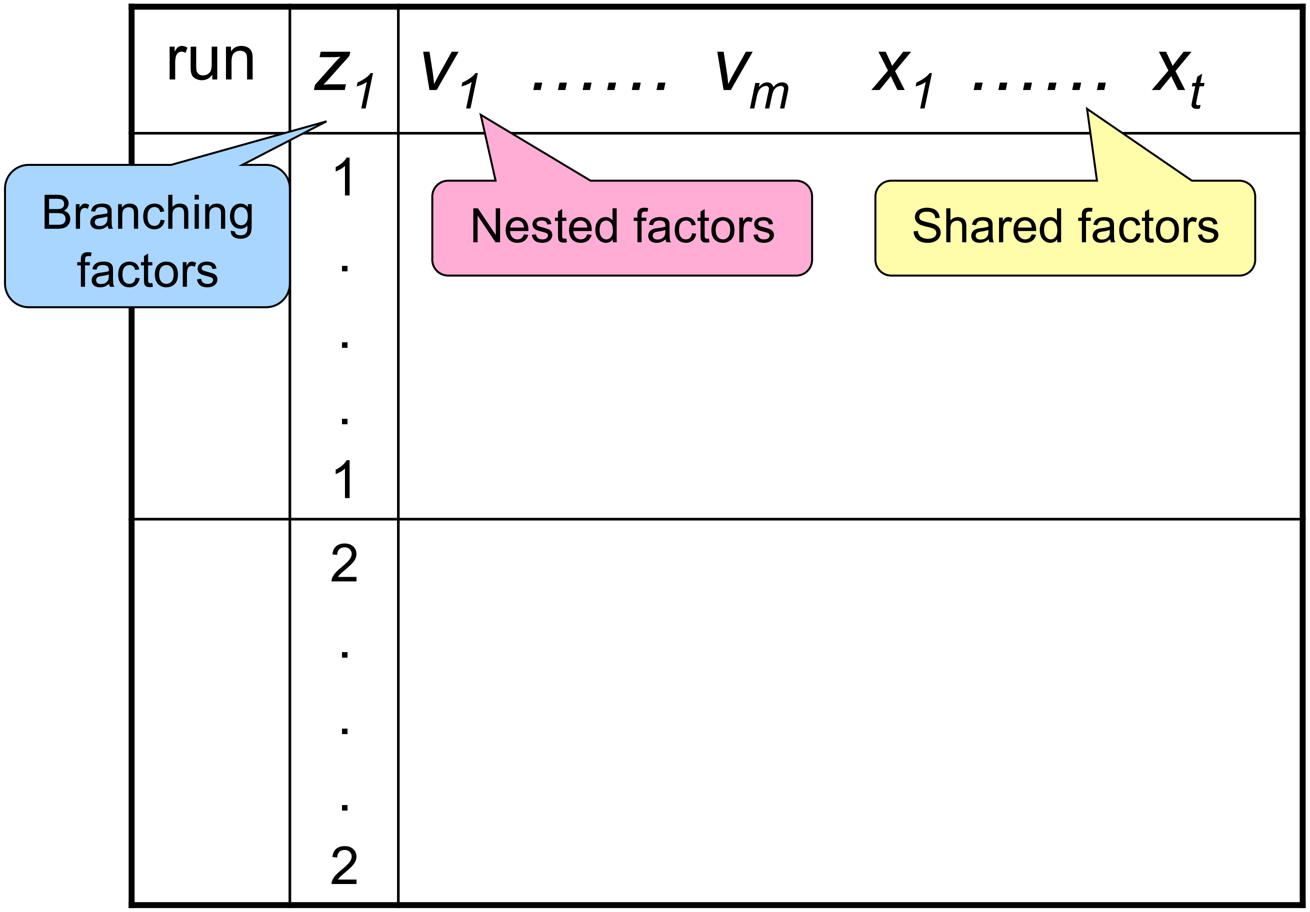
Design of Computer Experiments with Branching and Nested Factors

- Latin hypercube design (LHD).
  - McKay, Beckman, Conover (1979).
  - Easy to construct.
  - One-dimensional balance.
- LHD cannot be applied directly.

run	X1	X2	X3
1	1	2	3
2	2	4	5
3	3	5	1
4	4	1	2
5	5	3	4



A Naïve Design



run	z_1	v_1 …… v_m x_1 …… x_t
	1 . . . 1	
	2 . . . 2	

Branching factors

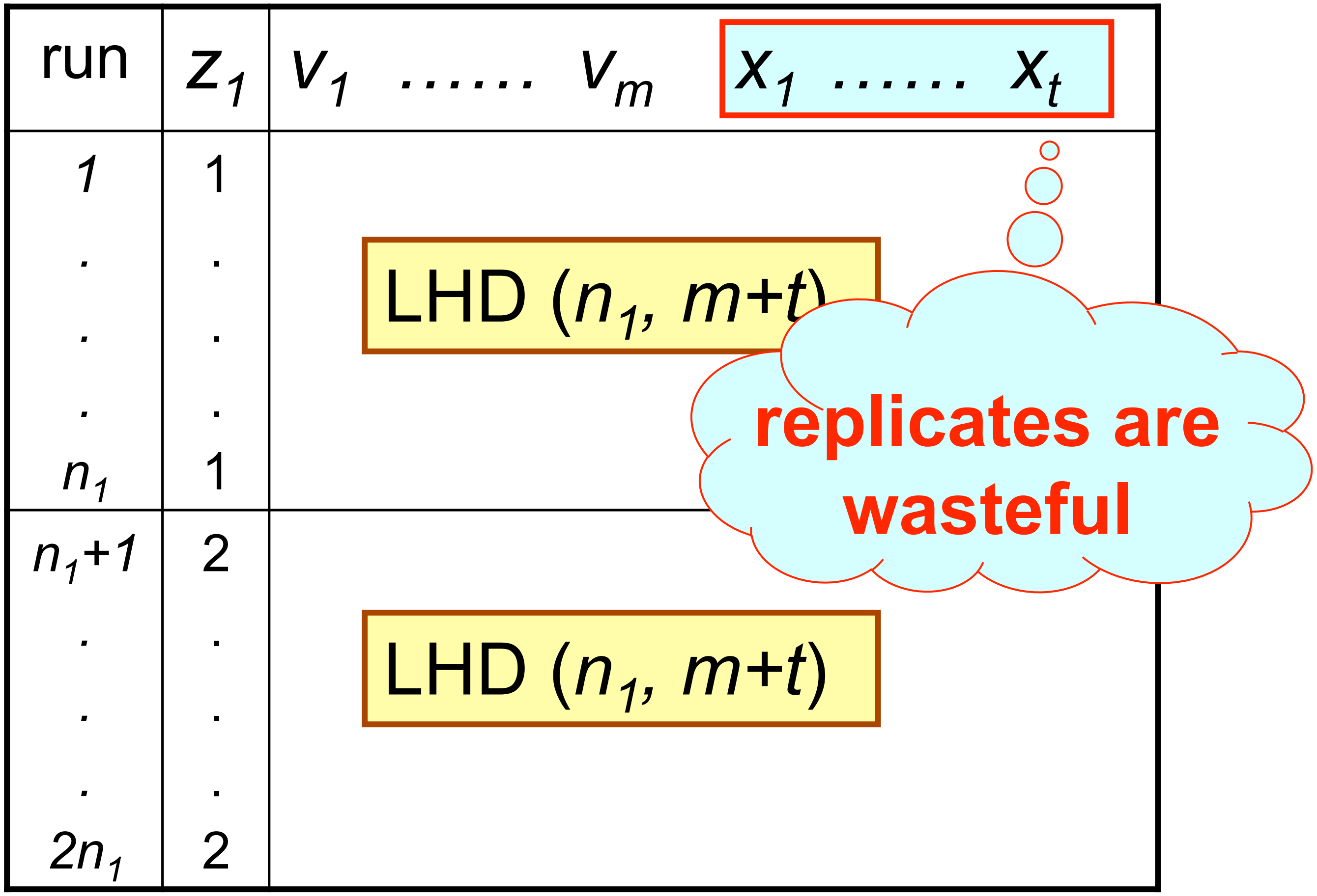
Nested factors

Shared factors

A Naïve Design

run	z_1	v_1 …… v_m x_1 …… x_t
1	1	
.	.	LHD (n_1, $m+t$)
.	.	
.	.	
n_1	1	
n_1+1	2	
.	.	LHD (n_1, $m+t$)
.	.	
.	.	
$2n_1$	2	

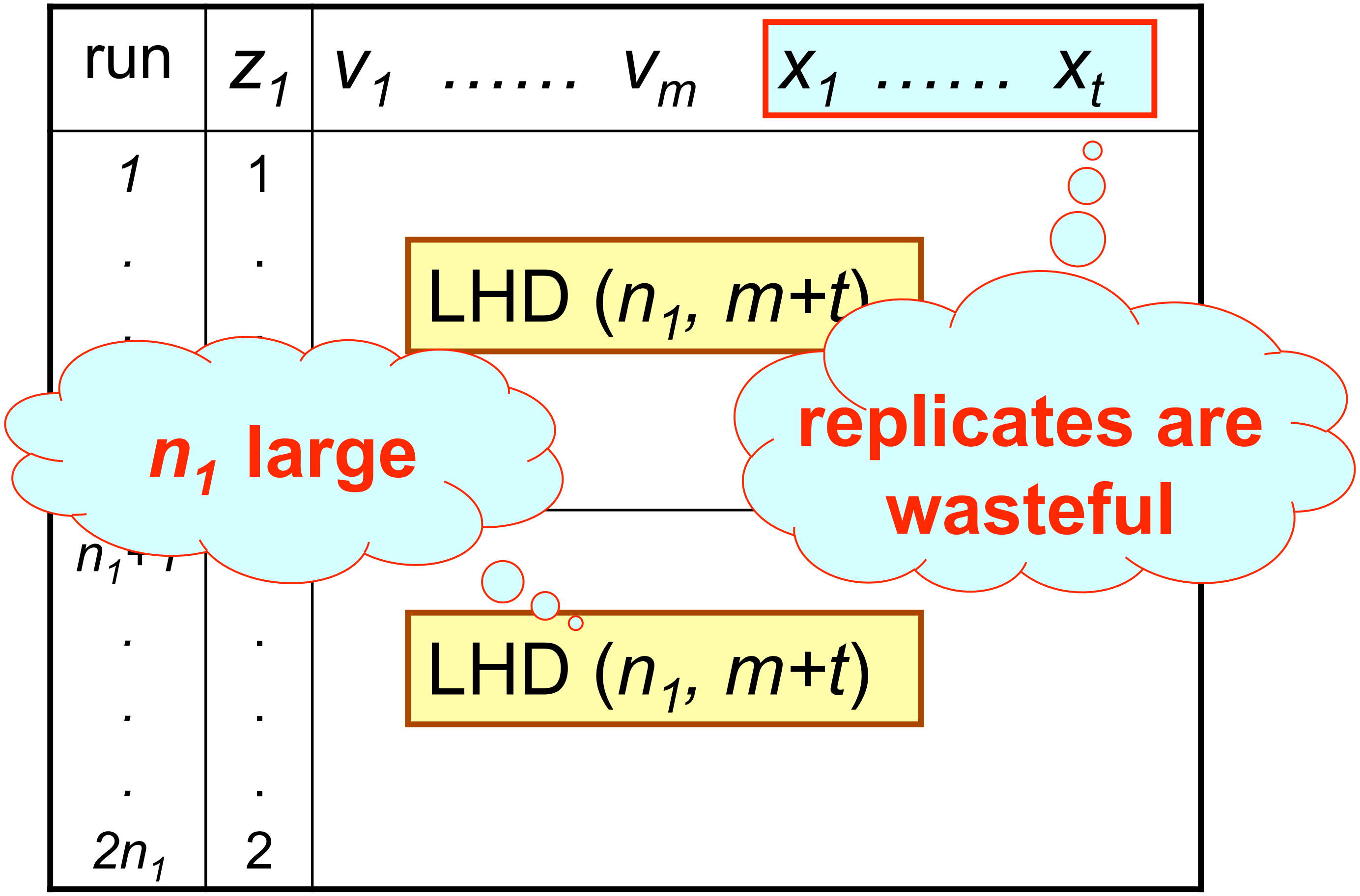
A Naïve Design



run	z_1	v_1 …… v_m	x_1 …… x_t
1	1		
.	.	LHD (n_1, $m+t$)	
.	.		
.	.		
n_1	1		
n_1+1	2		
.	.	LHD (n_1, $m+t$)	
.	.		
.	.		
$2n_1$	2		

replicates are wasteful

A Naïve Design



run

z_1

v_1 …… v_m

x_1 …… x_t

1

1

LHD (n_1, $m+t$)

n_1 large

replicates are wasteful

n_1+1

LHD (n_1, $m+t$)

$2n_1$

2

Branching Latin Hypercube Design (BLHD)

run	z_1	v_1 …… v_m	x_1 …… x_t
1	1		
.	.		
.	.		
.	.		
n_2	1		
n_2+1	2		
.	.		
.	.		
.	.		
$2n_2$	2		

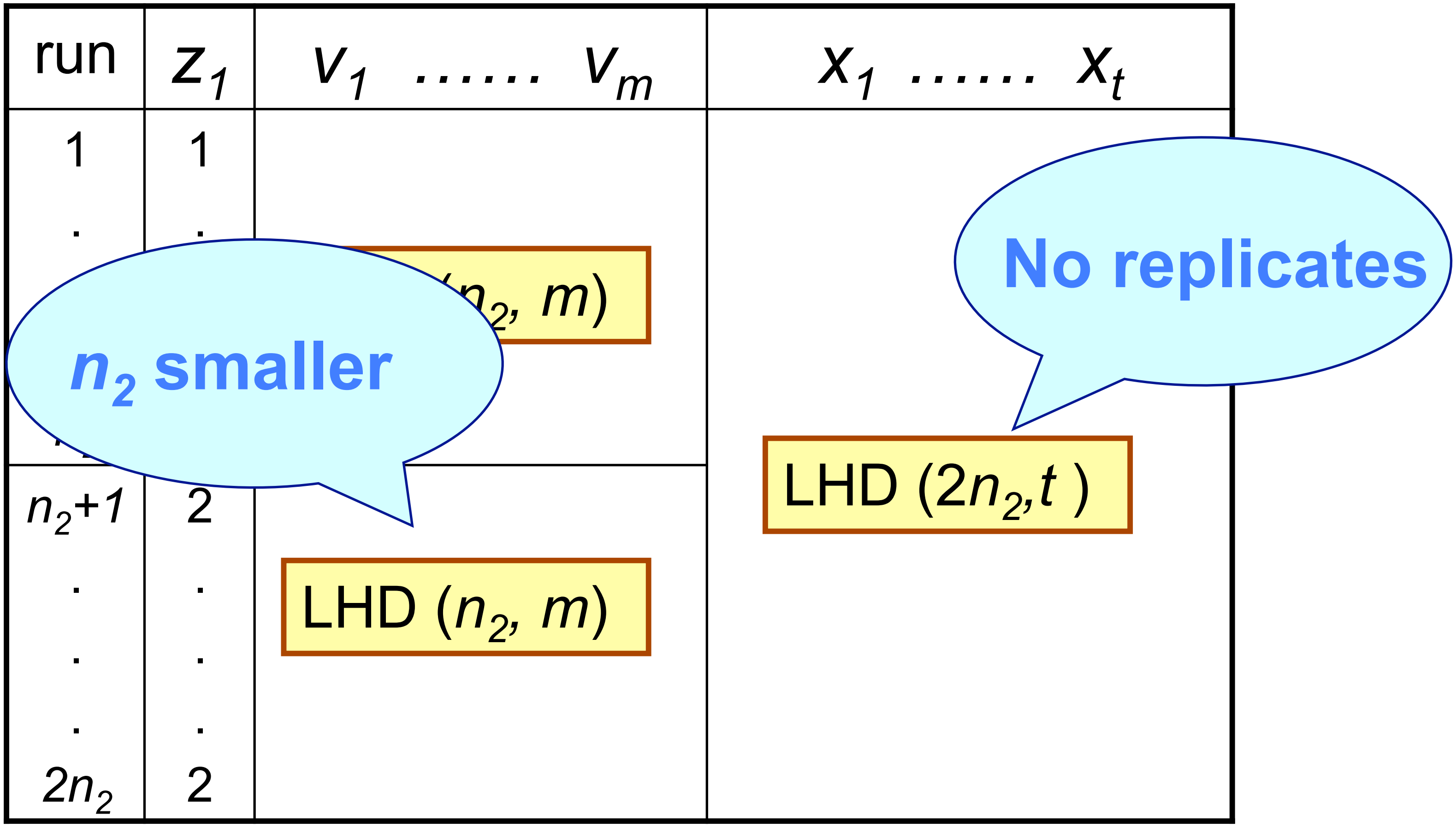
Branching Latin Hypercube Design (BLHD)

run	z_1	v_1 …… v_m	x_1 …… x_t
1	1		LHD $(2n_2, t)$
.	.		
.	.		
.	.		
n_2	1		
n_2+1	2		
.	.		
.	.		
.	.		
$2n_2$	2		

Branching Latin Hypercube Design (BLHD)

<table>
<tr><th>run</th><th>z_1</th><th>v_1 …… v_m</th><th>x_1 …… x_t</th></tr>
<tr><td>1
.
.
.
n_2</td><td>1
.
.
.
1</td><td>LHD (n_2, m)</td><td rowspan="2">LHD ($2n_2$,t)</td></tr>
<tr><td>n_2+1
.
.
.
$2n_2$</td><td>2
.
.
.
2</td><td>LHD (n_2, m)</td></tr>
</table>

Branching Latin Hypercube Design (BLHD)

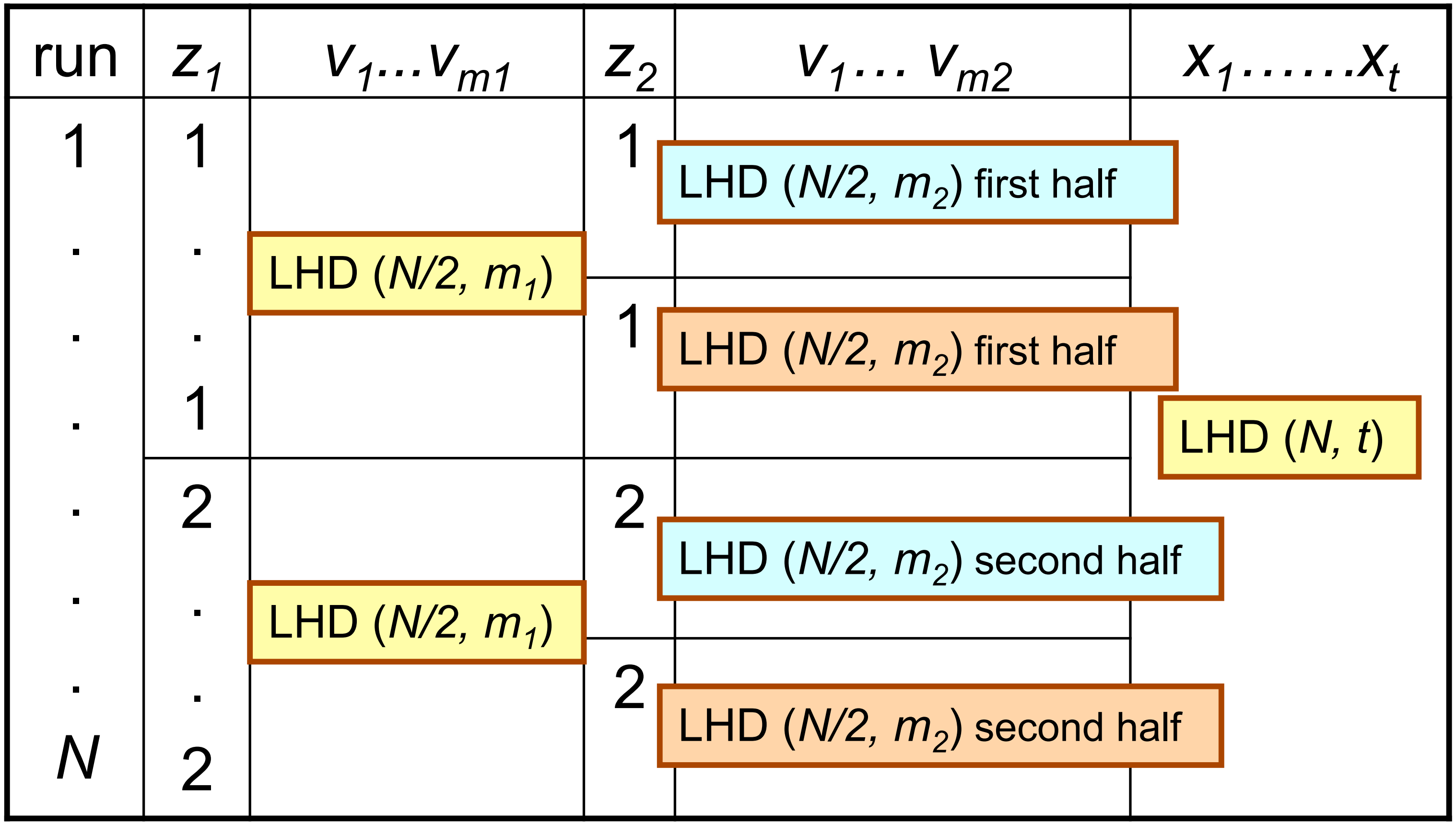


run	z_1	v_1 …… v_m	x_1 …… x_t
1	1		
.	.	(n_2, m)	
n_2+1	2		LHD ($2n_2$,t)
.	.	LHD (n_2, m)	
.	.		
.	.		
$2n_2$	2		

n_2 smaller

No replicates

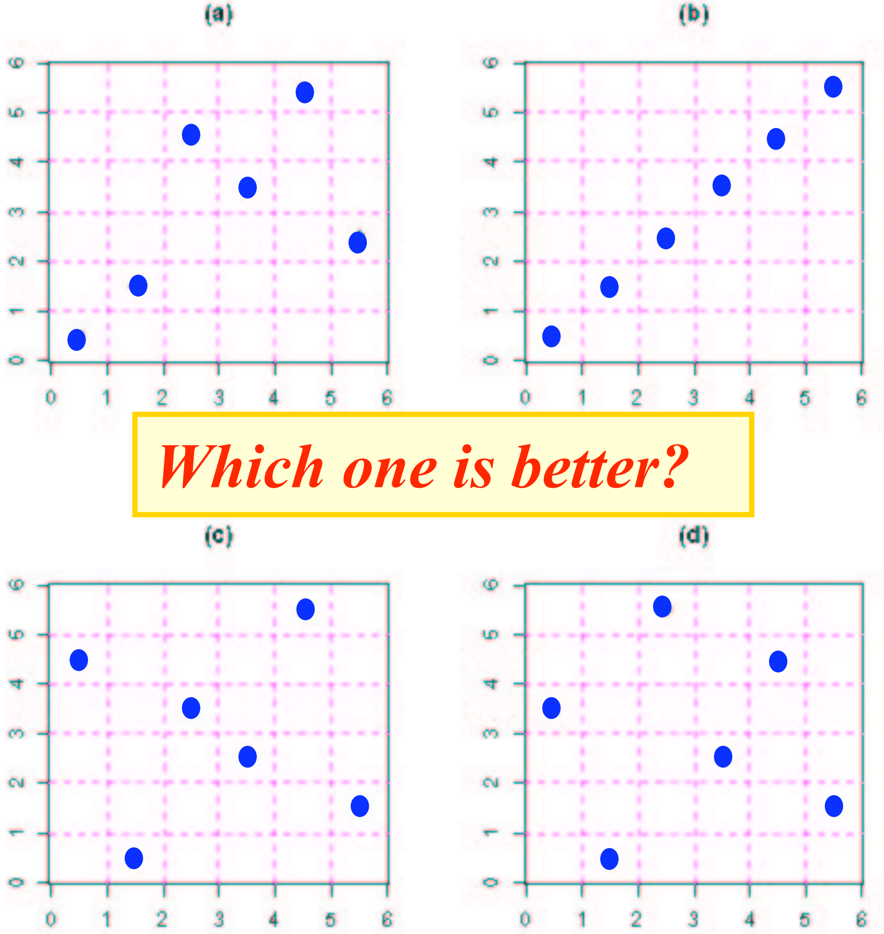
Branching Latin Hypercube Design (BLHD)



run	z_1	$v_1 \ldots v_{m1}$	z_2	$v_1 \ldots v_{m2}$	$x_1 \ldots\ldots x_t$
1	1		1	LHD ($N/2$, m_2) first half	
.	.	LHD ($N/2$, m_1)			
.	.		1	LHD ($N/2$, m_2) first half	
.	1				LHD (N, t)
.	2		2	LHD ($N/2$, m_2) second half	
.	.	LHD ($N/2$, m_1)			
.	.		2	LHD ($N/2$, m_2) second half	
N	2				

How to Find a "Good" Design?

- For n runs and k factors, we can obtain $(n!)^k$ LHDs.



Which one is better?

Minimize Correlation

- Iman and Conover (1982), Owen (1994), and Tang (1998) proposed to find designs minimizing correlations among factors.
- Owen (1994)

$$\rho^2 = \frac{\sum_{i=2}^{k} \sum_{j=1}^{i-1} \rho_{ij}^2}{k(k-1)/2},$$

where ρ_{ij} is the linear correlation between columns i and j.

- Figure (c) shows the optimal LHD found by Tang (1998).

Maximize Minimum Distance

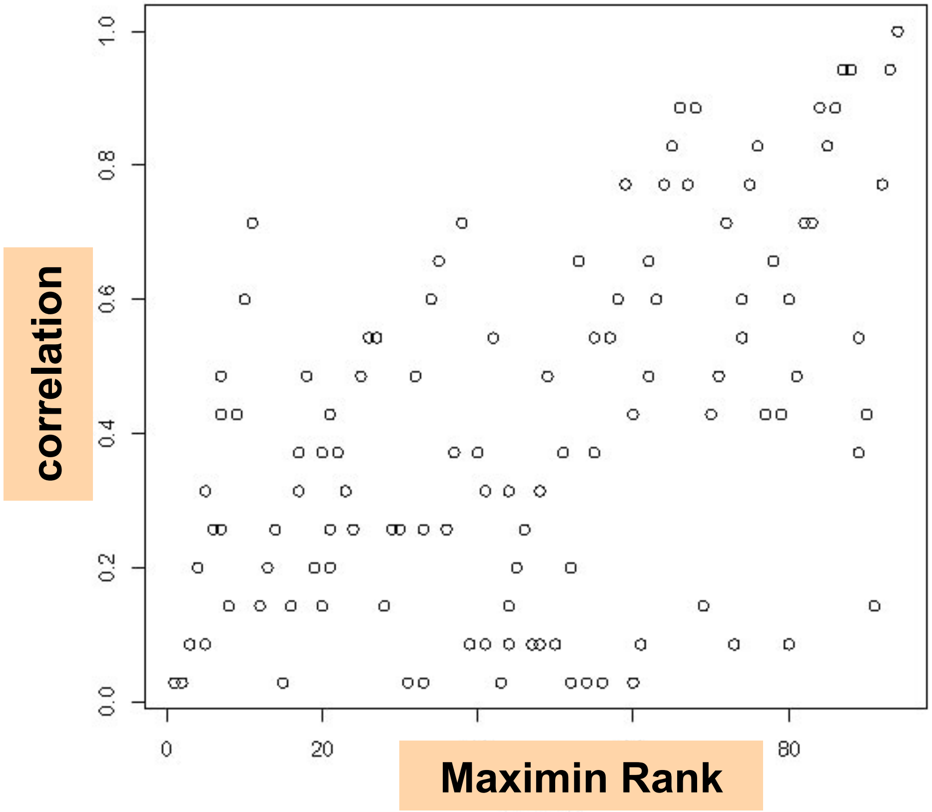
- Johnson, Moore, and Ylvisaker (1990) proposed the maximim distance criterion, which maximizes the minimum inter-site distance.
- Morris and Mitchell (1995) proposed to find the best LHD by maximizing the minimum distance between the points.
- Use a scalar-valued function to rank competing designs.

$$\phi_p = \left(\sum_{i=1}^{\binom{n}{2}} \frac{1}{d_i^p} \right)^{1/p}$$

✓ d_i is the (rectangular or Euclidean) distance between two design points.

Motivating Example

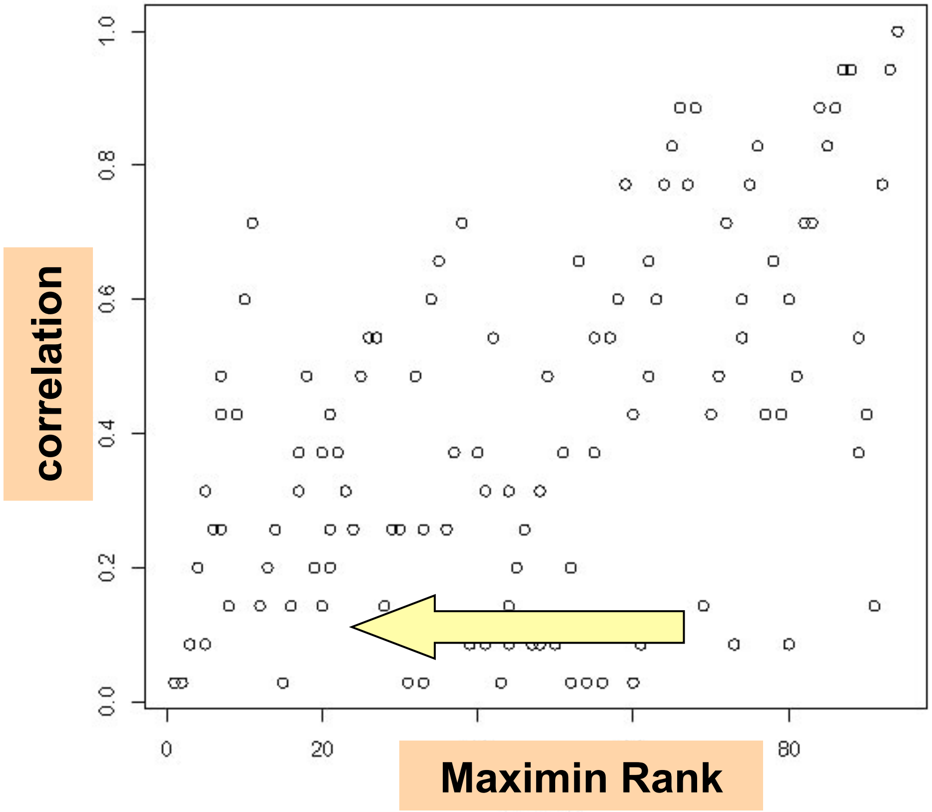
- Maximin rank vs. correlation in $n=6$, $k=2$ case.



- These two criteria can give conflicting results.
- Minimization of one criterion may not lead to minimization of the other.

Motivating Example

- Maximin rank vs. correlation in $n=6, k=2$ case.



- These two criteria can give conflicting results.
- Minimization of one criterion may not lead to minimization of the other.

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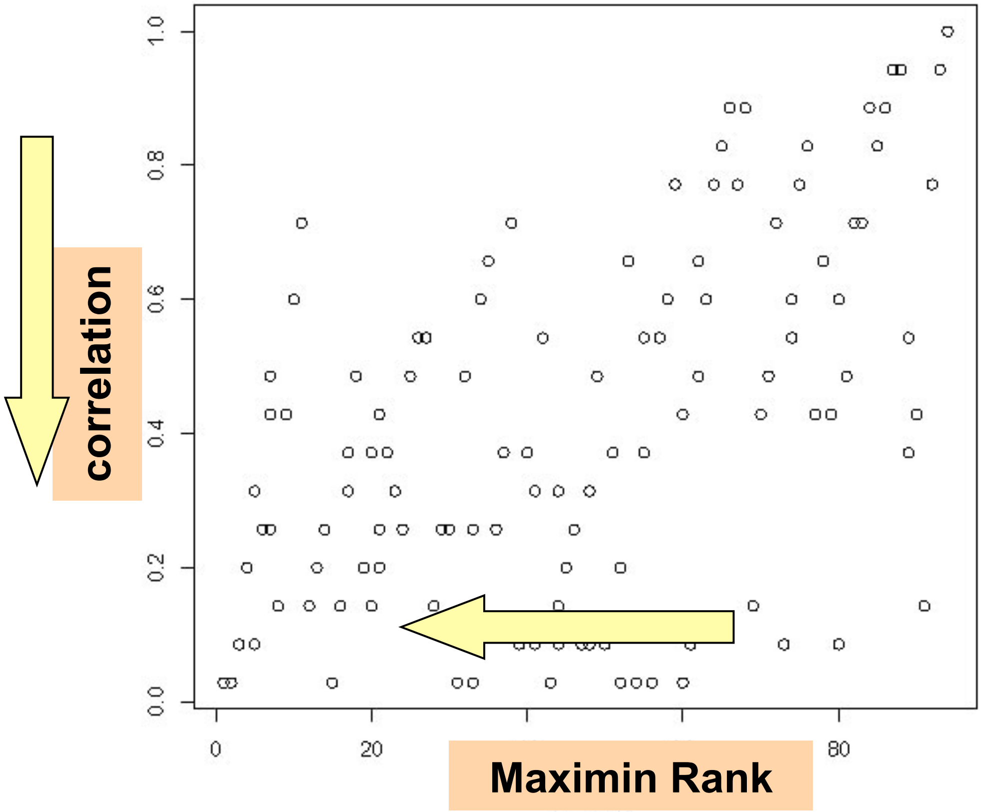

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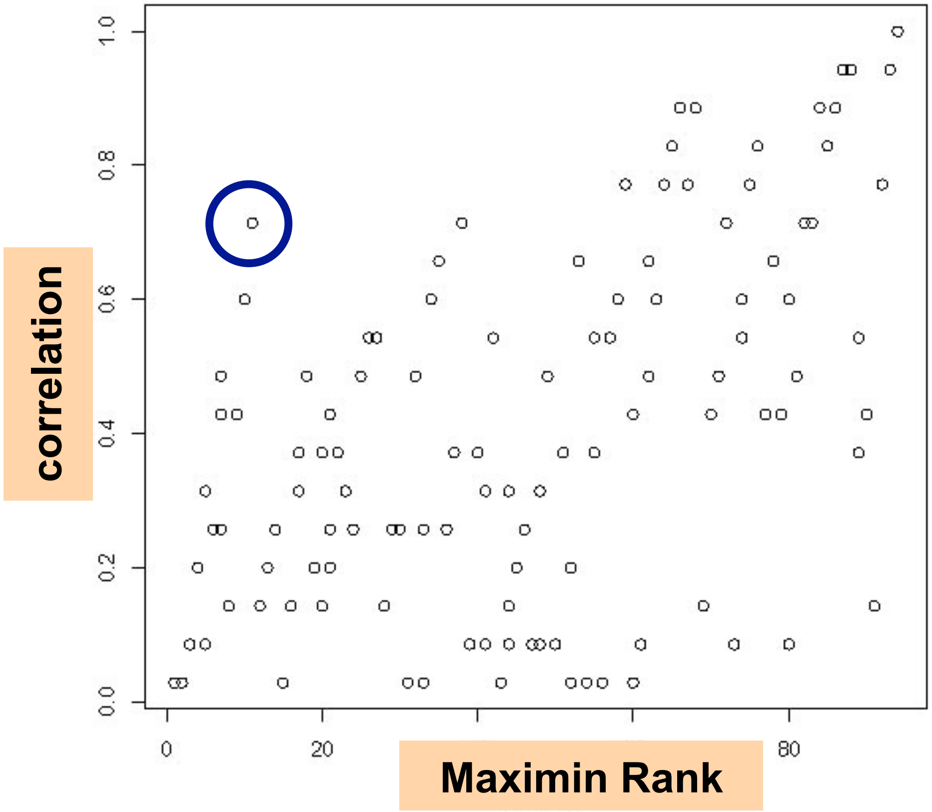

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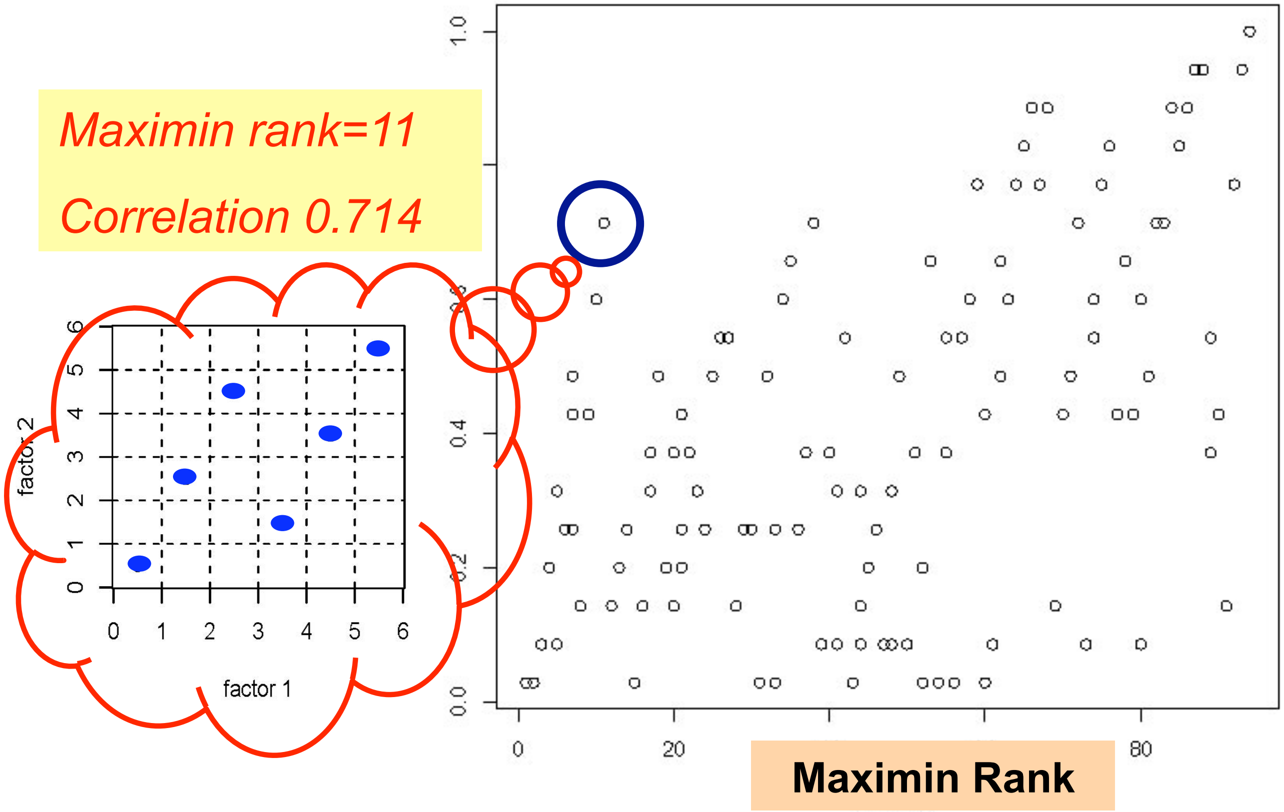

Maximin rank=11

Correlation 0.714

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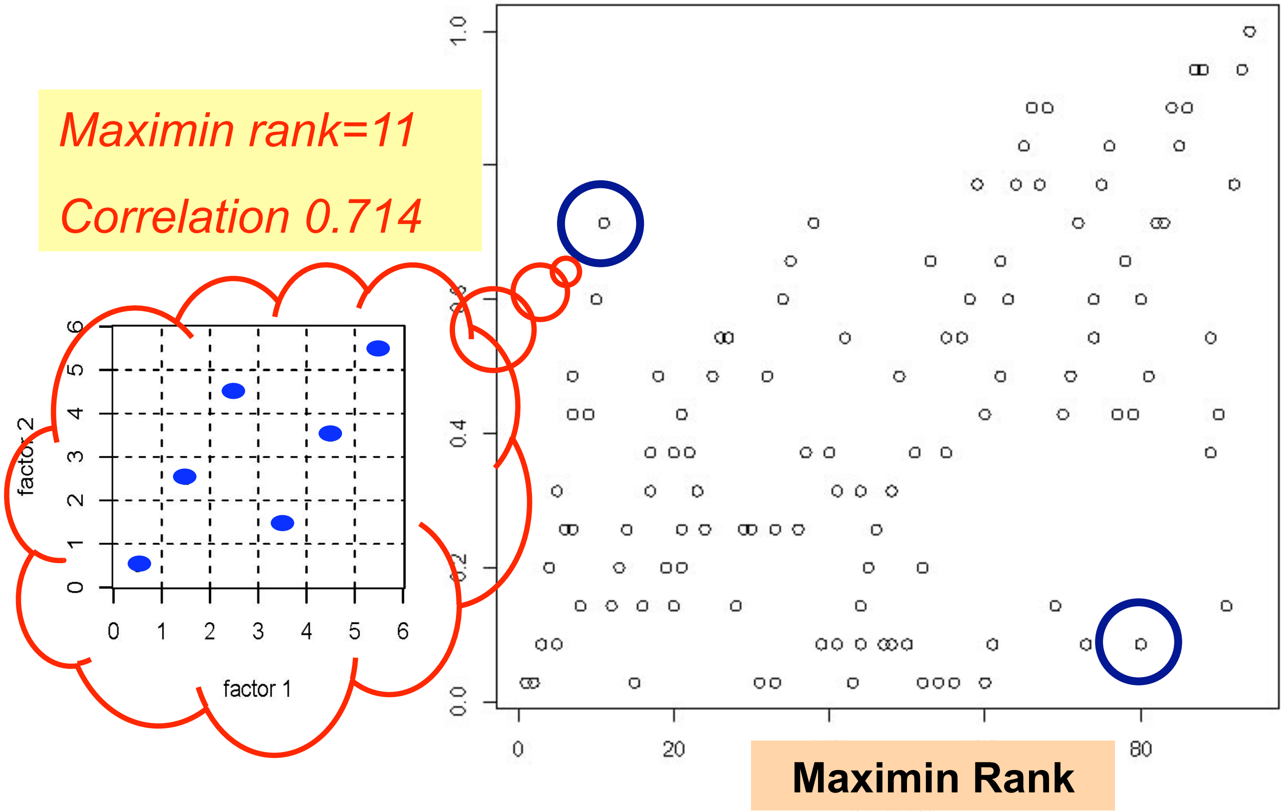

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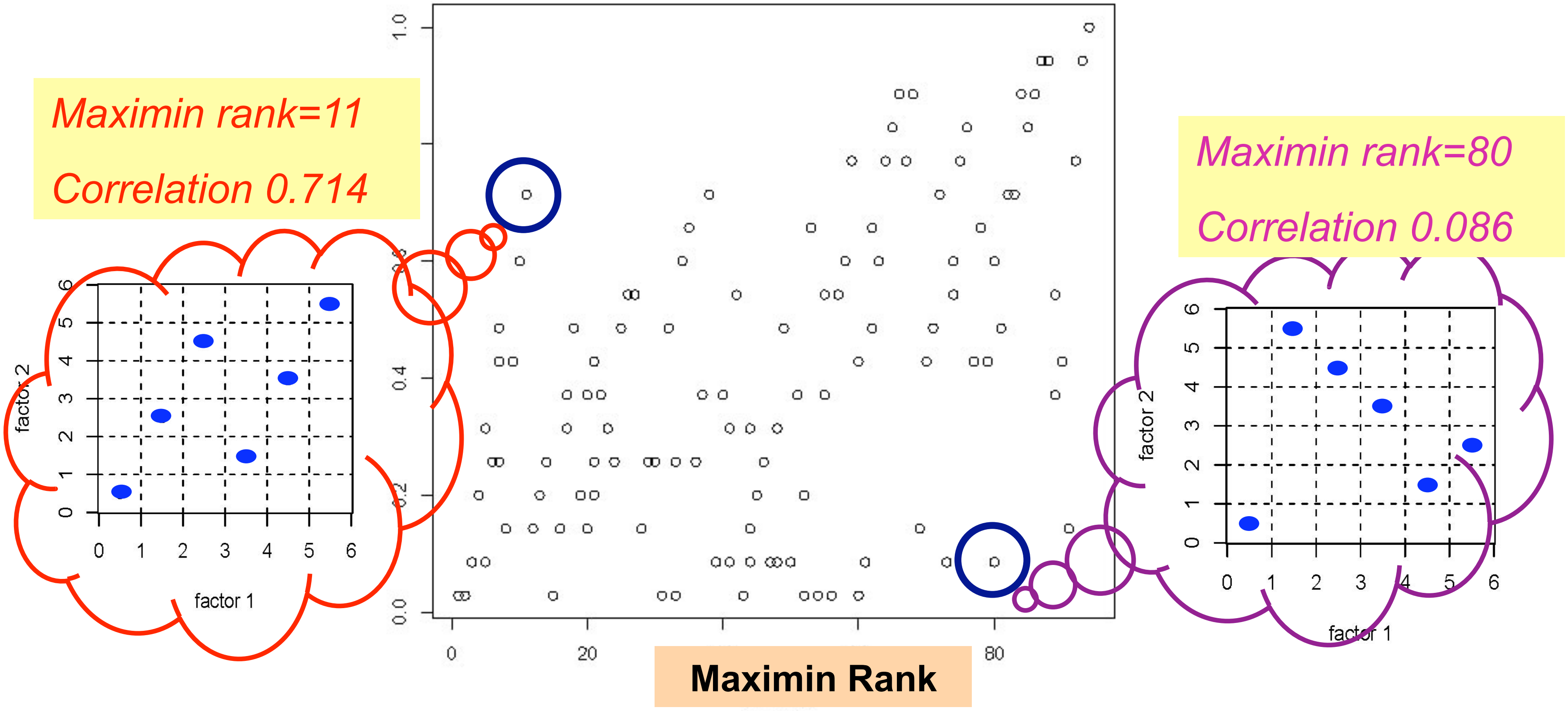

Maximin rank=11

Correlation 0.714

Maximin rank=80

Correlation 0.086

- These two criteria can give conflicting results.
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Orthogonal-Maximin Latin Hypercube Design

- Our objective is to find an LHD that minimizes both ρ^2 and ϕ_p.
- Proposition 1: For an $LHD(n,k)$, $\phi_{p,L} \leq \phi_p \leq \phi_{p,U}$.

$$\phi_{p,L} = \left\{ \binom{n}{2} \left(\frac{\lceil \bar{d} \rceil - \bar{d}}{\lfloor \bar{d} \rfloor^p} + \frac{\bar{d} - \lfloor \bar{d} \rfloor}{\lceil \bar{d} \rceil^p} \right) \right\}^{1/p} \quad \text{and} \quad \phi_{p,U} = \left\{ \sum_{i=1}^{n-1} \frac{(n-i)}{(ik)^p} \right\}^{1/p} .$$

- Define

$$\psi_p = w\rho^2 + (1-w)\frac{\phi_p - \phi_{p,L}}{\phi_{p,U} - \phi_{p,L}},$$

where $w \in (0,1)$.

- A design that minimizes ψ_p is called an orthogonal-maximin Latin hypercube design (OMLHD).

Reference: V. Roshan Joseph and Ying Hung (2008). Orthogonal-Maximin Latin Hypercube Designs, ***Statistica Sinica***, 18, 171-186.

Orthogonal-Maximin BLHD

- Orthogonal-Maximin BLHD

$$\rho^2 = \frac{\sum_{i=2}^{p}\sum_{j=1}^{i-1}\rho_{ij}^2+\sum_{i=1}^{t}\sum_{j=1}^{\alpha}\tilde{\rho}_{ij}^2}{(p(p-1)/2)+\alpha t},$$

⇨

$$\phi_P = \left(\sum_{g\neq h}\left[\frac{t}{d_x(\boldsymbol{g},\boldsymbol{h})}\right]^P + \sum_{i=1}^{k_1}\sum_{g_{t+1}=h_{t+1}=z_{1,i}}\left[\frac{1+t}{d_{v_1}(\boldsymbol{g},\boldsymbol{h})+d_x(\boldsymbol{g},\boldsymbol{h})}\right]^P\right)^{1/P},$$

run	z_1	v_1	x_1	x_2
1	1	1	4	1
2	1	2	3	8
3	1	3	8	5
4	1	4	2	3
5	2	1	7	2
6	2	2	1	6
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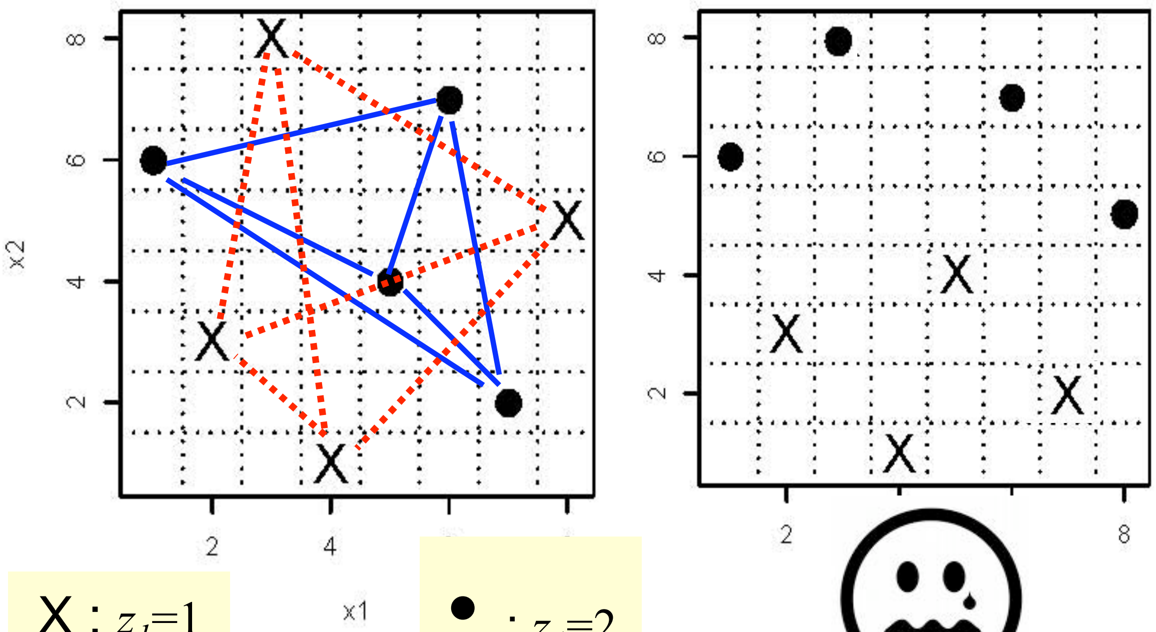
8	2	4	5	4



X : z_1=1

● : z_1=2

Orthogonal-Maximin BLHD

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- **Proposition 2:**

$$\phi_{P,L} = 6\kappa\left[t(N^2-1)+\sum_{i=1}^{k_1} m_1(n_1^2-1)\right]^{-1},$$

$$\phi_{P,U} = N\left[\sum_{i=1}^{k_1}\sum_{j=1}^{n_1-1}\frac{(n_1-j)(t+m_1)^P}{j^P(t+k_1m_1)^P}+\sum_{j=1}^{N-1}\frac{N-j}{j^P}\right]^{1/P}.$$

Orthogonal-Maximin BLHD

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- A multi-objective criterion is to minimize

$$\psi_P = w\rho^2+(1-w)\frac{\phi_P-\phi_{P,L}}{\phi_{P,U}-\phi_{P,L}}.$$

- Heuristic algorithm: simulated annealing algorithm(SAA)

Orthogonal-Maximin BLHD Example

run	z_1	v_1	x_1	x_2
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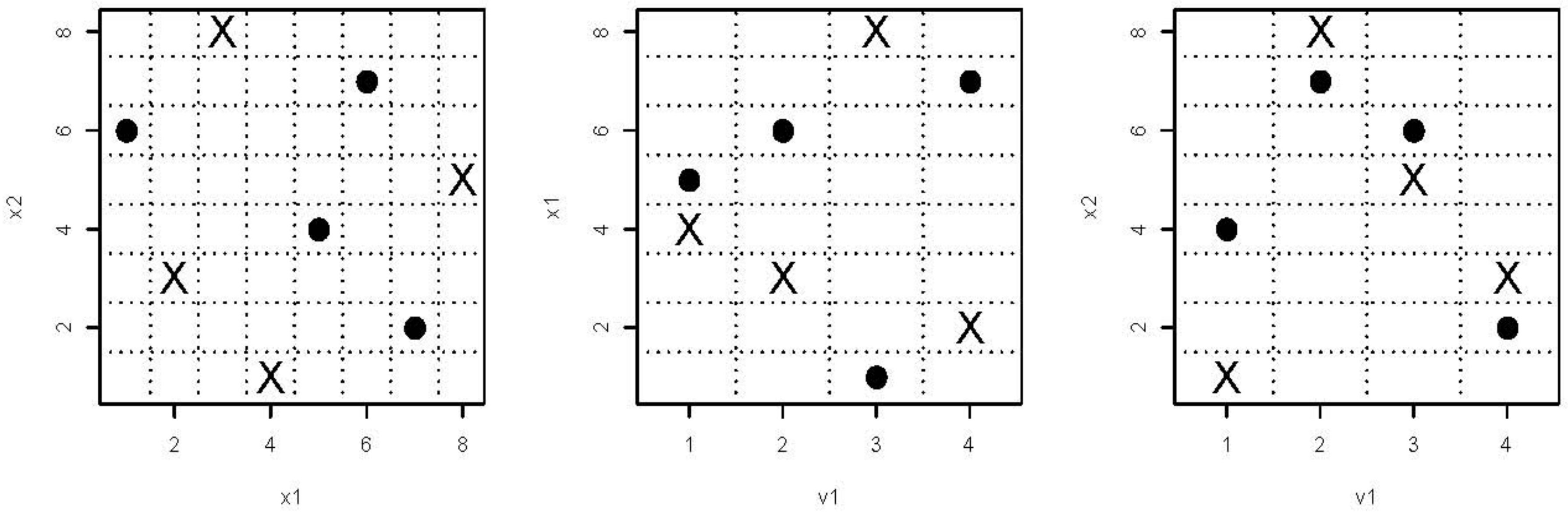

Model Fitting in Computer Experiments

- Kriging is first developed 40 years ago by G. Matheron and named in honor of D. Krige.
- Kriging is widely used in the analysis of computer experiments (Sacks et al. 1989; Santner et al. 2003) and in spatial statistics.
- Interpolating metamodel.
    - Interpolation property essential for *deterministic* computer experiments.
- Efficient in higher dimensions.

New Kriging Model with Branching and Nested Factors

- Kriging:

$$Y(\mathbf{x}) = \mathbf{v}(\mathbf{x})'\mu_m + Z(\mathbf{x}),$$

$Z(\mathbf{x})$ is assumed to be a weak stationary stochastic process with mean 0 and covariance function $\sigma_m^2\psi$

- Product correlation function:
  - ➢ $\boldsymbol{w}_1 = \left(x_{11}, x_{12}, z_{11}, v_{11}^{z_{11}}\right)$, $\boldsymbol{w}_2 = \left(x_{21}, x_{22}, z_{21}, v_{21}^{z_{21}}\right)$.
  - ➢ $\mathrm{cor}(\boldsymbol{Y}(\boldsymbol{w}_1), \boldsymbol{Y}(\boldsymbol{w}_2))$:

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- Gaussian correlation function for shared factors:

$$\psi(\boldsymbol{h}) = \exp(-\sum_{j=1}^{p}\theta_j h_j^2).$$

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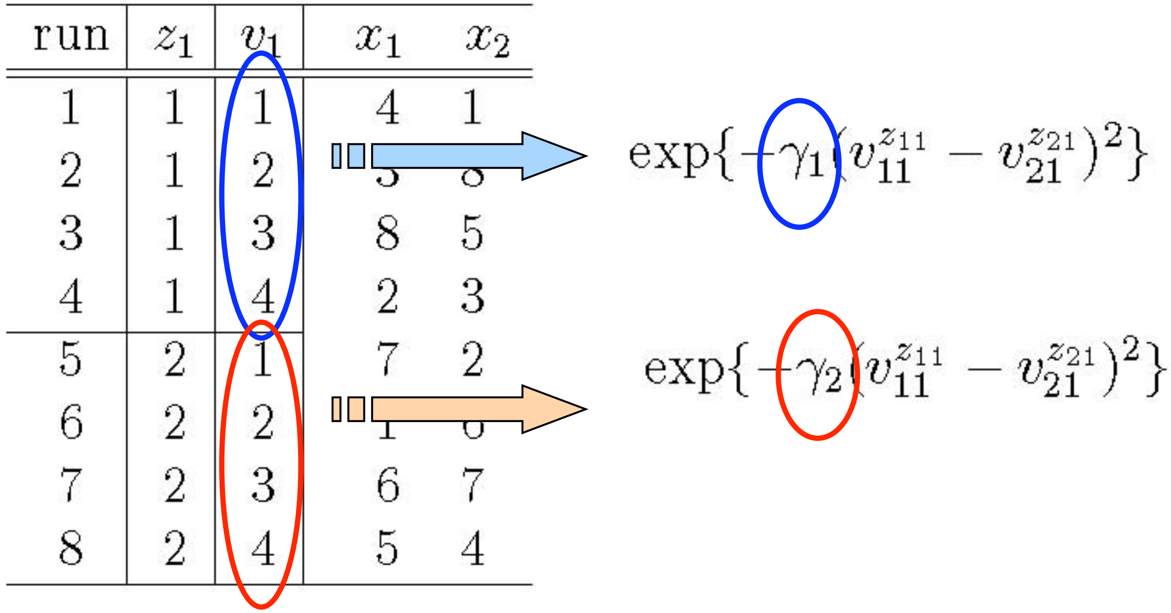
- Isotropic correlation for the branching factors:

$$\xi_1(z_{11}, z_{21}) = \exp\left\{ -\theta_1 I_{[z_{11} \neq z_{21}]} \right\}.$$

New correlation function for the nested factors

- Why not $\psi(\boldsymbol{h}) = \exp(-\sum_{j=1}^{p} \theta_j h_j^2)$.



run	z_1	v_1	x_1	x_2
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8	2	4	5	4

$$\exp\{-\gamma_1(v_{11}^{z_{11}} - v_{21}^{z_{21}})^2\}$$

$$\exp\{-\gamma_2(v_{11}^{z_{11}} - v_{21}^{z_{21}})^2\}$$

- Define new correlation function for nested factors:

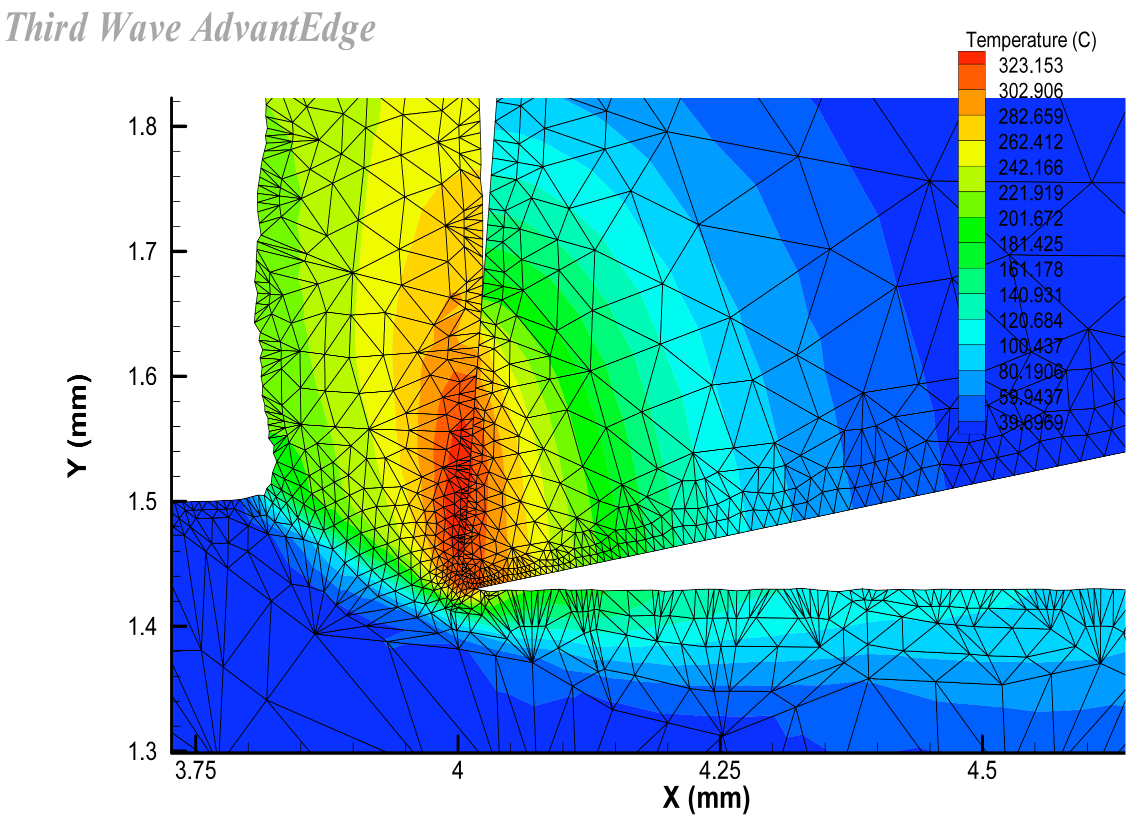
$$\varpi_1(v_{11}^{z_{11}}, v_{21}^{z_{21}}) = \exp\left\{ -\sum_{j=1}^{2} \gamma_j (v_{11}^{z_{11}} - v_{21}^{z_{21}})^2 I_{[z_{11}=z_{21}=j]} \right\}.$$

Computer Experiments in Machining

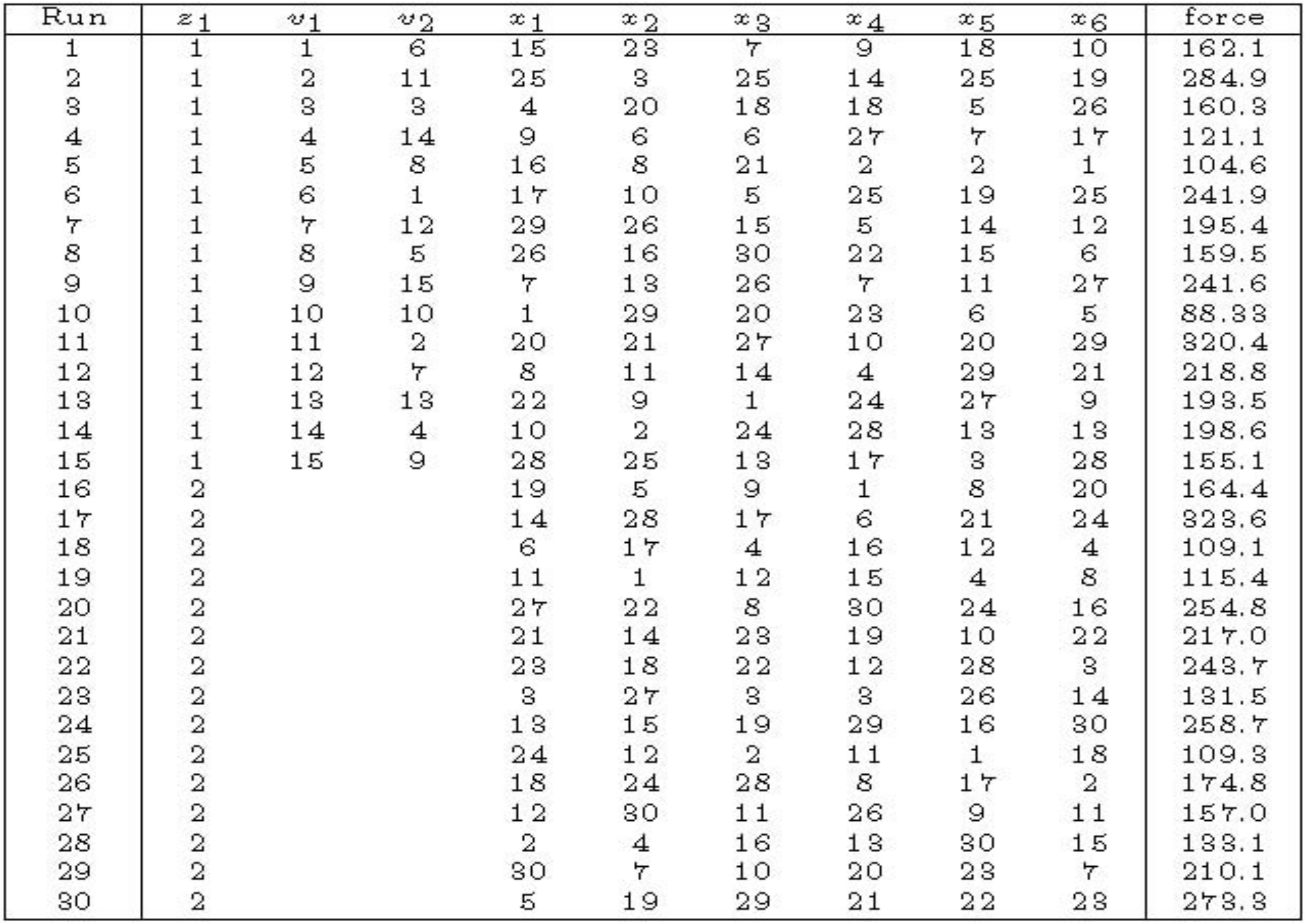
Type of Factor	Notation	Factor	Ranges
Branching factors	z_1	**Tool** (Cutting edge shape)	chamfer & hone
Nested factors	**$v_1 \| z_1$=chamfer**	**Angle**	17~ 20
	$v_2 \| z_1$=chamfer	**Length**	115~140
	$v_1 \| z_1$=hone	**None**	None
	$v_2 \| z_1$=hone	**None**	None
Shared factors	**x_1**	Cutting edge radius	5~25
	x_2	Rake angle	-15 ~ -5
	x_3	Tool nose radius	0.4 ~ 1.6
	x_4	Cutting speed	120 ~ 240
	x_5	Feed	0.05 ~ 0.15
	x_6	Depth of cut	0.1 ~ 0.25

Finite Element Based Simulation in Machining

- Hard turning experiments are simulated from *AdvantEdge*
- Time consuming: 12 hrs ~1 day per run



Finite Element Based Simulation in Machining



Run	z_1	v_1	v_2	x_1	x_2	x_3	x_4	x_5	x_6	force
1	1	1	6	15	23	7	9	18	10	162.1
2	1	2	11	25	3	25	14	25	19	284.9
3	1	3	3	4	20	18	18	5	26	160.3
4	1	4	14	9	6	6	27	7	17	121.1
5	1	5	8	16	8	21	2	2	1	104.6
6	1	6	1	17	10	5	25	19	25	241.9
7	1	7	12	29	26	15	5	14	12	195.4
8	1	8	5	26	16	30	22	15	6	159.5
9	1	9	15	7	13	26	7	11	27	241.6
10	1	10	10	1	29	20	23	6	5	88.33
11	1	11	2	20	21	27	10	20	29	320.4
12	1	12	7	8	11	14	4	29	21	218.8
13	1	13	13	22	9	1	24	27	9	193.5
14	1	14	4	10	2	24	28	13	13	198.6
15	1	15	9	28	25	13	17	3	28	155.1
16	2			19	5	9	1	8	20	164.4
17	2			14	28	17	6	21	24	323.6
18	2			6	17	4	16	12	4	109.1
19	2			11	1	12	15	4	8	115.4
20	2			27	22	8	30	24	16	254.8
21	2			21	14	23	19	10	22	217.0
22	2			23	18	22	12	28	3	243.7
23	2			3	27	3	3	26	14	131.5
24	2			13	15	19	29	16	30	258.7
25	2			24	12	2	11	1	18	109.3
26	2			18	24	28	8	17	2	174.8
27	2			12	30	11	26	9	11	157.0
28	2			2	4	16	13	30	15	133.1
29	2			30	7	10	20	23	7	210.1
30	2			5	19	29	21	22	23	273.3

Computer Experiments in Machining

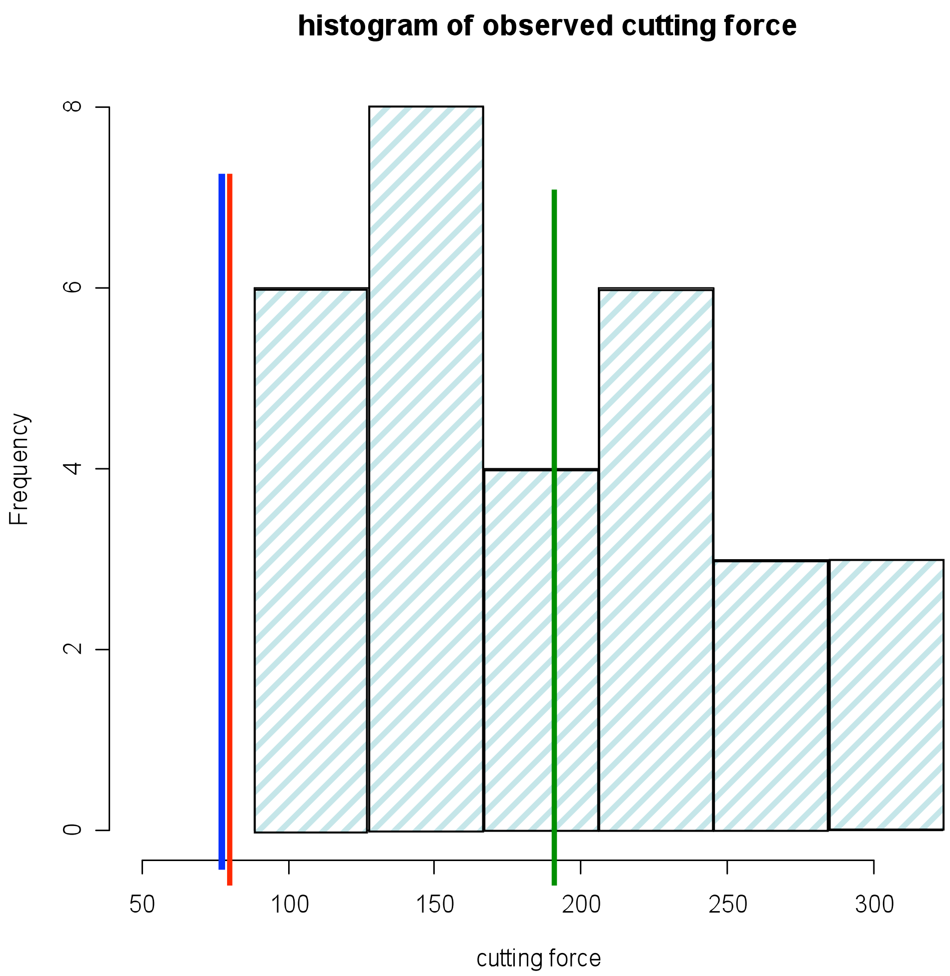
- Fitted kriging model:

$$\hat{y}(\mathbf{w}) = \mathbf{5.1} + \mathbf{0.2x_{51}} + \mathbf{0.2x_{61}} - \mathbf{0.12x_{11}x_{61}} + \hat{\psi}(\mathbf{w})'\hat{\mathbf{\Psi}}^{-1}(\mathbf{y} - \mathbf{V_3}\hat{\mu}_\mathbf{3}).$$

- Optimal setting:

Factors	setting
Cutting edge shape	Chamfer angle: 18.74, length 128.13
Cutting edge radius	5
Rake angle	-13.8
Tool nose radius	1.41
Cutting speed	222
Feed	0.067
Depth of cut	0.123

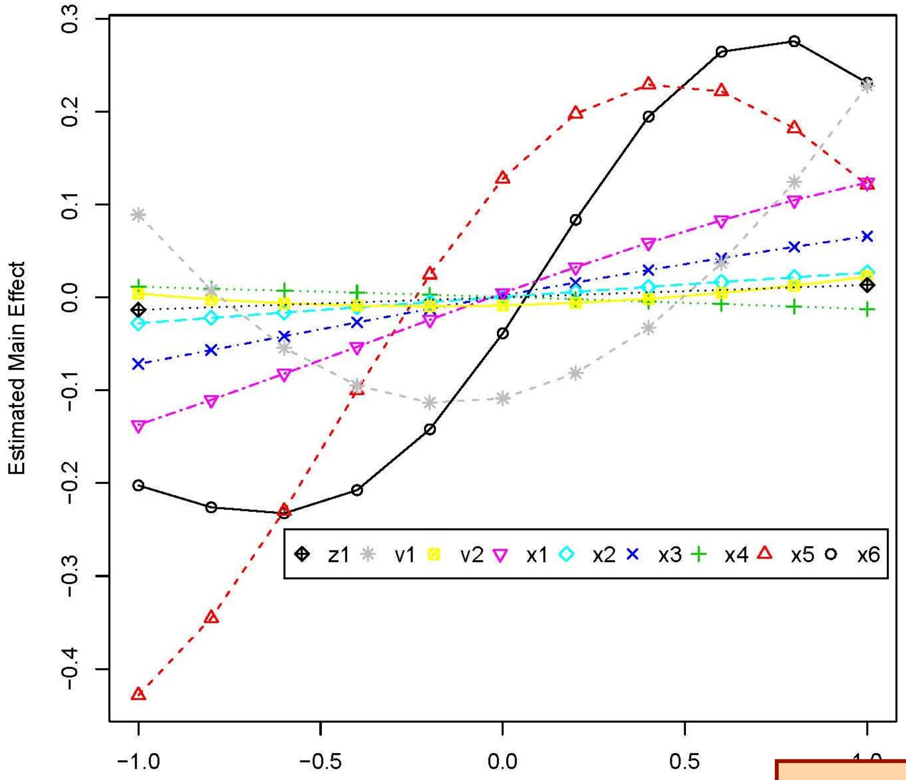
Computer Experiments in Machining



- Predicted minimum cutting force: 81 N (Lower than 191N, the observed average)
- Confirmation experiments: 79 N ⇒ Confirms the validity of the optimal setting.

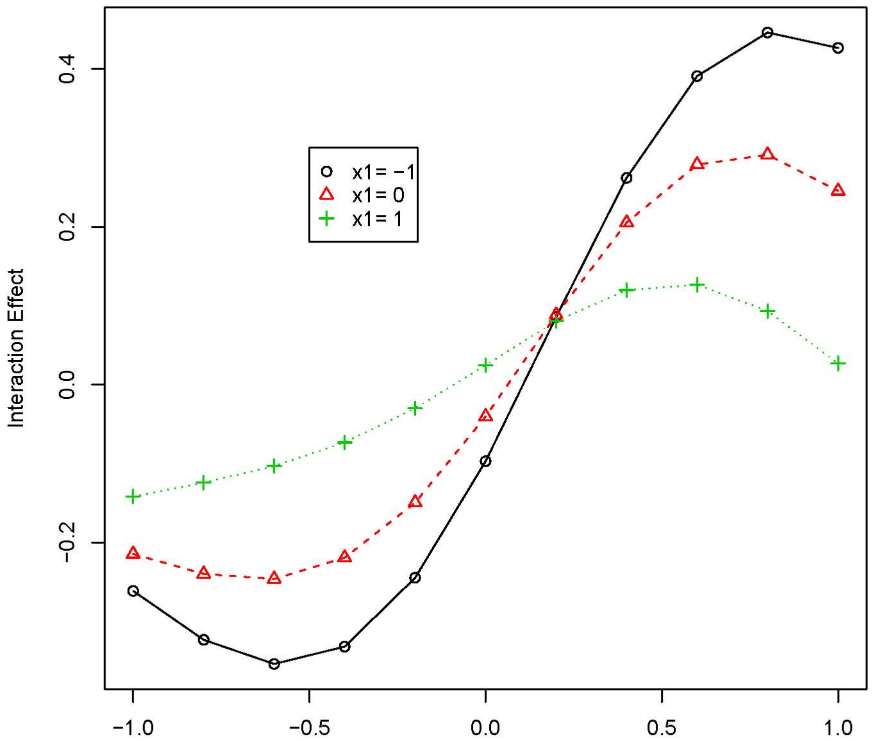
Sensitivity Analysis

Main effects plot



Interaction:

cutting edge radius & **depth of cut**



Feed, **depth of cut**
have significant effects

For small CER, increase of DOC produces increase of material deformation through shear

Concluding Remarks

- The first work in computer experiments with branching and nested factors.
- A new class of design, branching Latin hypercube design (BLHD), is proposed and optimal criteria are discussed.
- New metamodel: blind kriging and new correlation function.
- New method provides an efficient way to find optimal settings of branching factors, nested factors and shared factors simultaneously.

Thank you !