

## *Recent Advances in Design of Experiment*

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## **Design of Experiment**

*How to collect  
useful  
information?*

### **Design Objectives**

- ❖ Treatment Comparison
- ❖ Screening
- ❖ Model Building
- ❖ Parameter Estimation
- ❖ Optimization
- ❖ Prediction
- ❖ Confirmation
- ❖ Discovery (Random Shot)
- ❖ etc.



### **Design Methodology**

- Treatment Comparison
- Fractional & Full Factorial Design
- Orthogonal Arrays
- Combinatorics Design
- Coding Theory
- Response Surface Methodology
- ANOVA type Design
- Optimal Design
- Bayesian (Optimal) Design



## Design Methodology (Continued)

- Saturated (Minimal Point) Design
- Taguchi Product (Robust) Design
- Mixture Experiment
- Computer Experiment
- Supersaturated Design
- Uniform Design
- MicroArray Design



## Design of Experiment (Lin)

- Multiple Response Problems
  - ☞ Optimization: Kim and Lin (*JRSS-C*, 2000)
  - ☞ Design: Chang, Lo, Lin & Young (*JSPI*, 2001)
- Computer Experiment
  - ☞ Beattie and Lin (1999, 2005)
- Dispersion Effect
  - ☞ McGrath and Lin (*Technometrics*, 2002)
- Foldover Plan
  - ☞ Li and Lin (*Technometrics*, 2003)
- Supersaturated Designs
  - ☞ Lin (*Technometrics*, 1993, 1995, 2001) and others
- Uniform Designs
  - ☞ Fang, Lin, Winker & Yang (*Technometrics*, 1999)



## Dispersion Effect

McGrath and Lin (*JQT*, 2001)  
McGrath and Lin (*Technometrics*, 2002)

## Injection Molding Process

$Y$  = % shrinkage

$X_1$  (A) = mold temperature

$X_2$  (B) = screw speed

$X_3$  (C) = holding time

$X_4$  (D) = gate size



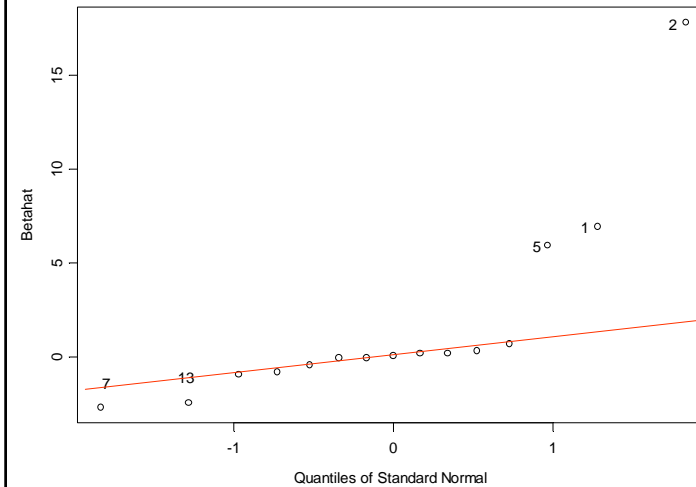
**Example: Injection Molding, Montgomery (1990)**

	A	B	C	D						E	G	F				
0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	y
1	-1	-1	-1	-1	1	1	1	1	1	1	-1	-1	-1	-1	1	6
1	1	-1	-1	-1	-1	-1	-1	1	1	1	1	1	1	-1	-1	10
1	-1	1	-1	-1	-1	1	1	-1	-1	1	1	1	-1	1	-1	32
1	1	1	-1	-1	1	-1	-1	-1	-1	1	-1	-1	1	1	1	60
1	-1	-1	1	-1	1	-1	1	-1	1	-1	-1	1	1	1	-1	4
1	1	-1	1	-1	-1	1	-1	-1	1	-1	-1	1	-1	1	1	15
1	-1	1	1	-1	-1	-1	1	1	-1	-1	1	1	-1	1	1	26
1	1	1	1	-1	1	1	-1	1	-1	-1	-1	-1	-1	-1	-1	60
1	-1	-1	-1	1	1	1	-1	1	-1	-1	1	1	1	1	-1	8
1	1	-1	-1	1	-1	-1	1	1	-1	1	-1	-1	1	1	1	12
1	-1	1	-1	1	-1	1	-1	1	-1	1	-1	1	-1	1	1	34
1	1	1	-1	1	1	-1	1	-1	1	-1	-1	-1	-1	-1	-1	60
1	-1	-1	1	1	1	-1	-1	-1	-1	1	1	-1	-1	-1	1	16
1	1	-1	1	1	-1	1	1	-1	1	-1	-1	1	-1	-1	-1	5
1	-1	1	1	1	-1	-1	1	1	1	-1	-1	-1	1	-1	-1	37
1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	52

$\hat{\beta} \rightarrow$

0	1	2	3	4	5	6	7	8
27.3125	6.9375	17.8125	-0.4375	0.6875	5.9375	-0.8125	-2.6875	-0.9375
9	10	11	12	13	14	15		
-0.0625	-0.0625	0.1875	0.0625	-2.4375	0.1875	0.3125		

Normal Probability Plot, Injection Molding Example



**Traditional Method of Identifying Dispersion Effects in Unreplicated Fractional Factorials**

Box and Meyer (1986b) and Montgomery (1990)

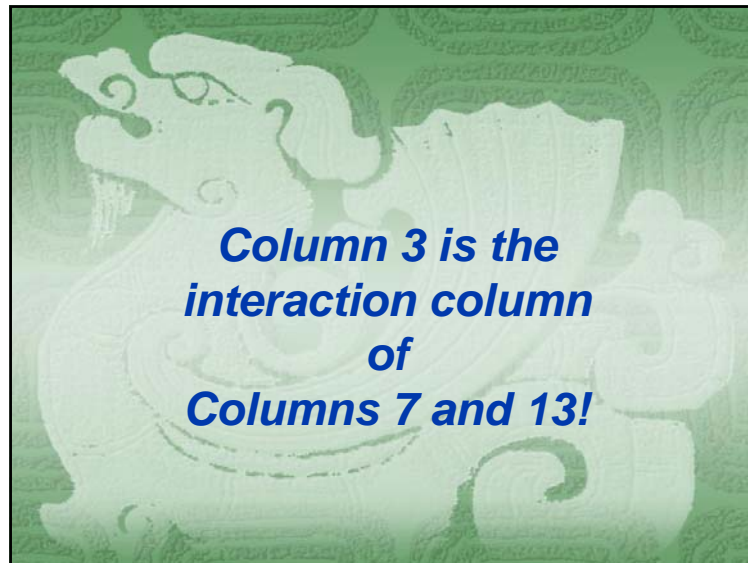
1. Identify location effects
2. Fit reduced model and calculate residuals
3. For column  $d$ , calculate  $F_d^* = \ln \frac{s_{d+}^2}{s_{d-}^2}$  (natural log of ratio of sample variance of residuals at  $d = \pm 1$ .)
4. Box and Meyer point out this statistic is *approximately* normally distributed with mean 0.
5. Montgomery (1990) use a normal probability plot of the  $F_d^*$  to identify dispersion effects.

**Two Feasible Models**

Model I:  $\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2 + \hat{\beta}_5 x_5$

Model II:  $\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2 + \hat{\beta}_5 x_5 + \hat{\beta}_7 x_7 + \hat{\beta}_{13} x_{13}$

Column	Model I			Model II		
	$s_{d+}^2$	$s_{d-}^2$	$F_d^*$	$s_{d+}^2$	$s_{d-}^2$	$F_d^*$
1	14.43	21.11	-0.38	3.26	2.19	0.40
2	16.11	19.43	-0.19	3.19	2.26	0.34
3	32.44	2.66	2.50	2.42	2.58	-0.06
4	21.55	12.91	0.51	1.98	2.39	-0.19
5	18.71	16.82	0.11	4.33	1.12	1.36
6	13.55	20.48	-0.41	1.95	1.99	-0.02
7	11.48	7.55	0.42	2.25	3.20	-0.35
8	14.80	18.73	-0.24	2.02	1.42	0.36
9	16.08	19.44	-0.19	2.08	3.35	-0.48
10	22.23	13.30	0.51	2.19	3.25	-0.39
11	17.41	18.05	-0.04	3.17	2.20	0.36
12	22.30	13.23	0.52	2.03	3.41	-0.52
13	12.23	9.73	0.23	1.29	4.16	-1.17
14	15.05	20.41	-0.30	1.16	4.21	-1.29
15	23.76	11.55	0.72	2.96	2.26	0.27



### FML, Testing in Presence of Multiple Dispersion Effects

1. Identify location effects.
2. Adapt the location effect model to include exactly the following  $a$  terms:
  - The overall mean ( $\beta_0$ ),
  - All active location effects and their interactions,
  - The location effects of the columns to be tested for dispersion and their interactions, and
  - The interactions of all of the above.
3. Identify the  $C_q$ s,  $q = 1, \dots, m$ , the  $m$  sets of residuals from rows that are identical for the above columns.
4. Calculate  $s_q^2$  as  $\sum_{e_i \in C_q} e_i^2 / (n/m - 1)$ , i.e. the sample variance of the residuals for each  $C_q$ . Each of these sample variance has  $d = (n - a)/m$  degrees of freedom.
5. 
$$F_j^{ML} = \left( \prod_{q: C_q \subset P_j} s_q^2 \prod_{q: C_q \subset M_j} s_q^{-2} \right)^{2/m}$$

### Multiple Dispersion Effects (McGrath and Lin, 2001)

Instead of

$$D_E^{BH} = \frac{\sum_{q: C_q \subset P_E} s_q^2}{\sum_{q: C_q \subset M_E} s_q^2} = \frac{s_1^2 + s_2^2}{s_3^2 + s_4^2}$$

use

$$F_E^{ML} = \frac{(\prod_{q: C_q \subset P_E} s_q^2)^{1/2}}{(\prod_{q: C_q \subset M_E} s_q^2)^{1/2}} = \frac{(s_1^2 \times s_2^2)^{1/2}}{(s_3^2 \times s_4^2)^{1/2}}$$

Then,

$$R_E^{ML} = \frac{(\Delta_E / \Delta_D \Delta_{DE})^{1/2} \times (\Delta_D \Delta_E \Delta_{DE})^{1/2}}{(\Delta_{DE} / \Delta_D \Delta_E)^{1/2} \times (\Delta_D / \Delta_E \Delta_{DE})^{1/2}} = \Delta_E$$

### Summary: Dispersion Effect

- Some Problems
  - (see Pan (1999), McGrath and Lin (2001), Breneman and Nair (2001))
  - ☞ unidentified location effects impact dispersion effect identification
  - ☞ dispersion effects impact location effect identification
  - ☞ multiple dispersion effects very complicated
- Some Solutions
  - (see also Bergman and Hynen (1997))
  - ☞ Minimal replication (McGrath (2002))
  - ☞ Joint confidence regions (McGrath and Lin (2001c))
  - ☞  $F^{ML}$  (McGrath and Lin (2002))
- Generalized linear models
  - Nelder and Lee (1991), Engel and Huele (1996), McCullagh and Nelder (1989)

## Uniform Designs

Fang, Lin, Winker & Yang  
(*Technometrics*, 1999)

Fang and Lin  
(Handbook of Statistics, Vol 22, 2003)

## Uniform Design

*A uniform design provides uniformly scatter design points in the experimental domain.*

<http://www.math.hkbu.edu.hk/UniformDesign>

## Uniform Design

$\hat{F}_n(x)$  = **Empirical** Cumulative Distribution Function

$F(x)$  = Uniform Cumulative Distribution Function

Find  $x = (x_1, x_2, \dots, x_n)$

such that  $\hat{F}_n(x)$  is closest to  $F(x)$ .

Discrepancy

$$D = \left[ \int_{\Omega} \|\hat{F}_n(x) - F(x)\|^p dx \right]^{1/p}$$

▪ Wang & Fang (1980)

*The centered  $L_p$ -discrepancy is invariant under exchanging coordinates from  $x$  to  $1-x$ . Especially, the centered  $L_2$ -discrepancy, denoted by  $CL_2$ , has the following computation formula:*

$$\begin{aligned} & (CL_2(P))^2 \\ &= \left(\frac{13}{12}\right)^s - \frac{2}{n} \sum_{k=li=1}^s \prod \left(1 + \frac{1}{2} |x_{ki} - \frac{1}{2}| - \frac{1}{2} |x_{ki} - \frac{1}{2}|^2\right) \\ &+ \frac{1}{n^2} \sum_{k=1}^n \sum_{j=li=1}^s \prod \left[1 + \frac{1}{2} |x_{ki} - \frac{1}{2}| + \frac{1}{2} |x_{ji} - \frac{1}{2}| - \frac{1}{2} |x_{ki} - x_{ji}|\right]. \end{aligned}$$

### Uniform Design Example

No.	1	2	3	4	$x_1$	$x_2$	$x_3$	$x_4$	$y$
1	11	8	2	10	5.0	40	1.5	60	0.1836
2	9	7	12	8	4.2	35	6.5	50	0.1739
3	8	2	3	2	3.8	10	2.0	20	0.0900
4	10	12	6	4	4.6	60	3.5	30	0.1176
5	1	10	4	7	1.0	50	2.5	45	0.0795
6	2	5	11	3	1.4	25	6.0	25	0.0118
7	4	6	1	5	2.2	30	1.0	35	0.0991
8	7	4	3	12	3.4	20	3.0	70	0.1319
9	6	9	8	1	3.0	45	4.5	15	0.0717
10	3	1	7	9	1.8	5	4.0	55	0.0109
11	5	11	10	11	2.6	55	5.5	65	0.1266
12	12	3	9	6	5.4	15	5.0	40	0.1424

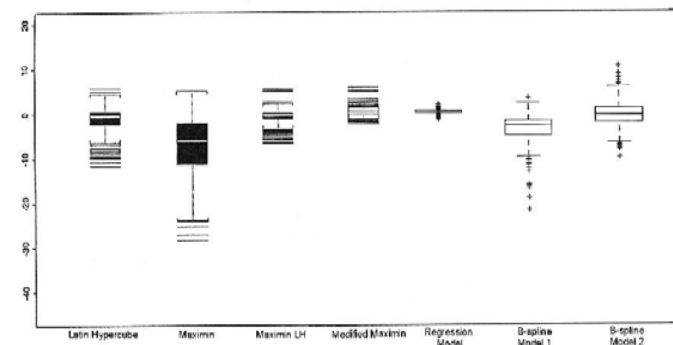
## Uniform Design

- *Uniformity*
- *Model Robustness*
- *Flexibility in experimental runs*
- *Flexibility in the number of levels*

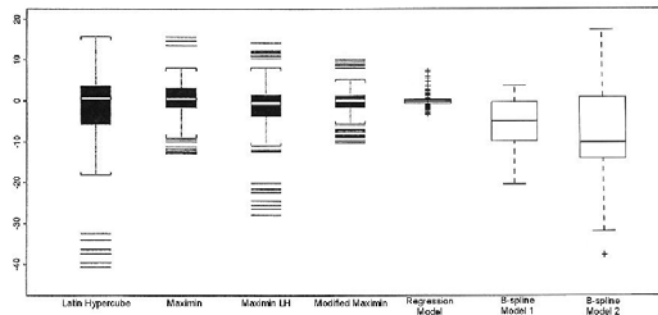
## Comparisons among different designs and models

- *Latin hypercube design*
- *maximin design*
- *maximin Latin hypercube design*
- *modified maximin design*
- *uniform design*

Prediction Errors at 400 Random Samples for Seven Design/Models



Prediction Errors at 256 Corner Points for Seven Design/Models



## More on Uniformity Criterion

- **Designs on computer experiments**
- **Factorial designs**
  - design isomorphism  
*Ma, Fang and Lin (2001, J. Complexity)*
  - consistent with minimum aberration  
*Fang and Mukerjee (2000, Biometrika)*
  - confounding  
*Hikernell and Liu (2000)*
  - orthogonality  
*Ma, Fang and Lin (2003, JPSI)*
  - Hadamard matrix equivalence  
*Fang and Ge (2001, accepted by MATH Computation)*
- **Supersaturated designs** (*Ma, Fang and Lin, 2000, JPSI*)

## Uniform Design: Summary

- Uniformity
- Model Robustness
- Flexibility in experimental runs
- Flexibility in the number of levels

### References

- Fang and Lin (2003)  
*Handbook of Statistics, Statistics in Industry (Vol.22).*
- Fang, Lin, Winker and Zhang  
*(Technometrics, 2000)*
- Website  
[www.math.hkbu.edu.hk/UniformDesign](http://www.math.hkbu.edu.hk/UniformDesign)

## Optimal Foldover Plan

*Li and Lin (Technometrics, 2003)*  
*Li, Ye and Lin (Technometrics, 2003)*

## Conclusion

*The classical wisdom on full foldover is unwise!*

## A crimp example

- Goal: determine the effect of post crimp stresses on the crimp resistance
- Design: 5=1234, 6=124
  - 1: crimp height, 2: pro-conditioning thermal shock, 3: dry heat soak, 4: fixture material, 5: thermal shock life test, 6: discoloration
- Original design: 16-run design
- How do we conduct the next 16-run design?

## Notations

- Factors: 1, 2, 3, 4
- Generators: 5=12, 6=134
- Defining relation: I=125=1346=23456
- Word length pattern:  $W=(0,0,1,1,1)$
- Resolution: III
- Foldover plan:  $\gamma^f=123456$
- WLP of the combined design:  $W=(0,0,0,1,0)$

## Resolution, Aberration and WLP

- Higher resolution implies less confounding
  - ⊗ Resolution III designs confound main effects and two-factor interactions
  - ⊗ Resolution IV designs confound two-factor interactions with some two-factor interactions
- WLP (Word Length Pattern) is used to further distinguish designs with same resolution--aberration criterion.





## Core foldover plans

- Core foldover plan: consists only of the generated factors
- Example:  $\gamma = 5$
- Theorem:** Any foldover plan is equivalent to a core foldover plan.
- Examples
  - $\gamma^f = 123456 \Leftrightarrow \gamma = 5$
  - $\gamma^* = 1 \Leftrightarrow \gamma^* = 56$
- There are essentially  $2^p$  choices.



## Foldover of resolution III designs

Table 3. Word Length Pattern Comparisons on Selected Foldover Resolution III Designs

Design $k-p$	Initial $W(\mathbf{d})$	$W(\mathbf{D}(\gamma^f))$ of full-foldover	$W(\mathbf{D}(\gamma^*))$ of optimal foldover	Optimal foldover plan ( $\gamma^*$ )
6-2.2	(1 1 1 0)	(0 1 0 0 0)	(0 0 1 0 0)	56
7-3.2	(2 3 2 0 0)	(0 3 0 0 0)	(0 1 2 0 0)	567
8-4.2	(3 7 4 0 1)	(0 7 0 0 0)	(0 3 4 0 0)	5678
8-4.4	(4 6 4 0 0)	(0 6 0 0 0)	(0 3 4 0 0)	567
9-5.1	(4 14 8 0 4)	(0 14 0 0 0)	(0 6 8 0 0)	5678
7-2.5	(1 1 0 0 1)	(0 1 0 0 0)	(0 0 0 0 1)	67
8-3.5	(1 2 3 1 0)	(0 2 0 1 0)	(0 0 2 1 0)	678
9-4.6	(1 5 6 2 1)	(0 5 0 2 0)	(0 1 4 2 0)	6789
9-4.7	(1 7 4 0 3)	(0 7 0 0 0)	(0 3 2 0 2)	67, ..., 69
9-4.8	(2 3 6 4 0)	(0 3 0 4 0)	(0 1 4 2 0)	6, 786, 789, 679
10-5.5	(1 14 7 0 7)	(0 14 0 0 0)	(0 6 4 0 4)	678, ..., 6910
11-6.6	(3 13 19 11 9)	(0 13 0 11 0)	(0 5 12 7 4)	678



## A Typical Example

- Factors: 1, 2, 3, 4
- Generators: 5=12, 6=134
- Defining relation:  $I=125=1346=23456$
- Word length pattern:  $W=(0,0,1,1,1,0)_{III}$
- Full Foldover plan:  $\gamma^f=123456$  [ $\gamma=5$ ]
- WLP of the combined design:  $W=(0,0,0,1,0,0)_{IV}$
- Optimal Foldover plan:  $\gamma^*=56$
- WLP of the combined design:  $W=(0,0,0,0,1,0)_{V}$



## Foldover of resolution IV designs

Li & Lin (2003)

Table 4. Word Length Pattern Comparisons on Selected Foldover Resolution IV Designs

Design $k-p$	Initial $W(\mathbf{d})$	$W(\mathbf{D}(\gamma^f))$ of full-foldover	$W(\mathbf{D}(\gamma^*))$ of optimal foldover	Optimal foldover plan ( $\gamma^*$ )
5-1.2	(0 1 0)	(0 1 0 0 0)	full factorial	5
6-2.1	(0 3 0 0)	(0 3 0 0 0)	(0 1 0 0 0)	5, 56, 6
7-3.1	(0 7 0 0 0)	(0 7 0 0 0)	(0 3 0 0 0)	5, ..., 7
8-4.1	(0 14 0 0 0)	(0 14 0 0 0)	(0 6 0 0 0)	56, ..., 78
7-2.1	(0 1 2 0 0)	(0 1 0 0 0)	(0 0 1 0 0)	6, 7
8-3.1	(0 3 4 0 0)	(0 3 0 0 0)	(0 1 2 0 0)	6, ..., 78
9-4.3	(0 9 0 6 0)	(0 9 0 6 0)	(0 3 0 4 0)	678, ..., 789
9-4.5	(0 14 0 0 0)	(0 14 0 0 0)	(0 6 0 0 0)	67, ..., 89
10-5.1	(0 10 16 0 0)	(0 10 0 0 0)	(0 4 8 0 0)	67, ..., 910
11-6.2	(0 26 0 24 0)	(0 26 0 24 0)	(0 10 0 16 0)	7810, ..., 8910 11



## Major results

- For most designs there exist better foldover plans than the full foldover plan
  - ↳ In 52 out of 77 designs have better foldover plans than full-foldover plans
  - ↳ Most (42) foldover plans are new
- Almost all minimum aberration designs have better foldover plans



## Summary *(Li & Lin, 2003)*

- Proposed a computer search method to construct optimal foldover plans that minimizes the WLP of the combined design.
- Tabulated optimal foldover plans for commonly-used 16-run and 32-run designs.
- Investigated optimal and full foldover plans by focusing on core foldover plans.
- Demonstrated that there exists a unique group of equivalent foldover plans.
- See also some work of Mee.
- Theory on optimal foldover—Fang, Lin and Qin(2003)



## Theoretical Support on Optimal Flodover (via Discrepancy)

## Fang, Lin and Qin (2003)

Discrepancy for Design D

$$(\text{CD}(\mathcal{D}))^2 = \left(\frac{13}{12}\right)^2 - \frac{1}{n} \sum_{k=1}^n \prod_{i=1}^r \left(1 - \frac{1}{2} |x_{ki} - \frac{1}{2}| - \frac{1}{2} |x_{ki} - \frac{1}{2}|^2\right) + \frac{1}{n^2} \sum_{k=1}^n \sum_{j=1}^n \prod_{i=1}^r \left(1 + \frac{1}{2} |x_{ki} - \frac{1}{2}| + \frac{1}{2} |x_{ji} - \frac{1}{2}| - \frac{1}{2} |x_{ki} - x_{ji}|\right)$$

Discrepancy for combined design under foldover plan  $\gamma$

$$(\text{CD}(T(\gamma)))^2 = c + \frac{1}{2n^2} \sum_{k=1}^n \sum_{j=1}^n \prod_{i=1}^r \left(\frac{5}{2} - \frac{1}{2} |x_{ki} - x_{ji}| - \frac{1}{2} |x_{ki} + (-1)^{d_i+1} x_{ji} - \delta_i|\right)$$

*This can be shown to be minimum among all designs of same size.*

## Future work

- Optimal foldover designs of non-regular designs
  - ↳ Generalized resolution criterion (Deng and Tang, 1999)
  - ↳ Allows “fractional” word length
  - ↳ Miller and Sitter (2001)
  - ↳ Li, Ye and Lin (2003)
- Optimal semi-foldover designs built on Mee and Peralta (2000) and this work
- Fold over high level designs
- Optimal follow-up experiment, in general.

## Supersaturated Designs

Lin (UTK Technical Report, 1991)  
 Lin (*Technometrics*, 1993, 1995, 2001)  
 Lin (*Handbook of Statistics*, Vol 22, 2003)  
 and others

## Supersaturated Design Example

Half Fraction of William's (1968) Data

Run	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	y
1	+	+	+	-	-	-	+	+	+	+	-	+	-	-	+	+	-	-	+	-	-	-	-	-	133
2	+	-	-	-	-	-	+	+	+	-	-	+	+	+	+	-	+	-	-	-	+	-	-	-	62
3	+	+	-	+	+	-	-	-	-	+	+	+	+	+	+	-	-	-	-	-	-	-	+	+	45
4	+	+	-	+	-	+	-	-	+	+	+	+	+	+	+	-	+	+	+	+	-	-	-	-	52
5	-	+	+	+	+	-	+	+	-	-	-	+	-	+	+	+	-	-	+	-	+	+	+	+	56
6	-	+	+	+	+	+	-	+	+	-	-	+	+	-	+	+	+	+	+	+	+	+	-	-	47
7	-	-	-	+	-	+	-	+	-	+	+	+	+	+	+	-	+	+	+	+	+	-	-	+	88
8	-	+	+	-	-	+	+	-	+	-	-	-	-	-	-	-	-	-	+	-	+	+	+	+	193
9	-	-	-	-	+	+	-	-	+	+	-	-	+	+	-	+	+	-	-	-	-	-	+	+	32
10	+	+	+	+	-	+	+	+	-	-	-	+	-	+	-	+	-	+	-	+	-	-	-	+	53
11	-	+	-	+	+	-	+	+	-	+	-	-	+	-	-	-	-	+	+	-	-	-	+	+	276
12	+	-	-	+	+	+	-	+	+	+	+	+	+	+	-	-	+	-	+	-	+	+	+	+	145
13	+	+	+	+	+	-	+	-	+	-	+	-	-	-	-	-	-	+	-	+	+	+	-	-	130
14	-	+	-	-	-	-	-	-	-	+	+	-	+	-	-	-	-	-	-	+	-	+	-	-	127

Lin (1993, *Technometrics*)

## SUPERSATURATED DESIGN

How can we study  $k$  parameters with  $n(<k)$  observations (experiments)?

A situation for using supersaturated design:

- A Small number of run is desired
- The number of potential factors is large
- Only a few active factors

## Design Criteria

### Supersaturated Design

- Booth and Cox (1962):  $E(s^2)$
- Wu (1993): Extension of classical optimalities ( $D_f, A_f$  etc)
- Deng and Lin (1994): 8 criteria
- Deng, Lin and Wang (1996): B-criterion
- Deng, Lin and Wang (1994): resolution rank
- Balkin and Lin (1997):  
Graphical Comparison (Harmonic mean of eigens)



## New Age SSD Criteria

- $E(f_{NOD})$
- Discrete Discrepancy
- Minimum Generalized Aberration (MGA)
- Generalized Minimum Aberration (GMA)
- Indicator Function
- Relationships/Connections Among criteria
- Probability of Correct Search



## Design Construction

### Supersaturated Design

- *Half Fraction of Hadamard Matrix*
- *Random Combined Design (Taguchi, 1986)*
- *Algorithmic Approach*
- *Combinatorial Approach*
- *Optimal Supersaturated Design*
- *Others*



Supersaturated Design From Hadamard Matrix of Order 12  
(Using 11 as the branching column)

Run	Factors											
No.	I	1	2	3	4	5	6	7	8	9	10	(11)
1	+	+	+	-	+	+	+	-	-	-	+	-
2	+	+	-	+	+	+	-	-	-	+	-	+
3	+	-	+	+	+	-	-	-	+	-	+	+
4	+	+	+	+	-	-	-	+	-	+	+	-
5	+	+	+	-	-	-	+	-	+	+	-	+
6	+	+	-	-	-	+	-	+	+	-	+	+
7	+	-	-	-	+	-	+	+	-	+	+	+
8	+	-	-	+	-	+	+	-	+	+	+	-
9	+	-	+	-	+	+	-	+	+	+	-	-
10	+	+	-	+	+	-	+	+	-	-	-	-
11	+	-	+	+	-	+	+	+	-	-	-	+
12	+	-	-	-	-	-	-	-	-	-	-	-



## Supersaturated Design Example

Half Fraction of William's (1968) Data

Run	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	y
1	+	+	+	-	-	-	+	+	+	+	-	-	-	+	+	-	-	+	-	-	-	-	-	-	133
2	+	-	-	-	-	-	+	+	+	-	-	-	+	+	+	+	-	+	-	-	-	+	+	-	62
3	+	+	-	+	+	-	-	-	-	+	-	+	+	+	+	+	+	-	-	-	-	-	+	+	45
4	+	+	-	+	-	+	-	-	-	+	+	-	+	-	+	-	+	-	+	+	+	-	-	-	52
5	-	-	+	+	+	+	-	+	+	-	-	-	+	-	+	+	+	-	-	+	-	+	+	+	56
6	-	-	+	+	+	+	-	+	+	-	-	-	+	-	+	+	+	+	+	+	+	-	-	-	47
7	-	-	-	-	-	-	+	+	+	-	-	+	+	+	+	+	+	+	+	+	+	-	-	+	88
8	-	+	+	-	-	+	-	+	-	+	-	-	-	-	-	-	-	-	-	-	-	+	+	+	193
9	-	-	-	-	-	+	-	+	-	-	-	+	-	+	-	+	+	-	-	-	-	-	+	+	32
10	+	+	+	+	-	+	+	+	+	-	-	+	-	+	-	+	-	+	-	+	-	-	+	+	53
11	-	+	-	+	+	-	-	+	+	-	+	-	-	+	-	-	+	+	-	-	-	-	+	+	276
12	+	-	-	-	+	+	-	+	+	+	+	+	-	-	+	-	-	+	-	+	+	+	+	+	145
13	+	+	+	+	+	-	-	+	-	-	-	+	-	-	-	-	-	-	-	+	+	+	+	-	130
14	-	-	+	-	-	-	-	-	-	-	+	-	+	-	-	-	-	-	-	+	+	-	-	-	127

Lin (1993, *Technometrics*)

## Half Fraction Hadamard Matrix

$$(n, k) = (2t, 4t - 2)$$



## Balanced Incomplete Block Design

$$v = 2t - 1$$

$$b = 4t - 2$$

$$r = 2t - 2$$

$$k = t - 2$$

Hedayat & Wallis  
(1978)

- $ave(s^2) = n^2 / (2n - 3)$   
proved to be  $E(s^2)$ -optimal!
- Non-isomorphic class exist!

## Half Fraction Hadamard Matrix

$$(n, k) = (2t, 4t - 2)$$



### Coding Binary Code

length  $n = 2t$

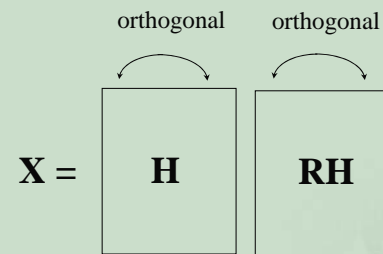
weight  $\omega = t$

distance  $d$

$$\frac{n}{3} \leq d \leq \frac{2n}{3}$$

if  $|\gamma| \leq 1/3$

- Find  $A[n, d, \omega]$ : maximum number of codewords.



not orthogonal  
Thus Permute rows of RH  
to minimize  $E(s^2)$ , say.

## Algorithmic

Supersaturated Design

Lin (1991, 1995): Pairwise Optimality

Nguyen (1996): Exchange Algorithm

Li and Wu (1997): Columnwise and Pairwise Algorithm

Church (1993): Projection Properties



UD

OD

SSD

$$U \oplus L = \begin{bmatrix} 1 & 1 \\ 2 & 7 \\ 3 & 3 \\ 4 & 9 \\ 5 & 5 \\ 6 & 6 \\ 7 & 2 \\ 8 & 8 \\ 9 & 4 \end{bmatrix} \oplus \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 \\ 0 & 2 & 2 & 2 \\ 1 & 0 & 1 & 2 \\ 1 & 1 & 2 & 0 \\ 1 & 2 & 0 & 1 \\ 2 & 0 & 2 & 1 \\ 2 & 1 & 0 & 2 \\ 2 & 2 & 1 & 0 \end{bmatrix} = X = \begin{bmatrix} 0 & 0 & 0 & 0 & | & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 & | & 2 & 0 & 2 & 1 \\ 0 & 2 & 2 & 2 & | & 0 & 2 & 2 & 2 \\ 1 & 0 & 1 & 2 & | & 2 & 2 & 1 & 0 \\ 1 & 1 & 2 & 0 & | & 1 & 1 & 2 & 0 \\ 1 & 2 & 0 & 1 & | & 1 & 2 & 0 & 1 \\ 2 & 0 & 2 & 1 & | & 0 & 1 & 1 & 1 \\ 2 & 1 & 0 & 2 & | & 2 & 1 & 0 & 2 \\ 2 & 2 & 1 & 0 & | & 1 & 0 & 1 & 2 \end{bmatrix}$$

Fang, Lin & Ma (2000)

## Data Analysis Methods

Supersaturated Design

- Pick-the-Winner
- Graphical Approach
- “PARC” (Practical Accumulation Record Computation)
- Compact Two-Sample Test
- Forward Selection
- Ridge Regression
- Normal Plot



## Design Analysis

Supersaturated Design

- *Classical Approaches*
- *Adjusted p-value*  
(Westfall, Young & Lin, *Statistica Sinica*, 1998)
- *Bayesian Approach*  
(Beattie, Fong & Lin, *Technometrics*, 2002)
- *Penalized Least Squares*  
(Li & Lin, 2002)



## SSD: Looking Ahead

### Supersaturated Design

- SSD is much more mature than ever
- Nano-Manufacturing Applications
- Micro-Array Design and Analysis
- Computer Experiment: Model Building (using SSD)
- Higher (and Mixed) Level SSD
- Spotlight Interaction Effects (Lin, 1998, QE)
- Combination Designs: Rotated FFD & SSD



## Computer Experiment

Beattie and Lin (1999 & 2005)

## Computer Experiment

- Expensive simulation
- When Monte Carlo study is infeasible, how to run simulation?
- Latin Hypercube



## Goals—Computer Experiment

- Confirmation
- Sensitivity Analysis
- Empirical Model Building
- Optimization
- Model Validation
- High Dimension Integration





## Statistics vs. Engineering Models

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

### Statistical Model

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

## Irrelevant Issues

- Replicates
- Blocking
- Randomization

*Question: How can a computer experiment be run in an efficient manner?*

## Current Approaches to Experimental Design

- Geometric (Frequentist) Designs
  - ☞ Full and Fractional Factorial Designs
  - ☞ Other Traditional Designs
  - ☞ Latin Hypercube Designs (McKay, Beckman, and Conover (1979))
- Computer-Generated (Bayesian) Designs
  - ☞ Maximin Distance Designs (Johnson, Moore, and Ylvisaker (1990))
- Combination Designs (Computer-Generated Geometric)
  - ☞ Maximin Latin Hypercube Designs (Morris and Mitchell (1992))
  - ☞ Orthogonal Array-based LHs (Tang (1993), Owen (1992))
  - ☞ Rotated Factorial Designs (Beattie and Lin (1999))

## Rotated Factorial Designs

- Computer experiments are gaining in popularity
  - ☞ main research area of the next 10 years
- Rotated factorial designs
  - ☞ good factorial design properties (orthogonality and structure)
  - ☞ good Latin hypercube properties (unique and equally-spaced projections)
  - ☞ easy to construct
  - ☞ comparable by Bayesian criteria
  - ☞ very suitable for computer experiments

$D = X \cdot V$

desirable design      factorial design      rotated matrix

1	1
2	1
⋮	⋮
p	1
1	2
2	2
⋮	⋮
p	2
⋮	⋮
1	p
2	p
⋮	⋮
p	p

$U_1$	$U_3$
$U_2$	$U_4$

*Beattie & Lin (1998):  
Rotating Full Factorials*

$D = X \cdot V$

desirable design      fractional factorial design (mostly two-level)      rotated matrix

$S_1$
$S_2$
⋮
$S_i$
⋮
$S_m$

*Bursztyn & Steinberg (2002):  
Rotating in Groups*

Now,  
Put these two ideas together!

- Grouping all design columns into groups,
- each forms a full factorial design,
- then rotate each group (in block).

*Steinberg and Lin (Biometrika, 2006)*

**Multiple Response Problems**

Optimization: Kim and Lin (*JRSS-C*, 2000)

Design: Chang, Lo, Lin & Young (*JSPI*, 2001)

## CGA Study

### Data:

Central Composite Design in  $x_1, x_2$  &  $x_3$ , with three outputs,  $y_1, y_2$  &  $y_3$  and three (3) replicates.

### Fitted "Location" Models

$$\hat{y}_{\mu_1}(x) = 4.95 + 0.82x_1 - 0.45x_2 - 0.15x_1^2 + 0.28x_2^2 - 0.11x_1x_2 + 0.07x_1x_3 \quad (R^2 = 0.91)$$

$$\hat{y}_{\mu_2}(x) = 0.46 + 0.13x_1 - 0.06x_2 + 0.05x_3 - 0.07x_1^2 - 0.04x_2^2 \quad (R^2 = 0.87)$$

$$\hat{y}_{\mu_3}(x) = 28.36 - 1.48x_1 + 2.33x_3 - 0.15x_1^2 - 1.42x_2^2 - 0.71x_1x_3 \quad (R^2 = 0.12)$$

### Objective:

Find  $x^*$  such that all  $y_1, y_2$  &  $y_3$  are simultaneously "optimized".



## CGA Study

### Fitted "Dispersion" Models

$$\hat{y}_{\sigma_1}(x) = 0.06 + 0.11x_2 + 0.06x_3 + 0.12x_1^2 + 0.11x_2^2 - 0.10x_1x_3 + 0.05x_2x_3 \quad (R^2 = 0.84)$$

$$\hat{y}_{\sigma_2}(x) = 0.02 - 0.01x_1 + 0.01x_2 - 0.01x_3 + 0.02x_1^2 - 0.01x_1x_3 + 0.02x_2x_3 \quad (R^2 = 0.83)$$

$$\hat{y}_{\sigma_3}(x) = 6.08 - 1.53x_1 + 0.50x_2 + 4.85x_3 + 2.26x_2^2 - 0.65x_1x_3 - 0.67x_1x_2x_3 \quad (R^2 = 0.95)$$

### Fitted "Location" Models

$$\hat{y}_{\mu_1}(x) = 4.95 + 0.82x_1 - 0.45x_2 - 0.15x_1^2 + 0.28x_2^2 - 0.11x_1x_2 + 0.07x_1x_3 \quad (R^2 = 0.91)$$

$$\hat{y}_{\mu_2}(x) = 0.46 + 0.13x_1 - 0.06x_2 + 0.05x_3 - 0.07x_1^2 - 0.04x_2^2 \quad (R^2 = 0.87)$$

$$\hat{y}_{\mu_3}(x) = 28.36 - 1.48x_1 + 2.33x_3 - 0.15x_1^2 - 1.42x_2^2 - 0.71x_1x_3 \quad (R^2 = 0.12)$$

### Objective:

Find  $x^*$  such that all  $y_1, y_2$  &  $y_3$  are simultaneously "optimized", when both location & dispersion responses are under concerned!



## MRS Optimization : Approaches

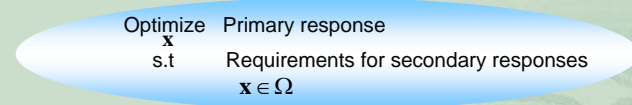
- Priority-based Approach
- Desirability Function Approach\*
- Generalized Distance Approach\*
- Loss Function Approach\*

\* dimensionality reduction strategy



## MRS Optimization : Priority – based Approach

- Primary response vs. Secondary responses
- Framework



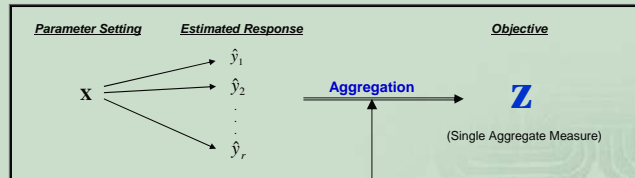
### Related Work

Hoerl (1959)  
Myers and Carter(1973)  
Biles (1975)  
Vining and Myers (1990)

Del Castillo and Montgomery (1993)  
Copeland and Nelson (1996)  
Semple (1997)  
Del Castillo, Fan, and Semple (1999)



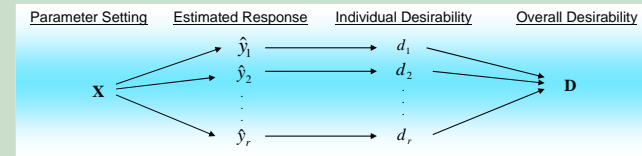
## Framework of Dimensionality Reduction Strategy



- Desirability Function Approach**  
 Harrington(1965), Derringer and Suich(1980), Derringer(1994), Del Castillo, Montgomery, and McCarville(1996), Kim and Lin(2000)
- Generalized Distance Approach**  
 Church(1978), Khuri and Conlon(1981)
- Loss Function Approach**  
 Pignatelli(1993), Reibeiro and Elsayed(1994), Ames et al.(1997), Lin and Tu(1995), Vining(1998)

## MRS Optimization : Desirability Function Approach

- Framework



- Find  $X^*$  to Maximize D

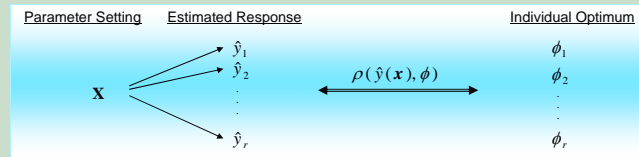
- Related work

Harrington (1965)  
 Derringer and Suich (1980)  
 Derringer (1994)  
 Goik, Liddy, and Taam (1994)

Kim and Lin (1998)  
 Kim and Lin (2000)  
 Del Castillo, Montgomery, and McCarville (1996)

## MRS Optimization : Generalized Distance Approach

- Framework



- $\rho(\hat{y}(x), \phi)$  = Distance between  $\hat{y}(x)$  and  $\phi$
- Find  $x^*$  to Minimize  $\rho(\hat{y}(x), \phi)$

- Related work

Church (1978)  
 Khuri and Conlon (1981)

## MRS Optimization : Generalized Distance Approach (cont'd)

- Khuri and Conlon (1981)

- Distance of Estimated Responses from Estimated "Ideal" Optimum

$$\rho[\hat{y}(x), \phi] = [(\hat{y}(x) - \phi)' \hat{\Sigma}^{-1} (\hat{y}(x) - \phi) / z'(x)(X'X)^{-1}z(x)]^{1/2},$$

where  $\phi = [\phi_1, \phi_2, \dots, \phi_r]$  is the ideal optimum,

$\hat{\Sigma}$  is the estimator of the common variance-covariance matrix of the random errors  $(\epsilon_1, \epsilon_2, \dots, \epsilon_r)$ ,

X is the design matrix, and

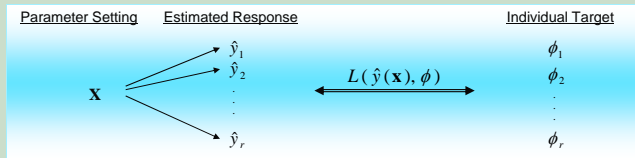
$z(x)$  is a column vector of the input variables of the given model.

- Assume All Response Functions

- Depend on the same set of input variables.
- Are of the same form.

## MRS Optimization : Loss Function Approach

### Framework



$L(\hat{y}(\mathbf{x}), \phi) = [\hat{y}(\mathbf{x}) - \phi]^T C [\hat{y}(\mathbf{x}) - \phi]$  (Multivariate squared error loss)

Find  $\mathbf{x}^*$  to minimize  $E(L)$

### Related Work

Pignatiello (1993)  
Ames et al. (1997)  
Vining (1998)

Ribeiro and Elsayed (1994)  
Lin and Tu (1995)



## Example : Colloidal Gas Aphrons (CGA) Study

- Characterization of CGA Properties (Jauregi et al. 1997)
- Responses : Stability ( $y_1$ , LTB), Volumetric Ratio ( $y_2$ , STB), Temperature ( $y_3$ , NTB)
- Input Variables : Concentration of Surfactant ( $x_1$ ), Concentration of Salt ( $x_2$ ), Time of Stirring ( $x_3$ )
- Design : CCD with 8 Factorial Points\*, 6 Axial Points\*, and a Center Point\*\*  
( \* Replicated twice, \*\* Replicated 6 times)



## Example : CGA Study (continued)

### Fitted "Location" Models

$$\hat{y}_{\mu_1}(x) = 4.95 + 0.82x_1 - 0.45x_2 - 0.15x_1^2 + 0.28x_2^2 - 0.11x_1x_2 + 0.07x_1x_3 \quad (R^2 = 0.91)$$

$$\hat{y}_{\mu_2}(x) = 0.46 + 0.13x_1 - 0.06x_2 + 0.05x_3 - 0.07x_1^2 - 0.04x_3^2 \quad (R^2 = 0.87)$$

$$\hat{y}_{\mu_3}(x) = 28.36 - 1.48x_1 + 2.33x_3 - 0.15x_1^2 - 1.42x_2^2 - 0.71x_1x_3 \quad (R^2 = 0.12)$$

### Linear Desirability Functions (for simplicity)

### Derringer and Suich (DS) Method :

$$\begin{aligned} &\text{Maximize} && \sqrt[3]{d_{\mu_1}(\hat{y}_{\mu_1})d_{\mu_2}(\hat{y}_{\mu_2})d_{\mu_3}(\hat{y}_{\mu_3})} \\ &\text{s.t} && -1 \leq x_i \leq 1 \quad (i = 1, 2, 3) \end{aligned}$$



## Example : CGA Study (continued)

	Responses		
	$y_1$	$y_2$	$y_3$
<b>Bounds and Target</b>			
$y_{\mu_j}^{\min}, \hat{y}_{\sigma_j}^{\min}$	3.00, <b>0.00</b>	0.10, <b>0.00</b>	15.00, <b>1.00</b>
$y_{\mu_j}^{\max}, \hat{y}_{\sigma_j}^{\max}$	7.00, <b>0.10</b>	0.60, <b>0.10</b>	45.00, <b>2.00</b>
$T_{\mu_j}, T_{\sigma_j}$	7.00, <b>0.00</b>	0.10, <b>0.00</b>	30.00, <b>1.00</b>
<b>Optimization Results</b>			
<b>DS Method</b>	$\mathbf{x}_{DS}^* = (-1.00, -1.00, -1.00)$		
$\hat{y}_{\mu_j}(\mathbf{x}_{DS}^*), \hat{y}_{\sigma_j}(\mathbf{x}_{DS}^*)$	4.66, <b>0.06</b>	0.24, <b>0.08</b>	25.38, <b>4.54</b>
$d_{\mu_j}(\hat{y}_{\mu_j}(\mathbf{x}_{DS}^*)), d_{\sigma_j}(\hat{y}_{\sigma_j}(\mathbf{x}_{DS}^*))$	0.41, <b>0.41</b>	0.72, <b>0.23</b>	0.69, <b>0.00</b>

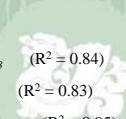
<sup>†</sup> The  $\hat{y}_{\sigma_j}$  and  $d_{\sigma_j}(\hat{y}_{\sigma_j})$  values for the standard deviation responses are computed *a posteriori* at the given  $\mathbf{x}_{DS}^*$ , and are written in italic.

### Fitted "Dispersion" Models

$$\hat{y}_{\sigma_1}(\mathbf{x}) = 0.06 + 0.11x_2 + 0.06x_3 + 0.12x_2^2 + 0.11x_3^2 - 0.10x_1x_3 + 0.05x_2x_3 \quad (R^2 = 0.84)$$

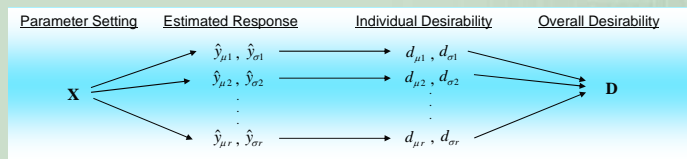
$$\hat{y}_{\sigma_2}(\mathbf{x}) = 0.02 - 0.01x_1 + 0.01x_2 - 0.01x_3 + 0.02x_2^2 - 0.01x_1x_3 + 0.02x_2x_3 \quad (R^2 = 0.83)$$

$$\hat{y}_{\sigma_3}(\mathbf{x}) = 6.08 - 1.53x_1 + 0.50x_2 + 4.85x_3 + 2.26x_2^2 - 0.65x_1x_3 - 0.67x_1x_2x_3 \quad (R^2 = 0.95)$$



## Proposed Approach\* : Framework

- Consideration of Both Location and Dispersion Effects
- “Maximizing” Desirability Functions
- Framework



$D = \text{Minimum} \{d_{\mu 1}, \dots, d_{\mu r}, d_{\sigma 1}, \dots, d_{\sigma r}\}$  → Find  $X^*$  to Maximize  $D$ .

\* Co-work with Kwang-Jae Kim

## Proposed Approach : Formulation

$$\begin{aligned} & \text{Maximize}_x \lambda \\ & \text{subject to } d_{\mu_j}(\hat{y}_{\mu_j}(\mathbf{x})) \geq \lambda, \quad j = 1, 2, \dots, r, \\ & \quad \quad \quad d_{\sigma_j}(\hat{y}_{\sigma_j}(\mathbf{x})) \geq \lambda, \quad j = 1, 2, \dots, r, \\ & \quad \quad \quad \mathbf{x} \in \Omega. \end{aligned}$$

## Example : CGA Study - Revisited

	Responses		
	$y_1$	$y_2$	$y_3$
<b>Bounds and Target</b>			
$y_{\mu_j}^{\min}, y_{\sigma_j}^{\min}$	3.00, <b>0.00</b>	0.10, <b>0.00</b>	15.00, <b>1.00</b>
$y_{\mu_j}^{\max}, y_{\sigma_j}^{\max}$	7.00, <b>0.10</b>	0.60, <b>0.10</b>	45.00, <b>2.00</b>
$T_{\mu_j}, T_{\sigma_j}$	7.00, <b>0.00</b>	0.10, <b>0.00</b>	30.00, <b>1.00</b>
<b>Optimization Results</b>			
DS Method	$x_{DS}^* = (-1.00, -1.00, -1.00)$		
$\hat{y}_{\mu_j}(x_{DS}^*), \hat{y}_{\sigma_j}(x_{DS}^*)$	4.66, <b>0.06</b>	0.24, <b>0.08</b>	25.38, <b>4.54</b>
$d_{\mu_j}(\hat{y}_{\mu_j}(x_{DS}^*)), d_{\sigma_j}(\hat{y}_{\sigma_j}(x_{DS}^*))$	0.41, <b>0.41</b>	0.72, <b>0.23</b>	0.69, <b>0.00</b>
Proposed Method	$x_p^* = (-0.21, -0.40, -1.00)$		
$\hat{y}_{\mu_j}(x_p^*), \hat{y}_{\sigma_j}(x_p^*)$	5.00, <b>0.06</b>	0.37, <b>0.05</b>	25.96, <b>1.64</b>
$d_{\mu_j}(\hat{y}_{\mu_j}(x_p^*)), d_{\sigma_j}(\hat{y}_{\sigma_j}(x_p^*))$	0.50, <b>0.36</b>	0.45, <b>0.50</b>	0.73, <b>0.36</b>

<sup>†</sup> The  $\hat{y}_{\sigma_j}$  and  $d_{\sigma_j}(\hat{y}_{\sigma_j})$  values for the standard deviation responses are computed *a posteriori* at the given  $x_{DS}^*$ , and are written in *italic*.

## Proposed Approach : General Properties

- Advantages
  - ☞ Good Balance among Responses on Both Location and Dispersion Effects
  - ☞ Robust to Potential Dependencies among Responses
  - ☞ Physical Interpretation of  $\lambda$
- Disadvantages
  - ☞ Unreasonable Solutions Possible
    - e.g. Let  $\mathbf{d} = (d_{\mu 1}, d_{\mu 2}, d_{\sigma 1}, d_{\sigma 2})$
    - $\mathbf{d}_1 = (0.5, 0.5, 0.5, 0.5)$  vs.  $\mathbf{d}_2 = (0.99, 0.99, 0.99, 0.49)$
    - $\mathbf{d}_1 = (0.5, 0.5, 0.5, 0.5)$  vs.  $\mathbf{d}_3 = (0.99, 0.99, 0.99, 0.50)$
  - ☞ Costs for Required Replication

## Micro-Array Design (SS Young)

- How do you pick the sequences that you are going to use.
  - ☞ They have to be unique vs other sub-sequences and they have to work at common temperature/chemical fluid concentrations.
- Placement of sub sequences on the chip and the number of rep spots.
- A no-no is possible reuse of chips. How to wash would be a good DOE problem.
  - ☞ Technically I think the chips can be reused, but contract requires only one use.
- There is very large variation in response among the sub-sequences within a gene. Does this relate to the sequence in some way?
  - ☞ If so, it would be of interest to try to figure out the factors influencing the among sub-sequence variation. So the question would be DOE on the selection of the subsequence and then DOE on the assay conditions.

## Where have all the Data gone?

- No need for data (Theoretical Development)
- Survey Sampling and Design of Experiment (Physical data collection)
- Computer Simulation (Experiment)
  - ☞ Statistical Simulation (Random Number generation)
  - ☞ Engineering Simulation
- Data from Internet
  - ☞ On-line auction
  - ☞ Search Engine

**STILL  
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## Send \$500 to

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