Supersaturated Design:

A Review and Some Research Potentials

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Screening: What for???

- Factor
- Group of Factors (Team)
- Methods
- Parameters (x_i/x_j vs $\beta_i/\beta_i/\beta_{ij}/\beta_i^2/\beta_j^2$)
- Graduate Students (Screening Exam)
- Faculty (Tenure Review)
- ...

Model Screening

- Given $f_i \in$ F

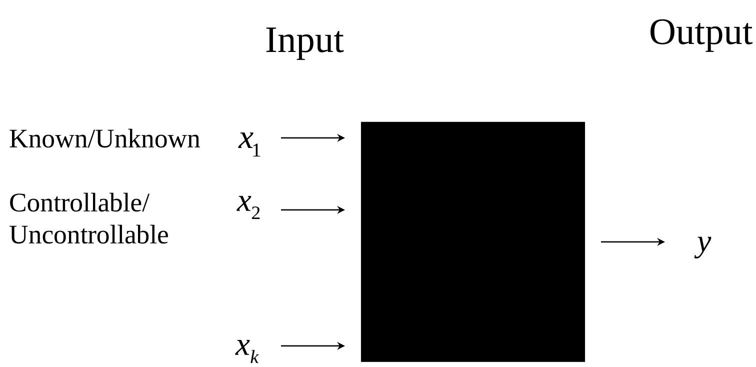
$$y=f_i(x)+\varepsilon$$

- Find $i=i^*$, such that

$$y=f_{i^*}(x)+\varepsilon$$

Which is most "appropriate".

Factor Screening



$$y = f(x_1, \ldots x_i, x_{i+1}, \ldots x_k) + \varepsilon$$

Situations: Good for Factor Screening

- Blood Tests
- Pareto Analysis
- Genetic Study
- Industrial Investigations
- Other Scientific Investigations
  - Physics, Chemistry, Biology
  - Human Resource, Business study etc.
- Others

Situations: Not Good for Factor Screening

Artificial Neural Network (ANN)
Drug Discovery
Others

First-Order Screening: Saturated Design

Lin (Handbook of Statistics, 2003)

- 2^{k-p} //R=III Design
- Plackett & Burman Design
- Optimal Design
- p-efficient Design
- Simplex Design
- T-optimal Design
- Uniform Design

Table 7
A summarized comparison on selected screening designs

Section	Design	Run	Level	Remarks
2.0	2_{III}^{k-p}	2^r	2	Orthogonal & symmetry
2.1	P&B	4t	2	Orthogonal & symmetry
2.2	Optimal	any	many	Nonorthogonal & asymmetry
2.3	p-eff	$k+1$	2	Nonorthogonal & symmetry
2.4	Simplex	$k+1$	many	Orthogonal & asymmetry
2.5	T-opt	$k+1$	many	Orthogonal & symmetry
2.6	Uniform	any	any	Symmetry

From Saturated
to
Supersaturated

No degree of freedom for σ
to
Negative degree of freedom for σ

Recent Applications in SSD

- (Nano-) Manufacturing
- Computer Experiments
- Numerical Analysis
- e-Business
- Marketing

Recent Advances in SSD

- Data Analysis Method:
  Panelized Least Squares
  (Li and Lin, 2003)
- Criterion:
  D-optimal Supersaturated Design
  (Nachtsheim, Jones and Lin, 2006, JSPI)
  Search Probability of Correct Identification
  (Shirakura, Takahashi and Srivastava, 1996)
- Construction:
  Combinatorial Approach
  (Fang, Ge and Liu, 2002 & 2004)

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*

Supersaturated Design —how to study *k* parameters with *n(<<k)* observations?

•*What for ?*

• *How to construct ?*

• *How to analyze ?*

• *Limitations ?*

• *Does it really work ?*

Life After Screening

- Follow-Up Experiment
- Projection Properties

A New Class of Supersaturated Designs

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Supersaturated designs are useful in situations in which the number of active factors is very small compared to the total number of factors being considered. In this article, a new class of supersaturated designs is constructed using half fractions of Hadamard matrices. When a Hadamard matrix of order N is used, such a design can investigate up to $N - 2$ factors in $N/2$ runs. Results are given for $N \leq 60$. Extension to larger N is straightforward. These designs are superior to other existing supersaturated designs and are easy to construct. An example with real data is used to illustrate the ideas.

KEY WORDS: Hadamard matrices; Plackett and Burman designs; Random balance designs.

UTK Technical Report, 1991

Most Popular Title

Optimal XYZ Supersaturated Designs

***XYZ* =**

- $E(s^2)$
- Weighing
- $E(f_{NOD})$
- Bayesian
- Minimum Moment Aberration
- Large
- Three-Level
- *s*-Level
- Multi-Level
- Discrepancy
- Uniform
- Cyclic BIBD
- k-circutant

Which Journals They Appeared?

- *Biometrika*
- *JRSS-B*
- *Statistical Science*
- *Annals of Statistics*
- *Communications in Statistics*
- *Journal of Statistical Planning & Inference*
- *Statistica Sinica*
- *Stat & Prob Letters*
- *Canadian Journal of Statistics*
- *Computational Statistics & Data Analysis*
- *Technometrics*
- *Journal of Quality Technology*
- *Quality and Reliability Engieerning, International*
- *Journal of Statistical Computation & Simulations*
- *Chinese Annals of Mathematics*
- *Metrika*
- *Discrete Mathematics*
- *Sceince in China*

In Random Order

Which Journals They Appeared?

- *Analytics Chimica Acta*
- *Trac-Trends in Analytical Chemistry*
- *Journal of AOAC International*
- *Journal of Analytical Atomic Spectrometry*
- *Journal of Environmental Monitoring*
- *Chemometrics & Intelligent Lab Systems*
- *Analytical Chemistry*
- *Journal of Pharmaceutical & Biomedical Analysis*
- *Computers & Industrial Engineering*

Supersaturated Design Example

Half Fraction of William's (1968) Data

	Factor																								
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

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

$\updownarrow$

Balanced Incomplete Block Design

$$\begin{aligned} \upsilon &= 2t - 1 \\ b &= 4t - 2 \\ \gamma &= 2t - 2 \\ k &= t - 2 \end{aligned}$$

Hedayat & Wallis (1978)

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

Half Fraction Hadamard Matrix

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

$\updownarrow$

Coding

Binary Code

length	$n = 2t$
weight	$\omega = t$
distance	d

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

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

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

$$H_{n\times n} = \begin{bmatrix} 1 & 1 & H_1 \\ 1 & -1 & H_2 \end{bmatrix}_{n\times n}$$

H_1 and H_2 are isormophic?
$(n-2)\times n/2$

Lin (1991)

$$X = \left[H_m, \quad H_{Int}\right]$$

H_m : Hadamard Matrix N

H_{Int} : Interaction Columns $\binom{N}{2}$

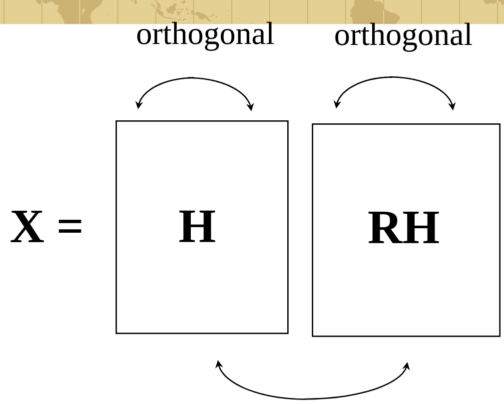
Wu (1993)

Table 34.1 Assignment Array

Class / Factor / Column — Experiment No.	Group I							Group II			
	A	B	C	D	E	F	G	H	J	L	M
	(9)	(10)	(12)	(13)	(5)	(1)	(2)	(3)	(5)	(1)	(2)
1—3	1	1	1	1	1	1	1	1	3	1	1
2—4	2	2	2	2	2	1	1	2	1	1	2
3—15	3	3	3	3	3	1	1	3	3	2	2
4—10	2	2	3	3	1	1	2	2	1	2	1
5—7	3	3	1	1	2	1	2	3	1	1	3
6—22	1	1	2	2	3	1	2	1	1	3	2
7—5	3	3	2	2	1	1	3	2	2	1	2
8—2	1	1	3	3	2	1	3	1	2	1	1
9—19	2	2	1	1	3	1	3	3	1	3	1
10—9	2	3	2	3	1	2	1	3	3	1	3
11—17	3	1	3	1	2	2	1	1	2	2	3
12—27	1	2	1	2	3	2	1	2	3	3	3
13—26	3	1	1	2	1	2	2	2	2	3	3
14—24	1	2	2	3	2	2	2	1	3	3	2
15—8	2	3	3	1	3	2	2	3	2	1	3
16—12	1	2	3	1	1	2	3	2	3	2	1
17—23	2	3	1	2	2	2	3	1	2	3	2
18—21	3	1	2	3	3	2	3	3	3	3	1
19—14	3	2	3	2	1	3	1	3	2	2	2
20—1	1	3	1	3	2	3	1	1	1	1	1
21—11	2	1	2	1	3	3	1	2	2	2	1
22—25	1	3	2	1	1	3	2	2	1	3	3
23—18	2	1	3	2	2	3	2	1	3	2	3
24—13	3	2	1	3	3	3	2	3	1	2	2
25—16	2	1	1	3	1	3	3	1	1	2	3
26—6	3	2	2	1	2	3	3	2	3	1	2
27—20	1	3	3	2	3	3	3	3	2	3	1

Random
Balance
Design

Taguchi (1986)



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

$X = [H \quad RHC]$

↑ matrix for column selection to get rid of fully aliased columns

EXAMPLES:

(1) R = D(h_i) product — Wu (1993)

(2) R = P permute — Tang & Wu (1993)

(3) R = PD(h_i)

(4) R = $\frac{1}{n} H a H'$

↑ nonequivalent Hadamard mx

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)
- Fang, Lin and Liu (2002):

Recent Design Criteria

Supersaturated Design

- Uniformity
- Generalized Minimum Aberration
- Majorization
- E(f_{NOD})
- Projection Properties (D_f, A_f, G_f, etc)
- E(χ^2), as an extension of E(s^2)
- Minimax s_{ij}
- Model Robustness

Recent Design Criteria

Supersaturated Design

- Minimum Moment Aberration
- E(d_2)
- G_2-Aberration
- Asymptotic Power Properties
- Orthogonal-Based
- Factor-Covering
- Marginally Over-saturated

Example: $E(f_{NOD})$

$$E(f_{NOD}) = \sum_{1 \le i < j \le m} f_{NOD}^{ij} \Big/ \binom{m}{2}$$

where $$f_{NOD}^{ij} = \sum_{u=1}^{q_i} \sum_{v=1}^{q_j} \left(n_{uv}^{(ij)} - \frac{n}{q_i q_j} \right)^2$$

Lower Bound of $E(f_{NOD})$

Theorem 1. *For any design* $\boldsymbol{X} \in \mathscr{U}(n; q_1, \ldots, q_m)$,

$$\begin{aligned} E(f_{NOD}) &= \frac{\sum_{k,l=1,k\neq l}^{n} \lambda_{kl}^2}{m(m-1)} + C(n, q_1, \ldots, q_m) \\ &\ge \frac{n(\sum_{j=1}^{m} n/q_j - m)^2}{m(m-1)(n-1)} + C(n, q_1, \ldots, q_m), \end{aligned}$$

where $C(n, q_1, \ldots, q_m) = \frac{nm}{m-1} - \frac{1}{m(m-1)} \left(\sum_{i=1}^{m} \frac{n^2}{q_i} + \sum_{i,j=1,j\neq i}^{m} \frac{n^2}{q_i q_j} \right)$

Connection with Previous Criteria

Corollary 1. *For any design* $\boldsymbol{X} \in \mathcal{U}(n; q^m)$,

$$E(f_{NOD}) \geq \frac{mn}{(m-1)(n-1)}\left(\frac{n}{q}-1\right)^2 + \frac{n}{m-1}\left(m-\frac{n}{q}\right) - \left(\frac{n}{q}\right)^2,$$

$$E(f_{NOD}) = \frac{n}{9}\text{ave } \chi^2, \ \text{when } q_i = 3$$

$$E(f_{NOD}) = \frac{1}{4}E(s^2), \ \text{when } q_i = 2,$$

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

Data Analysis Methods

Supersaturated Design

- *Satterthwaite (1959)*
- *Lin (1993): Forward Selection*
- *Westfall, Young and Lin (1998): Adjusted p-value*
- *Chen and Lin (1998): Identifiability*
- *Ryan and Lin (1997): Half Effect*
- *Contrasts-Based*
- *Staged Dimension Reduction*
- *Ye (1995): Generalized degree of freedom*

Design Analysis: Advances

Supersaturated Design

- *Sequential Analysis*
- *All Subsets Models*
- *Adjusted p-value*
  (Westfall, Young & Lin, Statistica Sinica, 1998)
- *Bayesian Approach*
  (Beattie, Fong & Lin, Technometrics, 2002)
- *Penalized Least Squares*
  (Li & Lin, 2002)

Algorithmic

Supersaturated Design

Lin (1991, 1995): Pair-wise Optimality

Nguyen (1996): Exchange Algorithm

Li and Wu (1997): Column-wise and Pair-wise Algorithm

Church (1993): Projection Properties

Jones (2000): JMP Product

Other Construction Methods

Table 1. Supersaturated designs derived from $L_{16}(4^5)$ (using **1** as the branching column)

$S(12;3^1 4^4)$	$S(8;2^1 4^4)$	Row	**1**	**2**	**3**	**4**	**5**
1		1	1	1	1	1	1
2		2	1	2	2	2	2
3		3	1	3	3	3	3
4		4	1	4	4	4	4
5	1	5	2	1	2	3	4
6	2	6	2	2	1	4	3
7	3	7	2	3	4	1	2
8	4	8	2	4	3	2	1
	5	9	3	1	3	4	2
	6	10	3	2	4	3	1
	7	11	3	3	1	2	4
	8	12	3	4	2	1	3
9		13	4	1	4	2	3
10		14	4	2	3	1	4
11		15	4	3	2	4	1
12		16	4	4	1	3	2

UD OD SSD

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

Fang, Lin & Ma (2000)

k-circulant Supersaturated Designs

Liu and Dean

Technometrics, 2004

Recent Advances in SSD

- Data Analysis Method:
  Panelized Least Squares
  (Li and Lin, 2003)
- Criterion:
  Search Probability of Correct Identification
  (Shirakura, Takahashi and Srivastava, 1996)
- Construction:
  Combinatorial Approach
  (Fang, Ge and Liu, 2002 & 2004)

Penalized Least Squares *(Li and Lin, 2003)*

Model

$$Y_i = \mathbf{x}_i^T \beta + \varepsilon_i$$

Penalized Likelihood (Fan and Li, 1999)

$$\frac{1}{n}\sum_{i=1}^{n} \log f(y_i, \mathbf{x}_i^T\beta) - \sum_{j=1}^{d} p_\lambda(|\beta_j|)$$

Becomes

$$Q(\beta) \equiv \frac{1}{2n}\sum_{i=1}^{n}(Y_i - \mathbf{x}_i^T\beta)^2 + \sum_{j=1}^{d} p_\lambda(|\beta_j|)$$

Choices of p_λ

$$Q(\beta) \equiv \frac{1}{2n}\sum_{i=1}^{n}(Y_i - \mathbf{x}_i^T\beta)^2 + \sum_{j=1}^{d} p_\lambda(|\beta_j|)$$

- L_1 penalty *(Donoho and Johnstone, 1994)*

$$p_\lambda(|\beta|) = \lambda|\beta|$$

- L_2 penalty & L_q penalty (Frank and Friedman, 1993)

$$p_\lambda(|\beta|) = \lambda\frac{|\beta|^2}{2}$$

- Hard Thresholding penalty

$$p_\lambda(|\beta|) = \lambda^2 - (|\beta| - \lambda)^2 I(|\beta| < \lambda)$$

Choices of p_λ

$$Q(\boldsymbol{\beta}) \equiv \frac{1}{2n}\sum_{i=1}^{n}(Y_i - \mathbf{x}_i^T\boldsymbol{\beta})^2 + \sum_{j=1}^{d} p_\lambda(|\beta_j|)$$

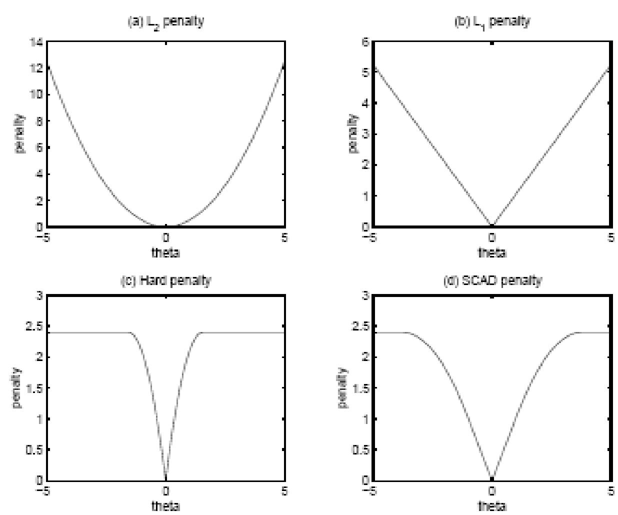
- SCAD (*Smoothly Clipped Absolute Deviation*, Fan, 1997)

$$p'_\lambda(\beta) = \lambda\left\{I(\beta \le \lambda) + \frac{(a\lambda - \beta)_+}{(a-1)\lambda} I(\beta > \lambda)\right\}$$

- λ is to be estimated (e.g., via GCV of Wahba, 1977)

$$\mathrm{GCV}(\lambda) = \frac{1}{n}\frac{\|\mathbf{y} - \mathbf{X}\widehat{\boldsymbol{\beta}}(\lambda)\|^2}{\{1 - e(\lambda)/n\}^2}$$

and $\widehat{\lambda} = \mathrm{argmin}_\lambda\{\mathrm{GCV}(\lambda)\}$



Various Examples: Real-life & Simulative

Li and Lin (2001)

Supersaturated Designs with High Searching Probability *(Chatterjee, Bhavana and Lin, 2006)*

$$\mathbf{y} = 1\mu + T_1(\zeta_0)\zeta_0 + \epsilon, \qquad V(\epsilon) = \sigma^2 I$$

Theorem

For any $\zeta_0 \subset \xi_2$ and $\zeta (\neq \zeta_0)$, we have

$$P(h(\zeta_0, \mathbf{y}) > h(\zeta, \mathbf{y})) = G_d(x, \rho)$$
$$= 1 - \Phi_d(\rho\sqrt{(n-x)/2}\,) - \Phi_d(\rho\sqrt{(n+x)/2}\,) + 2\Phi_d(\rho\sqrt{(n-x)/2}\,)\Phi_d(\rho\sqrt{(n+x)/2}\,)$$

where $x = t(\zeta_0)'t(\zeta)$, $\rho = \zeta_0/\sigma$ and Φ is the distribution function of $N(0,1)$.

Supersaturated Designs with High Searching Probability

(Chatterjee, Bhavana and Lin, 2006)

Searching Probabilities for Selected SSD

n	m	ρ = 1	1.2	1.4	1.6	1.8	2	Reference
6	10	0.9022	0.9477	0.9737	0.9875	0.9944	0.9976	L&D (2004)
8	21	0.9153	0.9537	0.9759	0.9881	0.9945	0.9977	L&D (2004)
10	15	0.9194	0.9548	0.9761	0.9882	0.9945	0.9977	B&C (2004)
12	16	0.975	0.9915	0.9974	0.9993	0.9998	0.9999	B&C (1962)
12	22	0.9207	0.9551	0.9761	0.9882	0.9945	0.9977	Lin(1993)
12	24	0.9207	0.9551	0.9761	0.9882	0.9945	0.9977	B&C (1962)
12	66	0.975	0.9915	0.9974	0.9993	0.9998	0.9999	Lin (1995)
14	19	0.9765	0.9917	0.9974	0.9993	0.9998	0.9999	B&C (2004)

Supersaturated Design via Combinatorial Construction

Fang, Ge and Liu, 2002 & 2004

- Constructing symmetrical SSDs from

  a. Resolvable balanced incomplete block designs, see Fang, Ge and Liu (2002b), Fang, Ge, Liu and Qin (2003);

  b. Room squares, see Fang, Ge and Liu (2002a);

  c. Resolvable packings and coverings, see Fang, Ge and Liu (2004) and Fang, Lu, Tang and Yin (2004);

  d. Super-simple resolvable t-designs, see Fang, Ge, Liu and Qin (2004b).

Summary: Combinatorial Construction

- The combinatorial approaches can be regarded as extensions of the methods of Nguyen (1996) and Liu and Zhang (2000) for 2-level SSDs.
- For $\lambda \geq 2$, the properties of the resulting optimal SSDs need further studies.
- How to construct optimal SSDs when $\lambda_{kl} = \lambda$ for all $k \neq l$ can not be satisfied?
- Data-analysis procedures and modelling methods for these SSDs need to be investigated.

SSD: Looking Ahead

There will be more and more factors & parameters in the future experimental investigations!!!

SSD: Looking Ahead

Supersaturated Design

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

Thanks Sue Lewis & Dave Woods and the Organization Committee for your kind invitation

Thanks also for those helped me in the past (and perhaps the future).

Send $500 to

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