Design for Order-of-Addition Experiments

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Design of Experiment

How to collect Useful Information?

Design of Experiment

Analyzing historical data is like listening to a lecture
Running a designed experiment is like conducting an interview

Randomization in Theory vs. Randomization in Reality

R.A. Fisher (1920)

Rao

How Should the Data be collected?

Randomly

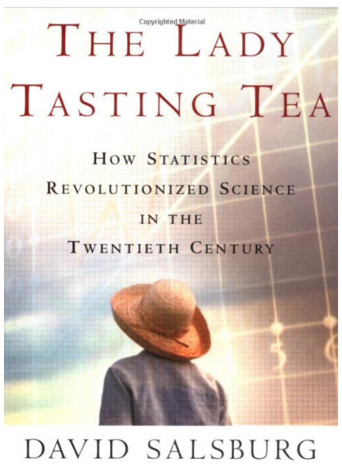
or

Systematically

Some Lin recent design projects

- Computer Experiment—LHC & UD
- Order of Addition Experiment
- Run Order Consideration
- t-covering array
- Design for On-Line Experiment
- New Type of Composite Design
- Fake Factors for estimate σ^2
- Meta-Analysis

Lady and Tea Tasting (Fisher)



UK

Milk → *Tea* or
Tea → *Milk*

Three-Cup Chicken

China

Three Cups：

酱油 **Soy Sauce**

米酒 **Wine**

麻油 **Sesame Oil**

Which first? Which last? Does it matter?

There are m! possible combinations, how could we run fraction of them?

1→2
2→1

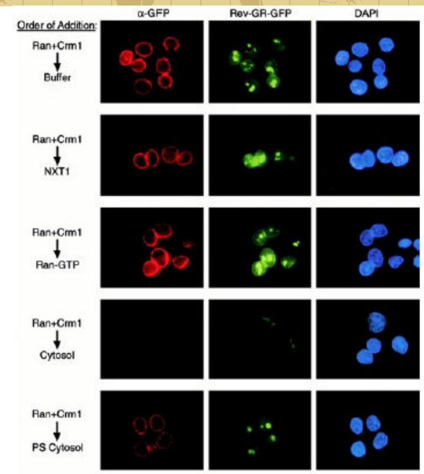
1→2→3
1→3→2
2→1→3
2→3→1
3→1→2
3→2→1

1234	1243	1423	4123
1324	1342	1432	4123
2134	2143	2413	4213
2314	2341	2431	4231
3124	3142	3412	4312
3214	3241	3421	4321

Order of addition (OofA) experiment:

the requirement for Ran, Crm1 and NXT1, etc

Journal of Cell Biology (2001)
—m is about 10.



- For three components, there are 3!=6 possible "treatments" to be tested.

$1 \to 2 \to 3$
$1 \to 3 \to 2$
$2 \to 1 \to 3$
$2 \to 3 \to 1$
$3 \to 1 \to 2$
$3 \to 2 \to 1$

- In general, there are m! treatments to be tested.
- for example, 10!=3,638,800.
  This may not be feasible.

OofA in Gnetics Areas

- The construction of phylogenetic trees depends on the order of taxa
- Many taxa (more than 10) are involved…
- Often, a set of random orders are tested (Olsen et al. 1994, Stewart et al. 2001)
- How to choose a subset of the orders?
  Randomly or systematically???

OofA in Different Areas

- Food science: Fuleki and Francis(1968)
- Bio-chemistry Science: Shinohara & Ogawa (1998)
- Food science: Jourdain et al. (2009)
- Nutritional science: Karim et al. (2000)
- Pharmaceutical science: Rajaonarivony et al. (1993)

Experiments are needed to find the optimal addition order!

Research Issues

How to run (small) n,
among those m! experiments,
to find out the "optimal"
sequence/order-of-addition (OofA)?

Note: 10!=3,628,800

Linking to conventional design…

- What are the experimental variables (X_i's)?
- What is the experimental unit?

Order-of-Addition Experiment

Outline

- Introduction (baby optimal design)
- Model Formulation (PWO)
- Optimality of the Full PWO Design
- orthogonality of a PWO Design
- Minimal-point PWO Design
- Optimal Fractional PWO Design
- Conclusion and Future Work

Brief on Optimal Design

Matrix Form

$$y_i = \beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i} + \ldots + \beta_k x_k + \varepsilon_i$$
$$i = 1, 2, \ldots, n$$

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} 1 & x_{11} & x_{21} & \cdots & x_{k1} \\ 1 & x_{12} & x_{22} & \cdots & x_{k2} \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & x_{1n} & x_{2n} & \cdots & x_{kn} \end{bmatrix} \cdot \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_k \end{bmatrix} + \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{bmatrix}$$

or $\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$

Estimation

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}$$

LSE / MLE under i.i.d. Normal

$$Var(\hat{\boldsymbol{\beta}}) = (\mathbf{X}'\mathbf{X})^{-1} \cdot \boldsymbol{\sigma}^2$$

Assuming (say) $\varepsilon_i \sim N(0, \sigma^2)$ *i.i.d*

Design Issue:
Now, suppose you have full control on the X matrix…

Choose **X** such that (**X'X**)$^{-1}$ is minimized—or **X'X** is maximized (in some senses).

Optimal Design—General Setting

- Given the model *y=f(x)+ε*,
- find its information matrix **I**,

The Optimal Design **X** is the design which "maximizes" the information matrix **I**.

- For Linear Model *y=Xβ+ε*,

the information matrix is **I=X'X**.

Optimality Theorem

the full PWO design is optimal under:

- D-criterion $= \arg\max\,[\det(\mathbf{M})]^{1/p}$, $p = \binom{m}{2} + 1$
- A-criterion $= \arg\min\,\mathrm{tr}\,(\mathbf{M}^{-1})$
- E-criterion $= \arg\max\,\lambda_{\min}\,(\mathbf{M})$
- $M.S.$-criterion $= \arg\min\,\mathrm{tr}\,(\mathbf{M}^{2})$

where, **M** *=Information Matrix*

Continuous Version

General estimator:

$$\hat{\theta}_{\zeta} = \int y(\mathbf{x})\zeta(d\mathbf{x}),$$

where $\zeta(d\mathbf{x})$ is a signed vector-measure.

$$\widehat{\theta}_{OLSE} = \int y(\mathbf{x}) M^{-1}(\xi) f(\mathbf{x})\xi(d\mathbf{x}),$$

where

$$M(\xi) = \int f(\mathbf{x}) f^{T}(\mathbf{x})\xi(d\mathbf{x}),$$

and $\xi(d\mathbf{x})$ is a design (probability measure for OLSE; a signed measure for SLSE). The covariance matrix of $\widehat{\theta}_{OLSE}$ is

$$\mathrm{Var}(\widehat{\theta}_{OLSE}) = \mathbf{M}(\xi)^{-1}\left[\int\int K(\mathbf{x},\mathbf{z})\mathbf{f}(\mathbf{x})\mathbf{f}^{T}(\mathbf{z})\xi(d\mathbf{x})\xi(d\mathbf{z})\right]\mathbf{M}(\xi)^{-1}$$

Model Formulation

for Order-of-Addition Experiment

Pairwise-order (PWO) model

Van Nostrand (1995)

- Suppose there are m components to be added, denoted by $1,2,\ldots,m$
- For any order $\boldsymbol{a}$ and $1 \le j < k \le m$, define the PWO factor

$$z_{jk}(\boldsymbol{a}) = \begin{cases} 1 & \text{if } j \text{ precedes } k \text{ in } \boldsymbol{a}, \\ -1 & \text{if } k \text{ precedes } j \text{ in } \boldsymbol{a}. \end{cases}$$

For example, $\boldsymbol{a}$=312 implies

$$z_{12} = +1,\; z_{13} = -1,\; and\; z_{23} = -1$$

Problem Formulation *(m=3 example)*

Sequence	$I_{1\to2}$	$I_{1\to3}$	$I_{2\to3}$
1 2 3	+	+	+
1 3 2	+	+	−
2 1 3	−	+	+
2 3 1	−	−	+
3 1 2	+	−	−
3 2 1	−	−	−

Model $y = M + \beta_{1,2}I_{1,2} + \beta_{1,3}I_{1,3} + \beta_{2,3}I_{2,3} + \varepsilon$

Test $H_0: \beta_{i,j} = 0$

PWO model

- For any order $\boldsymbol{a}$ affects the response via the Pairwise-order (PWO) effect

$$\tau(\boldsymbol{a}) = \beta_0 + \sum_{1\le j<k\le m} z_{jk}(\boldsymbol{a})\beta_{jk},$$

$\tau(\boldsymbol{a})$: expected response arising from $\boldsymbol{a}$

β_{jk}'s: linear coefficients to estimate

- With m components,

  there are $\binom{m}{2}$ PWO factors.

Research Issues

How to run (small) *n* among *m*! many experiments to test all $\binom{m}{2}$ pairwise order?

$$H_0: \beta_{i,j} = 0\ ?$$

Full PWO Design

- PWO design: $[z_{jk}(\boldsymbol{a}_i)]_{jk}$
- Full PWO design ($\mathbf{Z}_f$): representing all the permutations

Sequence	$I_{1\to2}$	$I_{1\to3}$	$I_{2\to3}$
1 2 3	+	+	+
1 3 2	+	+	−
2 1 3	−	+	+
2 3 1	−	−	+
3 1 2	+	−	−
3 2 1	−	−	−

As compared with 2^3 Full Factorial design, the treatment $(+-+)$ and $(-+-)$ are not feasible.

m=4

Index	Order	Pair-wise ordering factors $I_{1\to2}$	$I_{1\to3}$	$I_{2\to3}$	$I_{1\to4}$	$I_{2\to4}$	$I_{3\to4}$
1234	$1\to2\to3\to4$	1	1	1	1	1	1
2134	$2\to1\to3\to4$	−1	1	1	1	1	1
1324	$1\to3\to2\to4$	1	1	−1	1	1	1
2314	$2\to3\to1\to4$	−1	−1	1	1	1	1
3124	$3\to1\to2\to4$	1	−1	−1	1	1	1
3214	$3\to2\to1\to4$	−1	−1	−1	1	1	1
1243	$1\to2\to4\to3$	1	1	1	1	1	−1
2143	$2\to1\to4\to3$	−1	1	1	1	1	−1
1342	$1\to3\to4\to2$	1	1	−1	1	−1	1
2341	$2\to3\to4\to1$	−1	−1	1	−1	1	1
3142	$3\to1\to4\to2$	1	−1	−1	1	−1	1
3241	$3\to2\to4\to1$	−1	−1	−1	−1	1	1
1423	$1\to4\to2\to3$	1	1	1	1	−1	−1
2413	$2\to4\to1\to3$	−1	1	1	−1	1	−1
1432	$1\to4\to3\to2$	1	1	−1	1	−1	−1
2431	$2\to4\to3\to1$	−1	−1	1	−1	1	−1
3412	$3\to4\to1\to2$	1	−1	−1	−1	−1	1
3421	$3\to4\to2\to1$	−1	−1	−1	−1	−1	1
4123	$4\to1\to2\to3$	1	1	1	−1	−1	−1
4213	$4\to2\to1\to3$	−1	1	1	−1	−1	−1
4132	$4\to1\to3\to2$	1	1	−1	−1	−1	−1
4231	$4\to2\to3\to1$	−1	−1	1	−1	−1	−1
4312	$4\to3\to1\to2$	1	−1	−1	−1	−1	−1
4321	$4\to3\to2\to1$	−1	−1	−1	−1	−1	−1

Information matrix of PWO Design

The moment matrix (information matrix) of full PWO design:
$\mathbf{M}_f = \mathbf{X}_f^T\mathbf{X}_f/N$, with $\mathbf{X}_f = [\mathbf{1}, \mathbf{Z}_f]$ and $N = m!$

for $m = 4$, $\mathbf{M}_f = \text{diag}(1, \widetilde{\mathbf{M}}_f)$ and

$$\widetilde{\mathbf{M}}_f = \begin{bmatrix} 1 & 1/3 & 1/3 & -1/3 & -1/3 & 0 \\ 1/3 & 1 & 1/3 & 1/3 & 0 & -1/3 \\ 1/3 & 1/3 & 1 & 0 & 1/3 & 1/3 \\ -1/3 & 1/3 & 0 & 1 & 1/3 & -1/3 \\ -1/3 & 0 & 1/3 & 1/3 & 1 & 1/3 \\ 0 & -1/3 & 1/3 & -1/3 & 1/3 & 1 \end{bmatrix}$$

Main Challenge

- The moment matrix is complicated

$$\begin{bmatrix} 1 & 1/3 & 1/3 & -1/3 & -1/3 & 0 \\ 1/3 & 1 & 1/3 & 1/3 & 0 & -1/3 \\ 1/3 & 1/3 & 1 & 0 & 1/3 & 1/3 \\ -1/3 & 1/3 & 0 & 1 & 1/3 & -1/3 \\ -1/3 & 0 & 1/3 & 1/3 & 1 & 1/3 \\ 0 & -1/3 & 1/3 & -1/3 & 1/3 & 1 \end{bmatrix}$$

- The PWO design region is irregular, due to the transitive property
  - If $z_{jk} = +$ and $z_{kl} = +$ then z_{jl} must be $+$.
  - the level combination $(+,+,-)$ is invalid for the triplet (z_{jk}, z_{kl}, z_{kl})

Optimality Theorem

Theorem 1.

The moment matrix of PWO **full** design is ϕ-optimal among all full/**fractional** PWO design,

for any design optimality criterion ϕ which is concave and signed-permutation invariant.

Optimality Theorem

the full PWO design is optimal under:

- ***D***-criterion = $\arg\max\,[\det(\mathbf{M})]^{1/p}$, $p = \binom{m}{2} + 1$
- A-criterion = $\arg\min\,\mathrm{tr}\,(\mathbf{M}^{-1})$
- E-criterion = $\arg\max\,\lambda_{\min}\,(\mathbf{M})$
- $M.S.$-criterion = $\arg\min\,\mathrm{tr}\,(\mathbf{M}^{2})$

Explicit Values for the Optimality Criteria

- Explict values of the D-/A-/E-/$M.S.$-criteria are needed for comparative purpose
  - Benchmarks to assess the efficiency of any smaller design
- To derive such criteria, the eigen-structure of $\mathbf{M}_f$ is investigated

Explicit Values for the Optimality Criteria

Theorem 2

M_f *has eigenvalues* 1, $(m+1)/3$ *and* $1/3$, *with multiplicities* 1, $m-1$ *and* $\binom{m-1}{2}$, *respectively. Then for the full design:*

$$D\text{-criterion} = [\det(\mathrm{M}_f)]^{1/p} = \left[\frac{(m+1)^{m-1}}{3^q}\right]^{\frac{1}{p}},$$

$$A\text{-criterion} = tr(\mathrm{M}_f^{-1}) = 1 + \frac{3m(m-1)^2}{2(m+1)},$$

$$E\text{-criterion} = \lambda_{\min}(\mathrm{M}_f) = \frac{1}{3}, \text{ and}$$

$$M.S.\text{-criterion} = tr(\mathrm{M}_f^2) = 1 + \frac{(m-1)m(2m+5)}{18}.$$

p=(m¦2)+1

Optimality Theorem: A Catch!

a (fractional) PWO design is

D-/A-/$M.S.$-optimal

if and only if

it has the same moment matrix as the full PWO design.

Constraint on the Correlation

Lemma 1

For any (not full) PWO design with m components, and any $1 \le j < k < l \le m$, it always holds that

$$\widetilde{M}(jk, jl) - \widetilde{M}(jk, kl) + \widetilde{M}(jl, kl) = 1,$$

Note: $\widetilde{\mathbf{M}}(jk, jl)$ indicates the correlation between PWO factors Z_{jk} and Z_{jl}

Optimality Criteria: Another Catch!!

- PWO design can NOT be perfectly *orthogonal* —
  no regular fractional factorial design can be used as a PWO design.
- The maximum correlation ($r_{\max}$) is at least $1/3$.

A Bridge too far…

Primitive Idea—

- ***If*** there exist an appropriate 2^{k-p} design for OofA experiment…
- Applying Cheng and Li (1993, *Technometrics*), choose the fraction to avoid those infeasible runs (due to transitive property).
  "Constructing Orthogonal Fractional Factorial Designs When Some Factor-Level Combinations Are Debarred"

Peng, Mukerjee and Lin (2017)

Design of Order-of-addition Experiments

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Summary

In an order-of-addition experiment, each treatment is a permutation of m components. It is often unaffordable to test all the $m!$ treatments, and the design problem arises. We consider the model in which the response of a treatment depends on the pairwise orders of the components. The optimal design theory under this model is established, and the optimal values of the D-, A-, E-, and $M.S.$-criteria are derived. We identify a special constraint on the correlation structure of such designs. The closed-form construction of a class of optimal designs is obtained, with examples for illustration.

Minimal-point PWO Designs

There are *m!* possible runs,
the minimal point PWO design
requires $\binom{m}{2}+1$ runs

Two Extremes (and in-between)

Lowest Cost Minimal-Point PWO design Run size $n=\binom{m}{2}+1$	**In Between** ⇔	Highest Cost Full PWO design Run size $n=m!$

$m=3$ → $m!=6$ & $\binom{m}{2}+1=4$;
which (best) 4 among those 6 runs?

Index	Order	Pair-wise ordering factors $I_{1\to2}$	$I_{1\to3}$	$I_{2\to3}$
123	$1\to2\to3$	1	1	1
213	$2\to1\to3$	−1	1	1
132	$1\to3\to2$	1	1	−1
231	$2\to3\to1$	−1	−1	1
312	$3\to1\to2$	1	−1	−1
321	$3\to2\to1$	−1	−1	−1

$m=4$
→ $m!=24$
& $\binom{m}{2}+1=7$;

which (best) 7 among those 24 runs?

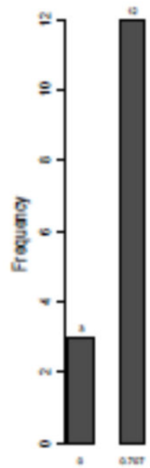
		Pair-wise ordering factors					
Index	Order	$I_{1\to2}$	$I_{1\to3}$	$I_{2\to3}$	$I_{1\to4}$	$I_{2\to4}$	$I_{3\to4}$
1234	$1\to2\to3\to4$	1	1	1	1	1	1
2134	$2\to1\to3\to4$	−1	1	1	1	1	1
1324	$1\to3\to2\to4$	1	1	−1	1	1	1
2314	$2\to3\to1\to4$	−1	−1	1	1	1	1
3124	$3\to1\to2\to4$	1	−1	−1	1	1	1
3214	$3\to2\to1\to4$	−1	−1	−1	1	1	1
1243	$1\to2\to4\to3$	1	1	1	1	1	−1
2143	$2\to1\to4\to3$	−1	1	1	1	1	−1
1342	$1\to3\to4\to2$	1	1	−1	1	−1	1
2341	$2\to3\to4\to1$	−1	−1	1	−1	1	1
3142	$3\to1\to4\to2$	1	−1	−1	1	−1	1
3241	$3\to2\to4\to1$	−1	−1	−1	−1	1	1
1423	$1\to4\to2\to3$	1	1	1	1	−1	−1
2413	$2\to4\to1\to3$	−1	1	1	−1	1	−1
1432	$1\to4\to3\to2$	1	1	−1	1	−1	−1
2431	$2\to4\to3\to1$	−1	−1	1	−1	1	−1
3412	$3\to4\to1\to2$	1	−1	−1	−1	−1	1
3421	$3\to4\to2\to1$	−1	−1	−1	−1	−1	1
4123	$4\to1\to2\to3$	1	1	1	−1	−1	−1
4213	$4\to2\to1\to3$	−1	1	1	−1	−1	−1
4132	$4\to1\to3\to2$	1	1	−1	−1	−1	−1
4231	$4\to2\to3\to1$	−1	−1	1	−1	−1	−1
4312	$4\to3\to1\to2$	1	−1	−1	−1	−1	−1
4321	$4\to3\to2\to1$	−1	−1	−1	−1	−1	−1

m=3 → m!=6 & $\binom{m}{2}+1=4$;

which (best) 4 among those 6 runs?

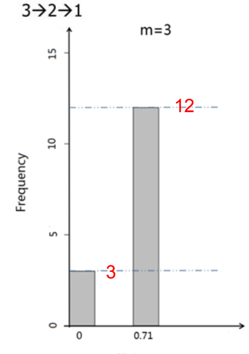
Index	Order	Pair-wise ordering factors $I_{1\to2}$	$I_{1\to3}$	$I_{2\to3}$
123	1 → 2 → 3	1	1	1
213	2 → 1 → 3	−1	1	1
132	1 → 3 → 2	1	1	−1
231	2 → 3 → 1	−1	−1	1
312	3 → 1 → 2	1	−1	−1
321	3 → 2 → 1	−1	−1	−1

There are $\binom{6}{4}$ =15 possibilities.



Minimal-Point Design (m=3)

1→2→3
1→3→2
2→1→3
2→3→1
3→1→2
3→2→1



Maximun D-efficiency: 0.71

Sample design: *123, 213, 132, 231*

	$I_{1\to2}$	$I_{1\to3}$	$I_{2\to3}$
123	+	+	+
213	−	+	+
132	+	+	−
231	−	−	+

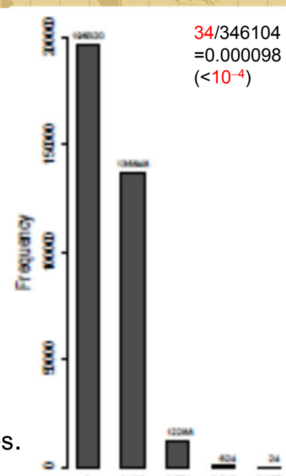
D-efficiency of full design: 0.88
Relative Efficiency: 0.71/0.88= 0.81

***m=4 →** m!=24 & $\binom{m}{2}+1=7$;*

which (best) 7 among those 24 runs?

Index	Order	Pair-wise ordering factors $I_{1\to2}$	$I_{1\to3}$	$I_{2\to3}$	$I_{1\to4}$	$I_{2\to4}$	$I_{3\to4}$
1234	1 → 2 → 3 → 4	1	1	1	1	1	1
2134	2 → 1 → 3 → 4	−1	1	1	1	1	1
1324	1 → 3 → 2 → 4	1	1	−1	1	1	1
2314	2 → 3 → 1 → 4	−1	−1	1	1	1	1
3124	3 → 1 → 2 → 4	1	−1	−1	1	1	1
3214	3 → 2 → 1 → 4	−1	−1	−1	1	1	1
1243	1 → 2 → 4 → 3	1	1	1	1	1	−1
2143	2 → 1 → 4 → 3	−1	1	1	1	1	−1
1342	1 → 3 → 4 → 2	1	1	−1	1	−1	1
2341	2 → 3 → 4 → 1	−1	−1	1	−1	1	1
3142	3 → 1 → 4 → 2	1	−1	−1	1	−1	1
3241	3 → 2 → 4 → 1	−1	−1	−1	−1	1	1
1423	1 → 4 → 2 → 3	1	1	1	1	−1	−1
2413	2 → 4 → 1 → 3	−1	1	1	−1	1	−1
1432	1 → 4 → 3 → 2	1	1	−1	1	−1	−1
2431	2 → 4 → 3 → 1	−1	−1	1	−1	1	−1
3412	3 → 4 → 1 → 2	1	−1	−1	−1	−1	1
3421	3 → 4 → 2 → 1	−1	−1	−1	−1	−1	1
4123	4 → 1 → 2 → 3	1	1	1	−1	−1	−1
4213	4 → 2 → 1 → 3	−1	1	1	−1	−1	−1
4132	4 → 1 → 3 → 2	1	1	−1	−1	−1	−1
4231	4 → 2 → 3 → 1	−1	−1	1	−1	−1	−1
4312	4 → 3 → 1 → 2	1	−1	−1	−1	−1	−1
4321	4 → 3 → 2 → 1	−1	−1	−1	−1	−1	−1

There are $\binom{24}{7}$ =346,104 possibilities.



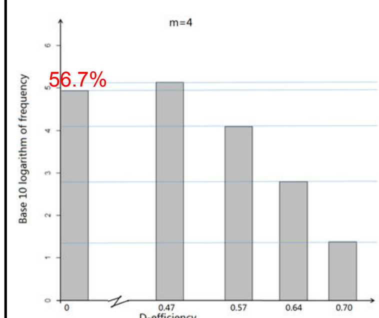
34/346104
=0.000098
($<10^{-4}$)

Minimal-Point Design (m=4)

Maximun D-efficiency: 0.70

Sample design:

1234, 2134,1324,3214,1243,2341,3142



	$I_{1\to2}$	$I_{1\to3}$	$I_{2\to3}$	$I_{1\to4}$	$I_{2\to4}$	$I_{3\to4}$
1234	+	+	+	+	+	+
2134	−	+	+	+	+	+
1324	+	+	−	+	+	+
3214	−	−	−	+	+	+
1243	+	+	+	+	+	−
2341	−	−	+	−	+	+
3142	+	−	−	+	−	+

D-efficiency of the full design(4!=24): 0.78 Relative Efficiency: 0.70/0.78= 0.90

For $m \geq 5$,

$$\binom{\binom{m}{2}+1}{m!} = \binom{120}{11} \text{ is too large!}$$

need a systematic construction method!

- Distribution of the D-efficiency of the 11- point designs for *m=5* is infeasible to search.
- Design with maximal D-efficiency 0.591 from 10^7 (10 millions) fractions of the PWO design

Q =

1	1	1	1	1	1	1	1	1	1
1	1	−1	1	1	1	1	1	1	−1
−1	−1	1	1	1	1	1	1	1	−1
−1	−1	1	−1	1	−1	−1	1	1	1
−1	−1	−1	−1	−1	1	−1	1	1	1
−1	1	1	−1	−1	−1	1	1	−1	1
1	1	−1	−1	−1	−1	1	−1	1	1
1	−1	−1	−1	−1	−1	−1	−1	−1	1
−1	1	1	1	1	−1	−1	−1	−1	−1
−1	−1	−1	−1	1	1	−1	−1	−1	−1
1	1	1	−1	−1	−1	−1	−1	−1	−1

Construction of minimal-point OofA designs ($m \geq 6$)

- Take H_1=(Q:1)

  then H is a minimal-point OofA design.

$$H = \begin{pmatrix} H_1 & H_2 \\ H_3 & H_4 \end{pmatrix}_{(\binom{m}{2}+1)\times\binom{m}{2}},$$

  - H_2 is a matrix with all elements=−1;
  - H_3 is a matrix with all elements=+1;
  - $H_4=(h_{ij})$ is a matrix with elements=+1, if $i \leq j$;

    and −1 otherwise.

- its d-efficieny is $D_e(H) = \left(4^{\binom{m}{2}-10}|H_1^T H_1|\right)^{1/(\binom{m}{2}+1)} \Big/ \left(\binom{m}{2}+1\right).$

Theorem 2. *For $m \geq 6$, let $H_1 = (Q : 1_{11})$ and*

$$H = \begin{pmatrix} H_1 & H_2 \\ H_3 & H_4 \end{pmatrix}_{(\binom{m}{2}+1)\times\binom{m}{2}},$$

where H_3 is a matrix of all elements -1, H_2 is a matrix of all elements 1 and $H_4 = (h_{ij})$ is an $(\binom{m}{2} - 10) \times (\binom{m}{2} - 11)$ matrix satisfying h_{ij} equals 1 when $i \leq j$, and -1 otherwise, then H is a minimal-point order of addition design with a D-efficiency

$$D_e(H) = \left(4^{\binom{m}{2}-10}|H_1^T H_1|\right)^{1/(\binom{m}{2}+1)} \Big/ \left(\binom{m}{2}+1\right). \quad (3.1)$$

D-efficiencies of the full PWO designs and the minimal-point designs

m	m!	$\binom{m}{2}+1$	$D_e(H)$	$D_e(F_m)$	$D_r(H)$
3	6	4	0.707	0.877	0.810
4	24	7	0.697	0.777	0.897
5	120	11	0.591	0.706	0.837
6	720	16	0.349	0.656	0.532
7	5040	22	0.232	0.618	0.375

Note: H represents the minimal-point order of addition design; F_m represents the pair-wise ordering design; $D_e(H)$, $D_e(F_m)$ and $D_r(H)$ are the D-efficiencies of H and F_m, and the relative D-efficiency of H, respectively.

Zhao, Lin and Liu (2017)

MINIMAL-POINT DESIGN FOR ORDER OF ADDITION EXPERIMENT

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Abstract: In Fisher (1971), a lady was able to tell whether the tea or the milk was first added by tasting. This is probably the first popular order of addition experiment. In general, there are m required components and we hope to determine the optimal sequence for adding these m components one after another. Knowing the optimal order of addition of components related in production is crucial. Order of addition, as an important factor affecting practical life, is involved in many areas including medical, food and film industry. However, references on this subject are rather primitive. In this paper, we provide some properties of the pair-wise ordering designs to study the orders of addition. A construction method of the minimal-point order of addition designs is proposed. It is shown that minimal-point order of addition designs can save significant amount of cost with higher relative D-efficiencies. Simulative studies are included to illustrate the ability of the minimal-point order of addition designs to distinguish the optimal

A Class of Optimal Fractional PWO Design

Information matrix of PWO Design

The moment matrix (information matrix) of full PWO design:

$\mathbf{M}_f = \mathbf{X}_f^T\mathbf{X}_f/N$, with $\mathbf{X}_f = [\mathbf{1}, \mathbf{Z}_f]$ and $N = m!$

for $m = 4$, $\mathbf{M}_f = \mathrm{diag}(1, \widetilde{\mathbf{M}}_f)$ and

$$\widetilde{\mathbf{M}}_f = \begin{bmatrix} 1 & 1/3 & 1/3 & -1/3 & -1/3 & 0 \\ 1/3 & 1 & 1/3 & 1/3 & 0 & -1/3 \\ 1/3 & 1/3 & 1 & 0 & 1/3 & 1/3 \\ -1/3 & 1/3 & 0 & 1 & 1/3 & -1/3 \\ -1/3 & 0 & 1/3 & 1/3 & 1 & 1/3 \\ 0 & -1/3 & 1/3 & -1/3 & 1/3 & 1 \end{bmatrix}$$

An example of Optimal PWO Design

For m=4 (m!=24), the following (half) fractional PWO design is "optimal."

1	2	3	4
2	1	4	3
4	3	1	2
3	4	2	1
1	3	2	4
3	1	4	2
4	2	1	3
2	4	3	1
1	4	2	3
4	1	3	2
3	2	1	4
2	3	4	1

$$\tilde{\mathbf{M}}_f = \begin{bmatrix} 1 & 1/3 & 1/3 & -1/3 & -1/3 & 0 \\ 1/3 & 1 & 1/3 & 1/3 & 0 & -1/3 \\ 1/3 & 1/3 & 1 & 0 & 1/3 & 1/3 \\ -1/3 & 1/3 & 0 & 1 & 1/3 & -1/3 \\ -1/3 & 0 & 1/3 & 1/3 & 1 & 1/3 \\ 0 & -1/3 & 1/3 & -1/3 & 1/3 & 1 \end{bmatrix}$$

It share the same moment matrix with the full PWO design.

An Example of Optimal Design

This design entails a partitioned structure:

1	2	3	4
2	1	4	3
4	3	1	2
3	4	2	1
1	3	2	4
3	1	4	2
4	2	1	3
2	4	3	1
1	4	2	3
4	1	3	2
3	2	1	4
2	3	4	1

$$\begin{bmatrix} \mathbf{B}_1 & \overline{\mathbf{B}}_1 \\ \ominus\overline{\mathbf{B}}_1 & \mathbf{B}_1 \\ \mathbf{B}_2 & \overline{\mathbf{B}}_2 \\ \ominus\overline{\mathbf{B}}_2 & \mathbf{B}_2 \\ \mathbf{B}_3 & \overline{\mathbf{B}}_3 \\ \ominus\overline{\mathbf{B}}_3 & \mathbf{B}_3 \end{bmatrix},$$

With $\mathbf{B}_1 = \begin{bmatrix} 1 & 2 \\ 2 & 1 \end{bmatrix}$, $\overline{\mathbf{B}}_1 = \begin{bmatrix} 3 & 4 \\ 4 & 3 \end{bmatrix}$,

$\mathbf{B}_2 = \begin{bmatrix} 1 & 3 \\ 3 & 1 \end{bmatrix}$, $\overline{\mathbf{B}}_2 = \begin{bmatrix} 2 & 4 \\ 4 & 2 \end{bmatrix}$,

$\mathbf{B}_3 = \begin{bmatrix} 1 & 4 \\ 4 & 1 \end{bmatrix}$, $\overline{\mathbf{B}}_3 = \begin{bmatrix} 2 & 3 \\ 3 & 2 \end{bmatrix}$

Extension to larger m

- Such a construction method can be extended to any larger, even m.

- **Theorem 3.**
  For any $m \geq 4$ and any $2 \leq r \leq m/2$, there exist optimal PWO designs with m components and $m!/r!$ runs.

Under Construction…

A Class of Optimal Fractional PWO Design

—an optimal PWD design with $2\cdot\binom{m}{2}$ *runs.*

Conclusion

- The optimality theory for PWO designs
- The explicit values of optimality criteria
- Description on the orthogonality of any PWO design
- Systematic construction of efficient minimal-point PWO designs
- Systematic construction of optimal fractional PWO designs

Order-of-Addition Experiments

- Data Analysis Strategies
- Beyond PWO system
  - Triple-wise order (TWO) system?
  - Travel Salesman Problem (TSP)
  - etc
- Run order consideration

Some (Very Selective) References

- Voelkel, J. (2017) "Design and Analysis of Order-of-Addition Experiments."
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