Design for Order-of-Addition Experiments: Some Recent Advances

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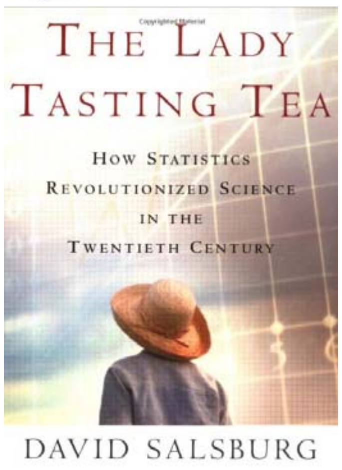
Order-of-Addition Experiment

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

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?

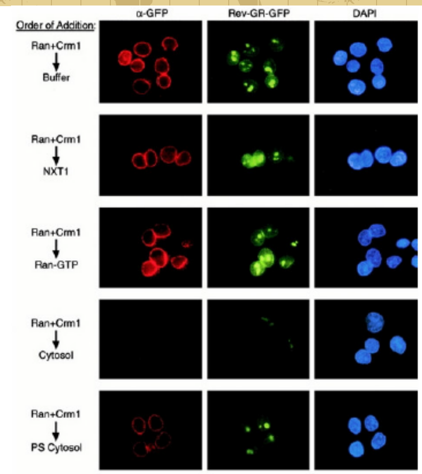
There are m! possible combinations, how could we run fraction of them?

1→2	1→2→3	1234	1243	1423	4123
2→1	1→3→2	1324	1342	1432	4123
	2→1→3	2134	2143	2413	4213
	2→3→1	2314	2341	2431	4231
	3→1→2	3124	3142	3412	4312
	3→2→1	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 → 2 → 3
  1 → 3 → 2
  2 → 1 → 3
  2 → 3 → 1
  3 → 1 → 2
  3 → 2 → 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?

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

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

Problem Formulation *(m=3 example)*

Sequence			$I_{1\to 2}$	$I_{1\to 3}$	$I_{2\to 3}$
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 $m = 4$, $\mathbf{M}_f = \mathrm{diag}(1, \widetilde{\mathbf{M}}_f)$ and

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

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

$\mathbf{M}_f$ 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:

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

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

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

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

p=(m¦2)+1

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!

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

		Pair-wise ordering factors		
Index	Order	$I_{1\to2}$	$I_{1\to3}$	$I_{2\to3}$
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?

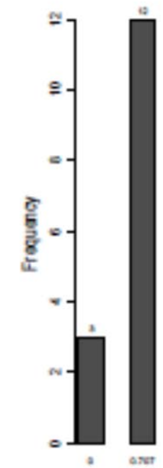
Index	Order	Pair-wise ordering factors $I_{1\to2}$	$I_{1\to3}$	$I_{2\to3}$	$I_{1\to4}$	$I_{2\to4}$	$I_{3\to4}$
1234	$1\to2\to3\to4$	1	1	1	1	1	1
2134	$2\to1\to3\to4$	−1	1	1	1	1	1
1324	$1\to3\to2\to4$	1	1	−1	1	1	1
2314	$2\to3\to1\to4$	−1	−1	1	1	1	1
3124	$3\to1\to2\to4$	1	−1	−1	1	1	1
3214	$3\to2\to1\to4$	−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

m=3 → *m!=6* & $\binom{m}{2}$+1=4;

which (best) 4 among those 6 runs?

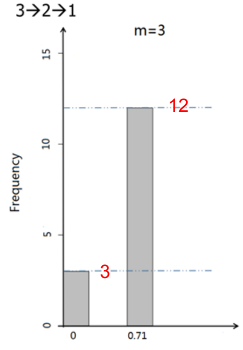
Index	Order	Pair-wise ordering factors $I_{1\to2}$	$I_{1\to3}$	$I_{2\to3}$
123	$1\to2\to3$	1	1	1
213	$2\to1\to3$	−1	1	1
132	$1\to3\to2$	1	1	−1
231	$2\to3\to1$	−1	−1	1
312	$3\to1\to2$	1	−1	−1
321	$3\to2\to1$	−1	−1	−1

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	−	−	+

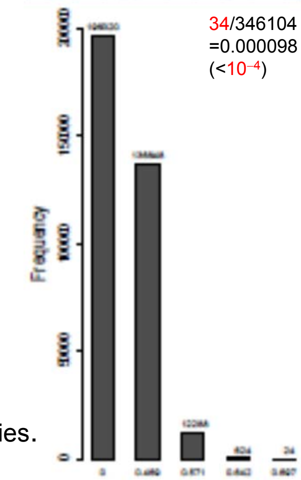
D-efficiency of full design: 0.88
Relative Efficiency: 0.71/0.88= 0.81

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	$1\to2\to3\to4$	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

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



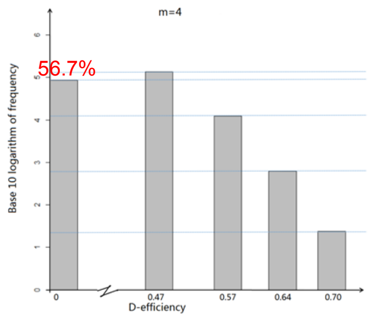
34/346104
=0.000098
(<10^{-4})

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 $m \geq 5$,

$$\left(\binom{m}{2}+1\right)^{m!} = \binom{120}{11} \text{ is too large!}$$

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

$$\mathbf{Q} = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & 1 & 1 & 1 & 1 & 1 & 1 & -1 \\ -1 & -1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & -1 \\ -1 & -1 & 1 & -1 & 1 & -1 & -1 & 1 & 1 & 1 \\ -1 & -1 & -1 & -1 & -1 & 1 & -1 & 1 & 1 & 1 \\ -1 & 1 & 1 & -1 & -1 & -1 & 1 & 1 & -1 & 1 \\ 1 & 1 & -1 & -1 & -1 & -1 & 1 & -1 & 1 & 1 \\ 1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & 1 \\ -1 & 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 & -1 \\ -1 & -1 & -1 & -1 & 1 & 1 & -1 & -1 & -1 & -1 \\ 1 & 1 & 1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 \end{pmatrix}$$

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

- Take H_1=(Q:1) then H is a minimal-point OofA design.

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

  - 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

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

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

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

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

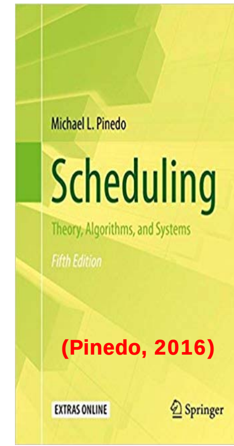
Extension to larger m

- 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.

Application—
Job Scheduling Problem

Real Application of OofA Experiments

- Job Scheduling
  - *"plays an important role in most manufacturing and production systems as well as in most information processing environments"* (Pinedo 2016)
- A wide class of scheduling problems is "permutation scheduling", which seeks an optimal order of m jobs



An Illustrative Example

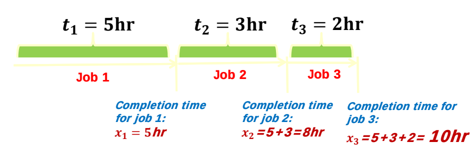
Job Scheduling

- The machine can process only one job at a time
- Process three jobs on a machine
- The process time is
  - 5 hours for the 1st job
  - 3 hours for the 2nd job
  - 2 hours for the 3rd job
- The three jobs must be processed one after one.
- The completion time (may be viewed as a "delay time") corresponds to a cost.
- The total cost function is known to be

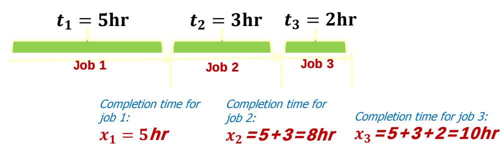
$$W = W_1 + W_2 + W_3, \quad \textit{e.g.,}\ W_1 = 6x_1^2,\ W_2 = 8x_2^2,\ W_3 = 7x_3^2$$

An Illustrative Example

- 3!=6 possible sequences of processing the jobs
- Consider the order 1->2->3



An Illustrative Example



- The total cost function is known to be

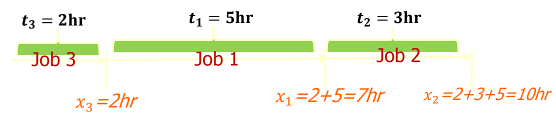
  $W = W_1 + W_2 + W_3,$

  where $W_1 = 6x_1^2,\ W_2 = 8x_2^2,\ W_3 = 7x_3^2$
- Thus the job-order 1->2->3 has a total cost of

  $W = W_1 + W_2 + W_3 = 6x_1^2 + 8x_2^2 + 7x_3^2$
  $= 6 \times 5^2 + 8 \times 8^2 + 7 \times 10^2 = \mathbf{1362}$

An Illustrative Example

- Consider a different order 3->1->2



- The order 3->1->2 has a total cost of
  $\boldsymbol{W} = 6 \times 7^2 + 8 \times 10^2 + 7 \times 2^2 = \mathbf{1122}$

An Illustrative Example

- Different orders yield different costs

Order	Completion times (x_1, x_2, x_3)	Total cost W
1→2→3	(5, 8, 10)	1362
1→3→2	(5, 10, 7)	1293
2→1→3	(8, 3, 10)	1156
2→3→1	(10, 3, 5)	847
3→1→2	(7, 10, 2)	1122
3→2→1	(10, 5, 3)	828

3→2→1 yields the minimum cost!

Single Machine Problem With Quadratic Cost: General Setup

- m jobs
- processed on a machine one after another
- Job-i has a process time of P_i
- Given a job-order $\boldsymbol{a} = a_1 \cdots a_m$, the completion time of job-a_j is

$$C_{a_j} = \sum_{i=1}^{j} P_{a_i}$$

- For any $k = a_j$, denote $C_k(a) = C_{a_j}$

Single Machine Problem With Quadratic Cost: General Setup

- The cost due to the completion times is

$$W_{\boldsymbol{a}} = \sum_{k=1}^{m} w_k C_k^2(\boldsymbol{a})$$

where w_k's being pre-specified weights

- The goal is to
  find a job-order such that W_a is minimized
- Like Travel Salesman Problem (TSP), this is an NP-Hard Problem.
- *This is also an Order-of-Addition problem!*

Single Machine Problem With Quadratic Cost

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THE SINGLE MACHINE PROBLEM WITH QUADRATIC PENALTY FUNCTION OF COMPLETION TIMES: A BRANCH-AND-BOUND SOLUTION*

W. TOWNSEND†

N jobs are to be sequenced on a single machine, each job carrying a penalty cost which is a quadratic function of its completion time. The objective is to find a sequence which minimizes the total penalty. Criteria are developed for ordering a pair of adjacent jobs in a sequence and these are incorporated into a branch-and-bound procedure.

- Existing approach: branch-and-bound
- The cost model $W_{\boldsymbol{a}} = \sum_{k=1}^{m} w_k C_k^2(\boldsymbol{a})$ is unknown
- Consider an approximate approach
  - o Fit an approximate model via testing a few job-orders
  - o Speculate the optimal order(s) from the approximate model

A Working Example

- *m=6* jobs
- P_i's: 1.19, 0.03, 1.76, 0.21, 0.03, 1.55 (generated from χ_1^2)
- w_i's: 3.86 0.55 1.31 1.07 1.80 0.08 (generated from χ_1^2)
- Suppose the underlying true model $W_{\boldsymbol{a}} = \sum_{k=1}^{m} w_k C_k^2(\boldsymbol{a})$ is unknown to us

A Working Example

- the PWO model is used as the approximate model
- Test the job orders in an optimal PWO design
- A 24-run optimal design from Voelkel (2017)

1	2	6	3	5	4	95.5
1	3	5	4	6	2	58.0
1	4	2	6	5	3	55.5
1	5	6	2	4	3	52.5
2	1	4	3	6	5	64.1
2	3	4	5	1	6	57.9
2	5	4	3	6	1	94.4
2	6	4	1	3	5	108.3
3	1	6	2	4	5	115.5
3	2	5	6	1	4	117.2
3	4	2	1	5	6	70.3
3	6	1	4	5	2	159.7
3	6	5	4	1	2	137.8
4	1	5	3	2	6	32.2
4	5	6	1	2	3	69.4
4	6	3	1	2	5	155.5
4	6	3	5	2	1	134.2
5	1	3	2	4	6	35.3
5	1	6	4	3	2	57.8
5	2	6	3	1	4	119.6
5	4	2	3	1	6	47.4
6	2	1	5	3	4	96.7
6	4	2	5	1	3	76.0
6	5	3	2	4	1	127.1

Obtain W_a's

A Working Example

- Model

$$E(Y|\boldsymbol{a}) = \beta_0 + \sum_{1\le j<k\le m} \beta_{jk} \cdot z_{jk}(\boldsymbol{a})$$

- Hypothesis Testing

$H_0\colon \beta_{jk} = 0$

$q = \binom{m}{2} = \binom{6}{2} = 15$ β_{ij}'s to be tested

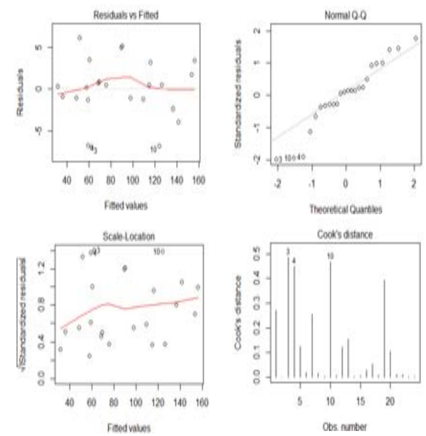
- An optimal order should be consistent with the favorable precedence patterns indicated by the significant variables

Significant variables	Signs of the effects	Favorable patterns
z_{12}	+	2 precedes 1
z_{13}	–	1 precedes 3
z_{14}	+	4 precedes 1
z_{15}	+	5 precedes 1
z_{16}	–	1 precedes 6
z_{35}	+	5 precedes 3
z_{36}	–	3 precedes 6
z_{56}	–	5 precedes 6

Model Diagnostics

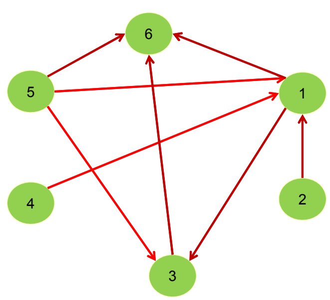
Regression diagnostics:

No assumption is obviously violated



A Working Example

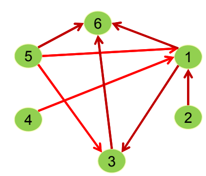
Favorable patterns
2 precedes 1
1 precedes 3
4 precedes 1
5 precedes 1
1 precedes 6
5 precedes 3
3 precedes 6
5 precedes 6



Optimal order(s) can be found by topological sorting in a directed graph:
Any favorable pattern "u precedes v" indicates an edge from u to v

A Working Example

Obtain 6 optimal orders using the (linear-time) topological sorting algorithm (Knuth and Szwarcfiter 1974)



Order	W_a
4→2→5→1→3→6	23.89
4→5→2→1→3→6	23.87
5→4→2→1→3→6	23.78
5→2→4→1→3→6	23.75
2→5→4→1→3→6	23.76
2→4→5→1→3→6	23.87

Confirmation

- Evaluate all possible order of the *m=6* jobs (a total of 6!=720 orders)
- Findings:
  - *The minimum among all 720 orders is W =23.73.*
  - *Our obtained orders rank the 3rd to 8th among all the 720 orders*

  –(nearly) optimal! The difference is insignificant!!

Order	W_a
4→2→5→1→3→6	23.89
4→5→2→1→3→6	23.87
5→4→2→1→3→6	23.78
5→2→4→1→3→6	23.75
2→5→4→1→3→6	23.76
2→4→5→1→3→6	23.87

OofA Model and Design in Real-life and Modern Scheduling Problems

- A large variety of job scheduling problems in practice: different job-machine setups/cost functions
- The OofA approach is potentially useful as
  - An effect approximate method for large-scale scheduling (usually NP-hard)
  - A generic approach for different types of scheduling problems;
    particularly useful when (1) the problem type might vary at any time – online scheduling (2) the cost function is unknown – black box
  - A method of determining initial points for existing heuristic algorithms, such as simulated annealing and genetic algorithm
  - A tool for challenging problems with stochastic process times

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

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