Order-of-Addition Experiments

to study the effect of treatment ordering

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Contents

Order-of-addition experiments investigate the effect of the order in which a set of treatments is applied

Experiment of Voelkel and Gallagher (2019)

Component	Abbreviation
Primary binding resin	R1
Secondary binder resin	R2
Flow and leveling additive	A1
Rheology modifier #1	M1
Crosslinking resin	X
Rheology modifier #2	M2

- 6 components of an automotive coating system
- In what order should they be added so that the coating is smooth and even?

An experimental design in 24 runs

Run	Order of addition						Run	Order of addition					
1	R1	R2	M2	A1	M1	X	13	R2	M2	R1	M1	A1	X
2	M1	R1	M2	R2	X	A1	14	R2	M1	R1	A1	X	M2
3	X	M1	M2	R1	R2	A1	15	R2	X	A1	M2	R1	M1
4	M2	R1	X	A1	R2	M1	16	R2	M1	X	M2	A1	R1
5	X	R1	M2	A1	M1	R2	17	M2	X	R2	M1	A1	R1
6	R1	M1	A1	M2	R2	X	18	M1	R2	M2	A1	X	R1
7	R1	X	M2	M1	A1	R2	19	X	M1	R2	A1	R1	M2
8	M1	X	R1	A1	R2	M2	20	A1	R2	M2	X	M1	R1
9	A1	R1	X	R2	M1	M2	21	M2	A1	R2	X	M1	R1
10	A1	X	R1	M2	R2	M1	22	A1	M1	R2	R1	X	M2
11	A1	M2	M1	R1	X	R2	23	A1	M1	X	M2	R2	R1
12	X	R2	R1	A1	M1	M2	24	M1	M2	X	A1	R2	R1

Key feature of a design

- m components
- m! possible permutations

- A design is a subset of these permutations.

A toy example

Run	Sequence
1	1 2 3
2	1 3 2
3	3 1 2
4	2 1 3
5	2 3 1
6	3 2 1

- Three components
- 3! = 6 possible sequences

Pairwise order model

Run	Sequence	O_{12}	O_{13}	O_{23}
1	1 2 3	1	1	1
2	1 3 2	1	1	−1
3	3 1 2	1	−1	−1
4	2 1 3	−1	1	1
5	2 3 1	−1	−1	1
6	3 2 1	−1	−1	−1

- Three components
- 3! = 6 possible sequences

- O_{ij} = 1 if i comes **before** j
- O_{ij} = −1 if i comes **after** j

- Main-effects model

$$y = \beta_0 + \sum_{i<j} \beta_{ij} O_{ij} + \varepsilon$$

Linear component position model

Run	Sequence	$p(b_1)$	$p(b_2)$	$p(b_3)$
1	1 2 3	−1	0	1
2	1 3 2	−1	1	0
3	3 1 2	0	1	−1
4	2 1 3	0	−1	1
5	2 3 1	1	−1	0
6	3 2 1	1	0	−1

- Three components
- 3! = 6 possible sequences

- $p(b_i)$: position for component i

Linear component position model

Run	Sequence	$p_1(b_1)$	$p_1(b_2)$	$p_1(b_3)$
1	1 2 3	$-\sqrt{3/2}$	0	$\sqrt{3/2}$
2	1 3 2	$-\sqrt{3/2}$	$\sqrt{3/2}$	0
3	3 1 2	0	$\sqrt{3/2}$	$-\sqrt{3/2}$
4	2 1 3	0	$-\sqrt{3/2}$	$\sqrt{3/2}$
5	2 3 1	$\sqrt{3/2}$	$-\sqrt{3/2}$	0
6	3 2 1	$\sqrt{3/2}$	0	$-\sqrt{3/2}$

- Three components
- 3! = 6 possible sequences

- $p_1(b_i)$ linear position factor for component i
- rows add up to 0
- Main-effects model

$$y = \gamma_0 + \sum_{i=1}^{m-1} \gamma_i p_1(b_i) + \varepsilon$$

Uniform design: optimality for PWO model

- m treatments, components,…
- m! orders
- the uniform design has all orders exactly once

Peng et al. (2019): uniform design is optimal for the main-effects PWO model according to many criteria, including D.

- main-effects PWO model matrix
  X_f =[$\mathbf{1}_{\mathbf{m!}}$ O_f]
- $M_f = X_f^T X_f / m!$

- Any design with N runs and
  $X^T X / N = X_f^T X_f / m!$
  is D-optimal for the main-effects PWO model

Uniform design: optimality for CP model

- m treatments, components,…
- m! orders
- the uniform design has all orders exactly once

Stokes and Xu (2022): uniform design is D-optimal for the linear CP model.

- linear position model matrix
  $L_f = [\mathbf{1}_{\mathbf{m!}}\ P_f]$
- $K_f = L_f^T L_f / m!$

- Any design with N runs and
  $$L^T L/N = L_f^T L_f / m!$$
  is D-optimal for the linear CP model

Optimality for PWO and linear CP model

- Peng et al. (2019): Any design with $X^T X/N = X_f^T X_f/m!$ is D-optimal for the main-effects PWO model

Stokes and Xu (2022): any design with $L^T L/N = L_f^T L_f/m!$ is D-optimal for the linear CP model

Schoen and Mee: any design with $X^T X/N = X_f^T X_f/m!$ is D-optimal for the linear CP model

An honorific name

- Any design with

  $(X^T X)/N = X_f^T X_f/m!$

  is called an order-of-addition orthogonal array (OA)….

  …but such a design is not orthogonal for the PWO main effects

- Here is the normalized information matrix for the full 4! design:

$$\frac{1}{3}\begin{pmatrix} 3 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 1 & 1 & -1 & -1 & 0 \\ 0 & 1 & 3 & 1 & 1 & 0 & -1 \\ 0 & 1 & 1 & 3 & 0 & 1 & 1 \\ 0 & -1 & 1 & 0 & 3 & 1 & -1 \\ 0 & -1 & 0 & 1 & 1 & 3 & 1 \\ 0 & 0 & -1 & 1 & -1 & 1 & 3 \end{pmatrix}$$

What run sizes are feasible for OAs?

$$\frac{1}{3}\begin{pmatrix} 3 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 1 & 1 & -1 & -1 & 0 \\ 0 & 1 & 3 & 1 & 1 & 0 & -1 \\ 0 & 1 & 1 & 3 & 0 & 1 & 1 \\ 0 & -1 & 1 & 0 & 3 & 1 & -1 \\ 0 & -1 & 0 & 1 & 1 & 3 & 1 \\ 0 & 0 & -1 & 1 & -1 & 1 & 3 \end{pmatrix}$$

- Run size *N* for 4 or more components must be a multiple of 2…
- and of 3 …
- and of 4.

- So N is multiple of 12

A challenge

$$
: \frac{1}{3}\begin{pmatrix} 3 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 1 & 1 & -1 & -1 & 0 \\ 0 & 1 & 3 & 1 & 1 & 0 & -1 \\ 0 & 1 & 1 & 3 & 0 & 1 & 1 \\ 0 & -1 & 1 & 0 & 3 & 1 & -1 \\ 0 & -1 & 0 & 1 & 1 & 3 & 1 \\ 0 & 0 & -1 & 1 & -1 & 1 & 3 \end{pmatrix}
$$

- Run size *N* for 4 or more components must be a multiple of 12.
- Can we enumerate OAs?
- Yes we can! We wrote an algorithm to enumerate all nonisomorphic Oas of given N and m.

Enumeration results

Run size *N*	Number of components *m*	Number of designs *d*
12	4	2
	5	2

- Complete enumeration of 12-run OAs

Enumeration results

Run size *N*	Number of components *m*	Number of designs *d*
12	4	2
	5	2
24	4	10
	5	8,642
	6	22,651
	7	2,906

- Complete enumeration of 12-run and 24-run OAs

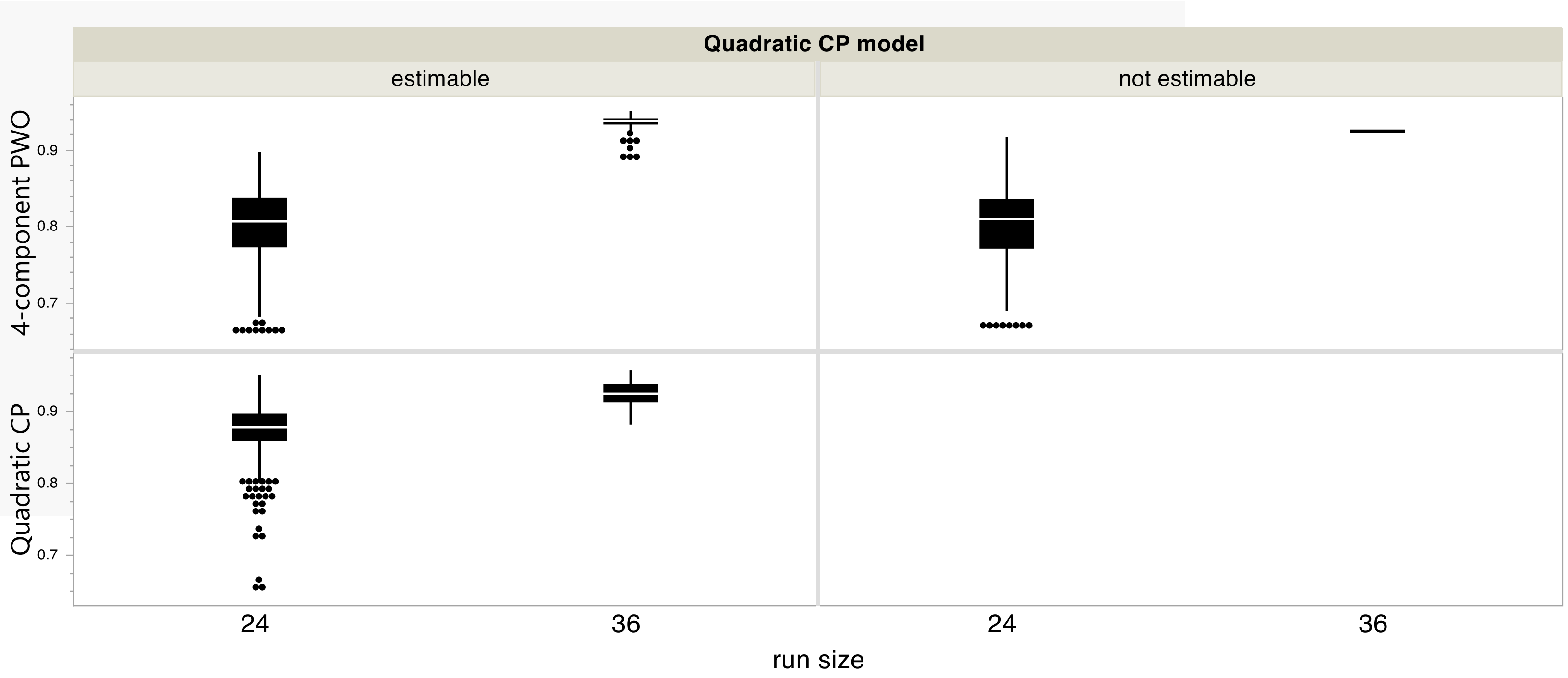
Enumeration results

Run size N	Number of components m	Number of designs d
12	4	2
	5	2
24	4	10
	5	8,642
	6	22,651
	7	2,906
36	4	30
	5	> 83,891,097
	6	> 309,655,722
	7	> 74

- Complete enumeration of 12-run and 24-run OAs
- Partial enumeration of 36-run OAs
- Can be characterized by additional criteria

D-efficiencies 7 component OAs

- Quadratic CP:
  D-efficiency for quadratic position model
- 4-component PWO: average D-eff for interaction model over all projections into 4 components



Concluding remarks

- The order in which treatments are applied can be modeled with pairwise order factors or component position factors
- It is possible to enumerate optimal designs for the model with main effects of the PWO factors
- Designs can be characterized further based on their efficiencies for more complex models

- Challenge: direct construction of efficient designs for realistic run sizes.

References

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Thank you for your attention