Factorial Experiments When Factor Levels Are Not Necessarily Reset

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Outline

- Example for experiments When Factor Levels Are Not Necessarily Reset
- Comparison of completely randomized experiment and a randomized run order and not reset experiment
- Conclusions

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Introduction

- An experiment is called a completely randomized experiment if it has a randomized run order and all factors in the experiment are reset at the beginning of each run (Ganju and Lucas (1997)).

$$\mathbf{X}_D = \begin{array}{c} \text{run} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \end{array} \begin{array}{c} \begin{array}{ccc} x_1 & x_2 & x_3 \end{array} \\ \begin{pmatrix} -1 & -1 & -1 \\ -1 & -1 & 1 \\ -1 & 1 & -1 \\ -1 & 1 & 1 \\ 1 & -1 & -1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \\ 1 & 1 & 1 \end{pmatrix} \end{array}.$$

- An experiment with a randomized run order and not reset experiment (RNR experiment).

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Introduction (cont.)

- In industry, the run order of experiment is often randomized, but not all factors are reset from one run to the next when they occur at the same level.
- For example, in an adhesive curing process the temperature of the curing dispenser is difficult to adjust. The temperature is left unadjusted at the current setting (i.e it is not reset). This is the situation we address in this paper.

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An Industrial Example

- This experiment was successful in improving the performance of a wrapper machine. Three factors, deemed important by engineers for creating a tight seal on the bag containing the product, were examined in this experiment. These factors were the spacing of the seal crimper, the speed at which the machine was run, and the temperature of the seal crimper.

  Because the mechanics of the machine, speed and spacing were physically hard to reset factors while temperature was easy to reset.

An Industrial Example (cont.)

The matrix in Table 1 displays the run order in which the experiment was carried out. Spacing and speed were not reset. Temperature was reset at the beginning of each run. The response, seal strength, is also listed. The lines represent restrictions on randomization due to spacing and speed not being reset.

TABLE 1. Wrapper Machine Example

Strength	Spacing	Speed	Temp
6.006	0	1	-1
9.170	0	1	1
9.235	0	0	0
6.450	1	0	1
8.110	1	0	-1
9.158	1	-1	0
5.010	1	1	0
5.800	-1	1	0
10.635	-1	-1	0
8.940	-1	0	-1
9.110	-1	0	1
8.090	0	0	0
9.100	0	-1	-1
10.150	0	-1	1
6.195	0	0	0

An Industrial Example (cont.)

- The experiment was analyzed using the fixed effects model, $y = X\beta + \varepsilon$,where the typical assumption of independent and identically distributed errors was made. All main effects, two-factor interactions, and squared terms were included in the model.
- The experimenters followed the very common industrial practice of using an ordinary least squares analysis, although they knew that the run order was not completely randomized.

An Industrial Example (cont.)

Another analysis using the mixed model $y = X\beta + Zu + \varepsilon$ was conducted.
For this example, the Z matrix is formed from matrices. That is, $Z=[Z_{spacing}|Z_{speed}]$, where ones in thematrices indicate successive runs where factors have the same level and are not reset .
For example, spacing is reset four times, and there are four columns in $Z_{spacing}$. The first three rows of the first column are ones because for the first three runs of the experiment spacing was not reset.

$$Z_{spacing} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \end{bmatrix};$$

and

$$Z_{speed} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

An Industrial Example (cont.)

The SAS output is shown in Table 3.
We note that the variables B_SPACE and B_SPEED are random effect s corresponding to the blocks formed by not resetting SPACING and SPEED. These are the blocks associated with the matrices Zspacing and Zspeed

TABLE 3. SAS Output for Wrapper Machine Example

Effect	Estimate	Std Error	DF	t	Pr > $\|t\|$
INTERCEPT	3.7411	0.7718	1.08	4.85	0.116
SPACING	-0.5012	0.7481	0.95	-0.67	0.620
SPEED	-2.1417	0.1656	1.11	-12.95	0.000
TEMP	1.4656	0.1397	4.00	10.49	0.001
SPACING*SPEED	0.2350	0.1976	4.00	1.19	0.300
SPACING*TEMP	0.0425	0.1976	4.00	0.22	0.840
SPEED*TEMP	0.7788	0.1976	4.00	3.94	0.017
SPACING*SPACING	-1.1176	1.0599	0.96	-1.05	0.469
SPEED*SPEED	0.0850	0.2078	4.00	0.41	0.700
TEMP*TEMP	-0.4711	0.2078	4.01	-2.28	0.081

Covariance Parameter Estimates (REML)	
B_SPACE	1.060
B_SPEED	0.000
Residual	0.156

Mixed model

- The mixed model $y = X\beta + Zu + \varepsilon$ is used to account for randomization restrictions in the experiment associated with c factors that are not reset. Where $Z = (Z_{x1} \mid \dots \mid Z_{xc})$ is the random effects design matrix for c not reset factors and u is the vector of random effects.
- For every factor x_i that is not reset from one run to the next in an L^k experiment, the standard random effects matrix Z_{xi} is defined as:

  $$\mathbf{Z}_{x_i} = \mathbf{j}_{L^{i-1}} \otimes \mathbf{I}_L \otimes \mathbf{j}_{L^{k-i}}$$

  where L is the number of levels of each factor, k is the number of factors, and j_L^{i-1} and j_L^{k-i} are column vectors of ones of sizes $L^{i-1} \times 1$ and $L^{k-i} \times 1$, respectively. The symbol $\otimes$ refers to Kronecker multiplication.

  $$A \otimes B = \begin{bmatrix} a_{11}B & \cdots & a_{1n}B \\ \vdots & \ddots & \vdots \\ a_{m1}B & \cdots & a_{mn}B \end{bmatrix}.$$

Mixed model (cont.)

For example, suppose the design matrix X_D and the standard random effects matrices Z_{x1} and Z_{x2} for the 2^3 factorial experiment are

$$\mathrm{X}_D = \begin{array}{c} \text{run} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \end{array} \begin{array}{c} \begin{array}{ccc} x_1 & x_2 & x_3 \end{array} \\ \begin{pmatrix} -1 & -1 & -1 \\ -1 & -1 & 1 \\ -1 & 1 & -1 \\ -1 & 1 & 1 \\ 1 & -1 & -1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \\ 1 & 1 & 1 \end{pmatrix} \end{array}, \quad \mathrm{Z}_{x_1} = \begin{bmatrix} 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \end{bmatrix},$$

and

$$\mathbf{Z}_{x_2} = \begin{bmatrix} 1 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \\ 1 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \end{bmatrix}.$$

The Expected Prediction Variance

- Experimenters are often interested in using the results of experiments for response prediction.
- An understanding of the properties of the prediction variance of factorial experiment that contain one or more factors that are not reset from one run to the next is valuable in comparing experiments.

The Expected Prediction Variance (cont.)

- The prediction variance of RNR experiments depends on how many factors are not reset and on where the lack of resetting occurs in the experiment. Therefore, it is not feasible to present all possible prediction variances for factorial experiments.
- Instead, we give the expected prediction variance for L^k factorial experiments, where the expectation is taken with respect to the discrete distribution of all possible $L^k!$ run orders.

Expected Variance-Covariance (EVC) Theorem

- The expected variance-covariance matrix V_E=E[Var(y)] of an L^k experiment with randomized run order when x1,x2,…,xc are factors that are not reset from one run to the next is

$$\mathbf{V}_E = \left[\sigma^2 + (1-p)\sum_{i=1}^{c}\sigma_i^2\right]\mathbf{I}_n + p\sum_{i=1}^{c}\sigma_i^2 \mathbf{Z}_{x_i}\mathbf{Z}'_{x_i},$$

where $p = 2/(L^{k-1}(L-1)+2)$.

$$\begin{aligned} E[\mathrm{Var}[\hat{\boldsymbol\beta}]] &= (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'E[\mathrm{Var}[\mathbf{y}]]\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1} \\ &= (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{V}_E\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1} \qquad (2) \end{aligned}$$

$$E[\mathrm{Var}[\hat{\mathbf{y}}]] = \mathbf{X}E[\mathrm{Var}[\hat{\boldsymbol\beta}]]\mathbf{X}'.$$

Expected Variance-Covariance (EVC) Theorem (cont.)

- The maximum prediction variance is a convenient criterion to use for comparison and is directly related to optimal design criterion.
- The maximum expected prediction variance of y_head, can be written as $\max_{x\in\mathcal{X}} E[\mathrm{Var}[\hat{\mathbf{y}}(\mathbf{x})]] = \mathbf{x}_0 E[\mathrm{Var}[\hat{\boldsymbol\beta}]]\mathbf{x}'_0$, where x_0 = [1,….,1]
- The EVC theorem allows a comparison to be made between RNR and completely randomized experiments based on the maximum prediction variance of the experimental design.

Compares completely randomized and RNR 2^k factorial experiments

- Table 4 compares completely randomized and RNR 2^k factorial experiments. Three models are considered: main effects; main effects and all 2-factor interactions; and full model.
- for a completely randomized experiment, the number of resets of the factor(s) that are not reset is the number of runs of the experiment
- the average number of resets for an L^k factorial experiment including one reset for the initial setup as L^k+1-L^{k-1}. For L =2, this reduces to $2^{k-1}+1$.

(Mood (1940))

Compares completely randomized and RNR 2^k factorial experiments (cont.)

- Each model contains c factors that are not reset, where $c \leqq k$. The multipliers of σ^2 and σ^2_j for the maximum prediction variance of a randomized design and the maximum expected prediction variance of a RNR design are given, where σ^2_j is the variance associated with not resetting the j factor, where $1 \leqq j \leqq c$.

Table 4

FACTORIAL EXPERIMENTS WHEN FACTOR LEVELS ARE NOT NECESSARILY RESET 7

TABLE 4. Average Number of Resets and Variance Multipliers of the Maximum Prediction Variance

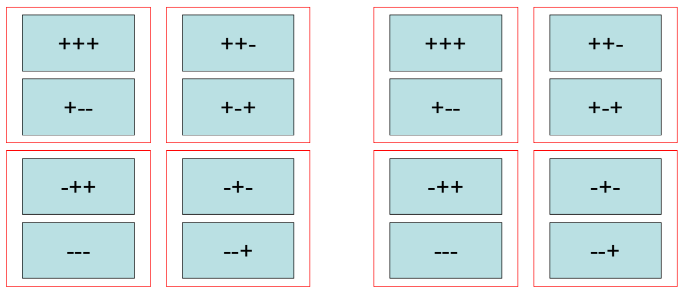
		Completely Randomized		RNR		
				Variance Multiplier		
2^k	Parameters in the Model	Variance Multiplier $\frac{\hat{y}}{\sigma^2 = \sigma_j^2}$	Avg. # Resets	σ^2	σ_j^2	Resets
	Main Effects	[illegible]	4c	[illegible]	[illegible]	3c
2^2	Main — 2 FI	[illegible]	4c	[illegible]	[illegible]	3c
	Full Model	[illegible]	4c	[illegible]	[illegible]	3c
	Main Effects	[illegible]	8c	[illegible]	[illegible]	5c
2^3	Main — 2 FI	[illegible]	8c	[illegible]	[illegible]	5c
	Full Model	[illegible]	8c	[illegible]	[illegible]	5c
	Main Effects	[illegible]	16c	[illegible]	[illegible]	9c
2^4	Main — 2 FI	[illegible]	16c	[illegible]	[illegible]	9c
	Full Model	[illegible]	16c	[illegible]	[illegible]	9c
	Main Effects	[illegible]	32c	[illegible]	[illegible]	17c
2^5	Main — 2 FI	[illegible]	32c	[illegible]	[illegible]	17c
	Full Model	[illegible]	32c	[illegible]	[illegible]	17c
	Main Effects	[illegible]	64c	[illegible]	[illegible]	[illegible]
2^6	Main — 2 FI	[illegible]	64c	[illegible]	[illegible]	[illegible]
	Full Model	[illegible]	64c	[illegible]	[illegible]	[illegible]
	Main Effects	[illegible]	128c	[illegible]	[illegible]	[illegible]
2^7	Main — 2 FI	[illegible]	128c	[illegible]	[illegible]	[illegible]
	Full Model	[illegible]	128c	[illegible]	[illegible]	[illegible]

Illustrating the information contained in Table 4

- we consider a 2^4 experiment, where the 11-parameter model contains main effects and all 2-factor interactions with c = 3.
- The maximum prediction variance for a completely randomized experiment in which each factor is reset is $(11/16)\sigma^2 + (11/16)\sigma^2_1 + (11/16)\sigma^2_2 + (11/16)\sigma^2_3$
- the maximum expected prediction variance for a RNR experiment is $(11/16)\sigma^2 + (12/16)\sigma^2_1 + (12/16)\sigma^2_2 + (12/16)\sigma^2_3$ which exceeds the maximum prediction variance for the completely randomized experiment by only $(1/16)(\sigma^2_1 + \sigma^2_2 + \sigma^2_3)$
- But the cost of resetting these factors in the completely randomized experiment is 16*3 = 48, while the RNR experiment requires only 9*3 = 27.

Industrial Example Revisited

- We suggest running 2 replicates of a full 2^3 factorial (the 3 factors are spacing (A), speed (B), and temperature (C))
- Each replication of the experiment is blocked on spacing using the relationship I=A=BC.



Industrial Example Revisited (cont.)

- It is better than a completely randomized 2 replications of a 2^3 design because it requires that spacing be reset only 8 times.
- Its maximum prediction variance is

  $(2/8)\ \sigma^2_A + (7/16)\ \sigma^2$

  while a randomized design has a variance of

  $(7/16) + (\sigma^2 + \sigma^2_A)$

Industrial Example Revisited (cont.)

- A second option is to block only on spacing using the relation I=A in each replicate.
- This gives a design with lower cost and less precision because it only requires 4 resets of spacing. Both of these designs are less expensive to run than a completely randomized design, both are easily analyzed, and both have good prediction variance properties.

+++	++-	-++	-+-	+++	++-	-++	-+-
+-+	+--	--+	---	+-+	+--	--+	---

Conclusions

- When there are one or two factors that are not reset, a blocked split-plot experiment is better than a randomized experiment because it can have a both lower cost and a smaller prediction variance.

- Thanks for your attention