Optimal two-level split-plot designs

Peter Goos

Universiteit Antwerpen

James M. Lucas

J.M. Lucas & Associates

Outline

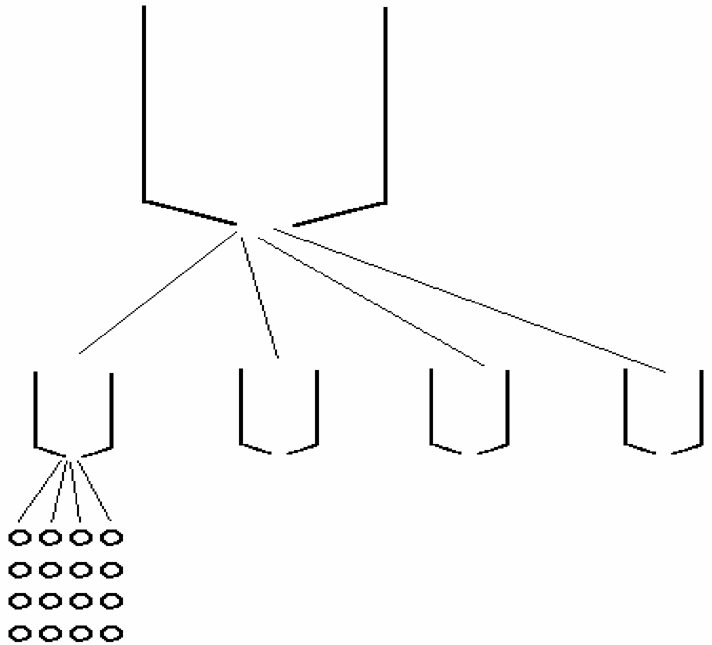
- types of split-plot designs
- number of possible designs
- illustration: 2^3 factorial design
  - main-effects model
  - main-effects + 2 f.i. model
- three simple design options
- comparison to completely randomized designs
- conclusion

Types of split-plot designs

- split-plot designs are used when independently resetting some of the factors for each run is impractical
- some terminology:
  - whole-plot vs. sub-plot factors
  - whole plots: subset of runs for which whole-plot factors are not reset
- examples:
  - mixture-process variable experiments
  - multi-stage experiments
  - experiments with hard-to-change variables

Multi-stage split-plot designs

Source: Eric Schoen



storage tanks / milk

batches / curds

cheeses

Mixture-process variable split-plot designs

Source: Jones & Goos (2006)

Whole-Plot Factors	Sub-Plot Factors
EPDM	Gas Type (3 levels)
Ethylene	Flow Rate
Tallow	Power
Mica	Reaction Time
Lubricant	
Stabilizer	
EVA	

Hard-to-change factors (version 1)

- time-consuming, hard, … to change factor levels
- physical constraints on whole-plot sizes, one-stage experiment
- example (Gilmour & Goos, 2006)
  - factors: pressure in drying chamber, heating temperature, initial solids content, slab thickness, freezing rate
  - response: amount of volatile components in freeze-dried coffee
  - 5 observations during each of 6 days

Freeze drying experiment

WP	Press	Temp	Solids	Thickn	Rate
1	1	0	0	0	1
1	1	0	0	1	0
1	1	-1	0	0	0
1	1	0	0	0	0
1	1	0	1	0	0
2	0	0	0	0	0
2	0	-1	1	-1	1
2	0	1	1	1	0
2	0	1	-1	-1	0
2	0	-1	-1	1	1
3	-1	0	0	0	0
3	-1	1	1	1	1
3	-1	-1	1	-1	-1
3	-1	-1	-1	1	-1
3	-1	1	-1	-1	1

WP	Press	Temp	Solids	Thickn	Rate
4	1	0	0	-1	0
4	1	1	0	0	0
4	1	0	0	0	-1
4	1	0	-1	0	0
4	1	0	0	0	0
5	-1	0	0	0	0
5	-1	1	1	-1	1
5	-1	1	-1	1	-1
5	-1	-1	1	1	-1
5	-1	-1	-1	-1	1
6	0	1	-1	1	1
6	0	0	0	0	0
6	0	1	1	-1	-1
6	0	-1	1	1	1
6	0	-1	-1	-1	-1

Hard-to-change factors (version 2)

- time-consuming, hard, … to change factor levels
- no physical constraints on whole-plot sizes, one-stage experiment
- example (Webb et al., JQT 2004)
  - factors: spacing seal crimper, machine speed, temperature
  - response: quality of air-tight bags
  - Box-Behnken design
  - spacing of seal crimper was reset only 4 times

Hard-to-change factors

wp	spacing	speed	temp	response
1	0	+1	−1	5.005
	0	+1	+1	9.170
	0	0	0	9.235
2	+1	0	+1	8.450
	+1	0	−1	5.110
	+1	−1	0	9.155
	+1	+1	0	5.010
3	−1	+1	0	5.800
	−1	−1	0	10.885
	−1	0	−1	5.940
	−1	0	+1	9.110
4	0	0	0	8.090
	0	−1	−1	9.100
	0	−1	+1	10.150
	0	0	0	8.195

Model

$$\gamma_i \sim N(0, \sigma_\gamma^2)$$

$$\varepsilon_{ij} \sim N(0, \sigma_\varepsilon^2)$$

$$\mathrm{cov}(\gamma_k, \varepsilon_{ij}) = 0, \forall i, j, k$$

$$y_{ij} = \mathbf{f}'(\mathbf{x}_{ij})\boldsymbol{\beta} + \gamma_i + \varepsilon_{ij}$$

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\boldsymbol{\gamma} + \boldsymbol{\varepsilon}$$

$$\mathbf{V} = \mathrm{diag}\,(\mathbf{V}_1, \mathbf{V}_2, \ldots, \mathbf{V}_b)$$

$$\eta = \frac{\sigma_\gamma^2}{\sigma_\varepsilon^2}$$

$$\mathbf{V}_i = \sigma_\varepsilon^2 \begin{bmatrix} 1+\eta & \eta & \cdots & \eta \\ \eta & 1+\eta & \cdots & \eta \\ \vdots & \ddots & \ddots & \vdots \\ \eta & \cdots & \cdots & 1+\eta \end{bmatrix}$$

Analysis and design

- GLS estimation

$$\hat{\beta} = \left(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X}\right)^{-1}\mathbf{X}'\mathbf{V}^{-1}\mathbf{y}$$

- variance-covariance matrix

$$\mathrm{var}(\hat{\beta}) = \left(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X}\right)^{-1}$$

Number of split-plot arrangements

- number of possible split-plot designs
  - given design with w whole-plot levels
  - n_i design points at whole-plot level i
- only partitioning matters
  - order of whole plots doesn't matter
  - neither does the order of the sub-plots within whole plots

$$N = \prod_{i=1}^{w} B_{n_i}$$

Number of split-plot arrangements

- number of possible split-plot designs
  - given design with w whole-plot levels
  - n_i design points at whole-plot level i
- only partitioning matters
  - order of whole plots doesn't matter
  - neither does the order of the sub-plots within whole plots

$$N = \prod_{i=1}^{w} B_{n_i}$$

$$\text{with } B_{n_i} = \sum_{\mathrm{k}=1}^{\mathrm{n_i}} S(n,k)$$

Number of split-plot arrangements

- number of possible split-plot designs
  - given design with w whole-plot levels
  - n_i design points at whole-plot level i
- only partitioning matters
  - order of whole plots doesn't matter
  - neither does the order of the sub-plots within whole plots

$$N = \prod_{i=1}^{w} B_{n_i}$$

$$\text{with } B_{n_i} = \sum_{\mathrm{k}=1}^{\mathrm{n_i}} S(n,k)$$

$$\text{and } S(n,k) = \frac{1}{k!} \sum_{i=0}^{k-1} (-1)^i \binom{k}{i} (k-i)^n$$

Number of split-plot arrangements with one hard-to-change factor x1

	x1	x2	x3
$n_1 = 4$	-	-	-
	-	-	+
	-	+	-
	-	+	+
$n_2 = 4$	+	-	-
	+	-	+
	+	+	-
	+	+	+

- $S(4,4)=1$ way to partition 4 runs in 4 subsets: {{1},{2},{3},{4}}
- $S(4,3)=6$ ways to partition them in 3 subsets: {{1}{2}{3,4},{{1}{3}{2,4},…}
- $S(4,2)=7$ ways to partition them in 2 subsets: {{1,2,3}{4},…,{1,4}{2,3}}
- $S(4,1)=1$ partition of a single subset: {1,2,3,4}
- 15 arrangements for each wp level
- $15 \times 15 =$ 225 possible designs

Number of possible designs

	$n_1 = \cdots = n_w$						
w	2	3	4	5	6	7	8
1	2	5	15	52	203	877	4140
2	4	25	225	2704	41209	769129	17139600
3	8	125	3375	140608	8365427	674526133	70957944000
4	16	625	50625	7311616	1698181681	5.91559E+11	2.93766E+14
5	32	3125	759375	380204032	3.44731E+11	5.18798E+14	1.21619E+18
6	64	15625	11390625	19770609664	6.99804E+13	4.54986E+17	5.03503E+21
7	128	78125	170859375	1.02807E+12	1.4206E+16	3.99022E+20	2.0845E+25
8	256	390625	2562890625	5.34597E+13	2.88382E+18	3.49943E+23	8.62984E+28

2 billion 562 million possibilities for a design with 8 whole-plot level combinations and 4 sub-plot level combinations

and that's just for a 2^5 factorial design with 3 hard-to-change variables and 2 easy-to-change variables !

The 2^3 factorial design revisited

x_1	x_2	x_3	D1	D2		D3		D4
-1	-1	-1	1	1	1	1	1	1
-1	-1	$+1$	2	2	2	1	2	1
-1	$+1$	-1	2	3	2	1	2	1
-1	$+1$	$+1$	1	1	3	1	1	1
$+1$	-1	-1	3	5	4	2	3	2
$+1$	-1	$+1$	4	4	5	3	3	2
$+1$	$+1$	-1	4	4	6	3	3	2
$+1$	$+1$	$+1$	3	6	4	2	3	2

D-optimal for **main-effects** model

(4 whole plots of size 2)

The 2^3 factorial design revisited

x_1	x_2	x_3	D1	D2		D3		D4
-1	-1	-1	1	1	1	1	1	1
-1	-1	$+1$	2	2	2	1	2	1
-1	$+1$	-1	2	3	2	1	2	1
-1	$+1$	$+1$	1	1	3	1	1	1
$+1$	-1	-1	3	5	4	2	3	2
$+1$	-1	$+1$	4	4	5	3	3	2
$+1$	$+1$	-1	4	4	6	3	3	2
$+1$	$+1$	$+1$	3	6	4	2	3	2

A-, G- and V-optimal for **main-effects** model

(2 whole plots of size 2 + 4 of size 1)

The 2^3 factorial design revisited

x_1	x_2	x_3	D1	D2		D3		D4
-1	-1	-1	1	1	1	1	1	1
-1	-1	$+1$	2	2	2	1	2	1
-1	$+1$	-1	2	3	2	1	2	1
-1	$+1$	$+1$	1	1	3	1	1	1
$+1$	-1	-1	3	5	4	2	3	2
$+1$	-1	$+1$	4	4	5	3	3	2
$+1$	$+1$	-1	4	4	6	3	3	2
$+1$	$+1$	$+1$	3	6	4	2	3	2

D-optimal for **main-effects + 2 f.i.** model when small correlation

(4 whole plots of size 2)

The 2^3 factorial design revisited

x_1	x_2	x_3	D1	D2		D3		D4
-1	-1	-1	1	1	1	1	1	1
-1	-1	$+1$	2	2	2	1	2	1
-1	$+1$	-1	2	3	2	1	2	1
-1	$+1$	$+1$	1	1	3	1	1	1
$+1$	-1	-1	3	5	4	2	3	2
$+1$	-1	$+1$	4	4	5	3	3	2
$+1$	$+1$	-1	4	4	6	3	3	2
$+1$	$+1$	$+1$	3	6	4	2	3	2

D-optimal for **main-effects + 2 f.i.** model when highly correlated observations

(2 whole plots of size 2 + 1 of size 4)

The 2^3 factorial design revisited

x_1	x_2	x_3	D1	D2		D3		D4
-1	-1	-1	1	1	1	1	1	1
-1	-1	$+1$	2	2	2	1	2	1
-1	$+1$	-1	2	3	2	1	2	1
-1	$+1$	$+1$	1	1	3	1	1	1
$+1$	-1	-1	3	5	4	2	3	2
$+1$	-1	$+1$	4	4	5	3	3	2
$+1$	$+1$	-1	4	4	6	3	3	2
$+1$	$+1$	$+1$	3	6	4	2	3	2

A-, G-, V- optimal for **main-effects + 2 f.i.** model

(4 whole plots of size 2)

The 2^3 factorial design revisited

x_1	x_2	x_3	D1	D2		D3		D4
-1	-1	-1	1	1	1	1	1	1
-1	-1	$+1$	2	2	2	1	2	1
-1	$+1$	-1	2	3	2	1	2	1
-1	$+1$	$+1$	1	1	3	1	1	1
$+1$	-1	-1	3	5	4	2	3	2
$+1$	-1	$+1$	4	4	5	3	3	2
$+1$	$+1$	-1	4	4	6	3	3	2
$+1$	$+1$	$+1$	3	6	4	2	3	2

D-optimal for saturated model with
main effect, 2 f.i.'s and 3 f.i.

(2 whole plots of size 4)

The 2^3 factorial design: conclusion

- all criteria lead to different designs
- the optimal designs strongly depend on the model
- unbalanced designs can be optimal
- the completely randomized design (CRD) is not optimal !
  - $\eta = 0.5$
    - 31/225 designs outperform the CRD in terms of D-eff.
    - 14/225 designs outperform it in terms of A- and V-eff.
    - 2/225 designs outperform it in terms of G-eff.
  - $\eta = 2$
    - 201/225 designs outperform the CRD in terms of D-eff.
    - 46/225 designs outperform it in terms of A- and V-eff.
    - 2/225 designs outperform it in terms of G-eff.

3 design strategies: Option I

- orthogonal main-effect plan
- option I
  - split runs at each whole-plot factor in 2 whole plots using highest-order sub-plot interaction contrast
  - 2^{m_w+1} whole plots of size 2^{m_s-1}
  - information matrix
    - diagonal
    - whole-plot terms (+ intercept): $\dfrac{n}{1+\eta\times 2^{m_s-1}}$
    - sub-plot terms: n

Option I: Illustration

x1	x2	x3	x2x3
-	-	-	+
-	-	+	-
-	+	-	-
-	+	+	+
+	-	-	+
+	-	+	-
+	+	-	-
+	+	+	+

Option I vs CRD

- D-efficiency

	m_s						
m_w	2	3	4	5	6	7	8
1	0.0000	0.0000	0.1143	0.2693	0.3802	0.4624	0.5255
2	0.6377	2.0000	2.9403	3.6041	4.0902	4.4584	4.7455
3	1.6180	4.1469	6.0000	7.3550	8.3723	9.1580	9.7805
4	3.0796	7.6682	11.2655	14.0000	16.1078	17.7679	19.1033
5	5.2223	13.3739	20.2439	25.6875	30.0000	33.4641	36.2927
6	8.3300	22.5511	35.4713	46.1584	54.8657	62.0000	67.9125

- A-, G-efficiency: CRD always better
- V-efficiency: CRD always better

3 design strategies: Option II

- orthogonal main-effect plan
- option II
  - create whole plots of size 2 by taking runs together which have opposite signs for sub-plot variables (*mirror-image pairs* (Tyssedal & Kulahci 2005))
  - n / 2 whole plots of size 2
  - information matrix
    - diagonal
    - whole-plot terms (+ intercept): $\dfrac{n}{1+\eta\times 2}$
    - sub-plot terms: n

Option II: Illustration

x1	x2	x3
-	-	-
-	-	+
-	+	-
-	+	+
+	-	-
+	-	+
+	+	-
+	+	+

Option II vs CRD: D-efficiency

- D-efficiency

	m_s						
m_w	2	3	4	5	6	7	8
1	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2	0.6377	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
3	1.6180	0.3924	0.0000	0.0000	0.0000	0.0000	0.0000
4	3.0796	0.9206	0.2827	0.0000	0.0000	0.0000	0.0000
5	5.2223	1.6180	0.6377	0.2207	0.0000	0.0000	0.0000
6	8.3300	2.5280	1.0776	0.4863	0.1810	0.0000	0.0000

- A-, G-efficiency: option II beats CRD if $m_w < m_s - 1$
- V-efficiency: option II beats CRD if $m_w < m_s - 3$

3 design strategies: Option III

- orthogonal main-effect plan
- option III
  - split entire design in two using highest-order interaction
  - run one half as a CRD
  - run other half as a split-plot design with 2^{m_w+1} whole plots
  - 2^{m_w} whole plots of size 2^{m_s-1} + 2^m of size 1
  - information matrix
    - diagonal
    - whole-plot terms (+ intercept): $\frac{n}{1+\eta} \times \frac{2+\eta\left(2^{m_s-1}+1\right)}{2+\eta \times 2^{m_s}}$
    - sub-plot terms: $\frac{n}{1+\eta} \times \left(1+\eta/2\right)$

Option III: Illustration

x1	x2	x3	x1x2x3
-	-	-	-
-	-	+	+
-	+	-	+
-	+	+	-
+	-	-	+
+	-	+	-
+	+	-	-
+	+	+	+

Option III vs CRD: D-efficiency

	m_s						
m_w	2	3	4	5	6	7	8
1	0.0000	0.3660	0.4733	0.4775	0.4449	0.4027	0.3616
2	0.3621	0.8000	0.8716	0.8186	0.7333	0.6483	0.5734
3	0.7870	1.3120	1.3333	1.2063	1.0556	0.9188	0.8042
4	1.2840	1.9151	1.8683	1.6471	1.4157	1.2170	1.0557
5	1.8646	2.6248	2.4879	2.1479	1.8182	1.5456	1.3297
6	2.5419	3.4593	3.2053	2.7170	2.2679	1.9077	1.6282

design option III performs reasonably well compared to the CRD when m_w is small

Option III vs CRD

- A-, G-efficiency: design option III is not too bad for small m_w

	m_s						
m_w	2	3	4	5	6	7	8
1	0.0000	0.6667	0.9091	0.9091	0.8235	0.7234	0.6324
2	0.6667	2.0000	2.2667	2.0000	1.6571	1.3684	1.1459
3	2.0000	6.0000	6.0000	4.4000	3.1892	2.4138	1.9084
4	6.0000	>>100	62.0000	14.0000	6.9302	4.4000	3.1587
5	>>100	>>100	>>100	>>100	30.0000	9.6364	5.5852
6	>>100	>>100	>>100	>>100	>>100	62.0000	12.3217

- V-efficiency: design option III is inferior to CRD in practical situations

Discussion

- relatively new design problem
  - most research on split-plot designs concentrates on different types of experiments
  - Webb, Lucas, Borkowski, … have looked at the average efficiency of using random run orders only
  - it is better to search for good run orders
- optimal numbers and sizes of whole plots heavily depend on model, optimality criterion, and variance ratio η

Discussion

- main-effects models
- several good arrangements of 2-level factorial design were presented
- designs that use mirror image pairs as whole plots perform very well with respect to all design criteria
  - + OLS and GLS are equivalent
  - – 2 f.i. coefficients are not estimated as efficiently as main effects
  - ± n/2 whole plots
    - expensive
    - whole-plot (and 2 f.i.) coefficients are estimated quite well

Optimal two-level split-plot designs

Peter Goos

Universiteit Antwerpen

James M. Lucas

J.M. Lucas & Associates