Response Surface Designs for Crossed and Nested Multi-Stratum Structures

In this document, we describe the algorithms used to construct designs, show how pure error degrees of freedom are calculated and give the designs obtained for the examples illustrated in the paper and their efficiencies. A brief sensitivity study is given to explore the dependence of designs on the criterion weights.

S1 Exchange Algorithms

The point and coordinate exchange algorithms for row-column designs are presented in Algorithm 1 and Algorithm 2, respectively. It should be noted that, except for the precise definition of the matrix $\mathbf{Q}$, the algorithms are essentially the same as for completely randomized or blocked designs.

Algorithm 1: Point Exchange Algorithm

Input : Number of factors `K`; candidate set `CAND`; number of rows `r`; number of columns `c`; model terms formula; number of random starting designs $Ntries$; weights for compound criteria $\kappa_D, \ldots, \kappa_{DF}$; weight vector for model parameters $\mathbf{W}$; significance levels α_{DP} and α_{LP}; logical flag for multiple comparisons correction `MC`

Output: Optimized design matrix $\mathbf{X}$

```
n ← r · c
N ← number of rows in CAND
T ← treatment labels for rows in CAND
Q ← matrix as defined in equation (6)
for m ← 1 to Ntries do
    det ← 0
    while det ≤ 0 do
        X ← model matrix (no intercept) for randomly sampled design from CAND
        det ← det(X^⊤ Q X)
    t ← treatment labels for the sampled design
    crit ← evaluate expression (7)
    improve ← 1
    while improve = 1 do
        improve ← 0
        for i ← 1 to n do
            for j ← 1 to N do
                if t[i] ≠ T[j] then
                    temp_X ← X
                    temp_t ← t
                    Exchange temp_X[i, 1 : K] ← CAND[j, ]
                    Exchange temp_t[i] ← T[j]
                    Complete columns of temp_X[i, ] according to model terms
                    crit_temp ← evaluate expression (7)
                    if crit_temp > crit then
                        improve ← 1
                        crit ← crit_temp
                        X[i, ] ← temp_X[i, ]
                        t[i] ← temp_t[i]
    if m = 1 then
        X_best ← X
        crit_best ← crit
    else
        if crit > crit_best then
            X_best ← X
            crit_best ← crit
return X_best
```

Algorithm 2: Coordinate Exchange Algorithm

Input : Number of factors K; candidate factor levels `levels[K][.]`; number of rows r; number of columns c; model terms formula; number of random starting designs *Ntries*; weights for compound criteria $\kappa_D, \ldots, \kappa_{DF}$; weight vector for model parameters $\mathbf{W}$; significance levels α_{DP} and α_{LP}; logical flag for multiple comparisons correction `MC`

Output: Optimized design matrix $\mathbf{X}$

```
n ← r · c
Q ← matrix as defined in equation (6)
for m ← 1 to N_tries do
    det ← 0
    while det ≤ 0 do
        X ← model matrix (no intercept) for randomly generated design
        det ← det(XᵀQX)
    t ← treatment labels for X[, 1 : K]
    crit ← evaluate expression (7)
    improve ← 1
    while improve = 1 do
        improve ← 0
        for i ← 1 to n do
            for j ← 1 to K do
                x_current ← X[i, j]
                foreach coordinate ∈ levels[j] do
                    if coordinate ≠ x_current then
                        temp_X ← X
                        Replace temp_X[i, j] ← coordinate
                        t ← treatment labels for temp_X[, 1 : K]
                        Complete columns of temp_X[i, ] according to model terms
                        crit_temp ← evaluate expression (7)
                        if crit_temp > crit then
                            improve ← 1
                            crit ← crit_temp
                            X[i, ] ← temp_X[i, ]
    if m = 1 then
        X_best ← X
        crit_best ← crit
    else
        if crit > crit_best then
            X_best ← X
            crit_best ← crit
return X_best
```

S2 Degrees of freedom in stratum s during design construction

For stratum s, in which at least one treatment factor will be applied, the *working* full model for the *responses* (fixed-effects model) is

$$\mathrm{E}(\mathbf{Y}_s) = \mathbf{Z}_s\mathbf{b}_s + \mathbf{T}_s\boldsymbol{\mu}_s = \mathbf{F}_s\boldsymbol{\theta}_s, \tag{S1}$$

where $\mathbf{F}_s = [\mathbf{Z}_s \parallel \mathbf{T}_s]$ ($\parallel$ is the operator representing stacking) and $\mathbf{Z}_s$ and $\mathbf{T}_s$ are indicator matrices for blocking units and treatments, respectively, all having m_s rows, the number of units in stratum s. The form of the matrix $\mathbf{Z}_s$ depends on the relationship between strata U_l for $l \in \{s-3,\ s-2,\ s-1,\ s\}$ as indicated in the flowchart in Figure 1 (main text).

The matrix $\mathbf{T}_s$ in equation (S1) depends on the relations between stratum s and higher strata. Let

$$\mathcal{K}(s) \subseteq \{\{1,\ldots,s-1|\ U_k \text{ has factors applied to its units}\} \cap U_k/U_s\}\}$$

and $\mathfrak{X}_k^s$ be the matrix of the treatment factor level combinations applied to stratum k ($k \in \mathcal{K}(S+1)$), with each row replicated as appropriate to form the matrix for the design in stratum s, i.e. a matrix with m_s units (rows). Then, the matrix of treatment factor level combinations that are applied to all strata up to stratum s, in which stratum s is nested, is

$$\mathcal{T}_s = \begin{cases} \left[\left(\parallel_{k\in\mathcal{K}(s)} \mathfrak{X}_k^s\right) \parallel \mathfrak{X}_s\right], & \text{if stratum } s \text{ has factors applied to its units;} \\ \left[\parallel_{k\in\mathcal{K}(s)} \mathfrak{X}_k^s\right], & \text{otherwise.} \end{cases} \tag{S2}$$

Therefore, the columns of $\mathbf{T}_s$ are indicators for the treatments in the matrix $\mathcal{T}_s$ defined in equation (S2).

Using standard linear model results, the number of degrees of freedom of the full model (equation (S1)) is the rank of the matrix $\mathbf{M}$ minus 1, where $\mathbf{M}$ is

$$\mathbf{M} = \mathbf{F}_s^\top\mathbf{F}_s = \begin{bmatrix} \mathbf{Z}_s^\top\mathbf{Z}_s & \mathbf{Z}_s^\top\mathbf{T}_s \\ \mathbf{T}_s^\top\mathbf{Z}_s & \mathbf{T}_s^\top\mathbf{T}_s \end{bmatrix} = \begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{B}^\top & \mathbf{D} \end{bmatrix}.$$

For such structured $\mathbf{M}$ matrix, the rank condition

$$rank(\mathbf{M}) = rank(\mathbf{A}) + rank(\mathbf{S})$$

is always satisfied, where $\mathbf{S} = \mathbf{D} - \mathbf{B}^\top\mathbf{A}^-\mathbf{B}$ is the generalized Schur complement of $\mathbf{A}$ and $\mathbf{A}^-$ is a generalized inverse of $\mathbf{A}$ (Searle, 1982, p.263). Thus, after allowing for the estimation of the blocking effects associated with $\mathbf{Z}_s$, the number of degrees of freedom remaining for treatments is

$$\begin{aligned} rank(\mathbf{S}) &= rank(\mathbf{M}) - rank(\mathbf{A}) \\ &= rank(\mathbf{F}_s^\top \mathbf{F}_s) - rank(\mathbf{Z}_s^\top \mathbf{Z}_s) \\ &= rank(\mathbf{Z}_s \| \mathbf{T}_s) - rank(\mathbf{Z}_s). \end{aligned}$$

Thus, the number of treatments from which effects can be estimated in stratum s, is

$$t_s = rank(\mathbf{S}) + 1.$$

Similarly, the number of degrees of freedom for the error term can be developed following standard results. It is given by

$$d_s = rank(\mathbf{I}_s - \mathbf{F}_s(\mathbf{F}_s^\top \mathbf{F}_s)^- \mathbf{F}_s) = m_s - rank(\mathbf{F}_s) = m_s - rank(\mathbf{Z}_s \| \mathbf{T}_s). \tag{S3}$$

S3 Degrees of freedom for the final design

Once the final design is obtained, the degrees of freedom for pure error are calculated following similar standard results, but now using the $\mathbf{Z}$'s and $\mathbf{T}$ matrices for the whole design with the total number of units or runs equal to $n = \prod_{s=1}^{S+1} n_s$. Thus, the columns of $\mathbf{T}$ are indicators of treatments formed by $\mathcal{T} = [\|_{k \in \mathcal{K}(S+1)} \mathfrak{X}_k]$ where $\mathcal{K}(S+1) \subseteq \{\{1, \ldots, S+1\} | \ U_k$ has factors applied to it units$\}$ and $\mathfrak{X}_k$ is the matrix of the treatment factor level combinations applied to stratum k ($k \in \mathcal{K}(S+1)$), with each row replicated as appropriate to form the matrix for the whole design with n units.

The number of pure error degrees of freedom in each stratum s will be denoted df_{PE_s} to explicitly indicate that it may be different from d_s in Equation (S3). They are calculated using Yates' procedure (Hinkelmann and Kempthorne, 2005), so they are exact for method of moments estimation of variance components and can be considered an approximation for REML estimation. For stratum s, df_{PE_s} is the number of degrees of freedom that correspond to the sum of squares for the current stratum blocking factor $\mathbf{Z}_s$, adjusted for treatments ($\mathbf{T}$), all higher blocking factors and all blocking factors crossed with the current stratum s (Stewart and Bradley, 1993; Hinkelmann and Kempthorne, 2005). Let $\mathcal{Z}_s$ and $\mathcal{Z}_{(-s)}$ be defined as the stack matrices

$$\mathcal{Z}_{(-s)} = [\|_{i \in \mathcal{I}(S)} \ \mathbf{Z}_i],$$

$$\mathcal{Z}_s = [\mathcal{Z}_{(-s)} \| \mathbf{Z}_s]$$

where $\mathcal{I}(S) \subseteq \{\{1, \ldots, S\} \cap \{i \neq s\} \cap \{U_i \times U_s \text{ or } U_i/U_s\}\}$, such that $\mathcal{Z}_{(-s)}$ is $\mathcal{Z}_s$ with $\mathbf{Z}_s$ removed. Therefore, in stratum s, the number of PE degrees of freedom is

$$df_{PE_s} = rank(\mathbf{T} \| \mathcal{Z}_s) - rank(\mathbf{T} \| \mathcal{Z}_{(-s)}). \tag{S4}$$

The total number of treatments is $t = rank(\mathbf{T})$. Note that the number of treatment degrees of freedom arising from the skeleton anova might be larger than $t-1$ since some effects can be estimated from intra-block information as well as from inter-block information. For stratum s, we redefine $\mathbf{T}_s$ as the column indicators for treatments in the matrix $\mathcal{T}_s$ such that

$$\mathcal{T}_s = \begin{cases} [(\|_{k \in \mathcal{K}(s-1)} \ \mathfrak{X}_k) \ \| \ \mathfrak{X}_s], & \text{if stratum } s \text{ has factors applied to its units;} \\ [\|_{k \in \mathcal{K}(s-1)} \ \mathfrak{X}_k], & \text{otherwise,} \end{cases} \tag{S5}$$

where $\mathcal{K}(s-1) \subseteq \{\{1, \ldots, s-1 | \ U_k \text{ has factors applied to it units}\} \cap U_k/U_s\}\}$. Then

$$df_{Treat_s} = rank(\mathcal{Z}_s \ \| \ \mathbf{T}_s) - rank(\mathcal{Z}_s).$$

The number of lack-of-fit degrees of freedom in each stratum is

$$df_{lof_s} = df_{Treat_s} - (p_s - 1).$$

The total degrees of freedom in each stratum is shown in the Hasse diagrams. For stratum s, it is calculated as

$$df_{Total_s} = (m_s - 1) - \sum_{\substack{j=1 \\ U_j/U_s}}^{s-1} (df_{Total_j} - 1).$$

Thus, the number of lack-of-fit degrees of freedom in stratum s but for effects from the lower strata, denoted $df_{lof_{s^+}}$, is

$$df_{lof_{s^+}} = df_{Total_s} - (p_s - 1 + df_{lof_s} + df_{PE_s}).$$

S4 Sensitivity Study

The literature on compound criteria recommends running the search for several weight patterns, calculating efficiencies of each property of interest and choosing the pattern that best suits the priorities of the experimenter (see, for example, Atkinson et al. (2007, Chapter 21), McGree et al. (2008); Gilmour and Trinca (2012); da Silva et al. (2017); de Oliveira et al. (2022); Egorova and Gilmour (2025)). Here we investigate the sensitivity of the designs on the weights for Example 3. Figure S1 shows D_S and $(DP)_S$

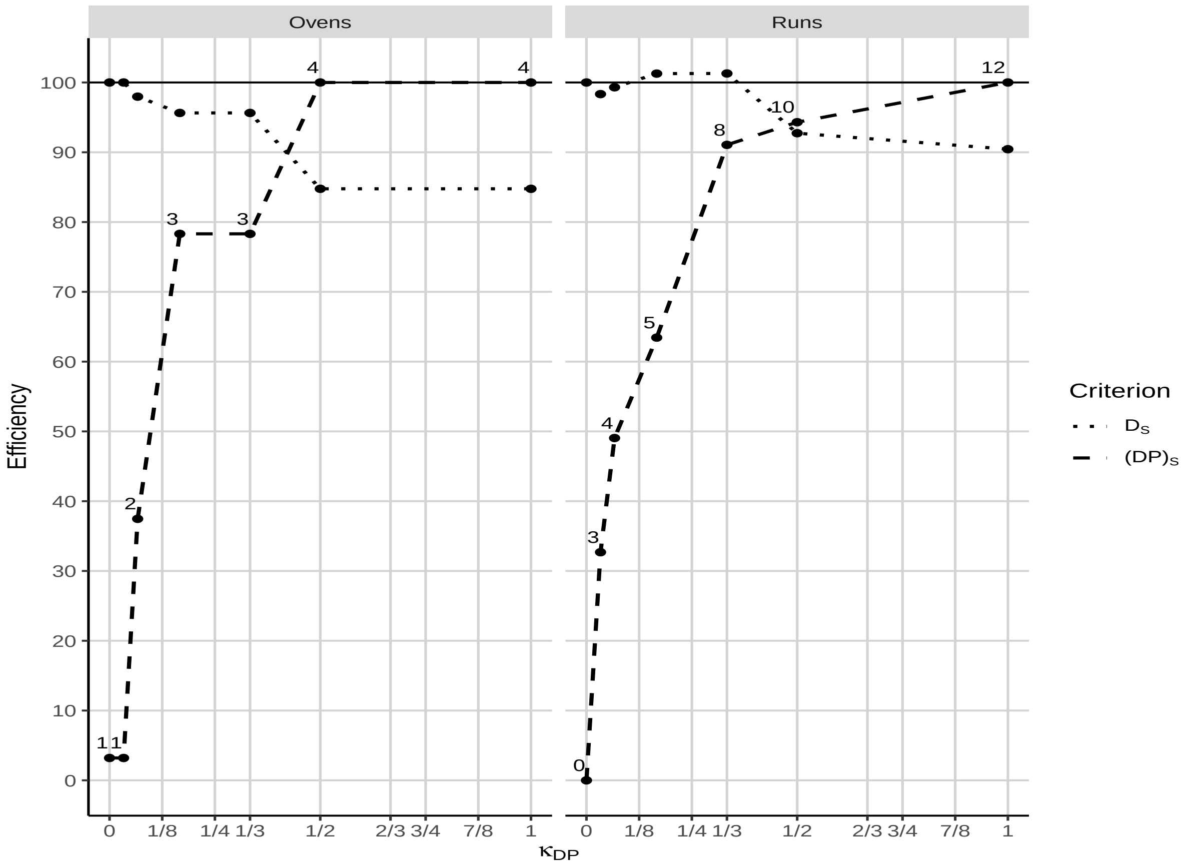

Figure S1: Efficiencies for designs in each stratum, as a function of the weight κ_{DP} in the compound criterion for Example 3.

efficiencies and pure error degrees of freedom, for each stratum, as the values of κ_{DP} were varied between 0 and 1. The design for $\kappa_D = 1$ is also included. For $0 < \kappa_{DP} < 1$ a compound criterion was used with κ_A fixed to $1/3$ and $\kappa_{DF} = 1 - (\kappa_{DP} + \kappa_A)$. Results show that small changes in the weights do not affect the properties of the design too much, except at zero weight for $(DP)_S$-optimality, where the requirement to have pure error degrees of freedom disappears.

Note that as the design in the Runs stratum is conditional on the design obtained in the Ovens stratum, it is possible to get a compromise design that is more D_S-efficient in the Runs stratum than the design obtained for $\kappa_D = 1$.

S5 Example 1

The designs constructed for Example 1 are presented in Table S1 in an unrandomized order. Randomization should be done by randomizing the Days labels to days and the Times labels to times of the day. The efficiencies of these designs, relative to the $D^\star$ design and for fixed levels of the ratios of variance components, are shown in Table S2.

Table S1: Designs for Example 1, a row×column structure Days(7)$*$Times(4), with three 3-level factors

Design $D^\star$

Days

Times		1			2			3			4			5			6			7	
1	0	-1	-1	-1	0	-1	0	0	0	-1	-1	1	1	1	0	1	-1	1	-1	1	1
2	-1	1	0	-1	-1	1	1	-1	-1	1	1	1	-1	0	-1	0	1	-1	1	-1	1
3	1	1	-1	1	-1	0	1	1	1	-1	1	-1	0	-1	1	-1	0	1	-1	-1	-1
4	1	0	1	0	1	1	-1	1	-1	0	0	0	1	-1	-1	-1	-1	0	1	1	-1

Design MSS_{D_S}

Days

Times		1			2			3			4			5			6			7	
1	1	1	1	-1	1	1	0	-1	-1	1	1	-1	1	-1	1	0	0	0	-1	0	1
2	-1	-1	1	0	-1	1	-1	1	0	-1	-1	-1	1	0	-1	1	-1	-1	1	1	1
3	-1	1	-1	-1	0	-1	1	1	-1	0	0	0	0	1	1	-1	-1	1	1	-1	0
4	1	-1	-1	1	1	0	1	0	1	-1	1	1	-1	-1	0	-1	0	1	0	1	-1

Design $\mathrm{MSS}_{(DP)_S}$

Days

Times		1			2			3			4			5			6			7	
1	-1	0	0	-1	-1	-1	-1	-1	1	0	1	0	1	-1	-1	-1	1	1	1	-1	1
2	1	1	1	1	-1	0	-1	1	-1	1	1	1	-1	1	-1	0	0	1	-1	-1	-1
3	1	-1	-1	0	0	1	0	1	0	-1	0	0	-1	-1	1	1	1	-1	-1	1	1
4	-1	-1	1	0	0	1	-1	0	0	1	-1	-1	0	1	0	1	-1	1	1	1	-1

Table S1: Designs for Example 1 (Continued)

Design MSS_{CP_κ}

Times	Days 1			2			3			4			5			6			7		
1	-1	0	-1	1	0	0	-1	-1	1	0	1	0	1	1	1	-1	1	1	0	-1	-1
2	0	1	0	-1	1	-1	1	1	1	-1	0	-1	1	-1	-1	1	-1	1	-1	-1	1
3	-1	1	1	0	-1	-1	0	0	1	1	1	-1	-1	1	-1	-1	-1	0	1	0	0
4	-1	-1	0	1	1	1	1	-1	-1	1	-1	1	0	0	1	1	1	-1	-1	1	-1

Table S2: D_S- and A_w-efficiencies, relative to the $D^\star$ design, of the row×column designs for Example 1

		Criterion							
		D_S				A_w			
		Designs				Designs			
η_{Days}	η_{Times}	D_S	$(DP)_S$	CP_κ	M_w[1]	D_S	$(DP)_S$	CP_κ	M_w[1]
1	1	99.87	84.49	93.23	82.75	100.46	78.46	90.67	75.23
1	10	99.70	83.65	93.04	82.52	100.27	77.41	90.41	74.89
1	100	99.68	83.55	93.01	82.49	100.25	77.28	90.37	74.85
10	1	99.97	83.02	92.19	82.11	100.52	76.76	89.36	74.94
10	10	99.80	82.18	91.99	81.88	100.33	75.75	89.07	74.61
10	100	99.78	82.08	91.97	81.86	100.31	75.62	89.04	74.57
100	1	99.98	82.83	92.06	82.03	100.53	76.54	89.18	74.90
100	10	99.81	81.99	91.86	81.80	100.34	75.53	88.89	74.57
100	100	99.79	81.89	91.83	81.77	100.32	75.40	88.86	74.53

[1]: Design I from Table 3 of Gilmour and Trinca (2003).

S6 Example 2

The designs constructed for Example 2 are presented in Table S3. Treatments are presented in an unrandomized order. To execute the experiment appropriate randomization is required. For that, randomize the Days labels to days and randomize the Periods labels to periods of the day.

The efficiencies of the designs, relative to the $D^\star$ design and for known values of the variance component ratios, are shown in Table S4.

Table S3: Designs for Example 2, a split-row×column structure Days(26)∗Periods(2), with 1 HS and 4 ES three-level factors

		$D^\star$							
		Morning				Afternoon			
Day	X_1	X_2	X_3	X_4	X_5	X_2	X_3	X_4	X_5
1	−1	−1	−1	−1	−1	1	1	1	−1
2	−1	−1	0	1	1	−1	1	−1	−1
3	−1	−1	1	1	−1	1	−1	1	1
4	−1	−1	0	0	−1	1	1	−1	0
5	−1	0	−1	−1	1	−1	−1	1	−1
6	−1	0	−1	1	0	1	0	−1	1
7	−1	1	−1	−1	−1	−1	1	−1	1
8	−1	1	−1	0	1	0	0	−1	−1
9	−1	1	−1	1	−1	−1	1	1	1
10	−1	1	1	−1	−1	0	−1	1	0
11	−1	1	1	1	1	−1	−1	−1	1
12	0	−1	−1	1	1	1	−1	−1	0
13	0	0	1	0	0	1	−1	1	−1
14	0	0	1	1	−1	−1	0	0	0
15	0	1	1	−1	1	−1	0	−1	−1
16	1	−1	−1	−1	1	1	1	−1	−1
17	1	−1	−1	1	−1	1	1	0	−1
18	1	−1	0	1	0	1	−1	−1	1
19	1	−1	1	−1	−1	1	1	1	1
20	1	−1	1	−1	1	0	−1	0	−1
21	1	1	−1	0	−1	−1	1	1	−1
22	1	1	−1	−1	0	0	1	0	1
23	1	1	−1	1	1	−1	−1	−1	−1
24	1	1	0	1	−1	−1	−1	1	1
25	1	1	1	−1	1	−1	1	1	1
26	1	1	1	1	−0.11	0	0	−1	1

		MSS_{D_S}							
		Morning				Afternoon			
Day	X_1	X_2	X_3	X_4	X_5	X_2	X_3	X_4	X_5
1	−1	−1	−1	−1	−1	1	1	1	−1
2	−1	−1	−1	0	1	1	−1	−1	−1
3	−1	−1	−1	1	−1	1	−1	−1	1
4	−1	−1	0	−1	−1	−1	−1	1	1
5	−1	−1	1	1	1	1	−1	1	−1
6	−1	1	−1	−1	0	−1	1	−1	1
7	−1	1	1	−1	−1	1	−1	1	1
8	−1	1	1	−1	1	−1	1	1	−1
9	−1	1	1	1	1	−1	−1	−1	1
10	0	−1	1	1	0	0	0	0	−1
11	0	0	−1	1	1	1	0	0	0
12	0	0	0	1	0	−1	1	0	−1
13	0	0	1	0	0	−1	0	1	1
14	0	1	−1	0	−1	−1	0	−1	0
15	0	1	−1	1	−1	0	1	−1	−1
16	0	1	0	0	−1	1	1	−1	1
17	0	1	1	1	−1	0	0	0	0
18	1	−1	−1	1	1	0	1	1	−1
19	1	−1	1	−1	−1	0	1	1	1
20	1	−1	1	−1	1	−1	−1	1	−1
21	1	−1	1	1	−1	1	−1	−1	−1
22	1	0	−1	1	−1	1	1	1	1
23	1	1	−1	−1	1	−1	1	1	1
24	1	1	−1	1	1	−1	−1	−1	−1
25	1	1	0	−1	1	1	−1	1	0
26	1	1	1	−1	−1	−1	−1	−1	1

Table S3: Designs for Example 2 (Continued)

		$\mathrm{MSS}_{(DP)_S}$							
		Morning				Afternoon			
Day	X_1	X_2	X_3	X_4	X_5	X_2	X_3	X_4	X_5
1	−1	−1	−1	−1	1	1	−1	1	−1
2	−1	−1	0	−1	−1	−1	1	0	1
3	−1	−1	0	−1	−1	−1	1	0	1
4	−1	0	−1	0	1	−1	1	1	0
5	−1	0	−1	0	1	−1	1	1	0
6	−1	1	−1	−1	0	−1	0	1	1
7	−1	1	1	0	−1	0	−1	1	0
8	−1	1	1	1	0	−1	1	−1	1
9	−1	1	1	1	1	−1	1	1	−1
10	0	−1	0	−1	1	0	1	−1	−1
11	0	−1	−1	1	1	0	0	0	−1
12	0	1	0	0	−1	−1	−1	0	−1
13	0	1	0	0	−1	−1	−1	0	−1
14	0	1	0	0	−1	−1	−1	0	−1
15	0	1	1	−1	1	1	−1	−1	−1
16	0	0	1	0	0	1	−1	−1	1
17	0	0	1	1	−1	1	0	0	0
18	1	−1	1	−1	−1	−1	−1	1	−1
19	1	−1	1	1	−1	−1	−1	−1	1
20	1	0	−1	−1	−1	1	1	1	−1
21	1	1	−1	1	−1	−1	1	1	1
22	1	1	1	−1	−1	1	−1	1	1
23	1	1	1	−1	−1	1	−1	1	1
24	1	1	1	−1	−1	1	−1	1	1
25	1	1	1	0	1	−1	0	0	0
26	1	1	1	0	1	−1	0	0	0

		MSS_{CP_κ}							
		Morning				Afternoon			
Day	X_1	X_2	X_3	X_4	X_5	X_2	X_3	X_4	X_5
1	−1	−1	1	−1	−1	1	−1	1	−1
2	−1	−1	1	1	−1	1	1	−1	1
3	−1	−1	1	1	1	0	−1	−1	−1
4	−1	0	0	0	1	1	1	0	−1
5	−1	0	0	0	1	1	1	0	−1
6	−1	1	−1	−1	1	0	0	0	−1
7	−1	1	1	−1	1	−1	−1	1	1
8	−1	1	1	1	1	−1	1	−1	1
9	−1	1	1	1	1	−1	1	−1	1
10	0	−1	−1	−1	−1	0	1	0	−1
11	0	−1	−1	−1	−1	0	1	0	−1
12	0	−1	−1	0	1	1	−1	1	1
13	0	−1	−1	0	1	1	−1	1	1
14	0	−1	−1	1	−1	1	0	−1	0
15	0	0	1	1	0	1	−1	0	1
16	0	1	−1	−1	−1	1	1	1	−1
17	0	1	−1	−1	−1	1	1	1	−1
18	1	−1	0	1	1	0	−1	−1	−1
19	1	−1	1	−1	−1	1	1	−1	1
20	1	−1	1	−1	1	−1	−1	1	0
21	1	0	−1	1	1	−1	0	1	−1
22	1	0	0	−1	0	0	1	1	1
23	1	0	0	−1	0	0	1	1	1
24	1	1	0	1	−1	−1	1	−1	0
25	1	1	1	−1	−1	1	−1	0	0
26	1	1	1	0	0	0	−1	−1	1

Table S4: D_S- and A_w-efficiencies, relative to the $D^\star$ design, given η's, of the split-row×column designs for Example 2

		Criterion							
		D_S Designs				A_w Designs			
η_{Days}	$\eta_{Periods}$	MSS$_{D_S}$	MSS$_{(DP)_S}$	MSS$_{CP_\kappa}$	CP[1]	MSS$_{D_S}$	MSS$_{(DP)_S}$	MSS$_{CP_\kappa}$	CP[1]
1	1	97.67	81.67	86.56	80.80	96.62	76.92	84.21	77.49
1	10	97.66	81.56	86.51	80.52	96.61	76.81	84.16	76.78
1	100	97.66	81.55	86.50	80.49	96.61	76.80	84.15	76.70
10	1	100.97	79.02	86.30	79.07	110.01	89.59	98.61	90.44
10	10	100.95	78.89	86.24	78.62	110.00	89.49	98.55	89.29
10	100	100.95	78.88	86.23	78.57	110.00	89.47	98.55	89.15
100	1	101.81	78.26	86.27	78.67	117.13	111.76	114.46	112.07
100	10	101.80	78.13	86.20	78.16	117.13	111.72	114.45	111.67
100	100	101.80	78.11	86.20	78.10	117.13	111.72	114.45	111.62

[1]: Design labeled as CP in Table 1 of Trinca and Gilmour (2017) with post-crossing.

S7 Example 3

The designs constructed for Example 3 are presented in Table S5. Treatments are presented in unrandomized order. To execute the experiment appropriate randomization is required. For that, randomize the Ovens labels to ovens, the Batches labels to batches and the Runs labels to runs within each combination of Oven×Batch. The efficiencies of the designs, relative to MSS_{D_S} and for known values of the variance components, are given in Table S6.

Table S5: Designs for Example 3, a strip-split-plot structure (Ovens(10)$*$Batches(3))/Runs(2), with two HS and three ES 3-level factors

Design $D^{\star}$

Oven		Batch 1			Batch 2			Batch 3		
X_1	X_2	X_3	X_4	X_5	X_3	X_4	X_5	X_3	X_4	X_5
-1	-1	-1	-1	1	1	-1	-1	0	0	-1
		-1	1	-1	1	-1	0	1	1	1
-1	-1	1	1	-1	-1	1	0	1	1	1
		1	-1	1	-1	0	1	-1	-1	-1
-1	1	-1	-1	-1	-1	1	1	-1	1	1
		0	1	-1	1	0	0	1	-1	1
-1	1	1	1	1	0	-1	1	1	-1	-1
		1	1	-1	-1	1	-1	-1	-1	0
0	1	1	1	-1	-1	-1	-1	-1	1	-1
		-1	0	1	1	-1	1	0	1	0
1	-1	-1	1	1	1	-1	1	0	-1	-1
		-1	-1	-1	1	1	-1	-1	0	1
1	-1	1	-1	0	-1	-1	1	-1	1	-1
		1	1	1	-1	-1	-1	1	0	-1
1	0	-1	1	-1	1	1	-1	1	0	1
		-1	-1	0	0	1	1	1	-1	-1
1	1	0	0	0	1	1	1	-1	-1	1
		1	-1	-1	-1	1	1	-1	1	-1
1	1	1	-1	1	-1	0	-1	1	1	0
		-1	1	1	0	-1	-1	-1	-1	1

Design MSS_{D_S}

Oven		Batch 1			Batch 2			Batch 3		
X_1	X_2	X_3	X_4	X_5	X_3	X_4	X_5	X_3	X_4	X_5
-1	-1	-1	1	0	-1	-1	-1	-1	-1	-1
		1	-1	1	-1	1	1	1	1	-1
-1	0	-1	-1	1	1	1	1	-1	1	-1
		1	-1	-1	1	-1	-1	1	0	0
-1	1	-1	1	1	-1	-1	0	0	-1	1
		1	1	-1	1	1	1	-1	1	-1
0	-1	0	1	-1	1	-1	1	-1	-1	1
		-1	0	1	1	1	-1	1	1	1
0	0	1	-1	0	0	1	1	1	1	0
		0	0	-1	1	0	0	0	0	-1
0	1	0	1	0	-1	0	0	1	-1	1
		-1	-1	-1	1	-1	-1	0	0	-1
1	-1	1	1	1	0	-1	1	-1	1	1
		-1	-1	-1	-1	1	-1	1	-1	-1
1	0	1	1	-1	1	-1	-1	1	0	-1
		-1	0	0	-1	1	-1	-1	-1	0
1	1	1	-1	1	0	-1	1	-1	1	1
		-1	1	1	1	1	-1	0	-1	-1
1	1	1	0	1	-1	-1	1	1	1	1
		-1	-1	-1	0	1	0	-1	1	-1

Table S5: Designs for Example 3 (Continued)

Design $\mathrm{MSS}_{(DP)_S}$

Oven		Batch								
		1			2			3		
X_1	X_2	X_3	X_4	X_5	X_3	X_4	X_5	X_3	X_4	X_5
-1	-1	1	1	-1	1	-1	-1	0	1	0
		-1	0	1	-1	1	-1	-1	-1	-1
-1	-1	-1	-1	-1	1	-1	-1	-1	1	-1
		0	1	0	1	1	1	1	1	1
-1	1	1	1	-1	1	1	1	1	0	-1
		1	-1	1	-1	-1	0	-1	1	1
-1	1	1	1	1	-1	1	1	1	-1	1
		-1	-1	0	1	0	-1	1	1	-1
0	0	0	-1	-1	-1	0	0	0	-1	-1
		-1	-1	1	0	-1	1	-1	-1	1
0	1	-1	-1	-1	1	1	-1	-1	0	1
		1	1	-1	-1	-1	-1	1	1	0
1	-1	1	1	-1	-1	1	1	-1	-1	0
		1	-1	1	1	0	-1	1	1	1
1	-1	-1	1	1	1	1	1	1	1	-1
		1	0	-1	-1	-1	0	1	-1	1
1	1	1	-1	-1	0	1	-1	-1	1	-1
		-1	1	0	1	-1	0	0	0	1
1	1	0	0	1	-1	-1	1	1	-1	-1
		-1	1	-1	1	1	0	-1	1	0

Design MSS_{CP_κ}

Oven		Batch								
		1			2			3		
X_1	X_2	X_3	X_4	X_5	X_3	X_4	X_5	X_3	X_4	X_5
-1	-1	1	0	1	-1	-1	1	-1	1	1
		-1	-1	-1	0	1	-1	1	-1	1
-1	-1	-1	-1	1	-1	1	-1	1	0	-1
		0	1	-1	1	-1	-1	0	-1	1
-1	1	-1	-1	-1	1	-1	1	-1	-1	-1
		-1	1	1	-1	1	-1	1	1	-1
-1	1	0	-1	0	-1	-1	-1	1	-1	1
		1	1	1	-1	1	1	-1	1	-1
0	-1	-1	1	-1	1	1	1	1	1	1
		0	-1	0	-1	0	-1	-1	0	-1
0	0	0	0	1	0	0	1	0	1	0
		1	-1	0	1	-1	0	1	0	-1
1	-1	-1	1	1	-1	-1	-1	1	1	-1
		1	1	-1	-1	1	1	-1	-1	-1
1	0	1	-1	1	1	-1	1	1	-1	1
		-1	-1	-1	0	1	0	0	1	0
1	1	1	-1	-1	1	0	0	0	1	1
		-1	0	0	-1	1	-1	-1	-1	0
1	1	-1	-1	1	0	-1	-1	1	0	0
		-1	1	-1	1	1	1	-1	-1	1

Table S6: D_S- and A_w-efficiencies, relative to the best fixed-effects D design obtained, the MSS_{D_S}, given η's, for the strip-split-plot designs for Example 3.

			D_S Designs			A_w Designs		
η_{Oven}	η_{Batch}	$\eta_{Oven*Batch}$	$D^\star$	$\text{MSS}_{(DP)_S}$	MSS_{CP_κ}	$D^\star$	$\text{MSS}_{(DP)_S}$	MSS_{CP_κ}
1	1	1	94.57	95.91	99.35	81.55	68.41	90.83
1	1	10	83.01	94.21	99.77	74.80	64.60	90.43
1	1	100	79.90	93.77	99.84	75.51	62.69	90.03
1	10	1	94.55	95.91	99.33	81.54	68.41	90.83
1	10	10	83.00	94.21	99.76	74.80	64.60	90.43
1	10	100	79.90	93.77	99.84	75.51	62.69	90.03
1	100	1	94.55	95.91	99.33	81.54	68.41	90.83
1	100	10	82.99	94.21	99.76	74.80	64.60	90.43
1	100	100	79.90	93.77	99.84	75.51	62.69	90.03
10	1	1	94.83	96.24	99.33	77.08	63.51	90.13
10	1	10	83.05	94.30	99.76	75.57	63.19	90.13
10	1	100	79.90	93.78	99.84	75.62	62.62	90.02
10	10	1	94.82	96.23	99.33	77.08	63.51	90.13
10	10	10	83.04	94.30	99.76	75.57	63.19	90.13
10	10	100	79.90	93.78	99.84	75.62	62.62	90.02
10	100	1	94.82	96.23	99.34	77.08	63.51	90.13
10	100	10	83.04	94.30	99.76	75.57	63.19	90.13
10	100	100	79.90	93.78	99.84	75.62	62.62	90.02
100	1	1	94.87	96.29	99.32	76.14	62.50	89.98
100	1	10	83.07	94.34	99.76	75.96	62.49	89.99
100	1	100	79.91	93.79	99.84	75.89	62.46	89.98
100	10	1	94.86	96.28	99.33	76.14	62.50	89.98
100	10	10	83.06	94.34	99.76	75.96	62.49	89.99
100	10	100	79.91	93.79	99.84	75.89	62.46	89.98
100	100	1	94.86	96.28	99.32	76.14	62.50	89.98
100	100	10	83.06	94.34	99.75	75.96	62.49	89.99
100	100	100	79.90	93.79	99.84	75.89	62.46	89.98

S8 Example 4

The designs for this example are stored, in an unrandomized order, in the `designs.zip` file (Supp). To randomize, we should randomize the Batch labels to batches, the Occasion labels to occasions and the Run labels to runs within each combination of Batch×Occasion. The efficiencies of designs, relative to the MSS_{D_S} design and for known values of the variance component ratios, are shown in Table S7.

Table S7: D_S- and A_w-efficiencies, relative to the MSS_{D_S} optimum design, given η's, for designs in Example 4

			Criterion			
			D_S Designs		A_w Designs	
$\eta_{Batches}$	η_{Occs}	$\eta_{Batches*Occs}$	$\text{MSS}_{(DP)_S}$	MSS_{CP_κ}	$\text{MSS}_{(DP)_S}$	MSS_{CP_κ}
1	1	1	86.11	90.96	75.42	96.44
1	1	10	85.80	90.73	77.63	93.03
1	1	100	85.75	90.69	79.16	91.30
1	10	1	86.11	90.96	88.50	98.55
1	10	10	85.80	90.73	84.69	95.51
1	10	100	85.75	90.69	80.46	91.92
1	100	1	86.11	90.96	98.18	99.79
1	100	10	85.80	90.73	96.31	99.01
1	100	100	85.75	90.69	87.97	95.28
10	1	1	86.10	90.95	75.78	95.75
10	1	10	85.79	90.72	77.67	92.94
10	1	100	85.75	90.69	79.15	91.30
10	10	1	86.10	90.95	87.83	98.11
10	10	10	85.79	90.72	84.43	95.36
10	10	100	85.75	90.69	80.44	91.92
10	100	1	86.10	90.95	97.96	99.71
10	100	10	85.79	90.72	96.14	98.95
10	100	100	85.75	90.69	87.93	95.27
100	1	1	86.10	90.95	77.21	93.32
100	1	10	85.79	90.72	77.90	92.44
100	1	100	85.75	90.69	79.08	91.32
100	10	1	86.10	90.95	84.07	95.61
100	10	10	85.79	90.72	82.69	94.31
100	10	100	85.75	90.69	80.28	91.89
100	100	1	86.10	90.95	96.03	99.01
100	100	10	85.79	90.72	94.53	98.36
100	100	100	85.75	90.69	87.47	95.10

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