Online Supplement:
Integer Programming Approaches to Find Row-Column Arrangements of Two-Level Orthogonal Experimental Designs

Nha Vo-Thanh
Institute of Crop Science, University of Hohenheim, Germany

Peter Goos
Faculty of Bioscience Engineering and Leuven Statistics Research Centre (LSTAT), KU Leuven, Belgium
Faculty of Business and Economics, University of Antwerp, Belgium

Eric D. Schoen
Faculty of Bioscience Engineering, KU Leuven, Belgium
TNO, Zeist, Netherlands

In this online supplement, we provide detailed results for a third kind of approach we utilized for arranging two-level orthogonal treatment designs in rows and columns. The third approach uses the output of the sequential approach as input for the simultaneous approach. The hope was that providing a good initial solution as input to the linearized quadratic programming approach and to the permutation-based approach would speed up the computations substantially.

The sequential approach's speed and its excellent performance in terms of the quality of the row-column arrangements suggest that using the row-column arrangement produced by the sequential approach as a starting solution for the simultaneous approach may lead to optimal row-column arrangements in less computing time. This is because many algorithms converge to good solutions more rapidly when provided with a high-quality starting solution. For all the designs problems considered earlier, we explored whether using the output of the sequential approach as input for the simultaneous approach indeed leads to computing time savings. Tables S1, S2 and S3 show our results for the treatment designs involving 24, 64 and 72 runs, respectively. The objective function values for the 24-run arrangements in Table S1 are not shown, because they are the same as those in Table 5 of the main paper.

Comparing the computing times in Table S1, obtained using the output of the sequential approach as input for the simultaneous approach, with those in Table 5 of the main paper shows that the computing time of the linearized quadratic model goes down for only seven of the 17 treatment designs. For design 12.1, the better starting solution leads to a drop in computing time of more than 12 minutes. In one case, the starting design led to an increase in computing time from about 36 seconds to about 147 seconds. Overall, the changes in computing time for the linearized quadratic model are minor. For the permutation-based approach, the better starting solution led to an improvement in computing time for nine of the 17 treatment designs. The largest improvement is again obtained for the treatment design with 12 factors. The original simultaneous approach based on the permutation-based model (without high-quality starting solution) was unable to confirm the optimality of the row-column arrangement it found for treatment design 12.1 within 10,000 seconds, while the permutation-based approach involving the better starting solution does establish the optimality of the row-column arrangement in about 4,000 seconds. Comparing the linearized quadratic model with the permutation-based model in Table S1, we can see the former is faster than the latter in all cases.

Table S1: Computing times for the linearized quadratic model (LQM) and the permutation-based model (PM) when arranging 24-run two-level treatment designs involving 4–13 factors in four rows and three columns when using the output of the sequential approach as a starting solution.

ID	LQM	PM
4.1	12.32	65.10
5.1	23.21	99.45
6.1	28.64	60.98
6.2	11.11	24.24
7.1	10.25	61.22
7.2	5.68	23.57
8.1	13.54	40.75
8.2	147.33	174.92
9.1	15.08	123.44
9.2	10.34	32.81
10.1	224.42	281.94
10.2	21.11	96.35
11.1	25.44	84.23
11.2	1448.41	2073.64
12.1	1401.90	4019.71
13.1	2.20	9.59
13.2	1.78	5.40

Table S2: Computing times and objective function values for the linearized quadratic model (LQM) and the permutation-based model (PM) when arranging 64-run two-level strength-3 designs involving 6–12 factors in four rows and four columns when using the output of the sequential approach as a starting solution. CT: computing time in seconds; Obj: objective function value.

ID	LQM		PM	
	CT	Obj	CT	Obj
6.1	2.34	0	2.45	0
7.1	0.78	0	1.08	0
8.3	0.36	0	0.64	0
9.1	0.42	0	0.75	0
9.2	0.41	0	0.78	0
10.1	0.33	0	0.78	0
11.1	0.66	0	1.22	0
11.2	84.57	0	88.90	0
11.3	0.28	0	0.80	0
11.4	109.34	0	112.65	0
12.1	44.80	0	46.85	0
12.2	107.25	0	102.06	0

Table S3: Computing times and objective function values for the linearized quadratic model (LQM) and the permutation-based model (PM) when arranging 72-run two-level strength-3 designs involving 6–12 factors in three rows and three columns when using the output of the sequential approach as a starting solution. CT: computing time in seconds; Obj: objective function value.

ID	LQM		PM	
	CT	Obj	CT	Obj
6.1	1.12	0	1.29	0
7.1	88.70	0	88.92	0
8.1	13018.32	0	20000	40048
9.1	1.17	0	1.47	0
10.1	1.00	0	1.59	0
11.1	1.17	0	1.90	0
12.1	0.31	0	1.12	0

Comparing the computing times for the 64-run designs in Table S2 with those in the top part of Table 6 of the main paper shows that the computing times for both the linearized quadratic model and the permutation-based model go down for eight of the 12 treatment designs considered. In each of these cases, the sequential approach obtained the optimal solution within a few seconds and the linearized quadratic model and the permutation-based model only need a few fractions of a second extra to confirm the optimality of the solution in terms of the objective function in Equations (19) and (40). For the remaining four treatment designs, the sequential approach fails to find solutions that are optimal in terms of the objective function in Equations (19) and (40) and it uses substantially more computing time. For each of these four cases, the computing times for the linearized quadratic model and the permutation-based model deteriorate much when using the output of the sequential approach as a starting solution. Comparing the linearized quadratic model with the permutation-based model in Table S2, we can see the former is faster than the latter in all but one case (treatment design 12.2).

Comparing the computing times for the 72-run designs in Table S3 with those in the bottom part of Table 6 in the main paper shows that the computing times of both the linearized quadratic model and the permutation-based model drop substantially (usually by at least one order of magnitude) for six of the seven 72-run treatment designs considered. Again, in each of these cases, the sequential approach obtained the optimal solution within a few seconds, and the linearized quadratic model and the permutation-based model only need a few fractions of a second extra to confirm the optimality in terms of the objective function in Equations (19) and (40). For treatment designs 9.1 and 10.1, the use of the starting solution reduced the computing time for the permutation-based model from about 6,000 seconds to about 1.5 seconds. For treatment design 7.1, the improvement is even more spectacular: the starting solution allows the linearized quadratic model and the permutation-based model to find an optimal row-column arrangement in less than 89 seconds (whereas these models did not allow the simultaneous approach to find the optimal solution within the computing time limit when not using the starting solution provided by the sequential approach). For the remaining treatment design 8.1, the sequential model fails to converge to optimality within 10,000 seconds. Using its output after 10,000 seconds as input for the linearized quadratic model results in an optimal solution after 3,000 more seconds. With the same input, the permutation-based model fails to find an optimal solution within the computing time limit.