Doubly Coupled Designs for Computer Experiments with both Qualitative and Quantitative Factors

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Supplementary Material

This supplementary material presents all the proofs, and tables of some possible DCDs produced by the proposed constructions.

S1 Proofs

Proof of Theorem 1. Since a DCD is a special MCD, part (a) follows from Proposition 1 of He et al. (2017). For part (b), when $\boldsymbol{D}_1 = \mathrm{OA}(n, q, s, 2)$, due to the property (ii) of a DCD that the rows in $\boldsymbol{D}_2$ corresponding to each of the s^2 level combinations of any two factors in $\boldsymbol{D}_1$ form an LHD with n/s^2 runs. This indicates that for $(\boldsymbol{z}_i, \boldsymbol{z}_j, \tilde{\tilde{\boldsymbol{d}}}_k)$, $1 \leq i \neq j \leq q$ and $1 \leq k \leq p$, each of all possible three-tuples occurs exactly once. $\square$

Proof of Theorem 2. We first show the necessity. If a DCD(n, s^q, p) exists, Condition (b) in Theorem 1 reveals that the rows in $\boldsymbol{D}_1$ corresponding to each level of $\tilde{\tilde{\boldsymbol{d}}}_k$ is an OA$(s^2, q, s, 2)$. Therefore, for a given k, according to the level of $\tilde{\tilde{\boldsymbol{d}}}_k$, $\boldsymbol{D}_1$ can be partitioned into n/s^2 OA$(s^2, p, s, 2)$'s, say $\boldsymbol{E}_1, \ldots, \boldsymbol{E}_{n/s^2}$. It remains to show that each $\boldsymbol{E}_i, i = 1, \ldots, n/s^2$, is a completely resolvable orthogonal array. From Condition (a) of Theorem 1, the rows in $\boldsymbol{D}_1$ corresponding to each level of $\tilde{\boldsymbol{d}}_k$ is an OA$(s, q, s, 1)$. Recall that the relationship $\tilde{\tilde{\boldsymbol{d}}}_k = \lfloor \tilde{\boldsymbol{d}}_k / s \rfloor$, which means each level in $\tilde{\tilde{\boldsymbol{d}}}_k$ corresponds to s levels in $\tilde{\boldsymbol{d}}_k$. Hence, each $\boldsymbol{E}_i$ can be divided into s OA$(s, q, s, 1)$'s, and by definition, it is a CROA$(s^2, q, s, 2)$.

Now, we show the sufficiency, that is, if $\boldsymbol{D}_1$ can be partitioned into n/s^2 CROA$(s^2, q, s, 2)$'s, then a DCD(n, s^q, p) exists. Note that $\boldsymbol{D}_1$ can be represented by $(\boldsymbol{E}_1^T, \ldots, \boldsymbol{E}_{n/s^2}^T)^T$ with $\boldsymbol{E}_i = (\boldsymbol{E}_{i,1}^T, \cdots, \boldsymbol{E}_{i,s}^T)^T$, where $\boldsymbol{E}_i$ is a CROA$(s^2, q, s, 2)$ and $\boldsymbol{E}_{i,j}$ is an OA$(s, q, s, 1)$, for $i = 1, \ldots, n/s^2$ and $j = 1, \ldots, s$. Since $\boldsymbol{E}_i$ is an OA$(s^2, q, s, 2)$, each level combination occurs once in any two columns of $\boldsymbol{E}_i$, and thus n/s^2 times in any two columns of $\boldsymbol{D}_1$. Likewise, each level appears once in any column of each $\boldsymbol{E}_{i,j}$, and thus n/s times in any column of $\boldsymbol{D}_1$. To show the existence of a DCD, given such a $\boldsymbol{D}_1$, we construct a $\boldsymbol{D}_2$. Let $\boldsymbol{d} = (\boldsymbol{g}_1^T, \cdots, \boldsymbol{g}_{n/s^2}^T)^T$, such that $\boldsymbol{g}_i = (\boldsymbol{g}_{i,1}^T, \cdots, \boldsymbol{g}_{i,s}^T)^T$, where $\boldsymbol{g}_{i,j} = ((i-1)s^2 + (j-1)s, \ldots, (i-1)s^2 + js - 1)^T$, for $i = 1, \ldots, n/s^2$ and $j = 1, \ldots, s$.

Next, we will explain that $(\boldsymbol{D}_1, \boldsymbol{d})$ is a DCD$(n, s^q, 1)$. Obviously, $\boldsymbol{d} = (0, 1, \ldots, n-1)^T$, which is an LH. Since $\lfloor \boldsymbol{g}_i/s^2 \rfloor = (i-1) \cdot \mathbf{1}_{s^2}$, where $\mathbf{1}_{s^2}$ is a column of s^2 ones, the rows in $\tilde{\tilde{\boldsymbol{d}}}$ corresponding to each level combination of any two factors in $\boldsymbol{D}_1$ are $(0, 1, \ldots, n/s^2-1)^T$, i.e., an LHD of n/s^2 runs. Moreover, $\lfloor \boldsymbol{g}_{i,j}/s \rfloor = ((i-1)s+j-1) \cdot \mathbf{1}_s$, so the rows in $\tilde{\boldsymbol{d}}$ corresponding to each level of any factor in $\boldsymbol{D}_1$ are $(0, 1, \ldots, n/s-1)^T$, which is an LHD of n/s runs. Thus, followed by Definition 1, $(\boldsymbol{D}_1, \boldsymbol{d})$ is a DCD$(n, s^q, 1)$. Besides, it can be easily checked that randomly permuting $\boldsymbol{g}_i$ in $\boldsymbol{d}$, randomly permuting $\boldsymbol{g}_{i,j}$ in $\boldsymbol{g}_i$ and randomly permuting the entries in $\boldsymbol{g}_{i,j}$ can generate additional columns of $\boldsymbol{D}_2$. □

Proof of Theorem 3. Let $\boldsymbol{D}_1 = (\boldsymbol{z}_1, \ldots, \boldsymbol{z}_q)$ be an OA$(n, q, s, 2)$, $\boldsymbol{B} = (\boldsymbol{b}_1, \ldots, \boldsymbol{b}_p)$ be an OA$(n, p, n/s^2, 1)$, and $\boldsymbol{C} = (\boldsymbol{c}_1, \ldots, \boldsymbol{c}_p)$ be an OA$(n, p, s, 1)$, such that for any $1 \le i \ne j \le q$ and $1 \le k \le p$, both $(\boldsymbol{z}_i, \boldsymbol{z}_j, \boldsymbol{b}_k)$ and $(\boldsymbol{z}_i, \boldsymbol{c}_k, \boldsymbol{b}_k)$ are OA$(n, 3, s^2\,(n/s^2), 3)$'s. Let $\widetilde{\boldsymbol{D}}_2 = s\boldsymbol{B} + \boldsymbol{C}$. To prove that the resulting design $\boldsymbol{D} = (\boldsymbol{D}_1, \boldsymbol{D}_2)$ is a DCD, it suffices to check the requirements in Theorem 1. As $(\boldsymbol{z}_i, \boldsymbol{c}_k, \boldsymbol{b}_k)$ is an OA$(n, 3, s^2\,(n/s^2), 3)$, it easily follows that $(\boldsymbol{z}_i, \tilde{\boldsymbol{d}}_k) = (\boldsymbol{z}_i, s\boldsymbol{b}_k + \boldsymbol{c}_k)$ is an OA$(n, 2, s\,(n/s), 2)$. Finally, note that $(\boldsymbol{z}_i, \boldsymbol{z}_j, \tilde{\tilde{\boldsymbol{d}}}_k)$ is an OA$(n, 3, s^2\,(n/s^2), 3)$, since $\tilde{\tilde{\boldsymbol{d}}}_k = \boldsymbol{b}_k$.

Conversely, if $(\boldsymbol{D}_1, \boldsymbol{D}_2)$ is a DCD(n, s^q, p), where $\widetilde{\boldsymbol{D}}_2 = s\boldsymbol{B} + \boldsymbol{C}$, i.e., $\tilde{\boldsymbol{d}}_k = s\boldsymbol{b}_k + \boldsymbol{c}_k$ and $\tilde{\tilde{\boldsymbol{d}}}_k = \boldsymbol{b}_k$, we will show that there exist three arrays, $\boldsymbol{D}_1 = (\boldsymbol{z}_1, \ldots, \boldsymbol{z}_q)$ is an

OA$(n, q, s, 2)$, $\boldsymbol{B} = (\boldsymbol{b}_1, \ldots, \boldsymbol{b}_p)$ is an OA$(n, p, n/s^2, 1)$, and $\boldsymbol{C} = (\boldsymbol{c}_1, \ldots, \boldsymbol{c}_p)$ is an OA$(n, p, s, 1)$, such that both $(\boldsymbol{z}_i, \boldsymbol{z}_j, \boldsymbol{b}_k)$ and $(\boldsymbol{z}_i, \boldsymbol{c}_k, \boldsymbol{b}_k)$ are OA$(n, 3, s^2\,(n/s^2), 3)$'s. Since $(\boldsymbol{D}_1, \boldsymbol{D}_2)$ is a DCD, we have that $\boldsymbol{D}_1$ is an OA$(n, q, s, 2)$ and $\boldsymbol{D}_2$ is an LH(n, p), which means that $\boldsymbol{B} = \tilde{\tilde{\boldsymbol{D}}}_2$ is an OA$(n, p, n/s^2, 1)$. Moreover, according to Theorem 1, $(\boldsymbol{z}_i, \tilde{\boldsymbol{d}}_k)$ forms an OA$(n, 2, s\,(n/s)\,, 2)$ and $(\boldsymbol{z}_i, \boldsymbol{z}_j, \tilde{\tilde{\boldsymbol{d}}}_k)$ is an OA$(n, 3, s^2\,(n/s^2)\,, 3)$, then it can be easily obtained that $(\boldsymbol{z}_i, \boldsymbol{c}_k, \boldsymbol{b}_k)$ is an OA$(n, 3, s^2\,(n/s^2)\,, 3)$, $\boldsymbol{C}$ is an OA$(n, p, s, 1)$ and $(\boldsymbol{z}_i, \boldsymbol{z}_j, \boldsymbol{b}_k)$ is an OA$(n, 3, s^2\,(n/s^2)\,, 3)$. □

Proof of Proposition 2. Stack λ $\boldsymbol{A}_1$'s row by row, and denote the resulting design by $\boldsymbol{A}_1^* = (\boldsymbol{a}_1^*, \ldots, \boldsymbol{a}_{q+1}^*)$, which is an OA$(\lambda s^2, q+1, s, 2)$. As $\boldsymbol{D}_1$ is from $\boldsymbol{A}_1^*$ by deleting the last column, we have that $\boldsymbol{D}_1 = (\boldsymbol{z}_1, \ldots, \boldsymbol{z}_q)$ is an OA $(\lambda s^2, q, s, 2)$ and $\boldsymbol{z}_i = \boldsymbol{a}_i^*$, for $1 \le i \le q$. From Step 2, it is easy to find that $\boldsymbol{B}$ is an OA$(\lambda s^2, p, \lambda, 1)$ and $(\boldsymbol{a}_i^*, \boldsymbol{a}_j^*, \boldsymbol{b}_k)$ is an OA $(\lambda s^2, 3, s^2 \times \lambda, 3)$, for any $1 \le i \ne j \le q+1$ and $1 \le k \le p$. In Step 3, note that $\boldsymbol{w}_k \otimes \boldsymbol{1}_s$ can be regarded as a level permutation of $\boldsymbol{x}_{q+1}$, where $\boldsymbol{x}_{q+1}$ represents the last column of $\boldsymbol{A}_1$, and thus $\boldsymbol{c}_k$ is a level permutation of $\boldsymbol{a}_{q+1}^*$. Clearly, $\boldsymbol{C}$ should be an OA$(n, p, s, 1)$. It is well-known that level permutations of any factor do not change the orthogonality, so $(\boldsymbol{a}_i^*, \boldsymbol{c}_k, \boldsymbol{b}_k)$ is also an OA$(\lambda s^2, 3, s^2 \times \lambda, 3)$, for any $1 \le i \ne j \le q$ and $1 \le k \le p$. Hence, $\boldsymbol{D}_1$, $\boldsymbol{B}$ and $\boldsymbol{C}$ are the needed arrays in Theorem 3. □

Proof of Proposition 3. Since $\boldsymbol{D}_1$ is a sub-array of $\boldsymbol{G}$, part (a) follows directly.

For (b), as $\boldsymbol{b}_k, \mathbf{a}^*$ and $\boldsymbol{b}'_k$ are three different columns of $\boldsymbol{G}$, i.e., $(\boldsymbol{b}_k, \mathbf{a}^*, \boldsymbol{b}_{k'})$ forms an $\mathrm{OA}(s^3, 3, s, 3)$, which implies that $(s\boldsymbol{b}_k + \mathbf{a}^*, \boldsymbol{b}_{k'})$ is an $\mathrm{OA}(s^3, 2, s^2 \times s, 2)$. Besides, level permutations of any factor do not alter the orthogonality. Thus, $(\tilde{\boldsymbol{d}}_k, \tilde{\boldsymbol{d}}_{k'}) = (s\boldsymbol{b}_k + \boldsymbol{c}_k, s\boldsymbol{b}_{k'} + \boldsymbol{c}_{k'})$ achieves $s^2 \times s$ and $s \times s^2$ grids stratification. Finally, $\widetilde{\widetilde{\boldsymbol{D}}}_2 = \boldsymbol{B} = (\boldsymbol{b}_1, \ldots, \boldsymbol{b}_p)$, the proof of (c) is similar to that of (a). □

Proof of Lemma 2. For any $k \in \{1, \ldots, (u-2)s^2\}$, there always exists a pair of integers v and f, such that $k = (f-1)(u-2) + v$, where $1 \leq v \leq u-2$ and $1 \leq f \leq s^2$. Then, $(\mathbf{a}_i, \mathbf{a}_j, \boldsymbol{b}_k) = (\mathbf{a}_i, \mathbf{a}_j, (\boldsymbol{r}_{1,f}, \ldots, \boldsymbol{r}_{u-2,f})\boldsymbol{t}_v)$ is an $\mathrm{OA}(s^u, 3, s^2(s^{u-2}), 3)$ due to Lemma 1(c). Part (b) is straightforward. □

Proof of Proposition 4. The resulting $\boldsymbol{D} = (\boldsymbol{D}_1, \boldsymbol{D}_2)$ is a DCD from Lemma 2 and Theorem 4. For (a), if $\lfloor (i-1)/(u-2) \rfloor = \lfloor (i'-1)/(u-2) \rfloor$, $\boldsymbol{b}_i$ and $\boldsymbol{b}_{i'}$ come from the same $\boldsymbol{B}_{\lfloor (i-1)/(u-2) \rfloor + 1}$. According to Equation ~~(4.4)~~ and Lemma 1(b), $\boldsymbol{b}_i$ and $\boldsymbol{b}_{i'}$ achieve the stratification on $s \times s$ grids. If $\lfloor (i-1)/(u-2) \rfloor \neq \lfloor (i'-1)/(u-2) \rfloor$, $\boldsymbol{b}_i$ and $\boldsymbol{b}_{i'}$ are from $\boldsymbol{B}_{\lfloor (i-1)/(u-2) \rfloor + 1}$ and $\boldsymbol{B}_{\lfloor (i'-1)/(u-2) \rfloor + 1}$, respectively. Similarly, part (b) follows from Lemma 1(d). □

S2 Tables of the DCDs

This section lists some examples of the DCDs generated by the proposed constructions. We omit the DCDs by Construction 2 since the results are very similar to that of Construction 1, ~~i.e., Table 3~~, except that the number of columns of the quantitative factors for Constructions 1 and 2 is $(s!)^{\lambda s} \cdot (s!)^{\lambda} \cdot \lambda!$ and $(s!)^{\lambda s} \cdot s! \cdot (\lambda!)^{s^2}$, respectively.

Table 1: DCDs produced by Construction 1, for $s \leq 11$ and a positive integer λ

s	$\boldsymbol{D}_1$	$\boldsymbol{D}_2$	Constraint
2	$OA(4\lambda, 2, 2, 2)$	$LH(4\lambda, p)$	$p \leq 2^{3\lambda} \cdot \lambda!$
3	$OA(9\lambda, 3, 3, 2)$	$LH(9\lambda, p)$	$p \leq 6^{4\lambda} \cdot \lambda!$
4	$OA(16\lambda, 4, 4, 2)$	$LH(16\lambda, p)$	$p \leq (4!)^{5\lambda} \cdot \lambda!$
5	$OA(25\lambda, 5, 5, 2)$	$LH(25\lambda, p)$	$p \leq (5!)^{6\lambda} \cdot \lambda!$
6	$OA(36\lambda, 2, 6, 2)$	$LH(36\lambda, p)$	$p \leq (6!)^{7\lambda} \cdot \lambda!$
7	$OA(49\lambda, 7, 7, 2)$	$LH(49\lambda, p)$	$p \leq (7!)^{8\lambda} \cdot \lambda!$
8	$OA(64\lambda, 8, 8, 2)$	$LH(64\lambda, p)$	$p \leq (8!)^{9\lambda} \cdot \lambda!$
9	$OA(81\lambda, 9, 9, 2)$	$LH(81\lambda, p)$	$p \leq (9!)^{10\lambda} \cdot \lambda!$
10	$OA(100\lambda, 3, 10, 2)$	$LH(100\lambda, p)$	$p \leq (10!)^{11\lambda} \cdot \lambda!$
11	$OA(121\lambda, 11, 11, 2)$	$LH(121\lambda, p)$	$p \leq (11!)^{12\lambda} \cdot \lambda!$

Table 2: DCDs produced by Case 1 of Construction 3, for $s \leq 10$

s	$\boldsymbol{D}_1$	$\boldsymbol{D}_2$	Constraint
2	$OA(8, q, 2, t)$	$LH(8, p)$	$q + p \leq 3$
3	$OA(27, q, 3, t)$	$LH(27, p)$	$q + p \leq 3$
4	$OA(64, q, 4, t)$	$LH(64, p)$	$q + p \leq 5$
5	$OA(125, q, 5, t)$	$LH(125, p)$	$q + p \leq 5$
6	$OA(216, q, 6, t)$	$LH(216, p)$	$q + p \leq 3$
7	$OA(343, q, 7, t)$	$LH(343, p)$	$q + p \leq 7$
8	$OA(512, q, 8, t)$	$LH(512, p)$	$q + p \leq 9$
9	$OA(729, q, 9, t)$	$LH(729, p)$	$q + p \leq 9$
10	$OA(1000, q, 10, t)$	$LH(1000, p)$	$q + p \leq 3$

The t refers to the strength of an orthogonal array. If $q < 3$, $t = q$, and if $q \geq 3$, $t = 3$.

Table 3: DCDs produced by Case 2 of Construction 3, for $s \leq 5$ and $n \leq 256$

s	u	$\boldsymbol{D}_1$	$\boldsymbol{D}_2$
2	3	$OA(8,2,2,2)$	$LH(8,4)$
2	4	$OA(16,2,2,2)$	$LH(16,8)$
2	5	$OA(32,2,2,2)$	$LH(32,12)$
2	6	$OA(64,2,2,2)$	$LH(64,16)$
2	7	$OA(128,2,2,2)$	$LH(128,20)$
2	8	$OA(256,2,2,2)$	$LH(256,24)$
3	3	$OA(27,3,3,2)$	$LH(27,9)$
3	4	$OA(81,3,3,2)$	$LH(81,18)$
3	5	$OA(243,3,3,2)$	$LH(243,27)$
4	3	$OA(64,4,4,2)$	$LH(64,16)$
4	4	$OA(256,4,4,2)$	$LH(256,32)$
5	3	$OA(125,5,5,2)$	$LH(125,25)$

Bibliography

He, Y., Lin, C. D. and Sun, F. (2017). On the construction of marginally coupled designs. *Statistica Sinica 27*, pp. 665-683.