

INTER-EFFECT ORTHOGONALITY AND OPTIMALITY IN HIERARCHICAL MODELS

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SUMMARY. It is shown that in hierarchical models if a fractional factorial plan allows inter-effect orthogonality then it is also universally optimal. It is also demonstrated that this phenomenon does not necessarily hold in non-hierarchical models. A combinatorial characterization for inter-effect orthogonality is given for hierarchical models and its applications are indicated.

1. Introduction

The study of optimal fractional factorial plans has received considerable attention over the last two decades. The universal optimality of plans based on orthogonal arrays was shown by Cheng (1980) and Mukerjee (1982). Various extensions of this result have also been reported in the literature; see Mukerjee (1995) for a brief review. Most of these results relate to situations where all factorial effects involving the same number of factors are considered equally important and, as such, the underlying model involves the general mean and all effects involving up to a specified number of factors.

The aforesaid presumption of equality in the importance of all factorial effects involving the same number of factors is, however, not tenable in many practical situations. For example, there may be a reason to believe that only one of the factors can possibly interact with the others and that interactions involving three or more factors are absent. The model then involves the general mean, all main effects and only some but not all two-factor interactions. The issue of optimality in situations of this kind for two-level factorials has been addressed recently by Hedayat and Pesotan (1992, 1997) and Chiu and John (1998); see also Wu and

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Chen (1992) and Sun and Wu (1994) in this connection. The present paper aims at further pursuing this line of research. This has been done for general factorials under the framework of hierarchical models which are defined in Section 2.

After presenting the preliminaries in Section 2, we show in Section 3 that in hierarchical models, inter-effect orthogonality implies universal optimality, and hence in particular, D -, A - or E -optimality. Interestingly, it is seen that this phenomenon is not guaranteed to hold in non-hierarchical models. A combinatorial characterization for inter-effect orthogonality is given in Section 4 for hierarchical models and some applications indicated.

2. Preliminaries

Consider the set up of an $m_1 \times \dots \times m_n$ factorial experiment involving n factors F_1, \dots, F_n appearing at m_1, \dots, m_n (≥ 2) levels respectively. The $v = \prod_{i=1}^n m_i$ treatment combinations are represented by ordered n -tuples $j_1 \dots j_n$ ($0 \leq j_i \leq m_i - 1$; $1 \leq i \leq n$). Let $\boldsymbol{\tau}$ denote the $v \times 1$ vector with elements $\tau(j_1 \dots j_n)$ arranged in the lexicographic order, where $\tau(j_1 \dots j_n)$ is the fixed effect of the treatment combination $j_1 \dots j_n$, and Ω denote the set of all binary n -tuples.

We represent the $a \times 1$ vector of all ones by $\mathbf{1}_a$ and the identity matrix of order a by I_a . For $1 \leq i \leq n$, let P_i be an $(m_i - 1) \times m_i$ matrix such that the $m_i \times m_i$ matrix $(m_i^{-\frac{1}{2}}\mathbf{1}_{m_i}, P_i')$ is orthogonal. For each $\mathbf{x} = x_1 \dots x_n \in \Omega$, let

$$P^{\mathbf{x}} = P_1^{x_1} \otimes \dots \otimes P_n^{x_n}, \quad \dots (2.1)$$

where for $1 \leq i \leq n$,

$$P_i^{x_i} = \begin{cases} m_i^{-\frac{1}{2}}\mathbf{1}'_{m_i} & \text{if } x_i = 0 \\ P_i & \text{if } x_i = 1, \end{cases} \quad \dots (2.2)$$

and \otimes denotes the Kronecker product. Then it is not hard to see that for each $\mathbf{x} = x_1 \dots x_n \in \Omega$, $\mathbf{x} \neq 00 \dots 0$, the elements of $P^{\mathbf{x}}\boldsymbol{\tau}$ represent a complete set of orthonormal contrasts belonging to the factorial effect $F_1^{x_1} \dots F_n^{x_n} \equiv F^{\mathbf{x}}$, say; cf. Gupta and Mukerjee (1989). Also $P^{00 \dots 0}\boldsymbol{\tau} = v^{\frac{1}{2}}\bar{\tau}$, where $\bar{\tau}$ is the general mean, and in this sense the general mean will be represented by $F^{00 \dots 0}$.

In this paper, we work with hierarchical factorial models. These are such that if a factorial effect $F^{\mathbf{x}}$ is included in the model then so is $F^{\mathbf{y}}$ for every $\mathbf{y} \in \Omega$ satisfying $\mathbf{y} \leq \mathbf{x}$, where $\mathbf{y} \leq \mathbf{x}$ means $y_i \leq x_i$ for $i = 1, \dots, n$. A hierarchical model is interesting in a factorial setting since it includes a factorial effect if and only if it includes all "ancestors" thereof.

Consider now an N -run fractional factorial plan d with reference to a hierarchical factorial model. Let R_d be a $v \times v$ diagonal matrix with diagonal elements representing, in the lexicographic order, the replication numbers of the

v treatment combinations in d . Also, let $\Gamma \subset \Omega$ be such that $F^{\mathbf{x}}$ is included in the model if and only if $\mathbf{x} \in \Gamma$. The parametric functions of interest are then represented by $P\boldsymbol{\tau}$, where

$$P = (\dots, (P^{\mathbf{x}})', \dots)'_{\mathbf{x} \in \Gamma}. \quad \dots (2.3)$$

As usual, assuming that the observations are homoscedastic and uncorrelated, the information matrix for $P\boldsymbol{\tau}$, under d , following Mukerjee (1995) is given by

$$\mathcal{I}_d = PR_dP'. \quad \dots (2.4)$$

The plan d is said to have inter-effect orthogonality if it keeps $P\boldsymbol{\tau}$ estimable and ensures

$$\text{Cov}(P^{\mathbf{x}}\hat{\boldsymbol{\tau}}, P^{\mathbf{y}}\hat{\boldsymbol{\tau}}) = 0, \text{ for every } \mathbf{x}, \mathbf{y} \in \Gamma, \mathbf{x} \neq \mathbf{y}, \quad \dots (2.5)$$

where $P^{\mathbf{x}}\hat{\boldsymbol{\tau}}$ is the best linear unbiased estimator of $P^{\mathbf{x}}\boldsymbol{\tau}$ in d . By (2.3)–(2.5), d has inter-effect orthogonality if and only if \mathcal{I}_d is positive definite and

$$P^{\mathbf{x}}R_d(P^{\mathbf{y}})' = 0, \text{ for every } \mathbf{x}, \mathbf{y} \in \Gamma, \mathbf{x} \neq \mathbf{y}. \quad \dots (2.6)$$

3. Orthogonality and Optimality

THEOREM 1. *If a fractional factorial plan has inter-effect orthogonality in a hierarchical model then it is universally optimal within the class of all plans involving the same number of runs.*

PROOF. Consider a hierarchical model specified by $\Gamma \subset \Omega$ as above. Let d be an N -run plan which has inter-effect orthogonality. Then (2.6) holds and by (2.3), (2.4) and (2.6), the information matrix for $P\boldsymbol{\tau}$, under d , is given by

$$\mathcal{I}_d = \text{diag}(\dots, P^{\mathbf{x}}R_d(P^{\mathbf{x}})', \dots)_{\mathbf{x} \in \Gamma}. \quad \dots (3.1)$$

We shall show that

$$P^{\mathbf{x}}R_d(P^{\mathbf{x}})' = (N/v)I_{\alpha(\mathbf{x})}, \text{ for all } \mathbf{x} \in \Gamma, \quad \dots (3.2)$$

where $\alpha(\mathbf{x})$ is the number of rows of $P^{\mathbf{x}}$.

Consider any fixed $\mathbf{x} \in \Gamma$. If $\mathbf{x} = 00 \dots 0$, then (3.2) holds trivially by (2.1) and (2.2). Next suppose $\mathbf{x} = x_1 \dots x_n \neq 00 \dots 0$ and, without loss of generality, let $x_1 = \dots = x_h = 1, x_{h+1} = \dots = x_n = 0$, where $1 \leq h \leq n$. Define

$$V = I_{m_1} \otimes \dots \otimes I_{m_h} \otimes \mathbf{1}'_{m_{h+1}} \otimes \dots \otimes \mathbf{1}'_{m_n}, \quad \dots (3.3)$$

$$a_1 = \prod_{i=1}^h m_i, \quad a_2 = \prod_{i=h+1}^n m_i, \quad \dots \quad (3.4)$$

$$\Gamma_1 = \{\mathbf{y} : \mathbf{y} \in \Omega, \mathbf{y} \leq \mathbf{x}\} = \{\mathbf{y} = y_1 \dots y_n : \mathbf{y} \in \Omega, y_{h+1} = \dots = y_n = 0\}. \quad \dots \quad (3.5)$$

Since $\mathbf{x} \in \Gamma$ and we are considering a hierarchical model, we have $\Gamma_1 \subset \Gamma$. Obviously, Γ_1 includes $00 \dots 0$. Writing $\mathbf{r}_d = R_d \mathbf{1}_v$, by (2.1), (2.2) and (2.6), then

$$P\mathbf{y}\mathbf{r}_d = v^{\frac{1}{2}} P\mathbf{y}R_d(P^{00\dots 0})' = 0, \quad \text{for all } \mathbf{y} \in \Gamma_1, \mathbf{y} \neq 00 \dots 0. \quad \dots \quad (3.6)$$

But for any $\mathbf{y} \in \Gamma_1, \mathbf{y} \neq 00 \dots 0$, by (2.1), (2.2), (3.3) and (3.4),

$$P\mathbf{y} = a_2^{-\frac{1}{2}} Q\mathbf{y}V, \quad (3.7)$$

where $Q\mathbf{y} = P_1^{y_1} \otimes \dots \otimes P_h^{y_h}$. Hence (3.6) implies that

$$QV\mathbf{r}_d = 0, \quad (3.8)$$

where

$$Q = [\dots, (Q\mathbf{y})', \dots]_{\mathbf{y} \in \Gamma_1, \mathbf{y} \neq 00 \dots 0}.$$

Since the matrix $(a_1^{-\frac{1}{2}} \mathbf{1}_{a_1}, Q')$ is orthogonal, from (3.8) it follows that the elements of $V\mathbf{r}_d$ are all equal. But by (3.3), the elements of $V\mathbf{r}_d$ represent, in the lexicographic order, the frequencies with which the level combinations of F_1, \dots, F_h appear in the N -run plan d . Therefore, by (3.4), $V\mathbf{r}_d = (N/a_1) \mathbf{1}_{a_1}$, so that $VR_dV' = (N/a_1) I_{a_1}$. Hence taking $\mathbf{y} = \mathbf{x}$ in (3.7) and recalling the definition of the matrices P_i ,

$$P\mathbf{x}R_d(P\mathbf{x})' = a_2^{-1} (P_1 \otimes \dots \otimes P_h) VR_dV' (P_1' \otimes \dots \otimes P_h') = (N/v) I_\alpha(\mathbf{x}),$$

by (3.4). This proves (3.2). By (3.1) and (3.2),

$$\mathcal{I}_d = (N/v) I_\alpha, \quad (3.9)$$

where $\alpha = \sum_{\mathbf{x} \in \Gamma} \alpha(\mathbf{x})$. Also, from (2.3) and (2.4), it is not hard to see that $\text{tr}(\mathcal{I}_{d'}) = (N\alpha/v)$ for every N -run plan d' ; cf. Mukerjee (1982). Hence by (3.9), following Kiefer (1975) and Sinha and Mukerjee (1982), the claimed universal optimality of d is established, completing the proof.

Thus inter-effect orthogonality entails universal optimality in hierarchical models. It may, however, be noted that, in contrast with Theorem 1, inter-effect orthogonality does not necessarily imply optimality, even under specific optimality criteria, in non-hierarchical models. The following example illustrates this point.

EXAMPLE 1. With reference to a 2×3^2 factorial, consider a non-hierarchical model which includes only the general mean and the two-factor interaction F_1F_2 . Let

$$d_0 = \{020, 021, 100, 111, 120, 121, 122\}$$

and

$$d_1 = \{000, 001, 010, 020, 100, 111, 122\},$$

be two plans, each of which involves $N = 7$ runs. Then from (2.3), (2.4) and (2.6), it can be checked that only d_0 and not d_1 has inter-effect orthogonality under the stated model. However, the eigenvalues of \mathcal{I}_{d_0} are $\frac{1}{6}, \frac{7}{18}, \frac{11}{18}$ and those of \mathcal{I}_{d_1} are $\frac{1}{3}, \frac{1}{3}, \frac{1}{2}$, so that under each of the $D-$, $A-$ and $E-$ criteria, d_1 dominates d_0 despite the inter-effect orthogonality of the latter.

4. A Combinatorial Characterization

In consideration of Theorem 1, it is appropriate to explore a combinatorial characterization for inter-effect orthogonality in hierarchical models. Consider a hierarchical model specified by $\Gamma \subset \Omega$ as in the last paragraph of Section 2. For any $\mathbf{x} = x_1 \dots x_n$ and $\mathbf{z} = z_1 \dots z_n$, both members of Γ , let $S(\mathbf{x}, \mathbf{z}) = \{i : \text{either } x_i = 1 \text{ or } z_i = 1\}$. Define

$$\bar{\Gamma} = \{\mathbf{x} : \mathbf{x} \in \Gamma, \text{ there does not exist } \mathbf{y} \in \Gamma \text{ such that } \mathbf{x} \leq \mathbf{y} \text{ and } \mathbf{x} \neq \mathbf{y}\}.$$

For example, if $n = 3$ and $\Gamma = \{000, 001, 010, 100, 110\}$ then $\bar{\Gamma} = \{001, 110\}$.

THEOREM 2. *Under a hierarchical model specified by Γ , a fractional factorial plan d has inter-effect orthogonality if and only if for every $\mathbf{x}, \mathbf{z} \in \bar{\Gamma}$, all level combinations of the factors $\{F_i : i \in S(\mathbf{x}, \mathbf{z})\}$ appear equally often in d .*

PROOF. “Only if” part. Let d have inter-effect orthogonality. Consider any $\mathbf{x}, \mathbf{z} \in \bar{\Gamma}$. First let $\mathbf{x} = \mathbf{z}$ and suppose, without loss of generality, $\mathbf{x} = x_1 \dots x_n$ with $x_1 = \dots = x_h = 1, x_{h+1} = \dots = x_n = 0$. Then $S(\mathbf{x}, \mathbf{z}) = \{1, \dots, h\}$ and, as shown while proving Theorem 1, all level combinations of F_1, \dots, F_h appear equally often in d . In fact, as in the proof of Theorem 1, we have

$$V\mathbf{r}_d = (N/a_1)\mathbf{1}_{a_1}, \tag{4.1}$$

where V and a_1 are as in (3.3) and (3.4).

Next suppose $\mathbf{z} \neq \mathbf{x}$. Let \mathbf{x} remain as before. By the definition of $\bar{\Gamma}$, then the set $\{i : x_i = 0, z_i = 1\}$ is nonempty and, without loss of generality, let this set be $\{h + 1, \dots, t\}$, where $h + 1 \leq t \leq n$. Then $S(\mathbf{x}, \mathbf{z}) = \{1, \dots, t\}$ and we have to show that all level combinations of F_1, \dots, F_t appear equally often in d . Let Γ_1 be as in (3.5) and define

$$\Gamma_2 = \{\mathbf{y} = y_1 \dots y_n : \mathbf{y} \in \Omega, \mathbf{y} \neq 00 \dots 0, y_1 = \dots = y_h = y_{t+1} = \dots = y_n = 0\}, \tag{4.2}$$

$$a_3 = \prod_{i=h+1}^t m_i, \quad a_4 = \prod_{i=t+1}^n m_i, \quad \dots (4.3)$$

$$P^{(1)} = [\dots, (P\mathbf{y})', \dots]'_{\mathbf{y} \in \Gamma_1}, \quad P^{(2)} = [\dots, (P\mathbf{y})', \dots]'_{\mathbf{y} \in \Gamma_2}. \quad \dots (4.4)$$

By (2.1), (2.2), (3.4), (3.5) and (4.2)–(4.4), analogously to (3.7),

$$P^{(1)} = (a_3 a_4)^{-\frac{1}{2}} A \otimes \mathbf{1}'_{a_3} \otimes \mathbf{1}'_{a_4}, \quad P^{(2)} = (a_1 a_4)^{-\frac{1}{2}} \mathbf{1}'_{a_1} \otimes B \otimes \mathbf{1}'_{a_4}, \quad \dots (4.5)$$

where A is an orthogonal matrix of order a_1 and B is an $(a_3 - 1) \times a_3$ matrix such that the matrix $(a_3^{-\frac{1}{2}} \mathbf{1}_{a_3}, B')$ is orthogonal.

By (3.5) and (4.2), Γ_1 and Γ_2 are disjoint. In view of the hierarchical model under consideration and the definitions of \mathbf{x} and \mathbf{z} , both of them are subsets of Γ . Since d has inter-effect orthogonality, by (2.6) and (4.4) it follows that $P^{(1)} R_d (P^{(2)})' = 0$. Hence use of (4.5) yields

$$(A \otimes \mathbf{1}'_{a_3}) R_d^* (\mathbf{1}_{a_1} \otimes B') = 0, \quad \dots (4.6)$$

where

$$R_d^* = (I_{a_1} \otimes I_{a_3} \otimes \mathbf{1}'_{a_4}) R_d (I_{a_1} \otimes I_{a_3} \otimes \mathbf{1}_{a_4}) \quad \dots (4.7)$$

is a diagonal matrix of order $a_1 a_3 = \prod_{i=1}^t m_i$ with diagonal elements representing, in the lexicographic order, the frequencies with which level combinations of F_1, \dots, F_t appear in d . Pre- and post-multiplying (4.6) by A' and B respectively, we get

$$(I_{a_1} \otimes \mathbf{1}'_{a_3}) R_d^* (\mathbf{1}_{a_1} \otimes (I_{a_3} - a_3^{-1} \mathbf{1}_{a_3} \mathbf{1}'_{a_3})) = 0. \quad \dots (4.8)$$

But by (3.3), (3.4), (4.1), (4.3) and (4.7),

$$(I_{a_1} \otimes \mathbf{1}'_{a_3}) R_d^* (\mathbf{1}_{a_1} \otimes \mathbf{1}_{a_3}) = (I_{a_1} \otimes \mathbf{1}'_{a_3} \otimes \mathbf{1}'_{a_4}) R_d \mathbf{1}_v = V \mathbf{r}_d = (N/a_1) \mathbf{1}_{a_1}.$$

Hence (4.8) yields

$$(I_{a_1} \otimes \mathbf{1}'_{a_3}) R_d^* (\mathbf{1}_{a_1} \otimes I_{a_3}) = \{N/(a_1 a_3)\} \mathbf{1}_{a_1} \mathbf{1}'_{a_3}. \quad \dots (4.9)$$

From (4.9), it is clear that every level combination of F_1, \dots, F_t appears $N/(a_1 a_3) = N/(m_1 \dots m_t)$ times in d . This proves the only if part.

“If” part. For any $\mathbf{x}, \mathbf{y} \in \Gamma$, not necessarily distinct, the stated condition implies that all level combinations of the factors $\{F_i : i \in S(\mathbf{x}, \mathbf{y})\}$ appear equally often in d . Hence from (2.1)–(2.4) the if part of the theorem follows. This completes the proof.

Under a hierarchical model, by Theorem 1, a plan d satisfying the condition of Theorem 2 is universally optimal in the class of plans involving the same number of runs. In particular, if the model consists of the general mean and all factorial effects involving up to $g \leq n/2$ factors, then this condition is equivalent to d

being represented by an orthogonal array of strength $2g$. This is in agreement with the findings in Cheng (1980) and Mukerjee (1982). Some more applications are indicated below. In what follows, $OA(N, \nu_1 \times \cdots \times \nu_t, 2)$ will denote an orthogonal array of strength two with N rows and t columns involving ν_1, \dots, ν_t symbols respectively; cf. Rao (1973) and Hedayat, Sloane and Stufken (1999).

EXAMPLE 2. Consider a hierarchical model consisting of the general mean, all main effects and only one two-factor interaction, say F_1F_2 . Then by Theorem 2, an N -run plan d has inter-effect orthogonality if and only if in d (i) all level combinations of F_1 , F_2 and F_i appear equally often, $3 \leq i \leq n$, and (ii) all level combinations of F_i and $F_{i'}$ appear equally often, $3 \leq i < i' \leq n$. This happens if and only if d can be constructed as follows. Start with an orthogonal array $OA(N, (m_1m_2) \times m_3 \times \cdots \times m_n, 2) \equiv L$, say, map the m_1m_2 symbols in the first column of L to the m_1m_2 level combinations of F_1 and F_2 and then interpret the rows of the resulting array as the treatment combinations in d . As an illustration, if $N = 18, n = 8, m_1 = 2, m_2 = \cdots = m_8 = 3$ then one can start with the array $OA(18, 6 \times 3^6, 2)$, constructed following Wang and Wu (1991) or Hedayat, Sloane and Stufken (1999, p.210), to get d .

EXAMPLE 3. Consider a hierarchical model consisting of the general mean, all main effects and exactly a pair of two-factor interactions. The case where these two-factor interactions have no common factor can be treated along the lines of Example 2. Now consider the other case and, without loss of generality, let F_1F_2 and F_1F_3 be the two-factor interactions included in the model. Then by Theorem 2, an N -run plan d has inter-effect orthogonality if and only if in d all level combinations of the following sets of factors appear equally often :

- (i) $\{F_1, F_2, F_i\}, \quad 3 \leq i \leq n;$
- (ii) $\{F_1, F_3, F_i\}, \quad 4 \leq i \leq n;$
- (iii) $\{F_i, F_{i'}\}, \quad 4 \leq i < i' \leq n.$

We shall show how the approach of Bose and Bush (1952) for the construction of orthogonal arrays can be modified to realize these conditions when $m_1 = \cdots = m_n = m$, where $m \geq 2$ is a prime or a prime power, and $N = m^k, k \geq 3$. Let e_1, \dots, e_k be the unit $k \times 1$ vectors over the Galois field $GF(m)$. Then there are

$$q = (m^k - 1)/(m - 1) - 2(m - 1) \tag{4.10}$$

distinct points in the finite projective geometry $PG(k - 1, m)$ which are not of the form $e_1 + \xi e_2$ or $e_1 + \xi e_3$ for some $\xi \in GF(m), \xi \neq 0$. Let C be a $k \times q$ matrix obtained by writing these q points as columns such that the first three columns of C are e_1, e_2 and e_3 . For example, if $m = k = 3$ then $q = 9$ and

$$C = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ 0 & 1 & 0 & 1 & 1 & 1 & 1 & 2 & 2 \\ 0 & 0 & 1 & 1 & 2 & 1 & 2 & 1 & 2 \end{bmatrix}.$$

The m^k vectors in the row space of C , when interpreted as treatment combinations, represent a plan d satisfying the equal frequency conditions stated in (i)–(iii) above. The plan d involves $N = m^k$ runs and $n = q$ factors. Using (4.10), by a simple count of the degrees of freedom, it is seen that d is saturated in the sense of allowing the estimability of the effects in the model with a minimum number of observations. For $n < q$, one has to just delete $q - n$ of the last $q - 3$ factors in d .

EXAMPLE 4. Consider a hierarchical model consisting of the general mean, all main effects and only those two-factor interactions that involve one particular factor, say F_1 . Then by Theorem 2, an N -run plan d has inter-effect orthogonality if and only if in d all level combinations of F_1, F_i and $F_{i'}$ appear equally often, $2 \leq i < i' \leq n$. This happens if and only if the levels of F_1 appear equally often in d and, in the subsdesign of d corresponding to every fixed level of F_1 , the level combinations of the other factors are represented by an orthogonal array of strength two. Thus the condition stated in Theorem 2 is met if the treatment combinations in d are of the form $j_1 \mathbf{l}_u$, $0 \leq j_1 \leq m_1 - 1$; $1 \leq u \leq N/m_1$, where the \mathbf{l}_u are the rows of an orthogonal array $OA(N/m_1, m_2 \times \cdots \times m_n, 2) \equiv L$, say. As an illustration, if $N = 20, n = 4, m_1 = 5, m_2 = m_3 = m_4 = 2$, then one can take L as $OA(4, 2^3, 2)$, derivable from a Hadamard matrix of order 4, to get d .

In each of these examples, the plan d is universally optimal by Theorem 1. We have already noted that d is saturated in Example 3. The same holds also in Examples 2 and 4 provided the orthogonal array L considered there attains Rao's bound. This happens indeed with the specific illustrations considered in these examples.

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