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ON ROBUST ESTIMATION OF VARIANCE COMPONENTS

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Abstract. Estimating functions of variance components is considered. The problem is to find an estimator, the variance of which changes as little as possible when the kurtosis of the underlying distribution runs over a given interval; such estimators are called *robust*. In the paper the existence of robust estimators is considered. The robust estimators with minimal variance are constructed. A comparison of robust and standard estimators is discussed.

1. Introduction. Consider a linear model

$$y = X\beta + \sum_{i=1}^{K} U_i \xi_i,$$

where y is an n-vector of observations; X is a known $(n\times p)$-matrix; β is a p-vector of unknown coefficients; U_i are known $(n\times n_i)$-matrices, $i = 1, \ldots, K$; $\xi_i = (\xi_{i1}, \ldots, \xi_{in_i})'$ are normally distributed random vectors such that $E\xi_i = 0$, $E\xi_i\xi_j' = 0$ for $i\neq j$, $E\xi_i\xi_i' = \sigma_i^2 I$, $\sigma_i^2 > 0$, $i, j = 1, \ldots, K$.

Let

$$V(\sigma) = \operatorname{Cov} y = \sum_{i=1}^{K} \sigma_i^2 V_i,$$

where $V_i = U_i U_i'$ and $\sigma = (\sigma_1^2, \ldots, \sigma_K^2)'$.

Let $f'\sigma = \sum f_i \sigma_i^2$ be an *invariantly estimable function*, i.e. a function for which there exists an estimator $y'Ay$ with $Ey'Ay = f'\sigma$, $A\in\mathscr{A} = \{A\colon AX = 0\}$. Let $\mathscr{G}$ denote the set of all such functions.

The problem is to estimate $f'\sigma$. The well-known optimal solution ([2, 3]), i.e. the solution minimizing

$$\operatorname{Var} y'Ay = 2\operatorname{tr} AV(\sigma)AV(\sigma), \quad A\in\mathscr{A},$$

will be denoted by $y'A_S y$ and will be referred to as the *standard estimator.*

It appears that statistical procedures based on the statistic $y'A_S y$ may be very bad when ξ_i are not normal (for example, see the Bartlett test in [1]). We are interested in estimators which are robust against nonnormality. Assume that the model under consideration is violated by letting the kurtosis $\gamma_{2i} = E\xi_{ij}^4/\sigma_i^4 - 3$, $j = 1, \ldots, n_i$, $i = 1, \ldots, K$, to change in a given interval

$$\Gamma = [\underline{\gamma}_{21}, \overline{\gamma}_{21}] \times [\underline{\gamma}_{22}, \overline{\gamma}_{22}] \times \ldots \times [\underline{\gamma}_{2K}, \overline{\gamma}_{2K}].$$

Now the variance of $y'Ay$, $A \in \mathscr{A}$, is given by

$$\text{(1)} \qquad \operatorname{Var} y'Ay = \sum_{i=1}^{K} \sigma_i^4 \gamma_{2i} a_i' a_i + 2 \operatorname{tr} AV(\sigma) AV(\sigma),$$

where a_i is the vector of diagonal elements of the matrix $U_i' A U_i$, $i = 1, \ldots, K$.

We are interested in an estimator, the variance of which changes as little as possible when the kurtosis $\gamma = (\gamma_{21}, \ldots, \gamma_{2K})$ runs over the interval Γ. Formally, given an estimator $y'Ay$, we consider a function on the parameter space of the model (cf. [8]) defined by

$$\text{(2)} \qquad r_A(\sigma) = \sup_{\gamma \in \Gamma} \operatorname{Var} y'Ay - \inf_{\gamma \in \Gamma} \operatorname{Var} y'Ay = \sum_{i=1}^{K} \sigma_i^4 (\overline{\gamma}_{2i} - \underline{\gamma}_{2i}) a_i' a_i.$$

Definition. An estimator $y'Ay$ ($A \in \mathscr{A}$) of $f'\sigma \in \mathscr{G}$ is said to be *robust*, if $Ey'Ay = f'\sigma$ and $r_A(\sigma) \leqslant r_B(\sigma)$ for all σ and $B \in \mathscr{A}$ such that $Ey'By = f'\sigma$.

In what follows, conditions for the existence of robust estimators for a function $f'\sigma \in \mathscr{G}$ are given. The problem of the existence of best robust estimators is considered and, if such exist, a comparison of those with the standard $y'A_S y$ is discussed.

The results remain valid if instead of the original Gaussian model one considers any model with fixed kurtosis.

The problem with $K = 1$ and $V = I$ was considered in [9].

2. Introductory results. In the paper we use the following basic facts and notation of the general theory of linear models (see [3]).

Let Z be a random element with values in an arbitrary Euclidean vector space $\mathscr{K}$ endowed with an inner product denoted by $(\cdot, \cdot)$. The expectation EZ and the covariance $\operatorname{Cov} Z$ are assumed to exist. The expectation EZ is assumed to be an element of a known subspace $\mathscr{E}$ of $\mathscr{K}$. Let Θ be the convex cone of self-adjoint, nonnegative defined (n.n.d.) linear operators from $\mathscr{K}$ to $\mathscr{K}$ (usually it is assumed that Θ is generated by $\operatorname{Cov} Z$). The problem is to estimate a linear function (A, EZ) defined on $\mathscr{E}$. We confine attention to the class of estimators of the form (B, Z) for $B \in \mathscr{K}_0$, where $\mathscr{K}_0$ is a given subspace of $\mathscr{K}$. The function (A, EZ) is said to be *$\mathscr{K}_0$-estimable* if there exists a $B \in \mathscr{K}_0$ such that $E(B, Z) = (A, EZ)$. The estimator (B, Z), $B \in \mathscr{K}_0$, is said to be *$(\mathscr{K}_0, \Theta)$-best for $\mathscr{K}_0$-estimable function* g, if $E(B, Z) = g$ and

$(B, \Gamma B) \leqslant (C, \Gamma C)$ for all $C \in \mathscr{K}_0$ such that $E(C, Z) = g$ and for all $\Gamma \in \Theta$.

Let $\Sigma \in \Theta$ be the maximal operator in Θ, i.e. an operator such that $\mathscr{N}(\Sigma) = \bigcap_{\Gamma \in \Theta} \mathscr{N}(\Gamma)$, where $\mathscr{N}(\Gamma)$ denotes the null space of the operator Γ. Such an operator exists in Θ (see [4]). Let $\mathscr{F} = \mathscr{E} + \mathscr{K}_0^{\perp}$.

LEMMA 1 ([3]). *For every $\mathscr{K}_0$-estimable function there exists the $(\mathscr{K}_0, \Theta)$-best estimator iff*

$$\Gamma\big(\mathscr{K}_0 \cap \Sigma^{-1}(\mathscr{F})\big) \subseteq \mathscr{F} \quad \text{for all } \Gamma \in \Theta.$$

LEMMA 2. *A $(\mathscr{K}_0, \Theta)$-best estimator is unique iff $\mathscr{N}(\Sigma) \cap \mathscr{F}^{\perp} = \{0\}$.*

This Lemma is a corollary from a well known Lehmann-Scheffé theorem.

LEMMA 3. *Let $\mathscr{K}_1$ be a subspace of $\mathscr{K}$ such that $\mathscr{K}_0 \subset \mathscr{K}_1$. Let us assume that for every $\mathscr{K}_0$-estimable function there exists a $(\mathscr{K}_1, \Theta)$-best estimator. Then a $(\mathscr{K}_1, \Theta)$-best estimator is $(\mathscr{K}_0, \Theta)$-best iff $\mathscr{K}_1 \cap \Sigma^{-1}(\mathscr{E} + \mathscr{K}_1^{\perp}) \subseteq \mathscr{K}_0$.*

Proof. A $(\mathscr{K}_1, \Theta)$-best estimator is $(\mathscr{K}_0, \Theta)$-best one iff the $(\mathscr{K}_1, \Theta)$-best estimator belongs to $\mathscr{K}_0$. It follows from the Lehmann-Scheffé theorem that the set of $(\mathscr{K}_1, \Theta)$-best estimators is of the form $\mathscr{K}_1 \cap \bigcap_{\Gamma \in \Theta} \Gamma^{-1}(\mathscr{E} + \mathscr{K}_1^{\perp})$. Hence we have to show that

$$\mathscr{K}_1 \cap \bigcap_{\Gamma \in \Theta} \Gamma^{-1}(\mathscr{E} + \mathscr{K}_1^{\perp}) = \mathscr{K}_1 \cap \Sigma^{-1}(\mathscr{E} + \mathscr{K}_1^{\perp}),$$

which follows from the proof of Theorem 3.1 in [3].

3. Existence of robust estimators. For every function $f'\sigma \in \mathscr{G}$ there exists a robust estimator iff the problem:

$$r_A(\sigma) = \min! \text{ for all } \sigma, \quad A \in \mathscr{A},\ Ey'Ay = f'\sigma$$

has a solution.

Let $(A, B) = \operatorname{tr} AB$ be the inner product in the space S_n of all symmetric $(n \times n)$-matrices. Let $\Phi_i\colon S_n \to S_n$ be a linear operator defined by $\Phi_i A = U_i\big(P(U_i' A U_i)\big)U_i'$ for each $A \in S_n$, where $PA = \operatorname{diag}(a_{11}, \ldots, a_{nn})$ is the orthogonal projection on the subspace of the diagonal matrices. Let

$$\Phi(\sigma) = \sum_{i=1}^{K} \sigma_i^4 (\overline{\gamma}_{2i} - \underline{\gamma}_{2i}) \Phi_i.$$

The function (2) can be written in the following way:

$$r_A(\sigma) = \sum_{i=1}^{K} \sigma_i^4 (\overline{\gamma}_{2i} - \underline{\gamma}_{2i})(A, \Phi_i A) = \big(A, \Phi(\sigma) A\big).$$

Let $\Theta = \operatorname{sp}\{\Phi_1, \ldots, \Phi_K\}^{+} = \{\sum_{i=1}^{K} \alpha_i \Phi_i\colon \alpha_i \geqslant 0\}$ and let Σ be maximal in Θ. Let $\mathscr{F} = \mathscr{E}+\mathscr{A}^{\perp}$, where $\mathscr{E} = \mathrm{sp}\{V_1, \ldots, V_K\}+\{X\Lambda X' : \Lambda = \Lambda'\}$ is a linear subspace generated by the expectations of yy'.

THEOREM 1. *For every invariantly estimable function there exists a robust estimator iff*

$$\Phi(\mathscr{A} \cap \Sigma^{-1}(\mathscr{F})) \subseteq \mathscr{F} \quad \textit{for all } \Phi \in \Theta.$$

Proof. For each $A, B \in S_n$ we have

$$(A, \Phi_i A) = \mathrm{tr}\, AU_i(P(U_i' AU_i))U_i' = \mathrm{tr}\, U_i' AU_i P(U_i' AU_i) = \mathrm{tr}\, P(U_i' AU_i) P(U_i' AU_i) \geqslant 0$$

and

$$(A, \Phi_i B) = \mathrm{tr}\, AU_i(P(U_i' BU_i))U_i' = \mathrm{tr}\, P(U_i' AU_i) P(U_i' BU_i) = \mathrm{tr}\, P(U_i' AU_i) U_i' BU_i = (\Phi_i A, B),$$

hence Φ_i is an n.n.d. and self-adjoint linear operator. The set Θ is a convex cone generated by $\Phi_1, \ldots, \Phi_K$. Theorem follows from Lemma 1.

From Lemma 2 we see that a robust estimator is unique iff $\mathscr{N}(\Sigma) \cap \mathscr{F}^{\perp} = \{0\}$.

4. Best robust estimators. Let $\mathscr{A}_R$ denote the set of all robust estimators. From Lehmann-Scheffé theorem it follows that $\mathscr{A}_R$ is a linear subspace. Let $\mathscr{G}_R \subseteq \mathscr{G}$ be the set of all robust estimable functions, i.e. $f'\sigma \in \mathscr{G}_R$ iff there exists an $A \in \mathscr{A}_R$ such that $Ey'Ay = f'\sigma$.

Let $f'\sigma \in \mathscr{G}_R$. We want to find the best robust estimator for $f'\sigma$. Due to (1) and due to the fact that $\Sigma\sigma_i^4(\bar{\gamma}_{2i}-\underline{\gamma}_{2i})a_i'a_i$, $i = 1, \ldots, K$, is the same for all $A \in \mathscr{A}_R$ such that $Ey'Ay = f'\sigma$, in order to find the best robust estimator one has to find a matrix A which minimizes $\mathrm{tr}\, AV(\sigma)AV(\sigma)$ uniformly in σ. Thus, we have to solve the following problem:

$$\mathrm{tr}\, AV(\sigma)AV(\sigma) = \min! \text{ for all } \sigma, \quad A \in \mathscr{A}_R,\ Ey'Ay = f'\sigma.$$

Let Σ_T be a linear operator defined by $\Sigma_T A = TAT$ for each $A \in S_n$. We can rewrite our problem as

$$(A, \Sigma_{V(\sigma)} A) = \min! \text{ for all } \sigma, \quad A \in \mathscr{A}_R,\ Ey'Ay = f'\sigma.$$

Let $\mathscr{V} = \mathrm{sp}\{\Sigma_{V_i} : i = 1, \ldots, K\}^{+}$. It is easy to see that $\mathscr{V}$ is a convex cone of n.n.d., self-adjoint linear operators. Let Ψ be maximal in $\mathscr{V}$ and let $\mathscr{F}_R = \mathscr{E}+\mathscr{A}_R^{\perp}$.

THEOREM 2. *For every function from $\mathscr{G}_R$ there exists a best robust estimator iff*

$$\Phi(\mathscr{A}_R \cap \Psi^{-1}(\mathscr{F}_R)) \subseteq \mathscr{F}_R \quad \textit{for all } \Phi \in \mathscr{V}.$$

Proof. Theorem 2 follows from Lemma 1.

Remark. Let $V_K = I$ and let Q denote the orthogonal projection on $\mathscr{A}_R$. Then for every function from $\mathscr{G}_R$ there exists a best robust estimator iff $\operatorname{sp}\{QV_1Q, \ldots, QV_KQ\}$ is a quadratic subspace.

5. Comparison with a standard estimator. Let A_R denote the matrix of the best robust estimator. If $I \in \mathscr{V}$, then Lemma 3 yields the following result:

LEMMA 4. $A_R = A_S$ *iff* $\mathscr{A} \cap (\mathscr{E} + \mathscr{A}^{\perp}) \subseteq \mathscr{A}_R$.

6. Examples. (6.1) Let $K = 1$, $U_1 = V_1 = I$. The only invariantly estimable functions are $c \cdot \sigma^2$, where $c \in R$. It is easy to see that for every such a function there exists the best robust estimator. This case is discussed in full details in [9].

(6.2) Consider a linear model "with two missing observations" ([7]):

	B_1	B_2	B_3
A_1	y_{11}	y_{12}	y_{13}
A_2	y_{21}		

The model is $y_{ij} = \alpha_i + b_j + e_{ij}$ $(i = 1, 2;\ j = 1, 2, 3)$, where the effects α_i are fixed, while the effects b_j and e_{ij} are random: $Eb_j = 0$, $Ee_{ij} = 0$, $\operatorname{var} b_j = \sigma_1^2, \operatorname{var} e_{ij} = \sigma_2^2$, $\operatorname{cov}(b_j, b_{j'}) = 0$ for $j \neq j'$, $\operatorname{cov}(e_{ij}, e_{i'j'}) = 0$ for $i \neq i'$ or $j \neq j'$, $\operatorname{cov}(b_{j'}, e_{ij}) = 0$ for all i, j', j. The vector model is

$$y = X\beta + U_1 a_1 + U_2 a_2,$$

where $\beta = (\alpha_1, \alpha_2)'$, $a_1 = (b_1, b_2, b_3)'$, $a_2 = (e_{11}, e_{12}, e_{13}, e_{21})'$, $U_2 = V_2 = I$,

$$X = \begin{pmatrix} 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad U_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, \quad V_1 = \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix}.$$

The number of observations is $n = 4$, rank of X is $p = 2$. The matrix $M = I - P$, where P is the ortoghonal projection on $\mathscr{R}(X)$, is of the form

$$M = \frac{1}{3}\begin{pmatrix} 2 & -1 & -1 & 0 \\ -1 & 2 & -1 & 0 \\ -1 & -1 & 2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

The rank of the matrix

$$G = \begin{pmatrix} \operatorname{tr} MV_1MV_1 & \operatorname{tr} MV_1 \\ \operatorname{tr} MV_1 & n-p \end{pmatrix} = \begin{pmatrix} 2 & 2 \\ 2 & 2 \end{pmatrix}$$

is equal to one, so we have $\mathcal{G} = \{c\cdot(\sigma_1^2+\sigma_2^2):\ c\in R\}$ (cf. [2]). Hence

$$\mathcal{E} = \left\{\begin{pmatrix} a+b+\lambda_1 & \lambda_1 & \lambda_1 & b+\lambda_2 \\ \lambda_1 & a+b+\lambda_1 & \lambda_1 & \lambda_2 \\ \lambda_1 & \lambda_1 & a+b+\lambda_1 & \lambda_2 \\ b+\lambda_2 & \lambda_2 & \lambda_2 & a+b+\lambda_3 \end{pmatrix}:\ a, b, \lambda_1, \lambda_2, \lambda_3 \in R\right\},$$

$$\mathcal{A} = \left\{\begin{pmatrix} 2a_{11} & -a_{11}-a_{22}+a_{33} & -a_{11}+a_{22}-a_{33} & 0 \\ -a_{11}-a_{22}+a_{33} & 2a_{22} & a_{11}-a_{22}-a_{33} & 0 \\ -a_{11}+a_{22}-a_{33} & a_{11}-a_{22}-a_{33} & 2a_{33} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}:\ a_{11}, a_{22}, a_{33} \in R\right\},$$

and

$$\mathcal{A}^{\perp} = \left\{\begin{pmatrix} 2b_{11} & -(b_{11}+b_{22}) & -(b_{11}+b_{33}) & b_{14} \\ -(b_{11}+b_{22}) & 2b_{22} & -(b_{22}+b_{33}) & b_{24} \\ -(b_{11}+b_{33}) & -(b_{22}+b_{33}) & 2b_{33} & b_{34} \\ b_{14} & b_{24} & b_{34} & b_{44} \end{pmatrix}:\ b_{11}, b_{22}, b_{33}, b_{14}, b_{24}, b_{34}, b_{44} \in R\right\}.$$

For every $f'\sigma$ from $\mathcal{G}$ there exist a unique robust estimator. We obtain

$$\mathcal{A}_R = \left\{\frac{c}{3}\begin{pmatrix} 2 & -1 & -1 & 0 \\ -1 & 2 & -1 & 0 \\ -1 & -1 & 2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}:\ c\in R\right\}.$$

Easy calculations show that $\mathcal{A}\cap(\mathcal{E}+\mathcal{A}^{\perp}) = \mathcal{A}_R$. From Lemma 4 it follows that $A_R = A_S$.

(6.3) Consider a linear model "with five missing observations":

	B_1	B_2	B_3
A_1+A_2	y_{11}		
A_1		y_{22}	y_{23}
0		y_{32}	

As in the previous case we assume that the A effects are fixed, and the B effects are random. The model is

$$y = X\beta + U_1 a_1 + U_2 a_2,$$

where $\beta = (\alpha_1, \alpha_2)'$, $a_1 = (b_1, b_2, b_3)'$, $a_2 = (e_{11}, e_{22}, e_{23}, e_{32})'$, $U_2 = V_2 = I$,

$$\mathbf{X} = \begin{pmatrix} 1 & 1 \\ 1 & 0 \\ 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad U_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad V_1 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \end{pmatrix}.$$

Now we have $n = 4$, $p = 2$ and

$$M = \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix}.$$

Because the rank of $G = \left(\begin{smallmatrix} 3 & 2 \\ 2 & 2 \end{smallmatrix}\right)$ is equal to two, all functions $f'\sigma = f_1\sigma_1^2 + f_2\sigma_2^2$ are invariantly estimable. We have

$$\mathscr{E} = \left\{ \begin{pmatrix} a+b+\lambda_1+2\lambda_2+\lambda_3 & \lambda_1+\lambda_2 & \lambda_1+\lambda_2 & 0 \\ \lambda_1+\lambda_2 & a+b+\lambda_1 & \lambda_1 & a \\ \lambda_1+\lambda_2 & \lambda_1 & a+b+\lambda_1 & 0 \\ 0 & a & 0 & b \end{pmatrix} : a, b, \lambda_1, \lambda_2, \lambda_3 \in R \right\};$$

$$\mathscr{A} = \left\{ \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & a_{22} & -a_{22} & a_{24} \\ 0 & -a_{22} & a_{22} & -a_{24} \\ 0 & a_{24} & -a_{24} & a_{44} \end{pmatrix} : a_{22}, a_{24}, a_{44} \in R \right\},$$

$$\mathscr{A}^{\perp} = \left\{ \begin{pmatrix} b_{11} & b_{12} & b_{13} & b_{14} \\ b_{12} & b_{22} & \tfrac{1}{2}(b_{22}+b_{33}) & b_{24} \\ b_{13} & \tfrac{1}{2}(b_{22}+b_{33}) & b_{33} & b_{34} \\ b_{14} & b_{24} & b_{34} & 0 \end{pmatrix} : b_{11}, b_{12}, b_{13}, b_{14}, b_{22}, b_{33}, b_{24}, b_{34} \in R \right\},$$

and

$$\mathscr{A} \cap (\mathscr{E} + \mathscr{A}^{\perp}) = \left\{ \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & a & -a & b \\ 0 & -a & a & b \\ 0 & b & -b & 2a \end{pmatrix} : a, b \in R \right\}.$$

For every function there exists a unique robust estimator and we get

$$\mathscr{A}_R = \left\{ \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & a & -a & b \\ 0 & -a & a & -b \\ 0 & b & -b & a \end{pmatrix} : a, b \in R \right\}.$$

Matrices A_R and A_S of the estimators of the function $f_1 \sigma_1^2 + f_2 \sigma_2^2$ are as follows:

$$A_R = \frac{1}{3} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & f_2 & -f_2 & \frac{3}{2}(f_1 - f_2) \\ 0 & -f_2 & f_2 & -\frac{3}{2}(f_1 - f_2) \\ 0 & \frac{3}{2}(f_1 - f_2) & -\frac{3}{2}(f_1 - f_2) & f_2 \end{pmatrix};$$

$$A_S = \frac{1}{4} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & f_2 & -f_2 & 2(f_1 - f_2) \\ 0 & -f_2 & f_2 & -2(f_1 - f_2) \\ 0 & 2(f_1 - f_2) & -2(f_1 - f_2) & 2f_2 \end{pmatrix}.$$

It is easy to see that the condition of Lemma 4, i.e. $\mathscr{A} \cap (\mathscr{E} + \mathscr{A}^{\perp}) \subseteq \mathscr{A}_R$, does not hold.

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