

Mean Driven Balance and Uniformly Best Linear Unbiased Estimators



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Introduction

When a model has mean vector $\mu = \mathbf{X}\beta$, with \mathbf{X} an incidence matrix, its observations vector can be partitioned into sub-models whose components have identical mean values. These will be the partitioned models.

We introduce a necessary and sufficient balance condition for partitioned mixed models to have Ordinary Least Squares Estimators, OLSE, for β that are Uniformly Best Unbiased Estimators, UBLUE, i.e., Best Linear Unbiased Estimators, BLUE, whatever the variance components.

Introduction

This condition is derived, from an extension of the identification of OLSE and Gauss-Markov Estimators, GME, in models with variance-covariance matrix $\mathbf{V}(\sigma^2) = \sigma^2\mathbf{M}$, when certain conditions hold.

The approach between this extension also leads to least squares like estimators of the variance components.

Introduction

We also consider special models to illustrate the applications range of the balance condition:

- Stair nesting
- Balanced cross-nesting

both class of models with OBS, having variance-covariance matrices that are all linear combinations, with non-negative coefficients, of known orthogonal projection matrices that are pairwise orthogonal, that add up to \mathbf{I}_n .

These models were introduced by Nelder, and play an important role in the theory of randomized block designs, see Caliński & Kageyama (2000, 2003). We also present a third model for which the balance condition holds but without OBS. This last example may be considered as a counter-example to the assumption that all models for which the balance condition holds are OBS.

Framework

We will put $\mathbf{y} \sim (\mathbf{X}\boldsymbol{\beta}, \sigma^2\mathbf{M})$ to indicate that vector \mathbf{y} has mean vector $\mathbf{X}\boldsymbol{\beta}$ and variance-covariance matrix $\sigma^2\mathbf{M}$. For those models the equality of the OLSE

$$\tilde{\boldsymbol{\beta}} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}$$

and GME

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}^\top \mathbf{M}^{-1} \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{M}^{-1} \mathbf{y}$$

has been studied as well as related subjects, by e.g., Kuskal (1968), Puntanen & Styan (1989), Krämer *et al.* (1996), Jaeger & Krämer (1998), Gotu (2001), Isotalo & Puntanen (2009) and Baksalary *et al.* (2013).

Framework

In this study, the Kruskal condition

$$\mathcal{R}(\mathbf{V}\mathbf{X}) \subseteq \mathcal{R}(\mathbf{X}),$$

with $\mathcal{R}(\mathbf{L})$ the range space for matrix \mathbf{L} , plays a central part. Since the GME are, for the models, BLUE, the question under study may be rephrased as obtaining conditions for the OLSE being BLUE. This new formulation may also be considered for models with more than one variance component, namely for models, $\mathbf{y} \sim (\mathbf{X}\boldsymbol{\beta}; \mathbf{V}(\boldsymbol{\sigma}^2))$, with variance-covariance matrices

$$\mathbf{V}(\boldsymbol{\sigma}^2) = \sum_{i=1}^w \sigma_i^2 \mathbf{M}_i$$

with $\sigma_i^2 \geq 0$ and $\mathbf{M}_i = \mathbf{X}_i \mathbf{X}_i^\top$, $i = 1, \dots, w$.

Framework

Besides the Kruskal condition we will consider the commutativity condition, in which \mathbf{T} , the orthogonal projection matrix on $\mathcal{R}(\mathbf{X})$, commutes with \mathbf{V} . This condition was considered by Zyskind (1967) and Zmyslony (1980). Taking $\sigma^2 = \sigma_0^2$ for a model $\mathbf{y} \sim (\mathbf{X}\beta; \mathbf{V}(\sigma_0^2))$, both conditions are necessary and sufficient for $\tilde{\beta}$ to be BLUE, thus they will be equivalent. Then

$$\mathcal{R}(\mathbf{V}(\sigma_0^2)) \subseteq \mathcal{R}(\mathbf{X})$$

if and only if

$$\mathbf{V}(\sigma_0^2) \mathbf{T} = \mathbf{T} \mathbf{V}(\sigma_0^2).$$

Framework

Proposition 1

The following statements for models $\mathbf{y} \sim (\mathbf{X}\boldsymbol{\beta}; \mathbf{V}(\boldsymbol{\sigma}^2))$, $\sigma_i^2 \geq 0$, $i = 1, \dots, w$, are equivalent:

- (a) whatever $\boldsymbol{\sigma}^2 \geq 0$, $\mathcal{R}(\mathbf{V}(\boldsymbol{\sigma}^2)\mathbf{X}) \subseteq \mathcal{R}(\mathbf{X})$;
- (b) whatever $\boldsymbol{\sigma}^2 \geq 0$, $\mathbf{V}(\boldsymbol{\sigma}^2)\mathbf{T} = \mathbf{T}\mathbf{V}(\boldsymbol{\sigma}^2)$;
- (c) $\tilde{\boldsymbol{\beta}}$ is UBLUE.

Balance

Let \mathbf{X} be a $n \times k$ incidence matrix. Since the reordering matrices are orthogonal and $\tilde{\beta}$ is invariant for orthogonal transformation $\overset{\circ}{\mathbf{y}} = \mathbf{P}\mathbf{y}$, with \mathbf{P} orthogonal, we can assume that the observations are grouped according to mean values in to sub-vectors with $r_1 \dots r_k$ components. Thus, with $\mathbf{D}(\dots)$ indicating a blockwise diagonal matrices, we will have $\mathbf{X} = \mathbf{D}(\mathbf{1}_{r_1} \dots \mathbf{1}_{r_k})$, and

$$\mathbf{T} = \mathbf{D} \left(\frac{1}{r_1} \mathbf{J}_{r_1} \dots \frac{1}{r_k} \mathbf{J}_{r_k} \right),$$

where $\mathbf{J}_r = \mathbf{1}_r \mathbf{1}_r^T$.

Let δ_i have all w components null but the i -th which is 1, then $\mathbf{V}(\delta_i) = \mathbf{M}_i$, $i = 1, \dots, w$, and so (a) holds whatever $\sigma_i^2 \geq 0$, $i = 1, \dots, w$, if and only if

$$\mathcal{R}(\mathbf{M}_i \mathbf{X}) \subseteq \mathcal{R} \mathbf{X}, i = 1, \dots, w.$$

Balance

Taking

$$\mathbf{M}_i = \begin{bmatrix} \mathbf{M}_{i,1,1} & \cdots & \mathbf{M}_{i,1,k} \\ \vdots & & \vdots \\ \mathbf{M}_{i,k,1} & \cdots & \mathbf{M}_{i,k,k} \end{bmatrix} \quad i = 1, \dots, w,$$

where $\mathbf{M}_{i,\ell,h}$ is $r_\ell \times r_h$, $\ell = 1, \dots, k$, $h = 1, \dots, k$, $i = 1, \dots, w$. It is now easy to see that (a) holds if and only if

$$\begin{cases} \mathbf{M}_{i,\ell,h} \mathbf{1}_{r_h} = \frac{t_{i,\ell,h}}{r_\ell} \mathbf{1}_{r_\ell} \\ \mathbf{1}_{r_\ell} \mathbf{M}_{i,\ell,h} = (\mathbf{M}_{i,h,\ell} \mathbf{1}_{r_\ell})^\top = \frac{t_{i,h,\ell}}{r_h} \mathbf{1}_{r_h}^\top = \frac{t_{i,h,\ell}}{r_h} \mathbf{1}_{r_h}^\top \end{cases}$$

with $t_{i,\ell,h}$ the sum of the elements of $\mathbf{M}_{i,\ell,h}$, $\ell = 1, \dots, k$, $h = 1, \dots, k$, $i = 1, \dots, w$.

Balance

Mean Driven Balance

Since the partition of matrices \mathbf{M}_i is carried out according to the mean values, the previous expressions convey a Mean Driven Balance.

Proposition 2

Models $\mathbf{y} \sim (\mathbf{X}\boldsymbol{\beta}; \mathbf{V}(\boldsymbol{\sigma}^2))$, with $\mathbf{X} = \mathbf{D}(\mathbf{1}_{r_1} \cdots \mathbf{1}_{r_k})$, have OLSE which are UBLUE if and only if they enjoy MDB.

Balance

Let us now assume that we had not grouped the observations according to their mean values and take $\mathcal{C}_1, \dots, \mathcal{C}_k$ to be the sets of indexes of observations with identical mean values.

Then $\mathbf{M}_{i,\ell,h}$ will be the sub-matrix of \mathbf{M}_i obtained selecting the elements with row and column indexes belonging to \mathcal{C}_ℓ and \mathcal{C}_h respectively.

Balance

We now consider a stronger version of MDB for which we establish the following proposition.

Proposition 3

The model has MDB whatever the sets $\mathcal{C}_1, \dots, \mathcal{C}_k$ if, with $\mathbf{M}_i = [m_{i,t,d}]$ we have $m_{i,t,t} = \overset{\circ}{m}_i$, $t = 1, \dots, n$ and $m_{i,t,d} = \tau_i \overset{\circ}{m}_i$, $t \neq d$, $i = 1, \dots, w$.

Variance components

With $\overset{\circ}{\mathbf{T}} = \mathbf{I}_n - \mathbf{T}$ the orthogonal projection matrix on the orthogonal complement Ω^\perp of Ω , $\overset{\circ}{\mathbf{y}} = \overset{\circ}{\mathbf{T}}\mathbf{y}$ will have the variance-covariance matrix

$$\mathbf{V}(\sigma^2) = \sum_{i=1}^w \sigma_i^2 \overset{\circ}{\mathbf{M}}_i$$

with

$$\overset{\circ}{\mathbf{M}}_i = \overset{\circ}{\mathbf{T}}\mathbf{M}_i\overset{\circ}{\mathbf{T}} = \begin{bmatrix} \overset{\circ}{m}_{i,1,1} & \cdots & \overset{\circ}{m}_{i,1,n} \\ \vdots & & \vdots \\ \overset{\circ}{m}_{i,n,1} & \cdots & \overset{\circ}{m}_{i,n,n} \end{bmatrix} \quad i = 1, \dots, n.$$

Variance components

Now the vector of principal elements of $\mathbf{V}(\sigma^2)$ will be σ^2 , with

$$\mathbf{B} = \begin{bmatrix} \overset{\circ}{m}_{1,1,1} & \cdots & \overset{\circ}{m}_{w,1,1} \\ \vdots & & \vdots \\ \overset{\circ}{m}_{1,n,n} & \cdots & \overset{\circ}{m}_{w,n,n} \end{bmatrix}.$$

The principal elements are the variance of the components $\overset{\circ}{y}_1 \cdots \overset{\circ}{y}_n$, of $\overset{\circ}{y}$, and, since they have null mean value, the mean values of their squares z_1, \dots, z_n . We thus get the OLSE like estimator

$$\tilde{\sigma}^2 = (\mathbf{B}^\top \mathbf{B})^{-1} \mathbf{BZ}.$$

Variance components

If \mathbf{y} and, consequently, $\overset{\circ}{\mathbf{y}}$ are normal, the variance-covariance matrix for \mathbf{Z} will be, see Schott (1997),

$$\mathbf{V}_{\mathbf{Z}}(\boldsymbol{\sigma}^2) = 2 \begin{bmatrix} \text{Var}(\overset{\circ}{\mathbf{y}}_1)^2 & \cdots & \text{Cov}(\overset{\circ}{\mathbf{y}}_1, \overset{\circ}{\mathbf{y}}_n)^2 \\ \vdots & & \vdots \\ \text{Cov}(\overset{\circ}{\mathbf{y}}_n, \overset{\circ}{\mathbf{y}}_1)^2 & \cdots & \text{Var}(\overset{\circ}{\mathbf{y}}_n)^2 \end{bmatrix}.$$

Thus we can apply the GLSE approach starting with $\tilde{\boldsymbol{\sigma}}_0^2 = \tilde{\boldsymbol{\sigma}}^2$ and successively complete the

$$\tilde{\boldsymbol{\sigma}}_{u+1}^2 = \left(\mathbf{B}^\top \mathbf{V}_{\mathbf{Z}}(\tilde{\boldsymbol{\sigma}}_u^2) \mathbf{B} \right)^{-1} \mathbf{B}^\top \mathbf{V}_{\mathbf{Z}}(\tilde{\boldsymbol{\sigma}}_u^2)^{-1} \mathbf{Z}$$

till $\left\| \tilde{\boldsymbol{\sigma}}_{u+1}^2 - \tilde{\boldsymbol{\sigma}}_u^2 \right\|$ is sufficiently null.

Stair nesting

In models with stair nesting a first fixed effects factor, with w levels, nests in succession k random effects factor.

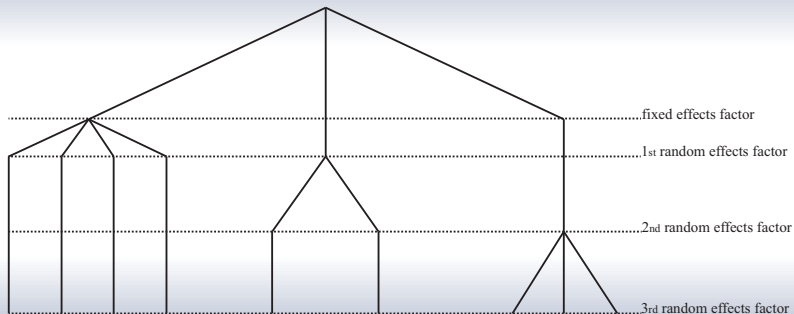


Figure: Stair nesting

Stair nesting

This model can be written as

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \sum_{i=1}^k \mathbf{X}_i \boldsymbol{\beta}_i,$$

with $\boldsymbol{\beta}$ fixed and the $\boldsymbol{\beta}_1, \dots, \boldsymbol{\beta}_k$ independent, with null mean vectors and variance-covariance matrices $\sigma_1^2 \mathbf{I}_{c_1}, \dots, \sigma_k^2 \mathbf{I}_{c_k}$. Moreover, we will have

$$\left\{ \begin{array}{l} \mathbf{X} = \mathbf{D} (\mathbf{1}_{r_1} \cdots \mathbf{1}_{r_k}) \\ \mathbf{X}_i = \mathbf{D} (\mathbf{I}_{r_1} \cdots \mathbf{I}_{r_i}, \mathbf{1}_{r_{i+1}} \cdots \mathbf{1}_{a_w}) \quad i = 1, \dots, w-1 \\ \mathbf{X}_w = \mathbf{D} (\mathbf{I}_{r_1} \cdots \mathbf{I}_{r_w}) = \mathbf{I}_n \end{array} \right.$$

where $n = \sum_{i=1}^w a_i$ is the number of observations.

Stair nesting

From the expression of \mathbf{X} above, we can see that the observations are grouped according to mean values. We also see that β_i has

$$c_i = \sum_{h=1}^i r_{h+w+i} \quad i = 1, \dots, w$$

components, and that the mean vector and variance-covariance of \mathbf{y} are

$$\begin{cases} \boldsymbol{\mu} = \mathbf{X}\boldsymbol{\beta} \\ \mathbf{V}(\boldsymbol{\sigma}^2) = \sum_{i=1}^r \sigma_i^2 \mathbf{M}_i \end{cases}$$

with

$$\begin{cases} \mathbf{M}_i = \mathbf{D}(\mathbf{I}_{r_1} \cdots \mathbf{I}_{r_i}, \mathbf{J}_{r_{i+1}} \cdots \mathbf{J}_{r_w}) & i = 1, \dots, k-1 \\ \mathbf{M}_w = \mathbf{D}(\mathbf{I}_{r_1}, \dots, \mathbf{I}_{r_w}) = \mathbf{I}_n. \end{cases}$$

Stair nesting

It is now straightforward to see that the condition for MDB holds since

$$\mathbf{M}_i = \begin{bmatrix} \mathbf{M}_{i,1,1} & \cdots & \mathbf{M}_{i,1,k} \\ \vdots & & \vdots \\ \mathbf{M}_{i,k,1} & \cdots & \mathbf{M}_{i,k,k} \end{bmatrix} \quad i = 1, \dots, k$$

with $\mathbf{M}_{i,\ell,\ell} = \mathbf{I}_{r_\ell}$, $\ell = 1, \dots, i$, $\mathbf{M}_{i,\ell,\ell} = \mathbf{J}_{r_\ell}$, $\ell = i + 1, \dots, w$, and $\mathbf{M}_{\ell,h} = \mathbf{0}_{r_\ell \times r_\ell}$, $\ell \neq h$. Thus we have established the following proposition.

Proposition 4

Stair nesting designs enjoy MDB, so their OLSE are UBLUE.

Balanced cross-nesting

Let there be u factors with b_1, \dots, b_u levels that cross and only one observation for each of the

$$n = \prod_{j=1}^u b_j$$

treatments. The first v factors are the ones with fixed effects and the factor levels will be $j_\ell = 1, \dots, b_\ell$, $\ell = 1, \dots, u$.

Balanced cross-nesting

So the treatments and the observations can be ordered according to the indexes

$$i(\mathbf{j}) = \sum_{\ell=1}^{k-1} (j_{\ell} - 1) \prod_{h=\ell+1}^u b_h + j_u,$$

so the densities will be grouped into

$$k = \prod_{\ell=1}^v b_{\ell}$$

sub-vectors each with

$$r = \prod_{\ell=v+1}^u b_{\ell}$$

observations with identical mean values.

Balanced cross-nesting

The parameters of this model correspond to the subsets \mathcal{C} of $\bar{u} = \{1, \dots, u\}$. To $\mathcal{C} = \emptyset$ is associated the general mean value $\mu = \beta(\emptyset)$. If $\#(\mathcal{C}) = 1$ [> 1], $\beta(\mathcal{C})$ will be constituted by the level effects [interactions between levels] of the factor or factors with indexes in \mathcal{C} . These sets and corresponding parameters may be ordered according to the indexes

$$k(\mathcal{C}) = 1 + \sum_{l \in \mathcal{C}} 2^{l-1},$$

these associated to the fixed [random] effects part having indexes $h = 1, \dots, 2^v$ [$h = 2^v + 1, \dots, 2^u$].

Balanced cross-nesting

Moreover, see Fonseca *et al.* (2003), the model may be written as

$$\mathbf{y} = \sum_{h=1}^{2^u} \mathbf{X}_h \boldsymbol{\beta}_h$$

with

$$\mathbf{X}_h = \bigotimes_{\ell=1}^u \mathbf{X}_{h,\ell} \quad h = 1, \dots, 2^u$$

where \otimes represents the Kronecker matrix product and $\mathbf{X}_{h,\ell} = \mathbf{1}_{b_\ell} [\mathbf{I}_{b_h}]$ when $\ell \in \mathcal{C}_h$ [$\ell \in \mathcal{C}_h$], $\ell = 1, \dots, u$, $h = 1, \dots, 2^u$.

Balanced cross-nesting

If the β_h , $h = 2^v + 1, \dots, 2^u$, are independent, with null mean vectors and variance-covariance matrices $\sigma_h^2 \mathbf{I}_{C_h}$, $h = 2^v + 1, \dots, 2^u$, we have

$$\mathbf{V}(\boldsymbol{\sigma}^2) = \sum_{h=2^v+1}^{2^u} \sigma_h^2 \mathbf{M}_h,$$

where

$$\mathbf{M}_h = \bigotimes_{\ell=1}^u \mathbf{M}_{h,\ell}, \quad h = 1, \dots, 2^u,$$

with $\mathbf{M}_{h,\ell} = \mathbf{J}_{b_\ell} [\mathbf{I}_{b_\ell}]$ when $\ell \notin \mathcal{C}_h$ [$\ell \in \mathcal{C}_h$], $\ell = 1, \dots, u$, $h = 1, \dots, 2^u$.

Balanced cross-nesting

Taking

$$\bigotimes_{\ell=1}^u \mathbf{M}_{h,\ell} = \begin{bmatrix} m_{h,1,1} & \cdots & m_{h,1,k} \\ \vdots & & \vdots \\ m_{h,k,1} & \cdots & m_{h,k,k} \end{bmatrix} \quad h = 1, \dots, 2^u,$$

we have

$$\mathbf{M}_h = \begin{bmatrix} m_{h,1,1} \mathbf{W}_h & \cdots & m_{h,1,k} \mathbf{W}_h \\ \vdots & & \vdots \\ m_{h,k,1} \mathbf{W}_h & \cdots & m_{h,k,k} \mathbf{W}_h \end{bmatrix} \quad h = 1, \dots, 2^u$$

with

$$\mathbf{W}_h = \bigotimes_{\ell=v+1}^u \mathbf{M}_{h,\ell} \quad h = 1, \dots, 2^u.$$

Balanced cross-nesting

We now have the following proposition

Proposition 4

The balanced cross nesting enjoys MDB.

On OBS

Now, see Mexia *et al.* (2010), a model

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \sum_{i=1}^w \mathbf{X}_i \boldsymbol{\beta}_i$$

with $\boldsymbol{\beta}$ fixed and the $\boldsymbol{\beta}_1, \dots, \boldsymbol{\beta}_w$ independent with null mean vectors and variance-covariance matrices $\sigma_1^2 \mathbf{I}_{c_1}, \dots, \sigma_w^2 \mathbf{I}_{c_w}$, has OBS if

$$\mathcal{R}([\mathbf{X}_1 \cdots \mathbf{X}_m]) = \mathbb{R}^n$$

and the matrices $\mathbf{M}_i = \mathbf{X}_i \mathbf{X}_i^\top$, $i = 1, \dots, w$, commute.

It is now easy to see that the models for stair nesting and balanced cross nesting enjoy OBS.

On OBS

To show that a model may have MDB without having OBS, we take, with

$$\mathbf{X} = \begin{bmatrix} \mathbf{1}_{r_1} & \mathbf{0}_{r_1} \\ \mathbf{0}_{r_2} & \mathbf{1}_{r_2} \end{bmatrix} \quad ; \quad \mathbf{X}_i = \begin{bmatrix} \mathbf{X}_{i,1} & \mathbf{0} \\ \mathbf{0} & \mathbf{X}_{i,2} \end{bmatrix} \quad i = 1, 2$$

$$\mathbf{X}_3 = \begin{bmatrix} \mathbf{I}_{r_1} & \mathbf{0} \\ \mathbf{0} & \mathbf{I}_{r_2} \end{bmatrix},$$

where the sub matrices $\mathbf{0}$ are null.

Assuming β to be fixed and the β_1, β_2 and β_3 to be independent with null mean vectors and variance-covariance matrices $\sigma_1^2 \mathbf{I}_{c_1}$, $\sigma_2^2 \mathbf{I}_{c_2}$ and $\sigma_3^2 \mathbf{I}_{c_3}$, if, with $\mathbf{M}_{i,\ell} = \mathbf{X}_{i,\ell} \mathbf{M}_{i,\ell}^\top$, $\ell = 1, 2$, $i = 1, 2$,

$$\mathbf{M}_{i,\ell} \mathbf{1}_{r_\ell} = t_{i,\ell} \mathbf{1}_{r_\ell} \quad \ell = 1, 2; i = 1, 2, 3,$$

the model will have MDB.

On OBS

But, if $M_{1,1}$ and $M_{2,2}$ do not commute, M_1 and M_2 don't commute and the model does not have OBS. For instance, taking

$$\mathbf{X}_{1,1} = \begin{bmatrix} 1 & 1 \\ 0 & 1 \\ 1 & 0 \end{bmatrix} ; \quad \mathbf{X}_{2,1} = \begin{bmatrix} 0 & 1 \\ 1 & 1 \\ 1 & 1 \end{bmatrix},$$

matrices $M_{1,1}$ and $M_{2,1}$ do not commute.

A final result

We established the equivalence of the Kruskal condition

$$\mathcal{R}(\mathbf{V}\mathbf{X}) \subseteq \mathcal{R}(\mathbf{X})$$

and the Zyskind & Zmysłony commutativity condition







$$\mathbf{V}\mathbf{T} = \mathbf{T}\mathbf{V}$$

using the fact that both were necessary and sufficient for the OLSE of models $\mathbf{y} \sim (\mathbf{X}\boldsymbol{\beta}; \sigma^2\mathbf{V})$ being Uniformly Minimum Variance Unbiased Estimator, UMVUE.







Proposition 6

We have $\mathcal{R}(\mathbf{V}\mathbf{X}) \subseteq \mathcal{R}(\mathbf{X})$ if and only if $\mathbf{V}\mathbf{T} = \mathbf{T}\mathbf{V}$.





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