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ON THE INVERSE OF CERTAIN PATTERNED MATRICES WITH KRONECKER PRODUCT STRUCTURES*

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Abstract. In this paper we derive explicit expressions for the entries of the inverse of a patterned matrix that is a sum of Kronecker products. This matrix keeps the Kronecker structure under matrix inversion. We also obtain a closed form inverse in terms of block matrices.

Key words. Inverse matrix, Kronecker product, sum of matrices, block matrix, covariance matrix

AMS subject classifications. 15A09, 15A27, 15A69

1. Introduction and examples. Matrices that can be presented as a linear combination of Kronecker products consisting of the identity matrix, I, and the matrix J with all elements equal to 1 often appear in statistics, in particular, in the analysis of linear models. A balanced s-factor linear mixed crossed-classification model can in matrix notation be expressed as

$$y = X\beta + Z\gamma + \epsilon, \tag{1.1}$$

where $y : n \times 1$ is a vector of random variables representing observations; both, X and Z consist of 0's and 1's: $X : n \times p$ is a known design matrix with Kronecker structure of the form $\mathbf{1} \otimes I$ specifying values of fixed effects for each observation (here $\mathbf{1}$ denotes a vector of ones); $Z : n \times q$ is a known incidence matrix with Kronecker structure of the form $I \otimes \mathbf{1}$ giving the values of random effects corresponding to each observation; $\beta = (\beta_1, \dots, \beta_\upsilon)' : p \times 1$ is a vector of unknown parameters (fixed effects); $\gamma = (\gamma_1, \dots, \gamma_s)' : q \times 1$ is a vector of unobservable random vectors γ_i (random effects), $E(\gamma) = 0$, $Var(\gamma) = G$; and $\epsilon : n \times 1$ is a vector of random errors, $E(\epsilon) = 0$, $Var(\epsilon) = R$, $R > 0$. It is assumed that the random vectors γ_i and γ_j ($i \neq j$, $i, j = 1, \dots, \nu$), and γ and ϵ are uncorrelated. Let Σ_s denote the variance-covariance matrix of y, i.e. $\Sigma_s = Var(y) = ZGZ' + R$, where G is a block-diagonal matrix with blocks $c_{0i}I_{n_i} + c_{1i}J_{n_i}$, $i = 1, \dots, s$, and $R = \sigma^2 I_n$. In this paper we will consider patterned matrices Σ_s of the following form

$$\Sigma_s = \sum_{\iota_s=0}^{1} \dots \sum_{\iota_1=0}^{1} v_{\iota_s \dots \iota_2 \iota_1} J_{n_s}^{\iota_s} \otimes \dots \otimes J_{n_2}^{\iota_2} \otimes J_{n_1}^{\iota_1}, \tag{1.2}$$

where

$$J_{n_i}^{\iota_i} \begin{cases} I_{n_i}, & \text{if } \iota_i = 0, \\ J_{n_i}, & \text{if } \iota_i = 1, \end{cases} \quad , i = 1, \dots, s, \tag{1.3}$$

I_{n_i} is an identity matrix of order n_i, J_{n_i} is an $n_i \times n_i$ matrix with all elements equal to 1, $v_{\iota_s \dots \iota_2 \iota_1}$'s are constants, and the symbol $\otimes$ denotes the Kronecker product operator. Properties of the Kronecker product can be found in, for example, [2], [4].

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The inverse Σ_s^{-1} of the covariance matrix Σ_s plays an important role in mixed model analysis, when estimating unknown parameters in the model (1.1), and in the variance-covariance matrix of the estimators. Thus, the inverses of matrices Σ_s have been studied extensively (see for example, [1], [3], [7], [8], [10], [13]-[15]). There have been proposed different algorithms (e.g., [3], [5], [9]-[11], [16]) for matrix inversion that handle sums of matrices with Kronecker structures similar to (1.2), though none of which appears to be optimal. Moreover, none of the proposed approaches takes into account the block structure of the matrix Σ_s.

In this work, alternative algorithms for inverting Σ_s given in (1.2) will be presented. We will also demonstrate how the block structure of Σ_s can be used.

The paper is organized as follows. The next section provides a brief survey of some existing results concerning the representation and the inversion of the class of patterned matrices that are sum of Kronecker products. In Section 3 new formulas for the inverse of this class of matrices are provided. Section 4 shows how to exploit the block structure of Σ_s to obtain an effective scheme for computing Σ_s^{-1}. Section 5 contains numerical examples.

2. Related work and preliminaries. In this section we establish some notation to be used throughout the paper and give a brief review of methods proposed be Searle and Henderson [10] and Jiang [3] concerning the inversion of Σ_s given in (1.2). First observe that [6]

LEMMA 2.1. *Any covariance matrix Σ_s can be expressed as*

$$\Sigma_s = (\sigma_{ij}) = \sum_{\substack{i_s,\dots,i_1 \\ j_s,\dots,j_1}} \sigma_{(i_s\dots i_2 i_1)(j_s\dots j_2 j_1)} (e_{s,i_s} e'_{s,j_s}) \otimes \cdots \otimes (e_{2,i_2} e'_{2,j_2}) \otimes (e_{1,i_1} e'_{1,j_1}), \quad (2.1)$$

where

$$\sigma_{(i_s\dots i_2 i_1)(j_s\dots j_2 j_1)} = cov(y_{i_s\dots i_2 i_1}, y_{j_s,\dots,j_1}) = \sigma_{ij}, \quad (2.2)$$

$$i = \sum_{h=1}^{s-1} (i_{s-h+1} - 1) n_{s-h} \cdot \ldots \cdot n_2 \cdot n_1 + i_1, \quad (2.3)$$

$$j = \sum_{h=1}^{s-1} (j_{s-h+1} - 1) n_{s-h} \cdot \ldots \cdot n_2 \cdot n_1 + j_1, \quad (2.4)$$

and e_{h,i_h} is the i_hth column of the identity matrix I_{n_h}; $i_h, j_h = 1, \dots, n_h$, $h = 1, \dots, s$.

The following notation will be used throughout the paper. For matrices $A_1, \dots, A_s$ the symbol $\bigotimes$ represents the operator of the following Kronecker product

$$\bigotimes_{h=s}^{1} A_h = A_s \otimes A_{s-1} \otimes \cdots \otimes A_1. \quad (2.5)$$

The next lemma shows an alternative way to present the matrix Σ_s defined in (1.2).

LEMMA 2.2. *The matrix Σ_s in (1.2) can be written as a linear combination of the components I_{n_h} and $(J_{n_h} - I_{n_h})$:*

$$\Sigma_s = \sum_{\iota_s=0}^{1} \dots \sum_{\iota_1=0}^{1} \tau_k \bigotimes_{i=s}^{1} (J_{n_i} - I_{n_i})^{\iota_i}, \quad (2.6)$$

where the index k is a function of $\iota_1, \dots, \iota_s$, i.e.

$$k(\iota_s, \dots, \iota_1) = \sum_{h=1}^{s} \iota_h \cdot 2^{h-1} + 1. \tag{2.7}$$

The constants τ_ν, $\nu = 1, \dots, 2^s$, are defined in the following way:

$$\tau_\nu = cov(y_{i_s \dots i_2 i_1}, y_{j_s \dots j_2 j_1}), \tag{2.8}$$

$$\nu = \sum_{h=1}^{s} 2^{h-1} \cdot 1_{\{i_h \neq j_h\}} + 1, \tag{2.9}$$

where $1_{\{\bullet\}}$ denotes the indicator function, and $i_h, j_h = 1, \dots, s$.

For example,

$$\begin{aligned} \Sigma_1 &= \tau_1 I_{n_1} + \tau_2 (J_{n_1} - I_{n_1}), \\ \Sigma_2 &= \tau_1 I_{n_2} \otimes I_{n_1} + \tau_2 I_{n_2} \otimes (J_{n_1} - I_{n_1}) \\ &\quad + \tau_3 (J_{n_2} - I_{n_2}) \otimes I_{n_1} + \tau_4 (J_{n_2} - I_{n_2}) \otimes (J_{n_1} - I_{n_1}). \end{aligned}$$

It worth to notice, that the matrix structures given by (1.2) or (2.6) carry over to their inverses [12], [10]. Therefore, the inverse of the matrix Σ_s in(1.2) can be presented in the following form:

$$\Sigma_s^{-1} = \sum_{\iota_s=0}^{1} \cdots \sum_{\iota_1=0}^{1} w_{\iota_s \dots \iota_2 \iota_1} J_{n_s}^{\iota_s} \otimes \cdots \otimes J_{n_2}^{\iota_2} \otimes J_{n_1}^{\iota_1}, \tag{2.10}$$

or

$$\Sigma_s^{-1} = \sum_{\iota_s=0}^{1} \cdots \sum_{\iota_1=0}^{1} \theta_k \bigotimes_{i=s}^{1} (J_{n_i} - I_{n_i})^{\iota_i}, \tag{2.11}$$

where $J_{n_h}^{\iota_h}$, $h = 1, \dots, s$, are defined in (1.3), $w_{\iota_s \dots \iota_2 \iota_1}$'s and θ_k are the constants.

Searle and Henderson [10] investigated spectral properties of Σ_s given in (1.2) and provided the expressions for $w_{\iota_s \dots \iota_2 \iota_1}$ in (2.10). A drawback of the obtained formulas is that they present results in terms of the coefficients $v_{\iota_s \dots \iota_2 \iota_1}$ in (1.2). As we can see the coefficients $v_{\iota_s \dots \iota_2 \iota_1}$ are not the elements of the matrix $\Sigma_s = (\sigma_{ij})$ but the linear combinations of them. For example,

$$\Sigma_1 = \begin{pmatrix} \tau_1 & \tau_2 & \tau_2 \\ \tau_2 & \tau_1 & \tau_2 \\ \tau_2 & \tau_2 & \tau_1 \end{pmatrix} = (\tau_1 - \tau_2) I_{n_1} + \tau_2 J_{n_1},$$

and

$$\Sigma_2 = \left(\begin{array}{cc|cc} \tau_1 & \tau_2 & \tau_3 & \tau_4 \\ \tau_2 & \tau_1 & \tau_4 & \tau_3 \\ \hline \tau_3 & \tau_4 & \tau_1 & \tau_2 \\ \tau_4 & \tau_3 & \tau_2 & \tau_1 \end{array} \right) = (\tau_1 - \tau_2 - \tau_3 + \tau_4) I_{n_2} \otimes I_{n_1} + (\tau_2 - \tau_4) I_{n_2} \otimes J_{n_1}$$
$$+ (\tau_3 - \tau_4) J_{n_2} \otimes I_{n_1} + \tau_4 J_{n_2} \otimes J_{n_1}.$$

Thus, when studying the spectral properties of the matrix Σ_s or the theoretical properties of Σ_s^{-1} it is not easy to see how they depend on the variance-covariance components of Σ_s which characterize dependencies among random factor levels. More explicit expressions for the coefficients $w_{\iota_s \ldots \iota_2 \iota_1}$ and the eigenvalues of Σ_s in terms of elements of Σ_s have been provided in [3] and [6], respectively.

First the following auxiliary lemma can be formulated [10], [6].

LEMMA 2.3. *Let $\lambda_{\alpha_s,\alpha_{s-1},\ldots,\alpha_1}$, $\alpha_h \in \{0, h\}$, $h = 1, \ldots, s$, be eigenvalues of Σ_s. Then the following relationship holds:*

$$\begin{pmatrix} \lambda_{0,0,\ldots,0} \\ \vdots \\ \lambda_{s,s-1,\ldots,1} \end{pmatrix} = \bigotimes_{i=s}^{1} \begin{pmatrix} 1 & 0 \\ 1 & n_i \end{pmatrix} \begin{pmatrix} v_{00\ldots0} \\ \vdots \\ v_{11\ldots1} \end{pmatrix}. \tag{2.12}$$

In the next theorem we derive the relationship between the coefficients $v_{\iota_s \ldots \iota_2 \iota_1}$ in (1.2) and Σ_s elements. This result will later be used when obtaining Σ_s^{-1}.

THEOREM 2.4. *The relationship between Σ_s elements τ_i given by (2.8), $i = 1, \ldots, 2^s$, and the coefficients $v_{\iota_s \ldots \iota_2 \iota_1}$ in (1.2) is the following:*

$$\begin{pmatrix} v_{00\ldots0} \\ \vdots \\ v_{11\ldots1} \end{pmatrix} = \bigotimes_{i=s}^{1} \begin{pmatrix} 1 & -1 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \tau_1 \\ \vdots \\ \tau_p \end{pmatrix}. \tag{2.13}$$

Proof. Using Lemma 2.3, Σ_s can be presented via its spectrum using the following relation [6]:

$$\begin{pmatrix} v_{00\ldots0} \\ \vdots \\ v_{11\ldots1} \end{pmatrix} = \bigotimes_{i=s}^{1} \begin{pmatrix} 1 & 0 \\ -\frac{1}{n_i} & \frac{1}{n_i} \end{pmatrix} \begin{pmatrix} \lambda_{0,0,\ldots,0} \\ \vdots \\ \lambda_{s,s-1,\ldots,1} \end{pmatrix}. \tag{2.14}$$

Finally, using some results in [6], we notice that

$$\begin{pmatrix} \lambda_{0,0,\ldots,0} \\ \vdots \\ \lambda_{s,s-1,\ldots,1} \end{pmatrix} = \bigotimes_{i=s}^{1} \begin{pmatrix} 1 & -1 \\ 1 & n_i - 1 \end{pmatrix} \begin{pmatrix} \tau_1 \\ \vdots \\ \tau_\nu \end{pmatrix}, \tag{2.15}$$

and hence

$$\begin{pmatrix} v_{00\ldots0} \\ \vdots \\ v_{11\ldots1} \end{pmatrix} = \bigotimes_{i=s}^{1} \begin{pmatrix} 1 & -1 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \tau_1 \\ \vdots \\ \tau_\nu \end{pmatrix}, \nu = 1, \ldots, 2^s.$$

□

COROLLARY 2.5. *The coefficients $v_{\iota_s \ldots \iota_1}$ in (1.2) are related to the elements of the matrix Σ_s in the following way:*

$$v_{\iota_s \ldots \iota_1} = \sum_{i_s=0}^{1} \cdots \sum_{i_1=0}^{1} \tau_k \prod_{h=1}^{s} (-1)^{1_{\{i_h > \iota_h\}}} \cdot 1_{\{i_h \geq \iota_h\}}, \tag{2.16}$$

where $1_{\{\bullet\}}$ is the indicator function, $\iota_h \in \{0, 1\}$, and k is given by (2.7).

We also will use the following result for obtaining the spectrum of Σ_s [6].

Theorem 2.6. *All eigenvalues of the matrix Σ_s given by (1.2) can be obtained by the following formula:*

$$\lambda_{\alpha_s,\dots,\alpha_1} = \sum_{\iota_s=0}^{1} \cdots \sum_{\iota_1=0}^{1} \tau_k \prod_{i=1}^{s} (n_{\alpha_i} - 1)^{\iota_i}, \tag{2.17}$$

where $\alpha_h = h \cdot \iota_h$, $\iota_h \in \{0,1\}$, $h = 1,\dots,s$, n_0=0, and k is given by (2.7).

3. Inverse of the matrix Σ_s. This section presents new formulas for obtaining the inverse of Σ_s. Our approach is different from those proposed by Searle and Henderson [10] and Jiang [3]. We will consider Σ_s given by (2.6) and provide explicitly the inverse Σ_s^{-1} of the form (2.11). The advantage of our approach is that the coefficients θ_k, $k = 1,\dots,2^s$, in the expression of Σ_s^{-1}, given by (2.11), are the elements of the matrix Σ_s^{-1} and not linear combinations of them as those $w_{\iota_s\dots\iota_1}$ in (3.1). Thus, the theoretical properties of Σ_s^{-1} could be investigated in a convenient manner. Another difference with the approach demonstrated in [3], [10] is that the algorithms developed in this paper cover random factors γ_i in (1.1) with the variance-covariance matrix of the form $Var(\gamma_i) = c_{0i}I_{n_i} + c_{1i}J_{n_i}$ and not restricting it to $Var(\gamma_i) = c_{0i}I_{n_i}$, $i = 1,\dots,\nu$, as in [3], [10].

First, we display a new algorithm for computing the coefficients $w_{\iota_s\dots\iota_1}$ in (3.1) which is very flexible, i.e. Σ_s^{-1} given by (2.10) can be obtained either in terms of Σ_s elements (τ_i, $i = 1,\dots,2^s$), coefficients $v_{\iota_s\dots\iota_1}$ given in (1.2), or the eigenvalues of Σ_s ($\lambda_{\alpha_s,\dots,\alpha_1}$, $\alpha_h \in \{0,h\}$, $h = 1,\dots,s$).

Theorem 3.1. *Let the matrix Σ_s be a linear combination of Kronecker products as defined in (1.2). Then its inverse Σ_s^{-1} has the Kronecker structure (2.10) with the coefficients*

$$\begin{pmatrix} w_{00\dots0} \\ \vdots \\ w_{11\dots1} \end{pmatrix} = \bigotimes_{i=s}^{1} \begin{pmatrix} 1 & 0 \\ -\frac{1}{n_i} & \frac{1}{n_i} \end{pmatrix} \begin{pmatrix} \lambda_{0,0,\dots,0}^{-1} \\ \vdots \\ \lambda_{s,s-1,\dots,1}^{-1} \end{pmatrix}, \tag{3.1}$$

and $\lambda_{0,0,\dots,0}^{-1}, \dots, \lambda_{s,s-1,\dots,1}^{-1}$ could be calculated using (2.12) or (2.17).

Corollary 3.2. *The coefficients $w_{\iota_s\dots\iota_1}$ in (3.1) can be computed in the following way:*

$$w_{\iota_s\dots\iota_1} = \sum_{i_s=0}^{1} \cdots \sum_{i_1=0}^{1} \lambda_{\alpha_s,\dots,\alpha_1}^{-1} \prod_{h=1}^{s} \frac{(-1)^{1_{\{\iota_h > i_h\}}}}{(n_h)^{\iota_h}} \cdot 1_{\{\iota_h \geq i_h\}}, \tag{3.2}$$

where $1_{\{\bullet\}}$ is the indicator function, α_h is defined in Theorem 2.6, $\iota_h \in \{0,1\}$, $h = 1,\dots,s$, and k is given by (2.7).

The next theorem gives an alternative method to obtain Σ_s^{-1}.

Theorem 3.3. *Let Σ_s be given by (2.6). Then*

$$\Sigma_s^{-1} = \sum_{\iota_s=0}^{1} \cdots \sum_{\iota_1=0}^{1} \theta_k \bigotimes_{i=s}^{1} (J_{n_i} - I_{n_i})^{\iota_i}, \tag{3.3}$$

where

$$\theta_k = \sum_{i_s=0}^{1} \cdots \sum_{i_1=0}^{1} \lambda_{\alpha_s,\dots,\alpha_1}^{-1} \prod_{h=1}^{s} \frac{(n_{\bar{\alpha}_h(\iota_h)} - 1)^{1-i_h}}{n_h}, \tag{3.4}$$

k is given by (2.7), $\alpha_h = h \cdot i_h$, $h = 1, \ldots, s$, $\bar{\alpha}_h(\iota_h) = h \cdot 1_{\{i_h=\iota_h=0\}}$, and $\lambda^{-1}_{\alpha_s,\ldots,\alpha_1}$ can be obtained using (2.17).

Proof. Let $\lambda_{0,0,\ldots,0}, \ldots, \lambda_{s,s-1,\ldots,1}$ be eigenvalues of Σ_s, and $\lambda^{-1}_{0,0,\ldots,0}, \ldots, \lambda^{-1}_{s,s-1,\ldots,1}$ be the eigenvalues of Σ_s^{-1}. Similar to the relationship (2.15) for Σ_s, we get that

$$\begin{pmatrix} \lambda^{-1}_{0,0,\ldots,0} \\ \vdots \\ \lambda^{-1}_{s,s-1,\ldots,1} \end{pmatrix} = \bigotimes_{i=s}^{1} \begin{pmatrix} 1 & -1 \\ 1 & n_i - 1 \end{pmatrix} \begin{pmatrix} \theta_1 \\ \vdots \\ \theta_\nu \end{pmatrix}, \nu = 1, \ldots, 2^s, \tag{3.5}$$

and

$$\begin{pmatrix} \theta_1 \\ \vdots \\ \theta_\nu \end{pmatrix} = \bigotimes_{i=s}^{1} \begin{pmatrix} \frac{n_i-1}{n_i} & \frac{1}{n_i} \\ -\frac{1}{n_i} & \frac{1}{n_i} \end{pmatrix} \begin{pmatrix} \lambda^{-1}_{0,0,\ldots,0} \\ \vdots \\ \lambda^{-1}_{s,s-1,\ldots,1} \end{pmatrix}. \tag{3.6}$$

Straightforward computation could be used to confirm the the relationship in (3.6) can be written as (3.4).□

4. Inverting a block matrix. In this section we show how to exploit the block structure of Σ_s given by (1.2) to obtain an efficient scheme for inverting Σ_s. We demonstrate how to perform a sequence of elementary blockwise inversion steps in order to get Σ_s^{-1}. It has been shown in [6] that Σ_s given by (1.2) or (2.6) can be written as

$$\Sigma_s = I_{n_s} \otimes \Sigma^{(1)}_{s-1} + (J_{n_s} - I_{n_s}) \otimes \Sigma^{(2)}_{s-1}, \tag{4.1}$$

where

$$\Sigma^{(i_h)}_0 = \tau_h, \quad h = 1, \ldots, 2^s, \tag{4.2}$$

$$\Sigma^{(i_k)}_k = I_{n_k} \otimes \Sigma^{(2i_k-1)}_{k-1} + (J_{n_k} - I_{n_k}) \otimes \Sigma^{(2i_k)}_{k-1},$$

$$i_k = 1, \ldots, 2^{s-k}, \; k = 1, \ldots, s-1,$$

and τ_h's are given by (2.8).
For example, the matrix Σ_2: 6×6

$$\Sigma_2 = \left(\begin{array}{cc|cc|cc} \tau_1 & \tau_2 & \tau_3 & \tau_4 & \tau_3 & \tau_4 \\ \tau_2 & \tau_1 & \tau_4 & \tau_3 & \tau_4 & \tau_3 \\ \hline \tau_3 & \tau_4 & \tau_1 & \tau_2 & \tau_3 & \tau_4 \\ \tau_4 & \tau_3 & \tau_2 & \tau_1 & \tau_4 & \tau_3 \\ \hline \tau_3 & \tau_4 & \tau_3 & \tau_4 & \tau_1 & \tau_2 \\ \tau_4 & \tau_3 & \tau_4 & \tau_3 & \tau_2 & \tau_1 \end{array}\right) \tag{4.3}$$

can be presented as

$$\Sigma_2 = \begin{pmatrix} \Sigma^{(1)}_1 & \Sigma^{(2)}_1 & \Sigma^{(2)}_1 \\ \Sigma^{(2)}_1 & \Sigma^{(1)}_1 & \Sigma^{(2)}_1 \\ \Sigma^{(2)}_1 & \Sigma^{(2)}_1 & \Sigma^{(1)}_1 \end{pmatrix}, \tag{4.4}$$

and hence

$$\Sigma_2 = I_3 \otimes \Sigma^{(1)}_1 + (J_3 - I_3) \otimes \Sigma^{(2)}_1, \tag{4.5}$$

where $n_1 = 2$, $n_2 = 3$ and

$$\Sigma^{(1)}_1 = \tau_1 I_2 + \tau_2(J_2 - I_2), \tag{4.6}$$

$$\Sigma^{(2)}_1 = \tau_3 I_2 + \tau_4(J_2 - I_2). \tag{4.7}$$

In general, the matrix Σ_s given by (1.2) or (2.6) has the following block-structure:

$$\Sigma_s = \begin{pmatrix} \Sigma_{s-1}^{(1)} & \Sigma_{s-1}^{(2)} & \cdots & \Sigma_{s-1}^{(2)} \\ \Sigma_{s-1}^{(2)} & \Sigma_{s-1}^{(1)} & \cdots & \Sigma_{s-1}^{(2)} \\ \vdots & \vdots & \ddots & \vdots \\ \Sigma_{s-1}^{(2)} & \Sigma_{s-1}^{(2)} & \cdots & \Sigma_{s-1}^{(1)} \end{pmatrix}. \tag{4.8}$$

In the next theorem, the block-structure (4.8) of Σ_s is used to get Σ_s^{-1}.

THEOREM 4.1. *Let the matrix Σ_s have a structure as defined in (4.1), and $|\Sigma_s| \neq 0$. The matrix Σ_s^{-1} can be obtained in a recursive form as*

$$\Sigma_s^{-1} = I_{n_s} \otimes \Sigma_{s-1,1}^{-1} + (J_{n_s} - I_{n_s}) \otimes \Sigma_{s-1,2}^{-1}, \tag{4.9}$$

where

$$\Sigma_{s-1,1}^{-1} = \Sigma_{s-1,2}^{-1} + \left(\Sigma_{s-1}^{(1)} - \Sigma_{s-1}^{(2)}\right)^{-1}, \tag{4.10}$$

$$\Sigma_{s-1,2}^{-1} = -\left(\Sigma_{s-1}^{(1)} + (n_s - 1)\Sigma_{s-1}^{(2)}\right)^{-1} \Sigma_{s-1}^{(2)} \left(\Sigma_{s-1}^{(1)} - \Sigma_{s-1}^{(2)}\right)^{-1}$$

$$\Sigma_0^{(i_h)} = \tau_h, \quad h = 1, \ldots, 2^s,$$

$$\Sigma_{k,i_k}^{-1} = I_{n_k} \otimes \Sigma_{k-1,2i_k-1}^{-1} + (J_{n_k} - I_{n_k}) \otimes \Sigma_{k-1,2i_k}^{-1},$$

$$i_k = 1, \ldots, 2^{s-k}, \; k = 1, \ldots, s-1,$$

the τ_h's are given by (2.8).

Proof. First, we notice that due to the structure of Σ_s in (1.2), and definition of matrices $\Sigma_{s-1}^{(h)}$, $h = 1, 2$, matrices $(J_{n_s} - I_{n_s})$, $\Sigma_{s-1}^{(1)}$ and $\Sigma_{s-1}^{(2)}$ in (4.1) commute. Since Σ_s^{-1} has the same form as Σ_s [10],[12], we need to solve

$$\Sigma_s \cdot \Sigma_s^{-1} = I_{n_s} \otimes I_{n_{s-1}}, \tag{4.11}$$

or

$$\left(I_{n_s} \otimes \Sigma_{s-1}^{(1)} + (J_{n_s} - I_{n_s}) \otimes \Sigma_{s-1}^{(2)}\right)\left(I_{n_s} \otimes \Sigma_{s-1,1}^{-1} + (J_{n_s} - I_{n_s}) \otimes \Sigma_{s-1,2}^{-1}\right) = I_{n_s} \otimes I_{n_{s-1}}. \tag{4.12}$$

After some calculations and regrouping the terms in (4.12) we get

$$I_{n_s} \otimes \left(\Sigma_{s-1}^{(1)}\Sigma_{s-1,1}^{-1} - \Sigma_{s-1}^{(1)}\Sigma_{s-1,2}^{-1} - \Sigma_{s-1}^{(2)}\Sigma_{s-1,1}^{-1} + \Sigma_{s-1}^{(2)}\Sigma_{s-1,2}^{-1}\right) \tag{4.13}$$

$$+ J_{n_s} \otimes \left(\Sigma_{s-1}^{(1)}\Sigma_{s-1,2}^{-1} + \Sigma_{s-1}^{(2)}\Sigma_{s-1,1}^{-1} + (n_s - 2)\Sigma_{s-1}^{(2)}\Sigma_{s-1,2}^{-1}\right) = I_{n_s} \otimes I_{n_{s-1}} \tag{4.14}$$

and therefore,

$$\Sigma_{s-1}^{(1)}\Sigma_{s-1,1}^{-1} - \Sigma_{s-1}^{(1)}\Sigma_{s-1,2}^{-1} - \Sigma_{s-1}^{(2)}\Sigma_{s-1,1}^{-1} + \Sigma_{s-1}^{(2)}\Sigma_{s-1,2}^{-1} = I_{n_{s-1}}, \tag{4.15}$$

$$\Sigma_{s-1}^{(1)}\Sigma_{s-1,2}^{-1} + \Sigma_{s-1}^{(2)}\Sigma_{s-1,1}^{-1} + (n_s - 2)\Sigma_{s-1}^{(2)}\Sigma_{s-1,2}^{-1} = \mathbf{0}_{n_{s-1}}, \tag{4.16}$$

where $\mathbf{0}_{n_{s-1}}$ is a square matrix of order n_{s-1} with elements equal to 0. From (4.15) it follows that

$$\Sigma_{s-1,1}^{-1} = \left(\Sigma_{s-1}^{(1)} - \Sigma_{s-1}^{(2)}\right)^{-1} + \Sigma_{s-1,2}^{-1}, \tag{4.17}$$

and from (4.16) we get

$$\Sigma_{s-1,2}^{-1} = -\left(\Sigma_{s-1}^{(1)} + (n_s - 1)\Sigma_{s-1}^{(2)}\right)^{-1} \Sigma_{s-1}^{(2)} \left(\Sigma_{s-1}^{(1)} - \Sigma_{s-1}^{(2)}\right)^{-1}. \tag{4.18}$$

Since $|\Sigma_s| \neq 0$, it is follows (see for example, Corollary 3.1 in [6]) that the inverses $\left(\Sigma_{s-1}^{(1)} + (n_s - 1)\Sigma_{s-1}^{(2)}\right)^{-1}$ and $\left(\Sigma_{s-1}^{(1)} - \Sigma_{s-1}^{(2)}\right)^{-1}$ exist. □

5. Examples. Let us consider

$$\Sigma_1 = \begin{pmatrix} \tau_1 & \tau_2 & \tau_2 & \tau_2 \\ \tau_2 & \tau_1 & \tau_2 & \tau_2 \\ \tau_2 & \tau_2 & \tau_1 & \tau_2 \\ \tau_2 & \tau_2 & \tau_2 & \tau_1 \end{pmatrix}, \tag{5.1}$$

which according to (4.1) can be written as

$$\Sigma_1 = I_{n_1} \otimes \Sigma_0^{(1)} + (J_{n_1} - I_{n_1}) \otimes \Sigma_0^{(2)}, \tag{5.2}$$

where $n_1 = 4$, $\Sigma_0^{(1)} = \tau_1$ and $\Sigma_0^{(2)} = \tau_2$. From Theorem 4.1 it follows that

$$\Sigma_1^{-1} = I_4 \otimes \Sigma_{0,1}^{-1} + (J_4 - I_4) \otimes \Sigma_{0,2}^{-1}, \tag{5.3}$$

where

$$\Sigma_{0,2}^{-1} = -\left(\Sigma_0^{(1)} + 3\Sigma_0^{(2)}\right)^{-1} \Sigma_0^{(2)} \left(\Sigma_0^{(1)} - \Sigma_0^{(2)}\right)^{-1} = -\frac{\tau_2}{\tau_1 + 3\tau_2} \cdot \frac{1}{\tau_1 - \tau_2}, \tag{5.4}$$

$$\Sigma_{0,1}^{-1} = \Sigma_{0,2}^{-1} + \left(\Sigma_0^{(1)} - \Sigma_0^{(2)}\right)^{-1} = \frac{\tau_1 + 2\tau_2}{(\tau_1 + 3\tau_2)(\tau_1 - \tau_2)}.$$

Thus,

$$\Sigma_1^{-1} = \frac{\tau_1 + 2\tau_2}{(\tau_1 + 3\tau_2)(\tau_1 - \tau_2)} I_4 - \frac{\tau_2}{(\tau_1 + 3\tau_2)(\tau_1 - \tau_2)} (J_4 - I_4). \tag{5.5}$$

Regrouping terms in (5.5) yields

$$\Sigma_1^{-1} = \frac{1}{\tau_1 - \tau_2} I_4 - \frac{\tau_2}{(\tau_1 + 3\tau_2)(\tau_1 - \tau_2)} J_4, \tag{5.6}$$

which can also be obtained using a well known formula [3], [9], [10].

Let us consider the matrix defined in (4.3) which is a linear combination of four Kronecker products, i.e.

$$\Sigma_2 = \sum_{\iota_2=0}^{1} \sum_{\iota_1=0}^{1} v_{\iota_2\iota_1} J_{n_2}^{\iota_2} \otimes J_{n_1}^{\iota_1} \tag{5.7}$$

$$= v_{00} I_{n_2} \otimes I_{n_1} + v_{01} I_{n_2} \otimes J_{n_1} + v_{10} J_{n_2} \otimes I_{n_1} + v_{11} J_{n_2} \otimes J_{n_1}.$$

The coefficients $v_{\iota_2\iota_1}$ in (5.7) are the linear combinations of the elements of Σ_2 as stated in Theorem 2.4, i.e.

$$\Sigma_2 = (\tau_1 - \tau_2 - \tau_3 + \tau_4) I_{n_2} \otimes I_{n_1} + (\tau_2 - \tau_4) I_{n_2} \otimes J_{n_1} \tag{5.8}$$

$$+ (\tau_3 - \tau_4) J_{n_2} \otimes I_{n_1} + \tau_4 J_{n_2} \otimes J_{n_1}.$$

Using available formulas [3], [10] one obtains Σ_2^{-1} in terms of coefficients $v_{\iota_2\iota_1}$'s, i.e.

$$\Sigma_s^{-1} = \frac{1}{v_{00}} I_{n_2} \otimes I_{n_1} - \frac{1}{n_1}\left(\frac{1}{v_{00}} - \frac{1}{v_{00} + n_1 v_{01}}\right) I_{n_2} \otimes J_{n_1} - \frac{1}{n_2}\left(\frac{1}{v_{00}} - \frac{1}{v_{00} + n_2 v_{10}}\right) J_{n_2} \otimes I_{n_1}$$

$$+ \frac{1}{n_1 n_2}\left(\frac{1}{v_{00}} - \frac{1}{v_{00} + n_1 v_{01}} - \frac{1}{v_{00} + n_2 v_{10}} + \frac{1}{v_{00} + n_1 v_{01} + n_2 v_{10} + n_1 n_2 v_{11}}\right) J_{n_2} \otimes J_{n_1}. \tag{5.9}$$

The disadvantage of this expression is that we cannot directly see how the elements of Σ_s^{-1} look like, unless the regrouping of the terms in (5.9) is done. Applying the alternative formula given in Theorem 3.3, we get directly expressions for Σ_2^{-1} elements:

$$\begin{aligned}\Sigma_2^{-1} = & \frac{1}{n_1 n_2}\left(\frac{(n_1-1)(n_2-1)}{\lambda_{00}} + \frac{(n_2-1)}{\lambda_{01}} + \frac{(n_1-1)}{\lambda_{20}} + \frac{1}{\lambda_{21}}\right) I_{n_2} \otimes I_{n_1} \\ & + \frac{1}{n_1 n_2}\left(-\frac{(n_2-1)}{\lambda_{00}} + \frac{(n_2-1)}{\lambda_{01}} - \frac{1}{\lambda_{20}} + \frac{1}{\lambda_{21}}\right) I_{n_2} \otimes (J_{n_1} - I_{n_1}) \\ & + \frac{1}{n_1 n_2}\left(-\frac{(n_1-1)}{\lambda_{00}} - \frac{1}{\lambda_{01}} + \frac{(n_1-1)}{\lambda_{20}} + \frac{1}{\lambda_{21}}\right) (J_{n_2} - I_{n_2}) \otimes I_{n_1} \\ & + \frac{1}{n_1 n_2}\left(\frac{1}{\lambda_{00}} - \frac{1}{\lambda_{01}} - \frac{1}{\lambda_{20}} + \frac{1}{\lambda_{21}}\right) (J_{n_2} - I_{n_2}) \otimes (J_{n_1} - I_{n_1}),\end{aligned}$$

where the eigenvalues $\lambda_{00}, \ldots, \lambda_{21}$ of Σ_s are obtained using (2.17), i.e.

$$\begin{aligned}\lambda_{00} &= \tau_1 - \tau_2 - \tau_3 + \tau_4, \\ \lambda_{01} &= \tau_1 + (n_1-1)\tau_2 - [\tau_3 + (n_1-1)\tau_4], \\ \lambda_{20} &= \tau_1 - \tau_2 + (n_2-1)[\tau_3 - \tau_4], \\ \lambda_{21} &= [\tau_1 + (n_1-1)\tau_2] + (n_2-1)[\tau_3 + (n_1-1)\tau_4].\end{aligned}$$

We can invert Σ_s recursively using its block structure in the following way. Let Σ_s be as defined in (4.5)–(4.7). From Theorem 4.1 it follows that

$$\Sigma_2^{-1} = I_3 \otimes \Sigma_{1,1}^{-1} + (J_3 - I_3) \otimes \Sigma_{1,2}^{-1}, \tag{5.10}$$

where

$$\Sigma_{1,1}^{-1} = \Sigma_{1,2}^{-1} + \left(\Sigma_1^{(1)} - \Sigma_1^{(2)}\right)^{-1} \tag{5.11}$$

$$\Sigma_{1,2}^{-1} = -\left(\Sigma_1^{(1)} + 2\Sigma_1^{(2)}\right)^{-1} \Sigma_1^{(2)} \left(\Sigma_1^{(1)} - \Sigma_1^{(2)}\right)^{-1}. \tag{5.12}$$

Matrices

$$\begin{aligned}\Sigma_1^{(1)} - \Sigma_1^{(2)} &= (\tau_1 - \tau_3) I_2 + (\tau_2 - \tau_4)(J_2 - I_2) \\ &= I_2 \otimes \Sigma_0^{(1)} + (J_2 - I_2) \otimes \Sigma_0^{(2)}\end{aligned}$$

and

$$\begin{aligned}\Sigma_1^{(1)} + 2\Sigma_1^{(2)} &= (\tau_1 + 2\tau_3) I_2 + (\tau_2 + 2\tau_4)(J_2 - I_2) \\ &= I_2 \otimes \Sigma_0^{(1)} + (J_2 - I_2) \otimes \Sigma_0^{(2)}\end{aligned} \tag{5.13}$$

have the structure defined in (4.1). Thus, we can use Theorem 4.1 in order to obtain their inverses, i.e.

$$\begin{aligned}\left(\Sigma_1^{(1)} - \Sigma_1^{(2)}\right)^{-1} &= I_2 \otimes \Sigma_{0,1}^{-1} + (J_2 - I_2) \otimes \Sigma_{0,2}^{-1} \\ &= \frac{\tau_1 - \tau_3}{(\tau_1 + \tau_2 - \tau_3 - \tau_4)} \cdot \frac{1}{(\tau_1 - \tau_2 - \tau_3 + \tau_4)} I_2 \\ &\quad - \frac{\tau_2 - \tau_4}{(\tau_1 + \tau_2 - \tau_3 - \tau_4)} \frac{1}{(\tau_1 - \tau_2 - \tau_3 + \tau_4)} (J_2 - I_2)\end{aligned}$$

$$\left(\Sigma_1^{(1)} + 2\Sigma_1^{(2)}\right)^{-1} = I_2 \otimes \Sigma_{0,1}^{-1} + (J_2 - I_2) \otimes \Sigma_{0,2}^{-1}$$
$$= \frac{\tau_1 + 2\tau_3}{(\tau_1 - \tau_2 + 2\tau_3 - 2\tau_4)} \cdot \frac{1}{(\tau_1 + \tau_2 + 2\tau_3 + 2\tau_4)} I_2$$
$$- \frac{\tau_2 + 2\tau_4}{(\tau_1 - \tau_2 + 2\tau_3 - 2\tau_4)} \frac{1}{(\tau_1 + \tau_2 + 2\tau_3 + 2\tau_4)} (J_2 - I_2) \quad .$$

Using (5.11)-(5.12) after some calculations we can obtain Σ_2^{-1} of the form (5.10). In spite of the complicated expressions for coefficients of matrices that should be inverted at each step, the blockwise structure of Σ_2^{-1} remains quite simple. Moreover, inverting Σ_2, as well as a general Σ_s, one repeats the same procedure all the time.

6. Conclusions. In this paper we have derived algorithms for the matrix inversion in the case when the matrix is a certain patterned sum of Kronecker products. This class of matrices often occurs in the analysis of linear mixed models. Proposed algorithms are helpful in the analysis of the linear model when constructing estimators or studying their statistical properties. These algorithms can easily be used when generating synthetic data sets with pre-specified properties which could be given via the variance-covariance matrix. Although there exist methods for inverting such a class of matrices, the available formulas do not completely elucidate the structure of the elements of the inverse matrix. Moreover, we have worked out the inversion techniques that employs block-structure of this class of matrices.

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