

Further techniques on a polynomial positivity question of Collins, Dykema, and Torres-Ayala

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ABSTRACT. We prove that the coefficient of t^2 in $\text{trace}((A + tB)^6)$ is a sum of squares in the entries of the symmetric matrices A and B .

1. Introduction

In [5], Collins, Dykema, and Torres-Ayala asked the following question:

Conjecture 1. *If A and B are symmetric matrices of the same size, then for all $m \geq r$ where m and r are even, the coefficient of t^r in $\text{trace}((A + tB)^m)$ is non-negative.*

The question was a variant of the following question (in the version stated below, given by Lieb and Seiringer in [9]).

Conjecture 2. *If A and B are positive semidefinite matrices of the same size, then for all integers $m \geq r \geq 0$, the coefficient of t^r in $\text{trace}((A + tB)^m)$ is non-negative.*

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This conjecture is neither stronger than nor weaker than Conjecture 1 as the statement relaxes the evenness conditions on m and r , but requires A and B to be positive semidefinite. Conjecture 2 was formulated by Lieb and Seiringer because it is equivalent to the following conjecture from 1975 by Bessis, Moussa, and Villani in [2]:

Statement 1. *Given an $n \times n$ Hermitian matrix A and an $n \times n$ positive semidefinite matrix B , the function $t \mapsto \text{trace}(\exp(A - tB))$ is the Laplace transform of a positive measure supported in $[0, \infty)$.*

This was proved by Stahl (see [16]) and simplified by Eremenko (see [6]). Collins, Dykema, and Torres-Ayala (see [5]) and Burgdorf et al. (see [3, 4]) prove the special case of Conjecture 1 when $(m, r) = (4, 2)$ by expressing the coefficient of t^r in $\text{trace}((A + tB)^m)$ as a sum of squares of non-commutative variables A and B .

In [7], the special case of Conjecture 1 when $(m, r) = (4, 2)$ is proved by expressing the coefficient of t^r in $\text{trace}((A + tB)^m)$ as a sum of squares in the $2n + 2\binom{n}{2}$ commutative variables $a_{\{i,j\}}$ and $b_{\{i,j\}}$, the entries of A and B . The article [7] also examines the special case of Conjecture 1 when $(m, r) = (8, 4)$ for small n . The focus of [7] was on cases of Conjecture 1 when r is a power of 2 and $m = 2r$. The first natural case this leaves out is $(m, r) = (6, 2)$, which we examine in Theorem 1.

Theorem 1. *If A and B are $n \times n$ symmetric matrices, then the coefficient of t^2 in $\text{trace}((A + tB)^6)$ is a sum of squares of polynomials in the variables $a_{\{i,j\}}$ and $b_{\{i,j\}}$: there exist positive semidefinite matrices U and R and vectors y and $z_{(i,j)}$ such that the coefficient of t^2 in $\text{trace}((A + tB)^6)$ is equal to*

$$y^T U y + \sum_{1 \leq i < j \leq n} z_{(i,j)}^T R z_{(i,j)}. \tag{1}$$

In our proof of Theorem 2.1 we use well known results (see, e.g., [8, 13, 14]) to show, given appropriate matrices and vectors, $\text{trace}((A + tB)^6)$ is non-negative. In our proof we will use two matrices U and R , along with vectors y and $z_{(i,j)}$ to prove each term from the expression above, $y^T U y, z_{(1,2)}^T R z_{(1,2)}, \dots, z_{(n-1,n)}^T R z_{(n-1,n)}$ is non-negative, therefore proving the whole expression non-negative.

Three large questions arise that will be answered in the following three sections. We set out to provide index based descriptions of all previously mentioned matrices and vectors in Section 2. In Section 3 we prove

$y^T U y + \sum_{1 \leq i < j \leq n} z_{(i,j)}^T R z_{(i,j)}$ equals the coefficient of t^2 in $\text{trace}((A + tB)^6)$ by exhaustion. In Section 4 we provide a proof that R is positive semidefinite using the generalized Schur complement and other various methods. In Section 5 we provide descriptions of U, U^2, U^3 , and U^4 to show U satisfies a polynomial μ , which is a multiple of the minimum polynomial of U . We then use Descartes' Law of Signs so show μ has no negative roots, therefore proving U is positive semidefinite.

1.1. Notation for block constant matrices

When defining the matrix R and subsequent analysis, it will be helpful to introduce notation for block matrices which have constant value within each block. Throughout this paper, whenever a non-negative integer appears outside the presentation of what appears to be a small matrix, such a row heading (respectively, column heading) indicates the number of rows (respectively, columns) in a block, while the entry within the brackets indicates the entry throughout the block. For example,

$$\begin{array}{c} 3 \quad 4 \\ 1 \quad 2 \end{array} \begin{bmatrix} 5 & 6 \\ 7 & 8 \end{bmatrix} = \begin{bmatrix} 5 & 5 & 5 & 6 & 6 & 6 & 6 \\ 7 & 7 & 7 & 8 & 8 & 8 & 8 \\ 7 & 7 & 7 & 8 & 8 & 8 & 8 \end{bmatrix}.$$

2. Definitions of relevant matrices and vectors

Throughout the following section we define vectors y and $z_{(i,j)}$, and matrices U and R .

2.1. Definition of y

In this section, we define a vector y of size $3 \cdot \binom{n}{3} + n(n - 1) + n^2$. The vector y is partitioned into three blocks. The first block has $3 \cdot \binom{n}{3}$ entries indexed by all possible ordered pairs of the form (T, ℓ) where T is a 3-element subset of $[n]$ and $\ell \in T$. The monomial at index $(\{i, j, k\}, \ell)$ is $a_{\{i,j\}} a_{\{i,k\}} b_{\{j,k\}}$. The second block of the vector y has $n(n - 1)$ entries indexed by all possible ordered pairs (i, j) such that $i \neq j$ and $i, j \leq n$. The monomial at index (i, j) is $a_{\{i,j\}} a_{\{i,i\}} b_{\{i,j\}}$. The third block of the vector y has n^2 entries indexed by all possible ordered pairs (\hat{i}, \hat{j}) , where $\hat{i}, \hat{j} \leq n$. The monomial at index (\hat{i}, \hat{j}) is $a_{\{\hat{i}, \hat{j}\}} a_{\{\hat{i}, \hat{j}\}} b_{\{\hat{i}, \hat{i}\}}$.

2.2. Definition of U

We now define a symmetric block matrix U with $3 \cdot \binom{n}{3} + n(n-1) + n^2$ rows and columns, of the form

$$U = \begin{bmatrix} S_1 & S_{12} & S_{13} \\ S_{12}^T & S_2 & S_{23} \\ S_{13}^T & S_{23}^T & S_3 \end{bmatrix}.$$

Six submatrices are described below, with the remaining three blocks below the block diagonal automatically given by transposition. Each submatrix is indexed the same way as the vector y . Moreover, the blocks in y determine the submatrices of U .

The S_1 submatrix

The entry in the $(\{i, j, k\}, \ell)$ -row $(\{i', j', k'\}, \ell')$ -column of S_1 is $6(|\{i, j, k\} \cap \{i', j', k'\}| + |\{\ell\} \cap \{\ell'\}|)$, where $\ell \in \{i, j, k\}$ and $\ell' \in \{i', j', k'\}$.

The S_2 submatrix

The entry in the (i, j) -row (i', j') -column of S_2 is $6|\{j\} \cap \{j'\}| + 30|\{i\} \cap \{i'\}| + 12|\{i\} \cap \{j'\}| + 12|\{j\} \cap \{i'\}|$.

The S_3 submatrix

The entry in the (\hat{i}, \hat{j}) -row (\hat{i}', \hat{j}') -column of S_3 is:

- $3(|\{\hat{i}, \hat{j}\} \cap \{\hat{i}', \hat{j}'\}| + |\{\hat{i}\} \cap \{\hat{i}'\}|)$ if $\hat{i} \neq \hat{j}$ and $\hat{i}' \neq \hat{j}'$,
- $3(3|\{\hat{i}\} \cap \{\hat{i}'\}| + 2|\{\hat{j}\} \cap \{\hat{j}'\}|)$ if $\hat{i} = \hat{j}$ or $\hat{i}' = \hat{j}'$.

The S_{12} submatrix

The rows of S_{12} are indexed as in S_1 , with a typical index being of the form $(\{i, j, k\}, \ell)$, where $\ell \in \{i, j, k\}$. The columns of S_{12} are indexed as in S_2 with a typical index being of the form (i', j') with $i' \neq j'$. The entry in row $(\{i, j, k\}, \ell)$ column (i', j') is $12|\{i'\} \cap \{i, j, k\}| + 6|\{j'\} \cap \{i, j, k\}| + 6|\{i'\} \cap \{\ell\}|$.

The S_{13} submatrix

The rows of S_{13} are indexed as in S_1 , with a typical index being of the form $(\{i, j, k\}, \ell)$, where $\ell \in \{i, j, k\}$. The columns of S_{13} are indexed as in S_2 with a typical index being of the form (\hat{i}, \hat{j}) . The entry in row $(\{i, j, k\}, \ell)$ column (\hat{i}, \hat{j}) is $6|\{\hat{i}\} \cap \{i, j, k\}| + 3|\{\hat{j}\} \cap \{i, j, k\}| + 3|\{\hat{j}\} \cap \{\ell\}|$.

The S_{23} submatrix

The rows of S_{23} are indexed as in S_2 , with a typical index being of the form (i, j) with $i \neq j$. The columns of S_{23} are indexed as in S_3 , with a typical index being of the form (\hat{i}, \hat{j}) . The entry in the (i, j) row (\hat{i}, \hat{j}) column of S_{23} is:

- 15 if $i = \hat{i}$ and $j = \hat{j}$.
- Otherwise, 21 if $i = \hat{i}$ and $i = \hat{j}$.
- Otherwise, 12 if $i = \hat{i}$ and $i \neq j$ and $j \neq \hat{i}$ and $i \neq \hat{j}$.
- Otherwise, 15 if $j = \hat{i}$ and $i = \hat{j}$.
- Otherwise, 9 if $i = \hat{j}$ and $j \neq \hat{i}$ and $i \neq \hat{i}$.
- Otherwise, 9 if $\hat{i} = \hat{j}$ and $j = \hat{i}$.
- Otherwise, 6 if $j = \hat{i}$ and $i \neq \hat{j}$ and $j \neq \hat{j}$.
- Otherwise, 3 if $j = \hat{j}$ and $\hat{i} \neq \hat{j}$.
- Otherwise 0.

2.3. Definition of $z_{(i,j)}$

Let $z_{(i,j)}$ be a vector of size $3n^2 - 2n$, broken up into six blocks as described below.

- The first block contains a single monomial $a_{\{i,j\}}^2 b_{\{i,j\}}$ with index (1).
- The second block has size $n - 1$, and consists of the single monomial $a_{\{i,i\}} a_{\{i,j\}} b_{\{i,i\}}$ with index (2, 1), followed by $n - 2$ monomials of the form $a_{\{i,j\}} a_{\{i,k\}} b_{\{i,k\}}$ with index (2, 2, k), where $k \leq n$ and $k \neq i, j$.
- The third block has the $n - 1$ monomials of the form $a_{\{i,j\}} a_{\{j,k\}} b_{\{j,k\}}$ with index (3, k), where $k \leq n$ and $k \neq i$.
- The fourth block has size $(n - 1)^2$, and consists of the single monomial $a_{\{i,i\}} a_{\{j,j\}} b_{\{i,j\}}$ with index (4, 1), followed by $n - 2$ monomials of the form $a_{\{i,i\}} a_{\{j,k\}} b_{\{i,k\}}$ with index (4, 2, k), then $n - 2$ monomials of the form $a_{\{i,k\}} a_{\{j,j\}} b_{\{j,k\}}$ with index (4, 3, k), then $n - 2$ monomials of the form $a_{\{i,k\}} a_{\{j,k\}} b_{\{k,k\}}$ with index (4, 4, k). Finally, $n^2 - 5n + 6$ monomials of the form $a_{\{i,k\}} a_{\{j,l\}} b_{\{k,l\}}$ with index (4, 5, k, l), where $k \neq i, j, l$ and $l \neq i, j, k$.

- The fifth block has size $n(n-1)$, starting with monomials $a_{\{i,i\}}a_{\{i,i\}}b_{\{i,j\}}$ with index $(5, 1)$ and $a_{\{i,i\}}a_{\{i,j\}}b_{\{j,j\}}$ with index $(5, 2)$. Then follow $n-2$ monomials of the form $a_{\{i,i\}}a_{\{i,k\}}b_{\{k,j\}}$ with index $(5, 3, k)$, then $n-2$ monomials of the form $a_{\{i,k\}}a_{\{i,k\}}b_{\{i,j\}}$ with index $(5, 4, k)$, then $n-2$ monomials of the form $a_{\{i,k\}}a_{\{j,k\}}b_{\{j,j\}}$ with index $(5, 5, k)$, and $n-2$ monomials of the form $a_{\{i,k\}}a_{\{k,k\}}b_{\{j,k\}}$ with index $(5, 6, k)$, where $k \neq i, j$. Finally, there are $n^2 - 5n + 6$ monomials of the form $a_{\{i,k\}}a_{\{k,l\}}b_{\{j,l\}}$ with index $(5, 7, k, l)$, where $k \neq i, j, l$ and $l \neq i, j, k$.
- The sixth block has size $n(n-1)$, starting with monomials $a_{\{j,j\}}a_{\{i,j\}}b_{\{i,i\}}$ with index $(6, 1)$ and $a_{\{j,j\}}a_{\{j,j\}}b_{\{i,j\}}$ with index $(6, 2)$. Then follow $n-2$ monomials of the form $a_{\{j,j\}}a_{\{k,j\}}b_{\{i,k\}}$ with index $(6, 3, k)$, then $n-2$ monomials of the form $a_{\{j,k\}}a_{\{i,k\}}b_{\{i,i\}}$ with index $(6, 4, k)$, then $n-2$ monomials of the form $a_{\{j,k\}}a_{\{j,k\}}b_{\{i,j\}}$ with index $(6, 5, k)$, and $n-2$ monomials of the form $a_{\{j,k\}}a_{\{k,k\}}b_{\{i,k\}}$ with index $(6, 6, k)$, where $k \neq i, j$. Finally, there are $n^2 - 5n + 6$ monomials of the form $a_{\{j,k\}}a_{\{k,l\}}b_{\{i,l\}}$ with index $(6, 7, k, l)$, where $k \neq i, j, l$ and $l \neq i, j, k$.

For our use of the index language, in what follows, we will write, for example, the $(2, 2, 3)$ -entry of $z_{(1,2)}$ is the monomial $a_{\{1,2\}}a_{\{1,3\}}b_{\{2,3\}}$.

2.4. Definition of R

Just as the indexing of the vector y determined U , the blocks of $z_{(i,j)}$ determine R . The description of R is simple compared to U . Using the notation introduced in Section 1.1, for a fixed n , the matrix R is the $(3n^2 - 2n) \times (3n^2 - 2n)$ symmetric matrix

$$\begin{matrix}
 & 1 & n-1 & n-1 & (n-1)^2 & n(n-1) & n(n-1) \\
 \begin{matrix} 1 \\ n-1 \\ n-1 \\ (n-1)^2 \\ n(n-1) \\ n(n-1) \end{matrix} & \begin{bmatrix} 30 & 21 & 21 & 12 & 9 & 9 \\ 21 & 18 & 12 & 9 & 3 & 9 \\ 21 & 12 & 18 & 9 & 9 & 3 \\ 12 & 9 & 9 & 6 & 3 & 3 \\ 9 & 3 & 9 & 3 & 6 & 0 \\ 9 & 9 & 3 & 3 & 0 & 6 \end{bmatrix} & .
 \end{matrix}$$

2.5. Examples of matrices and vectors for $n = 4$

$$y = \begin{bmatrix} a_{\{1,2\}} a_{\{1,3\}} b_{\{2,3\}} \\ a_{\{1,2\}} a_{\{2,3\}} b_{\{1,3\}} \\ a_{\{1,3\}} a_{\{2,3\}} b_{\{1,2\}} \\ a_{\{1,2\}} a_{\{1,4\}} b_{\{2,4\}} \\ a_{\{1,2\}} a_{\{2,4\}} b_{\{1,4\}} \\ a_{\{1,4\}} a_{\{2,4\}} b_{\{1,2\}} \\ a_{\{1,3\}} a_{\{1,4\}} b_{\{3,4\}} \\ a_{\{1,3\}} a_{\{3,4\}} b_{\{1,4\}} \\ a_{\{1,4\}} a_{\{3,4\}} b_{\{1,3\}} \\ a_{\{2,3\}} a_{\{2,4\}} b_{\{3,4\}} \\ a_{\{2,3\}} a_{\{3,4\}} b_{\{2,4\}} \\ a_{\{2,4\}} a_{\{3,4\}} b_{\{2,3\}} \\ a_{\{1,1\}} a_{\{1,2\}} b_{\{1,2\}} \\ a_{\{1,1\}} a_{\{1,3\}} b_{\{1,3\}} \\ a_{\{1,1\}} a_{\{1,4\}} b_{\{1,4\}} \\ a_{\{1,2\}} a_{\{2,2\}} b_{\{1,2\}} \\ a_{\{2,2\}} a_{\{2,3\}} b_{\{2,3\}} \\ a_{\{2,2\}} a_{\{2,4\}} b_{\{2,4\}} \\ a_{\{1,3\}} a_{\{3,3\}} b_{\{1,3\}} \\ a_{\{2,3\}} a_{\{3,3\}} b_{\{2,3\}} \\ a_{\{3,3\}} a_{\{3,4\}} b_{\{3,4\}} \\ a_{\{1,4\}} a_{\{4,4\}} b_{\{1,4\}} \\ a_{\{2,4\}} a_{\{4,4\}} b_{\{2,4\}} \\ a_{\{3,4\}} a_{\{4,4\}} b_{\{3,4\}} \\ a_{\{1,1\}}^2 b_{\{1,1\}} \\ a_{\{1,2\}}^2 b_{\{1,1\}} \\ a_{\{1,3\}}^2 b_{\{1,1\}} \\ a_{\{1,4\}}^2 b_{\{1,1\}} \\ a_{\{1,2\}}^2 b_{\{2,2\}} \\ a_{\{2,2\}}^2 b_{\{2,2\}} \\ a_{\{2,3\}}^2 b_{\{2,2\}} \\ a_{\{2,4\}}^2 b_{\{2,2\}} \\ a_{\{1,3\}}^2 b_{\{3,3\}} \\ a_{\{2,3\}}^2 b_{\{3,3\}} \\ a_{\{3,3\}}^2 b_{\{3,3\}} \\ a_{\{3,4\}}^2 b_{\{3,3\}} \\ a_{\{1,4\}}^2 b_{\{4,4\}} \\ a_{\{2,4\}}^2 b_{\{4,4\}} \\ a_{\{3,4\}}^2 b_{\{4,4\}} \\ a_{\{4,4\}}^2 b_{\{4,4\}} \end{bmatrix}$$

$$z_{(1,2)} = \begin{bmatrix} a_{\{1,2\}}^2 b_{\{1,2\}} \\ a_{\{1,1\}} a_{\{1,2\}} b_{\{1,1\}} \\ a_{\{1,2\}} a_{\{1,3\}} b_{\{1,3\}} \\ a_{\{1,2\}} a_{\{1,4\}} b_{\{1,4\}} \\ a_{\{1,2\}} a_{\{2,2\}} b_{\{2,2\}} \\ a_{\{1,2\}} a_{\{2,3\}} b_{\{2,3\}} \\ a_{\{1,2\}} a_{\{2,4\}} b_{\{2,4\}} \\ a_{\{1,1\}} a_{\{2,2\}} b_{\{1,2\}} \\ a_{\{1,1\}} a_{\{2,3\}} b_{\{1,3\}} \\ a_{\{1,1\}} a_{\{2,4\}} b_{\{1,4\}} \\ a_{\{1,1\}} a_{\{3,3\}} b_{\{1,3\}} \\ a_{\{1,1\}} a_{\{3,4\}} b_{\{1,4\}} \\ a_{\{1,3\}} a_{\{2,2\}} b_{\{2,3\}} \\ a_{\{1,3\}} a_{\{2,3\}} b_{\{3,3\}} \\ a_{\{1,3\}} a_{\{2,4\}} b_{\{3,4\}} \\ a_{\{1,3\}} a_{\{3,3\}} b_{\{3,3\}} \\ a_{\{1,3\}} a_{\{3,4\}} b_{\{3,4\}} \\ a_{\{1,4\}} a_{\{2,2\}} b_{\{2,4\}} \\ a_{\{1,4\}} a_{\{2,3\}} b_{\{3,4\}} \\ a_{\{1,4\}} a_{\{2,3\}} b_{\{3,4\}} \\ a_{\{1,1\}}^2 b_{\{1,2\}} \\ a_{\{1,1\}} a_{\{1,2\}} b_{\{2,2\}} \\ a_{\{1,1\}} a_{\{1,3\}} b_{\{2,3\}} \\ a_{\{1,1\}} a_{\{1,4\}} b_{\{2,4\}} \\ a_{\{1,1\}}^2 a_{\{1,3\}} b_{\{1,2\}} \\ a_{\{1,1\}}^2 a_{\{1,4\}} b_{\{1,2\}} \\ a_{\{1,3\}} a_{\{2,3\}} b_{\{2,2\}} \\ a_{\{1,4\}} a_{\{2,4\}} b_{\{2,2\}} \\ a_{\{1,3\}} a_{\{3,3\}} b_{\{2,3\}} \\ a_{\{1,4\}} a_{\{3,4\}} b_{\{2,4\}} \\ a_{\{1,3\}} a_{\{3,4\}} b_{\{2,4\}} \\ a_{\{1,4\}} a_{\{3,4\}} b_{\{2,3\}} \\ a_{\{1,2\}} a_{\{2,2\}} b_{\{1,1\}} \\ a_{\{2,2\}}^2 b_{\{1,2\}} \\ a_{\{2,2\}} a_{\{2,3\}} b_{\{1,3\}} \\ a_{\{2,2\}} a_{\{2,4\}} b_{\{1,4\}} \\ a_{\{1,3\}} a_{\{2,3\}} b_{\{1,1\}} \\ a_{\{1,4\}} a_{\{2,4\}} b_{\{1,1\}} \\ a_{\{2,3\}}^2 b_{\{1,2\}} \\ a_{\{2,4\}}^2 b_{\{1,2\}} \\ a_{\{2,3\}} a_{\{3,3\}} b_{\{1,3\}} \\ a_{\{2,4\}} a_{\{3,4\}} b_{\{1,4\}} \\ a_{\{2,3\}} a_{\{3,4\}} b_{\{1,4\}} \\ a_{\{2,4\}} a_{\{3,4\}} b_{\{1,3\}} \end{bmatrix}$$

3. Proof of relevance to (1)

Starting with the notation and setup of Theorem 1, the coefficient of t^2 in $\text{trace}((A + tB)^6)$ is a polynomial p in the variables $a_{\{i,j\}}$ and $b_{\{i,j\}}$. Note that p is a multivariate polynomial where each term has total degree 6. Moreover, each term as a -degree 4 and b -degree 2. Since $m = 6$, if $n \geq 6$, the number of monomials up to type (under \mathfrak{S}_n -action $a_{\{i,j\}} \mapsto a_{\{\sigma(i),\sigma(j)\}}$ and $b_{\{i,j\}} \mapsto b_{\{\sigma(i),\sigma(j)\}}$) remains constant as $n \rightarrow \infty$.

For each n , the monomial types may be obtained by exhaustion, examining the terms of p . For example, when $n = 3$, there are exactly 80 monomial types. When $n = 6$, there are exactly 169 monomial types. Therefore, for all $n \geq 6$, the number of monomial types is 169. Moreover, for all n , every term is equivalent (up to \mathfrak{S}_n -action) to one of these 169 monomials:

$$\begin{aligned}
 & a_{11}^4 b_{11}^2, a_{11}^2 a_{12}^2 b_{11}^2, a_{12}^4 b_{11}^2, a_{12}^2 a_{13}^2 b_{11}^2, a_{11} a_{12}^2 a_{22} b_{11}^2, a_{12}^2 a_{22}^2 b_{11}^2, a_{11} a_{12} a_{13} a_{23} b_{11}^2, \\
 & a_{12} a_{13} a_{22} a_{23} b_{11}^2, a_{12}^2 a_{23}^2 b_{11}^2, a_{13} a_{14} a_{23} a_{24} b_{11}^2, a_{11}^3 a_{12} b_{11} b_{12}, a_{11} a_{12}^3 b_{11} b_{12}, \\
 & a_{11} a_{12} a_{13}^2 b_{11} b_{12}, a_{11}^2 a_{12} a_{22} b_{11} b_{12}, a_{12}^3 a_{22} b_{11} b_{12}, a_{12} a_{13}^2 a_{22} b_{11} b_{12}, a_{11} a_{12} a_{22}^2 b_{11} b_{12}, \\
 & a_{12} a_{22}^3 b_{11} b_{12}, a_{11}^2 a_{13} a_{23} b_{11} b_{12}, a_{12}^2 a_{13} a_{23} b_{11} b_{12}, a_{13}^3 a_{23} b_{11} b_{12}, a_{13} a_{14}^2 a_{23} b_{11} b_{12}, \\
 & a_{11} a_{13} a_{22} a_{23} b_{11} b_{12}, a_{13} a_{22}^2 a_{23} b_{11} b_{12}, a_{11} a_{12} a_{23}^2 b_{11} b_{12}, a_{12} a_{22} a_{23}^2 b_{11} b_{12}, \\
 & a_{13} a_{23}^3 b_{11} b_{12}, a_{14} a_{23}^2 a_{24} b_{11} b_{12}, a_{12} a_{23}^2 a_{33} b_{11} b_{12}, a_{11} a_{13} a_{23} a_{33} b_{11} b_{12}, \\
 & a_{13} a_{22} a_{23} a_{33} b_{11} b_{12}, a_{12} a_{23}^2 a_{33} b_{11} b_{12}, a_{13} a_{23} a_{33}^2 b_{11} b_{12}, a_{12} a_{13} a_{14} a_{34} b_{11} b_{12}, \\
 & a_{11} a_{14} a_{23} a_{34} b_{11} b_{12}, a_{14} a_{22} a_{23} a_{34} b_{11} b_{12}, a_{12} a_{23} a_{24} a_{34} b_{11} b_{12}, a_{14} a_{23} a_{33} a_{34} b_{11} b_{12}, \\
 & a_{13} a_{24} a_{33} a_{34} b_{11} b_{12}, a_{13} a_{23} a_{34}^2 b_{11} b_{12}, a_{15} a_{24} a_{34} a_{35} b_{11} b_{12}, a_{11}^4 b_{12}^2, a_{11}^2 a_{12}^2 b_{12}^2, \\
 & a_{12}^4 b_{12}^2, a_{11}^2 a_{13}^2 b_{12}^2, a_{12}^2 a_{13}^2 b_{12}^2, a_{13}^4 b_{12}^2, a_{13}^2 a_{14}^2 b_{12}^2, a_{11}^3 a_{22} b_{12}^2, a_{11} a_{12}^2 a_{22} b_{12}^2, \\
 & a_{11} a_{13}^2 a_{22} b_{12}^2, a_{11}^2 a_{22}^2 b_{12}^2, a_{13}^2 a_{22}^2 b_{12}^2, a_{11} a_{12} a_{13} a_{23} b_{12}^2, a_{13}^2 a_{23}^2 b_{12}^2, a_{14}^2 a_{23}^2 b_{12}^2, \\
 & a_{13} a_{14} a_{23} a_{24} b_{12}^2, a_{11} a_{13}^2 a_{33} b_{12}^2, a_{13}^2 a_{22} a_{33} b_{12}^2, a_{12} a_{13} a_{23} a_{33} b_{12}^2, a_{13}^2 a_{33}^2 b_{12}^2, \\
 & a_{11} a_{13} a_{14} a_{34} b_{12}^2, a_{13} a_{14} a_{22} a_{34} b_{12}^2, a_{12} a_{14} a_{23} a_{34} b_{12}^2, a_{13} a_{14} a_{33} a_{34} b_{12}^2, a_{13}^2 a_{34}^2 b_{12}^2, \\
 & a_{14} a_{15} a_{34} a_{35} b_{12}^2, a_{11}^2 a_{12} a_{13} b_{12} b_{13}, a_{12}^3 a_{13} b_{12} b_{13}, a_{12} a_{13} a_{14}^2 b_{12} b_{13}, \\
 & a_{11} a_{12} a_{13} a_{22} b_{12} b_{13}, a_{12} a_{13} a_{22}^2 b_{12} b_{13}, a_{11}^3 a_{23} b_{12} b_{13}, a_{11} a_{12}^2 a_{23} b_{12} b_{13}, \\
 & a_{11} a_{14}^2 a_{23} b_{12} b_{13}, a_{11}^2 a_{22} a_{23} b_{12} b_{13}, a_{12}^2 a_{22} a_{23} b_{12} b_{13}, a_{12}^2 a_{22} a_{23} b_{12} b_{13}, \\
 & a_{14}^2 a_{22} a_{23} b_{12} b_{13}, a_{11} a_{12}^2 a_{23} b_{12} b_{13}, a_{12}^3 a_{23} b_{12} b_{13}, a_{12} a_{13} a_{23}^2 b_{12} b_{13}, a_{11} a_{23}^3 b_{12} b_{13}, \\
 & a_{22} a_{23}^3 b_{12} b_{13}, a_{11} a_{13} a_{14} a_{24} b_{12} b_{13}, a_{13} a_{14} a_{22} a_{24} b_{12} b_{13}, a_{12} a_{14} a_{23} a_{24} b_{12} b_{13}, \\
 & a_{12} a_{13} a_{24}^2 b_{12} b_{13}, a_{11} a_{23} a_{24}^2 b_{12} b_{13}, a_{22} a_{23} a_{24}^2 b_{12} b_{13}, a_{12} a_{13} a_{22} a_{33} b_{12} b_{13}, \\
 & a_{11} a_{22} a_{23} a_{33} b_{12} b_{13}, a_{22}^2 a_{23} a_{33} b_{12} b_{13}, a_{13} a_{14} a_{24} a_{33} b_{12} b_{13}, a_{23} a_{24}^2 a_{33} b_{12} b_{13}, \\
 & a_{11}^2 a_{24} a_{34} b_{12} b_{13}, a_{12}^2 a_{24} a_{34} b_{12} b_{13}, a_{14}^2 a_{24} a_{34} b_{12} b_{13}, a_{15}^2 a_{24} a_{34} b_{12} b_{13}, \\
 & a_{11} a_{22} a_{24} a_{34} b_{12} b_{13}, a_{22}^2 a_{24} a_{34} b_{12} b_{13}, a_{23}^2 a_{24} a_{34} b_{12} b_{13}, a_{34}^2 a_{34} b_{12} b_{13},
 \end{aligned}$$

$a_{14}a_{15}a_{25}a_{34}b_{12}b_{13}$, $a_{24}a_{25}^2a_{34}b_{12}b_{13}$, $a_{22}a_{24}a_{33}a_{34}b_{12}b_{13}$, $a_{14}^2a_{23}a_{44}b_{12}b_{13}$,
 $a_{13}a_{14}a_{24}a_{44}b_{12}b_{13}$, $a_{23}a_{24}^2a_{44}b_{12}b_{13}$, $a_{11}a_{24}a_{34}a_{44}b_{12}b_{13}$, $a_{22}a_{24}a_{34}a_{44}b_{12}b_{13}$,
 $a_{24}a_{34}a_{44}^2b_{12}b_{13}$, $a_{14}a_{15}a_{23}a_{45}b_{12}b_{13}$, $a_{13}a_{15}a_{24}a_{45}b_{12}b_{13}$, $a_{23}a_{24}a_{25}a_{45}b_{12}b_{13}$,
 $a_{11}a_{25}a_{34}a_{45}b_{12}b_{13}$, $a_{22}a_{25}a_{34}a_{45}b_{12}b_{13}$, $a_{25}a_{34}a_{44}a_{45}b_{12}b_{13}$, $a_{24}a_{34}a_{45}^2b_{12}b_{13}$,
 $a_{26}a_{35}a_{45}a_{46}b_{12}b_{13}$, $a_{11}^2a_{12}^2b_{11}b_{22}$, $a_{12}^4b_{11}b_{22}$, $a_{12}^2a_{13}^2b_{11}b_{22}$, $a_{11}a_{12}^2a_{22}b_{11}b_{22}$,
 $a_{11}a_{12}a_{13}a_{23}b_{11}b_{22}$, $a_{13}^2a_{23}^2b_{11}b_{22}$, $a_{13}a_{14}a_{23}a_{24}b_{11}b_{22}$, $a_{12}a_{13}a_{23}a_{33}b_{11}b_{22}$,
 $a_{12}a_{14}a_{23}a_{34}b_{11}b_{22}$, $a_{11}a_{12}^2a_{13}b_{13}b_{22}$, $a_{12}^2a_{13}a_{22}b_{13}b_{22}$, $a_{11}^2a_{12}a_{23}b_{13}b_{22}$,
 $a_{12}a_{22}^2a_{23}b_{13}b_{22}$, $a_{11}a_{13}a_{23}^2b_{13}b_{22}$, $a_{12}a_{13}a_{14}a_{24}b_{13}b_{22}$, $a_{11}a_{14}a_{23}a_{24}b_{13}b_{22}$,
 $a_{14}a_{22}a_{23}a_{24}b_{13}b_{22}$, $a_{12}a_{23}a_{24}^2b_{13}b_{22}$, $a_{11}a_{12}a_{23}a_{33}b_{13}b_{22}$, $a_{14}a_{23}a_{24}a_{33}b_{13}b_{22}$,
 $a_{12}^2a_{14}a_{34}b_{13}b_{22}$, $a_{14}a_{24}^2a_{34}b_{13}b_{22}$, $a_{15}a_{24}a_{25}a_{34}b_{13}b_{22}$, $a_{14}a_{23}a_{24}a_{44}b_{13}b_{22}$,
 $a_{15}a_{23}a_{24}a_{45}b_{13}b_{22}$, $a_{11}a_{12}a_{13}a_{14}b_{14}b_{23}$, $a_{12}a_{13}a_{14}a_{22}b_{14}b_{23}$, $a_{12}^2a_{14}a_{23}b_{14}b_{23}$,
 $a_{11}^2a_{13}a_{24}b_{14}b_{23}$, $a_{12}^2a_{13}a_{24}b_{14}b_{23}$, $a_{13}^3a_{24}b_{14}b_{23}$, $a_{13}a_{14}^2a_{24}b_{14}b_{23}$, $a_{13}a_{15}^2a_{24}b_{14}b_{23}$,
 $a_{11}a_{13}a_{22}a_{24}b_{14}b_{23}$, $a_{13}a_{14}a_{15}a_{25}b_{14}b_{23}$, $a_{11}a_{13}a_{24}a_{33}b_{14}b_{23}$, $a_{13}a_{22}a_{24}a_{33}b_{14}b_{23}$,
 $a_{12}a_{23}a_{24}a_{33}b_{14}b_{23}$, $a_{11}a_{15}a_{25}a_{34}b_{14}b_{23}$, $a_{15}a_{25}a_{33}a_{34}b_{14}b_{23}$, $a_{12}a_{24}a_{25}a_{35}b_{14}b_{23}$,
 $a_{15}a_{25}a_{35}a_{45}b_{14}b_{23}$, $a_{16}a_{26}a_{35}a_{45}b_{14}b_{23}$, $a_{15}a_{25}a_{34}a_{55}b_{14}b_{23}$, $a_{16}a_{25}a_{34}a_{56}b_{14}b_{23}$.

For each monomial type, every monomial of the given type may be considered. (This can be completed by exhaustion, applying every element of \mathfrak{S}_n to the fixed monomial type.)

For each monomial, we state which entries of U and which entries (in which copy) of R addresses said monomial. Mentioning every entry in full this way is exhaustive, but by examining the mentioned entries by their indexes, we have a finite-length (albeit long) description of showing that each matrix entry is used exactly once. The verification in the case of $n = 6$, when replacing constant indices with variables, is a computer-aided verification (in 169 cases) that for all n , the coefficient of t^2 in $\text{trace}((A+tB)^6)$ is (1), as desired. Details of this verification (for $n = 3, 4, 5, 6$) and accompanying sage code (see [15]) are found at

<https://edward-kim-math.github.io/cdta-m6r2>

but for the sake of illustration, in the case when $n = 3$, the following three monomials are the only monomials of p appearing together in a type class (up to \mathfrak{S}_3 -action), namely, $a_{12}^2a_{13}^2b_{11}^2$ and $a_{12}^2a_{23}^2b_{22}^2$ and $a_{13}^2a_{23}^2b_{33}^2$. Each of these three monomials appears in p with coefficient 18. The list below describes which entries of U and which entries in which copy of R address each monomial:

- Monomial $a_{12}^2 a_{13}^2 b_{11}^2$
 - The $(\hat{1}, \hat{2})$ -row $(\hat{1}, \hat{3})$ -column entry of U is 6, addresses $(a_{12}^2 b_{11})(a_{13}^2 b_{11})$.
 - The $(\hat{1}, \hat{3})$ -row $(\hat{1}, \hat{2})$ -column entry of U is 6, addresses $(a_{13}^2 b_{11})(a_{12}^2 b_{11})$.
 - The $(2, 3)$ -copy of R whose entry 6 is addressed by $(a_{12} a_{13} b_{11})(a_{12} a_{13} b_{11})$.
- Monomial $a_{12}^2 a_{23}^2 b_{22}^2$
 - The $(\hat{2}, \hat{1})$ -row $(\hat{2}, \hat{3})$ -column entry of U is 6, addresses $(a_{12}^2 b_{22})(a_{23}^2 b_{22})$.
 - The $(\hat{2}, \hat{3})$ -row $(\hat{2}, \hat{1})$ -column entry of U is 6, addresses $(a_{23}^2 b_{22})(a_{12}^2 b_{22})$.
 - The $(1, 3)$ -copy of R whose entry 6 is addressed by $(a_{12} a_{23} b_{22})(a_{12} a_{23} b_{22})$.
- Monomial $a_{13}^2 a_{23}^2 b_{33}^2$
 - The $(\hat{3}, \hat{1})$ -row $(\hat{3}, \hat{2})$ -column entry of U is 6, addresses $(a_{13}^2 b_{33})(a_{23}^2 b_{33})$.
 - The $(\hat{3}, \hat{2})$ -row $(\hat{3}, \hat{1})$ -column entry of U is 6, addresses $(a_{23}^2 b_{33})(a_{13}^2 b_{33})$.
 - The $(1, 2)$ -copy of R whose entry 6 is addressed by $(a_{13} a_{23} b_{33})(a_{13} a_{23} b_{33})$.

4. Proof of positive semidefiniteness of R

Fix an integer $n \geq 4$. Our proof that R is positive semidefinite makes use of the generalized Schur complement, which relies on the Moore-Penrose pseudo-inverse (see [1, 10, 12]). For a matrix C with real entries, its pseudo-inverse C^+ satisfies $CC^+C = C$ and $C^+CC^+ = C^+$ and $(CC^+)^t = CC^+$ and $(C^+C)^t = C^+C$. Given the matrix

$$R = \begin{bmatrix} F & G^t \\ G & E \end{bmatrix},$$

the generalized Schur complement (see [17]) of E in R is $H - G^t E^+ G$.

Lemma 1. *Suppose C is an $s \times s$ matrix with every entry c . Then the pseudo-inverse of C is an $s \times s$ matrix with every entry $d = \frac{1}{s^2 c}$.*

Proof. Let C be an $s \times s$ matrix with every entry being c . Let D be an $s \times s$ matrix with every entry d . Then $(CD)^t = CD$ and $(DC)^t = DC$ are obvious since C and D are themselves symmetric.

We need $CDC = C$. Note CD has every entry scd . So $(CD)C$ is a matrix where each entry is $s(sc d)c$ and for this to equal c , we need $d = \frac{1}{s^2 c}$. Similarly, for $DCD = D$ to be true, we again need $d = \frac{1}{s^2 c}$. \square

The submatrix of R consisting of all rows and columns from block 5 is the $n(n - 1) \times n(n - 1)$ with every entry 6, so its pseudo-inverse is the $n(n - 1) \times n(n - 1)$ matrix with every entry $\frac{1}{6n^2(n-1)^2}$. Let E be the submatrix of R consisting of all rows and columns from blocks 5 and 6. That is, E is the $2n(n - 1) \times 2n(n - 1)$ matrix

$$\begin{matrix} & n(n - 1) & n(n - 1) \\ n(n - 1) & \left[\begin{array}{cc} 6 & 0 \\ 0 & 6 \end{array} \right] \\ n(n - 1) & & \end{matrix}$$

Using the notation introduced in Section 1.1 for block constant matrices.

Corollary 1. *The pseudo-inverse E^+ of E is*

$$\begin{matrix} & n(n - 1) & n(n - 1) \\ n(n - 1) & \left[\begin{array}{cc} \frac{1}{6n^2(n-1)^2} & 0 \\ 0 & \frac{1}{6n^2(n-1)^2} \end{array} \right] \\ n(n - 1) & & \end{matrix}$$

In what follows, we make regular use of the fact that a square matrix with all entries $c \geq 0$ is positive semidefinite since such a matrix is clearly a Gram matrix.

Now we make use of the generalized Schur complement. We decompose the matrix R as

$$R = \begin{bmatrix} F & G^t \\ G & E \end{bmatrix}, \tag{2}$$

where E has all rows and columns from blocks 5 and 6, while F has all rows and columns from blocks 1, 2, 3, and 4, with G having the appropriate rows and columns. It is known (see [17]) that a matrix R with the block decomposition as shown in (2) is positive semidefinite if and only if E is positive semidefinite and $(I - EE^T)G = 0$ and $F - G^t E^+ G$ is positive semidefinite.

Lemma 2. *E is positive semidefinite.*

Proof. Note E is a block diagonal matrix, and E is 6 as each entry in the two diagonal blocks, so each block is a Gram matrix. □

Lemma 3. *Let I be the $2n(n - 1) \times 2n(n - 1)$ identity matrix, and let E and G be as defined before. Then $(I - EE^+)G$ is the $2n(n - 1) \times [1 + 2(n - 1) + (n - 1)^2]$ matrix of all zeroes.*

Proof. It follows from Corollary 1 that EE^+ is a $2n(n-1) \times 2n(n-1)$ matrix whose upper left block and lower right blocks are $n(n-1) \times n(n-1)$ matrices with every entry $n(n-1) \cdot 6 \cdot \frac{1}{6n^2(n-1)^2} = \frac{1}{n(n-1)}$, and whose upper right block and lower left block are all zeroes. Thus, the (i, j) -entry of $H = I - EE^+$ is

$$H_{i,j} = \begin{cases} 1 - \frac{1}{n(n-1)} & \text{if } i = j, \\ -\frac{1}{n(n-1)} & \text{if } i \neq j \text{ and } (i, j \leq n \text{ or } i, j > n), \\ 0 & \text{otherwise.} \end{cases}$$

Every column of G is a vector with $2n(n-1)$ entries, where the first $n(n-1)$ entries are identical (either 3 or 9), and the second $n(n-1)$ entries are identical (either 3 or 9). Every one of these combinations occurs: that is, there is a column of all 9s, but there is also a column of G where the first half is all 3s and the second half is all 9s, and so on.

Now we prove $HG = 0$. For this, consider an arbitrary row of H and an arbitrary column of G , and we will consider the result of the dot product. For the chosen column of G , let us say that the first $n(n-1)$ entries are ρ and the second $n(n-1)$ entries are τ . For the selected row of H , either the 0s are the second-half entries or the first-half entries. If the second-half entries are 0, then the product is

$$\begin{aligned} (1 - \frac{1}{n(n-1)})\rho + (n(n-1) - 1)(\frac{1}{n(n-1)})\rho + n(n-1) \cdot 0 \cdot \tau = \\ n(n-1) \cdot \frac{1}{n(n-1)} \cdot \rho - \rho = 0. \end{aligned}$$

If the chosen row of H is in the second half (so the 0 entries are in the first half, then the expression is similar to the one just shown, except that the ρ s and the τ s are switched. In particular, the result is still 0, so every entry of HG is 0. □

Lemma 4. *The generalized Schur complement $F - G^tE^+G$ is positive semidefinite.*

Proof. The indexing for E^+ follows the indexing for E . Thus, E^+G has rows from blocks 5 and 6, and columns from blocks 1, 2, 3, 4. For each entry from row block 5 and column block 1, the entry of E^+G is $n(n-1) \cdot \frac{1}{6n^2(n-1)^2} \cdot 9 + n(n-1) \cdot 0 \cdot 9 = \frac{9}{6n(n-1)}$. Each entry of E^+G is similarly computed. Thus, E^+G is the product of the following two

block constant matrices

$$\begin{matrix} n(n-1) & n(n-1) \\ n(n-1) \end{matrix} \begin{bmatrix} \frac{n(n-1)}{6n^2(n-1)^2} & 0 \\ 0 & \frac{1}{6n^2(n-1)^2} \end{bmatrix} \begin{matrix} 1 & n-1 & n-1 & (n-1)^2 \\ n(n-1) \end{matrix} \begin{bmatrix} 9 & 3 & 9 & 3 \\ 9 & 9 & 3 & 3 \end{bmatrix}$$

which simplifies to

$$\begin{matrix} n(n-1) \\ n(n-1) \end{matrix} \begin{bmatrix} \frac{1}{9} & \frac{n-1}{6n(n-1)} & \frac{n-1}{6n(n-1)} & \frac{(n-1)^2}{6n(n-1)} \\ \frac{6n(n-1)}{9} & \frac{6n(n-1)}{9} & \frac{6n(n-1)}{3} & \frac{6n(n-1)}{3} \end{bmatrix}.$$

We now examine $G^t(E^+G)$. For example, the (only) entry whose row block is 1 and whose column block is 1 has value $n(n-1) \cdot 9 \cdot \frac{9}{6n(n-1)} + n(n-1) \cdot 9 \cdot \frac{9}{6n(n-1)} = \frac{9 \cdot 9 + 9 \cdot 9}{6} = 27$. The remaining entries are found the same way. Thus, $G^t(E^+G)$ is the product of the following two block constant matrices

$$\begin{matrix} n(n-1) & n(n-1) \\ 1 & n-1 \\ n-1 & n-1 \\ (n-1)^2 \end{matrix} \begin{bmatrix} 9 & 9 \\ 3 & 9 \\ 9 & 3 \\ 3 & 3 \end{bmatrix},$$

$$\begin{matrix} n(n-1) \\ n(n-1) \end{matrix} \begin{bmatrix} \frac{1}{9} & \frac{n-1}{6n(n-1)} & \frac{n-1}{6n(n-1)} & \frac{(n-1)^2}{6n(n-1)} \\ \frac{6n(n-1)}{9} & \frac{6n(n-1)}{9} & \frac{6n(n-1)}{3} & \frac{6n(n-1)}{3} \end{bmatrix},$$

which simplifies to

$$\begin{matrix} 1 & n-1 & n-1 & (n-1)^2 \\ n-1 & n-1 & n-1 & (n-1)^2 \\ n-1 & n-1 & n-1 & (n-1)^2 \\ (n-1)^2 & n-1 & n-1 & (n-1)^2 \end{matrix} \begin{bmatrix} \frac{9 \cdot 9 + 9 \cdot 9}{6} & \frac{9 \cdot 3 + 9 \cdot 9}{6} & \frac{9 \cdot 9 + 9 \cdot 3}{6} & \frac{9 \cdot 3 + 9 \cdot 3}{6} \\ \frac{3 \cdot 9 + 9 \cdot 9}{6} & \frac{3 \cdot 3 + 9 \cdot 9}{6} & \frac{3 \cdot 9 + 9 \cdot 3}{6} & \frac{3 \cdot 3 + 9 \cdot 3}{6} \\ \frac{9 \cdot 9 + 3 \cdot 9}{6} & \frac{9 \cdot 3 + 3 \cdot 9}{6} & \frac{9 \cdot 9 + 3 \cdot 3}{6} & \frac{9 \cdot 3 + 3 \cdot 3}{6} \\ \frac{3 \cdot 9 + 3 \cdot 9}{6} & \frac{3 \cdot 3 + 3 \cdot 9}{6} & \frac{3 \cdot 9 + 3 \cdot 3}{6} & \frac{3 \cdot 3 + 3 \cdot 3}{6} \end{bmatrix} =$$

$$\begin{matrix} 1 & n-1 & n-1 & (n-1)^2 \\ 1 & n-1 & n-1 & (n-1)^2 \\ n-1 & n-1 & n-1 & (n-1)^2 \\ n-1 & n-1 & n-1 & (n-1)^2 \\ (n-1)^2 & n-1 & n-1 & (n-1)^2 \end{matrix} \begin{bmatrix} 27 & 18 & 18 & 9 \\ 18 & 15 & 9 & 6 \\ 18 & 9 & 15 & 6 \\ 9 & 6 & 6 & 3 \end{bmatrix}.$$

Then $F - G^t E^+ G$ is

$$\begin{aligned}
 & \begin{matrix} & 1 & n-1 & n-1 & (n-1)^2 \\ & 1 & \left[\begin{matrix} 30 & 21 & 21 & 12 \\ 21 & 18 & 12 & 9 \\ 21 & 12 & 18 & 9 \\ 12 & 9 & 9 & 6 \end{matrix} \right] \\ n-1 & \\ n-1 & \\ (n-1)^2 & \end{matrix} & - & \\
 & \begin{matrix} & 1 & n-1 & n-1 & (n-1)^2 \\ & 1 & \left[\begin{matrix} 27 & 18 & 18 & 9 \\ 18 & 15 & 9 & 6 \\ 18 & 9 & 15 & 6 \\ 9 & 6 & 6 & 3 \end{matrix} \right] \\ n-1 & \\ n-1 & \\ (n-1)^2 & \end{matrix} & = & n^2 \begin{bmatrix} 3 \end{bmatrix}.
 \end{aligned}$$

Therefore $F - G^t E^+ G$ is positive semidefinite since it is an $n^2 \times n^2$ matrix with every entry 3. □

5. Proof of positive semidefiniteness of U

Fix an integer $n \geq 4$. In the following subsections, we describe the entries of U, U^2, U^3 , and U^4 based on the indexing of rows and columns. In each of these four matrices, due to symmetry of an \mathfrak{S}_n action, we only need to present one entry up to index type. Moreover, the size of this information does not grow as n increases, and this is all that is needed to show that U satisfies a certain polynomial whose degree is bounded universally in n .

We describe the matrix U defined in Section 2.2 by index type. While this expands on information which is essentially already provided by Section 2.2, formatting the information in this expanded form (and in this order, matching the next several subsections) will be useful in proving that U satisfies a certain polynomial. In the list below, the indexing applies only when it makes sense. For example, discussing the $(\{4, 5, 6\}, 4)$ -column does not apply when $n = 4$.

Exhaustive information on the entries of U, U^2, U^3 , and U^4 by entry-type is found at <https://edward-kim-math.github.io/cdta-m6r2/>. The data is stored in `appendix-min-poly-U-data.sage`. For instance, the $(\{1, 2, 3\}, 1)$ -row $(\{1, 2, 3\}, 1)$ -column entry of U is 24, and the entry of U^2 is $216n^2 + 1026n - 432$. Detailed proofs for selected entries of U^2 are given at <https://edward-kim-math.github.io/cdta-m6r2/>, and the code there verifies that the entries are as claimed.

5.1. The minimal polynomial of U

Fix $n \geq 4$. Let $b = -3n(4n - 3)$ and $c = 54[2\binom{n+2}{4} + 5\binom{n+1}{4} + \binom{n}{4}]$ and $d = 15n(2n - 1)$. Note $c = 18n^4 - 27n^3 + 9n^2$. Let $f = b - d$ and $g = c - bd$ and $h = -cd$. Note $f = -42n^2 + 24n$ and $g = 378n^4 - 477n^3 + 144n^2$ and $h = -540n^6 + 1080n^5 - 675n^4 + 135n^3$.

Define $\mu(x) = x(x - d)(x^2 + bx + c)$. Then $\mu(x) = x^4 + fx^3 + gx^2 + hx$. For example, when $n = 4$, then $\mu(x) = x(x - 420)(x^2 - 156x + 3024) = x^4 - 576x^3 + 68544x^2 - 1270080x$, and when $n = 5$, then $\mu(x) = x(x - 675)(x^2 - 255x + 8100) = x^4 - 930x^3 + 180225x^2 - 5467500x$.

It turns out that $U^4 + fU^3 + gU^2 + hU = 0$. For instance, the $(\{1, 2, 3\}, 1)$ -row $(\{1, 2, 3\}, 1)$ -column entry of $U^4 + fU^3 + gU^2 + hU$ is $(22032n^6 + 1506276n^5 - 2246778n^4 + 1093824n^3 - 173664n^2) + (-42n^2 + 24n)(2160n^4 + 44496n^3 - 43254n^2 + 9828n) + (378n^4 - 477n^3 + 144n^2)(216n^2 + 1026n - 432) + (-540n^6 + 1080n^5 - 675n^4 + 135n^3)(24)$, which is equal to 0. A similar calculation has been verified for every entry type, which the reader may check using the provided code. Thus, $\mu(U) = 0$.

We note $f < 0$ and $g > 0$ and $h < 0$, since $b < 0$ and $c > 0$ and $d > 0$. By Descartes' Law of Signs, μ has no negative real roots. Thus μ is (a multiple of) the minimum polynomial of U . Since U is symmetric (and thus all eigenvalues of U are real), this proves that U is positive semidefinite. (For $n \leq 3$, the positive semidefiniteness of U was directly verified.)

5.2. Remarks

Since μ is (a multiple of) the minimum polynomial of U , the distinct eigenvalues of U are 0, the integer $d = 15n(2n - 1)$, and the roots of $q(x) = x^2 + bx + c$. While our proof only shows that μ is a multiple of the minimum polynomial of U , but through computation for many values of n , we believe that μ is the minimum polynomial of U .

While the linear coefficient of $q(x)$ had a relatively nice formula $b = -3n(4n - 3)$, the constant term $c = 54[2\binom{n+2}{4} + 5\binom{n+1}{4} + \binom{n}{4}]$ deserves some explanation. The values of $\frac{1}{54}c$ starting at $n = 4$ are 56, 150, 330, 637, 1120, 1836, and so on. This sequence is every other term of A181474 (see [11]). Thus, $\frac{1}{54}c$ is the coefficient of x^{2n-3} in the generating

function

$$\gamma(x) = \frac{1 + x + 4x^2 + x^3 + x^4}{(1 - x)^5(1 + x)^4}.$$

After applying Taylor expansion to $\frac{1}{(1-x^2)^4}$ and then to $\frac{1}{(1-x^2)^4(1-x)}$, the result of multiplying by $1 + x + 4x^2 + x^3 + x^4$ yielded that the coefficient of x^{2n-3} in $\gamma(x)$, and thus the value of $\frac{1}{54}c$, is the following weighted sum of binomial coefficients:

$$2\binom{n+2}{4} + 5\binom{n+1}{4} + \binom{n}{4}.$$

Though we already showed that U is positive-semidefinite in the previous subsection via alternating coefficients on the minimal polynomial, we have computational evidence which suggests the following additional spectral data:

First, recall that U is a square matrix of size $3\binom{n}{3} + n(n-1) + n^2$. It appears that the integer d is an eigenvalue of U with multiplicity 1, while 0 is an eigenvalue of multiplicity $w = 3\binom{n}{3} + 2n^2 - 3n + 1$ and the two distinct roots of $q(x)$ appear as eigenvalues of multiplicity $n-1$ each. That is to say, it appears that the characteristic polynomial of U is $\chi(x) = x^w(x-d)(x^2+bx+c)^{n-1}$.

Eigenvectors of U

Let $e_{(\{i,j,k\},i)}$ denote the standard unit basis vector for the $(\{i,j,k\},i)$ -entry in block 1. Likewise, $e_{(i,j)}$ denotes the standard basis vector in block 2, and $e_{(\hat{i},\hat{j})}$ denotes the standard basis vector in block 3.

For a fixed n , the vector

$$\sum_{(\{i,j,k\},i)} e_{(\{i,j,k\},i)} + \sum_{(i,j)} e_{(i,j)} + \frac{1}{2} \sum_{(\hat{i},\hat{j})} e_{(\hat{i},\hat{j})}$$

is an eigenvector of U corresponding to $\lambda = d$.

We present below a set of linearly independent eigenvectors of U corresponding to $\lambda = 0$:

- $e_{(\{i,j,k\},i)} - e_{(\hat{j},\hat{n})} - e_{(\hat{k},\hat{n})} - 2e_{(\hat{n},\hat{i})} + 2e_{(\hat{n},\hat{n})}$ whenever $i, j, k \neq n$;
- $e_{(i,j)} - e_{(\hat{i},\hat{n})} - e_{(\hat{j},\hat{n})} - 2e_{(\hat{n},\hat{i})} + 2e_{(\hat{n},\hat{n})}$ whenever $i, j \neq n$;

- $e_{(\{i,j,n\},i)} - e_{(\hat{i},\hat{n})} - e_{(\hat{j},\hat{n})} - 2e_{(\hat{n},\hat{j})} + e_{(\hat{n},\hat{n})}$ whenever $i, j \neq n$;
- $e_{(i,n)} - e_{(\hat{i},\hat{n})} - 2e_{(\hat{n},\hat{i})} + e_{(\hat{n},\hat{n})}$ whenever $i \neq n$;
- $e_{(\{i,j,n\},n)} - e_{(\hat{i},\hat{n})} - e_{(\hat{j},\hat{n})}$ whenever $i, j \neq n$;
- $e_{(n,i)} - e_{(\hat{i},\hat{n})} - e_{(\hat{n},\hat{n})}$ whenever $i \neq n$;
- $e_{(\hat{i},\hat{j})} - e_{(\hat{i},\hat{n})} - e_{(\hat{n},\hat{j})} + e_{(\hat{n},\hat{n})}$ whenever $i, j \leq n$.

Based on the coordinates of the seven types of vectors mentioned above, this gives $3\binom{n-1}{3} + 2\binom{n-1}{2} + 2\binom{n-1}{2} + (n-1) + \binom{n-1}{2} + (n-1) + (n-1)^2$ of linearly independent eigenvectors of U corresponding to $\lambda = 0$, thus the geometric multiplicity of $\lambda = 0$ matches the algebraic multiplicity $w = 3\binom{n}{3} + 2n^2 - 3n + 1$.

Diagonalization for each n would be complete if we could, for each n , obtain exact representations of $n - 1$ linearly independent eigenvectors of U for each root of $q(x) = x^2 + bx + c$. The sum of the eigenspaces corresponding to the two roots of q form a $2(n - 1)$ -dimensional subspace of $\mathbb{R}^{3\binom{n}{3} + n(n-1) + n^2}$. Say that $c_1, \dots, c_{2(n-1)}$ is a basis for this subspace. We make use of the fact that each c_i is orthogonal to the eigenvectors corresponding to $\lambda = 0$ and $\lambda = d$. Thus, a concrete way to find obtain a basis is to place the eigenvectors for 0 and d as the rows of a matrix and find a basis for its kernel. We denote by V the $(3\binom{n}{3} + n(n - 1) + n^2) \times 2(n - 1)$ matrix whose columns are the vectors $c_1, \dots, c_{2(n-1)}$ generating the kernel. Fix λ to be a root of $q(x)$. Then finding a non-zero $x \in \mathbb{R}^{3\binom{n}{3} + n(n-1) + n^2}$ satisfying $Ux = \lambda x$ is the same as finding a parameter vector $\alpha \in \mathbb{R}^{2(n-1)}$ satisfying $W\alpha = 0$, where $x = V\alpha$ and $W = UV - \lambda V$. Finding an exact representation for a vector α in the kernel of $UV - \lambda V$ can be done for fixed n , and then $x = V\alpha$ is an eigenvector of U corresponding to λ .

For concreteness, we describe this process for $n = 4$. In this case, U is a 40×40 matrix, and the roots of $q(x) = x^2 - 156x + 3024$ are $78 \pm 6\sqrt{85}$. Let us fix $\lambda = 78 + 6\sqrt{85}$. A minimal generating set of eigenvectors for 0 and d consists of 34 vectors. These vectors can be the rows of a 34×40 matrix, and a basis for the kernel of this matrix is found as the columns of

$$V = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ -1 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & -1 & 0 & 0 & 1 \\ 1 & 0 & -1 & -1 & 1 & 1 \\ -1 & -1 & 1 & 0 & -1 & -1 \\ 0 & -1 & 0 & 0 & -1 & -1 \\ 0 & -1 & 0 & -1 & 0 & -1 \\ 0 & 2 & 0 & 1 & 1 & 1 \\ 1 & 2 & -1 & 0 & 1 & 2 \\ 0 & 2 & -1 & 1 & 1 & 2 \\ 0 & 0 & 1 & 1 & 0 & -1 \\ 0 & -1 & 1 & 0 & -1 & -2 \\ -1 & -1 & 1 & 1 & -1 & -2 \\ 1 & 0 & 0 & -1 & 0 & 1 \\ 0 & -1 & 1 & -1 & -1 & -1 \\ 0 & -1 & 0 & -1 & -1 & 0 \\ 0 & 0 & -1 & 0 & 1 & 1 \\ -1 & -1 & 0 & 0 & 0 & -1 \\ 0 & -1 & -1 & -1 & 0 & 0 \\ \frac{1}{2} & \frac{3}{2} & -\frac{1}{2} & \frac{1}{2} & 1 & \frac{3}{2} \\ \frac{1}{2} & \frac{1}{2} & 0 & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 & \frac{1}{2} & 1 \\ \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & 0 & 1 & 1 \\ -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & 0 & -\frac{1}{2} \\ -\frac{1}{2} & -\frac{1}{2} & 1 & \frac{1}{2} & -\frac{1}{2} & -\frac{3}{2} \\ -\frac{1}{2} & -\frac{1}{2} & 1 & 0 & -\frac{1}{2} & -1 \\ -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & 0 & 0 & -1 \\ \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & 0 & -\frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & 0 & -1 & -\frac{1}{2} & 0 \\ -\frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & -1 & 0 & 0 \\ -\frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & 0 & \frac{1}{2} \\ -\frac{1}{2} & -\frac{1}{2} & 0 & \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & -\frac{1}{2} & 0 & 0 & -\frac{1}{2} & 0 \\ -\frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & 0 & 0 & 0 \end{bmatrix}.$$

Let $W = UV - (78 + 6\sqrt{85})V$. Instead of describing a complete basis for the eigenspace of $78 + 6\sqrt{85}$, we summarize what happens with one vector. For any vector α satisfying $W\alpha = 0$, the vector $x = V\alpha$ is an eigenvector of U corresponding to $\lambda = 78 + 6\sqrt{85}$ given with exact coordinates. Displaying α and x requires large-format paper, and both are available at

<https://www.overleaf.com/read/xhmyxkywrqhb>

While we have an alternate proof that U is positive semidefinite, what remains open (and interesting) is finding, for all n , exact representations of eigenvectors corresponding to both roots of $q(x)$.

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