Symmetrisable matrices, quotients, and the trace problem

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Abstract

Symmetrisable matrices are those that are a real diagonal change of basis away from being symmetric. Restricting to matrices that have integer entries (symmetrisable integer matrices — SIMs) we enter the worlds of combinatorics and number theory. It is known that quotients of equitable partitions of graphs provide examples of SIMs (with all entries nonnegative). We note a converse result, that every SIM comes from a quotient of an equitable partition of a signed graph (in the nonnegative case, a graph). There is a beautiful well-known combinatorial description of SIMs, which leads to a necessary combinatorial/number-theoretic property of their symmetrisations. We show that this property in fact classifies the matrices that are symmetrisations of SIMs. We then turn to the trace problem for totally positive algebraic integers. The analogous problem for eigenvalues of positive definite integer symmetric matrices (ISMs) was recently solved. We extend this to SIMs, showing that if A is a connected positive definite $n \times n$ SIM, then $\operatorname{tr}(A) \geq 2n-1$, and that if equality holds then A must in fact be symmetric. We explore the structure of minimal-trace examples, in both the symmetric and asymmetric cases.

Keywords: Symmetrisable matrices, equitable partitions, trace problem
2010 MSC: 15A18, 15B36, 11C99

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1. Introduction

The theory of symmetrisable matrices was developed largely in the context of Lie theory: generalised Cartan matrices are important special cases of symmetrisable matrices. There is a beautiful combinatorial classification of these matrices as those that are sign symmetric and satisfy a certain cycle condition (Proposition 11, [3, Corollary 15.15]).

We shall explore connections with equitable partitions of signed graphs. It will transpire that symmetrisable integer matrices (SIMs) are precisely those that occur as quotient matrices for these equitable partitions. It is known that equitable partitions of graphs provide examples of symmetrisable matrices (for example, this is implicit in [4, Lemma 9.3.1] along with the preceding discussion), but the converse (even for graphs) does not appear to have been noted before.

The Schur-Siegel-Smyth trace problem [2, Open Problem 17] concerning the absolute traces of totally positive algebraic integers remains open. See also the survey paper [1] of Aguirre and Peral. The analogous problem for characteristic polynomials of positive definite integer symmetric matrices was recently settled [5]. Moving to symmetrisable matrices there are many more possible characteristic polynomials, but here we shall establish the same trace bound as for the symmetric case. Moreover we shall see that this bound can only be attained by symmetric matrices, so that for symmetrisable but asymmetric matrices a stronger bound holds. We shall describe a structure theory for minimal-trace examples in both the symmetric and asymmetric cases.

2. Statement of main results

We start with the definition of a symmetrisable matrix. In fact there are at least two other equivalent definitions in the literature, but the one we give here seems the most natural.

Definition 1. An $n \times n$ real matrix B is said to be **symmetrisable** if there is a real diagonal matrix $D = \mathrm{diag}(d_1, \dots, d_n)$ with each $d_i > 0$ such that

$$S = D^{-1}BD \tag{1}$$

is symmetric. We call S the **symmetrisation** of B.

If the entries of a symmetrisable matrix B are integers, then we call B a **SIM** (symmetrisable integer matrix).

Our next definition describes a property of a matrix which combines combinatorics and number theory.

Definition 2. Let $S = (s_{ij})$ be real symmetric $n \times n$ matrix. We say that S satisfies the **rational cycle condition** if for every $t \geq 2$ and every sequence $i_1, \ldots, i_t$ of elements of $\{1, \ldots, n\}$ there holds

$$s_{i_1 i_2} s_{i_2 i_3} \cdots s_{i_{t-1} i_t} s_{i_t i_1} \in \mathbb{Q}\,. \tag{2}$$

We also define

$$\sqrt{\mathbb{N}_0} = \{a \in \mathbb{R} \mid a^2 \in \mathbb{N}_0\} = \{0,\ 1,\ -1,\ \sqrt{2},\ -\sqrt{2},\ \sqrt{3},\ -\sqrt{3}, \ldots\}\,. \tag{3}$$

With these definitions, we can now state our first preliminary result.

Proposition 1. *Let $S = (s_{ij})$ be a symmetric matrix with entries in $\sqrt{\mathbb{N}_0}$ that satisfies the rational cycle condition. Then there exists some SIM B such that S is the symmetrisation of B.*

We shall define below (Definition 6) what it means to say that a matrix is the quotient matrix of an equitable partition of a signed graph. Then we shall establish the following characterisation of SIMs.

Theorem 2. *A matrix is a SIM if and only if it is the quotient matrix of an equitable partition of a signed graph.*

A matrix with all entries non-negative is a SIM if and only if it is the quotient matrix of an equitable partition of a graph.

In the final part of the paper, we turn to the SIM analogue of the trace problem. We start by proving the following general trace bound.

Theorem 3. *Let A be an $n \times n$ positive definite connected SIM. Then $\operatorname{tr} A \geq 2n - 1$. If moreover A is asymmetric, then $\operatorname{tr} A \geq 2n$.*

There is an immediate consequence regarding possible *minimal* polynomials of SIMs.

Corollary 4. *Let m be a monic irreducible polynomial with integer coefficients, degree n, and with all roots real and strictly positive. If the trace of m is strictly less than $2n - 1$, then m is not the minimal polynomial of a SIM.*

We can also settle the analogue of the trace problem for SIMs.

Definition 3. The **absolute trace** of an $n \times n$ matrix A, is defined to be $\mathrm{tr}(A)/n$, where $\mathrm{tr}(A)$ is the usual trace (the sum of the diagonal entries).

Corollary 5. *Let X be the set of absolute traces of connected positive definite SIMs, and let Y be the set of absolute traces of connected positive definite real symmetric matrices that have entries in $\sqrt{\mathbb{N}_0}$ and satisfy the rational cycle condition* (2)*. Then $X = Y$, and the smallest limit point of X is* 2*.*

3. Definitions and elementary remarks

The final section of the paper develops a structure theory for minimal-trace SIMs, and for this endeavour it will be convenient to work up to a suitable notion of equivalence. In this section we define the relevant concept of equivalence for matrices generally and show that any matrix that is equivalent to a SIM is itself a SIM (Lemma 8). The results in this section are elementary, and are surely essentially known, but as we could find no explicit reference we give all the proofs.

A symmetrisable matrix (Definition 1) can be transformed to a symmetric matrix by a diagonal change of basis. In particular, all the eigenvalues of a symmetrisable matrix are real, since they equal those of the symmetrisation. Note that if B is symmetrisable then the corresponding D is certainly not uniquely determined, as we may scale all the entries by any positive real number, but any such scaling preserves $D^{-1}BD$.

It feels artificial to require that all the diagonal entries of D in (1) are positive, but we lose no generality in doing so. If $D^{-1}BD = S$ is symmetric, where now D is an arbitrary invertible diagonal real matrix, then define the diagonal matrix E that has as its diagonal entries the signs of those of D:

$$E = \mathrm{diag}\big(\mathrm{sgn}(d_1), \ldots, \mathrm{sgn}(d_n)\big) .$$

Then DE has all diagonal entries strictly positive, $E^{-1} = E$, and the matrix

$$(DE)^{-1}B(DE) = ESE$$

is symmetric. One convenience of restricting to positive diagonal entries as a canonical choice is that this makes the symmetrisation matrix unique.

Lemma 6. *If $B = (b_{ij})$ is symmetrisable then then it has a unique symmetrisation.*

Proof. Let $S = D^{-1}BD = (s_{ij})$ be any symmetrisation of B, with

$$D = \operatorname{diag}(d_1, \dots, d_n)$$

and each $d_i > 0$. We have

$$s_{ij} = d_i^{-1} b_{ij} d_j \,. \tag{4}$$

One immediate consequence of (4) is that the signs of the entries of B and S agree:

$$\operatorname{sgn}(s_{ij}) = \operatorname{sgn}(b_{ij}) \text{ for all } i \text{ and } j \,. \tag{5}$$

Using (4) and the symmetry of S we have

$$s_{ij}^2 = s_{ij} s_{ji} = d_i^{-1} b_{ij} d_j d_j^{-1} b_{ji} d_i = b_{ij} b_{ji} \,. \tag{6}$$

Hence $|s_{ij}|$ is determined by B. Together with (5) this shows that S is uniquely determined by B. □

Lemma 7. *If B is symmetrisable, then so is B^{T}, and the symmetrisations of B and B^{T} are the same.*

Proof. If B is symmetrisable, then there is diagonal D with positive diagonal entries such that $S = D^{-1}BD$ is symmetric. Transposing we see that

$$S = D^{\mathsf{T}} B^{\mathsf{T}} (D^{\mathsf{T}})^{-1}$$

so that B^{T} is indeed symmetrisable, and with the same symmetrisation. □

When the symmetrisable matrix B has integer entries (i.e., B is a SIM) we shall see below in Lemma 9 that the diagonal entries of D in (1) can be chosen to be square-roots of positive integers.

Definition 4. We shall say that two $n \times n$ matrices A and B are *equivalent* if A can be transformed to $\pm B$ by conjugating by an element of $O_n(\mathbb{Z})$.

Note that $O_n(Z)$ is the set of *signed permutation matrices*, namely those matrices P for which row and each column contain precisely one nonzero entry, and that each nonzero entry is either 1 or -1.

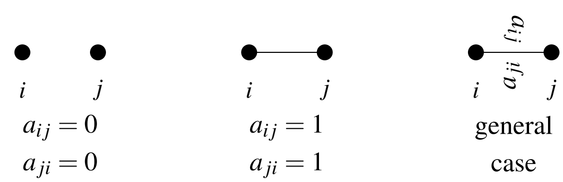
Lemma 8. *If an integer matrix B is symmetrisable, then so is any matrix equivalent to B.*

Proof. Suppose that $D^{-1}BD = S$, where D is diagonal with positive diagonal entries, and let P be any signed permutation matrix of the same size. Then we compute that $P^{-1}DP = P^{\mathsf{T}}DP$ is also diagonal with positive diagonal entries. Since

$$(P^{-1}D^{-1}P)(P^{-1}BP)(P^{-1}DP) = P^{\mathsf{T}}SP$$

is symmetric, we see that $P^{-1}BP$ is symmetrisable. Moreover $D^{-1}(-B)D = -S$ is symmetric, so that the negative of a symmetrisable matrix is symmetrisable. Hence any matrix equivalent to B is symmetrisable. □

We shall have occasion to represent SIMs as digraphs, and to apply the language of graph theory to properties of matrices. To any square matrix $A = (a_{ij})$ with entries in $\mathbb{R}$, we associate a digraph, also called A. (We shall refer to A interchangeably as a digraph and as a matrix, sometimes within the same sentence.) To the ith row of the matrix A we associate a vertex i of the digraph. The diagonal entry a_{ii} represents a *charge* on the vertex i. The only charges of interest to us will be integral ones, and the only ones we shall need to draw are 0, 1 and -1, which we draw as $\bullet$, $\oplus$ and $\ominus$ respectively. The directed edge weights a_{ij} (from i to j) are arbitrary real numbers. We represent the pairs of directed edges (a_{ij}, a_{ji}) by drawing a single labelled edge (or no edge) as shown (here picturing all the vertices with zero charge).



In the general case, the value a_{ij} is written on the *left* of the edge as we travel from i to j (and a_{ji} is on the left as we travel from j to i).

Given a digraph A, the matrix A is determined only once the vertices have been given an ordering, but we regard all possible such matrices as equivalent (Definition 4).

4. The structure of symmetrisable matrices

Both our characterisation of SIMs as quotients of equitable partitions of signed graphs (Section 6) and our work on the trace problem (Section 7) require some detail of the structure of symmetrisable matrices. In this section we recall the classical characterisation Proposition 11, giving the detail which will be needed later. In particular we highlight a balancing condition (9) that is equivalent to symmetrisability (Lemma 10).

Definition 5. A real $n \times n$ matrix $B = (b_{ij})$ is called **sign symmetric** if

$$\operatorname{sgn}(b_{ij}) = \operatorname{sgn}(b_{ji}) \tag{7}$$

holds for all i, $j \in \{1, \ldots, n\}$.

Let B be a symmetrisable matrix, with symmetrisation S. One immediate consequence of (5), together with symmetry of S, is that any symmetrisable matrix is sign symmetric.

Lemma 9. *If B is an $n \times n$ SIM, then we can choose $D = \operatorname{diag}(d_1, \ldots, d_n)$ in (1) to have all entries being positive square-roots of integers (i.e., $d_i \in \{1, \sqrt{2}, \sqrt{3}, \ldots\}$ for each i).*

Proof. Writing $B = (b_{ij})$, $D = \operatorname{diag}(d_1, \ldots, d_n)$ and $S = (s_{ij})$, we get from symmetry of S and (11) that

$$d_j^2 = (b_{ji}/b_{ij})d_i^2 \text{ when } b_{ij} \neq 0\,. \tag{8}$$

Thus for all indices i, k in the same connected component of B, we see by considering a chain of such identities that d_i^2/d_k^2 is rational. Thus on fixing some i in this component, for an appropriate positive integer N we can scale by N/d_i all the d_k in this component to make the d_k^2 all integers. The relation $S = D^{-1}BD$ is preserved by this scaling. Doing this for all connected components of B makes D a diagonal matrix with all its diagonal entries being (positive) square-roots of integers. □

From (8) we get the condition

$$b_{ij}d_j^2 = b_{ji}d_i^2, \qquad (1 \leq i \leq n,\ 1 \leq j \leq n)\,. \tag{9}$$

Lemma 10. *An $n \times n$ matrix $B = (b_{ij})$ is symmetrisable if and only if there exist $d_1 > 0$, $\ldots$, $d_n > 0$ such that (9) holds.*

Proof. We have seen that if B is symmetrisable then (9) holds for some $d_1 > 0$, $\ldots$, $d_n > 0$. Conversely, suppose that there exist $d_1 > 0$, $\ldots$, $d_n > 0$ such that (9) holds, and let $D = \operatorname{diag}(d_1, \ldots, d_n)$. Then $S = D^{-1}BD = (s_{ij})$ is symmetric (for $s_{ij} = d_i^{-1}b_{ij}d_j$, and then (9) gives $s_{ij} = s_{ji}$), and hence B is symmetrisable. □

Suppose that B is an $n \times n$ symmetrisable matrix. Take any $i_1, i_2, \ldots, i_t \in \{1, \ldots, n\}$. Multiplying (9) for $(i, j) = (i_1, i_2)$, (i_2, i_3), $\ldots$, (i_{t-1}, i_t), (i_t, i_1), then dividing by the (nonzero) product of all the $d_{i_j}^2$ we get

$$b_{i_1i_2}b_{i_2i_3}\cdots b_{i_{t-1}i_t}b_{i_ti_1} = b_{i_2i_1}b_{i_3i_2}\cdots b_{i_ti_{t-1}}b_{i_1i_t} \tag{10}$$

for all sequences $i_1, i_2, \ldots, i_t$ of elements of $\{1, \ldots, n\}$.

An $n \times n$ real matrix $B = (b_{ij})$ is said to satisfy the **cycle condition** if (10) holds for all sequences $i_1, i_2, \ldots, i_t$ of elements of $\{1, \ldots, n\}$.

Thus any symmetrisable matrix is sign symmetric and satisfies the cycle condition. In fact that these two conditions together are sufficient for a matrix to be symmetrisable.

Proposition 11 (Essentially [3, Corollary 15.15])**.** *An $n \times n$ real matrix B is symmetrisable if and only if it is sign symmetric and satisfies the cycle condition.*

Proof. We have seen that any symmetrisable matrix is sign symmetric and satisfies the cycle condition.

Now suppose that $B = (b_{ij})$ satisfies both these conditions. For simplicity suppose that B is connected (else treat each component separately). Set $d_1 = 1$. For each neighbour i of vertex 1, sign symmetry gives both b_{1i} and b_{i1} non-zero, so that we can define $d_i = d_1\sqrt{b_{1i}/b_{i1}} = \sqrt{b_{1i}/b_{i1}}$. Then the balancing condition (9) holds when $j = 1$ (if any b_{1j} in (9) is zero, then both sides are zero). Next for neighbours k of neighbours i of 1, define d_k by $d_k = d_i\sqrt{b_{ik}/b_{ki}}$. By the cycle condition, any vertex k for which d_k has been defined more than once will have received the same value each time. The balancing condition now holds for $j = 1$ and for j any neighbour of 1. And so on, we grow our labelling to all the vertices (consistently, thanks to (10)), and produce positive numbers d_i such that (9) holds, and hence B is symmetrisable by Lemma 10. $\square$

5. The symmetrisation map

We have seen that if B is symmetrisable, then its symmetrisation S is uniquely determined. We saw in the proof of Lemma 6 that the entries in S can be computed without knowledge of D.

Lemma 12. *For B an $n \times n$ real matrix that is sign symmetric, define the real $n \times n$ matrix $\varphi(B)$ by*

$$\varphi\big((b_{ij})\big) = \big(\operatorname{sgn}(b_{ij})\sqrt{b_{ij}b_{ji}}\big)\,. \tag{11}$$

Then $\varphi(B)$ is symmetric. If in addition B is symmetrisable, then $\varphi(B)$ is its symmetrisation.

Proof. It is clear that $\varphi(B)$ is symmetric. The rest follows from the proof of Lemma 6. $\square$

When applied to symmetrisable matrices, we call the map φ in Lemma 12 the **symmetrisation map**. Generally we have a fixed n in mind, but we may view φ as being defined on the set of all sign symmetric matrices of any size – even on matrices that are not symmetrisable (because they do not satisfy the cycle condition).

Lemma 13. *If B is a SIM, then its symmetrisation has all entries in $\sqrt{\mathbb{N}_0}$ (defined in* (3)*).*

Proof. Clear from (11). $\square$

The cycle condition for SIMs implies a corresponding cycle condition for their symmetrisations, namely the rational cycle condition (2).

Lemma 14. *If B is a symmetrisable integer matrix, then $\varphi(B)$ satisfies the rational cycle condition.*

Proof. Let $S = (s_{ij}) = \varphi(B)$, where $B = (b_{ij})$ is an $n \times n$ symmetrisable integer matrix. Take any $t \geq 2$ and any $i_1, \ldots, i_t \in \{1, \ldots, n\}$. From (11) we have

$$s_{i_1 i_2} s_{i_2 i_3} \cdots s_{i_{t-1} i_t} s_{i_t i_1} = \pm\sqrt{b_{i_1 i_2} b_{i_2 i_1} \cdots b_{i_t i_1} b_{i_1 i_t}}\,.$$

By (10) this is rational, indeed in $\mathbb{Z}$, given that the b_{ij} are all in $\mathbb{Z}$. $\square$

Lemma 15. *If $C = (c_{ij})$ is any matrix satisfying the rational cycle condition* (2)*, then its diagonal entries are all rational.*

Proof. Taking $t = 2$ and $i_1 = i_2 = i$ in the rational cycle condition gives $c_{ii}^2 \in \mathbb{Q}$. Taking $t = 3$ and $i_1 = i_2 = i_3 = i$ gives $c_{ii}^3 \in \mathbb{Q}$. Hence $c_{ii} \in \mathbb{Q}$. $\square$

It is easily possible that a matrix B fails the cycle condition whilst $\varphi(B) = S$ satisfies the rational cycle condition. For example, consider

$$B_1 = \begin{pmatrix} 0 & 1 & -2 \\ 3 & 0 & 1 \\ -3 & 2 & 0 \end{pmatrix}.$$

The matrix B_1 is sign symmetric, and even has all eigenvalues real, but it fails the cycle condition and is not symmetrisable. Yet $\varphi(B_1)$ satisfies the rational cycle condition. Proposition 1 is rather more positive: it shows that if a symmetric matrix S with entries in $\sqrt{\mathbb{N}_0}$ satisfies the rational cycle condition then there is at least one SIM B such that $\varphi(B) = S$. For example, the symmetrisable matrix

$$B_2 = \begin{pmatrix} 0 & 1 & -2 \\ 3 & 0 & 2 \\ -3 & 1 & 0 \end{pmatrix}$$

has the same image under φ as the nonsymmetrisable B_1 above.

We now prove Proposition 1, which shows that the symmetrisation map from the set of all SIMs to the set of symmetric matrices with entries in $\sqrt{\mathbb{N}_0}$ and satisfying the rational cycle condition is surjective.

Proof of Proposition 1. We are given that S is symmetric, and may suppose that S is connected. If not, then tackle each component in turn and glue things together. By Lemma 15 the diagonal entries of S lie in $\mathbb{Q} \cap \sqrt{\mathbb{N}_0} = \mathbb{N}_0$. For each i and j, define positive integers d_{ij} and non-negative integers e_{ij} by $s_{ij}^2 = d_{ij}e_{ij}^2$, with d_{ij} square-free (if $s_{ij} = 0$, then $d_{ij} = 1$ and $e_{ij} = 0$). Define

$$A_0 = \big(\operatorname{sgn}(s_{ij})e_{ij}\big)\,.$$

Since S is symmetric, so is A_0. Note that the diagonal entries of A_0 agree with those of S (see Lemma 15).

Choose a spanning tree T for the underlying graph G of S (or of A_0: the underlying graphs are the same), and choose some vertex v as the root.

For each prime p, define a colouring (depending on p) of the vertices of G as follows. Colour the root vertex v red. For each other vertex of G, there is a unique path in T to the root; if an odd number of edges (i, j) on this path have $p \mid d_{ij}$, then colour the vertex blue; if an even number, then red. Then for nonzero d_{ij}, we have that $p \mid d_{ij}$ if and only if the vertices i and j have different colours. This is clear if the edge between i and j is in the tree T. If not, consider the closed walk in G defined as follows: start at i, use the edge from i to j, then follow the unique path in T to v, then follow the unique path in T to i. By the rational cycle condition, this closed walk uses an even number of edges xy with p dividing d_{xy}. If $p \mid d_{ij}$, then the edge from i to j is one of this even number, and there must be an odd number in the rest of the closed walk; but that part of the closed walk is in T, and hence i and j must have opposite colours. If $p \nmid d_{ij}$, then there is an even number of edges xy in the rest of the closed walk for which $p \mid d_{xy}$, and since all these edges are in T we deduce that i and j have the same colour.

Now for each (i, j) with $p \mid d_{ij}$ do the following:

- if vertex i is red and vertex j is blue, multiply $(A_0)_{ij}$ by p;
- if vertex i is blue and vertex j is red, multiply $(A_0)_{ji}$ by p.

Repeat this for each prime p dividing any of the d_{ij}, and let $A = (a_{ij})$ be the final matrix produced from A_0 having done all the required multiplications of elements.

If $i_1, i_2, \ldots, i_t, i_1$ is any closed walk in G, then for each prime p the number of changes from red to blue (using the colouring for p) must equal the number of changes from blue to red (since the walk is closed). Hence each side of (10) is divisible by the same power of p. Since this holds for all p, the matrix A satisfies the cycle condition (and sign symmetry is trivial from the initial construction of A_0), and A is in M_1. $\square$

Note that the colouring of the vertices in this construction (given A_0 and p) is independent of the spanning tree chosen, and of the root, except that the colours red and blue might be swapped. There could easily be elements in the fibre of φ over S that cannot be generated by the above procedure, but in any event this fibre is finite. For we must have $b_{ij}b_{ji} = s_{ij}^2$, giving a finite number of possibilities for each b_{ij}. The force of the Lemma is that provided S satisfies the rational cycle condition, there is at least one choice of these b_{ij} that makes B symmetrisable.

6. Equitable partitions of signed graphs

Our goal in the section is to prove Theorem 2.

Let G be a signed graph (edges may have weight $+1$ or -1), with vertex set $V = \{1,\dots,n\}$. Thus its adjacency matrix A has all entries in $\{-1,0,1\}$. A *partition* of V is simply a partitioning of the vertex set as a disjoint union of nonempty subsets: $V = V_1 \cup \cdots \cup V_r$, where $V_i \cap V_j = \varnothing$ if $i \neq j$ and $V_i \neq \varnothing$ for any i. An arbitrary partition may not be very informative. By contrast, an *equitable partition* reflects a strong symmetry within the signed graph.

Definition 6. A partition $V = V_1 \cup \cdots \cup V_r$ is **equitable** if there are constants b_{ij} (i, $j \in \{1,\dots,r\}$) such that for any i and j in $\{1,\dots,r\}$ (perhaps $i = j$), and any vertex $x \in V_i$, the sum of the weights of the edges from x to vertices in V_j is b_{ij}. (If G is a graph (only positive edges) then b_{ij} is simply the number of neighbours that $x \in V_i$ has in V_j.)

The matrix $B = (b_{ij})$ is called the **quotient matrix** of the equitable partition. We briefly describe any such matrix as 'a quotient matrix'.

In this section we show that quotient matrices are precisely symmetrisable integer matrices (Theorem 2). It is easy to see that quotient matrices are symmetrisable (Lemma 16; this is certainly known for graphs, and the extension to signed graphs is trivial). However, the reverse implication that every symmetrisable integer matrix is in fact a quotient (Lemma 17) requires a little more work (and does not even appear to have been known for graphs).

If the vertices are ordered to reflect an equitable partition of G, then the adjacency matrix A of G has block form

$$A = \begin{pmatrix} A_{11} & A_{12} & \cdots & A_{1r} \\ A_{21} & A_{22} & \cdots & A_{2r} \\ \vdots & \vdots & \ddots & \vdots \\ A_{r1} & A_{r2} & \cdots & A_{rr} \end{pmatrix} \tag{12}$$

where each submatrix A_{ij} has constant row sum b_{ij}.

Since A is symmetric, we have $A_{ji} = A_{ij}^{\mathsf{T}}$, and A_{ii} is always square. If $|V_i| = c_i$, then A_{ij} is a $c_i \times c_j$ matrix. Since $A_{ij} = A_{ji}^{\mathsf{T}}$, each A_{ij} also has constant column sum, namely b_{ji}.

While A is symmetric, has zeros on the diagonal, and has all off-diagonal entries in the set $\{-1,0,1\}$, none of these properties need hold for the quotient matrix (b_{ij}). Certainly the b_{ij} are all integers, but the matrix need not be symmetric, and there are no general bounds on any of the entries.

Recall that if B is a quotient matrix for an equitable partition of a signed graph G with adjacency matrix A then (after permuting rows/columns so that the order of the vertices reflects the partition) A has block structure as in (12) with A_{ij} having constant row sum b_{ij}. If V_i contains c_i vertices, then the sum of all the entries in $A_{ij} = A_{ji}^{\top}$ can be computed either as $c_i b_{ij}$ or as $c_j b_{ji}$:

$$c_i b_{ij} = c_j b_{ji}\,. \tag{13}$$

Comparing with (9) setting $d_i = 1/\sqrt{c_i}$, and using Lemma 10, we see that if B is a quotient matrix then it is symmetrisable. We record this as a Lemma.

Lemma 16. *Let B be the quotient matrix of an equitable partition of a signed graph. Then B is symmetrisable.*

Since quotient matrices are symmetrisable, they must satisfy the sign symmetry condition (7) and the cycle condition (10). We now show that the existence of c_i such that (13) holds is sufficient to imply that B is a quotient matrix.

Lemma 17. *Let $B = (b_{ij})$ be an $r \times r$ integer matrix. If there are positive integers $c_1, \ldots, c_r$ such that* (13) *holds for all $1 \le i,\ j \le r$, then B is the quotient matrix of an equitable partition of a signed graph. If in addition the entries of B are all nonnegative, then B is the quotient matrix of an equitable partition of a graph.*

Proof. Suppose that we have $B = (b_{ij})$ and $c_1, \ldots, c_r$ as in the hypothesis of the lemma. Define

$$M = \prod_{i=1}^{r}(1+|b_{ii}|) \prod_{1\le i,j\le r,\ i\ne j} \max(1,|b_{ij}|)\,. \tag{14}$$

For $1 \le i \le r$, put $c_i' = Mc_i$. We shall define a signed graph G on $n = c_1' + \cdots + c_r'$ vertices which has an equitable partition for which B is the quotient matrix. The construction will be such that if all the b_{ij} are nonnegative then the signed graph is actually a graph.

Take disjoint sets $V_1, \ldots, V_r$ with $|V_i| = c_i'$. The elements of these will be the vertices of G, and we shall now describe how to allocate signed edges so as to achieve our desired equitable partition.

For each i, split V_i (arbitrarily) into subsets of size $1+|b_{ii}|$ (note from (14) that $1+|b_{ii}|$ divides c_i'). Within each subset, put signed edges between every pair of vertices in the subset, all with the same sign $\operatorname{sgn}(b_{ii})$. These will be the only edges between vertices in the same V_i, so the sum of the weights of the edges between any one vertex in V_i and all other vertices in V_i is the constant b_{ii}.

For each $i < j$ for which $b_{ij} \neq 0$, split V_i into subsets $U_{i1}, \ldots, U_{ik}$ of size $|b_{ji}|$. We have $k = c_i'/|b_{ji}| = Mc_i/|b_{ji}| = Mc_j/|b_{ij}| = c_j'/|b_{ij}|$, using (13) (which implies that $b_{ji} \neq 0$ too; and note from (14) that k is a positive integer). Hence with the same k we can split V_j into subsets $W_{j1}, \ldots, W_{jk}$ of size $|b_{ij}|$. For each $1 \leq l \leq k$, we put signed edges, all of sign $\operatorname{sgn}(b_{ij})$, between every vertex in U_{il} and every vertex in W_{jl}. Hence the sum of the weights of the edges between any vertex in V_i and all vertices in V_j is the constant b_{ij}, and the sum of the weights of the edges between any vertex in V_j and all vertices in V_i is the constant b_{ji}.

We have therefore constructed a signed graph G that admits an equitable partition of its vertices as $V_1 \cup \cdots \cup V_r$ such that the quotient matrix is B, and if all entries of B are nonnegative then the construction produces a graph. $\square$

Combining this with Lemma 16 gives Theorem 2: SIMs and quotients of signed graphs are precisely the same objects.

7. The trace problem for symmetrisable matrices

A SIM is called **positive definite** if all its eigenvalues are real and strictly positive. Naturally we speak of a SIM, or a real symmetric matrix, as being **connected** if the associated digraph is connected. For a digraph associated to a real symmetric matrix, the properties of being connected or strongly connected coincide. By sign symmetry, the same is true for the digraphs associated to SIMs.

SIMs admit more possibilities for their characteristic polynomials than do integer symmetric matrices. For example, $x^2 - d$ is the characteristic polynomial of a SIM for any integer $d \geq 0$, whereas $x^2 - d$ is the characteristic polynomial of an integer symmetric matrix if and only if d can be written as a sum of two squares of integers.

In [5] it was shown that if A is a positive definite connected integer $n \times n$ symmetric matrix, then its trace is at least $2n - 1$. We revisit this question in the context of the larger class of characteristic polynomials of SIMs: perhaps we can manage to make the trace smaller. It turns out that we cannot. Moreover if the trace of an $n \times n$ positive definite connected SIM is $2n - 1$, then in fact the matrix must be symmetric. In the asymmetric case, the lower bound on the trace can be improved to $2n$.

Given n, we define a chain of sets of $n \times n$ integer matrices

$$M_0 \supseteq M_1 \supseteq M_2 \supseteq M_2^+$$

by imposing increasingly stringent conditions on the matrices.

- The set M_0 comprises those $n \times n$ integer matrices $A = (a_{ij})$ that satisfy the sign symmetry condition (7).
- M_1 is the set of $n \times n$ SIMs: those matrices in M_0 that additionally satisfy the cycle condition (10).
- We define M_2 to be the subset of M_1 comprising those SIMs that are connected.
- Let M_2^+ be the subset of M_2 comprising the positive definite matrices in M_2.

Thus M_0 is the set of $n \times n$ integer matrices for which the symmetrisation map φ is defined. The set M_1 has been our primary object of study until now, but in this section we switch our focus to M_2^+.

Note that membership of M_0, M_1, or M_2 is completely independent of the values of the diagonal entries: these can be varied freely without affecting whether or not the matrix is in any given M_i. In particular we can add any multiple of the identity matrix without affecting whether or not a matrix is connected, or satisfies either or both of (7) and (10). On the other hand, the diagonal entries certainly affect whether or not a matrix is in M_2^+.

We now define a parallel chain

$$Q_0 \supseteq Q_1 \supseteq Q_2 \supseteq Q_2^+$$

of sets of $n \times n$ matrices whose entries come from the larger set $\sqrt{\mathbb{N}_0}$. All the matrices in $Q_0, \ldots, Q_2^+$ will be symmetric.

- The set Q_0 comprises symmetric $n \times n$ matrices with elements from $\sqrt{\mathbb{N}_0}$ whose diagonal entries are in $\mathbb{Z}$.
- Q_1 is the set of those $B = (b_{ij})$ in Q_0 that satisfy the rational cycle condition (2).

- The set Q_2 comprises those elements of Q_1 that are connected.

- Q_2^+ is the set of those elements of Q_2 that are positive definite.

One easily sees that $\varphi : M_0 \to Q_0$ is surjective, and Proposition 1 says that $\varphi : M_1 \to Q_1$ is surjective. Since φ preserves connectedness and eigenvalues, $\varphi : M_2 \to Q_2$ and $\varphi : M_2^+ \to Q_2^+$ are also surjective.

Our first result in this section is stronger than the statement that any element of Q_2^+ has trace at least $2n-1$, as the hypothesis involves a weakened form of the rational cycle condition.

Proposition 18. *Let $B = (b_{ij})$ be a connected symmetric $n \times n$ matrix with entries in $\sqrt{\mathbb{N}_0}$. Suppose also that B is positive definite, and satisfies the* rational triangle condition *(a special case of the rational cycle condition):*

$$\forall i_1, i_2, i_3 \in \{1, \ldots, n\}, \quad b_{i_1 i_2} b_{i_2 i_3} b_{i_3 i_1} \in \mathbb{Q}. \tag{15}$$

Then $\mathrm{tr}(B) \geq 2n-1$.

In particular, this Proposition applies to all matrices in Q_2^+. Note that by Lemma 15, the condition (15) implies that each diagonal entry is in $\mathbb{Z}$.

Using the symmetrisation map φ that sends each M_i to the corresponding Q_i, we shall deduce Theorem 3.

To help with the proof of Proposition 18, we shall use the following lemma.

Lemma 19. *Suppose that $B = (b_{ij})$ is a connected symmetric positive definite $n \times n$ matrix with entries in $\sqrt{\mathbb{N}_0}$ that satisfies the rational triangle condition* (15). *Let* $\mathbf{e}_1$, *…,* $\mathbf{e}_n$ *be a basis for $\mathbb{R}^n$, and let $\langle \cdot, \cdot \rangle$ be the positive definite symmetric bilinear form defined via $\langle \mathbf{e}_i, \mathbf{e}_j \rangle = b_{ij}$. Define*

$$\mathbf{e}_2' = \mathbf{e}_2 - b_{12}\mathbf{e}_1 \,,$$

and let B' be the matrix of $\langle \cdot, \cdot \rangle$ with respect to the basis $\mathbf{e}_1$, $\mathbf{e}_2'$, $\mathbf{e}_3$, *…,* $\mathbf{e}_n$. *Then:*

- *B' is positive definite;*
- *B' has all entries in $\sqrt{\mathbb{N}_0}$;*
- *B' satisfies the rational triangle condition.*

Before commencing the proof, we define the **core** of a positive integer n, written $\mathrm{core}(n)$ as follows. Write $n = rs^2$ with r square-free. Then $\mathrm{core}(n) = r$.

Proof. The form is positive definite, so B' is positive definite.

The only entries of B' that are not simply copied from B are those in the second row and column. The new diagonal entry is

$$\langle \mathbf{e}_2 - b_{12}\mathbf{e}_1, \mathbf{e}_2 - b_{12}\mathbf{e}_1 \rangle = b_{22} - (2 - b_{11}) b_{12}^2 \in \mathbb{Z}\,. \tag{16}$$

For the new off-diagonal entries b'_{2i} ($i \neq 2$) we have

$$b'_{2i} = b_{2i} - b_{12} b_{1i}\,. \tag{17}$$

The rational triangle condition gives

$$b_{12} b_{2i} b_{i1} \in \mathbb{Q}\,,$$

and hence $\operatorname{core}(b_{2i}^2) = \operatorname{core}(b_{12}^2 b_{i1}^2)$, whence $b'_{2i} \in \sqrt{\mathbb{N}_0}$.

Moreover, either $b'_{2i} = 0$ or $\operatorname{core}(b'_{2i}) = \operatorname{core}(b_{2i})$, and hence B' satisfies the rational triangle condition. $\square$

Proof of Proposition 18. We suppose that $B = (b_{ij})$ is a minimal counterexample to the Proposition, in the following strong sense: B is $n \times n$, symmetric, connected, positive definite, has trace less than $2n-1$, with n minimal, and moreover with the trace minimal for this n. By Lemma 15, each $b_{ij} \in \mathbb{N}$. We have that B has entries in $\sqrt{\mathbb{N}_0}$ and satisfies the rational triangle condition (15). Since B is positive definite, each b_{ii} is strictly positive.

Given $\operatorname{tr}(B) \leq 2n-2$, at least two of the diagonal entries must equal 1. In particular, $n \geq 2$, and we may reorder the rows and columns to achieve $b_{11} = 1$ and $b_{12} \neq 0$.

Let $\mathbf{e}_1, \ldots, \mathbf{e}_n$ be a basis for $\mathbb{R}^n$. The matrix B defines a positive definite symmetric bilinear form $\langle \cdot, \cdot \rangle$ on $\mathbb{R}^n \times \mathbb{R}^n$ via $\langle \mathbf{e}_i, \mathbf{e}_j \rangle = b_{ij}$.

Perform the base change of Lemma 19. By that lemma, the matrix B' of $\langle \cdot, \cdot \rangle$ with respect to this new basis is positive definite, has all entries in $\sqrt{\mathbb{N}_0}$, and satisfies the rational triangle condition. Moreover from (16) we see that the new diagonal entry b'_{22} is strictly smaller than b_{22}, so B' has smaller trace than B.

By our minimality conditions in choosing B, we must have that B' is not connected.

Using B and B' to refer to either the matrix or the corresponding digraph, the only possible changes to edge weights when we move from B to B' are those involving vertex 2. We shall show that every vertex in B' is in the same connected component as one of the vertices 1 or 2, and hence that B' (being disconnected) has exactly two components. The argument here follows that in [5].

Let K_1, K_2 be the components of B' containing vertices 1, 2 respectively. *A priori* we might have $K_1 = K_2$, but once we have shown that every vertex is in either K_1 or K_2 then since B' is not connected these components must be distinct.

Take any $j \in \{3, 4, \ldots, n\}$. Taking language from graph theory, there is a path in B from j to 2 (B is connected). If all of the edges of this path lie in B' then $j \in K_2$. Otherwise, the path in B must finish with an edge from some vertex i to the vertex 2 that is not present in B' (no other edges in the path can involve the vertex 2). Then from (17) we see that $b_{1i} \neq 0$ (else $b'_{2i} = b_{2i} \neq 0$). Then we can follow our path along edges in B' from j as far as i, and from there to 1, to see that $j \in K_1$. Hence, as claimed, B' has exactly two components (and the components K_1 and K_2 must be different).

The matrix of each component is positive definite (since the form is positive definite), and of course each component is connected. If K_1, K_2 have r_1, r_2 vertices respectively ($r_1 + r_2 = n$), and their matrices have traces t_1, t_2 respectively, then (recall that B' has smaller trace than B) $t_1 + t_2 < t < 2n-1$, so $t_1 + t_2 \leq 2(r_1 + r_2) - 3$. Thus either $t_1 < 2r_1 - 1$ or $t_2 < 2r_2 - 1$, and one of the two components would give a counterexample to the Proposition, contradicting our minimality assumptions on B. □

On applying the map φ, the first part of Theorem 3 follows immediately from Proposition 18. If A is a connected symmetrisable matrix that is positive definite, i.e., if $A \in M_2^+$, then $\varphi(A) \in Q_2^+$ has the same trace as A. Being in $Q_2^+ \subseteq Q_1$, $\varphi(A)$ certainly satisfies the rational triangle condition, and the Proposition applies to give $\mathrm{tr}(\varphi(A)) \geq 2n-1$, and hence $\mathrm{tr}(A) \geq 2n-1$.

For the second part of Theorem 3, we need a further lemma.

Lemma 20. *Let S be an $n \times n$ matrix satisfying the hypotheses of Proposition 18. Suppose that* $\mathrm{tr}(S) = 2n-1$ *(the minimal possible trace, given Proposition 18). Then every off-diagonal entry of S is either* -1*,* 0*, or* 1.

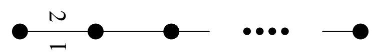
Proof. At least one diagonal entry of $S = (s_{ij})$ is 1, and we may suppose that $s_{11} = 1$. If $n = 1$ then there is nothing to prove. If $n \geq 2$, then vertex 1 is connected to at least one other vertex, which we may suppose is vertex 2: $s_{12} = s_{21} \neq 0$. As in the proof of Proposition 18, we make a change of basis that transforms S to a disconnected matrix $S' = (s'_{ij})$, trace $2n - 1 - s_{12}^2$. As in that proof, one argues that S' has exactly two components, say on r and s vertices ($r + s = n$), and by Proposition 18 these have traces at least $2r-1$ and $2s-1$ respectively. Then $2n-1-s_{12}^2 \geq 2r-1+2s-1 = 2n-2$, so $s_{12} = \pm 1$. Moreover each of the two components of S' has minimal trace for its size. By an inductive argument, each off-diagonal entry of each component of S' has modulus at most 1, and hence the same holds for all off-diagonal entries of S'. Moreover vertices 1 and 2 are in different components of S', so that if $s'_{2i} \neq 0$ then $s'_{1i} = s_{1i} = 0$. Therefore, for $i \neq 2$,

$$s_{2i} = s'_{2i} + s_{12}s_{1i} = \begin{cases} s_{12}s_{1i} & \text{if } s'_{2i} = 0\,, \\ s'_{2i} & \text{if } s'_{2i} = \pm 1\,. \end{cases}$$

We see inductively that all off-diagonal entries of S have modulus at most 1. □

Now we complete the proof of Theorem 3. Suppose that B is an $n \times n$ positive definite connected SIM that has trace $2n-1$. The symmetrisation $S = \varphi(B) = (s_{ij})$ also has trace $2n-1$, and satisfies the hypotheses of Lemma 20. By that lemma, all off-diagonal entries of $\varphi(B)$ are 0, -1, or 1. This implies that the same holds for B itself ($b_{ij}b_{ji} = s_{ij}^2$), which implies that B is symmetric. Hence we get an improved lower bound for the trace in the asymmetric case, namely $2n$, completing the proof of the theorem.

The lower bound of $2n$ in the asymmetric case of Theorem 3 is best-possible. Let B be the adjacency matrix of the weighted digraph



on n vertices. Then $B+2I$ is positive definite, symmetrisable, connected, and has trace $2n$.

We get an immediate corollary concerning possible traces of *minimal* polynomials.

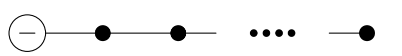
Corollary 21. *Let m be a monic irreducible polynomial with integer coefficients, degree n, and with all roots real and strictly positive. If the trace of m is strictly less than* $2n-1$*, then m is not the minimal polynomial of a SIM, and nor is m the minimal polynomial of any symmetric matrix with entries in* $\sqrt{\mathbb{N}_0}$ *that satisfies the rational cycle condition* (2)*.*

Proof. Let $t < 2n-1$ be the trace of m. If m were the minimal polynomial of a SIM, then it would be the minimal polynomial of its symmetrisation, so we may suppose by way of contradiction that m is the minimal polynomial of a symmetric matrix S with entries in $\sqrt{\mathbb{N}_0}$ that satisfies the rational cycle condition. Since m is irreducible, the characteristic polynomial of S must be m^r for some r. If S is not connected, then m is the minimal polynomial of each component; moving to a component we may suppose that S is connected. Then S has trace rt, and is positive definite. From Theorem 3, $rt \geq 2nr-1 \geq r(2n-1)$, contradicting $t < 2n-1$. □

We can also settle the analogue of the trace problem in our setting, namely Corollary 5.

Proof of Corollary 5. If $B \in M_2^+$, then $\varphi(B) \in Q_2^+$ has the same absolute trace. Conversely, if $S \in Q_2^+$, then by Lemma 1 there is a symmetrisable matrix $B \in M_1$ with $\varphi(B) = S$. Since φ preserves the eigenvalues of symmetrisable matrices, and preserves the underlying graph, $B \in M_2^+$ and has the same absolute trace as S. Thus $X = Y$.

Let A be the adjacency matrix of the n-vertex path with one negatively charged vertex at one end:



One checks that $A+2I$ is positive definite, connected, symmetric (hence symmetrisable), and has absolute trace $2-1/n$, so that 2 is a limit point of X. It will be enough to show that for any $\varepsilon > 0$, only finitely many positive definite connected SIMs have absolute trace below $2-\varepsilon$. Suppose that B is such a SIM. By Theorem 3, n is bounded. The trace is then also bounded, and hence the set of possible diagonals for B is finite. Positive definiteness of each principal 2×2 submatrix then bounds the off-diagonal entries, so there are finitely many possibilities for those too, and we are done. □

One consequence of Theorem 3 is that if a symmetrisable positive definite connected $n \times n$ integer matrix has trace $2n-1$ then it is in fact symmetric. Thus, for example, if A is the matrix in the proof of Corollary 5, and the characteristic polynomial of $A+2I$ is presented as the characteristic polynomial of a positive definite connected SIM B, then B must in fact be symmetric.

The argument in the proof of Theorem 3 is a proof by contradiction, showing that no counterexamples exist. The idea of that proof can be put to constructive use, to generate all examples that have minimal trace from smaller ones. We explore this in the final section of the paper.

8. The structure of minimal-trace examples

We have seen already that an $n \times n$ positive definite connected SIM that has trace $2n-1$ must in fact be symmetric, and moreover all the off-diagonal entries have modulus at most 1. Note that one can have a diagonal entry as large as n:

$$\begin{pmatrix} n & 1 & 1 & 1 & \cdots & 1 \\ 1 & 1 & 0 & 0 & \cdots & 0 \\ 1 & 0 & 1 & 0 & \cdots & 0 \\ 1 & 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 0 & 0 & 0 & \cdots & 1 \end{pmatrix}.$$

We now describe a method to glue together minimal-trace symmetric examples to produce larger minimal-trace symmetric examples. Then we shall show that working up to equivalence all minimal-trace symmetric examples can be produced this way (starting from the trivial 1×1 case).

Suppose that $A = (a_{ij})$ and $B = (b_{ij})$ are positive definite connected integer symmetric matrices, A is $r \times r$ with trace $2r-1$, and B is $s \times s$ with trace $2s-1$. At least one diagonal entry of A must equal 1, and we suppose that $a_{11} = 1$. The construction is asymmetric in A and B, and we do not care whether or not $b_{11} = 1$.

Pick a basis $\mathbf{e}_1, \ldots, \mathbf{e}_r, \mathbf{f}_1, \ldots, \mathbf{f}_s$ for $\mathbb{R}^{r+s}$, and define a symmetric bilinear form

$\langle\cdot,\cdot\rangle$ on $\mathbb{R}^{r+s}\times\mathbb{R}^{r+s}$ via

$$\begin{aligned}
\langle \mathbf{e}_i,\mathbf{e}_j\rangle &= a_{ij}\,, \quad 1\le i\le r,\ 1\le j\le r\,,\\
\langle \mathbf{f}_i,\mathbf{f}_j\rangle &= b_{ij}\,, \quad 1\le i\le s,\ 1\le j\le s\,,\\
\langle \mathbf{e}_i,\mathbf{f}_j\rangle &= 0\,, \quad 1\le i\le r,\ 1\le j\le s\,.
\end{aligned}$$

This bilinear form is positive definite, since the eigenvalues of its matrix with respect to this basis pool those of A and B. The matrix with respect to this basis has trace $2(r+s)-2$, and is not connected: there are two components, corresponding to A and B.

Change basis, replacing $\mathbf{f}_1$ by $\mathbf{f}_1+\mathbf{e}_1$. The matrix $C=(c_{ij})$ of the bilinear form with respect to this new basis is positive definite, and now connected. Most diagonal entries are unchanged, but $\langle \mathbf{f}_1,\mathbf{f}_1\rangle$ has been replaced by

$$\langle \mathbf{f}_1+\mathbf{e}_1,\mathbf{f}_1+\mathbf{e}_1\rangle = \langle \mathbf{f}_1,\mathbf{f}_1\rangle + 1\,.$$

Hence C has trace $2(r+s)-1$, and is another minimal-trace example.

We give a gory description of the entries of $C=(c_{ij})$, as it will be convenient later to indicate which small details change as we vary the construction.

$$c_{ij} = \begin{cases}
a_{ij} & 1\le i\le r,\ 1\le j\le s\,,\\
b_{i-r,j-r} & r+1\le i\le r+s,\ r+1\le j\le r+s,\\
 & (i,j)\neq(r+1,r+1)\,,\\
b_{r+1,r+1}+1 & i=r+1,\ j=r+1\,,\\
a_{1,j} & i=r+1,\ 1\le j\le r\,,\\
a_{i,1} & 1\le i\le r,\ j=r+1\,,\\
0 & \text{otherwise.}
\end{cases} \tag{18}$$

Now we claim that every minimal-trace example that has at least two rows can be grown in this way (working up to equivalence: Definition 4). Suppose that $C=(c_{ij})$ is an $n\times n$ positive definite connected integer *symmetric* matrix, having trace $2n-1$, and $n\ge 2$. We may assume that $c_{11}=1$, and that $c_{12}\neq 0$, indeed by our bound on off-diagonal entries we may assume that $c_{12} = \pm 1$. Working up to equivalence we may assume that $c_{12} = 1$. Performing the change of basis idea in the proof of Proposition 18, we produce a new matrix with two components A and B. To comply with the trace bound of Theorem 3, A and B both have minimal trace for their size. Then, after shuffling rows, C is formed from A and B by our growing construction above.

The asymmetric case is more delicate. Let $C = (c_{ij})$ be an $n \times n$ positive definite connected SIM that is *not* symmetric, and has trace $2n$ (necessarily $n \geq 2$).

We can no longer assume that there is a diagonal entry equal to 1, and deal first with the special case where every diagonal entry equals 2. Take two vertices in the digraph corresponding to C that are as far apart as possible in terms of the minimal length of a path between them. Unless $n = 2$, deleting a suitable choice of one of these vertices will leave a subgraph that is not only connected but remains asymmetric (if there is only one asymmetric edge it must be an isthmus, by the cycle condition). The matrix corresponding to this subgraph is connected, positive definite, and has minimal trace in this asymmetric case (all diagonal entries equal 2). Hence, working up to equivalence, we can 'grow' all minimal-trace examples in this subcase from smaller ones, starting from the 2×2 cases

$$\begin{pmatrix} 2 & 2 \\ 1 & 2 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} 2 & 3 \\ 1 & 2 \end{pmatrix},$$

or their transposes.

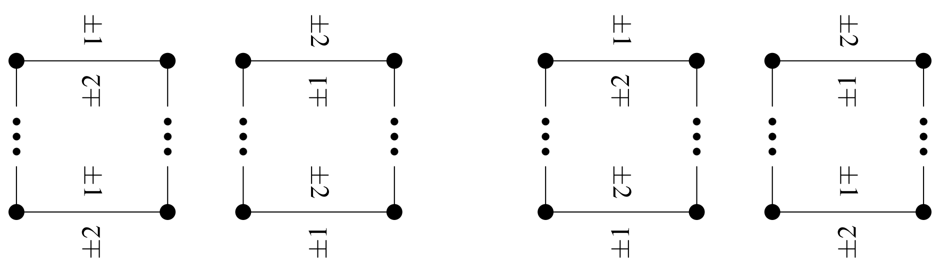
Now consider the case where C has some diagonal entry equal to 1. Working up to equivalence, we may assume that $c_{11} = 1$ and $c_{12} > 0$. Let $S = (s_{ij})$ be the symmetrisation of C. Performing the basis change of the proof of Proposition 18, the matrix S changes to S', where $\mathrm{tr}(S') < \mathrm{tr}(S)$. The argument in the proof of that Proposition shows that S' has at most two components, and there are two possibilities: $\mathrm{tr}(S') = 2n-2$ or $\mathrm{tr}(S') = 2n-1$.

If $\mathrm{tr}(S') = 2n-2$, then it is not connected and must decompose into exactly two components, say A $(r \times r)$ and B $(s \times s)$, where $\mathrm{tr}(A) = 2r-1$, $\mathrm{tr}(B) = 2s-1$. Then A and B are symmetric minimal-trace examples (the last part of Theorem 3). We have in this case that $s_{12} = \sqrt{2}$ (since $\mathrm{tr}(S') = \mathrm{tr}(S) - 2$ and $\mathrm{sgn}(s_{12}) = \mathrm{sgn}(c_{12})$). After permuting, we see that S is built from A and B in essentially the same way as in our symmetric construction (18), but with

$$s_{ij} = \begin{cases} b_{r+1,r+1} + 2 & i = r+1,\ j = r+1\,, \\ a_{1,j}\sqrt{2} & i = r+1,\ 1 \le j \le r\,, \\ a_{i,1}\sqrt{2} & 1 \le i \le r,\ j = r+1\,. \end{cases} \tag{19}$$

Note the factors of $\sqrt{2}$ (the change of basis here is to replace $\mathbf{f}_1$ by $\mathbf{f}_1 + \sqrt{2}\mathbf{e}_1$), and the addition of 2 to the $(r+1, r+1)$ diagonal entry rather than 1. We need to recover C from its symmetrisation S. The subgraph corresponding to A must be symmetric, by its trace, and similarly for B (adjusting the special diagonal entry does not break the symmetry). Thus the only asymmetry comes in the $(r+1)$th row and column. Here we have $c_{i,r+1}c_{r+1,i} = s_{i,r+1}^2 = 2a_{i,r+1}^2$, which is either 0 or 2. If 2, then we need to choose which of $c_{i,r+1}$ and $c_{r+1,i}$ is $2\,\mathrm{sgn}(s_{i,r+1})$ and which is $\mathrm{sgn}(s_{i,r+1})$. Since A and B are symmetric, we must either always put the factor of 2 in the row, or always in the column, to satisfy the cycle condition (10):

vertical paths are symmetric; horizontal edges have sign symmetry



these satisfy the cycle condition these fail the cycle condition

Hence the values for c_{ij} are as for s_{ij} in (19) except for

$$c_{ij} = \begin{cases} 2a_{1,j} & i = r+1,\ 1 \le j \le r\,, \\ a_{i,1} & 1 \le i \le r,\ j = r+1\,, \end{cases}$$

or the transpose of this.

If $\mathrm{tr}(S') = 2n-1$, then $s_{12} = 1$. Note that *a priori* S' might be connected in this case. But if so, then being minimal trace all off-diagonal entries would have modulus at most 1, so would equal 0, 1 or -1, and reversing the change of basis would produce the same conclusion for S (as in the proof of Lemma 20), implying that C was symmetric, which it is not. So we still must have S' falling into two components, say A' $(r \times r)$ and B' $(s \times s)$, with the first vertex of S' corresponding to the first vertex of A'. Let A and B be the subgraphs of C corresponding to A', B' respectively. We permute rows/vertex labels so that the first r rows of C correspond to A (and with $a_{11} = 1$) and the final s rows correspond to B. Our challenge is to complete the first r entries in row $r+1$ and column $r+1$. There are two subcases: $\mathrm{tr}(A') = 2r-1$, $\mathrm{tr}(B') = 2s$, or $\mathrm{tr}(A') = 2r$, $\mathrm{tr}(B') = 2s-1$.

If $\mathrm{tr}(A') = 2r-1$, then A must be symmetric, and the formula for C is as in (18). (Here B must be asymmetric, else C would be symmetric.)

If $\mathrm{tr}(A') = 2r$, then it is a minimal-trace asymmetric example with a 1 on the diagonal. We have a formula analogous to (18) for the s_{ij}, and in particular

$$s_{r+1,i} = s_{1,i}\ (1 \le i \le r), \quad s_{i,r+1} = s_{i,1}\ (1 \le i \le r). \tag{20}$$

For $1 \le i \le r$ we have $c_{r+1,i}c_{i,r+1} = s_{1,i}s_{i,1} = s_{1,i}^2$, which is known, and the signs of the $c_{i,j}$ are all known, but in the asymmetric case this formula does not tell us how the factors of $s_{1,i}^2$ are to be shared between $c_{r+1,i}$ and $c_{i,r+1}$. The cycle condition for C for the triangle 1, i, $r+1$ gives

$$c_{1,i}c_{i,r+1}c_{r+1,1} = c_{i,1}c_{r+1,i}c_{1,r+1}\,,$$

which with $c_{1,r+1} = c_{r+1,1} = 1$ gives $c_{1,i}c_{i,r+1} = c_{i,1}c_{r+1,i}$. Together with (20) and sign symmetry, we find that $c_{r+1,i} = c_{1,i} = a_{1,i}$ and $c_{i,r+1} = c_{i,1} = a_{i,1}$ $(1 \le i \le r)$, so that (18) holds in this case too.

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