Electronic Journal of Linear Algebra, ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 39, pp. 154-163, April 2023.

CENTERED PSD MATRICES WITH THIN SPECTRUM ARE M-MATRICES*

KAREL DEVRIENDT†

Abstract. We show that real, symmetric, centered (zero row sum) positive semidefinite matrices of order n and rank $n-1$ with eigenvalue ratio $\lambda_{\max}/\lambda_{\min} \leq n/(n-2)$ between the largest and smallest nonzero eigenvalue have nonpositive off-diagonal entries, and that this eigenvalue criterion is tight. The result is relevant in the context of matrix theory and inverse eigenvalue problems, and we discuss an application to Laplacian matrices.

Key words. Inverse eigenvalue problem, Laplacian matrix, Nonnegative matrices.

AMS subject classifications. 15A29, 15A42, 15B35.

1. Introduction. A central theme in linear algebra and matrix theory is to understand how certain structures of matrices are reflected in their spectra and vice versa. This is perhaps most clearly manifested in the multitude of inverse eigenvalue problems (IEPs) [3, 5] which ask to specify the conditions that a list σ of real numbers with possible repeats (i.e. a multiset) must satisfy such that they can be the spectrum of a matrix with some given structure X – both necessary and sufficient conditions are widely studied. Here, X can for instance prescribe a specific pattern for the matrix entries (e.g. Toeplitz, circulant, or tridiagonal), restrict the sign of the entries (e.g. everywhere nonnegative, positive diagonal or nonpositive off-diagonal), or be a combination of such requirements.

As the main result of this article, we show that if a centered positive semidefinite real, symmetric, centered (zero row sum), and positive semidefinite matrix satisfies a spectral property which we will call "thin spectrum", then this guarantees that the matrix has nonpositive off-diagonal entries; in other words, that it is an M-matrix. We furthermore show how to interpret our result in the context of Laplacian matrices of graphs, where the sign property has a natural meaning as positive edge weights.

The article is organized as follows: Section 2 introduces the relevant class of matrices, states the main result, Theorem 2.2, and provides a brief discussion of the implications. Section 3 describes an application to Laplacian matrices and an application to the inverse singular M-matrix problem. Section 4 finally proves the main result, and Section 5 concludes the article with a brief summary.

2. Main result and discussion. We fix an integer $n \geq 3$ throughout the article and consider real symmetric $n \times n$ (order n) matrices A which are

- positive semidefinite (PSD): all eigenvalues of A are real and nonnegative
- centered: the row and column sums of A equal zero
- have rank $n-1$: all but one eigenvalues are zero

We remark that positive semidefinite also implies that A is symmetric. To be concise, we will call a matrix

*Received by the editors on March 26, 2022. Accepted for publication on March 23, 2023. Handling Editor: K.C. Sivakumar. Corresponding Author: Karel Devriendt.

†Mathematical Institute, University of Oxford, Oxford UK and Alan Turing Institute, London, UK (karel.devriendt@mis.mpg.de).

Electronic Journal of Linear Algebra, ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 39, pp. 154-163, April 2023.

with these properties "a centered PSD_n^{n-1} matrix," where the sub and superscript indicate the order and rank of the matrix and where we leave the real entries and symmetry implicit. Alternatively, one might use "centered corank 1 PSD matrix."

Since A is PSD, it has nonnegative real eigenvalues $\{\lambda_i\}_{i=1}^n$ and can be diagonalized by an orthonormal set of eigenvectors. Being centered furthermore means that $Au = 0$ with all-one vector $u = (1, \dots, 1)^T$ and thus that A has at least one zero eigenvalue and that u is in the zero eigenspace. Moreover, since $\mathrm{rank}(A) = n - 1$ this is the only zero eigenvalue and u spans the kernel of A. We may thus order the eigenvalues as $0 = \lambda_1 < \lambda_2 \leq \cdots \leq \lambda_n$ and introduce

$$\lambda_{\min} := \lambda_2 = \min\{\lambda_i : 1 \leq i \leq n, \lambda_i \neq 0\}, \quad \lambda_{\max} := \lambda_n = \max\{\lambda_i : i \leq 1 \leq n\}.$$

Since $n \geq 3$, both $\lambda_{\min}$ and $\lambda_{\max}$ are positive, and we can consider the ratio $\lambda_{\max}/\lambda_{\min}$ which can be thought of as the condition number of A for pseudoinversion (i.e. inversion in $\ker(A)^\perp$). We define the following eigenvalue property:

Definition 2.1 (Thin spectrum). *A centered PSD $_n^{n-1}$ matrix has a thin spectrum (is spectrally thin) if $\lambda_{\max}/\lambda_{\min} \leq n/(n-2)$.*

Roughly speaking, the thin spectrum condition says that the eigenvalues of a matrix must be of the same order. For n large, we find that the ratio tends to $n/(n-2) \approx 1 + \frac{2}{n}$. $\lambda_{\max}/\lambda_{\min} \approx 1 + \frac{2}{n}$.

We are now ready to state the main result of this article which will be proven in Section 4 after a brief discussion of the Theorem in the remainder of this section.

Theorem 2.2. *All real, symmetric, centered, positive semidefinite matrices of order n and rank $n-1$ and $\lambda_{\max}/\lambda_{\min} \leq n/(n-2)$ have nonpositive off-diagonal entries. The eigenvalue ratio criterion is tight.*

A matrix with nonpositive off-diagonal entries is also called a Z-matrix and a Z-matrix with nonnegative eigenvalues (or nonnegative real parts of eigenvalues) is called an M-matrix [2]. Theorem 2.2 can be thus be summarized more succinctly as "*centered PSD_n^{n-1} matrices with thin spectrum are M-matrices.*" The eigenvalue criterion being tight means that there exists at least one centered PSD_n^{n-1} matrix with eigenvalue ratio $\lambda_{\max}/\lambda_{\min} > n/(n-2)$ which has positive off-diagonal entries. In the proof of Theorem 2.2, we explicitly construct such an example.

While not necessarily formulated as such, Theorem 2.2 gives a "spectral recipe" to construct a subclass of M-matrices: the matrix

$$\sum_{k=1}^{n-1} \lambda_k z_k z_k^T \text{ with } \{z_k\}_{k=1}^{n-1} \text{ an orthonormal basis for } \mathrm{span}(u)^\perp, \text{ and } \lambda_k > 0 \text{ and } \lambda_{\max}/\lambda_{\min} \leq n/(n-2),$$

has nonpositive off-diagonal entries. A second construction starts from a given centered PSD_n^{n-1} matrix A with thin spectrum. In this case, the matrix OAO^T with O any orthogonal matrix ($O^TO = I$) that satisfies $Ou = u$ (u-invariant) is again a centered PSD_n^{n-1} matrix with thin spectrum and thus an M-matrix. In terms of the spectral decomposition above, this corresponds to the orthogonal transformation of the eigenvectors $\{z_k\}_{k=1}^n$ of A by O. We note two further observations.

Remark 2.3. If $\lambda_{\max}/\lambda_{\min} \leq n/(n-2)$, then also $(1/\lambda)_{\max}/(1/\lambda)_{\min} = (1/\lambda_{\min})/(1/\lambda_{\max}) = \lambda_{\max}/\lambda_{\min} \leq n/(n-2)$. Consequently, the Moore–Penrose pseudoinverse – which is obtained by inverting all nonzero eigenvalues – of a centered PSD_n^{n-1} matrix with thin spectrum is again a centered PSD_n^{n-1} matrix with thin

Electronic Journal of Linear Algebra, ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 39, pp. 154-163, April 2023.

spectrum, and thus an M-matrix. In other words, this is a class of matrices where the M-matrix property is invariant under Moore–Penrose pseudoinversion. We note that the Moore–Penrose pseudoinverse of a real symmetric matrix corresponds to the group inverse of the matrix [11, Sec. 2.4].

Remark 2.4. Let $f(A)$ be a function of a centered PSD_n^{n-1} matrix determined by a function $f:\mathbb{R}^+\to\mathbb{R}^+$ acting on its nonzero eigenvalues. If this function satisfies $f(a)/f(b)<a/b$ for all $a>b$, then the matrix sequence $A, f(A), f^2(A),\dots$ will have a decreasing eigenvalue ratio which eventually will result in a thin spectrum. By Theorem 2.2, this means that the matrix sequence $(f^k(A))_{k\in\mathbb{N}}$ will eventually have all off-diagonal entries nonpositive. An example is the function $f:x\mapsto x^\alpha$ for $\alpha\in(0,1)$ or $\alpha\in(-1,-\infty)$.

Remark 2.5. As n grows large, the matrices with a thin spectrum make up a vanishingly small fraction of all centered PSD_n^{n-1} matrices. Let $\lambda_n=1$ be fixed, then the centered PSD_n^{n-1} matrices are determined by sequences of eigenvalues $0<\lambda_2\le\cdots\le\lambda_{n-1}\le 1$, while the eigenvalues of the centered PSD_n^{n-1} matrices are determined by $1-\frac{2}{n}\le\lambda_2\le\cdots\le\lambda_{n-1}\le 1$. These sets of possible eigenvalues form $(n-2)$-dimensional simplices[1] in $\mathbb{R}^n$, with vertices $(0,0,\dots,0,1),(0,0,\dots,1,1),\dots,(0,1,\dots,1,1)$ in the general case and vertices $(0,1-\frac{2}{n},\dots,1-\frac{2}{n},1),(0,1-\frac{2}{n},\dots,1,1),\dots,(0,1,\dots,1,1)$ in the thin spectrum case. In particular, these two simplices are congruent with scale factor $2/n$. As a result, the volume ratio between the two $(n-2)$-dimensional simplices, which equals the fraction of centered PSD_n^{n-1} matrices that have a thin spectrum, is $\left(\frac{2}{n}\right)^{n-2}$. The fraction of spectrally thin matrices thus tends to zero exponentially fast with increasing order.

3. Application to Laplacian matrices. A *weighted graph* $G=(V,E,c)$ consists of a set of $n<\infty$ vertices V and a set of edges E which connect (unordered, distinct) pairs of vertices, and positive weights $c:E\to\mathbb{R}^+$ defined on the edges; we write $\{i,j\}\in E$ for an edge between i and j, and c_{ij} for its weight. One approach to study graphs is to represent their structure in a matrix and then try to understand properties of the graphs through the lens of linear algebra or matrix theory; this approach is called algebraic/spectral graph theory, see for instance [6]. One of the best studied examples is the *Laplacian matrix* of a graph G, which is the $n\times n$ matrix Q with entries

$$(Q)_{ij}=\begin{cases}k_i & \text{if } j=i\\ -c_{ij} & \text{if } \{i,j\}\in E\\ 0 & \text{otherwise,}\end{cases}\tag{3.1}$$

where $k_i=\sum_{(i,j)\in E}c_{ij}$ is the *weighted degree* of a vertex i. From its definition, the Laplacian is real, symmetric, and centered, and it furthermore holds[2] that Q is PSD and has $\mathrm{rank}(Q)=n-1$ if G is connected [6, 8]. However, as shown in [8], these properties alone are not enough to guarantee that the off-diagonal entries of Q are nonnegative (corresponding to positive edge weights). Instead, a necessary and sufficient condition is "centered + PSD_n^{n-1} + nonpositive off-diagonal," but this characterization involves both spectral and nonspectral information. Theorem 2.2 implies a new sufficient and exclusively spectral condition: "centered + PSD_n^{n-1} + thin spectrum $\Rightarrow$ Laplacian." Following the introduced terminology, we can call these Laplacians "spectrally thin." These spectrally thin Laplacians are similar to the Laplacian of the complete graph $Q_K=nI-uu^T$, which has one eigenvalue equal to 0 and all others equal to n, and thus $\lambda_{\max}/\lambda_{\min}=1$.

[1] For simplicity, we ignore the fact that these should be open sets in the case of general centered PSD_n^{n-1} matrices (where $\lambda_1>0$ is strict). The inclusion of these faces does not change the volume of the simplex and thus does not affect the ratio we are interested in.

[2] A quick proof follows by the decomposition $Q=\sum_{(i,j)\in E}c_{ij}(e_i-e_j)(e_i-e_j)^T$ as a sum of PSD matrices which is again PSD.

Electronic Journal of Linear Algebra, ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 39, pp. 154-163, April 2023.

In terms of applications, we may consider spectral perturbations of a Laplacian matrix: assume that the eigenvalues $\{\lambda_k\}_{k=1}^{n-1}$ of a given Laplacian Q are perturbed as $\{\lambda_k+\epsilon_k\}_{k=1}^{n-1}$ (i.e. with the zero eigenvalue of Q unperturbed); this can be for instance due to approximation errors when calculating the eigenvalues, or finite precision errors when storing or representing the eigenvalues on a computer. From Theorem 2.2, we then know that if $\epsilon_{\max}/\epsilon_{\min} \leq n/(n-2)$ then the resulting matrix with the same eigenvectors but perturbed eigenvalues will still have nonpositive off-diagonal entries (and thus will still be Laplacian), while if this ratio is larger we may have positive off-diagonal entries; indeed this follows from

$$\sum_{k=1}^{n-1}(\lambda_k+\epsilon_k)z_kz_k^T = \sum_{k=1}^{n-1}\lambda_k z_k z_k^T + \sum_{k=1}^{n-1}\epsilon_k z_k z_k^T = Q + Q_\epsilon,$$

where Q is the unperturbed Laplacian and Q_ϵ is a Laplacian following Theorem 2.2. We note one further observation.

Remark 3.1. Following the observation in Section 2 that the centered, PSD_n^{n-1} and thin spectrum properties are invariant with respect to u-invariant orthogonal transformations, Theorem 2.2 may be used to formulate a continuous set of Laplacian matrices: $\mathcal{Q}_O = \{OQO^T : O \text{ is orthogonal, } u\text{-invariant}\}$ where the "base" Laplacian Q is spectrally thin.

3.1. Application to the inverse singular M-matrix problem. We recall that an M-matrix is a matrix with nonpositive off-diagonal entries and with eigenvalues with nonnegative real parts. In the symmetric case, these are PSD matrices with nonpositive off-diagonal entries. One property of nonsingular M matrices is that their inverse has nonnegative entries [2, Ch. 6]; for singular M matrices, this has raised the analogous question "*when is the Moore–Penrose pseudoinverse of a singular M-matrix again a singular M-matrix?*" [7], [11, Question 3.3.8]. Making use of the fact that the Laplacian matrix of a graph is an M-matrix, this problem was studied for weighted trees in [10], for distance-regular graphs in [4] and for path graphs in [1].

Following Following Remark 2.3 in Section 2, we know that the Moore–Penrose pseudoinverse of a spectrally thin Laplacian matrix is again a Laplacian (i.e. with nonpositive off-diagonal entries). This means that Theorem 2.2 can be used to construct some examples of singular M matrices whose Moore–Penrose pseudoinverse is again an M-matrix, based on some simple graphs with known spectrum; the following examples were suggested by an anonymous referee:

Example 3.2 (Complete graph). The complete graph is the graph on n vertices, where every pair of vertices is connected by an edge. The Laplacian spectrum of the complete graph is $\{0^{(1)}, n^{(n-1)}\}$ where the superscripts indicate multiplicity. Since $\lambda_{\max}/\lambda_{\min} = 1 < n/(n-2)$ for all $n \geq 2$, it follows that the Moore–Penrose pseudoinverse of the complete graph Laplacian is again a Laplacian matrix (and thus a singular M-matrix). This result is also easily obtained by noticing that the Moore–Penrose pseudoinverse of the complete graph Laplacian amounts to rescaling the Laplacian by n^{-2}.

Example 3.3 (Star graph). The star graph consists of a distinguished central vertex which is connected to all other vertices, and no edges otherwise. The Laplacian spectrum of the star graph on n vertices is $\{0^{(1)}, 1^{(n-2)}, n^{(1)}\}$. Since $\lambda_{\max}/\lambda_{\min} = n$, the star graph Laplacian is spectrally thin if and only if $n \leq 3$. Applying Theorem 2.2 thus says that the Moore–Penrose pseudoinverse of the Laplacian of the star graph on 3 vertices is again a Laplacian. In [10], Kirkland and Neumann show that the Moore–Penrose pseudoinverse Laplacian of a star graph on n vertices is an M-matrix for any n. This illustrates that Theorem 2.2 generally only provides sufficient criteria.

Electronic Journal of Linear Algebra, ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 39, pp. 154-163, April 2023.

Example 3.4 (Path graph). The path graph consists of n vertices that can be labeled $1, 2, \ldots, n$ such that all consecutive vertices are connected by an edge as $E = \bigcup_{i=1}^{n-1}\{i, i+1\}$. The Laplacian spectrum of the path graph is $\left\{2\left(1-\cos\left(\frac{k\pi}{n}\right)\right)\right\}_{k=0}^{n-1}$. Since $\lambda_{\max}/\lambda_{\min} = (1+\cos(\pi/n))/(1-\cos(\pi/n))$, the Laplacian of the path graph is spectrally thin if and only if $n \leq 3$. We note that for $n \leq 3$, the path graph corresponds to the star graph, and we thus have the same result as Example 3.3.

4. Proof of main result, Theorem 2.2. We exclude order $n = 1, 2$ from the Theorem because in these cases the eigenvalue ratio $\lambda_{\max}/\lambda_{\min}$ is not well defined or the statement is satisfied trivially. For $n = 1, 2$, we find that centered PSD_n^{n-1} matrices satisfy the sign property "automatically": for $n = 1$, the only centered PSD_n^{n-1} matrix is $A = 0$ which has no off-diagonal entries and for $n = 2$, all centered PSD_n^{n-1} matrices can be parametrized as:

$$M = \begin{pmatrix} \mu & -\mu \\ -\mu & \mu \end{pmatrix} \text{ with } \mu \geq 0,$$

which has nonpositive off-diagonals $-\mu$.

We now continue with the main result where $n \geq 3$. Let A be a centered PSD_n^{n-1} matrix with $\lambda_{\min}/\lambda_{\max} \leq n/(n-2)$. We can write the off-diagonal entries of A as $(A)_{ij} = e_i^T A e_j$ for $i \neq j$ and where e_i is the i^{th} unit vector, with entries $(e_i)_k = 1$ if $k = i$ and zeroes otherwise. Since A is centered and thus $Au = 0$, we can also write this as:

$$(A)_{ij} = v^T A w \text{ with } v := (e_i - u/n) \text{ and } w := (e_j - u/n),$$

where v and w are now vectors orthogonal to the constant vector u. Next, we normalize these vectors as:

$$\frac{(A)_{ij}}{\|v\|.\|w\|} = \tilde{v}^T A \tilde{w} \text{ with } \tilde{v} := v/\|v\| \text{ and } \tilde{w} := w/\|w\|,$$

where the norms equal $\|v\| = \|w\| = \sqrt{1-1/n}$. Next, we decompose the vector $\tilde{w}$ into a component parallel to $\tilde{v}$ and some orthogonal component $\tilde{v}_\perp$, that is, which satisfies $\tilde{v}^T\tilde{v}_\perp = 0$ and which is normalized as $\tilde{v}_\perp^T\tilde{v} = 1$. We thus write

$$\frac{(A)_{ij}}{\|v\|^2} = \alpha\tilde{v}^T A\tilde{v} + \beta\tilde{v}^T A\tilde{v}_\perp \text{ with } \tilde{w} = \alpha\tilde{v} + \beta\tilde{v}_\perp,$$

for some scalars α, β, which can be calculated as:

$$\left.\begin{array}{l} \tilde{w}^T\tilde{v} = \frac{(e_i-u/n)^T(e_j-u/n)}{\|v\|.\|w\|} \\ \tilde{w}^T\tilde{v} = \alpha \end{array}\right\} \Rightarrow \alpha = -1/(n-1)$$

$$\left.\begin{array}{l} \tilde{w}^T\tilde{w} = 1 \\ \tilde{w}^T\tilde{w} = \alpha^2 + \beta^2 \end{array}\right\} \Rightarrow \beta = \sqrt{n(n-2)}/(n-1).$$

We remark that $\alpha < 0$ and that since we can always swap $\tilde{v}_\perp$ with $(-\tilde{v}_\perp)$, we can assume $\beta > 0$. Dividing both sides by $|\alpha| = 1/(n-1)$ and using $\|v\|^2 = (n-1)/n$ we then find

$$n(A)_{ij} = -\tilde{v}^T A\tilde{v} + \gamma\tilde{v}^T A\tilde{v}_\perp \text{ with } \gamma := \sqrt{n(n-2)}. \tag{4.2}$$

At this point, we may introduce the eigendecomposition of A – which, we recall, is a centered PSD_n^{n-1} matrix – as:

$$A = \sum_{k=1}^{n-1} \lambda_k z_k z_k^T + 0.uu^T/n,$$

Electronic Journal of Linear Algebra, ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 39, pp. 154-163, April 2023.

where the $(n-1)$ eigenvalues λ_k are positive and where the eigenvectors $\{z_k\}_{k=1}^{n-1}$ determine an orthonormal basis of $\operatorname{span}(u)^\perp$. We can rewrite (4.2) using this eigendecomposition as:

$$n(A)_{ij} = \sum_{k=1}^{n-1} \lambda_k[-(x_k)^2 + \gamma x_k y_k] \text{ where } x_k := z_k^T \tilde{v},\ y_k := z_k^T \tilde{v}_\perp,$$

In other words, x_k and y_k are the projections of $\tilde{v}$ and $\tilde{v}_\perp$ onto z_k, respectively. As both $\tilde{v}$ and $\tilde{v}_\perp$ are orthogonal to u, the transformation $\tilde{v} \to x = (x_1, \dots, x_{n-1})^T$ and $\tilde{v}_\perp \to y = (y_1, \dots, y_{n-1})^T$ is a change of basis (orthogonal transformation) which retains the vector *norms* $\|\tilde{v}\|^2, \|\tilde{v}_\perp\|^2 = 1 \Rightarrow \|x\|^2, \|y\|^2 = 1$, as well as the *angles* between vectors, that is, $\tilde{v}^T \tilde{v}_\perp = 0 \Rightarrow x^T y = 0$. Next, we split the sum on the right-hand side in two terms as:

$$\begin{gathered} n(A)_{ij} = \sum_{k \in K^+} \lambda_k[-(x_k)^2 + \gamma x_k y_k] + \sum_{k \in K^-} \lambda_k[-(x_k)^2 + \gamma x_k y_k] \\ \text{where } \begin{cases} K^+ := \{k : -(x_k)^2 + \gamma x_k y_k > 0\} \\ K^- := \{k : -(x_k)^2 + \gamma x_k y_k \leq 0\}. \end{cases} \end{gathered}$$

We remark that the normalization of x and $x^T y = 0$ means that

$$\sum_{k \in K^+} (x_k)^2 + \sum_{k \in K^-} (x_k)^2 = 1 \quad \text{and} \quad \sum_{k \in K^+} x_k y_k + \sum_{k \in K^-} x_k y_k = 0. \tag{4.3}$$

Since we now know the sign of each term involving the nonzero eigenvalues, we can upper-bound the right-hand side using the largest and smallest nonzero eigenvalues $\lambda_{\max}, \lambda_{\min}$ as:

$$\begin{aligned} n(A)_{ij} &\leq \lambda_{\max} \sum_{k \in K^+} [-(x_k)^2 + \gamma x_k y_k] + \lambda_{\min} \sum_{k \in K^-} [-(x_k)^2 + \gamma x_k y_k] \\ &= (\lambda_{\max} - \lambda_{\min}) \sum_{k \in K^+} [-(x_k)^2 + \gamma x_k y_k] - \lambda_{\min} \text{ (invoking (4.3))}. \end{aligned} \tag{4.4}$$

We remark that we can always find a bound of this form because $\operatorname{rank}(A) \geq 2$. Since $(\mu_{\max} - \mu_{\min}) \geq 0$, we can further upper-bound this expression by finding an upper-bound for its associated factor. We consider the following optimization problem:

$$\begin{aligned} &\max_{x, y \in \mathbb{R}^{n-1}} \sum_{k \in K} [-(x_k)^2 + \gamma x_k y_k] \\ &\text{subj. to } \|x\|^2 = \|y\|^2 = 1 \text{ and } x^T y = 0, \end{aligned} \tag{4.5}$$

for some subset $K \subseteq [1, n]$ of the vector indices, where we recall that $\gamma = \sqrt{n(n-2)}$ is some positive number. Writing the vectors in block-form as $x = (a, b)^T$ and $y = (c, d)^T$ with $a, c \in \mathbb{R}^{|K|}$ and $b, d \in \mathbb{R}^{n-1-|K|}$ translates the problem to

$$\begin{aligned} &\max_{a,b,c,d} \{-\|a\|^2 + \gamma a^T c\} \\ &\text{subj. to } \|a\|^2 + \|b\|^2 = 1 \\ &\qquad\quad \|c\|^2 + \|d\|^2 = 1 \\ &\qquad\quad a^T c + b^T d = 0. \end{aligned} \tag{4.6}$$

Electronic Journal of Linear Algebra, ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 39, pp. 154-163, April 2023.

If we isolate the variable c, we can consider the problem:

$$\begin{aligned}&\max_c\{-\|a\|^2+\gamma a^Tc\}\\&\text{subj. to } \|c\|^2+\|d\|^2=1 \text{ and } a^Tc=-b^Td.\end{aligned}$$

where a,b,d are then simply fixed constants. From the Lagrangian function

$$\mathcal{L}(c,\ell_1,\ell_2)=-\|a\|^2+\gamma a^Tc+\ell_1(\|c\|^2+\|d\|^2-1)+\ell_2(a^Tc+b^Td),$$

with Lagrangian multipliers ℓ_1,ℓ_2, we find the optimality criteria:

$$\begin{cases}\frac{d\mathcal{L}}{dc}=0\Leftrightarrow \ell_1c=(1+\gamma)a\\ \frac{d\mathcal{L}}{d\ell_1}=0\Leftrightarrow \|c\|^2+\|d\|^2=1\\ \frac{d\mathcal{L}}{d\ell_2}=0\Leftrightarrow a^Tc=-b^Td.\end{cases}\Leftrightarrow\begin{cases}c=\ell a \text{ for some scalar } \ell\\ \ell^2\|a\|^2+\|d\|^2=1\\ \ell\|a\|^2=-(b^Td)\end{cases}\Leftrightarrow\begin{cases}c=\ell a\\ \|a\|^2(1-\|d\|^2)=(b^Td)^2.\end{cases}$$

We may then rewrite the original optimization problem (4.6) using $a^Tc=-b^Td$ to eliminate c from the objective function and replacing the two equality constraints involving c by their equivalent $\|a\|^2(1-\|d\|^2)=(b^Td)^2$ to eliminate c from the constraints. This yields

$$\begin{aligned}&\max_{a,b,d}\{-\|a\|^2-\gamma b^Td\}\\&\text{subj. to } \|a\|^2+\|b\|^2=1 \text{ and } \|a\|^2(1-\|d\|^2)=(b^Td)^2.\end{aligned}\tag{4.7}$$

Using the same approach, we can isolate variable b and obtain the problem:

$$\begin{aligned}&\max_b\{-\|a\|^2-\gamma b^Td\}\\&\text{subj. to } \|a\|^2+\|b\|^2=1 \text{ and } \|a\|^2(1-\|d\|^2)=(b^Td)^2.\end{aligned}$$

The same approach using Lagrangian multipliers yields that $b=\theta d$ for some scalar θ which, introduced into the equality constraints, yields

$$\begin{cases}\|a\|^2+\theta^2\|d\|^2=1\\ \|a\|^2(1-\|d\|^2)=\theta^2\|d\|^4\end{cases}\Leftrightarrow\begin{cases}\theta^2\|d\|^2=1-\|a\|^2\\ \theta^2\|d\|^4=\|a\|^2(1-\|d\|^2)\end{cases}\Leftrightarrow\|d\|^2(1-\|a\|^2)=\|a\|^2(1-\|d\|^2),$$

which implies that $\|a\|^2=\|d\|^2$. To eliminate b from the objective function, we may use the constraint $(b^Td)^2=\|a\|^2(1-\|d\|^2)$ from which it follows that $b^Td=\pm\sqrt{\|a\|^2(1-\|a\|^2)}$ where the $+$ solution will result in a larger value for the objective function and should thus be chosen. The optimization problem (4.7) is then rewritten as:

$$\begin{aligned}&\max_a\{-\|a\|^2+\gamma\sqrt{\|a\|^2(1-\|a\|^2)}\}\\&\text{subj. to } 0\le\|a\|^2\le 1.\end{aligned}$$

This problem only depends on the norm of a and, introducing introducing $\mathcal{A}:=\|a\|^2$, we may write the optimization as:

$$\max_{0\le\mathcal{A}\le 1}\left\{-\mathcal{A}+\gamma\sqrt{\mathcal{A}(1-\mathcal{A})}\right\}.$$

Electronic Journal of Linear Algebra, ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 39, pp. 154-163, April 2023.

To solve this optimization problem, we calculate the first and second derivatives of the objective function $f(\mathcal{A}) = -\mathcal{A} + \gamma\sqrt{\mathcal{A}(1-\mathcal{A})}$ with respect to the variable $\mathcal{A}$ as:

$$\frac{df}{dx} = -1 + \frac{\gamma(1-2\mathcal{A})}{2\sqrt{\mathcal{A}(1-\mathcal{A})}} \qquad \text{and} \qquad \frac{d^2 f}{d\mathcal{A}^2} = \frac{-\gamma(\mathcal{A}^2+2\mathcal{A}-1)}{2\sqrt{\mathcal{A}(1-\mathcal{A})}}.$$

Since the second derivative is negative on $[-1,1]$, the objective function f is concave and the optimal value $\mathcal{A}^\star$ can be calculated from $\frac{df}{d\mathcal{A}}(\mathcal{A}^\star) = 0$, which yields

$$\mathcal{A}^\star = \frac{1}{2} - \frac{1}{2}\sqrt{\frac{1}{\gamma^2+1}} \text{ with } f(\mathcal{A}^\star) = -\frac{1}{2} + \frac{1}{2}\sqrt{\gamma^2+1}.$$

Introducing $\gamma = \sqrt{n(n-2)}$ we find that the optimum equals $f(\mathcal{A}^\star) = (n-2)/2$. Returning to the original optimization problem (4.5), we have thus shown that

$$\sum_{k\in K^+} [-(x_k)^2 + \gamma x_k y_k] \leq (n-2)/2.$$

For the bound (4.4) for the off-diagonal entries of A, this then implies that

$$n(A)_{ij} \leq (\lambda_{\max} - \lambda_{\min})(n-2)/2 - \lambda_{\min}, \text{ and thus } \frac{2n(A)_{ij}}{(n-2)\lambda_{\min}} \leq \lambda_{\max}/\lambda_{\min} - n/(n-2). \tag{4.8}$$

Hence, whenever $\lambda_{\max}/\lambda_{\min} \leq n/(n-2)$ we know that $(A)_{ij} \leq 0$ for all $i \neq j$ which completes the first part of the proof.

Next, we show that **the eigenvalue criterion is tight** by constructing an example with positive entries whenever the criterion is not met. Fix two numbers $1 \leq i \neq j \neq n$ and let $z_1, z_2 \in \mathbb{R}^n$ be the vectors defined as:

$$(z_1)_k := \begin{cases} \sqrt{\dfrac{n-2}{2n}} \text{ if } k = i,j \\ -\sqrt{\dfrac{2}{n(n-2)}} \text{ otherwise} \end{cases} \qquad (z_2)_k := \begin{cases} \dfrac{1}{\sqrt{2}} \text{ if } k = i \\ \dfrac{-1}{\sqrt{2}} \text{ if } k = j \\ 0 \text{ otherwise} \end{cases}.$$

These vectors have unit norm, are pairwise orthogonal, and are both orthogonal to u. Let $\{z_k\}_{k=3}^{n-1}$ be an orthonormal basis of $\operatorname{span}(u, z_1, z_2)^\perp$ with $(z_k)_i = (z_k)_j = 0$ for all $3 \leq k \leq n-1$. In other words, if we let i, j be the first two indices, these basis vectors are of the form $(0, 0, \tilde{z}_k)$ and $\{\tilde{z}_k\}_{k=3}^{n-1}$ is an orthonormal basis of $\operatorname{span}(\tilde{u})^\perp$ (where $\tilde{u}$ is the $(n-2)\times 1$ all-one vector), since u, z_1, z_2 are constant in this subspace. Finally, we fix some $\lambda > 0$ let $n \geq 3$ and construct the matrix B_ϵ as:

$$B_\epsilon = \underbrace{\lambda\left(\frac{n}{n-2} + \epsilon\right)}_{\lambda_{\max}} z_1 z_1^T + \underbrace{\lambda}_{\lambda_{\min}} \sum_{k=2}^{n-1} z_k z_k^T \text{ for some } \epsilon > 0.$$

By construction, this matrix is centered and PSD (since $B_\epsilon u = 0$ following $z_k^T u = 0$), has rank $n-1 \geq 2$ and eigenvalue ratio $\lambda_{\max}/\lambda_{\min} = n/(n-2) + \epsilon > n/(n-2)$. Furthermore, we find that

$$\begin{aligned}(B_\epsilon)_{ij} &= \lambda\left(\frac{n}{n-2} + \epsilon\right)(z_1)_i(z_1)_j + \lambda(z_2)_i(z_2)_j \\ &= \lambda\left(\frac{n}{n-2} + \epsilon\right)\frac{n-2}{2n} - \frac{1}{2}\lambda \\ &= \frac{\lambda\epsilon(n-2)}{2n} > 0.\end{aligned}$$

Electronic Journal of Linear Algebra, ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 39, pp. 154-163, April 2023.

In other words, for a given n and $\lambda_{\max}/\lambda_{\min} > n/(n-2)$ we have at least one centered PSD_n^{n-1} matrix B_ϵ which has a positive off-diagonal entry. This proves that the eigenvalue criterion is tight. □

The vectors z_1, z_2 that are used to construct the example that proves tightness are Soules vectors. These vectors were introduced by G.W. Soules in [12] in the context of the inverse eigenvalue problem and used in [9] to construct Laplacian matrices with any nonnegative spectrum.

4.1. Another application of the proof technique. One of the main steps in the proof of Theorem 2.2 is to solve the optimization problem (4.5). This is a geometric optimization problem asking how much two orthogonal and unit-norm vectors $x, y \in \mathbb{R}^n$ can overlap in a certain subspace (given by K) relative to the norm of one of the vectors in that subspace. This proof technique seems more broadly applicable and to illustrate, we show how it can be used to retrieve the following result[3]:

PROPOSITION 4.1. *Let A be a real symmetric matrix with eigenvalues in $[\lambda_{\min}, \lambda_{\max}]$ and $\lambda_{\min} > 0$, then $(A)_{ij} \leq \frac{1}{2}(\lambda_{\max} - \lambda_{\min})$ for all $i \neq j$.*

Proof: Since A is a real, symmetric matrix, it has an orthonormal basis of eigenvectors $\{z_k\}_{k=1}^n$. The off-diagonal entries of A can be written as:

$$\begin{aligned}
(A)_{ij} &= \sum_{k=1}^{n} \lambda_k (z_k)_i (z_k)_j \\
&= \sum_{k=1}^{n} \lambda_k x_k y_k, \text{ where } x_k := z_k^T e_i, y_k := z_k^T e_j \\
&= \sum_{k \in K^+} \lambda_k x_k y_k + \sum_{k \in K^-} \lambda_k x_k y_k, \;\; \text{where } K^{\pm} := \{k : \lambda_k \gtrless 0\} \\
&\leq \lambda_{\max} \sum_{k \in K^+} x_k y_k + \lambda_{\min} \sum_{k \in K^-} x_k y_k \\
&= (\lambda_{\max} - \lambda_{\min}) \sum_{k \in K^+} x_k y_k \quad (\text{since } e_i^T e_j = 0 \Rightarrow x^T y = 0).
\end{aligned}$$

Following the same steps as in the Proof of Theorem 2.2, we then find that optimizing $\sum_{k \in K} x_k y_k$ translates to $\max_{0 \leq \mathcal{A} \leq 1} \sqrt{\mathcal{A}(1-\mathcal{A})} = \frac{1}{2}$ which completes the proof. □

5. Conclusion. The main result in this article, Theorem 2.2, states that centered positive semidefinite matrices with one-dimensional kernel and with a thin spectrum have nonpositive off-diagonal entries, that is, they are M-matrices. The tight condition on the eigenvalue ratio is a clear example of how spectral properties can guarantee certain (sign) properties of matrices. The proof of Theorem 2.2 involves solving what is essentially a geometric optimization problem; we believe it would be interesting to find alternative proofs using different techniques. Finally, we also describe the connection to Laplacian matrices, where the sign property relates to positivity of edge weights.

Acknowledgment. The author was supported by The Alan Turing Institute under the EPSRC grant EP/N510129/1 and is grateful to Piet Van Mieghem for helpful discussions and to an anonymous referee for pointing out the applications related to the inverse nonsingular M-matrix problem.

[3]Prof. Van Mieghem noted that this bound is known and can also be derived by using the identity $2(z_k)_i(z_k)_j = (z_k)_i^2 + (z_k)_j^2 - [(z_k)_i - (z_k)_j]^2$ (private communication).

Electronic Journal of Linear Algebra, ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 39, pp. 154-163, April 2023.

REFERENCES

[1] E. Bendito, A. Carmona, A. M. Encinas, and M. Mitjana. The M-matrix inverse problem for singular and symmetric Jacobi matrices. *Linear Algebra Appl.*, 436(5):1090–1098, 2012.

[2] A. Berman and R.J. Plemmons. *Nonnegative Matrices in the Mathematical Sciences.* Classics in Applied Mathematics. SIAM, Philadelphia, PA, 1994.

[3] D. Boley and G.H. Golub. A survey of matrix inverse eigenvalue problems. *Inverse problems*, 3(4):595–622, 1987.

[4] A. Carmona, E. Bendito, A.M. Encinas, and M. Mitjana. On the Moore-Penrose inverse of distance–regular graphs. *Electronic Notes Discr. Math.*, 38:227–232, 2011.

[5] M.T. Chu and G.H. Golub. Structured inverse eigenvalue problems. *Acta Numer.*, 11:1–71, 2002.

[6] F.R.K. Chung. *Spectral Graph Theory.* Regional Conference Series in Mathematics. AMS, Providence, RI, 1997.

[7] E. Deutsch and M. Neumann. Derivatives of the Perron root at an essentially nonnegative matrix and the group inverse of an M-matrix. *J. Math. Anal. Appl.*, 102(1):1–29, 1984.

[8] K. Devriendt. Effective resistance is more than distance: Laplacians, Simplices and the Schur complement. *Linear Algebra Appl.*, 639:24–49, 2022.

[9] K. Devriendt, R. Lambiotte, and P. Van Mieghem. Constructing Laplacian matrices with Soules vectors: Inverse eigenvalue problem and applications, arXiv:1909.11282, 2019.

[10] S.J. Kirkland and M. Neumann. The M-matrix group generalized inverse problem for weighted trees. *SIAM J. Matrix Anal. Appl.*, 19(1):226–234, 1998.

[11] S.J. Kirkland and M. Neumann. *Group Inverses of M-matrices and Their Applications.* Chapman & Hall/CRC Applied Mathematics and Nonlinear Science Series. CRC Press, Boca Raton, FL, 2013.

[12] G.W. Soules. Constructing symmetric nonnegative matrices. *Linear Multilinear Algebra*, 13(3):241–251, 1983.