Advanced Course on
Combinatorial Matrix Theory

Number 72 / June 2015
Advanced Course on

Combinatorial Matrix Theory

June, 29 to July 3, 2015
Acknowledgements. The Advanced Course on Combinatorial Matrix Theory is supported by the DGI MICIN MTM2011-28800-C02-01 and MTM2011-28800-C02-02.
Contents

Foreword v

Advanced Course

Richard A. Brualdi, University of Wisconsin-Madison ............ 5

Combinatorial matrix theory

Angeles Carmona Mejías, Universitat Politècnica de
Catalunya-BarcelonaTech ............................................. 79

Boundary value problems of finite networks

Stephen J. Kirklan, University of Manitoba ...................... 119

The group inverse of the Laplacian matrix of a graph

Dragan Stevanović, Serbian Academy of Sciences and Arts
(SANU) ................................................................. 141

Spectral radius of graphs

Pauline van den Driessche, University of Victoria .............. 163

Sign pattern matrices
The notes contained in this booklet were printed directly from files supplied by the authors before the course.
Foreword

The present volume contains the notes prepared by the professors of the Advanced Course *Combinatorial Matrix Theory* organized by the Centre de Recerca Matemàtica (CRM) in Bellaterra from June 29 to July 3, 2015. This Advanced Course consists of five different series of four lectures each one, delivered by Richard A. Brualdi (University of Wisconsin-Madison) on *Combinatorial Matrix Theory*, Ángeles Carmona (Universitat Politècnica de Catalunya) on *Boundary value problems on Finite Networks*, Stephen Kirkland (University of Manitoba) on *The Group Inverse for the Laplacian Matrix of a Graph*, Dragan Stevanovic (Serbian Academy of Sciences and Arts) on *Spectral Raddious of Graphs*, and Pauline van den Driessche (University of Victoria) on *Sign Pattern Matrices*.

Combinatorial matrix theory is a rich branch of matrix theory; it is both an active field of research and a widespread toolbox for many scientists. Combinatorial properties of matrices are studied based on qualitative rather than quantitative information, so that the ideas developed can provide consistent information about a model even when the data is incomplete or inaccurate. The theory behind qualitative methods can also contribute to the development of effective quantitative matrix methods. In this volume we present the following set of notes:

*Combinatorial Matrix Theory* by Richard A. Brualdi: Combinatorial Matrix Theory (CMT) is concerned with the interplay of combinatorics/graph theory and matrix theory/linear algebra. It’s a two way street, with linear algebra providing a means to prove combinatorial theorems, and combinatorics providing more detailed and refined information in linear algebra. In addition, in CMT classes of matrices (adjacency matrices of bipartite graphs, or in the symmetric case, graphs) are investigated with the goal of understanding such classes and investigation of combinatorial or linear algebraic invariants over the class. In these lectures many aspects of CMT will be discussed.

*Boundary value problems on Finite Networks* by Ángeles Carmona: The aim of these lectures is to analyze self–adjoint boundary value problems on finite networks. The starting point is the description of the basic difference operators: the derivative, gradient, divergence, curl and laplacian, or more generally, Schrodinger operators. Then, it is proved that the above operators satisfy analogue properties to those exhibited by their continuous counterpart. The next step is to define the discrete analogue of a manifold with boundary, which includes the concept of outer normal field and prove the Green Identities in order to establish the variational formulation of boundary value problems. At that point, the focus is located on some aspects of discrete Potential Theory by proving the discrete version of the Dirichlet, the maximum and the condenser principles. In this framework, another useful tool is the concept of Resolvent Kernel associated with a boundary value problem. So, the discrete analogous of the Green and Poisson Kernels will be defined and their main properties as well as their relationship with the so-called Dirichlet–to–Neuman map established.
Finally, some applications to Matrix Theory and to Organic Chemistry, as the $M$-inverse problem or the Kirchhoff Index computation will be considered.

The Group Inverse for the Laplacian Matrix of a Graph by Stephen Kirkland: Laplacian matrices for undirected graphs have received a good deal of attention, in part because the spectral properties of the Laplacian matrix are related to a number of features of interest of the underlying graph. It turns out that a certain generalised inverse - the group inverse - of a Laplacian matrix also carries information about the graph in question. This series of lectures will explore the group inverse of the Laplacian matrix and its relationship with graph structure. Connections with algebraic connectivity and resistance distance will be made, and the computation of the group inverse of a Laplacian matrix will also be considered from a numerical viewpoint.

Spectral radius of graphs by Dragan Stevanovic: Eigenvalues and eigenvectors of graph matrices have become standard mathematical tools nowadays due to their wide applicability in network analysis and computer science, with the most prominent graph matrices being the adjacency and the Laplacian matrix. In these lectures, lower and upper limits of the spectral radius of adjacency and Laplacian matrices, with special attention to testing techniques and common properties of shapes of the boundaries are studied. Some interesting approximate formulas for the spectral radius of adjacency matrix will be discussed as well.

Sign Pattern Matrices by Pauline van den Driessche: An $n \times n$ sign pattern (matrix) $A^* = (\alpha_{ij})$ has entries from the set $\{+,-,0\}$ with an associated sign pattern class of real $n \times n$ matrices $\{A = (a_{ij}) : \text{sign}(a_{ij}) = \alpha_{ij} \text{ for all } i,j\}$. These lectures will survey some important classes of sign patterns, including sign patterns that allow all possible spectra, those that allow all possible inertias, those that allow stability, and those that may give rise to Hopf bifurcation in associated dynamical systems. Then some classes will be explored in more detail using techniques from matrix theory, graph theory and analysis, and open problems will be suggested.

The scientific committee of the course is composed by Andrés M. Encinas (Universitat Politècnica de Catalunya), Carlos da Fonseca (Kuwait University) and Margarida Mitjana (Universitat Politècnica de Catalunya). The program is being made possible not only by the support of the CRM, but also by the support of Elsevier, publisher of the journal Linear Algebra and its Applications, the Societat Catalana de Matemàtiques and the Real Sociedad Matemática Española.

We also acknowledge the financial support from the research projects DGI MICIIN MTM2011-28800-C02-01 and MTM2011-28800-C02-02.

Bellaterra, June 19, 2015
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Advanced Course
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Combinatorial matrix theory
Combinatorial Matrix Theory

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CRM - Summer School

Barcelona

June 29 – July 3, 2015

1 Permutations, Tuesday, 9:30 – 11:00
   • Permutation Matrices
   • Bruhat Order
     • Matrix Bruhat Decomposition
     • Flags
   • Nonnegative Integral matrices
   • Permutations and Symmetric Matrices

   • Origins of ASMs
   • Additional Properties of ASMs
   • ASM Completions: Patterns of the \(-1\)s in ASMs
   • Spectral Radius
   • ASM Generalization

3 Tournaments: Friday 9:30 – 11:00
   • Tournament matrices
   • Multi-Tournaments
   • Loopy Tournaments
   • Hankel Tournaments
   • Combinatorially skew-Hankel Tournaments
Permutations

$\mathfrak{S}_n$: the set of all permutations $\sigma = (i_1, i_2, \ldots, i_n)$ of \{1, 2, \ldots, n\}.

**Example:** $n = 5$ and $\sigma = (3, 5, 4, 2, 1)$.

Each permutation $\sigma$ of \{1, 2, \ldots, n\} can be identified with an $n \times n$ permutation matrix $P = [p_{ij}]$ where

$$p_{i_1} = p_{i_2} = \cdots = p_{i_n} = 1 \text{ and } p_{ij} = 0, \text{ otherwise.}$$

**Example:** $P = \begin{bmatrix} 1 & 1 \\ 1 & 1 \\ 1 & \end{bmatrix}$.

Ascents and Descents in Permutations

$\sigma = (i_1, i_2, \ldots, i_n)$

**Ascent:** A pair $k, k+1$ with $i_k < i_{k+1}$. **Occurs** at position $k$.

**Descent:** A pair $k, k+1$ with $i_k > i_{k+1}$. **Occurs** at position $k$.

**Example:** $\sigma = (3, 5, 4, 2, 1)$ and $P = \begin{bmatrix} 1 \\ 1 \\ 1 \\ \end{bmatrix}$.

The number of ascents plus the number of descents equals $n - 1$. In the example,

$$1 + 3 = 4.$$
Inversions in Permutations

\[ \sigma = (i_1, i_2, \ldots, i_n) \]

**Inversion:** A pair \( k, l \) of positions with with \( k < l \) such that \( i_k > i_l \) (out of the natural order \( 1, 2, \ldots, n \)).

**Example:** \( \sigma = (3, 5, 4, 2, 1) \) with \( P = \begin{bmatrix} 1 & 1 \\ 1 & 1 \\ 1 & 1 \end{bmatrix} \) has 8 inversions (count them!) The identity \( I_n \) has no inversions. The **anti-identity** \( L_n \) has the maximum number \( \binom{n}{2} \) of inversions; e.g.

\[ L_5 = \begin{bmatrix} 1 & 1 \\ 1 & 1 \\ 1 & 1 \end{bmatrix} \quad (\sigma = (5, 4, 3, 2, 1)). \]

Inversions in Permutations

An inversion in a permutation matrix \( P \) corresponds to a \( 2 \times 2 \) submatrix

\[ P[i, j|k, l] = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = L_2 \quad (i < j, k < l). \]

Replacing this submatrix with

\[ I_2 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \]

gives a new permutation with fewer inversions, maybe a lot fewer:

\[ L_5 = \begin{bmatrix} 1 & 1 \\ 1 & 1 \\ 1 & 1 \end{bmatrix} \rightarrow \begin{bmatrix} 1 & 1 \\ 1 & 1 \\ 1 & 1 \end{bmatrix} \quad (10 \rightarrow 3). \]

\( (5, 4, 3, 2, 1) \rightarrow (1, 4, 3, 2, 5) \)

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Inversions in Permutations

But if the inversion takes place in a submatrix like

\[
\begin{array}{ccc}
1 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
1 & 0 & 0 \\
\end{array}
\]

\[
\begin{array}{ccc}
1 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 1 \\
\end{array}
\]

\((a \rightarrow a - 1),\)

(in particular in two consecutive positions), then the number of inversions is decreased by exactly 1.

For instance,

\[
\ldots, 8, 2, 1, 9, 3 \ldots \rightarrow \ldots, 3, 2, 1, 9, 8 \ldots
\]

<3 or >8

François Bruhat (8 April 1929 - 17 July 2007)

A French mathematician who worked on algebraic groups.

A third generation member of Bourbaki.

An Officer of the Légion d’Honneur and the national order of merit. He was also made Commandeur des Palmes Académiques.

Bruhat Order $\leq_B$ of Permutations

$\sigma$ and $\tau$: permutations of $\{1, 2, \ldots, n\}$: Then $\sigma \leq_B \tau$, $\sigma$ is less than $\tau$ in the Bruhat order provided $\sigma$ can be obtained from $\tau$ by a sequence of inversion-reducing transformations. Thus the identity $\iota_n$ is the smallest permutation in the Bruhat order (no inversions) and the anti-identity $\ell_n$ is the largest permutation in the Bruhat order (all possible inversions).

$\sigma$ is covered in the Bruhat order by $\tau$ provided the number of inversion is decreased by exactly 1.

The Bruhat order on $S_n$ is a partial order graded by the number of inversions.

Hasse Diagram of the Bruhat Order of $S_3$

$$L_3 = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix} : (3, 2, 1)$$

$$(2, 3, 1): \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}$$

$$(2, 1, 3): \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$I_3 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} : (1, 2, 3)$$
Gaussian Elimination: $A = PLU$ decomposition

A an $n \times n$ nonsingular complex matrix. Then there exist (not necessarily unique) a permutation matrix $P$, and lower and upper triangular matrices $L$ and $U$ such that

$$A = PLU.$$

$$\begin{bmatrix} 1 & 2 \\ 1 & 1 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}.$$

(Gaussian elimination can usually be carried out in many ways: Apply a permutation matrix to $A$ so that all the pivots are on the main diagonal.)

Matrix Bruhat Decomposition for $A$ nonsingular

$A = LPU$ or $A = LPL$ where $L, U$ are nonsingular.

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

Using elementary row operations (multiplying on the left by a lower triangular matrix) and elementary column operations (multiplying on the right by an upper triangular matrix), $A$ can be reduced to a permutation matrix, and this gives $A = LPU$. Here is how:
Consider the first nonzero in row 1. Postmultiplication by an upper triangular matrix makes all subsequent entries 0 and "pivot" element 1.

Premultiplication by a lower triangular matrix makes all elements below the pivot 1 equal to 0.

Find a new pivot entry in row 2, and proceed recursively.

At the end we have a permutation matrix $P$ (since $A$ is nonsingular) and so $P = L'AU'$ where $L'$ is lower triangular and $U'$ is upper triangular.

Then $A = LP$ where $L = (L')^{-1}$ and $U = (U')^{-1}$.

Take $A$ nonsingular and $Q_n = \begin{bmatrix} 0 & 0 & \cdots & 0 & 1 \\ 0 & 0 & \cdots & 1 & 0 \\ \vdots \\ 0 & 1 & \cdots & 0 & 0 \\ 1 & 0 & \cdots & 0 & 0 \end{bmatrix}$ where $Q_n$ is a symmetric permutation matrix with $Q_n^2 = I$.

Then $AQ_n = L_1PU$ and

$$A = L_1PUQ_n = L_1PQ_n^2UQ_n = L_1(PQ_n)(Q_nUQ_n) = L_1P_1L_2.$$
Uniqueness of $P$ in $A = LPU$ and so in $A = LPL$

Let: $P = P_\sigma$.
Consider initial parts of rows of $A$:
\[
r_i(A, j) = A[i|\{1, 2, \ldots, j\}] \quad (j = 1, 2, \ldots, n), \text{ for } i = 1, 2, \ldots, n.
\]

Let:

(**) $\rho(A : i)$ be the minimal $j$ such that $r_i(A, j)$ is not in the span of
{$r_1(A, j), \ldots, r_{i-1}(A, j)$}.

For $P$ we obviously have that $\rho(P : i) = \sigma(i)$.
But property (***) is preserved under multiplication on the left by a	nonsingular lower triangular matrix and on the right by a nonsingular
upper triangular matrix. Thus $P$ is uniquely determined by $A$.

Non-Uniqueness of $L, U$ in $A = LPU$

Again, let $Q_n$ be the $n \times n$ permutation matrix corresponding to the
permutation $(n, \ldots, 2, 1)$. So, for instance,
\[
Q_3 = \begin{bmatrix}
0 & 0 & 1 \\
0 & 1 & 0 \\
1 & 0 & 0
\end{bmatrix}
\]

We have that $Q_n^2 = I_n$. If $L$ is lower triangular, then $U = Q_nLQ_n$ is upper
triangular. Then defining $A$ by
\[
A = LQ_nU,
\]
we also have
\[
A = LQ_nU = LQ_n(Q_nLQ_n) = L(Q_n^2)LQ_n = L^2Q_n = L^2Q_nI_n,
\]
two different decompositions (with the same permutation matrix $Q_n$).
Bruhat Decomposition formalized

$GL_n$: the linear group of $n \times n$ nonsingular complex matrices. Then

$$GL_n = \mathcal{L}_n S_n \mathcal{L}_n$$

where $\mathcal{L}_n$ is the subgroup of (nonsingular) lower triangular matrices and $S_n$ is the subgroup of $n \times n$ permutation matrices.

This is a partition (since the permutation matrix $P$ is unique in the matrix Bruhat decomposition $LPL$) of $GL_n$ into double cosets parametrized by the $n \times n$ permutation matrices.

(Note: $GL_n$ can be replaced by a wider class of groups, and $\mathcal{L}_n$ and $S_n$ replaced by a wider class of its subgroups.)

(Complete) Flags in $\mathbb{C}^n$

$\mathcal{F}: F_0 = \{0\} \subset F_1 \subset F_2 \subset \cdots \subset F_n = \mathbb{C}^n$ where $\dim F_k = k$ for all $k$.

These correspond to $n \times n$ nonsingular complex matrices $A$ with row vectors $v_1, v_2, \ldots, v_n$: $F_k = \langle v_1, v_2, \ldots, v_k \rangle$.

Under the action of $GL_n$ (a nonsingular linear transformation) there is only one flag: Every basis of $\mathbb{C}^n$ can be brought to the standard basis and thus all the flags become

$$\{0\} \subset \langle e_1 \rangle \subset \langle e_1, e_2 \rangle \subset \cdots \subset \langle e_1, e_2, \ldots, e_n \rangle,$$

where $e_i$ is the standard $i$th unit vector.
Pairs of Flags $F^{(1)}, F^{(2)}$ in $\mathbb{C}^n$

These correspond to two $n \times n$ nonsingular complex matrices $A_1$ and $A_2$ with row vectors $v_1, v_2, \ldots, v_n$ and $w_1, w_2, \ldots, w_n$, respectively:

$$F^{(1)}_k = \langle v_1, v_2, \ldots, v_k \rangle \quad \text{and} \quad F^{(2)}_k = \langle w_1, w_2, \ldots, w_k \rangle.$$ 

Under the action of $GL_n$: There exists a nonsingular matrix $C$ such that $A_2 = CA_1$, where $C$ has a matrix Bruhat decomposition $C = L_1 P L_2$. Thus

$$A_2 = CA_1 = L_1 P L_2 A_1 \implies L_1^{-1} A_2 = P L_2 A_1.$$ 

Thus, under a change of basis (determined by the nonsingular lower triangular matrices $L_1^{-1}$ and $L_2$), the configuration type of $F^{(1)}, F^{(2)}$ consists of the pair of flags $B^{(1)}, B^{(2)}$ with

$$B^{(1)}_k = \langle u_1, u_2, \ldots, u_k \rangle \quad \text{and} \quad B^{(2)}_k = \langle u_{\sigma(1)}, u_{\sigma(2)}, \ldots, u_{\sigma(k)} \rangle;$$

configuration types of double flags are indexed by permutations $\sigma$.

We have that $\dim(B^{(1)}_i \cap B^{(2)}_j) = |\{1, 2, \ldots, i\} \cap \{\sigma(1), \sigma(2), \ldots, \sigma(j)\}|$.

---

Pairs of Flags $F^1, F^2$ with $\sigma = (n, n-1, \ldots, 2, 1)$

Recall that $Q_n$ is the $n \times n$ permutation matrix corresponding to the permutation $\sigma = (n, n-1, \ldots, 2, 1)$. Thus if $n = 6$,

$$Q_n = \begin{bmatrix} \ & \ & 1 \\ \ & 1 & \ \\ \ & 1 & \ \\ 1 & \ & \ \\ 1 & \ & \ \\ 1 & \ & \ \\ \end{bmatrix}$$

and then we get

$$\dim(B^1_i \cap B^2_j) = |\{1, 2, \ldots, i\} \cap \{\sigma(1), \sigma(2), \ldots, \sigma(j)\}| = (i + j - n)^+,$$

the number of 1s of $Q_n$ in the leading $i \times j$ submatrix of $Q_n$. This is the smallest possible dimension of the intersection of an $i$-dimensional subspace $U$ and a $j$-dimensional subspace $W$ in an $n$-dimensional space:

$$\dim(U \cap W) \geq (i + j - n)^+.$$ 

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Pairs of Flags $B^1, B^2$ in $C_n$

Thus we can say that the pair of flags $B^1, B^2$, where

$$B^1 : <0 > <u_1 > <u_1, u_2 > <\cdots <u_1, u_2, \ldots, u_n >$$

$$B^2 : <0 > <u_n > <u_n, u_{n-1} > <\cdots <u_n, u_{n-1}, \ldots, u_1 >$$

is the most generic pair of flags.

[In general, $\dim(B^1 \cap B^2) = |\{1, 2, \ldots, i\} \cap \{\sigma(1), \sigma(2), \ldots, \sigma(j)\}|$, and the larger these intersections, the less generic the flag pairs are.]

$(B^1, B^2)$ degenerates to $B^3, B^4$ if there is a continuous sequence of flags $B^1, B^2$ indexed by a parameter $\tau \in C$ such that for $\tau \neq 0$, $B^1, B^2$ has the same type as $B^1, B^2$ but has the type of $B^3, B^4$ for $\tau = 0$.]

Bruhat Order: The $\Sigma$-way

For an $m \times n$ matrix $A = [a_{ij}]$, define $\Sigma(A) = [\sigma_{ij}(A)]$ by

$$\sigma_{ij} = \sigma_{ij}(A) = \sum_{1 \leq k \leq i, 1 \leq l \leq j} a_{ij}, \quad (1 \leq i \leq m, 1 \leq j \leq n)$$

the sum of the entries of the leading $i \times j$ submatrix of $A$. (If $A$ is a permutation matrix, this is the same as the rank of the leading $i \times j$ submatrix of $A$.)

Example: $A = \begin{bmatrix} 1 & 3 & 2 & 4 \\ 0 & 3 & 1 & 2 \\ 3 & 5 & 1 & 2 \end{bmatrix}$ $\rightarrow \Sigma(A) = \begin{bmatrix} 1 & 4 & 6 & 10 \\ 1 & 7 & 10 & 16 \\ 4 & 15 & 19 & 27 \end{bmatrix}$

Theorem: [More about this to come] For $n \times n$ permutation matrices $P$ and $Q$, we have

$$P \preceq_B Q \text{ if and only if } \Sigma(P) \succeq \Sigma(Q) \text{ (entrywise).}$$
Bruhat Order: Example

\[ P = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \quad Q = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \]

\[ \Sigma(P) = \begin{bmatrix} 0 & 1 & 1 & 1 \\ 0 & 1 & 2 & 2 \\ 1 & 2 & 2 & 3 \\ 1 & 2 & 3 & 4 \end{bmatrix} \quad \Sigma(Q) = \begin{bmatrix} 0 & 0 & 1 & 1 \\ 0 & 1 & 2 & 2 \\ 1 & 2 & 3 & 3 \\ 1 & 2 & 3 & 4 \end{bmatrix} \]

\[ P \] and \[ Q \] are unrelated in the Bruhat order.

---

Pairs of Flags \( B^1, B^2 \) and the Bruhat order

Thus the orbits of pairs of flags in \( C^n \) under the action of \( GL_n \) are indexed by permutations \( \sigma \):

\[ B^{(1)}_k = \langle u_1, u_2, \ldots, u_k \rangle \quad \text{and} \quad B^{(2)}_k = \langle u_{\sigma(1)}, u_{\sigma(2)}, \ldots, u_{\sigma(k)} \rangle, \]

A configuration of type \( \sigma \) (or \( P_\sigma \)) is a degeneration of a configuration of type \( \rho \) (or \( P_\rho \)) exactly if \( P_\sigma \preceq_B P_\rho \), that is, when \( \Sigma(P_\sigma) \geq \Sigma(P_\rho) \); geometrically, this means that the configuration of type \( \sigma \) has larger intersections among its subspaces than the configuration of type \( \rho \).

If \( \sigma \) is the identity permutation \( (1, 2, \ldots, n) \), then a configuration of type \( \sigma \) is a degeneration of all configurations of pairs of flags. If \( \sigma = (n, n-1, \ldots, n, 1) \), a configuration of type \( \sigma \) degenerates to all configurations of pairs of flags.
Bruhat Order: $P \preceq_B Q$ if and only if $\Sigma(P) \geq \Sigma(Q)$

One direction is easy:

- $P \preceq_B Q \implies \Sigma(P) \geq \Sigma(Q)$: 
  
  \[
  \begin{bmatrix}
  0 & 1 \\
  * & * \\
  1 & 0
  \end{bmatrix} \rightarrow 
  \begin{bmatrix}
  1 & 0 \\
  * & * \\
  0 & 1
  \end{bmatrix}.
  \]

- $\Sigma(P) \geq \Sigma(Q) \implies P \preceq_B Q$: Not so obvious.

In fact, this equivalence is true more generally.

Nonnegative Integral Matrices with specified Row and Column Sum Vectors

Replace $\mathcal{S}_n$ by the set $\mathcal{N}(R, S)$ of all $m \times n$ nonnegative, integral matrices with row sum vector $R = (r_1, r_2, \ldots, r_m)$ and column sum vector $S = (s_1, s_2, \ldots, s_n)$. Thus $\mathcal{S}_n$ is the special case with $m = n$ and $R = S = (1, 1, \ldots, 1)$.

**Fact:** $\mathcal{N}(R, S) \neq \emptyset$ if and only if $\sum_{i=1}^{m} r_i = \sum_{j=1}^{n} s_j$.

**Example:** $R = (3, 5, 4)$ and $S = (2, 4, 3, 3)$, 

\[
\begin{bmatrix}
2 & 1 & 0 & 0 \\
0 & 3 & 2 & 0 \\
0 & 0 & 1 & 3
\end{bmatrix} \in \mathcal{N}(R, S).
\]
Bruhat Order on $\mathcal{N}(R, S)$

$A_1, A_2 \in \mathcal{N}(R, S)$: $A_1 \preceq_B A_2$ if and only if $A_1$ can be gotten from $A_2$ by a sequence of moves of the form

\[
\begin{bmatrix}
a & * & b \\
* & * & * \\
c & * & d + 1
\end{bmatrix} \rightarrow \begin{bmatrix}
a + 1 & * & b - 1 \\
* & * & * \\
c - 1 & * & d + 1
\end{bmatrix},
\]

that is, by adding \( \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \) to a $2 \times 2$ submatrix of $A_2$ where $b, c \geq 1$.

These moves keep one in $\mathcal{N}(R, S)$, and it is immediate that

$$A_1 \preceq_B A_2 \implies \Sigma(A_1) \geq \Sigma(A_2).$$

\[\Sigma(A_1) \geq \Sigma(A_2) \implies \Sigma(A_1) \geq \Sigma(A_2), \quad A_1, A_2 \in \mathcal{N}(R, S)\]

**Proof Outline:** Let $A, A' \in \mathcal{N}(R, S)$ with $\Sigma(A) > \Sigma(A')$.

- Choose $(k_0, l_0)$ the lex. first position with $a_{k_0l_0} > a'_{k_0l_0}$. So $a_{k_0l_0} > 0$ and $\sigma_{k_0l_0}(A) > \sigma_{k_0l_0}(A')$.
- Choose $k_1 > k_0$ and $l_1 > l_0$ as large as possible so that $\sigma_{ij}(A) > \sigma_{ij}(A')$ for $k_0 \leq i \leq k_1 - 1$ and $l_0 \leq j \leq l_1 - 1$.
- Using $\Sigma(A) > \Sigma(A')$, one can find an $(i_1, j_1)$ such that $a_{i_1j_1} > 0$. Take $(i_1, j_1)$ lex. minimal so that $a_{ij} = 0$ for $k_0 + 1 \leq i \leq i_1, l_0 + 1 \leq j \leq j_1, (i, j) \neq (i_1, j_1)$.
- One can then find a position $(i_0, j_0)$ with $i_0 = k_0$ such that $i_0 < i_1, j_0 < j_1$, and $a_{ij} = 0$ for $i_0 \leq i \leq i_1, j_0 \leq j \leq j_1$ but $(i, j) \neq (i_0, j_0), (i_1, j_0), (i_0, j_1), (i_1, j_1)$ and $\sigma_{ij}(A) > \sigma_{ij}(A')$ for $i_0 \leq i \leq i_1 - 1, j_0 \leq j \leq j_1 - 1$.
- Now one can add $\begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix}$ to $A[i_0, i_1 | j_0, j_1]$ and proceed recursively.
Here is what is found in $A$: a submatrix

$$
\begin{bmatrix}
a & 0 & \cdots & 0 & b \\
0 & \ddots & \ddots & \ddots & 0 \\
\vdots & & \ddots & \ddots & \vdots \\
c & 0 & \cdots & 0 & d
\end{bmatrix}
\rightarrow
\begin{bmatrix}
a - 1 & 0 & \cdots & 0 & b + 1 \\
0 & \ddots & \ddots & \ddots & 0 \\
\vdots & & \ddots & \ddots & \vdots \\
c + 1 & 0 & \cdots & 0 & d - 1
\end{bmatrix}
$$

to get us to a matrix $A_1 \in \mathcal{N}(R, S)$ closer to $A'$:

$$\Sigma(A) > \Sigma(A_1) \geq \Sigma(A').$$

In fact, this is what characterizes the cover relation in the Bruhat order on $\mathcal{N}(R, S)$.
Bruhat Order on $\mathcal{N}(R, S)$: Minimal & Maximal Elements

Recursively choosing the position in the northwest corner (so starting with position $(1, 1)$), we get the unique minimal element in the Bruhat order on $\mathcal{N}(R, S)$ . (By recursively choosing the northwest corner and inserting $\min\{r_i, s_j\}$ in that position, we are always obtaining the maximum value of $\sigma_{ij}$ possible for the given $R$ and $S$.)

Similarly, recursively choosing the position in the northeast corner (so starting with position $(1, n)$), we get the unique maximal element. In case of $S_n$, this gives $I_n$ and $L_n$, respectively.

Example: $R = (3, 5, 4)$ and $S = (2, 4, 3, 3)$

\[
\begin{bmatrix}
0 & 0 & 0 & 3 & | & 3 \\
0 & 2 & 3 & 0 & | & 5 \\
2 & 2 & 0 & 0 & | & 4 \\
2 & 4 & 3 & 3 & | & 3
\end{bmatrix}
\]

Pairs of Partial Flags and $\mathcal{N}(R, S)$

Let $b = (b_1, b_2, \ldots, b_q)$, positive integers with $\sum b_i = n$.
Let $c = (c_1, c_2, \ldots, c_r)$, positive integers with $\sum c_i = n$.

(partial flag) $B : \{0\} = B_0 \subset B_1 \subset \cdots \subset B_q$, subspaces of $C_n$ with $\dim B_i / B_{i-1} = b_i$, $i = 1, 2, \ldots, r$.

(partial flag) $C : \{0\} = C_0 \subset C_1 \subset \cdots \subset C_q$, subspaces of $C_n$ with $\dim C_i / C_{i-1} = c_i$, $i = 1, 2, \ldots, r$.

Action of $GL_n$ on partial flags: Orbits $\mathcal{F}_M$ of $\text{Flag}(b) \times \text{Flag}(c)$ are indexed by $q \times r$ nonnegative integral matrices $M = [m_{ij}]$ with row sum vector $b$ and column sum vector $c$ as follows:

Take a basis of $n$ vectors: $(v_{ijk} : 1 \leq i \leq q, 1 \leq j \leq r, 1 \leq k \leq m_{ij})$ and let

$B_i = \langle v_{i'j}^i : 1 \leq i' \leq i \rangle$ and $C_j = \langle v_{j'k}^j : 1 \leq j' \leq j \rangle$. As the basis varies we get the orbit $\mathcal{F}_M$. Note that

$\dim(B_i \cap B_j) = r_{ij}(M) := \sum_{k \leq i, l \leq j} m_{kl}$ (rank numbers).

The Bruhat order on integral matrices (in its two equivalent characterizations) describes the degeneration order on the partial flags.
References I


**Involution**

A permutation $\sigma \in S_n$ is an **involution** provided $\sigma^2 = I_n$. In terms of $n \times n$ permutation matrices $P$, this means

$$P^2 = I_n.$$

The permutation matrix $P$ is an involution if and only if $P$ is symmetric.

**Example:**

$$\begin{pmatrix}
1 & 1 & 1 \\
1 & 1 & 1 \\
1 & 1 & 1
\end{pmatrix} \quad (3, 6, 1, 4, 5, 2).$$
**Descents**

Recall that for a permutation $\pi = (i_1, i_2, \ldots, i_n)$ of $\{1, 2, \ldots, n\}$:

- **Ascent**: A pair $k, k+1$ with $i_k < i_{k+1}$. Occurs at position $k$.
- **Descent**: A pair $k, k+1$ with $i_k > i_{k+1}$. Occurs at position $k$.

An ascent in a permutation $\sigma$ becomes a descent in $\sigma^{-1}$ so we just consider descents. Let $I(n, k)$ ($k = 1, 2, \ldots, n - 1$) equal the number of permutations of $\mathfrak{S}_n$ with exactly $k$ descents and let

$$I_n(t) = \sum_{k=1}^{n-1} I(n, k) t^k$$

be its *generating polynomial*.

**Fact**: The polynomial is symmetric and unimodal, for instance,

$$I_5(t) = 1 + 6t + 12t^2 + 6t^3 + t^4.$$ 

**Nonnegative Integral Symmetric Matrices**

Let $T(n, k)$ denote the set of $k \times k$ nonnegative integral, symmetric matrices without zero rows or columns and with sum of entries equal to $n$. For example,

$$\begin{bmatrix} 1 & 0 & 3 & 1 \\ 0 & 4 & 2 & 1 \\ 3 & 2 & 0 & 2 \\ 1 & 1 & 2 & 3 \end{bmatrix} \in T(26, 4)$$

Let $T(n, k) = |T(n, k)|$.

There is a connection between involutions ($n \times n$ symmetric permutation matrices) with $k$ descents - the $I(n, k)$ - and $k \times k$ nonnegative integral symmetric matrices with sum of entries equal to $n$ - the $T(n, k)$.
Nonnegative Integral Symmetric Matrices

**Theorem:** \( \sum_{k=0}^{n-1} I(n, k) t^k + 1 (1 + t)^{n-1-k} = \sum_{i=1}^{n} T(n, i) t^i. \)

Equivalently,

\[
T(n, i) = \sum_{k=0}^{i-1} I(n, k) \binom{n-1-k}{i-1-k} \quad (i = 1, 2, \ldots, n).
\]

Every consecutive pair of indices in a permutation is either a descent or ascent. Thus if a permutation has \( k \) descents, it has \( n-1-k \) ascents. Thus \( I(n, k) = I'(n, n-1-k) \) where the prime refers to ascents. Doing this replacement and using the fact that \( \binom{n-1-k}{i-1-k} = \binom{n-1-k}{n-i} \), we get

\[
T(n, i) = \sum_{k=0}^{i-1} I'(n, n-1-k) \binom{n-1-k}{n-i}.
\]

Finally, letting \( j = n-1-k \), we get the above equation is equivalent to:

\[
\text{CRM - Barcelona, June 29 – July 3, 2015}
\]

Nonnegative Integral Symmetric Matrices

\[
T(n, i) = \sum_{j=n-i}^{n-1} I'(n, j) \binom{j}{n-i} \quad (j = 1, 2, \ldots, n)
\]

where recall that \( I'(n, j) \) equals the number of permutations of \( \mathfrak{S}_n \) with exactly \( j \) ascents.

In this form, it suggests that there is a mapping \( F_{n-i} \) from the set of all \( n \times n \) symmetric permutation matrices \( P \) with \( j \geq n-i \) ascents onto the subsets of the set of \( i \times i \) nonnegative integral symmetric matrices without zero rows or columns whose entries sum to \( n \) such that

\[
|F_{n-i}(P)| = \binom{j}{n-i}
\]

where the \( F_{n-i}(P) \) partition \( T(n, i). \)
Illustration of the Mapping $F_{n-i} (|F_{n-i}(P) = (\binom{j}{n-i})$)

**Example:** Let $n = 8$ and consider the involution $(5, 7, 8, 6, 1, 4, 2, 3)$ with corresponding symmetric permutation matrix

$$P = \begin{bmatrix}
1 & 1 & & & & & & \\
 & 1 & & & & & & \\
1 & & 1 & & & & & \\
 & & & 1 & & & & \\
 & & & & 1 & & & \\
 & & & & & 1 & & \\
 & & & & & & 1 & \\
 & & & & & & & 1
\end{bmatrix}.$$  

The ascents occur in the pairs of positions (row indices) $\{1, 2\}$, $\{2, 3\}$, $\{5, 6\}$, and $\{7, 8\}$. Choose any subset of these, say pairs $\{1, 2\}$, $\{2, 3\}$, and $\{7, 8\}$, we obtain by combining consecutive pairs, the partition $U_1 = \{1, 2, 3\}$, $U_2 = \{4\}$, $U_3 = \{5\}$, $U_4 = \{6\}$, $U_5 = \{7, 8\}$ of $\{1, 2, \ldots, 8\}$ with corresponding partition of $P$ given by:

Adding the entries in each block gives the symmetric matrix

$$A = \begin{bmatrix}
0 & 0 & 1 & 0 & 2 \\
0 & 0 & 1 & 0 & \\
1 & 0 & 0 & 0 & \\
0 & 1 & 0 & 0 & \\
2 & 0 & 0 & 0 & 0
\end{bmatrix}.$$
Inverting the Mapping $F_{n-i}$

Take an $i \times i$ symmetric, nonnegative integral matrix $A$ with no zero rows and columns whose sum of entries equals $n$. Let $r_k$ be the sum of the entries in row (and column) $k$ of $A$. If $A$ is to result from an $n \times n$ symmetric permutation matrix $P$ by our procedure, then, since $P$ has exactly one 1 in each row and column, it must use the partition of the row and column indices of $P$ into the sets:

$$U_1 = \{1, \ldots, r_1\}, U_2 = \{r_1 + 1, \ldots, r_1 + r_2\}, \ldots$$

$$\ldots, U_i = \{r_1 + r_2 + \cdots + r_{i-1} + 1, r_1 + r_2 + \cdots + r_i\}.$$

There must be a string of $(r_k - 1)$ consecutive ascents corresponding to the positions in each $U_k$. There may be ascents or descents in the position pairs:

$$(r_1, r_1+1), (r_1+r_2, r_1+r_2+1), \ldots, (r_1+r_2+\cdots+r_{i-1}, r_1+r_2+\cdots+r_{i-1}+1).$$

One needs to show that there is exactly one involution (symmetric permutation matrix) with these restrictions.

Illustration of Inverting the Mapping $F_{n-i}$

$$A = \begin{bmatrix} 0 & 2 & 0 \\ 2 & 1 & 3 \\ 0 & 3 & 0 \end{bmatrix} \quad (n = 11, r_1 = 2, r_2 = 6, r_3 = 3).$$

We seek an $11 \times 11$ symmetric permutation matrix of the form

$$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

with 1 ascent in rows 1 and 2, 5 in rows 3 to 8, and 2 in rows 9,10,11.
Illustration of Inverting the Mapping $F_{n-i}$

The only possibility is

\[
\begin{bmatrix}
0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 \\
1 & 1 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 & 1 & 1 \\
0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 \\
\end{bmatrix},
\]

equivalently, the involution

\[3, 4; 1, 2, 5, 9, 10, 11; 6, 7, 8.\]

Notice that the pairs of positions which could be either ascents or descents, namely $\{2, 3\}$ and $\{8, 9\}$, are both descents in this case.

References II

- M. Barnabei, F. Bonetti and M. Silimbani, The descent statistic on involutions is not log-concave, European J. Combin. 30(1)(2009), 11–16.
What is an ASM?

An $n \times n$ $(0, 1, -1)$-matrix such that, ignoring 0s, in each row and column the 1’s and $-1$’s alternate, beginning and ending with a 1.

**Examples:**
- Permutation matrices, for example
  \[
  \begin{bmatrix}
  0 & 1 & 0 \\
  0 & 0 & 1 \\
  1 & 0 & 0 \\
  \end{bmatrix}
  \]

- \[
  \begin{bmatrix}
  0 & 1 & 0 \\
  1 & -1 & 1 \\
  0 & 1 & 0 \\
  \end{bmatrix} \rightarrow \begin{bmatrix}
  0 & + & 0 \\
  + & - & + \\
  0 & + & 0 \\
  \end{bmatrix} \rightarrow \begin{bmatrix}
  + & + & + \\
  + & - & + \\
  + & + & + \\
  \end{bmatrix}
  \]
  (the only non-permutation $3 \times 3$)

Let $\mathfrak{A}_n$ denote the set of all $n \times n$ ASMs. The diamond ASM $D_5 \in \mathfrak{A}_5$ on the left has the largest number of nonzeros in $\mathfrak{A}_5$. 
Basic Properties of ASMs

- The first/last row/column contain a unique +1 and no −1.
- The number of ±1’s in each row and column is odd.
- All row and column sums equal 1.
- The partial row (column) sums starting from the first or last entry in a row (column) equal 0 or 1.
- The number of nonzeros in rows and columns is entrywise bounded by

\[(1, 3, 5, 7 \ldots, 7, 5, 3, 1)\]

The ASM property is preserved under the dihedral group of order 8 (symmetries of a square), but not under arbitrary (simultaneous) row and columns permutations.

The diamond ASM $D_6$. stark

CRM - Barcelona, June 29 – July 3, 2015
ASMs as Column Sum (0, 1)-Matrices (CSMs)

Sum rows 1, 2, \ldots, i of an $n \times n$ ASM for $i = 1, 2, \ldots, n$.

\[
\begin{bmatrix}
0 & 0 & 1 & 0 \\
0 & 1 & -1 & 1 \\
1 & -1 & 1 & 0 \\
0 & 1 & 0 & 0
\end{bmatrix} \rightarrow \begin{bmatrix}
0 & 0 & 1 & 0 \\
0 & 1 & 0 & 1 \\
1 & 0 & 1 & 1 \\
1 & 1 & 1 & 1
\end{bmatrix} \rightarrow \begin{bmatrix}
0 & 0 & 1 & 0 \\
0 & 1 & -1 & 1 \\
1 & -1 & 1 & 0 \\
0 & 1 & 0 & 0
\end{bmatrix}
\]

- Sums must be 0 or 1 by alternating property.
- Row sums of the resulting (0, 1)-matrix must be 1, 2, \ldots, $n$, since the rows of an ASM sum to 1.
- Reconstruction of the ASM: Let $r_1, r_2, \ldots, r_n$ be the rows of the CSM. Then row $i$ of the ASM is $r_i - r_{i-1}$ with row 1 being $r_1$.

ASMs as Monotone Triangles (MTs)

A monotone triangle (MT) is a triangular arrangement of $n(n+1)/2$ integers $t_{ij}$ taken from $\{1, 2, \ldots, n\}$ of shape 1, 2, \ldots, $n$ such that

- $t_{ij} < t_{i,j+1}$ for $1 \leq j \leq i$, (strictly increasing in rows)
- $t_{ij} \leq t_{i-1,j} \leq t_{i,j+1}$ for $1 \leq j \leq i - 1$.

\[
\begin{bmatrix}
0 & 0 & 1 & 0 \\
0 & 1 & -1 & 1 \\
1 & -1 & 1 & 0 \\
0 & 1 & 0 & 0
\end{bmatrix} \rightarrow \begin{bmatrix}
0 & 0 & 1 & 0 \\
0 & 1 & 0 & 1 \\
1 & 0 & 1 & 1 \\
1 & 1 & 1 & 1
\end{bmatrix} \rightarrow \begin{bmatrix}
0 & 0 & 1 & 0 \\
0 & 1 & 0 & 1 \\
1 & 0 & 1 & 1 \\
1 & 1 & 1 & 1
\end{bmatrix}
\]

The integers in the MT record the column indices of the 1s in the CSM of the ASM.
MacNeille Completion

Theorem (MacNeille 1937): Let \((P, \leq_P)\) be a finite partially ordered set. Then there exists a unique minimal lattice \((L, \leq_L)\) such that \(P \subseteq L\) and for \(a, b \in P\), \(a \leq_P b\) if and only if \(a \leq_L b\).

\((L, \leq_L)\) is the MacNeille completion of \((P, \leq)\).

Theorem (Lascoux & Schützenberger 1996): The MacNeille completion of \((\mathfrak{S}_n, \leq_B)\) is \((\mathfrak{A}_n, \leq_B)\) where \(\leq_B\) in \((\mathfrak{S}_n, \leq_B)\) is the Bruhat order on \(\mathfrak{A}_n\) defined by

\[ A_1 \leq_B A_2 \text{ iff } \Sigma(A_1) \geq \Sigma(A_2) \text{ (entrywise).} \]

In particular, the elements of the MacNeille completion of the \(n \times n\) permutation matrices with the Bruhat partial order are the \(n \times n\) ASMs.

Hasse diagram of \((\mathfrak{A}_3, \leq_B)\)

\[ L_3 = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix} \]

\[ D_3 \text{ where } D_3 = \begin{bmatrix} 0 & 1 & 0 \\ 1 & -1 & 1 \\ 0 & 1 & 0 \end{bmatrix} \]

\[ I_3 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \]
The $\lambda$-determinant arises by starting with
\[
\det_\lambda \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} = a_{11}a_{22} + \lambda a_{21}a_{22} \quad (\text{or with } \det_\lambda [a_{11}] = a_{11})
\]
and adapting the well-known Dodgson’s condensation formula for determinants (which iteratively expresses a determinant in terms of $2 \times 2$ determinants) to the $\lambda$-determinant using the rule
\[
\det_\lambda A = \frac{\det_\lambda A_{UL}\det_\lambda A_{LR} + \lambda\det_\lambda A_{UR}\det_\lambda A_{LL}}{\det_\lambda A_C}.
\]
($A_{UL}$ is the $(n-1) \times (n-1)$ submatrix in upper left, $A_{LR}$ in lower right, etc. and $A_C$ is the $(n-2) \times (n-2)$ submatrix in the center.)

If $\lambda = -1$, we get Dodgson’s formula for the ordinary determinant.
The $\lambda$-determinant

If $n = 2$, we get

$$\det_\lambda \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} = a_{11}a_{22} + \lambda a_{12}a_{21}.$$  

(if $\lambda = -1$, we get the ordinary determinant)

If $n = 3$, we get

$$\det_\lambda (A) = a_{11}a_{22}a_{33} + \lambda a_{12}a_{21}a_{33} + \lambda a_{11}a_{23}a_{32} + (\lambda^2 + \lambda)a_{12}a_{21}a_{22}^{-1}a_{23}a_{32} +$$

$$+ \lambda^2 a_{13}a_{21}a_{32} + \lambda^2 a_{12}a_{23}a_{31} + \lambda^3 a_{13}a_{22}a_{31}. \quad (n = 3)$$

(if $\lambda = -1$, we get the ordinary determinant)

The $\lambda$-determinant and ASMs

$$\det_\lambda (A) = a_{11}a_{22}a_{33} + \lambda a_{12}a_{21}a_{33} + \lambda a_{11}a_{23}a_{32} + (\lambda^2 + \lambda)a_{12}a_{21}a_{22}^{-1}a_{23}a_{32} +$$

$$+ \lambda^2 a_{13}a_{21}a_{32} + \lambda^2 a_{12}a_{23}a_{31} + \lambda^3 a_{13}a_{22}a_{31}. \quad (n = 3)$$

If for each of the seven terms we replace entries in $A$ by the corresponding power we get the seven $3 \times 3$ ASMs. For instance,

$$(\lambda^2 + \lambda)a_{12}a_{21}a_{22}^{-1}a_{23}a_{32} \rightarrow \begin{bmatrix} 0 & 1 & 0 \\ 1 & -1 & 1 \\ 0 & 1 & 0 \end{bmatrix},$$

and the other terms give the six $3 \times 3$ permutation matrices.

If $A = [a_{ij}]$ is an $n \times n$ matrix, then $\det_\lambda A$ is of the form

$$\sum_{B=[b_{ij}] \in \text{ASM}_{n \times n}} p_B(\lambda) \prod_{i,j=1}^n a_{ij}^{b_{ij}}$$

where $p_B(\lambda)$ is a (known) polynomial in $\lambda$.  

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Enumeration of ASMs

The $\lambda$-determinant led to the question: How many $n \times n$ ASMs are there? (How many terms in the expansion of the $\lambda$-determinant?)

- For small $n$, the number of $n \times n$ ASMs is: 1, 2, 7, 42, 429, 7436, . . . .
- **Celebrated Theorem**: The number of $n \times n$ ASMs is

\[
\frac{1!4!7! \cdots (3n-2)!}{n!(n+1)!(n+2)! \cdots (2n-1)!}.
\]


- This sequence occurred earlier in another context: Totally Symmetric Self-Complementary Plane Partitions.

TSSCPP

**TSSCPP** = **T**otally **S**ymmetric **S**elf-**C**omplementary **P**lane-**P**artitions.

**Example**: (Stack to form a $4 \times 4 \times 4$ configuration)

\[
\begin{array}{ccc|ccc|ccc}
11 & 5 & 10 & 6 & 6 & 10 & 5 & 11 \\
\hline
x & x & x & x & x & x & x & x & x \\
x & x & x & x & y & x & x & x & y \\
x & x & x & y & x & x & y & y & y \\
x & y & y & y & x & y & y & y & y \\
\end{array}
\]
Number of TSSCPP

Andrews (1994) showed that the number of TSSCPPs in a $2n \times 2n \times 2n$ configuration equals

$$
\prod_{j=0}^{n-1} \frac{(3j + 1)!}{(n + j)!}
$$

the same number that was conjectured for the number of $n \times n$ ASMs.

No bijection between ASMs and TSSCPPs is known.

ASMs and Square Ice

There is a 1-1 correspondence between ASMs and something called "square ice" configurations: a system of water (H$_2$O) molecules frozen in a square lattice.
Square Ice I

There are oxygen atoms at each vertex of an $n \times n$ lattice, with hydrogen atoms between successive oxygen atoms in a row or column, and on either vertical side of the lattice, but not on the two horizontal sides. E.G. $n = 4$:

\[
\begin{array}{cccccccc}
H & O & H & O & H & O & H \\
H & H & H & H \\
H & O & H & O & H & O & H \\
H & H & H & H \\
H & O & H & O & H & O & H \\
H & H & H & H \\
\end{array}
\]

Each $O$ is to be attached to two $H$s (a water molecule $H_2O$) in a one to two bijection. There are six possible configurations in which an oxygen atom can be attached to two hydrogen atoms:

\[
\begin{array}{cccccccc}
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\end{array}
\]

Square Ice II

\[
\begin{array}{cccccccc}
H \\
\uparrow \\
H & \leftrightarrow & O & \rightarrow & H \\
\downarrow \\
H \\
\end{array}
\]

\[
\begin{array}{cccccccc}
H & H & O & \rightarrow & H & H & \leftrightarrow & O \\
\uparrow & \uparrow & \downarrow & \downarrow \\
H & \leftrightarrow & O & \rightarrow & H & H \\
\end{array}
\]

Let the top left (horizontal) configuration correspond to $1$ and the top right (vertical) configuration correspond to $-1$. Let the other four (skew) configurations correspond to $0$.  

\[
\begin{array}{cccccccc}
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\end{array}
\]
Square Ice III

\((n = 4)\)

\[
\begin{array}{cccc}
H & \leftrightarrow & O & H \\
\downarrow & & \downarrow & \downarrow \\
H & & H & H \\
\uparrow & & \uparrow & \uparrow \\
H & \leftrightarrow & O & \rightarrow H \\
\downarrow & & \downarrow & \downarrow \\
H & & H & H \\
\uparrow & & \uparrow & \uparrow \\
H & \leftrightarrow & O & \rightarrow H \\
\downarrow & & \downarrow & \downarrow \\
H & & H & H \\
\uparrow & & \uparrow & \uparrow \\
H & \leftrightarrow & O & \rightarrow H \\
\end{array}
\]

and this corresponds to the ASM:

\[
\begin{pmatrix}
0 & 0 & 1 & 0 \\
1 & 0 & -1 & 1 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0
\end{pmatrix}
\]

Maximal ASMs I

An extension of an \(n \times n\) ASM \(A = [a_{ij}]\) is an \(n \times n\) ASM \(B = [b_{ij}]\) such that \(B \neq A\) and

\[a_{ij} \neq 0 \text{ implies } b_{ij} = a_{ij} \quad (1 \leq i, j \leq n).\]

A maximal ASM is an ASM without any extensions.

Examples:

\[
\begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1
\end{pmatrix}
\]
is maximal.

\[
\begin{pmatrix}
0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 \\
1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0 & 0
\end{pmatrix}
\]
is not:

\[
\begin{pmatrix}
0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 \\
1 & -1 & 1 & 0 & 0 \\
0 & 1 & -1 & 0 & 1 \\
0 & 0 & 1 & 0 & 0
\end{pmatrix}
\]
Maximal ASMs II

An **elementary extension** of an ASM is an ASM extension obtained by replacing a $2 \times 2$ zero submatrix by

$$T = \pm \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}.$$ 

Recall that permutation matrices are ASMs.

**Theorem:** A permutation matrix is not a maximal ASM iff it has an elementary ASM extension.

Maximal ASMs III

It is sometimes possible to add $T = \pm \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$ to a $2 \times 2$ nonzero submatrix of an ASM with the result being an ASM. E.G.

$$\begin{bmatrix} 0 & 0 & +1 & 0 & 0 \\ 0 & +1 & 0 & 0 & 0 \\ +1 & 0 & -1 & 0 & +1 \\ 0 & 0 & 0 & +1 & 0 \\ 0 & 0 & +1 & 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & +1 & 0 \\ 0 & 0 & +1 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix} =$$

$$\begin{bmatrix} 0 & 0 & +1 & 0 & 0 \\ 0 & +1 & -1 & +1 & 0 \\ +1 & 0 & 0 & -1 & +1 \\ 0 & 0 & 0 & +1 & 0 \\ 0 & 0 & +1 & 0 & 0 \end{bmatrix}$$
ASM Interchanges

Call this operation of adding \( T = \pm \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \) to a \( 2 \times 2 \) (not necessarily zero) submatrix of an ASM an ASM interchange. ASM interchanges generalize transpositions of permutations. The reason is that a permutation interchange in terms of the corresponding permutation matrix can be gotten by an ASM interchange:

\[
\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + \begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}.
\]

Generating ASMs

The following theorem generalizes the basic fact that the permutations of \( \{1, 2, \ldots, n\} \) can be generated from the identity permutation by a sequence of transpositions:

**Theorem:** Any \( n \times n \) ASM can be gotten from the identity matrix \( I_n \) by a sequence of ASM interchanges.
**ASM Recall**

An **ASM** is an $n \times n$ $(0, 1, -1)$-matrix such that, ignoring 0s, in each row and column the 1's and $-1$'s alternate beginning and ending with a 1. For example,

\[
\begin{bmatrix}
+ & - & + \\
- & + & - \\
+ & - & + \\
+ & - & + \\
\end{bmatrix}
\]

\[
\begin{bmatrix}
+ & - & + \\
- & + & - \\
+ & - & + \\
+ & + \\
\end{bmatrix}
\]

**(0, $-1$)-matrices**

A an $n \times n$ $(0, -1)$-matrix.

Completion of $A$: an $n \times n$ $(0, +1, -1)$-matrix $B$ obtained from $A$ by replacing some 0s with $+1$s. If $B$ is an ASM, then $B$ is an **ASM completion** of $A$.

Example:

\[
A = \begin{bmatrix}
-1 \\
-1 & -1 \\
-1 & -1 \\
-1 & -1 \\
\end{bmatrix}
\]

Can $A$ be completed to an ASM?
Any completion of \( A \) to an ASM must include +1s as shown in

\[
A' = \begin{bmatrix}
  & & & +1 \\
  & +1 & -1 & +1 \\
  +1 & -1 & -1 & +1 \\
  +1 & -1 & -1 & +1 \\
  +1 & -1 & +1 \\
  & & & +1
\end{bmatrix}
\]

For an ASM completion, +1s are required between four pairs of \(-1\)s, but the result is never an ASM. Note that if we put a \(-1\) in the middle position of \( A \), then there is a unique completion to an ASM:
Necessary conditions for an ASM completion

A = \([a_{ij}]\) an \(n \times n\) \((0, -1)\)-matrix. For \(A\) to have an ASM completion, the following must hold:

1. \(A\) does not have any \(-1\)s in its first and last row and column.
2. There do not exist consecutive \(-1\)s in a row or column.
3. If \(U = (u_1, u_2, \ldots, u_n)\) and \(V = (v_1, v_2, \ldots, v_n)\) record the number of \(-1\)s in the rows and columns of \(A\), then \(U, V \leq (0, 1, 2, 3, \ldots, 3, 2, 1, 0)\) (entrywise).

Bordered-Permutation \((0, -1)\)-Matrix

An \(n \times n\) \((0, -1)\)-matrix \(A\) such that

- The first and last rows and columns contain only zeros, and
- The middle \((n - 2) \times (n - 2)\) submatrix

\[
A[\{2, 3, \ldots, n - 1\}|\{2, 3, \ldots, n - 1\}] = -P
\]

where \(P\) is a permutation matrix.

Example:

\[
\begin{bmatrix}
\phantom{-1} & -1 & \\
-1 & -1 & \\
-1 & & \\
\end{bmatrix}
\rightarrow
\begin{bmatrix}
+1 & -1 & +1 \\
+1 & -1 & +1 \\
+1 & -1 & +1 \\
\end{bmatrix}
\]

(ASM)
In general, there is a 1-1 correspondence between the set of ASM completions of a $(0, -1)$-matrix $A$ and the set of perfect matchings of a bipartite graph $G(A) \subseteq K_{n+\sigma,n+\sigma}$ where $\sigma$ is the number of $-1$s of $A$. In particular, $A$ has a completion to an ASM iff the bipartite graph $G(A)$ has a perfect matching (so there is a polynomial algorithm to determine an ASM completion).

This is illustrated by the previous example where $n = 5$, $\sigma = 3$, and $G(A) \subseteq K_{8,8}$ (horizontal partition of empty positions versus vertical partition):

\[
\begin{pmatrix}
+1 & & & & +1 \\
-1 & -1 & & & +1 \\
& +1 & -1 & +1 & \\
+1 & -1 & & +1 & \\
& & & & +1
\end{pmatrix}
\]

**Theorem:** Let $n \geq 2$. An $n \times n$ bordered-permutation $(0, -1)$-matrix $A$ can be completed to an ASM.

**Corollary:** An $n \times n$ $(0, -1)$-matrix such that the first and last rows and columns are zero rows and zero columns, respectively, and $A[[2, 3, \ldots, n-1]|\{2, 3, \ldots, n-1\}]$ has at most one $-1$ in each row and column. Then $A$ has an ASM completion.
Example: Bordered-perm. \((0, -1)\)-matrix with another \(-1\)

\[
\begin{bmatrix}
-1 & & & & \\
-1 & -1 & & & \\
-1 & & -1 & & \\
& & & & \\
& & & & \\
\end{bmatrix}
\]

. To complete must have:

\[
\begin{bmatrix}
+1 & & & & \\
+1 & -1 & +1 & & \\
+1 & -1 & +1 & +1 & \\
+1 & -1 & +1 & & \\
+1 & -1 & +1 & & \\
\end{bmatrix}
\]

and this is not further completable to an ASM.

Monotone Decomposition

An \(n \times n\) bordered-permutation \((0, -1)\)-matrix \(A\) has a monotone decomposition provided \(A\) contains a position with \(-1\) (a central position or central \(-1\)) that partitions \(A\) as

\[
\begin{bmatrix}
A_{11} & & A_{12} \\
& -1 & \\
A_{21} & & A_{22}
\end{bmatrix},
\tag{1}
\]

where the \(-1\)s in \(A_{11}\) and \(A_{22}\) are monotone decreasing, and those in \(A_{12}\) and \(A_{21}\) are monotone increasing (e.g. the \(-1\)s in \(A_{11}, A_{12},\) and the central \(-1\) are “concave up”).
**Example**

A monotone decomposition of a $9 \times 9$ bordered-permutation $(0, -1)$-matrix:

$$A = \begin{bmatrix}
\end{bmatrix}.$$  

The $-1$ in position $(5, 6)$ is the central $-1$ of the monotone decomposition.

**CRM - Barcelona, June 29 – July 3, 2015**

**Example continued**

It has a unique ASM completion which is easily determined to be

$$\begin{bmatrix}
\end{bmatrix}.$$  

**CRM - Barcelona, June 29 – July 3, 2015**
**Theorem**

Let $n \geq 3$. An $n \times n$ bordered-permutation $(0, -1)$-matrix $A$ has a unique completion to an ASM if and only if $A$ has a monotone decomposition.

Proof is fairly long and uses induction

**A Conjecture**

Let $E_m$ be the $m \times m$ $(0, -1)$-matrix with $-1$s in positions $(2, m), (3, m - 1), \ldots, (m, 2)$ and let $F_m$ be the $m \times m$ $(0, -1)$-matrix with $-1$s in positions $(1, m - 1), (2, m - 2), \ldots, (m - 1, 1)$.

**Conjecture** If $n \geq 4$ is even, then

$$E_{n/2} \oplus F_{n/2}$$

is the $n \times n$ bordered-permutation $(0, -1)$-matrix with the largest number of ASM completions. If $n \geq 5$ is odd, then

$$E_{(n-1)/2} \oplus (-I_1) \oplus F_{(n-1)/2}$$

is the $n \times n$ bordered-permutation $(0, -1)$-matrix with the largest number of ASM completions.
Example of the Conjecture I

For instance, with $n = 10$ we have

$$E_5 \oplus F_5 = \begin{bmatrix}
-1 \\
-1 \\
-1 \\
-1 \\
-1 \\
-1 \\
-1 \\
-1 \\
-1 \\
-1 \\
\end{bmatrix}.$$

Example of the Conjecture II

Every completion of $E_5 \oplus F_5$ to an ASM must have $+1$s as shown in

$$\begin{bmatrix}
+1 & -1 \\
+1 & -1 \\
+1 & -1 \\
+1 & -1 \\
-1 & +1 \\
-1 & +1 \\
-1 & +1 \\
-1 & +1 \\
+1 & \\
\end{bmatrix}.$$
Example of the Conjecture III

Our conjecture asserts that the matrix

\[
\begin{bmatrix}
1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 \\
\end{bmatrix}
\]

has the largest permanent among the permanents of all the adjacency matrices of bipartite graphs \(G(A)\) where \(A\) is a 10 \(\times\) 10 bordered-permutation \((0, -1)\)-matrix. More generally, in the even case, it asserts that the largest permanent is obtained by the \((n - 2) \times (n - 2)\) \((0, 1)\)-Hankel matrix with an equal number of bands of 1s to the left and below the upper right corner.

Some Basics

- \(\mathcal{A}_n = \{\text{all } n \times n \text{ ASMs}\}\).
- \(\rho(X)\) is the spectral radius of the square matrix \(X\), that is, the maximum absolute value of an eigenvalue of \(X\).
- \(\rho_n = \max\{\rho(A) : A \in \mathcal{A}\}\).
- Since all row and column sums of an ASM equal 1, 1 is an eigenvalue of every ASM with corresponding eigenvector equal to a vector of all 1s. Thus \(\rho(A) \geq 1\) for every ASM.
- Equality holds for permutation matrices but can also hold for ASMs that are not permutation matrices.
Example

\[ A = \begin{bmatrix}
0 & 0 & +1 & 0 & 0 \\
+1 & 0 & -1 & +1 & 0 \\
0 & 0 & +1 & -1 & +1 \\
0 & 0 & 0 & +1 & 0 \\
0 & +1 & 0 & 0 & 0
\end{bmatrix}. \]

Characteristic polynomial of \( A \) is

\[(\lambda - 1)^2(\lambda + 1)(\lambda^2 - \lambda + 1)\]

and hence \( A \) has eigenvalues

\[ 1, 1, -1, \frac{1 \pm \sqrt{-3}}{2} \]

all of which have absolute value equal to 1. Therefore \( \rho(A) = 1 \). (Note that \( A^6 = I_6 \) also shows that \( \rho(A) = 1 \).)

Diamond ASM \( D_n : n \) odd

\[ D_7 = \begin{bmatrix}
+ & - & + & - & - & + & - \\
+ & - & + & - & - & + & - \\
+ & - & + & - & - & + & - \\
+ & - & + & - & - & + & - \\
+ & - & + & - & - & + & - \\
+ & - & + & - & - & + & - \\
+ & - & + & - & - & + & - \\
\end{bmatrix} \quad (n \text{ odd : } \frac{n^2 + 1}{2} \text{ nonzeros}). \]
Diamond ASM $D_n$: $n$ odd, again

$$D_7 = E_7$$

where $E_7 = \text{diag}(1, -1, 1, -1, 1, -1, 1)$. In general, $D_n$ is diagonally similar to $|D_n|$ and has the same spectrum as $|D_n|$ ($n$ odd). In particular, $\rho(D_n) = \rho(|D_n|)$.

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Diamond ASM $D_n$: $n$ even

Similarly,

$$D_6 = \begin{bmatrix} + & + & + \cr + & + & + \cr + & + & + \cr + & + & + \cr + & + & + \cr + & + & + \cr \end{bmatrix} \quad (n \text{ even}; \frac{n^2}{2} \text{ nonzeros}).$$

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Diamond ASM $D_n$: $n$ even again

$$D_6 = E_6 \begin{bmatrix}
| & | & | & + & | \\
| & + & + & + & | \\
| & + & + & + & + |
+ + + + + \\
| + + + | \\
| + | \\
\end{bmatrix} E_6$$

where $E_6 = \text{diag}(1, -1, 1, -1, 1, -1)$. In general, $D_n$ is diagonally similar to $|D_n|$ and has the same spectrum as $|D_n|$ ($n$ even). In particular, $\rho(D_n) = \rho(|D_n|)$.

Two Negative Observations (1)

Not every ASM is signature similar to its absolute value, e.g.

$$\begin{bmatrix}
0 & 0 & +1 & 0 \\
+1 & 0 & -1 & +1 \\
0 & 0 & +1 & 0 \\
0 & +1 & 0 & 0
\end{bmatrix} \text{ is not sig. similar to } \begin{bmatrix}
0 & 0 & 1 & 0 \\
1 & 0 & 1 & 1 \\
0 & 0 & 1 & 0 \\
0 & 1 & 0 & 0
\end{bmatrix}. $$

(They have the same eigenvalues, namely 0, 1, 1, −1, but they have different Jordan canonical forms.)
Two Negative Observations (2)

- Not every $n \times n$ ASM $A$ satisfies $|A| \leq Q|D_n|Q^T$ for some permutation matrix $Q$ for some permutation matrix $Q$, e.g.

$$A = \begin{bmatrix} 0 & +1 & 0 & 0 & 0 & 0 \\ +1 & -1 & +1 & 0 & 0 & 0 \\ 0 & +1 & -1 & +1 & 0 & 0 \\ 0 & 0 & +1 & -1 & +1 & 0 \\ 0 & 0 & 0 & +1 & -1 & +1 \\ 0 & 0 & 0 & 0 & +1 & 0 \end{bmatrix}$$

is such that $|A|$ is not permutation similar to a matrix $B \leq |D_6|$.

Maximum Spectral Radius

$\rho_n = \rho(D_n)$ and for $A$ an $n \times n$ ASM, $\rho(A) = \rho(D_n)$ iff $A = D_n$

By negative observation (1) this does not directly reduce to an application of the Perron-Frobenius theory of nonnegative matrices.

By negative observation (2) and the fact that $\rho(X) \leq \rho(|X|) \leq \rho(D_n)$ if $|X| \leq |D_n|$, this does not directly reduce to application of the Perron-Frobenius theory of nonnegative matrices.
Maximum Spectral Radius: $n$ odd (easy case)

Let $X_n = |D_n|^2$; e.g. $X_7 = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 3 & 3 & 3 & 3 & 3 & 1 \\ 1 & 3 & 5 & 5 & 5 & 5 & 1 \\ 1 & 3 & 5 & 7 & 5 & 3 & 1 \\ 1 & 3 & 5 & 5 & 5 & 5 & 1 \\ 1 & 3 & 3 & 3 & 3 & 3 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix}$. Note that the middle row of $X_n$ bounds the number of nonzeros in the rows and columns of an ASM, and it follows that for $A$ an $n \times n$ ASM, $|A|^2 \leq X_n$ with equality iff $A = D_n$.

So by (PF)

$$\rho(|A_n|^2) \leq \rho(X_n) = \rho(|D_n|^2)$$

with equality if and only if $|A_n|^2 = |D_n|^2$. Since $\rho(|A_n|^2) = \rho(|A_n|)^2$, we get $\rho(A_n) \leq \rho(D_n)$ with equality iff $A_n = D_n$.

Maximum Spectral Radius: $n$ even (harder case), 1

Outline: Define $X_n$ like the matrix in the odd case but now there is no middle row, e.g.

$$X_8 = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 3 & 3 & 3 & 3 & 3 & 1 \\ 1 & 3 & 5 & 5 & 5 & 5 & 1 \\ 1 & 3 & 5 & 7 & 5 & 3 & 1 \\ 1 & 3 & 5 & 7 & 7 & 5 & 3 \\ 1 & 3 & 5 & 5 & 5 & 5 & 1 \\ 1 & 3 & 3 & 3 & 3 & 3 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix}.$$

If $E_n$ is the anti-identity matrix, then $|D_n|^2 = X_n - E_n$. 
Maximum Spectral Radius: $n$ even (harder case), II

$$|D_8|^2 = X_8 - E_8 = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 0 \\ 1 & 3 & 3 & 3 & 3 & 3 & 2 & 1 \\ 1 & 3 & 5 & 5 & 4 & 3 & 1 \\ 1 & 3 & 5 & 7 & 6 & 5 & 3 & 1 \\ 1 & 3 & 5 & 6 & 7 & 5 & 3 & 1 \\ 1 & 3 & 4 & 5 & 5 & 5 & 3 & 1 \\ 1 & 2 & 3 & 3 & 3 & 3 & 3 & 1 \\ 0 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix}.$$

Spectral Radius

Spectral Radius of the Diamond ASM

For large $n$, $\rho(D_n)$ is essentially $\frac{2}{\pi}n$:

$$\rho_n = \frac{2}{\pi}n + O(1).$$

CRM - Barcelona, June 29 – July 3, 2015

Generalized ASMs

$u = (u_1, u_2, \ldots, u_n), u' = (u'_1, u'_2, \ldots, u'_n), v = (v_1, v_2, \ldots, v_m), \text{ and } v' = (v'_1, v'_2, \ldots, v'_m)$ are vectors of $\pm1$s.

A $(u, u'|v, v')$-ASM is an $m \times n$ $(0, \pm1)$-matrix $A$ such that the $+1$s and $-1$s in rows $1, 2, \ldots, m$ and columns $1, 2, \ldots, n$ of the $(m + 2) \times (n + 2)$ $(0, \pm1)$-matrix $A'$ below alternate:

$$A' = \begin{bmatrix}
0 & u_1 & u_2 & \cdots & u_{n-1} & u_n & 0 \\
v_1 \\
v_2 \\
\vdots \\
v_{m-1} \\
v_m \\
0 & u'_1 & u'_2 & \cdots & u'_{n-1} & u'_n & 0
\end{bmatrix}$$

(2) $A = A'[1, 2, \ldots, m|1, 2, \ldots, n]$. 

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Examples

\[
A' = \begin{pmatrix}
+ & - & - & + \\
- & + & - & + \\
+ & - & + & - \\
- & + & - & + \\
\end{pmatrix}, \quad A' = \begin{pmatrix}
+ & - & - & - \\
- & + & - & - \\
+ & - & + & - \\
- & + & - & + \\
\end{pmatrix}
\]

Remarks

- \( u = (+1, +1), \ u' = (-1, +1), \ v = (+1, +1), \ v' = (+1, -1) \): a \((u, u'|v, v')\)-ASM does not exist:

\[
\begin{pmatrix}
+ & + \\
- & + \\
- & + \\
\end{pmatrix}
\]

(Impossible to get alternating signs).

- \( u = u' = v = v' = (-1, -1, \ldots, -1) \): a \((u, u'|v, v')\)-ASM is an ordinary ASM.

- If \( A \) is any \((0, \pm 1)\)-matrix in which the +1s and −1s alternate in each row and column, then we may choose \( u, u', v, v' \) so that \( A \) is a \((u, u'|v, v')\)-ASM.
When does a \((u, u'|v, v')\)-ASM exist?

Some Notation

For \(k = 1, 2, \ldots, m\) and \(l = 1, 2, \ldots, n\), let
\[
\begin{align*}
    r^+_k &= r^+_k(v, v') \text{ is the number of } i \leq k \text{ such that } v_i = v'_i = +1, \\
    r^-_k &= r^-_k(v, v') \text{ is the number of } i \leq k \text{ such that } v_i = v'_i = -1, \\
    c^+_i &= c^+_i(u, u') \text{ is the number of } j \leq l \text{ such that } u_j = u'_j = +1, \\
    c^-_i &= c^-_i(u, u') \text{ is the number of } j \leq l \text{ such that } u_j = u'_j = -1.
\end{align*}
\]

So,
\[
\begin{align*}
    r^+_m &= r^+_m(v, v') \text{ is the total number of } i \text{ such that } v_i = v'_i = +1, \\
    r^-_m &= r^-_m(v, v') \text{ is the total number of } i \text{ such that } v_i = v'_i = -1, \\
    c^+_n &= c^+_n(u, u') \text{ is the total number of } j \text{ such that } u_j = u'_j = +1, \\
    c^-_n &= c^-_n(u, u') \text{ is the total number of } j \text{ such that } u_j = u'_j = -1.
\end{align*}
\]

Let
\[
\begin{align*}
    u^+ &= |\{j : u_j = +1\}|, \\
    u^- &= |\{j : u_j = -1\}|, \\
    v^+ &= |\{i : v_i = +1\}|, \\
    v^- &= |\{i : v_i = -1\}|.
\end{align*}
\]
Necessary Conditions

Necessary conditions for existence are

\[ r_m^- (v, v') - r_m^+ (v, v') = c_n^- (u, u') - c_n^+ (u, u'), \]
\[ -v^+ \leq r_k^- (v, v') - r_k^+ (v, v') \leq v^- \quad (k = 1, 2, \ldots, m), \]
\[ -u^+ \leq c_l^- (u, u') - c_l^+ (u, u') \leq u^- \quad (l = 1, 2, \ldots, n). \]

**Theorem.** A \((u, u'|v, v')\)-ASM exists if and only if these conditions are satisfied.

The proof contains an algorithm to construct a \((u, u'|v, v')\)-ASM when these conditions are satisfied.

---

Questions

- The number of \((u, u'|v, v')\)-ASMs?
- The minimum and maximum number of nonzeros in an \((u, u'|v, v')\)-ASM,?

For classical ASMs, these numbers are, respectively, \(n\) (the permutation matrices) and \(n^2/2\) (\(n\) even) and \((n^2 + 1)/2\) (\(n\) odd) (the diamond ASMs). If \(u = u' = v = v'\) with the +1s and −1s alternating, then there is a \((u, u'|v, v')\)-ASM with \(n\) nonzeros in a permutation set of places and \(n\) is clearly the minimum number of nonzeros; the maximum number is \(n^2\) if \(n\) is odd and \(n^2 - n\) if \(n\) is even.
References IIa


References IIb

Tournaments

A tournament $T_n$ of order $n$ is an orientation of the complete graph $K_n$ of order $n$: For each unordered pair $\{p, q\}$ of distinct integers from $\{1, 2, \ldots, n\}$ one chooses an ordering of first element and second element, e.g. $(q, p)$, usually denoted as $q \to p$.

Ex. $K_6$ and orientation of it giving a $T_6$.

$4, 3, 3, 2, 2, 1$ is the score vector

e.g. $1 \to 2, 1 \to 3, 1 \to 4, 1 \to 6, \text{ but } 5 \to 1$

Tournament Matrices

A tournament has an $n \times n$ adjacency matrix $T = [t_{ij}]$ where $t_{ii} = 0$ for all $i$ and $t_{ij} + t_{ji} = 1$ for all $i \neq j$. Thus

$$T + T^t = J_n - I_n$$

where $J_n$ is the $n \times n$ matrix of all 1s.

Example: $T = \begin{bmatrix} 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{bmatrix}$.

The score vector of a tournament $T$ is the vector $R = (r_1, r_2, \ldots, r_n)$ of row sums of $T$. In the example, $R = (2, 1, 1, 1)$. WLOG, $R$ is nondecreasing: $r_1 \leq r_2 \leq \cdots \leq r_n$. In the example, interchange vertices 1 and 4 (interchange rows 1 and 4, and interchange columns 1 and 4).
Tournaments Matrices

A tournament has an $n \times n$ adjacency matrix $T = [t_{ij}]$ where $t_{ii} = 0$ for all $i$ and $t_{ij} + t_{ji} = 1$ for all $i \neq j$. Thus

$$T + T^t = J_n - I_n$$

where $J_n$ is the $n \times n$ matrix of all 1s.

**Example:**

$$T = \begin{bmatrix}
0 & 1 & 0 & 1 \\
0 & 0 & 1 & 0 \\
1 & 0 & 0 & 1 \\
0 & 1 & 0 & 0
\end{bmatrix} \quad \longrightarrow \quad \begin{bmatrix}
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
1 & 0 & 0 & 1 \\
1 & 1 & 0 & 0
\end{bmatrix}$$

The score vector of a tournament $T$ is the vector $R = (r_1, r_2, \ldots, r_n)$ of row sums of $T$. In the example, $R = (2, 1, 2, 1)$. WLOG $R$ is nondecreasing: $r_1 \leq r_2 \leq \cdots \leq r_n$. In the example, interchange vertices 2 and 3 (interchange rows 2 and 3, and interchange columns 2 and 3).

Inverse problem: Theorem of Landau (1953) on Score Vectors of Tournaments

**Theorem:** Let $R = (r_1, r_2, \ldots, r_n)$ be a vector of nondecreasing, nonnegative integers. Then $R$ is the score vector of a tournament if and only if

$$\sum_{i=1}^{k} r_i \geq \binom{k}{2} \quad (k = 1, 2, \ldots, n),$$

with equality for $k = n$.

(These conditions are obviously necessary.)

Let $T(R)$ denote the set of all tournaments (tournament matrices) with score vector $R$.
Ryser’s Theorem on $\mathcal{T}(R)$: Generating $\mathcal{T}(R)$

Given $T_1, T_2 \in \mathcal{T}(R)$, there is a sequence of motions of three types which transform $T_1$ to $T_2$. These are the $\Delta$-interchange which interchanges a certain $3 \times 3$ principal submatrix for another as shown:

$$C = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix} \leftrightarrow \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} = C'$$ (i.e. reversing arcs of a 3-cycle).

and two types of double-interchanges, replacing a $4 \times 4$ principal submatrix for another as shown where $a$ and $b = 0$ or $1$ (two 3-cycle reversals does this):

$$D_1 = \begin{bmatrix} 0 & a & 1 & 0 \\ 1 - a & 0 & 0 & 1 \\ 0 & 1 & b & 0 \\ 1 & 0 & 1 - b & 0 \end{bmatrix} \leftrightarrow \begin{bmatrix} 0 & a & 0 & 1 \\ 1 - a & 0 & 1 & 0 \\ 1 & 0 & 0 & b \\ 0 & 1 & 1 - b & 0 \end{bmatrix} = D_1'.$$

and

$$D_2 = \begin{bmatrix} 0 & 1 & 0 & a \\ 0 & 0 & b & 1 \\ 1 & 1 - b & 0 & 0 \\ 1 - a & 0 & 1 & 0 \end{bmatrix} \leftrightarrow \begin{bmatrix} 0 & 0 & 1 & a \\ 0 & 1 & 0 & b \\ 1 & 0 & 1 - b & 0 \\ 1 - a & 1 & 0 & 0 \end{bmatrix} = D_2'.$$

Multi-Tournaments

Replace $K_n$ by any multigraph on $n$ vertices and choose an orientation for each edge. Equivalently, take an $n \times n$ symmetric, nonnegative integral matrix $C = [c_{ij}]$ with zero diagonal, and for each $i < j$, choose nonnegative integral $a_{ij}$ and $a_{ji}$ with $a_{ij} + a_{ji} = c_{ij}$ giving an $n \times n$ nonnegative integral matrix $A = [a_{ij}]$ with $A + A^t = C$, called a $C$-tournament. If $C = J_n - I_n$, then we get the tournament matrices as previously defined.

**Example:**

$$C = \begin{bmatrix} 0 & 5 & 1 \\ 5 & 0 & 2 \\ 1 & 2 & 0 \end{bmatrix} \rightarrow A = \begin{bmatrix} 0 & 2 & 1 \\ 3 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}.$$

The row (column) sum vector of $C$ gives the number of games played by each team. In the example it is $(6, 7, 3)$.

The score vector is the row sum vector $R$ of $A$; the loss vector is the column sum vector $S$ of $A$. In the example. $R = (3, 4, 1)$ and $S = (3, 3, 2)$.
Hakimi’s 1965 Theorem (Unaware of Landau’s Theorem) and Cruse 1978 (Unaware of Hakimi’s Theorem)

Let $C = [c_{ij}]$ be an $n \times n$ symmetric, nonnegative integral matrix with 0s on the main diagonal. A vector $R = (r_1, r_2, \ldots, r_n)$ of nonnegative integers is the score vector of a $C$-tournament if and only if

$$r(J) \geq c(J) \quad (J \subseteq \{1, 2, \ldots, n\}) \text{ with equality if } J = \{1, 2, \ldots, n\}.$$  

Here $r(J) = \sum_{j \in J} r_j$ and $c(J) = \sum_{i,j \in J, i < j} c_{ij}$. Note that $c(J)$ is the total number of games played amongst the players in $J$ so that the above condition is surely necessary.

Let $\mathcal{T}_C(R)$ be the set of all $C$-tournaments with score vector $R$.

Generating $\mathcal{T}_C(R)$

Given any $C$-tournament $T_1$ in $\mathcal{T}_C(R)$, then by a sequence of reversals of the arcs of directed cycles, one get from $T_1$ to any other $C$-tournament $T_2$ in $\mathcal{T}_C(R)$ with all intermediate tournaments in $\mathcal{T}_C(R)$. In the case of classical tournaments (that is, $C = J - I$), reversals of arcs of 3-cycles suffices.

Reason: Difference of two tournaments in $\mathcal{T}_C(R)$ is a digraph in which the outdegree of each vertex equals its indegree, and so can be partitioned into directed cycles. Now reverse each of those directed cycles.
Loopy Tournaments: Motivations

- **From the matrix point of view:** there is no reason to have 0’s on the main diagonal.
- **From the game point of view:** Before the round-robin competition begins, each player $i$ flips a coin after calling heads or tails. If player $i$ calls the coin correctly, the player gets a win, and we set $t_{ii} = 1$; otherwise, we set $t_{ii} = 0$. A correct call adds 1 to a player’s score. As before, the score vector $R = (r_1, r_2, \ldots, r_n)$ equals the number of 1s in each row of the resulting loopy tournament $T$. The score vector still determines the losing vector $S = (s_1, s_2, \ldots, s_n)$ since $r_i + s_i = n$ for all $i$. But now $S$ is not in general the vector of column sums of $T$. If $S' = (s'_1, s'_2, \ldots, s'_n)$ is the column sum vector of $T$, then $r_i + s'_i = n - 1$ or $n + 1$ depending on whether $t_{ii} = 0$ or $t_{ii} = 1$.

Note that every tournament is also a loopy tournament (all calls of the coin are wrong!).

Example of a Loopy Tournament

\[
T = \begin{bmatrix}
0 & 1 & 1 & 0 & 0 \\
0 & 1 & 1 & 0 & 1 \\
0 & 0 & 0 & 1 & 1 \\
1 & 1 & 0 & 0 & 1 \\
1 & 0 & 0 & 0 & 1
\end{bmatrix}, \quad \text{where} \quad T + T^t = \begin{bmatrix}
0 & 1 & 1 & 1 & 1 \\
1 & 2 & 1 & 1 & 1 \\
1 & 1 & 0 & 1 & 1 \\
1 & 1 & 1 & 0 & 1 \\
1 & 1 & 1 & 1 & 2
\end{bmatrix}.
\]

The score vector of $T$ is $(2, 3, 2, 3, 2)$; the losing vector is $(3, 2, 3, 2, 3)$. The column sum vector of $T$ is $(2, 3, 2, 1, 4)$. 

CRM - Barcelona, June 29 – July 3, 2015
Weakening of Landau’s Conditions for $\mathcal{T}(R) \neq \emptyset$

Let $k$ be a nonnegative integer. A vector $R = (r_1, r_2, \ldots, r_n)$ is \textit{k-nearly nondecreasing} provided there is a vector $u = (u_1, u_2, \ldots, u_n)$ such that $u_i \in \{0, 1, \ldots, k\}$ with $R - u$ nondecreasing.

Thus $R$ is $k$-nearly nondecreasing if and only if $r_j \geq r_i - k$ for $1 \leq i < j \leq n$. If $k = 0$, then $R$ is nondecreasing. If $k = 1$, then we use \textit{nearly nondecreasing} instead of $k$-nearly nondecreasing. For example, $(3, 2, 3, 4, 3, 4)$ is nearly nondecreasing.

\textbf{Lemma:} Let $R = (r_1, r_2, \ldots, r_n)$ be a $2$-nearly nondecreasing vector of nonnegative integers. Assume that $R$ satisfies Landau’s inequalities

$$\sum_{i=1}^{k} r_i \geq \binom{k}{2}$$

with equality if $k = n$.

Then the nondecreasing rearrangement of $R$ also satisfies Landau’s inequalities. (Proof is by algebraic manipulation.) \textbf{So it suffices to assume $R$ is $2$-nearly nondecreasing in Landau’s theorem.}

\textbf{Landau-like Theorem for Loopy Tournaments}

\textbf{Theorem:} Let $R = (r_1, r_2, \ldots, r_n)$ be a vector of nonnegative integers with $r_1 \leq r_2 \leq \cdots \leq r_n$. Then there exists an loopy tournament with score vector $R$ if and only if there is an integer $t$ with $0 \leq t \leq n$ such that

$$\sum_{i=1}^{k} r_i \geq \binom{k}{2} + (k-t)^+, (k = 1, 2, \ldots, n),$$

with equality when $k = n$.

When these conditions are satisfied, the number of $1$s on the main diagonal of the loopy tournament is $n - t$ and these can be taken to be in the last $(n - t)$ positions on the main diagonal (i.e. the “best” teams call the coin correctly).

For sufficiency, subtract 1 from the $(n - t)$ largest $r_i$ getting a nearly nondecreasing sequence and then use the strengthening of Landau’s theorem. Finally, replace the last $(n - t)$ 0’s on the main diagonal with 1’s.
$T^\ell(R)$ denotes the set of all loopy tournaments with score vector $R$. Thus to construct a tournament in $T^\ell(R)$, we can subtract 1 from the largest $n - t$ components of $R$, giving a nearly nondecreasing $R'$ which satisfies Landau's conditions, construct a tournament in $T(R')$, and then change the 0s in the last $n - t$ positions on the main diagonal to 1s.

A Bijection

Let $R = (r_1, r_2, \ldots, r_n)$ be a nondecreasing vector of nonnegative integers such that
\[
\sum_{i=1}^{n} r_i = \binom{n}{2} + (n - t)^+ \text{ for some } 0 \leq t \leq n.
\]

Let $R' = (t, r_1, r_2, \ldots, r_n)$. A bijection between $T^\ell(R)$ and $T(R')$ is:

Given $T \in T^\ell(R)$, then $T' \in T(R')$ is obtained from $T$ by horizontally moving the entries $((n - t)$ 1’s and $t$ 0’s) on the main diagonal to column 0, vertically moving 1 minus the entries on the main diagonal to row 0 (giving a row sum of $t$), and putting 0s everywhere on the main diagonal of the resulting $(n + 1) \times (n + 1)$ matrix. This mapping is reversible.
Example of the Bijection

\[
\begin{bmatrix}
0 & 1 & 0 & 1 & 0 \\
0 & 1 & 0 & 1 & 1 \\
1 & 1 & 0 & 1 & 0 \\
0 & 0 & 0 & 1 & 1 \\
1 & 0 & 1 & 0 & 0 \\
\end{bmatrix}
\rightarrow
\begin{bmatrix}
0 & 1 & 0 & 1 & 0 \\
0 & 0 & 1 & 0 & 1 \\
1 & 0 & 0 & 1 & 1 \\
0 & 1 & 1 & 0 & 1 \\
1 & 0 & 0 & 0 & 1 \\
0 & 1 & 0 & 1 & 0 \\
\end{bmatrix}.
\]

Generating \(T^\ell(R)\)

Recall that \(T(R')\) can be generated starting from any \(T' \in T(R')\) and performing 3-cycle switches. Using the bijection between \(T^\ell(R)\) and \(T(R')\) this leads to:

\(T^\ell(R)\) can be generated starting from any \(T \in T^\ell(R)\) by a sequence of 3-cycle switches and

\[
\begin{bmatrix}
0 & 1 & 0 \\
0 & 0 & 1 \\
1 & 0 & 0 \\
\end{bmatrix}
\rightarrow
\begin{bmatrix}
0 & 0 & 1 \\
1 & 0 & 0 \\
0 & 1 & 0 \\
\end{bmatrix}
\]

and edge-loop switches (if the 3-cycle switch uses the new row/column):

\[
\begin{bmatrix}
i & j \\
0 & 1 \\
j & 0 \\
\end{bmatrix}
\rightarrow
\begin{bmatrix}
i & j \\
1 & 0 \\
j & 1 \\
\end{bmatrix}
\]

reversing the direction of an edge from a non-loop vertex \(i\) to a loop-vertex \(j\) and moving the loop from \(j\) to \(i\).
The Hankel-diagonal (anti-diagonal) of an $n \times n$ matrix consists of the positions $\{(i, n+1-i) : 1 \leq i \leq n\}$:

\[
\begin{array}{|c|c|c|c|c|c|}
\hline
  &  &  & 1 &  & \\
\hline
  &  &  &  &  & \\
\hline
  &  &  &  &  & \\
\hline
\end{array}
\]

If $A = [a_{ij}]$ is an $n \times n$ matrix, then we define its Hankel transpose to be the matrix $A^h = [a'_{ij}]$ obtained from $A$ by transposing across the Hankel diagonal and thus for which $a_{ij} = a'_{n+1-j,n+1-i}$ for all $i$ and $j$.

A Hankel tournament is defined to be a tournament $T$ for which $T^h = T$. Thus a $(0,1)$-matrix $T = [t_{ij}]$ is a Hankel tournament if and only if

\[t_{n+1-j,n+1-i} = t_{ij} = 1 - t_{ji} = 1 - t_{n+1-i,n+1-j} \text{ for all } i \neq j.\]

In general one entry determines three others, except when the entry is on either of the diagonals.

The set of all Hankel tournaments with score vector $R$ is denoted by $T_H(R)$.
Example of a Hankel Tournament

\[
T = \begin{bmatrix}
0 & 0 & 0 & 1 & 1 \\
1 & 0 & 0 & 0 & 1 \\
1 & 1 & 0 & 0 & 0 \\
0 & 1 & 1 & 0 & 0 \\
0 & 0 & 1 & 1 & 0
\end{bmatrix}
\]

**Combinatorially anti-symmetric** (0 ↔ 1) about the main diagonal. **Symmetric** about the Hankel diagonal.

The entries on the Hankel diagonal of a Hankel tournament can be 0 or 1 but, by the combinatorial skew-symmetry of a tournament, there must be \( \frac{n}{2} \) 1s on the Hankel diagonal; if \( n \) is odd, then the entry \( t_{(n+1)/2,(n+1)/2} \) on the Hankel diagonal equals 0, since \( T \) is a tournament.

Consequence of a Hankel Tournament

Row \( i \) of a Hankel tournament \( T \) determines column \( i \) (tournament property), and determines row and column \( n + 1 - i \) (Hankel property).

Let \( T \) be an \( 8 \times 8 \) Hankel tournament with row 3 given. Then the entries in column 3, and row and column \( 8 + 1 - 3 = 6 \) are determined as shown in

\[
\begin{array}{cccccc}
0 & 1 - a & & & & \\
0 & 1 - b & & & & \\
& & a & b & 0 & c \\
1 - c & 0 & & & & d \\
1 - d & & & & 0 & c \\
1 - g & 1 - f & 1 - e & 1 - d & 1 - c & 0 & 1 - b & 1 - a \\
& & & & & & & & \\
& & & & & & 1 - f & b & 0 \\
& & & & & & 1 - g & a & 0
\end{array}
\]

where the 0s on the main diagonal have been inserted and the Hankel diagonal has been shaded.
Score Vector of a Hankel Tournament

Let \( R = (r_1, r_2, \ldots, r_n) \) be the score vector of a Hankel tournament \( T \), and let \( S = (s_1, s_2, \ldots, s_n) \) be the column sum vector of \( T \). Since \( T \) is symmetric about the Hankel diagonal,

\[ r_i = s_{n+1-i}. \]

Since \( T \) is a tournament,

\[ r_{n+1-i} = (n-1) - s_{n+1-i} = (n-1) - r_i \]

and thus the score vector \( R \) satisfies the Hankel property

\[ r_i + r_{n+1-i} = n - 1 \text{ for all } i = 1, 2, \ldots, n. \]

In particular, if \( n \) is odd, \( r_{(n+1)/2} = \frac{n-1}{2} \).

It can be shown, by permutations preserving the tournament and Hankel properties, that there is no loss of generality in assuming that \( R \) is nondecreasing.

Algorithm to construct a Hankel tournament with score vector \( R \) (omitted here).

Nonemptiness of \( T_H(R) \)

**Theorem:** Let \( R = (r_1, r_2, \ldots, r_n) \) be a vector of nonnegative integers with \( r_1 \leq r_2 \leq \cdots \leq r_n \). Then there exists a Hankel tournament with score vector \( R \) if and only if

\[ r_i + r_{n+1-i} = n - 1, \quad (i = 1, 2, \ldots, n) \]

and

\[ \sum_{i=1}^{k} r_i \geq \binom{k}{2}, \quad (k = 1, 2, \ldots, n), \text{ with equality if } k = n. \]

Thus besides Landau’s conditions, the only other condition needed is that the score vector satisfy the Hankel property. (Actually it suffices to assume here that \( R \) is 2-nearly nondecreasing.)

Proof proceeds by choosing a minimal counterexample (\( n \) minimum and then \( r_1 \) minimum.)

Algorithm to construct a Hankel tournament with score vector \( R \) (omitted here).
There are three kinds of switches needed to generate all Hankel tournaments in $T_H(R)$, with all intermediate tournaments also in $T_H(R)$, from any one such Hankel tournament. Briefly they are:

- **3-cycle Hankel switches**: a 3-cycle switch on indices $i, (n + 1)/2, n + 1 - i$ ($n$ odd);

- **pairs consisting of a pure 3-cycle switch on indices $i, j, k$ and its complementary 3-cycle switch in the reverse order on indices $n + 1 - i, n + 1 - j, n + 1 - k$**

Here **pure** means that $\{i, j, k\} \cap \{n + 1 - i, n + 1 - j, n + 1 - k\} = \emptyset$;

- **4-cycle Hankel switches**: a 4-cycle switch on indices $i, j, n + 1 - j, n + 1 - i$ that reverses the cycle $i \rightarrow j \rightarrow n + 1 - j \rightarrow n + 1 - i \rightarrow i$.

---

**Combinatorially skew-Hankel Tournaments**

A **combinatorially skew-Hankel tournament** is an $n \times n$ $(0, 1)$-matrix which is combinatorially skew-symmetric about both the main diagonal and the Hankel diagonal, and which has only 0s on both its main diagonal and its Hankel diagonal.

Let $D_n$ be the $n \times n$ $(0, 1)$-matrix with 1s on the main diagonal and on the Hankel diagonal and 0s elsewhere. The $n \times n$ $(0, 1)$-matrix $T = [t_{ij}]$ is a combinatorially skew-Hankel tournament if and only if $T^t = J_n - D_n - T$ and $T^h = J_n - D_n - T$; so $T^t = T^h$ or, put another way, $T^{th} = T$.

Thus $T$ is a combinatorially skew-Hankel tournament if and only if

$$t_{ij} = t_{i, n+1-i} = 0 \text{ for all } i,$$

$$t_{ji} = 1 - t_{ij} \text{ and } t_{n+1-j, n+1-i} = 1 - t_{ij} \text{ for all } j \neq i, n + 1 - i.$$

Thus if $T$ is a combinatorially skew-Hankel tournament, then $t_{ij} = t_{n+1-i, n+1-j}$ for all $i$ and $j$. 

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CRM - Barcelona, June 29 – July 3, 2015
Example of a Combinatorially skew-Hankel Tournament

\[
\begin{bmatrix}
0 & 1 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 1 \\
1 & 0 & 0 & 0 & 1 \\
1 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 \\
\end{bmatrix}
\]

where the four shaded entries determine all the other entries off the main and Hankel diagonals. (Invariant under a rotation by 180 degrees.)

Not a real tournament because skew-symmetry does not hold for symmetrically opposite elements on the Hankel diagonal. Viewing \( T \) with respect to either its main diagonal or its Hankel diagonal, we have a round-robin tournament in which for each \( i \), players \( i \) and \( n+1-i \) do not play a game.

The set of all combinatorially skew-Hankel tournaments with a prescribed score vector is denoted by \( T_{H^*}(R) \).

CRM - Barcelona, June 29 – July 3, 2015

Score Vector of a Combinatorially skew-Hankel Tournament

Let \( T = [t_{ij}] \) be an \( n \times n \) combinatorially skew-Hankel tournament, and let the score vector of \( T \) be \( R = (r_1, r_2, \ldots, r_n) \). Since \( T \) is invariant under a rotation by 180 degrees, we have that for each \( i \), row \( n+1-i \) is obtained by reversing row \( i \), and thus the score vector of \( T \) is palindromic, that is,

\[
R = (r_1, r_2, r_3, \ldots, r_3, r_2, r_1).
\]

Since \( T \) is combinatorially skew with respect to the main diagonal, row \( i \) of \( T \) not only determines row \( n+1-i \) but it also determines columns \( i \) and \( n+1-i \).
Property of a Combinatorially skew-Hankel Tournament

Let $T$ be an $8 \times 8$ combinatorially skew-Hankel tournament with row 3 given. Then the entries in column 3, and row and column $8 + 1 - 3 = 6$ are determined as shown in

\[
\begin{array}{cccccccc}
0 & 1-a & & 1-f & & & & 0 \\
0 & 1-b & & 1-e & & & & 0 \\
a & b & 0 & c & d & 0 & e & f \\
1-c & 0 & 0 & 1-d & & & & \\
1-d & 0 & 0 & 1-c & & & & \\
f & e & 0 & d & c & 0 & b & a \\
0 & 1-e & & 1-b & & & & 0 \\
0 & 1-f & & 1-a & & & & 0 \\
\end{array}
\]

where the 0s on the main and Hankel diagonals have been inserted and shaded.

Another Example of a Combinatorially skew-Hankel Tournament

A $7 \times 7$ combinatorially skew-Hankel tournament with palindromic score vector $R = (1, 3, 4, 2, 4, 3, 1)$ is given by

\[
\begin{bmatrix}
0 & 0 & 1 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 1 & 0 & 0 & 1 \\
0 & 1 & 0 & 1 & 0 & 1 & 1 \\
1 & 0 & 0 & 0 & 0 & 0 & 1 \\
1 & 1 & 0 & 1 & 0 & 1 & 0 \\
1 & 0 & 0 & 1 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 \\
\end{bmatrix}
\]
Nonemptiness of $\mathcal{T}_{H^*}$: $n$ even

**Theorem:** Let $n$ be an even integer, and let $R = (r_1, r_2, \ldots, r_{n/2}, r_{n/2}, \ldots, r_2, r_1)$ be a vector of nonnegative integers such that $(r_1, r_2, \ldots, r_{n/2})$ is nondecreasing (WLOG). Then there exists a combinatorially skew-Hankel tournament with score vector $R$ if and only if

$$\sum_{i=1}^{k} r_i \geq k(k - 1), \ (k = 1, 2, \ldots, \frac{n}{2}), \text{ with equality for } k = \frac{n}{2}. \quad (1)$$

Actually “nondecreasing” above may be replaced by “3-nearly nondecreasing.”

$X_1$ is $k \times k$ with 0’s on its main diagonal; $X_2$ is $k \times k$ with 0’s on its Hankel diagonal. The sums of the entries of $X_1$ and $X_2$ are each $\binom{k}{2}$ and together the sum is $k(k - 1)$. Thus

$$\sum_{i=1}^{k} r_i \geq k(k - 1). \quad (2)$$
Nonemptiness of $\mathcal{T}_{H^\ast}$: $n$ odd

**Theorem:** Let $n$ be an odd integer, and let

$$R = (r_1, \ldots, r_{(n-1)/2}, r_{(n+1)/2}, r_{(n-1)/2}, \ldots, r_1)$$

be a vector of nonnegative integers such that $(r_1, r_2, \ldots, r_{(n-1)/2})$ is nondecreasing WLOG. Then there exists a combinatorially skew-Hankel tournament with score vector $R$ if and only if $r_{(n+1)/2} \leq n - 1$ and

$$\sum_{i=1}^{k} r_i \geq k(k - 1) + \left(k - \frac{r_{(n+1)/2}}{2}\right)^+, \quad \left(k = 1, 2, \ldots, \frac{n-1}{2}\right),$$

with equality if $k = \frac{n-1}{2}$.

**Algorithm to construct a combinatorially skew-Hankel tournament with score vector $R$ (omitted here).**

---

Generating $\mathcal{T}_{H^\ast}$

There are two kinds of switches needed to generate all combinatorially skew-Hankel tournaments in $\mathcal{T}_{H}(R)$, with all intermediate combinatorially skew-Hankel tournaments also in $\mathcal{T}_{H}(R)$, from any one such combinatorially skew-Hankel tournament. Briefly they are:

- **pairs consisting of a pure 3-cycle switch on indices $i, j, k$ and its complementary 3-cycle switch in the reverse order on indices $n + 1 - i, n + 1 - j, n + 1 - k$** (Here ‘pure’ means that $\{i, j, k\} \cap \{n + 1 - i, n + 1 - j, n + 1 - k\} = \emptyset$);
- **4-cycle skew-Hankel switches:** a 4-cycle switch on indices $i, j, n + 1 - i, n + 1 - j$ that reverses the cycle

$$i \rightarrow j \rightarrow n + 1 - i \rightarrow n + 1 - j \rightarrow i.$$
Hankel and Combinatorially skew-Hankel Loopy Tournaments

Nothing is gained here since, in both cases, it can be shown that the score vector \( R \) determines which diagonal elements are 1 and which are 0. Also, by reversing the order of columns, combinatorially skew-Hankel H-loopy (i.e. 1s allowed on the Hankel diagonal) tournaments are equivalent to combinatorially skew-Hankel loopy tournaments.

We may also consider \textit{combinatorially skew-Hankel doubly-loopy tournaments}, that is, combinatorially skew-Hankel tournaments \( T = [t_{ij}] \) with possible 1s on both the main diagonal and the Hankel diagonal. But again it can be shown that there is nothing essentially new here.

**Tournament Summary**

- Necessary and sufficient conditions for the existence of tournaments with additional structures: loopy tournaments, Hankel tournaments, and combinatorially skew-Hankel tournaments with a prescribed score vector.
- Algorithms for their construction when these conditions are satisfied.
- Identification of moves from one tournament to another tournament in the same class given by switches and pairs of switches. The moves used in each case are:
  
  (a) loopy tournaments: \( \rightarrow ij \); \( \triangle_{i,j,k} \)
  
  (b) Hankel tournaments: \( \triangle_{i,j,k} \) followed by \( \triangle_{k,j,i} \); \( \triangle_{i,(n+1)/2,n+1-i} \); \( \square_{i,j,n+1-j,n+1-i} \)
  
  (c) combinatorially skew-Hankel tournaments: \( \triangle_{i,j,k} \) followed by \( \triangle_{i,j,k} \); \( \square_{i,j,n+1-i,n+1-j} \).
References III

Angeles Carmona Mejías

Boundary value problems of finite networks
LECTURE I: DISCRETE VECTOR CALCULUS

Abstract. We first motivate the series of Lectures that compose the course through a well–known matrix problem. Specifically, the $M$–matrix inverse problem. Then, we aim at introducing the basic terminology and results on discrete vector calculus on finite networks. After defining the tangent space at each vertex of a network, we introduce the basic difference operators that mimetize the usual differential operators. Specifically we define the derivative, gradient, divergence, curl and laplacian operators; or more generally Schödinger operator. Moreover, we prove that the above defined operators satisfy properties that are analogues to those satisfied by their continuous counterpart.

1. Motivation

The matrices\footnote{2000 Mathematics Subject Classification: Keywords: Symmetric and Circulant Matrices, Inverses, Chebyshev polynomials.} that can be expressed as $L = kI - A$, where $k > 0$ and $A \geq 0$, appear in relation with systems of equations or eigenvalue problems in a broad variety of areas including finite difference methods for solving partial differential equations, input–output production and growth models in economics or Markov processes in probability and statistics. Of course, the combinatorial community can recognize within this type of matrices, the combinatorial Laplacian of a $k$–regular graph where $A$ is the adjacency matrix.

If $k$ is at least the spectral radio of $A$, then $L$ is called an $M$–matrix, which satisfy monotonicity properties that are the discrete counterpart of the minimum principle, and this makes them suitable for the resolution of large sparse systems of linear equations by iterative methods. In fact, the properties of $M$-matrices are the discrete analogue of the properties of elliptic operators of second order. These Lecture are motivated by this analogy.

A well–known property of an irreducible non–singular $M$–matrix is that its inverse is positive, \cite{5}. However, when the matrix is an irreducible and
Combinatorial Matrix Theory. Boundary Value Problems on Networks

singular $M$–matrix it is known that it has a generalized inverse which is non–negative, but this is not always true for any generalized inverse. For instance, the Moore–Penrose inverse of the combinatorial Laplacian of a path always has some negative off–diagonal entries.

The difficulty of characterizing all nonnegative matrices whose inverses are $M$–matrices has led to the study of the general properties of inverse $M$–matrices and to the identification of particular classes of such matrices.

Let us begin with some notation and bibliographic revision.

Let $c_{ij} \geq 0$, $1 \leq i < j \leq n$, and the symmetric matrix that we always assume irreducible

$$A = \begin{bmatrix}
0 & c_{12} & \cdots & c_{1n-1} & c_{1n} \\
c_{12} & 0 & \cdots & c_{2n-1} & c_{2n} \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
c_{1n-1} & c_{2n-1} & \cdots & 0 & c_{n-1n} \\
c_{1n} & c_{2n-1} & \cdots & c_{n-1n} & 0
\end{bmatrix}$$

and consider the $Z$–matrix

$$M = \begin{bmatrix}
d_1 & -c_{12} & \cdots & -c_{1n-1} & -c_{1n} \\
-c_{12} & d_2 & \cdots & -c_{2n-1} & -c_{2n} \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
-c_{1n-1} & -c_{2n-1} & \cdots & d_{n-1} & -c_{n-1n} \\
-c_{1n} & -c_{2n-1} & \cdots & -c_{n-1n} & d_n
\end{bmatrix} = D - A$$

The different problems that we can raise in this framework are:

(i) (Characterization of Symmetric $M$–Matrices) For which values $d_1, \ldots, d_n > 0$ is $M$ an $M$–matrix?

(ii) (Inverse $M$–Matrix Problems: Non–Singular Case) When $M$ is invertible (Stieltjes matrix), then $M^{-1} > 0$. So, if we consider $K > 0$ is irreducible, symmetric and invertible, when $K = M^{-1}$?

(iii) (Inverse $M$–Matrix Problems: Singular Case) If $M$ is singular, what can we say about $M^\dagger$? When is $M^\dagger$ an $M$–matrix?

There have been many contributions to solve these problems along the years. For instance T.L. Markham proved in [10] that if $K = (a_{\min\{i,j\}})$, $0 < a_1 < \cdots < a_n$, then $K^{-1}$ is a Jacobi $M$–matrix. S. Martínez et al. in [11] showed that if $K$ is a strictly ultrametric matrix, then $K^{-1}$ is a strictly d.d. Stieltjes matrix. On the other hand, M. Fiedler proved in [8] that a Stieltjes and d.d. matrix, $M$, then $M^{-1}$ is a resistive inverse matrix. Moreover, Chen et al. proved that the Moore–Penrose inverse of a singular and d.d. Jacobi $M$–matrix is an $M$–matrix, then $n \leq 4$, see [6]. Kirkland & Neumann proved characterized all weighted trees whose Laplacian ha a group inverse which is ab $M$–matrix, see [9]. Our research group has also worked in this framework obtaining a generalization of some of the above results. Specifically, we have proved that any irreducible Stieltjes matrix is a resistive inverse and that for any $n$, there exist singular, symmetric and Jacobi $M$–matrices of order $n$ whose Moore–Penrose inverse is also an $M$–matrix, see [1, 2, 3].
The techniques we used are based on the study of Potential Theory associated with semidefinite positive Schrödinger operator on a finite network and can be seen as the discrete counterpart of the Potential Theory associated with elliptic operators. The connection between finite networks and matrices comes from the following definition.

Given \( c_{ij} \geq 0, 1 \leq i < j \leq n \), and the irreducible and symmetric matrix

\[
A = \begin{bmatrix}
0 & c_{12} & \cdots & c_{1n-1} & c_{1n} \\
c_{12} & 0 & \cdots & c_{2n-1} & c_{2n} \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
c_{1n-1} & c_{2n-1} & \cdots & 0 & c_{n-1n} \\
c_{1n} & c_{2n} & \cdots & c_{n-1n} & 0 \\
\end{bmatrix}
\]

we can define a network, \( \Gamma = (V, E, c) \), whose vertex set is \( V = \{x_1, \ldots, x_n\} \) and where \( c(x_i, x_j) = c_{ij} \); i.e., \( \{x_i, x_j\} \in E \iff c_{ij} > 0 \). Moreover, \( \kappa_i = \kappa(x_i) = \sum_{j=1}^{n} c_{ij} \) is the degree of \( x_i \). The fact that \( A \) is irreducible is equivalent to be \( \Gamma \) connected.

Using this definition we can parametrize all the \( Z \)-matrices having the same off–diagonal elements as the matrices

\[
M = \begin{bmatrix}
\kappa_1 & -c_{12} & \cdots & -c_{1n-1} & -c_{1n} \\
-c_{12} & \kappa_2 & \cdots & -c_{2n-1} & -c_{2n} \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
-c_{1n-1} & 0 & \cdots & \kappa_{n-1} & -c_{n-1n} \\
-c_{1n} & 0 & \cdots & -c_{n-1n} & \kappa_n \\
\end{bmatrix} + \begin{bmatrix}
q_1 & 0 & \cdots & 0 & 0 \\
0 & q_2 & \cdots & 0 & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & \cdots & q_{n-1} & 0 \\
0 & 0 & \cdots & 0 & q_n \\
\end{bmatrix},
\]

where \( d_1, \ldots, d_n \in \mathbb{R} \). As we will see these are the matrices associated with Schrödinger operators on \( \Gamma \) where \( q_i \) represent the corresponding potential. Clearly, when \( q_i \geq 0 \) then \( M \) is d.d and hence positive semidefinite.

2. Preliminaries

Throughout these notes, \( \Gamma = (V, E) \) denotes a simple connected and finite graph without loops, with vertex set \( V \) and edge set \( E \). Two different vertices, \( x, y \in V \), are called adjacent, which is represented by \( x \sim y \), if \( \{x, y\} \in E \). In this case, the edge \( \{x, y\} \) is also denoted as \( e_{xy} \) and the vertices \( x \) and \( y \) are called incidents with \( e_{xy} \). In addition, for any \( x \in V \) the value \( k(x) \) denote the number of vertices adjacent to \( x \). When, \( k(x) = k \) for any \( x \in V \) we say that the graph is \( k \)-regular.

We denote by \( \mathcal{C}(V) \) and \( \mathcal{C}(V \times V) \), the vector spaces of real functions defined on the sets that appear between brackets. If \( u \in \mathcal{C}(V) \) and \( f \in \mathcal{C}(V \times V) \), \( uf \) denotes the function defined for any \( x, y \in V \) as \( (uf)(x, y) = u(x)f(x, y) \). If \( u \in \mathcal{C}(V) \), the support of \( u \) is the set \( \text{supp}(u) = \{x \in V : u(x) \neq 0\} \). For any \( u \in \mathcal{C}(V) \) we denote by \( \int_V u \, dx \) the value \( \sum_{x \in V} u(x) \).

Throughout the paper we make use of the following subspace of \( \mathcal{C}(V \times V) \):

\[
\mathcal{C}(\Gamma) = \{f \in \mathcal{C}(V \times V) : f(x, y) = 0, \text{ if } x \not\sim y\}.
\]
We call conductance on $\Gamma$ a function $c \in \mathcal{C}(\Gamma)$ such that $c(x, y) > 0$ iff $x \sim y$. The pair $(\Gamma, c)$ is called network. In what follows we consider fixed the network $(\Gamma, c)$ and we refer to it simply by $\Gamma$. The function $\kappa \in \mathcal{C}(V)$ defined as $\kappa(x) = \int_V c(x, y) \, dy$ for any $x \in V$ is called the (generalized) degree of $\Gamma$. Moreover, the resistance of $\Gamma$ is the function $r \in \mathcal{C}(\Gamma)$ defined as $r(x, y) = \frac{1}{c(x, y)}$ when $x \sim y$.

Next we define the tangent space at a vertex of a graph. Given $x \in V$, we call the real vector space of formal linear combinations of the edges incident with $x$, tangent space at $x$ and we denote it by $T_x(\Gamma)$. So, the set of edges incident with $x$ is a basis of $T_x(\Gamma)$, that is called coordinate basis of $T_x(\Gamma)$ and hence, $\dim T_x(\Gamma) = k(x)$. Note that, in the discrete setting, the dimension of the tangent space varies with each vertex except when the graph is regular.

We call any application $f : V \rightarrow \bigcup_{x \in V} T_x(\Gamma)$ such that $f(x) \in T_x(\Gamma)$ for each $x \in V$, vector field on $\Gamma$. The support of $f$ is defined as the set $\text{supp}(f) = \{x \in V : f(x) \neq 0\}$. The space of vector fields on $\Gamma$ is denoted by $\mathcal{X}(\Gamma)$.
If \( f \) is a vector field on \( \Gamma \), then \( f \) is uniquely determined by its components in the coordinate basis. Therefore, we can associate with \( f \) the function \( f \in C(\Gamma) \) such that for each \( x \in V \), \( f(x) = \sum_{y \sim x} f(x, y) e_{xy} \) and hence \( \mathcal{X}(\Gamma) \) can be identified with \( C(\Gamma) \).

A vector field \( f \) is called a flow when its component function satisfies that \( f(x, y) = -f(y, x) \) for any \( x, y \in V \), whereas \( f \) is called symmetric when its component function satisfies that \( f(x, y) = f(y, x) \) for any \( x, y \in V \). Given a vector field \( f \in \mathcal{X}(\Gamma) \), we consider two vector fields, the symmetric and the antisymmetric fields associated with \( f \), denoted by \( f^s \) and \( f^a \), respectively, that are defined as the fields whose component functions are given respectively by

\[
(1) \quad f^s(x, y) = \frac{f(x, y) + f(y, x)}{2} \quad \text{and} \quad f^a(x, y) = \frac{f(x, y) - f(y, x)}{2}.
\]

Observe that \( f = f^s + f^a \) for any \( f \in \mathcal{X}(\Gamma) \).

If \( u \in C(V) \) and \( f \in \mathcal{X}(\Gamma) \) has \( f \in C(\Gamma) \) as its component function, the field \( uf \) is defined as the field whose component function is \( uf \).

If \( f, g \in \mathcal{X}(\Gamma) \) and \( f, g \in C(\Gamma) \) are their component functions, the expression \( \langle f, g \rangle \) denotes the function in \( C(V) \) given by

\[
(2) \quad \langle f, g \rangle(x) = \sum_{y \sim x} f(x, y)g(x, y)r(x, y), \quad \text{for any} \ x \in V.
\]

Clearly, for any \( x \in V \), \( \langle \cdot, \cdot \rangle(x) \) determines an inner product on \( T_x(\Gamma) \). Therefore, on a network we can consider the following inner products on \( C(V) \) and on \( \mathcal{X}(\Gamma) \),

\[
(3) \quad \langle u, v \rangle = \int_V u v \, dx, \quad u, v \in C(V) \quad \text{and} \quad \frac{1}{2} \int_V \langle f, g \rangle \, dx, \quad f, g \in \mathcal{X}(\Gamma),
\]

where the factor \( \frac{1}{2} \) is due to the fact that each edge is considered twice.

**Lemma 2.1.** Given \( f, g \in \mathcal{X}(\Gamma) \), then

\[
\int_V \langle f, g \rangle \, dx = \int_V \langle f^s, g^s \rangle \, dx + \int_V \langle f^a, g^a \rangle \, dx.
\]

In particular, if \( f \) is symmetric and \( g \) is a flow, then \( \int_V \langle f, g \rangle \, dx = 0 \).

### 3. Difference Operators on Networks

Our objective in this section is to define the discrete analogues of the fundamental first and second order differential operators on Riemannian manifolds, specifically the derivative, gradient, divergence, curl and the laplacian. The last one is called **second order difference operator** whereas the former are generically called **first order difference operators**. From now on we suppose fixed the network \( (\Gamma, c) \) and also the associated inner products on \( C(V) \) and \( \mathcal{X}(\Gamma) \).

We call **derivative operator** the linear map \( \text{d} : C(V) \to \mathcal{X}(\Gamma) \) that assigns to any \( u \in C(V) \) the flow \( \text{d}u \), called **derivative of** \( u \), given by

\[
(4) \quad \text{d}u(x) = \sum_{y \sim x} \left( u(y) - u(x) \right) e_{xy}.
\]
We call gradient the linear map \( \nabla : \mathcal{C}(V) \rightarrow \mathcal{X}(\Gamma) \) that assigns to any \( u \in \mathcal{C}(V) \) the flow \( \nabla u \), called gradient of \( u \), given by
\[
\nabla u(x) = \sum_{y \sim x} c(x, y)(u(y) - u(x)) e_{xy}.
\]

Clearly, it is verified that \( du = 0 \), or equivalently \( \nabla u = 0 \), iff \( u \) is a constant function.

We define the divergence operator as \( \text{div} = -\nabla^* \), that is the linear map \( \text{div} : \mathcal{X}(\Gamma) \rightarrow \mathcal{C}(V) \) that assigns to any \( f \in \mathcal{X}(\Gamma) \) the function \( \text{div} f \), called divergence of \( f \), determined by the relation
\[
\int_V u \text{div} f \, dv = -\frac{1}{2} \int_V \langle \nabla u, f \rangle \, dx, \quad \text{for an } u \in \mathcal{C}(V).
\]

Therefore, taking \( u \) constant in the above identity, we obtain that
\[
\int_V \text{div} f \, dx = 0 \quad \text{for any } f \in \mathcal{X}(\Gamma).
\]

**Proposition 3.1.** If \( f \in \mathcal{X}(\Gamma) \), for any \( x \in V \) it holds
\[
\text{div} f(x) = \sum_{y \sim x} f^a(x, y).
\]

Proof. For any \( z \in V \) consider \( u = \varepsilon_z \), the Dirac function at \( z \). Then, from Identity (6) we get that
\[
\text{div} f(z) = -\frac{1}{2} \int_V \langle \nabla \varepsilon_z, f \rangle \, dx = -\frac{1}{2} \sum_{x \in V} (\nabla \varepsilon_z, f)(x)
\]

Given \( x \in V \), we get that
\[
\langle \nabla \varepsilon_z, f \rangle(x) = \sum_{y \sim x} c(x, y)(\varepsilon_z(y) - \varepsilon_z(x)) f(x, y) r(x, y)
\]
\[
= \sum_{y \in V} (\varepsilon_z(y) - \varepsilon_z(x)) f(x, y) = f(x, z) - \sum_{y \in V, y \neq z} \varepsilon_z(y) f(x, y)
\]

and hence when \( x \neq z \), then \( \langle \nabla \varepsilon_z, f \rangle(x) = f(x, z) \), whereas \( \langle \nabla \varepsilon_z, f \rangle(z) = -\sum_{y \in V, y \neq z} f(z, y) \). Therefore,
\[
\text{div} f(z) = -\frac{1}{2} \sum_{x \in V} (\nabla \varepsilon_z, f)(x) = \frac{1}{2} \left[ \sum_{y \in V} f(z, y) - \sum_{x \in V, x \neq z} f(x, z) \right] = \sum_{x \in V} f^a(z, x). \quad \Box
\]

We call curl the linear map \( \text{curl} : \mathcal{X}(\Gamma) \rightarrow \mathcal{X}(\Gamma) \) that assigns to any \( f \in \mathcal{X}(\Gamma) \) the symmetric vector field \( \text{curl} f \), called curl of \( f \), given by
\[
\text{curl} f(x) = \sum_{y \sim x} r(x, y) f^s(x, y) e_{xy}.
\]

In the following result we show that the above defined difference operators satisfy properties that are mimetic to the ones satisfied by their differential analogues.
**Proposition 3.2.** \( \text{curl}^* = \text{curl}, \; \text{div} \circ \text{curl} = 0 \) and \( \text{curl} \circ \nabla = 0 \).

Proof. Let \( f, h \in \mathcal{X}(\Gamma) \), then

\[
\int_V \langle \text{curl} f, h \rangle \, dx = \int_V \langle \text{curl} f, h^s \rangle \, dx = \sum_{x,y \in V} r(x,y)^2 f^s(x,y) h^s(x,y)
= \int_V \langle f^s, \text{curl} h \rangle \, dx = \int_V \langle f, \text{curl} h \rangle \, dx.
\]

The other two equalities follows directly from the definition of the involved operators. \( \square \)

Now we introduce the fundamental second order difference operator on \( \mathcal{C}(V) \) which is obtained by composition of two first order operators. Specifically, we consider the endomorphism of \( \mathcal{C}(V) \) given by \( \mathcal{L} = -\text{div} \circ \nabla \), that we call the \textit{Laplace operator} or \textit{combinatorial Laplacian of} \( \Gamma \).

**Proposition 3.3.** For any \( u \in \mathcal{C}(V) \) and for any \( x \in V \) we get that

\[
\mathcal{L}(u)(x) = \sum_{y \in V} c(x,y)(u(x) - u(y)).
\]

Moreover, given \( u, v \in \mathcal{C}(V) \), the following properties hold:

(i) First Green Identity

\[
\int_V v \mathcal{L}(u) \, dx = \frac{1}{2} \int_V \langle \nabla u, \nabla v \rangle \, dx = \frac{1}{2} \int_{V \times V} c(x,y) (u(x) - u(y))(v(x) - v(y)) \, dx dy.
\]

(ii) Second Green Identity

\[
\int_V v \mathcal{L}(u) \, dx = \int_V u \mathcal{L}(v) \, dx.
\]

(iii) Gauss Theorem

\[
\int_V \mathcal{L}(u) \, dx = 0.
\]

Proof. The expression for the Laplacian of \( u \) follows from the expression of the divergence keeping in mind that \( \nabla u \) is a flow. On the other hand, given \( v \in \mathcal{C}(V) \) from the definition of divergence we get that

\[
\int_V v \mathcal{L}(u) \, dx = -\int_V v \text{div} (\nabla u) \, dx = \frac{1}{2} \int_V (\nabla u, \nabla v) \, dx
= \frac{1}{2} \int_{V \times V} c(x,y)(u(x) - u(y))(v(x) - v(y)) \, dx dy
\]

and the First Green Identity follows. The proof of the Second Green Identity and the Gauss Theorem are straightforward consequence of (i). \( \square \)

**Corollary 3.4.** The Laplacian of \( \Gamma \) is self–adjoint and positive semi–definite. Moreover \( \mathcal{L}(u) = 0 \) iff \( u \) is constant.
Remark: Suppose that $V = \{x_1, \ldots, x_n\}$ and consider $c_{ij} = c(x_i, x_j) = c_{ji}$. Then, each $u \in \mathcal{C}(V)$ is identified with $(u(x_1), \ldots, u(x_n))^T \in \mathbb{R}^n$ and the Laplacian of $\Gamma$ is identified with the irreducible matrix

$$L = \begin{bmatrix}
\kappa_1 & -c_{12} & \cdots & -c_{1n} \\
-c_{21} & \kappa_2 & \cdots & -c_{2n} \\
\vdots & \vdots & \ddots & \vdots \\
-c_{n1} & -c_{n2} & \cdots & \kappa_n
\end{bmatrix}$$

where $\kappa_i = \sum_{j=1}^n c_{ij}$, $i = 1, \ldots, n$. Clearly, this matrix is symmetric and diagonally dominant and hence it is positive semi–definite. Moreover, it is singular and 0 is a simple eigenvalue whose associated eigenvectors are constant.

3.1. Schrödinger operators. A Schrödinger operator on $\Gamma$ is a linear operator $\mathcal{L}_q : \mathcal{C}(V) \rightarrow \mathcal{C}(V)$ that assigns to each $u \in \mathcal{C}(V)$ the function $\mathcal{L}_q(u)(x) = \mathcal{L}(u)(x) + q(x)u(x)$, where $q \in \mathcal{C}(V)$ is called the potential. The bilinear form $\mathcal{E}_q(u, v) = \langle u, \mathcal{L}_q(v) \rangle$ is called the energy of $\mathcal{L}_q$. Notice that from the first Green Identity

$$\mathcal{E}_q(u, v) = \frac{1}{2} \int_{V \times V} c(x, y)(u(x) - u(y))(v(x) - v(y)) \, dx \, dy + \int_V q(x)u(x)v(x) \, dx.$$

The fundamental problem in this framework is to determine when $\mathcal{E}_q$ is positive semi–definite; that is, when $\mathcal{E}_q(u) = \mathcal{E}_q(u, u) \geq 0$ for any $u \in \mathcal{C}(V)$. Observe that the matrix associated with $\mathcal{L}_q$ is

$$\mathcal{L}_q = \begin{bmatrix}
\kappa_1 + q(x_1) & -c_{12} & \cdots & -c_{1n} \\
-c_{12} & \kappa_2 + q(x_2) & \cdots & -c_{2n} \\
\vdots & \vdots & \ddots & \vdots \\
-c_{n1} & -c_{n2} & \cdots & \kappa_n + q(x_n)
\end{bmatrix}$$

which is an irreducible and symmetric $Z$–matrix. Therefore, the fundamental problem is equivalent to determine when $\mathcal{L}_q$ is an $M$–matrix. Of course, this happens when $q \geq 0$ and $\mathcal{L}_q$ is a non–singular $M$–matrix when in addition $q$ is non–null.

In order to obtain the necessary and sufficient condition for the positive semi definiteness of Schrödinger operators, it will be useful to consider the so–called Doob transform which is a common tool in the framework of Dirichlet forms. We introduce the following concept: A weight is a function $\omega \in \mathcal{C}(V)$ such that $\omega > 0$ on $V$ and $(\omega, \omega) = 1$. The set of weights is denoted by $\Omega(V)$. Given a weight $\omega$, we define the potential associated with $\omega$ as the function $q_\omega = -\omega^{-1}\mathcal{L}(\omega)$. 


Therefore, for any \( x \in V \),
\[
q_\omega(x) = -\frac{1}{\omega(x)} \sum_{y \in V} c(x, y) (\omega(x) - \omega(y)) = -\kappa(x) + \frac{1}{\omega(x)} \sum_{y \in V} c(x, y) \omega(y).
\]

Since \( \int_V \omega q_\omega \, dx = 0 \), \( q_\omega \) takes positive and negative values, except when \( \omega \) is constant in which case \( q_\omega = 0 \) and the corresponding Schrödinger operator coincides with the Laplacian. Moreover, we prove that any potential \( q \) is closely related with a potential of the form \( q_\omega \).

**Lemma 3.5.** Given \( q \in \mathcal{C}(V) \), there exist unique \( \omega \in \Omega(V) \) and \( \lambda \in \mathbb{R} \) such that \( q = q_\omega + \lambda \).

**Proof.** If we consider the matrix \( M = tI - L_q \), for \( t \in \mathbb{R} \) large enough, then \( M \) is an irreducible, symmetric and non–negative matrix. From Perron–Frobenius’ Theorem, the biggest eigenvalue of \( M \), \( \mu \), is simple and positive and has an associated eigenvector that is also positive, \( \omega \). Therefore, \( L_q(\omega) = (t - \mu) \omega \) and it suffices to take \( \lambda = t - \mu \).

Suppose that there exist \( \alpha \in \mathbb{R} \) and \( \sigma \in \Omega(V) \), such that \( q = q_\sigma + \lambda = q_\sigma + \alpha \). Therefore, \( L_q(\omega) = \lambda \omega \) and \( L_q(\sigma) = \alpha \sigma \), hence applying the second Green’s Identity
\[
(\lambda - \sigma) \int_V \sigma \omega \, dx = 0,
\]
which implies that \( \lambda = \sigma \). Considering again \( M = tI - L_q \), we get that \( M(\sigma) = (t - \lambda) \sigma \) and \( M(\omega) = (t - \lambda) \omega \) and hence \( \sigma = \omega \) since \( M \) is an irreducible, symmetric and non–negative matrix. \( \square \)

**Proposition 3.6 (Doob Transform).** Given \( \omega \in \Omega(V) \), then for any \( u \in \mathcal{C}(V) \) the following identity holds:
\[
\mathcal{L}(u)(x) = \frac{1}{\omega(x)} \int_V c(x, y) \omega(x) \omega(y) \left( \frac{u(x)}{\omega(x)} - \frac{u(y)}{\omega(y)} \right) dy - q_\omega(x) u(x), \quad x \in V
\]

In addition, for any \( u, v \in \mathcal{C}(V) \) we get that
\[
\mathcal{E}(u, v) = \frac{1}{2} \int_V \int_V c(x, y) \omega(x) \omega(y) \left( \frac{u(x)}{\omega(x)} - \frac{u(y)}{\omega(y)} \right) \left( \frac{v(x)}{\omega(x)} - \frac{v(y)}{\omega(y)} \right) dxdy
- \int_V q_\omega u v.
\]

**Proof.** First observe that
\[
\omega(x)(u(x) - u(y)) = \omega(x) \omega(y) \left( \frac{u(x)}{\omega(x)} - \frac{u(y)}{\omega(y)} \right) + (\omega(x) - \omega(y)) u(x),
\]
for any $x, y \in V$. So, if $x \in V$, then
\[ L(u)(x) = \frac{1}{\omega(x)} \int_V c(x, y) \omega(x) \left( \frac{u(x)}{\omega(x)} - \frac{u(y)}{\omega(y)} \right) dy \]
\[ + \frac{u(x)}{\omega(x)} \int_V c(x, y)(\omega(x) - \omega(y)) dy \]
\[ = \frac{1}{\omega(x)} \int_V c(x, y) \omega(x) \omega(y) \left( \frac{u(x)}{\omega(x)} - \frac{u(y)}{\omega(y)} \right) dy \]
\[ = \frac{1}{\omega(x)} \int_V c(x, y) \omega(x) \omega(y) \left( \frac{u(x)}{\omega(x)} - \frac{u(y)}{\omega(y)} \right) dy - q_{\omega}(x) u(x). \]

Finally, we get that
\[ E(u, v) = \int_V v(x) \frac{v(x)}{\omega(x)} \int_V c(x, y) \omega(x) \omega(y) \left( \frac{u(x)}{\omega(x)} - \frac{u(y)}{\omega(y)} \right) dy dx - \int_V q_{\omega} u v \]
\[ = \int_V \int_V c(x, y) \omega(x) \omega(y) \omega(x) \omega(y) \left( \frac{u(x)}{\omega(x)} - \frac{u(x)}{\omega(y)} \right) dx dy - \int_V q_{\omega} u v. \]

Therefore, the last claim is consequence of the following identities,
\[ \int_V \int_V c(x, y) \omega(x) \omega(y) \omega(x) \omega(y) \left( \frac{u(x)}{\omega(x)} - \frac{u(y)}{\omega(y)} \right) dx dy \]
\[ = \int_V \int_V c(y, x) \omega(y) \omega(x) \omega(y) \omega(y) \left( \frac{u(x)}{\omega(y)} - \frac{u(x)}{\omega(x)} \right) dy dx \]
\[ = - \int_V \int_V c(x, y) \omega(x) \omega(y) \omega(y) \omega(y) \left( \frac{u(x)}{\omega(x)} - \frac{u(y)}{\omega(y)} \right) dx dy, \]
where we have taken into account the symmetry of $c$.

\[ \Box \]

**Corollary 3.7 (Energy Principle).** If $q = q_{\omega} + \lambda$, $\omega \in \Omega(V)$ and $\lambda \in \mathbb{R}$, then $L_q$ is positive semi–definite iff $\lambda \geq 0$ and positive definite iff $\lambda > 0$. Moreover, when $\lambda = 0$, $L_q(u) = 0$ iff $u = a \omega$, $a \in \mathbb{R}$.

**Proof.** Since $q = q_{\omega} + \lambda$, from the above proposition, we get that
\[ E_q(u) = \frac{1}{2} \int_V \int_V c(x, y) \omega(x) \omega(y) \left( \frac{u(x)}{\omega(x)} - \frac{u(y)}{\omega(y)} \right) + \lambda \int_V u^2. \]

In particular, $E_q(\omega) = \lambda$. Therefore, $L_q$ is positive semi–definite iff $\lambda \geq 0$ and positive definite iff $\lambda > 0$. When $\lambda = 0$, $L_q(u) = 0$ iff
\[ 0 = E_q(u) = \frac{1}{2} \int_V \int_V c(x, y) \omega(x) \omega(y) \left( \frac{u(x)}{\omega(x)} - \frac{u(y)}{\omega(y)} \right)^2; \]
that is iff $u = a \omega$ since $\Gamma$ is a connected network.

Observe that $\min_{(u, u) = 1} \{ E_q(u) \} \geq \lambda$, and $E_q(u) = \lambda$ iff $u = \pm \omega$. Therefore, $L_q(\omega) = \lambda \omega$, $\lambda$ is the lowest eigenvalue of $L_q$ and it is simple.
Throughout the Lecture we have proved that

\[
M = \begin{bmatrix}
  d_1 & -c_{12} & \cdots & -c_{1n} \\
-\frac{c_{12}}{\omega_1} & d_2 & \cdots & -c_{2n} \\
  \vdots & \vdots & \ddots & \vdots \\
-\frac{c_{1n}}{\omega_1} & -\frac{c_{2n}}{\omega_1} & \cdots & d_n
\end{bmatrix}
\]

is an \(M\)-matrix iff there exists \(\omega \in \Omega(V)\) and \(\lambda \geq 0\) such that

\[
d_i = \lambda + \frac{1}{\omega_i} \sum_{j=1, j \neq i}^{n} c_{ij} \omega_j,
\]

where \(c_{ij} = c_{ji}\) when \(i > j\). Moreover, \(M\) is invertible iff \(\lambda > 0\). Equivalently, \(M\) is an \(M\)-matrix iff there exists \(\sigma \in \Omega(V)\) such that

\[
d_i \geq \frac{1}{\sigma_i} \sum_{j=1, j \neq i}^{n} c_{ij} \sigma_j.
\]

The concept of Schrödinger operator encompasses other widely used discrete operators as the normalized Laplacian introduced by F. Chung and R. Langlands in [7], that is defined as

\[
\Delta(u)(x) = \frac{1}{\sqrt{\kappa(x)}} \sum_{y \in V} \frac{c(x, y)}{\sqrt{\kappa(y)}} \left( \frac{u(x)}{\sqrt{\kappa(x)}} - \frac{u(y)}{\sqrt{\kappa(y)}} \right)
\]

As we can see the normalized Laplacian is nothing else but a Schrödinger operator associated with a new network. Specifically, if we denote by \(\hat{\mathcal{L}}\) the combinatorial laplacian of the network \(\hat{\Gamma} = (V, E, \hat{c})\) where \(\hat{c} = \frac{c(x, y)}{\sqrt{\kappa(x)} \sqrt{\kappa(y)}}\), then Identity (3.6) implies that \(\Delta = \hat{\mathcal{L}}_{q, \omega}\) where \(\omega = \frac{1}{2m} \sqrt{\kappa}\) and \(m\) denotes the size of \(\Gamma\).

4. Glossary

Let \(M = (m_{ij})\) be a symmetric square matrix of order \(n\). See [4] for all the definition given here. Then,

(i) (Irreducible) \(M\) is reducible if there exists a permutation matrix \(P\) such that \(P^T M P = \begin{bmatrix} A & 0 \\ 0 & B \end{bmatrix}\). Then, \(M\) is irreducible if it is not reducible.

(ii) (Positive) \(M\) is a non-negative matrix; i.e., \(M \geq 0\) iff \(m_{ij} \geq 0\). \(M\) is a positive matrix; i.e., \(M > 0\) iff \(m_{ij} > 0\).

(iii) (\(Z\)-matrix) \(M\) is a \(Z\)-matrix iff \(m_{ij} \leq 0\) for any \(i \neq j\).

(iv) (\(M\)-matrix) \(M\) is an \(M\)-matrix if it is a positive semidefinite \(Z\)-matrix. In particular, \(m_{ii} \geq 0\), for any \(i\).

(v) (Jacobi matrix) \(M\) is a Jacobi matrix if it is a tridiagonal matrix.

(vi) (Stieltjes matrix) \(M\) is a Stieltjes matrix if it is a positive definite \(M\)-matrix.
(vii) (Diagonal dominant (d.d.) matrix) \( M \) is d.d. matrix iff \( |m_{ii}| \geq \sum_{j=1 \atop j \neq i}^{n} |m_{ij}| \) and it is strictly diagonally dominant if \( |m_{ii}| > \sum_{j=1 \atop j \neq i}^{n} |m_{ij}| \), for any \( i \).

(viii) (Strictly ultrametric matrix) \( M \) is a strictly ultrametric matrix iff \( M \) is non-negative and \( m_{ij} \geq \min\{m_{ik}, m_{jk}\} \) for any \( i, j, k \).

\( m_{ii} > m_{ij} \) for all \( i \neq j \).

(ix) (Generalized inverse) Given \( M \), \( M^g \) is a generalized inverse of \( M \) iff \( MM^g M = M \).

(x) (Moore–Penrose Inverse) Given \( M \), \( M^\dagger \) is the Moore–Penrose inverse of \( M \) iff

\[
\begin{align*}
(i) \quad MM^\dagger M &= M, \\
(ii) \quad M^\dagger MM^\dagger &= M^\dagger, \\
(iii) \quad (M^\dagger M)^\top &= M^\dagger M, \\
(iv) \quad (MM^\dagger)^\top &= MM^\dagger.
\end{align*}
\]

Moreover, \( M \) is symmetric iff \( M^\dagger \) is symmetric and then, \( MM^\dagger = M^\dagger M \).

(xi) (Group inverse) Given \( M \), \( M^\# \) is the Group inverse of \( M \) iff

\[
\begin{align*}
(i) \quad MM^\# M &= M, \\
(ii) \quad M^\# MM^\# &= M^\#, \\
(iii) \quad M^\# M &= MM^\#.
\end{align*}
\]

In general the inverse group matrix does not exists for any squared matrix. But when \( M \) is a symmetric matrix, then \( M^\# \) exists and \( M^\# = M^\dagger \).

References


Abstract. We aim here at introducing the basic terminology and results on self-adjoint boundary value problems on finite networks. Firstly we define the discrete analogue of a manifold with boundary, which includes the concept of outer normal field. Then, we prove the Green Identities in order to establish the variational formulation of boundary value problems. Moreover, we prove the discrete version of the Dirichlet Principle.

1. Networks with boundary

Throughout these notes we follow the notations and definitions given in the notes Lecture I: Discrete vector calculus. From now on we suppose fixed the weighted network $(\Gamma, c)$ and also the associated inner products on $C(V)$ and $X(\Gamma)$.

Given a vertex subset $F \subset V$, we denote by $F^c$ its complement in $V$ and by $\chi_F$ its characteristic function. For any $x \in V$, $\varepsilon_x$ denotes the characteristic function of $\{x\}$. Moreover, we define the sets

$$\overset{\circ}{F} = \{x \in F : \{y \sim x\} \subset F\}$$

interior of $F$

$$\delta(F) = \{x \in F^c : \text{exists } y \in F \text{ such that } y \sim x\}$$

(>vertex<) boundary of $F$

$$\bar{F} = F \cup \delta(F)$$

closure of $F$.

In Figure 1 we have display the above sets for a given network and $F$.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure1.png}
\caption{Blue: $F$, Green: $\delta(F)$, Circle: $\overset{\circ}{F}$}
\end{figure}

If $F \subset V$ is a proper subset, we say that $F$ is connected if for any $x, y \in V$ there exists a path joining $x$ and $y$ whose vertices are all in $F$. It is easy to prove that $\bar{F}$ is connected when $F$ is. In the sequel we always assume that $F$ is a connected set. Moreover, if $F \subset V$, $C(F)$ denotes the subspace of $C(V)$ formed by the functions whose support is contained in $F$.

We are also interested in the Divergence Theorem and the Green’s Identities, that play a fundamental role in the analysis of boundary value problems. These results are given on a finite vertex subset, the discrete equivalent to a
compact manifold with boundary, so we need to define the discrete analogous of the outer normal vector field to the set.

The normal vector field to $F$ is defined as $n_F = -d\chi_F$. Therefore, the component function of $n_F$ is given by $n_F(x,y) = 1$ when $y \sim x$ and $(x,y) \in \delta(F) \times \delta(F)$, $n_F(x,y) = -1$ when $y \sim x$ and $(x,y) \in \delta(F) \times \delta(F^c)$ and $n_F(x,y) = 0$, otherwise. In consequence, $n_{Fc} = -n_F$ and $\text{supp}(n_F) = \delta(F^c) \cup \delta(F)$.

Of course networks do not have boundaries by themselves, but starting from a network we can define a network with boundary as $\Gamma = (\bar{F}, c_F)$ where $F$ is a connected proper subset and $c_F = c \cdot \chi_{(\bar{F} \times \bar{F}) \setminus (\delta(F) \times \delta(F))}$.

**Corollary 1.1 (Divergence Theorem).** For any $f \in \chi(\Gamma)$, it is verified that

$$\int_F \text{div} f \, dx = \int_{\delta(F)} (f^a, n_F) \, dx,$$

where $(f, g)(x) = \sum_{y \in V} f(x,y)g(x,y)$, denotes the standard inner product on $T_x(\Gamma)$.

**Proof.** Taking $u = \chi_F$ in the definition of $\text{div}$ we get

$$\int_F \text{div} (f) \, dx = \int_V \chi_F \text{div} (f) \, dx = -\frac{1}{2} \int_V (f, \nabla \chi_F) \, dx = -\frac{1}{2} \int_V (f^a, \nabla \chi_F) \, dx$$

$$= \frac{1}{2} \int_V (f^a, n_F) \, dx = \frac{1}{2} \int_{\delta(F)} (f^a, n_F) \, dx + \frac{1}{2} \int_{\delta(F^c)} (f^a, n_F) \, dx.$$

The result follows taking into account that

$$(f^a, n_F) \, dy = \sum_{y \in \delta(F^c)} \sum_{x \in \delta(F)} f^a(y,x)n_F(y,x)$$

$$= \sum_{x \in \delta(F)} \sum_{y \in \delta(F^c)} f^a(x,y)n_F(x,y) = \int_{\delta(F)} (f^a, n_F) \, dx.$$

$\square$
Recall that the Laplacian of $\Gamma$ is the linear operator $L: C(\bar{F}) \to C(\bar{F})$ that assigns to each $u \in C(\bar{F})$ the function

$$L(u)(x) = \sum_{y \in \bar{F}} c(x, y) (u(x) - u(y)), \ x \in \bar{F}.$$  

Given $q \in C(\bar{F})$ the Schrödinger operator on $\Gamma$ with potential $q$ is the linear operator $L_q: C(\bar{F}) \to C(\bar{F})$ that assigns to each $u \in C(\bar{F})$ the function $L_q(u) = L(u) + qu$.

For each $u \in C(\bar{F})$ we define the normal derivative of $u$ on $F$ as the function in $C(\delta(F))$ given by

$$\left(\frac{\partial u}{\partial n_F}\right)(x) = (\nabla u, n_F)(x) = \sum_{y \in F} c(x, y) (u(x) - u(y)), \text{ for any } x \in \delta(F).$$

The normal derivative on $F$ is the operator $\frac{\partial}{\partial n_F}: C(\bar{F}) \to C(\delta(F))$ that assigns to any $u \in C(\bar{F})$ its normal derivative on $F$.

The relation between the values of the Schrödinger operator with potential $q$ on $F$ and the values of the normal derivative at $\delta(F)$ is given by the following identities.

**Proposition 1.2.** Given $u, v \in C(\bar{F})$ the following properties hold:

(i) First Green Identity

$$\int_F vL_q(u)\,dx = \frac{1}{2} \int_{F \times F} c(x, y)(u(x) - u(y))(v(x) - v(y))\,dxdy$$

$$+ \int_F quv\,dx - \int_{\delta(F)} v \frac{\partial u}{\partial n_F} \,dx.$$

(ii) Second Green Identity

$$\int_F (vL_q(u) - uL_q(v))\,dx = \int_{\delta(F)} \left(u \frac{\partial v}{\partial n_F} - v \frac{\partial u}{\partial n_F}\right) \,dx.$$

(iii) Gauss’ Theorem

$$\int_F L(u)\,dx = -\int_{\delta(F)} \frac{\partial u}{\partial n_F} \,dx.$$

**Proof.** We get that

$$\int_F vL(u)\,dx = \int_F \int_F c(x, y)v(x)(u(x) - u(y))\,dy\,dx$$

$$= \int_F \int_F c(x, y)v(x)(u(x) - u(y))\,dy\,dx$$

$$- \int_{\delta(F)} \int_F c(x, y)v(x)(u(x) - u(y))\,dy\,dx$$
\[
\int_{\bar{F} \times \bar{F}} c(x, y)v(x)(u(x) - u(y))dydx - \int_{\delta(F)} v \frac{\partial u}{\partial n_F} \; dx
\]

\[
= \frac{1}{2} \int_{\bar{F} \times \bar{F}} c(x, y)(u(x) - u(y))(v(x) - v(y))dydx - \int_{\delta(F)} v \frac{\partial u}{\partial n_F} \; dx
\]

and the First Green Identity follows. The proof of the Second Green Identity and the Gauss’ Theorem are straightforward consequence of (i). \(\square\)

2. Self–adjoint boundary value problems

Given \(\delta(F) = H_1 \cup H_2\) a partition of \(\delta(F)\) and functions \(q \in C(F \cup H_1), \; g \in C(F), \; g_1 \in C(H_1), \; g_2 \in C(H_2)\), a boundary value problem on \(F\) consists in finding \(u \in C(\bar{F})\) such that

(3) \(L_q(u) = g\) on \(F\), \(\frac{\partial u}{\partial n_F} + qu = g_1\) on \(H_1\) and \(u = g_2\) on \(H_2\).

The associated homogeneous boundary value problem consists in finding \(u \in C(\bar{F})\) such that

(4) \(L_q(u) = 0\) on \(F\), \(\frac{\partial u}{\partial n_F} + qu = 0\) on \(H_1\) and \(u = 0\) on \(H_2\).

It is clear that the set of solutions of the homogeneous boundary value problem is a vector subspace of \(C(F \cup H_1)\) that we denote by \(V\). Moreover if Problem (3) has solution and \(u\) is a particular one, then \(u + V\) describes the set of all its solutions.

Problem (3) is generically known as a mixed Dirichlet–Robin problem, specially when \(H_1, H_2 \neq \emptyset\) and \(q \neq 0\) on \(H_1\), and summarizes the different boundary value problems that appear in the literature with the following proper names:

(i) Dirichlet problem: \(\emptyset \neq H_2 = \delta(F)\) and hence \(H_1 = \emptyset\).
(ii) Robin problem: \(\emptyset \neq H_1 = \delta(F)\) and \(q \neq 0\) on \(H_1\).
(iii) Neumann problem: \(\emptyset \neq H_1 = \delta(F)\) and \(q = 0\) on \(H_1\).
(iv) Mixed Dirichlet–Neumann problem: \(H_1, H_2 \neq \emptyset\) and \(q = 0\) on \(H_1\).
(v) Poisson equation on \(V\): \(H_1 = H_2 = \emptyset\) and hence \(F = V\).

Applying the Second Green Identity, we can show that the raised boundary value problem has some sort of symmetry. In addition, we obtain the conditions that assure the existence and uniqueness of solutions of the boundary value problem (3).

**Proposition 2.1.** The boundary value problem (3) is self–adjoint; that is, for any \(u, v \in C(F \cup H_1)\) such that \(\frac{\partial u}{\partial n_F} + qu = \frac{\partial v}{\partial n_F} + qv = 0\) it is satisfied that

\[
\int_F vL_q(u)dx = \int_F uL_q(v)dx.
\]
Proposition 2.2 (Fredholm Alternative). The boundary value problem (3) has solution iff
\[ \int_F g v \, dx + \int_{H_1} g_1 v \, dx = \int_{H_2} g_2 \frac{\partial v}{\partial n_F} \, dx, \quad \text{for each } v \in \mathcal{V}. \]

In addition, when the above condition holds, then there exists a unique solution \( u \in \mathcal{C}(\bar{F}) \), such that \( \int_F u v \, dx = 0 \), for any \( v \in \mathcal{V} \).

Proof. First, observe that problem (3) is equivalent to the boundary value problem
\[ L_q(u) = g - L(g_2) \text{ on } F, \quad \frac{\partial u}{\partial n_F} + qu = g_1 - \frac{\partial g_2}{\partial n_F} \text{ on } H_1 \text{ and } u = 0 \text{ on } H_2 \]
in the sense that \( u \) is a solution of this problem iff \( u + g_2 \) is a solution of (3).

Consider now the linear operator \( \mathcal{F} : \mathcal{C}(F \cup H_1) \rightarrow \mathcal{C}(F \cup H_1) \) defined as
\[
\mathcal{F}(u) = \begin{cases} 
L(u) + qu & \text{on } F, \\
\frac{\partial u}{\partial n_F} + qu & \text{on } H_1.
\end{cases}
\]

Then, \( \ker \mathcal{F} = \mathcal{V} \) and moreover, by applying Proposition 2.1 for any \( u, v \in \mathcal{C}(F \cup H_1) \) it is verified that
\[
\int_{F \cup H_1} v \mathcal{F}(u) \, dx = \int_F v L_q(u) \, dx + \int_{\delta(F)} v \left( \frac{\partial u}{\partial n_F} + qu \right) \, dx
\]
\[
= \int_F u L_q(v) \, dx + \int_{\delta(F)} u \left( \frac{\partial v}{\partial n_F} + qv \right) \, dx
\]
\[
= \int_{F \cup H_1} u \mathcal{F}(v) \, dx.
\]

Therefore the operator \( \mathcal{F} \) is self-adjoint with respect to the inner product induced in \( \mathcal{C}(F \cup H_1) \) and hence \( \text{Im} \mathcal{F} = \mathcal{V}^\perp \) by applying the classical Fredholm Alternative. Consequently Problem (3) has a solution iff \( \tilde{g} \in \mathcal{C}(F \cup H_1) \) given by \( \tilde{g} = g - L(g_2) \) on \( F \) and \( \tilde{g} = g_1 - \frac{\partial g_2}{\partial n_F} \) on \( H_1 \) verifies that
\[
0 = \int_{F \cup H_1} \tilde{g} v \, dx = \int_F g v \, dx + \int_{H_1} g_1 v \, dx - \int_{H_2} g_2 \frac{\partial v}{\partial n_F} \, dx - \int_{\delta(F)} g_2 v \, dx
\]
\[
= \int_F g v \, dx + \int_{H_1} g_1 v \, dx - \int_F g_2 L(v) \, dx - \int_{\delta(F)} g_2 \frac{\partial v}{\partial n_F} \, dx
\]
\[
= \int_F g v \, dx + \int_{H_1} g_1 v \, dx - \int_{H_2} g_2 \frac{\partial v}{\partial n_F} \, dx,
\]
for any \( v \in \mathcal{V} \).
Finally, when the necessary and sufficient condition is attained there exists a unique \( w \in \mathcal{V} \) such that \( \mathcal{F}(w) = \bar{g} \). Therefore, \( u = w + g_2 \) is the unique solution of Problem (3) such that for any \( v \in \mathcal{V} \)

\[
\int_{\bar{F}} uv \, dx = \int_{F \cup H_1} uv \, dx = \int_{F \cup H_1} wv \, dx = 0,
\]

since \( v = 0 \) on \( H_2 \) and \( g_2 = 0 \) on \( F \cup H_1 \).

Observe that as a by–product of the above proof, we obtain that uniqueness is equivalent to existence for any data.

Next, we establish the variational formulation of the boundary value problem (3), that represents the discrete version of the weak formulation for boundary value problems. Prior to describe the claimed formulation, we give some useful definitions. The bilinear form associated with the boundary value problem (3) is \( B: \mathcal{C}(\bar{F}) \times \mathcal{C}(\bar{F}) \rightarrow \mathbb{R} \) given by

\[
B(u, v) = \int_{\bar{F}} v\mathcal{L}_q(u) \, dx + \int_{\partial(F)} v \frac{\partial u}{\partial n_F} \, ds + \int_{H_1} q uv \, dx,
\]

and hence, from the Second Green Identity, \( B(u, v) = B(v, u) \) for any \( u, v \in \mathcal{C}(\bar{F}) \), that is \( B \) is symmetric. In addition by applying the First Green Identity, we obtain that

\[
B(u, v) = \frac{1}{2} \int_{F \times F} c(x, y) \left( u(x) - u(y) \right) \left( v(x) - v(y) \right) \, dxdy + \int_{\bar{F}} q uv \, dx + \int_{H_1} q uv \, dx.
\]

Associated with any pair of functions \( g \in \mathcal{C}(F) \) and \( g_1 \in \mathcal{C}(H_1) \) we define the linear functional \( \ell: \mathcal{C}(\bar{F}) \rightarrow \mathbb{R} \) as \( \ell(v) = \int_{\bar{F}} gv \, dx + \int_{H_1} g_1 v \, dx \), whereas for any function \( g_2 \in \mathcal{C}(H_2) \) we consider the convex set \( K_{g_2} = g_2 + \mathcal{C}(F \cup H_1) \).

**Proposition 2.3 (Variational Formulation).** Given \( g \in \mathcal{C}(F) \), \( g_1 \in \mathcal{C}(H_1) \) and \( g_2 \in \mathcal{C}(H_2) \), then \( u \in K_{g_2} \) is a solution of Problem (3) ifff \( B(u, v) = \ell(v) \), for any \( v \in \mathcal{C}(F \cup H_1) \)

and in this case, the set \( w = \{ w \in \mathcal{C}(F \cup H_1) : B(w, v) = 0, \text{ for any } v \in \mathcal{C}(F \cup H_1) \} \)
describes all solutions of (3).

**Proof.** A function \( u \in K_{g_2} \) satisfies that \( B(u, v) = \ell(v) \) for any \( v \in \mathcal{C}(F \cup H_1) \)

\[
\int_{\bar{F}} v(\mathcal{L}_q(u) - g) \, dx + \int_{H_1} v \left( \frac{\partial u}{\partial n_F} + qu - g_1 \right) \, dx = 0.
\]

Then, the first result follows by taking \( v = \varepsilon_x \), \( x \in F \cup H_1 \). Finally, \( u^* \in K_{g_2} \) is another solution of (3) ifff \( B(u^*, v) = \ell(v) \) for any \( v \in \mathcal{C}(F \cup H_1) \) and hence ifff \( B(u - u^*, v) = 0 \) for any \( v \in \mathcal{C}(F \cup H_1) \).

Observe that the equality \( B(u, v) = \ell(v) \) for any \( v \in \mathcal{C}(F \cup H_1) \) assures that the condition of existence of solution given by the Fredholm Alternative
holds, since for any \( v \in \mathcal{C}(F \cup H_1) \) it is verified that
\[
\int_F g v dx + \int_{H_1} g_1 v dx = B(u, v) = \int_F u \mathcal{L}_q(v) dx + \int_{\partial(F)} u \frac{\partial v}{\partial n} dx + \int_{H_1} q uv dx.
\]
In particular if \( v \in \mathcal{V} \) we get that
\[
\int_F g v dx + \int_{H_1} g_1 v dx = \int_{H_2} g_2 \frac{\partial v}{\partial n} dx.
\]
On the other hand, we note that the vector subspace
\[
\{ w \in \mathcal{C}(F \cup H_1) : B(w, v) = 0, \text{ for any } v \in \mathcal{C}(F \cup H_1) \}
\]
is precisely the set of solutions of the homogeneous boundary value problem associated with (3). So, Problem (3) has solution for any data \( g, g_1 \) and \( g_2 \) iff it has a unique solution and this occurs iff \( w = 0 \) is the unique function in \( \mathcal{C}(F \cup H_1) \) such that \( B(w, v) = 0 \), for any \( v \in \mathcal{C}(F \cup H_1) \). Therefore, to assure the existence (and hence the uniqueness) of solutions of Problem (3) for any data it suffices to provide conditions under which \( B(w, w) = 0 \) with \( w \in \mathcal{C}(F \cup H_1) \), implies that \( w = 0 \). In particular, this occurs when \( B \) is positive definite on \( \mathcal{C}(F \cup H_1) \).

The quadratic form associated with the boundary value problem (3) is the function \( \mathcal{Q} : \mathcal{C}(F) \rightarrow \mathbb{R} \) given by \( \mathcal{Q}(u) = B(u, u) \); that is,
\[
(7) \quad \mathcal{Q}(u) = \frac{1}{2} \int_{F \times F} c(x, y) (u(x) - u(y))^2 \, dxdy + \int_F q u^2 dx + \int_{H_1} q u^2 dx.
\]

**Corollary 2.4 (Dirichlet Principle).** Assume that \( \mathcal{Q} \) is positive semi–definite on \( \mathcal{C}(F \cup H_1) \). Let \( g \in \mathcal{C}(F) \), \( g_1 \in \mathcal{C}(H_1) \), \( g_2 \in \mathcal{C}(H_2) \) and consider the quadratic functional \( \mathcal{J} : \mathcal{C}(F) \rightarrow \mathbb{R} \) given by
\[
\mathcal{J}(u) = \mathcal{Q}(u) - 2\ell(u).
\]
Then \( u \in K_{g_2} \) is a solution of problem (3) iff it minimizes \( \mathcal{J} \) on \( K_{g_2} \).

**Proof.** Firstly note that when \( u \in K_{g_2} \), then \( K_{g_2} = u + \mathcal{C}(F \cup H_1) \).

If \( u \) is a minimum of \( \mathcal{J} \) on \( K_{g_2} \) then for any \( v \in \mathcal{C}(F \cup H_1) \) the function \( \varphi_v : \mathbb{R} \rightarrow \mathbb{R} \) given by
\[
\varphi_v(t) = \mathcal{J}(u + tv) = \mathcal{J}(u) + t^2 \mathcal{Q}(v) + 2t[B(u, v) - \ell(v)]
\]
attains a minimum value at \( t = 0 \) and hence \( 0 = \varphi_v'(0) = B(u, v) - \ell(v) \).

Therefore, from Proposition 2.3, \( u \) is a solution of Problem (3). Conversely if \( u \in K_{g_2} \) is a solution of Problem (3), then \( B(u, v) = \ell(v) \) for any \( v \in \mathcal{C}(F \cup H_1) \) and hence we get that
\[
\mathcal{J}(u + v) = \mathcal{J}(u) + \mathcal{Q}(v) + B(u, v) - \ell(v) = \mathcal{J}(u) + \mathcal{Q}(v) \geq \mathcal{J}(u);
\]
since \( \mathcal{Q} \) is positive semi–definite; that is \( u \) is a minimum of \( \mathcal{J} \) on \( K_{g_2} \).

Notice that if \( \mathcal{Q} \) is not positive semi–definite on \( F \cup H_1 \), then \( \mathcal{J} \) cannot attain any minimum, since if there exists \( v \in \mathcal{C}(F \cup H_1) \) such that \( \mathcal{Q}(v) < 0 \), then \( \lim_{t \rightarrow +\infty} \mathcal{J}(u + tv) = -\infty \).
The adaptation of the Doob–transform to networks with boundary allows us to establish an easy sufficient condition to assure that $B$ is positive semi–definite. Given a weight $\omega \in \Omega(\bar{F})$, we define the potential associated with $\omega$ as the function

$$q_\omega = -\omega^{-1}L(\omega) \text{ on } F \text{ and } q_\omega = -\omega^{-1}\frac{\partial \omega}{\partial n_F} \text{ on } \delta(F).$$

**Proposition 2.5 (Doob Transform).** Given $\omega \in \Omega(\bar{F})$, then for any $u \in C(\bar{F})$ the following identities hold:

$$L(u)(x) = \frac{1}{\omega(x)}\int_{\bar{F}} c(x,y)\omega(x)\omega(y) \left( \frac{u(x)}{\omega(x)} - \frac{u(y)}{\omega(y)} \right) dy - q_\omega(x) u(x), \quad x \in F,$$

$$\left( \frac{\partial u}{\partial n_F} \right)(x) = \frac{1}{\omega(x)}\int_{F} c(x,y)\omega(x)\omega(y) \left( \frac{u(x)}{\omega(x)} - \frac{u(y)}{\omega(y)} \right) dy - q_\omega(x) u(x), \quad x \in \delta(F).$$

In addition, for any $u \in C(\bar{F})$ we get that

$$Q(u) = \frac{1}{2} \int_{\bar{F}} \int_{\bar{F}} c(x,y)\omega(x)\omega(y) \left( \frac{u(x)}{\omega(x)} - \frac{u(y)}{\omega(y)} \right)^2 dxdy$$

$$+ \int_{F \cup H_1} (q - q_\omega)u^2 - \int_{H_2} q_\omega u^2.$$

**Corollary 2.6 (Energy Principle).** If there exist $\omega \in \Omega(\bar{F})$ such that $q \geq q_\omega$ on $F \cup H_1$, then the Energy $Q$ is positive semi–definite on $C(F \cup H_1)$. Moreover, it is not strictly definite iff $H_2 = \emptyset$ and $q = q_\omega$, in which case $Q(v) = 0$ iff $v = a\omega$, $a \in \mathbb{R}$. 
LECTURE III: MONOTONICITY AND RESOLVENT KERNELS

Abstract. In this lecture we aim at analyzing the fundamental properties of positive semi–definite Schödinger operator on networks both with boundary or not. We prove the properties of monotonicity and the minimum principle which allows us to define the Green and Poisson operators associated with the Schrödinger operators. In the case of network with boundary or when $F = V$ but $q \neq q_\omega$, the Green operator can be thought as the inverse matrix of $L_q$; whereas when $F = V$ and $q = q_\omega$ it can be seen as the Moore–Penrose inverse. After analyzing the properties and relation of both operator we define the associated kernels as well as the Dirichlet–to–Robin map.

1. Monotonicity and minimum principle

In this lecture we are concerned with either the Poisson equation or the Dirichlet problem. The main results can be found in [1, 2, 3]. So, following the notation of the preceding lectures, we consider $\Gamma$ either a network as in Lecture I and hence $\Gamma = (V,c)$, or a network with boundary as in Lecture II, and hence $\Gamma = (\bar{F},c)$. If $q \in C(V)$ is a potential, recall that the Poisson equation consist in given $f \in C(V)$, finding $u \in C(V)$ such that

$$L_q(u) = f \text{ on } V,$$

whereas the Dirichlet Problem consist in given $f \in C(F)$ and $g \in C(\delta(F))$, finding $u \in C(\bar{F})$ such that

$$L_q(u) = f \text{ on } F \text{ and } u = g \text{ on } \delta(F).$$

We can treat both problems (1) and (2) in an unified manner considering that Poisson equation corresponds to the limit case of Dirichlet problem when $F = V$; or equivalently, when $\delta(F) = \emptyset$.

According with the Energy Principles in Lectures I and II, from now on we assume that the potential satisfies that $q \geq q_\omega$ for some weight $\omega \in \Omega(\bar{F})$, so that $L_q$ is positive semi–definite on $C(\bar{F})$.

A function $u \in C(\bar{F})$ is called $q$–harmonic, $q$–superharmonic or $q$–subharmonic on $F$ iff $L_q(u) = 0$, $L_q(u) \geq 0$ or $L_q(u) \leq 0$ on $F$, respectively. Moreover, $u \in C(V)$ is called strictly $q$–superharmonic or strictly $q$–subharmonic on $F$ iff $L_q(u) > 0$ or $L_q(u) < 0$ on $F$.

Proposition 1.1 (Hopf’s minimum principle). Let $u \in C(\bar{F})$ $q$–superharmonic on $F$ and suposse that there exists $x^* \in F$ satisfying

$$u(x^*) \leq 0 \text{ and } \frac{u(x^*)}{\omega(x^*)} = \min_{y \in F} \left\{ \frac{u(y)}{\omega(y)} \right\},$$

then $u = a\omega$, $a \leq 0$, on $\bar{F}$, $u$ is $q$–harmonic on $F$ and either $u = 0$ or $q = q_\omega$ on $F$. 

99
Proof. As \( u(x^*) \leq 0 \),
\[
0 \leq \mathcal{L}_q(u)(x^*) = \int_F c(x^*, y)\omega(y)\left(\frac{u(x^*)}{\omega(x^*)} - \frac{u(y)}{\omega(y)}\right)dy + (q(x^*) - q_\omega(x^*))u(x^*) \leq 0
\]
which implies that
\[
0 = \int_F c(x^*, y)\omega(y)\left(\frac{u(x^*)}{\omega(x^*)} - \frac{u(y)}{\omega(y)}\right)dy = (q(x^*) - q_\omega(x^*))u(x^*).
\]
From the first identity \( \frac{u(y)}{\omega(y)} = \frac{u(x^*)}{\omega(x^*)} \) for all \( y \in \bar{F} \) such that \( y \sim x^* \). Hence \( u = a\omega \), \( a \in \mathbb{R} \), since \( \bar{F} \) is connected. Moreover, \( a \leq 0 \), since \( u(x^*) \leq 0 \).

On the other hand,
\[
0 \leq \mathcal{L}_q(u) = a\mathcal{L}_q(\omega) = a(q - q_\omega)\omega \leq 0 \quad \text{on} \quad F,
\]
which implies that \( \mathcal{L}_q(u) = 0 \) on \( F \) and either \( a = 0 \) or \( q = q_\omega \) on \( F \). □

**Proposition 1.2** (Monotonicity Principle). If \( u \in \mathcal{C}(\bar{F}) \) is \( q \)-superharmonic on \( F \) the following results hold:

(i) If \( \delta(F) \neq \emptyset \) and \( u \geq 0 \) on \( \delta(F) \) then either \( u > 0 \) on \( F \) or \( u = 0 \) on \( F \).

(ii) If \( \delta(F) = \emptyset \) and \( q \neq q_\omega \) then either \( u > 0 \) on \( V \) or \( u = 0 \) on \( V \).

(iii) If \( \delta(F) = \emptyset \) and \( q = q_\omega \), then \( u = a\omega \), \( a \in \mathbb{R} \) and hence \( u \) is \( q \)-harmonic.

Proof. Let \( x^* \in F \) such that \( \frac{u(x^*)}{\omega(x^*)} = \min_{y \in F} \left\{ \frac{u(y)}{\omega(y)} \right\} \).

If \( \delta(F) = \emptyset \) and \( q = q_\omega \), then
\[
0 \leq \mathcal{L}_q(u)(x^*) = \int_F c(x^*, y)\omega(y)\left(\frac{u(x^*)}{\omega(x^*)} - \frac{u(y)}{\omega(y)}\right)dy \leq 0
\]
which implies that \( u = a\omega \), \( a \in \mathbb{R} \), since \( \bar{F} \) is connected. Moreover, \( u \) is \( q \)-harmonic.

If \( u(x^*) > 0 \), then \( u > 0 \) on \( F \). Otherwise, suppose that \( u(x^*) \leq 0 \). Then, from Hopf’s minimum principle \( u = a\omega \), \( a \leq 0 \), on \( F \), \( \mathcal{L}_q(u) = 0 \) on \( F \) and either \( u = 0 \) or \( q = q_\omega \) on \( F \).

When \( \delta(F) \neq \emptyset \), necessarily \( u = 0 \) on \( \delta(F) \) since \( u \geq 0 \) on \( \delta(F) \) and hence \( u = 0 \) on \( \bar{F} \).

The next result shows that strictly \( q_\omega \)-superharmonic functions cannot have local minima on \( F \), a well-known fact for the continuous case.

**Proposition 1.3.** If \( u \in \mathcal{C}(\bar{F}) \) is strictly \( q_\omega \)-superharmonic on \( F \), then for any \( x \in F \) there exists \( y \in \bar{F} \) such that \( c(x, y) > 0 \) and \( \frac{u(y)}{\omega(y)} < \frac{u(x)}{\omega(x)} \).

Proof. Let \( x \in F \) and suppose that for all \( y \in \bar{F} \) such that \( c(x, y) > 0 \), \( \frac{u(y)}{\omega(y)} \geq \frac{u(x)}{\omega(x)} \). Then,
\[
0 < \mathcal{L}_{q_\omega}(u)(x) = \int_F c(x, y)\omega(y)\left(\frac{u(x)}{\omega(x)} - \frac{u(y)}{\omega(y)}\right)dy \leq 0,
\]
which is a contradiction.
In the case of networks with boundary, i.e., $\delta(F) \neq \emptyset$, the Monotonicity Principle for $q_\omega$-superharmonic functions is equivalent to the following minimum principle.

**Proposition 1.4 (Minimum Principle).** Let $\Gamma = (\bar{F}, c)$ a network with boundary and $u \in C(\bar{F})$, $q_\omega$-superharmonic on $F$. Then
\[
\min_{x \in \delta(F)} \left\{ \frac{u(x)}{\omega(x)} \right\} \leq \min_{x \in \bar{F}} \left\{ \frac{u(x)}{\omega(x)} \right\}
\]
and the equality holds iff $u$ coincides on $\bar{F}$ with a multiple of $\omega$.

**Proof.** Consider $m = \min_{x \in \delta(F)} \left\{ \frac{u(x)}{\omega(x)} \right\}$ and $v = u - mw$. Then, $v$ is $q_\omega$-superlinebreak harmonic on $F$, since $\mathcal{L}_{q_\omega}(\omega) = 0$, and moreover $v \geq 0$ on $\delta(F)$. Therefore the claims follows from Proposition 1.2 (i). □

Now, we obtain a new proof of the existence and uniqueness of solution for the Dirichlet and Poisson problems, which includes a property of the support of the solution.

**Corollary 1.5.** Let $\Gamma$ a network such that when $F = V$ then $q \neq q_\omega$. For each $f \in C(F)$ there exists a unique $u \in C(F)$ such that $\mathcal{L}_{q}(u) = f$ on $F$. In addition, if $f \in C^+(F)$, then $u \in C^+(F)$ and $\text{supp}(f) \subset \text{supp}(u)$.

**Proof.** Consider the endomorphism $F: C(F) \rightarrow C(F)$ given by $F(u) = \mathcal{L}_{q}(u)|_{\bar{F}}$. By Proposition 1.2, $F$ is a monotone operator; that is, if $F(u) \geq 0$, then $u \geq 0$. Therefore, if $F(u) = 0$, it is also verified that $F(-u) = 0$, and hence $u, -u \geq 0$ which implies that $u = 0$. So, $F$ is injective and this implies that it is an isomorphism and moreover, $u \in C^+(F)$ when $f = \mathcal{L}_{q}(u)|_{\bar{F}} \in C^+(F)$.

Besides, if $u(x) = 0$, then $f(x) = \mathcal{L}_{q}(u)(x) = -\int_{\bar{F}} c(x, y) u(y) dy \leq 0$ and hence $f(x) = 0$. □

**2. Green and Poisson kernels**

In this section we assume that the potential satisfies that $q \geq q_\omega$ for some weight $\omega \in \Omega(\bar{F})$, so that $\mathcal{L}_{q}$ is positive semi-definite and then, we build the kernels associated with the inverse operators which correspond either to a semihomogeneous Dirichlet problem or to a Poisson equation. In the same way that in the continuous case, such operators will be called Green operators. In addition, for any proper subset, we will also consider the kernel associated with the inverse operator of the boundary value problem in which the equation is homogeneous and the boundary data is prescribed. Such integral operator will be called Poisson operator.

Here, we study the properties of the above-mentioned integral operators. Firstly we establish the basic notions about integral operators and their associated kernels. Then, we prove the existence and uniqueness of Green and Poisson operators for each proper subset $F$, we show some of their properties and we build the associated Green or Poisson kernels. On the other hand, under hypothesis $q \neq q_\omega$ we make an analogous study for the Green operator.
for $V$. Moreover, we consider also the singular case; that is, when $F = V$ and $q = q_\omega$ simultaneously and we construct the Green operators that represent the Moore–Penrose inverse of the matrix associated with the boundary value problem.

Given $S, T \subset V$, we define
\[ \mathcal{C}(S \times T) = \{ f : V \times V \rightarrow \mathbb{R} : f(x, y) = 0 \text{ if } (x, y) \notin S \times T \}. \]
In particular, any function $K \in \mathcal{C}(F \times F)$ is called a kernel on $F$.

If $K$ is a kernel on $F$, for each $x, y \in F$ we denote by $K^x$ and $K^y$ the functions of $\mathcal{C}(F)$ defined by $K^x(y) = K^y(x) = K(x, y)$. The integral operator associated with $K$ is the endomorphism $\mathcal{K} : \mathcal{C}(F) \rightarrow \mathcal{C}(F)$ that assigns to each $f \in \mathcal{C}(F)$, the function $\mathcal{K}(f)(x) = \int_F K(x, y) f(y) \, dy$ for all $x \in V$. Conversely, given an endomorphism $\mathcal{K} : \mathcal{C}(F) \rightarrow \mathcal{C}(F)$, the associated kernel is given by $K(x, y) = \mathcal{K}(\varepsilon_y)(x)$. Clearly, kernels and operators can be identified with matrices, after giving a label on the vertex set. In addition, a function $u \in \mathcal{C}(F)$ can be identified with the kernel $K(x, x) = u(x)$ and $K(x, y) = 0$ otherwise and hence with a diagonal matrix, that will be denoted by $D_u$.

When $K$ is a kernel on $\bar{F}$, for each $x \in \delta(F)$ and each $y \in \bar{F}$, we denote by \( \partial K \) \( \frac{\partial K^y}{\partial n_x} \) \( (x, y) \) \( \frac{\partial K^y}{\partial n_x} \) \( (x) \), whereas for each $x \in \bar{F}$ and each $y \in \delta(F)$ we denote by \( \frac{\partial K^y}{\partial n_x} \) \( (x, y) \) \( \frac{\partial K^y}{\partial n_x} \) \( (y) \) \( \frac{\partial K^y}{\partial n_x} \) \( (y) \). Clearly, \( \frac{\partial K^y}{\partial n_x} \) \( \in \mathcal{C}(\delta(F) \times \bar{F}) \) \( \frac{\partial K^y}{\partial n_x} \) \( \in \mathcal{C}(\delta(F) \times \bar{F}) \) and \( \frac{\partial K^y}{\partial n_x} \) \( \in \mathcal{C}(\bar{F} \times \delta(F)) \) \( \frac{\partial K^y}{\partial n_x} \) \( \in \mathcal{C}(\bar{F} \times \delta(F)) \) and hence both are kernels on $\bar{F}$.

**Lemma 2.1.** If $K$ is a kernel on $\bar{F}$, then it satisfies \( \frac{\partial^2 K}{\partial n_x \partial n_y} = \frac{\partial^2 K}{\partial n_y \partial n_x} \) \( \in \mathcal{C}(\delta(F) \times \delta(F)) \). Moreover, for any $x, y \in \delta(F)$
\[
\left( \frac{\partial^2 K}{\partial n_x \partial n_y} \right)(x, y) = \kappa(x)\kappa(y)K(x, y) - \kappa(x) \int_F c(y, z)K(x, z) \, dz
\]
\[ - \kappa(y) \int_F c(x, z)K(z, y) \, dz + \int_F \int_F c(x, u)c(y, z)K(u, z) \, du \, dz. \]
In addition, \( \left( \frac{\partial^2 K}{\partial n_x \partial n_y} \right) \) \( \text{is a symmetric kernel when } K \text{ is.} \)

Now we are ready to introduce the concept of Green operator and kernel. Firstly, we consider the case in which $\Gamma$ is either a network with boundary or when $F = V$, then $q \neq q_\omega$. Recall that in this situation, the endomorphism $\mathcal{F}$ defined in the proof of Corollary 1.5 as $\mathcal{F}(u) = \mathcal{L}_q(u)|_\mu$ is an isomorphism. Its inverse is named **Green operator of** $\Gamma$ and denoted by $\mathcal{G}$. Therefore, when $\Gamma$ is a network with boundary, for any $f \in \mathcal{C}(F)$, $u = \mathcal{G}(f)$ is the unique solution of the Dirichlet problem $\mathcal{L}_q(u) = f$ on $F$ and $u = 0$ on $\delta(F)$, whereas when $F = V$, for any $f \in \mathcal{C}(V)$, $u = \mathcal{G}(f)$ is the unique solution of the Poisson equation $\mathcal{L}_q(u) = f$ on $V$. 

Observe that the matrix associated with the operator $F$ is $L_q(F; F)$ and its inverse, $G$, is the matrix associated with $G$.

When $\Gamma = (\bar{F}, c)$ is a network with boundary, we call the linear operator $\mathcal{P} : \mathcal{C}(\delta(F)) \rightarrow \mathcal{C}(\bar{F})$ that assigns to each $g \in \mathcal{C}(\delta(F))$ the unique function $\mathcal{P}(g) \in \mathcal{C}(\bar{F})$ such that $L_q(\mathcal{P}(g)) = 0$ on $F$ and $\mathcal{P}(g) = g$ on $\delta(F)$ the Poisson operator of $\Gamma$. In particular, when $q = q_\omega$, then $\mathcal{P}(\omega) = \omega$.

In the following result we investigate formal properties of the Green and Poisson operators.

**Proposition 2.2.** If $\Gamma$ is either a network with boundary or $q \neq q_\omega$ when $F = V$, then the Green and the Poisson operators of $\Gamma$ are formally self–adjoint in the sense that

$$
\int_F g \mathcal{G}(f) \, dy = \int_F f \mathcal{G}(g) \, dy, \quad \text{for all } f, g \in \mathcal{C}(F),
$$

$$
\int_{\delta(F)} g \mathcal{P}(f) \, dy = \int_{\delta(F)} f \mathcal{P}(g) \, dy, \quad \text{for all } f, g \in \mathcal{C}(\delta(F)).
$$

Proof. Given $f, g \in \mathcal{C}(F)$, consider $u = \mathcal{G}(f)$ and $v = \mathcal{G}(g)$. Then $u, v \in \mathcal{C}(F)$ and $L_q(u) = f$ and $L_q(v) = g$ on $F$. In addition since both the Dirichlet problem and the Poisson equation are formally self–adjoint we get that

$$
\int_F g \mathcal{G}(f) \, dy = \int_F u \mathcal{L}_q(v) \, dy = \int_F v \mathcal{L}_q(u) \, dy = \int_F f \mathcal{G}(g) \, dy.
$$

On the other hand, $\mathcal{P}$ is self–adjoint since it coincides with the identity operator on $\mathcal{C}(\delta(F))$. \hfill \Box

The Green and Poisson operators of $\Gamma$ are integral operators on $F$ and $\bar{F}$, respectively, so the kernels associated with them will be called Green and Poisson kernels of $\Gamma$, and denoted by $G$ and $P$, respectively.

It is clear that $\mathcal{G} \in \mathcal{C}(F \times F)$ and $\mathcal{P} \in \mathcal{C}(\bar{F} \times \delta(F))$. Moreover, if $f \in \mathcal{C}(F)$ and $g \in \mathcal{C}(\delta(F))$, then the functions given by

$$
u(x) = \int_F G(x, y) f(y) \, dy \quad \text{and} \quad v(x) = \int_{\delta(F)} P(x, y) g(y) \, dy,
$$

are the solutions of the semihomogeneous boundary value problems $L_q(u) = f$ on $F$, $u = 0$ on $\delta(F)$ and $L_q(v) = 0$ on $F$ and $v = g$ on $\delta(F)$, respectively. In particular, for each $g \in \mathcal{C}(\delta(F))$ we have that $g(x) = \int_{\delta(F)} P(x, y) g(y) \, dy$ for all $x \in \delta(F)$. So, $1 = \int_{\delta(F)} P(x, y) \, dy$ for all $x \in \delta(F)$ and $\omega(x) = \int_{\delta(F)} P(x, y) \omega(y) \, dy$ for all $x \in \bar{F}$ when $q = q_\omega$.

Now, the relation between an integral operator and its associated kernel enables us to characterize the Green and Poisson kernels as solutions of suitable boundary value problems.

**Proposition 2.3.** If $\Gamma$ is either a network with boundary or $q \neq q_\omega$ when $F = V$, then for all $y \in F$, the function $G_y$ is characterized by $L_q(G_y) = \varepsilon_y$ on
Moreover, $G$ is symmetric on $F$, $P(x, y) = \varepsilon_y(x) - \left( \frac{\partial G}{\partial n_y} \right) (x, y)$ for all $x \in \tilde{F}$ and $y \in \delta(F)$ and

$$\left( \frac{\partial P}{\partial n_x} \right) (x, y) = \varepsilon_y(x) \kappa(x) - \left( \frac{\partial^2 G}{\partial n_x \partial n_y} \right) (x, y)$$

for all $x, y \in \delta(F)$. Therefore, $\left( \frac{\partial P}{\partial n_x} \right)$ is symmetric on $\delta(F)$.

Proof. For each $y \in F$, $G_y = \mathcal{G}(\varepsilon_y)$ and hence $\mathcal{L}_q(G_y) = \varepsilon_y$. In the same way if $y \in \delta(F)$, then $P_y = P(\varepsilon_y)$ is the unique solution of the boundary value problem $\mathcal{L}_q(P_y) = 0$ on $F$ and $P_y = \varepsilon_y$ on $\delta(F)$.

Moreover, from Proposition 2.2

$$G(x, y) = G_y(x) = \int_F \varepsilon_x \mathcal{G}(\varepsilon_y) \, dz$$

$$= \int_F \varepsilon_y \mathcal{G}(\varepsilon_x) \, dz = G_x(y) = G(y, x), \text{ for all } x, y \in F.$$

On the other hand, $u = P_y$ is the unique solution of the boundary value problem $\mathcal{L}_q(u) = 0$ on $F$ and $u = \varepsilon_y$ on $\delta(F)$. This problem is equivalent to the semihomogeneous one $\mathcal{L}_q(v) = -\mathcal{L}_q(\varepsilon_y)$ on $F$ with $v \in \mathcal{C}(F)$ and hence $u = P_y = \varepsilon_y - \mathcal{G}(\mathcal{L}(\varepsilon_y))$, for all $y \in \delta(F)$. Since for all $x \in F$, $\mathcal{L}(\varepsilon_y)(x) = \int_V c(x, z) (\varepsilon_y(x) - \varepsilon_y(z)) \, dz = -c(x, y)$, we get that for all $x \in F$, and all $y \in \delta(F)$,

$$\mathcal{G}(\mathcal{L}(\varepsilon_y)|_F)(x) = -\int_F G(x, z) c(z, y) \, dz$$

$$= \int_F c(y, z) \left( G(x, y) - G(x, z) \right) \, dz = \left( \frac{\partial G}{\partial n_y} \right) (x, y).$$

As, $\left( \frac{\partial \varepsilon_y}{\partial n_x} \right) (x, y) = \varepsilon_y(x) \kappa(x)$, the expression for the normal derivative of $P_y$ follows and hence its symmetry from Lemma 2.1. 

\textbf{Proposition 2.4.} If $\Gamma$ is either a network with boundary or $q \neq q_\omega$ when $F = V$, then for all $y \in F$, it is satisfied that $G_y > 0$ on $F$ for any $y \in F$, and $0 < P_y < \frac{\omega}{\omega(y)}$ on $F$ for any $y \in \delta(F)$. Moreover, for all $y \in F$, such that $F \setminus \{y\}$ is connected, $G_y < \frac{G_y(y)}{\omega(y)} \omega$ on $F \setminus \{y\}$.

Proof. A direct consequence of the Monotonicity Principle given in Proposition 1.2 is that $G_y > 0$ on $F$ for any $y \in F$ and that $P_y > 0$ on $F$ for any $y \in \delta(F)$. Moreover, taking $u = \frac{\omega}{\omega(y)} - P_y$, we get that

$$\mathcal{L}_q(u) = (q - q_\omega) \frac{\omega}{\omega(y)} \geq 0 \text{ on } F, \quad u(y) = 0, \quad u > 0 \text{ on } \delta(F) \setminus \{y\}$$

and hence by the Monotonicity Principle $u > 0$ on $F$. 


Finally, we consider \( y \in F \), such that \( H = F \setminus \{y\} \) is connected and \( v = \frac{G_y(y)}{\omega(y)} \omega - G_y \). Applying the Monotonicity Principle to the network with boundary \((H \cup \delta(H), c)\) where \( \delta(H) = \delta(F) \cup \{y\} \), we get that

\[
\mathcal{L}_q(v) = \frac{G_y(y)}{\omega(y)} (q - q_\omega) \omega \geq 0 \quad \text{on} \quad H, \quad v(y) = 0, \quad v > 0 \quad \text{on} \quad \delta(H) \setminus \{y\}
\]

and hence \( v > 0 \) on \( H \). \( \square \)

Next, we define the concept of Green operator and Green kernel when \( F = V \) and \( q = q_\omega \). For this, we will consider the vectorial subspace \( V = \ker(\mathcal{L}_q) \) and \( \pi \) the orthogonal projection on it. We already know that \( V \) is the subspace generated by \( \omega \), and hence \( \pi(f) = \langle f, \omega \rangle \omega \). Recall that, \( \mathcal{L}_q \) is an isomorphism of \( V^\bot \). Moreover, for each \( f \in C(V) \) there exists \( u \in C(V) \) such that \( \mathcal{L}_q(u) = f - \pi(f) \) and then \( u + V \) is the set of all functions such that \( \mathcal{L}_q(v) = f - \pi(f) \).

We call \textit{Green operator for} \( \Gamma \), the operator \( \mathcal{G} \) of \( C(V) \) that assigns to each \( f \in C(V) \) the unique function \( \mathcal{G}(f) \in V^\bot \) satisfying that \( \mathcal{L}_q(\mathcal{G}(f)) = f - \pi(f) \). Its associated kernel will be denoted by \( G \). In this case, the matrix associated with \( \mathcal{G} \) is nothing else but the Moore–Penrose inverse of \( \mathcal{L}_q \), usually denoted by \( \mathcal{L}_q^\dagger \).

**Proposition 2.5.** If \( F = V \) and \( q = q_\omega \), then the Green operator \( \mathcal{G} \) is self–adjoint and positive semi–definite. Moreover, \( \langle \mathcal{G}(f), f \rangle = 0 \) iff \( f = a\omega \), \( a \in \mathbb{R} \).

**Proof.** Let \( f, g \in C(V) \), \( u = \mathcal{G}(f) \) and \( v = \mathcal{G}(g) \). Then \( u, v \in V^\bot \), \( \mathcal{L}_q(u) = f - \pi(f) \), \( \mathcal{L}_q(v) = g - \pi(g) \) and hence

\[
\int_V g \mathcal{G}(f) \, dx = \int_V (g - \pi(g)) u \, dx = \int_V u \mathcal{L}_q(v) \, dx = \int_V v \mathcal{L}_q(u) \, dx
\]

\[
= \int_V (f - \pi(f)) v \, dx = \int_V f \mathcal{G}(g) \, dx.
\]

Moreover, \( \langle \mathcal{G}(f), f \rangle = \int_V f \mathcal{G}(f) \, dx = \int_V u \mathcal{L}_q(u) \, dx \geq 0 \), with equality iff \( u = 0 \), which implies that \( f = \pi(f) \) and hence \( f = a\omega \). \( \square \)

If \( G \) is the Green kernel for \( \Gamma \), then \( G \in C(V \times V) \) is symmetric and moreover, if \( f \in C(V) \) then the function given by \( u(x) = \int_V G(x, y) f(y) \, dy \) for all \( x \in V \) is the unique solution in \( V^\bot \) of the Poisson equation \( \mathcal{L}_q(u) = f - \pi(f) \). The relation between an integral operator and its associated kernel enables us again to characterize the Green kernel for \( \Gamma \) as solutions of suitable boundary value problems.

**Proposition 2.6.** For all \( y \in V \), the function \( G_y \) is characterized by equations

\[
\mathcal{L}_q(G_y) = \varepsilon_y - \omega(y) \omega \quad \text{and} \quad \int_V \omega G_y \, dx = 0.
\]

Moreover, \( G_y(y) > 0 \) and \( G_y < \frac{G_y(y)}{\omega(y)} \omega \) on \( V \setminus \{y\} \), for any \( y \in V \) such that \( V \setminus \{y\} \) is connected.
Proof. Observe that \( \pi(\varepsilon_y) = \omega(y)\omega \) for any \( y \in V \). Moreover, \( G_y = G(\varepsilon_y) \) and hence \( \mathcal{L}_q(G_y) = \varepsilon_y - \omega(y)\omega \). As \( G_y(y) = \langle \varepsilon_y, G(\varepsilon_y) \rangle > 0 \); since \( G \) is positive semi–definite and \( \varepsilon_y \) is not a multiple of \( \omega \). On the other hand, if \( F = V \setminus \{ y \} \) and \( u = \frac{G_y(y)}{\omega(y)}\omega - G_y \), we get that \( u(y) = 0 \) and \( \mathcal{L}_q(u) = \omega(y)\omega > 0 \) on \( F \). Applying the Monotonicity Principle we get that \( u > 0 \) on \( F \). \( \square \)

### 3. The Dirichlet–Robin map

In this section we define the **Dirichlet–Robin map** on general networks and we study its main properties. This map is naturally associated with a Schrödinger operator, and generalizes the concept of **Dirichlet–Neumann map** for the case of the combinatorial Laplacian. Through this section we suppose that \( \Gamma = (\bar{F}, c) \) is a network with boundary and that \( q = q_\sigma + \lambda \chi_{\delta(F)} \), so that \( q \geq q_\sigma \) and then the Energy Principle is in force, see Corollary 2.6 of Lecture 2.

Recall that the Energy is given by \( \mathcal{E}_q : \mathcal{C}(\bar{F}) \times \mathcal{C}(\bar{F}) \longrightarrow \mathbb{R} \) given for any \( u, v \in \mathcal{C}(\bar{F}) \) by

\[
\mathcal{E}_q(u, v) = \frac{1}{2} \int_{\bar{F}} \int_{\bar{F}} c_F(x, y) \left( u(x) - u(y) \right) \left( v(x) - v(y) \right) \, dx \, dy + \int_{\bar{F}} q u \, v.
\]

From the First Green Identity, for any \( u, v \in \mathcal{C}(\bar{F}) \) we get that

\[
\mathcal{E}_q(u, v) = \int_{\bar{F}} v \mathcal{L}_q(u) + \int_{\delta(F)} v \left[ \frac{\partial u}{\partial n_F} + qu \right].
\]

Under the above hypothesis, for any \( g \in \mathcal{C}(\delta(F)) \), the Dirichlet problem

\[
\mathcal{L}_q(u) = 0 \quad \text{on} \quad F \quad \text{and} \quad u = g \quad \text{on} \quad \delta(F)
\]

has \( u_q = \mathcal{P}_q(g) \) as its unique solution.

The map \( \Lambda_q : \mathcal{C}(\delta(F)) \longrightarrow \mathcal{C}(\delta(F)) \) that assigns to any function \( g \in \mathcal{C}(\delta(F)) \) the function \( \Lambda_q(g) = \frac{\partial u_q}{\partial n_F} + qg \) is called **Dirichlet–Robin map**.

The Poisson kernel is directly related to the Dirichlet–Robin map \( \Lambda_q \), as it is shown on the proposition below.

**Proposition 3.1.** The Dirichlet–Robin map, \( \Lambda_q \), is a self–adjoint, positive semi–definite operator whose associated quadratic form is given by

\[
\int_{\delta(F)} g \Lambda_q(g) = \mathcal{E}_q(u_g, u_g).
\]

Moreover, \( \lambda \) is the lowest eigenvalue of \( \Lambda_q \) and its associated eigenfunctions are multiple of \( \sigma \). In addition, the kernel \( N \in \mathcal{C}(\delta(F) \times \delta(F)) \) of \( \Lambda_q \) is

\[
N = \frac{\partial \mathcal{P}_q}{\partial n_x} + q = \kappa + q - \frac{\partial^2 G_q}{\partial x \partial n_y},
\]

which is symmetric, negative off–diagonal and positive on the diagonal.
Monotonicity and Resolvent Kernels

PROOF. From (4) we get that for any \( f, g \in C(\delta(F)) \),
\[
\int_{\delta(F)} f \Lambda_q(g) = \mathcal{E}_q(u_f, u_g) = \mathcal{E}_q(u_g, u_f) = \int_{\delta(F)} g \Lambda_q(f)
\]
and hence \( \Lambda_q \) is self-adjoint and positive semi-definite. Moreover, for every \( x \in \delta(F) \), using that \( P_q(\sigma \chi_{\delta(F)}) = \sigma \) on \( F \) it is easily seen that
\[
\Lambda_q(\sigma \chi_{\delta(F)})(x) = \frac{\partial \sigma}{\partial \nu_F}(x) + q_\sigma(x)\sigma(x) + \lambda\sigma(x) = \lambda\sigma(x),
\]
since \( q_\sigma = -\sigma^{-1} \frac{\partial \sigma}{\partial \nu_F} \) on \( \delta(F) \).

On the other hand, from Proposition 2.5 of Lecture II and taking into account that \( u_g = g \) on \( \delta(F) \), we get
\[
\mathcal{E}_q(u_g, u_g) = \frac{1}{2} \int_F \int_F c_F(x, y)\sigma(x)\sigma(y) \left( \frac{u_g(x)}{\sigma(x)} - \frac{u_g(y)}{\sigma(y)} \right)^2 \, dx dy + \lambda \int_{\delta(F)} g^2 \geq \lambda \int_{\delta(F)} g^2.
\]
The equality holds iff \( u_g = a\sigma \); that is, iff \( g = a\sigma \).

Suppose that \( g \) is a non-zero eigenfunction corresponding to the eigenvalue \( \alpha \). Then, by the definition of eigenvalue and the first part of the proposition, we have
\[
\alpha \int_{\delta(F)} g^2 = \int_{\delta(F)} g \Lambda_q(g) = \mathcal{E}_q^F(u_g, u_g) \geq \lambda \int_{\delta(F)} g^2
\]
which implies that \( \alpha \geq \lambda \).

The expression and the symmetry property for the kernel follows from Proposition 2.3. Finally, for any \( x, y \in \delta(F) \) with \( x \neq y \), notice that \( P_q(x, y) = \varepsilon_y(x) = 0 \). In this case, we get that
\[
N(x, y) = \Lambda_q(\varepsilon_y)(x) = \frac{\partial P_q}{\partial \nu_x}(x, y) = \sum_{z \in F} c(x, z)(P_q(x, y) - P_q(z, y)) = -\sum_{z \in F} c(x, z)P_q(z, y) < 0,
\]
since \( P_q(z, y) > 0 \). Moreover, as \( \Lambda_q(\sigma) = \lambda\sigma \) on \( \delta(F) \), then for any \( y \in \delta(F) \)
\[
\sum_{x \in \delta(F)} \Lambda_q(\varepsilon_y)(x)\sigma(x) = \lambda\sigma(y),
\]
and hence
\[
\Lambda_q(\varepsilon_y)(y) = \lambda - \sigma(y)^{-1} \sum_{x \in \delta(F)} \Lambda_q(\varepsilon_y)(x)\sigma(x) > 0,
\]
where we used the fact that \( \Lambda_q(\varepsilon_y)(x) < 0 \) for any \( x, y \in \delta(F) \) and \( x \neq y \) as shown above.

The kernel of Dirichlet–to–Robin map is closely related to the Schur complement of \( (L_q)_F \) in \( L_q \); see [5] and [4, Theorem 3.2] for the combinatorial
Laplacian and the Dirichlet–to–Neumann map. Notice that the Robin problem

\[ \mathcal{L}_q(u) = f \text{ on } F, \quad \frac{\partial u}{\partial n_F} + qu = g \text{ on } \delta(F), \]

has the following matrix expression

\[
\begin{bmatrix}
D & -C \\
-C^T & M
\end{bmatrix}
\begin{bmatrix}
v_{\delta} \\
v
\end{bmatrix}
= \begin{bmatrix}
g \\
f
\end{bmatrix},
\]

where \( D \) is the diagonal matrix whose diagonal entries are given by \( \kappa + q \), \( C = (c(x,y))_{x \in \delta(F)} \), \( M \) is the matrix associated with \( (\mathcal{L}_q)_{|F} \), \( v_{\delta} \), \( v \), \( f \), \( g \) are the vectors determined by \( u_{|\delta(F)} \), \( u_{|F} \), \( f \) and \( g \), respectively. Then, \( M \) is invertible and \( M^{-1} = \left( G_q(x,y) \right)_{x,y \in F} \). Moreover, the Schur complement of \( M \) in \( L \) is

\[
L/M = D - CM^{-1}C^T = \left( N(x,y) \right)_{x,y \in \delta(F)},
\]

since we have the equality given for \( N \) in Proposition 5 and the following equality from Lemma 2.1

\[
CM^{-1}C^T = \left( \frac{\partial^2 G_q}{\partial n_x \partial n_y} \right)_{x,y \in \delta(F)},
\]

where we have taken into account that \( G_q \) is symmetric and zero on \( \delta(F) \times F \).

**References**


LECTURE IV: APPLICATIONS TO MATRIX THEORY

Abstract. In this lecture we present an application of the results displayed in the previous lectures to Matrix Theory. Firstly, we introduce the concept of effective resistance and Kirchhoff index with respect to a parameter and a weight and we find the relation between effective resistances and Green functions. These definitions have allowed us to extend the $M$–matrix inverse problem to non diagonally dominant matrices and to give a characterization of when a singular symmetric and irreducible $M$–matrix has a Moore–Penrose inverse that is also an $M$–matrix.

1. Kirchhoff Index and Effective resistances

The Kirchhoff Index was introduced in Chemistry as a better alternative to other parameters used for discriminating among different molecules with similar shapes and structures; see [11]. Since then, a new line of research with a considerable amount of production has been developed and the Kirchhoff Index has been computed for some classes of graphs with symmetries; see for instance [1] and the references therein. This index is defined as the sum of all effective resistances between any pair of vertices of the network and it is also known as the Total Resistance; [10] and coincides with the Kemeny constant when considering the Markov chain associated with the network. We have introduced a generalization of the Kirchhoff Index of a finite network that consists in defining the effective resistance between any pair of vertices with respect to a value $\lambda \geq 0$ and a weight $\omega$ on the vertex set. It turns out that $\lambda$ is the lowest eigenvalue of a suitable semi–definite positive Schrödinger operator and $\omega$ is the associated eigenfunction. Then, we prove that the effective resistance, with respect to $\lambda$ and $\omega$, define a distance on the network as in the standard case and hence it can be also used with the same aims. Actually, we show that the generalized effective resistance verifies analogous properties to those verified in the classical case. In particular, we obtain the relation between the Kirchhoff Index with respect to $\lambda$ and $\omega$ and the eigenvalues of the associated Schrödinger operator as well as the relation between the effective resistances with respect to $\lambda$ and $\omega$ and the eigenvalues and eigenfunctions of the mentioned operator.

In the standard setting, the effective resistance between vertices $x$ and $y$ is defined through the solution of the Poisson equation $L(u) = f$ when the data is the dipole with poles at $x$ and $y$; that is, $f = \varepsilon_x - \varepsilon_y$. The knowledge of the effective resistance can be used to deduce important properties of electrical networks, see for instance [10, 11, 12].

In the sequel we work only with semi–definite positive Schrödinger operators. Therefore, we will consider fixed a value $\lambda \geq 0$, a weight $\omega \in \Omega(V)$ and their associated potential $q = q_\omega + \lambda$. 109
We can generalize the concept of effective resistance in the following way. Given \( x, y \in V \), the \( \omega \)-dipole between \( x \) and \( y \) is the function \( f_{xy} = \frac{1}{\omega}(\varepsilon_x - \varepsilon_y) \).

Clearly, for any \( x, y \in V \) it is verified that \( \pi(f_{xy}) = 0 \) and hence the Poisson equation

\[
L_q(v) = f_{xy}
\]

is solvable and any solution maximizes the functional

\[
J_{x,y}(u) = \int_V u L_q(u) \, dx;
\]

see Lecture II Corollary 2.4.

Given \( x, y \in V \), the Effective Resistance between \( x \) and \( y \) with respect to \( \lambda \) and \( \omega \), is the value

\[
R_{\lambda,\omega}(x,y) = \max_{u \in C(V)} \{ J_{x,y}(u) \}.
\]

Moreover the Kirchhoff Index of \( \Gamma \), with respect to \( \lambda \) and \( \omega \), is the value

\[
K(\lambda, \omega) = \frac{1}{2} \sum_{x,y \in V} R_{\lambda,\omega}(x,y) \omega^2(x) \omega^2(y).
\]

The kernel \( R_{\lambda,\omega}: V \times V \to \mathbb{R} \) is called the Effective Resistance of the network \( \Gamma \), with respect to \( \lambda \) and \( \omega \).

**Proposition 1.1.** If \( u \in C(V) \) is a solution of the Poisson equation \( L_q(u) = f_{xy} \), then

\[
R_{\lambda,\omega}(x,y) = \int_V u L_q(u) \, dx = \frac{u(x)}{\omega(x)} - \frac{u(y)}{\omega(y)}.
\]

Therefore, \( R_{\lambda,\omega} \) is symmetric, non-negative and moreover \( R_{\lambda,\omega}(x,y) = 0 \) iff \( x = y \).

Proof. Given \( u \in C(V) \) we get that \( J_{x,y}(u) = J_{y,x}(-u) \) and hence \( R_{\lambda,\omega}(x,y) = R_{\lambda,\omega}(y,x) \) for any \( x, y \in V \). Moreover, we know that \( R_{\lambda,\omega}(x,x) = 0 \) for any \( x \in V \) and also that \( R_{\lambda,\omega}(x,y) = 0 \) iff \( \langle L_q(u), u \rangle = 0 \) for any solution of the Poisson equation \( L_q(u) = f_{xy} \). So, \( u = a \omega \), where \( a = 0 \) if \( \lambda > 0 \), that in any case implies that \( L_q(u) = 0 \) and hence \( f_{xy} = 0 \) or equivalently \( x = y \). \( \square \)

The effective resistance is closely related with the Green function of \( \Gamma \), \( G \).

Recall that \( G = L_q^{-1} \) when \( \lambda > 0 \), whereas \( G = L_q^\dagger \) when \( \lambda = 0 \).

**Corollary 1.2.** For any \( x, y \in V \), it is satisfied that

\[
R_{\lambda,\omega}(x,y) = \frac{G(x,x)}{\omega^2(x)} + \frac{G(y,y)}{\omega^2(y)} - \frac{2G(x,y)}{\omega(x)\omega(y)}.
\]

In particular,

\[
k(\lambda, \omega) = \text{tr}(G) - \lambda^\dagger,
\]

where \( \lambda^\dagger = \lambda^{-1} \) if \( \lambda > 0 \) and \( \lambda^\dagger = 0 \), otherwise.
Proof. If \( u = \mathcal{G}(f_{xy}) \), then \( \mathcal{L}_q(u) = f_{xy} \). Therefore, for any \( z \in V \),

\[
u(z) = \int_V G(z,t) f_{xy}(t) \, dt = \frac{G(z,x)}{\omega(x)} - \frac{G(z,y)}{\omega(y)}.
\]

The result follows from the identity \( R_{\lambda,\omega}(x,y) = \frac{u(x)}{\omega(x)} - \frac{u(y)}{\omega(y)} \) taking into account the symmetry of \( G \).

On the other hand,

\[
k(\lambda,\omega) = \frac{1}{2} \sum_{x,y \in V} \left( \frac{G(x,x)}{\omega^2(x)} + \frac{G(y,y)}{\omega^2(y)} - 2 \frac{G(x,y)}{\omega(x)\omega(y)} \right) \omega(x)^2 \omega(y)^2
\]

\[
= \frac{1}{2} \sum_{x,y \in V} G(x,x)\omega^2(y) + \frac{1}{2} \sum_{x,y \in V} G(y,y)\omega^2(x) - \sum_{x,y \in V} G(x,y)\omega(x)\omega(y)
\]

\[
= \sum_{x \in V} G(x,x) - \langle \mathcal{G}(\omega),\omega \rangle = \text{tr}(\mathcal{G}) - \lambda^1. \quad \square
\]

2. Characterization of symmetric \( M \)-matrices as resistive inverses

The proof of the main result in this lecture is based in a commonly used technique in the context of electrical networks and Markov Chains, that in fact is used in [7, 8]. We remark that in the probabilistic context, the function \( q \) is usually called the potential (vector) of the operator \( \mathcal{L}_q \), see for instance [8].

Given \( \mathcal{L}_q \), a positive definite Schrödinger operator on \( \Gamma \), the method consists of embedding the given network into a suitable host network. The new network is constructed by adding a new vertex, that represents an absorbing state, joined with each vertex in the original network through a new edge whose conductance is the diagonal excess after the use of the \( h \)-transform; i.e. Doob transform.

Given \( \lambda > 0, \omega \in \Omega(V) \) and \( \hat{x} \notin V \), we consider the network \( \Gamma_{\lambda,\omega} = (V \cup \{\hat{x}\}, c_{\lambda,\omega}) \) where \( c_{\lambda,\omega}(x,y) = c(x,y) \) when \( x,y \in V \) and \( c_{\lambda,\omega}(\hat{x},x) = c_{\lambda,\omega}(x,\hat{x}) = \lambda \omega(x) \) for any \( x \in V \). We denote by \( \mathcal{L}^{\lambda,\omega} \) its combinatorial Laplacian and by \( \hat{\omega} \in \Omega(V \cup \{\hat{x}\}) \) the weight given by \( \hat{\omega}(x) = \frac{\sqrt{2}}{2} \omega(x) \) when \( x \in V \) and \( \hat{\omega}(\hat{x}) = \frac{\sqrt{3}}{2} \). See Figure 1.

The next result establishes the relationship between the original Schrödinger operator \( \mathcal{L}_q \) and a new semidefinite Schrödinger operator on \( \Gamma_{\lambda,\omega} \).

**Proposition 2.1.** If \( q = q_\omega + \lambda \) and we define \( \hat{q} = -\frac{1}{\hat{\omega}} \mathcal{L}^{\lambda,\omega}(\hat{\omega}) \), then \( \hat{q}(\hat{x}) = \lambda \left( 1 - \langle \omega,1 \rangle \right) \) and \( \hat{q} = q - \lambda \omega \) on \( V \). Moreover, for any \( u \in C(V \cup \{\hat{x}\}) \) we get that \( \mathcal{L}^{\lambda,\omega}_q(u)(\hat{x}) = \lambda \left( u(\hat{x}) - \langle \omega, u_\hat{\nu} \rangle \right) \) and

\[
\mathcal{L}^{\lambda,\omega}_q(u) = \mathcal{L}_q(u_\hat{\nu}) - \lambda \omega u(\hat{x}) = \mathcal{L}_q(u_\hat{\nu}) - \lambda \mathcal{P}_\omega(u_\hat{\nu}) - \omega \mathcal{L}^{\lambda,\omega}_q(u)(\hat{x}) \quad \text{on} \ V.
\]
Figure 1. Host network

Proof. Given $u \in C(V \cup \{\hat{x}\})$, then for any $x \in V$ we get that
\[ L^{\lambda,\omega}(u)(x) = L(u_{|V})(x) + \lambda \omega(x)u(x) - \lambda \omega(x)u(\hat{x}). \]
In particular, taking $u = \hat{\omega}$ we obtain that
\[ -\hat{q}(x) = -q + \lambda \omega \text{ on } V \]
and hence
\[ L^{\lambda,\omega}(\hat{\omega})(\hat{x}) = \lambda(\omega,1) \]
which, in particular, implies that
\[ -\hat{q}(\hat{x}) = L^{\lambda,\omega}(\hat{\omega})(\hat{x}) = \lambda(\omega,1) - 1. \]
Therefore, for any $u \in C(V \cup \{\hat{x}\})$ we get that
\[ L^{\lambda,\omega}(u)(\hat{x}) = \lambda(u(\hat{x}) - (\omega, u_{|V})), \]
which is equivalent to \( \lambda \omega u(\hat{x}) = L^{\lambda,\omega}(u)(\hat{x}) - \lambda \omega u(\hat{x}) \) and the second identity for the value of $L^{\lambda,\omega}(u)$ on $V$ follows. \( \square \)

We end this lecture with the matrix counterpart of the main results in [2]. So, we characterize the inverse of any irreducible symmetric $M$–matrix, singular or not, in terms of the effective resistances of a suitable network, or equivalently, we prove that any irreducible symmetric $M$–matrix is a resistive inverse.

**Theorem 2.2.** Let $M$ be an irreducible Stieltjes matrix of order $n$ and $M^{-1} = (g_{ij})$ its inverse. Then there exist a network $\Gamma = (V,c)$ with $|V| = n$, a value $\lambda > 0$ and a weight $\omega \in \Omega(V)$ such that $M = L_\omega + \lambda I$. Moreover, if we consider the host network $\Gamma_{\lambda,\omega} = (V \cup \{x_{n+1}\}, 1\varsigma_{\omega})$ and $\hat{R}_{ij}$, $i,j = 1, \ldots, n+1$ are the effective resistances of $\Gamma_{\lambda,\omega}$ with respect to $\hat{\omega}$, then
\[
L_{\omega} = \begin{bmatrix}
M & -Mw \\
-w^*M & w^*Mw
\end{bmatrix} = \begin{bmatrix}
M & -\lambda w \\
-\lambda w^* & n\lambda
\end{bmatrix},
\]
where $w \in \mathbb{R}^n$ is the vector indetified with $\omega$, and
\[
g_{ij} = \frac{\omega_{ij}}{2} \left( \hat{R}_{in+1} + \hat{R}_{jn+1} - \hat{R}_{ij} \right), \text{ for any } i,j = 1, \ldots, n.
\]

The above theorem generalizes the main result obtained by M. Fiedler in [9] where the inverses of weakly diagonal dominant Stieltjes matrices were characterized.
Theorem 2.3. Let $M$ be a singular irreducible and symmetric $M$–matrix of order $n$ and consider $M^\dagger = (g_{ij})$ its Moore–Penrose inverse. Then there exist a network $\Gamma = (V,c)$ with $|V| = n$ and a weight $\omega \in \Omega(V)$ such that $M = L_\omega$. Moreover, if $R_{ij}$, $i,j = 1,\ldots,n$ are the effective resistances of $\Gamma$ with respect to $\omega$, then

$$g_{ij} = -\frac{\omega_i \omega_j}{2} \left( R_{ij} - \frac{1}{n} \sum_{k=1}^{n} (R_{ik} + R_{jk}) \omega_k^2 + \frac{1}{n^2} \sum_{k,l=1}^{n} R_{kl} \omega_k^2 \omega_l^2 \right).$$

Finally, the problem of knowing when the Moore–Penrose inverse of a singular irreducible and symmetric $M$–matrix is also a $M$–matrix, it a difficult problem. We have the following general result, see [3], that is a consequence of the minimum principle.

Proposition 2.4. Let $M$ a singular irreducible and symmetric $M$–matrix. Then, $M^\dagger = (g_{ij})$ is a $M$–matrix iff $g_{ij} \leq 0$ for any $j \sim i$.

Proof. If $M$ a singular irreducible and symmetric $M$–matrix, there exists a network $\Gamma = (V,c)$ and a weight $\omega \in \Omega(V)$ such that $M = L_\omega$ and $M^\dagger = G$. For any $y \in V$, consider $u_y(x) = -G(x,y)$. Then, $u_y$ is a $q_\omega$–superharmonic on $F = V \setminus \{y\} \cup N(y)$ and hence $\min_{z \sim y} \left\{ \frac{u_y(z)}{\omega(z)} \right\} \leq \min_{z \in F} \left\{ \frac{u_y(z)}{\omega(z)} \right\}$, since $\delta(F) = N(y)$. Therefore, $\max_{z \sim y} \left\{ \frac{G(z,y)}{\omega(z)} \right\} \geq \frac{G(x,y)}{\omega(x)}$ for any $x \neq y$. □

We focus now on singular irreducible and symmetric Jacobi $M$–matrix. Given $c_1,\ldots,c_{n-1} > 0$ and $d_1,\ldots,d_n \geq 0$ such that the tridiagonal matrix

$$M = \begin{bmatrix}
d_1 & -c_1 & \cdots & \cdots & \cdots \\
-c_1 & d_2 & -c_2 & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots \\
& \cdots & \cdots & \cdots & \cdots \\
& & \cdots & \cdots & \cdots \\
\vdots & \cdots & \cdots & \cdots & \cdots \\
c_{n-2} & d_{n-1} & -c_{n-1} & \cdots & \cdots \\
& c_{n-1} & d_n & -c_n & \cdots \\
& & & \cdots & \cdots \\
& & & & \cdots \\
& & & & \cdots \\
0 & & & & \cdots \\
\end{bmatrix}$$

is a singular $M$–matrix, we aim here at determining when its Moore–Penrose inverse $M^\dagger$ is also an $M$–matrix.

We have proved that the matrix given in (3) is a singular $M$–matrix iff there exists $\omega_1,\ldots,\omega_n > 0$ such that $\omega_1^2 + \ldots + \omega_n^2 = 1$ and

$$d_1 = \frac{c_1 \omega_2}{\omega_1}, \quad d_n = \frac{c_{n-1} \omega_n - 1}{\omega_n} \quad \text{and} \quad d_j = \frac{1}{\omega_j} (c_j \omega_{j+1} + c_{j-1} \omega_{j-1})$$

for any $j = 2,\ldots,n-1$. Moreover, the weight is uniquely determined by $(d_1,\ldots,d_n)$ and $(c_1,\ldots,c_{n-1})$.

In the sequel the matrix given in (3), where $c = (c_1,\ldots,c_{n-1}) \in (0,\infty)^{n-1}$ is a conductance, $\omega \in \Omega(V)$ and the diagonal entries are given by (4), is denoted by $M(c,\omega)$ and hence its Moore–Penrose inverse is denoted by $M^\dagger(c,\omega)$.

Throughout the lecture, we use the conventions $\sum_{i=1}^{j} a_i = 0$ and $\prod_{i=1}^{j} a_i = 1$ when $j < i$. In addition we denote by $e_j$ the $j$-th vector in the standard basis of $\mathbb{R}^n$ and by $e$ the vector $e = e_1 + \cdots + e_n$. 
Proposition 2.5. The Moore–Penrose inverse of $M(c, \omega)$ is $M^\dagger(c, \omega) = (g_{ij})$, where
\[
g_{ji} = g_{ij} = \omega_i \omega_j \left[ \sum_{k=1}^{i-1} \left( \sum_{l=1}^{k} \omega_l^2 \right)^2 + \sum_{k=i}^{n-1} \left( \sum_{l=k+1}^{n} \omega_l^2 \right)^2 - \sum_{k=1}^{j-1} \left( \sum_{l=k+1}^{n} \omega_l^2 \right)^2 \right]
\]
for any $1 \leq i \leq j \leq n$.

Notice that $g_{1n} = -\sum_{k=1}^{n-1} \left( \sum_{l=k+1}^{n} \omega_l^2 \right)^2 < 0$ and hence the Moore–Penrose inverse of any path always has a negative entry.

The Moore–Penrose inverse for the normalized Laplacian; that is, when $\omega$ is the square root of the generalized degree, was obtained in [6, Theorem 9].

If we take into account that the Moore–Penrose inverse of a symmetric and positive semi–definite matrix is itself symmetric and positive semi–definite, as a by–product of the expression of $M^\dagger(c, \omega)$ we can easily characterize when it is an $M$–matrix.

Theorem 2.6. $M^\dagger(c, \omega)$ is an $M$–matrix iff $g_{ii+1} \leq 0$ for any $i = 1, \ldots, n-1$, that is; iff
\[
\left( \sum_{l=i+1}^{n} \omega_l^2 \right) \left( \sum_{l=1}^{i} \omega_l^2 \right)^2 \geq \sum_{k=1}^{i-1} \left( \sum_{l=k+1}^{n} \omega_l^2 \right)^2 + \sum_{k=i+1}^{n-1} \left( \sum_{l=k+1}^{n} \omega_l^2 \right)^2, \quad i = 1, \ldots, n-1.
\]

The conclusion of the above Theorem for $\omega$ constant was given in [5, Lemma 3.1], where it is proved that $n \leq 4$. For general weights, the above characterization involves a highly non–linear system of inequalities on the off–diagonal entries of the matrix. The problem can be solved explicitly for $n \leq 3$, but for $n \geq 4$ the system becomes much more complicated and the key idea to solve it is to apply well–known properties of general $M$–matrices to the coefficient matrix of the system. Our main result establishes that for any $n$, there exist singular, symmetric and tridiagonal $M$–matrices of order $n$ whose Moore–Penrose inverse is also an $M$–matrix; see [4] for a complete study.

References


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The group inverse of the Laplacian matrix of a graph
THE GROUP INVERSE OF THE LAPLACIAN MATRIX OF A GRAPH

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1. Preamble

What follows is a short tour through some of the connections between weighted graphs and the group inverses of their associated Laplacian matrices. The presentation below draws heavily from chapter 7 of [7], and the interested reader can find further results on the topic in that book. We have assumed that the student has a working knowledge of matrix theory, and knows the basics of graph theory. References to specialised results are included as needed in these notes and a notation sheet is included at the end of the notes for the reader’s convenience.

2. The Laplacian matrix

Let \( G = (V, E) \) be an undirected graph on vertices labelled 1, \ldots, \( n \). Suppose also that for each edge \( e \in E \) there is an associated weight – i.e., a positive number \( w(e) \). We think of the graph \( G \), along with the associated weight function \( w \) as a weighted graph; in the case that each edge weight is 1 we say that \( G \) is unweighted. When vertices \( i \) and \( j \) are adjacent in \( G \), we use the notation \( i \sim j \) to denote the edge between them.

Build the \( n \times n \) matrix \( A = [a_{i,j}]_{i,j=1,...,n} \) from the weighted graph as follows:

\[
a_{i,j} = \begin{cases} 
w(e), & \text{if } i \text{ is adjacent to } j \text{ and } e \text{ is the edge between them} \\0, & \text{if not.}
\end{cases}
\]

Set \( D = \text{diag}(A1) \), where \( 1 \) is the all–ones vector in \( \mathbb{R}^n \). The Laplacian matrix for the weighted graph \( G \) is

\[
L = D - A.
\]

Throughout we will typically suppress the explicit dependence on the weight function \( w \), and simply refer to ‘the weighted graph \( G \').

Observations.

1. For \( i, j = 1, \ldots, n \), we have

\[
l_{i,j} = \begin{cases} 
-w(e), & \text{if } i \text{ is adjacent to } j, e = i \sim j \\
0, & \text{if } i \neq j \text{ and } i, j \text{ are not adjacent} \\
\sum_{e \in E, \ e \text{ incident with } j} w(e), & \text{if } i = j.
\end{cases}
\]
2. Let \( L = \sum_{e \in E, e = i \sim j} w(e)(e_i - e_j)(e_i - e_j)^\top. \)

3. Impose any orientation on \( G \) (i.e., replace edges \( i \sim j \) by directed arcs \( i \rightarrow j \)). Construct the corresponding oriented incidence matrix \( Q \) as follows: rows of \( Q \) are indexed by vertices of \( G \), columns of \( Q \) are indexed by edges of \( G \); for each \( e \in E \), the column of \( Q \) corresponding to \( e \) is \( \sqrt{w(e)}(e_i - e_j) \), where \( i \rightarrow j \) is the directed arc arising from the orientation of the edge \( e \). From 2. it follows readily that \( L = QQ^\top. \)

4. \( L \) is positive semidefinite – i.e., for each \( x \in \mathbb{R}^n, x^\top Lx \geq 0. \)

5. \( L \) is singular, with 1 as a null vector.

6. Consider the case that \( G \) is connected and let \( x \) be a null vector for \( L \). Then \( Q^\top x = 0 \), from which we deduce that \( x_i = x_j \) whenever \( i \) is adjacent to \( j \) in \( G \). It follows that for any pair of vertices \( p, q \), we must have \( x_p = x_q \), since there is a path from \( p \) to \( q \) in \( G \), say \( p = p_0 \sim p_1 \sim \cdots \sim p_k = q \), so \( x_{p_0} = x_{p_1} = \cdots = x_{p_k} \). Hence \( x \) is a scalar multiple of 1.

7. If \( G \) has \( k \) connected components, say \( G_1, \ldots, G_k \), then the nullity of \( L \) is \( k \). Further, the null space of \( L \) is spanned by the vectors \( z^{G_j}, j = 1, \ldots, k \) with

\[
\tilde{z}_{ip}^{G_j} = \begin{cases} 1 & \text{if } p \in G_j \\ 0 & \text{if not.} \end{cases}
\]

Denote the eigenvalues of \( L \) by \( 0 = \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n \). From 6. above we see that \( \lambda_2 > 0 \) if and only if \( G \) is connected. Suppose that \( x \in \mathbb{R}^n \) with \( x^\top x = 1 \) and \( x^\top 1 = 0 \). Let \( v_2, \ldots, v_n \) be an orthonormal collection of eigenvectors of \( L \) corresponding to \( \lambda_2, \lambda_n \), respectively, each of which is orthogonal to 1. Then there are scalars \( c_j, j = 2, \ldots, n \) such that \( x = \sum_{j=2}^n c_j v_j \). Hence

\[
x^\top Lx = \sum_{j=2}^n c_j^2 v_j^\top L v_j = \sum_{j=2}^n c_j^2 \lambda_j v_j^\top v_j = \sum_{j=2}^n \frac{c_j^2}{\lambda_j} \geq \lambda_2 \sum_{j=2}^n \frac{c_j^2}{\lambda_2} = \lambda_2.
\]

We deduce that

\[
\lambda_2 = \min\{x^\top Lx \mid x^\top x = 1, x^\top 1 = 0\}.
\]

As our next result shows, \( \lambda_2 \) is a nondecreasing function of the weight of any edge in the graph.

**Proposition 2.1.** Let \( G \) be a weighted graph and form \( H \) from \( G \) by either adding a weighted edge \( e \) to \( G \), or by increasing the weight of an existing edge. Denote the second smallest eigenvalues of the Laplacian matrices of \( G \) and \( H \) by \( \lambda_2 \) and \( \hat{\lambda}_2 \), respectively. Then \( \hat{\lambda}_2 \geq \lambda_2 \).

**Proof.** Let \( L \) and \( \hat{L} \) denote the Laplacian matrices for \( G \) and \( H \), respectively. We have \( \hat{L} = L + w(e_i - e_j)(e_i - e_j)^\top \) where \( w > 0 \) and \( i \sim j \) is the edge that is either added or whose weight is increased. Let \( y \) be a vector such that
Let $G$ be an unweighted non-complete graph on $n$ vertices with vertex connectivity $p$. Then the algebraic connectivity of $G$ is at most $p$.

Proof. Suppose that by deleting vertices $n - p + 1, \ldots, n$, from $G$, we have a disconnected graph $G_1 \cup G_2$; let $L_1, L_2$ denote the Laplacian matrices for $G_1, G_2$, respectively. Adding edges to $G$ if necessary, we find that the algebraic connectivity of $G$ is bounded above by that of the graph whose Laplacian matrix is

$$
\tilde{L} \equiv \begin{bmatrix}
L_1 + pI & 0 & -J \\
0 & L_2 + pI & -J \\
-J & -J & nI - J
\end{bmatrix}
$$

(here $J$ denotes an all-ones matrix whose order can be determined from the context). Suppose that $m_1, m_2$ are the numbers of vertices in $G_1, G_2$ respectively. Consider the vector

$$
x = \frac{1}{\sqrt{m_1m_2(m_1 + m_2)}} \begin{bmatrix}
m_21 \\
-m_11 \\
0
\end{bmatrix}.
$$

Observe that $x^T x = 1, x^T 1 = 0$, and $x^T \tilde{L} x = p$. From the development above, we see that the algebraic connectivity for $G$ is bounded above by $p$. □

The following result, attributed to Kirchhoff, illustrates how the algebraic properties of the Laplacian matrix can reflect the combinatorial properties of the underlying graph.

**Theorem 2.1.** Suppose that $G$ is an unweighted graph on $n$ vertices with Laplacian matrix $L$. Select a pair of indices $i, j$ between 1 and $n$, and let $\mathcal{L}$ denote the matrix formed from $L$ by deleting the $i$-th row and $j$-th column. Then

$$
\det(\mathcal{L}) = (-1)^{i+j} \times \{\text{the number of spanning trees in } G\}.
$$

Note that in Theorem 2.1, it doesn’t matter which indices $i$ and $j$ we choose! This is the Matrix Tree Theorem, and a proof can be found in [2].
3. The group inverse

Suppose that $M$ is a real square matrix of order $n$. Suppose further that $M$ is singular, with 0 as a semi-simple eigenvalue (i.e., the algebraic and geometric multiplicities of 0 coincide). Of course $M$ is not invertible, but it has a group inverse, which we now define.

The group inverse of $M$ is the unique matrix $X$ satisfying the following three properties: i) $MX = XM$, ii) $XM = M$ and iii) $XMX = X$. We denote this group $X$ by $M^\#$. One way of computing $M^\#$ is to work with a full rank factorisation of $M$: if $M$ has rank $k$, then there is an $n \times k$ matrix $U$ and a $k \times n$ matrix $V$ such that $M = UV$ (see section 0.4 of [5]). In that case, $M^\#$ can be written as $M^\# = U(VU)^{-2}V$.

**Remark 3.1.** Consider the special case that 0 is a simple eigenvalue of $M$, say with $u$ and $v^\top$ as right and left null vectors, normalised so that $v^\top u = 1$. In this case, $X$ is the group inverse iff $MX = XM = I - uv^\top$, $Xu = 0$ and $v^\top X = 0$.

**Example 3.1.** Consider the $n \times n$ matrix $M = \begin{bmatrix} I_{n-1} & -1_{n-1} \\ -1_{n-1} & n-1 \end{bmatrix}$. (Evidently $M$ is the Laplacian matrix of the star on $n$ vertices.) Then

$$M^\# = \frac{1}{n^2} \begin{bmatrix} n^2 I_{n-1} - (n + 1)J & -1_{n-1} \\ -1_{n-1} & n-1 \end{bmatrix}.$$ 

(Just check that the expression for $M^\#$ satisfies i)–iii) above.)

Next we give some expressions for the group inverse of the Laplacian matrix of a graph.

**Theorem 3.1.** Let $L$ be the Laplacian matrix of a connected weighted graph $G$ on $n$ vertices. Denote the eigenvalues of $L$ by $0 = \lambda_1 < \lambda_2 \leq \cdots \leq \lambda_n$, and let $Q$ be an orthogonal matrix (of eigenvectors) such that $L = Q \text{diag}(\begin{bmatrix} 0 & \lambda_2 & \cdots & \lambda_n \end{bmatrix}) Q^\top$. Then $L^\# = Q \text{diag}(\begin{bmatrix} 0 & \frac{1}{\lambda_2} & \cdots & \frac{1}{\lambda_n} \end{bmatrix}) Q^\top$.

**Corollary 3.1.1.** Suppose that $L$ is as in Theorem 3.1 and that $t \neq 0$ is given. Then $L^\# = (L + \frac{t}{n}J)^{-1} - \frac{1}{tn}J$.

**Proof.** Observe that $\frac{t}{n}J = Q \text{diag}(\begin{bmatrix} t & 0 & \cdots & 0 \end{bmatrix}) Q^\top$, so that $(L + \frac{t}{n}J)^{-1} - \frac{1}{tn}J = Q \left( \text{diag}(\begin{bmatrix} t & \lambda_2 & \cdots & \lambda_n \end{bmatrix}) \right)^{-1} Q^\top - Q \text{diag}(\begin{bmatrix} \frac{1}{t} & 0 & \cdots & 0 \end{bmatrix}) Q^\top$. The conclusion now follows readily. \( \square \)

Evidently $L$, and hence $L^\#$, carries information about the associated weighted graph $G$. Our goals in this series of lectures are to an a) determine how the combinatorial structure of $G$ is reflected in $L^\#$, and b) use $L^\#$ to get information about $G$. 
4. ANOTHER EXPRESSION FOR $L^#$

**Theorem 4.1.** Suppose that $G$ is a connected weighted graph on $n$ vertices with Laplacian matrix $L$. Denote the leading principal submatrix of $L$ of order $n - 1$ by $L_{(n)}$, and let $B = L_{(n)}^{-1}$. Then

$$L^# = \frac{1}{n^2}B1\top J + \begin{bmatrix} B - \frac{1}{n}BJ - \frac{1}{n}JB \top & -\frac{1}{n}B1 \top \\ -\frac{1}{n}1\top B & 0 \end{bmatrix}. $$

**Proof.** Note that $L$ can be written as

$$L = \begin{bmatrix} L_{(n)} & -L_{(n)}1 \top \\ -1\top L_{(n)} & 1\top L_{(n)}1 \top \end{bmatrix}.$$ 

This yields the full rank factorisation $L = UV$, where

$$U = \begin{bmatrix} L_{(n)} \\ -1\top L_{(n)} \end{bmatrix}, V = \begin{bmatrix} I & -1 \end{bmatrix}.$$ 

Note that $VU = (I + J)L_{(n)}$, so that $(VU)^{-1} = L_{(n)}^{-1}(I + J)^{-1} = B(I - \frac{1}{n}J)$. The expression for $L^#$ now follows from the fact that $L^# = U(VU)^{-2}V$.  

**Example 4.1.** Consider the unweighted graph in Figure 1, whose Laplacian matrix is given by

$$L = \begin{bmatrix} 2 & -1 & 0 & 0 & -1 \\ -1 & 2 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & 1 & -1 \\ -1 & -1 & -1 & -1 & 4 \end{bmatrix}.$$ 

In the notation of Theorem 4.1, we have

$$B = \begin{bmatrix} \frac{2}{3} & \frac{1}{3} & 0 & 0 \\ \frac{1}{3} & \frac{2}{3} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix},$$

and it now follows that

$$L^# = \begin{bmatrix} \frac{32}{75} & \frac{7}{75} & -\frac{6}{25} & -\frac{6}{25} & -\frac{1}{25} \\ \frac{7}{75} & \frac{32}{75} & -\frac{6}{25} & -\frac{6}{25} & -\frac{1}{25} \\ -\frac{6}{25} & -\frac{6}{25} & \frac{19}{25} & -\frac{6}{25} & -\frac{1}{25} \\ -\frac{6}{25} & -\frac{6}{25} & -\frac{6}{25} & \frac{19}{25} & -\frac{1}{25} \\ -\frac{1}{25} & -\frac{1}{25} & -\frac{1}{25} & -\frac{1}{25} & \frac{4}{25} \end{bmatrix}.$$
The matrix $B$ in Theorem 4.1 is known as the \textit{bottleneck matrix based at vertex} $n$ for the weighted graph. Using the adjugate formula for the inverse (see section 0.8 of [5]), we see that for each $i, j = 1, \ldots, n - 1$, 

\begin{equation}
\begin{align*}
    b_{i,j} &= (-1)^{i+j} \frac{\det(L_{(j,n),\{i,n\})}}{\det(L_{\{n\})}},
\end{align*}
\end{equation}

where $L_{(j,n),\{i,n\}}$ is the $(n-2) \times (n-2)$ matrix formed from $L$ by deleting rows $j,n$ and columns $i,n$. Earlier, we saw in Theorem 2.1 that for an unweighted graph, $\det(L_{\{n\}})$ counts the number of spanning trees in the graph – in fact a more general result, the \textit{all minors matrix tree theorem} [3], will assist us. First, we need a little notation. Let $G$ be a weighted graph, and let $H$ be a subgraph of $G$. Let $w(H)$ denote the product of the weights of the edges in $H$. The set of spanning trees of $G$ is denoted by $S$, and for each $i,j,k = 1, \ldots, n$, we let $S^{(i,j)}_{k,i,j}$ denote the set of spanning forests of $G$ consisting of just two trees, one of which contains vertex $k$ and the other of which contains vertices $i$ and $j$. With this in hand, we have the following facts, both of which are consequences of the all minors matrix tree theorem.

\textbf{Fact 1}: $\det(L_{\{n\}}) = \sum_{T \in S} w(T)$. 

\textbf{Fact 2}: $\det(L_{(j,n),\{i,n\}}) = (-1)^{i+j} \sum_{F \in S^{(i,j)}_{k}} w(F)$. 

As usual we interpret an empty sum as 0 in Facts 1 and 2.

We remark that for each $k = 1, \ldots, n$, we can analogously define the bottleneck matrix based at vertex $k$ as the inverse of $L_{\{k\}}$, the principal submatrix of the Laplacian formed by deleting its $k$–th row and column. Thus an analogue of Theorem 4.1 using the bottleneck matrix based at any vertex $k$ also holds.

\textbf{Example 4.2}. We revisit Example 4.1. Since the graph in question is unweighted, every edge weight is equal to 1. Our graph has three spanning trees (each formed by deleting one edge of the three–cycle through vertices 1, 3 and 5), so $\det(L_{\{5\}}) = 3$. Observe that $S^{(1,1)}_{5}$ consists of two forests: the one formed by deleting the edges $1 \sim 5$ and $1 \sim 2$, and the one formed by deleting the edges $1 \sim 5$ and $2 \sim 5$. Hence $\det(L_{\{1,5\},\{1,5\}}) = 2$. Similarly, $S^{(1,2)}_{5}$ contains a single forest, formed by deleting the edges $1 \sim 5$ and $2 \sim 5$, so that $\det(L_{\{1,5\},\{2,5\}}) = -1$. Noting that for $j = 3,4, S^{(1,1)}_{5} = \emptyset$, it now follows that the first row of the bottleneck matrix based at vertex $n$ is given by

\begin{figure}[h]
\centering
\includegraphics[width=0.25\textwidth]{example41.png}
\caption{Graph for Example 4.1}
\end{figure}
\[
\begin{bmatrix}
\frac{2}{3} & \frac{1}{3} & 0 & 0 \\
\frac{1}{3} & \frac{1}{3} & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0
\end{bmatrix}
\]. Analogous arguments can be used to determine the rest of the entries in that bottleneck matrix.

5. \( L^\# \) FOR WEIGHTED TREES

If our graph is a weighted tree, we have the following especially simple expression for the entries in the bottleneck matrix.

**Theorem 5.1.** Let \( T \) be a weighted tree on \( n \) vertices, and let \( B \) denote the corresponding bottleneck matrix based at vertex \( n \). For each index \( k \) between 1 and \( n - 1 \), let \( P_{k,n} \) denote the path from vertex \( k \) to vertex \( n \) in \( T \). Then for each \( i, j = 1, \ldots, n - 1 \),

\[
 b_{i,j} = \sum_{e \in P_{i,n} \cap P_{j,n}} \frac{1}{w(e)}.
\]

**Proof.** Fix indices \( i, j \) between 1 and \( n - 1 \), and note that the spanning forests with exactly two trees are precisely those graphs that arise by deleting a single edge from \( T \). It now follows that a spanning forest \( F \) is in \( \mathcal{S}_n^{(i,j)} \) if and only if it is formed from \( T \) by deleting a single edge, say \( e_F \in P_{i,n} \cap P_{j,n} \) from \( T \). Observing that the weight of such a forest is \( w(F) = \frac{w(T)}{w(e_F)} \), the conclusion now follows from (1) and Facts 1 and 2. \( \square \)

We can represent the bottleneck vertex based at vertex \( n \) for a weighted tree \( T \) in an alternate format, as follows. For each edge \( e \) of \( T \), define the vector \( u(e) \in \mathbb{R}^{n-1} \) via

\[
 u(e)_j = \begin{cases} 
 1, & \text{if } j \text{ is in the component of } T \setminus e \text{ without vertex } n \\
 0, & \text{otherwise.} 
\end{cases}
\]

It then readily follows from Theorem 5.1 that the bottleneck matrix based at vertex \( n \) is given by \( B = \sum_{e \in E} \frac{1}{w(e)} u(e) u(e)\top \).

Next we want to develop expressions for the entries in \( L^\# \) when \( L \) is the Laplacian matrix of a weighted tree on \( n \) vertices. We introduce the following notation: for each edge \( e \) of \( T \) and any vertex \( k = 1, \ldots, n \), let \( \beta_k(e) \) denote the set of vertices in the connected component of \( T \setminus e \) not containing vertex \( k \). Observe that with this notation and any edge \( e \), \( 1\top u(e) = |\beta_n(e)| \). From Theorem 4.1, we find that \( l_{i,n}^\# = \frac{1}{n} \frac{1}{w(e)} (1\top u(e))^2 = \frac{1}{n^2} \sum_{e \in E} \frac{|\beta_n(e)|^2}{w(e)} \).

Next we consider off–diagonal entries in \( L^\# \). Fix an index \( i \neq n \), and consider \( l_{i,n}^\# \). From Theorem 4.1, \( l_{i,n}^\# = l_{i,n}^\# - \frac{1}{n} e_i \top B1 \). Note that \( e_i \top B1 = \sum_{e \in E} \frac{1}{w(e)} u(e)_i |\beta_n(e)| \). Observing that \( u(e)_i = 1 \) if and only if \( e \in P_{i,n} \) and is 0 otherwise, we find that \( e_i \top B1 = \sum_{e \in P_{i,n}} \frac{1}{w(e)} |\beta_n(e)| \). Assembling the above, it follows that \( l_{i,n}^\# = \frac{1}{n^2} \sum_{e \in E} \frac{|\beta_n(e)|^2}{w(e)} - \frac{1}{n} \sum_{e \in P_{i,n}} \frac{1}{w(e)} |\beta_n(e)| \). As noted above, we can construct \( L^\# \) using the bottleneck matrix based at any vertex of our graph. Consequently, we have the following. For each \( k = 1, \ldots, n, l_{k,k}^\# = \frac{1}{n^2} \sum_{e \in E} \frac{|\beta_k(e)|^2}{w(e)} \), and for any \( i, j = 1, \ldots, n - 1 \) with \( i \neq j \), \( l_{i,j}^\# = \frac{1}{n^2} \sum_{e \in E} \frac{|\beta_i(e)|^2}{w(e)} - \frac{1}{n} \sum_{e \in P_{i,j}} \frac{1}{w(e)} |\beta_n(e)| \).
We have one more alternate expression for $L#$ for a weighted tree $T$. For each edge $e$ of $T$, denote the connected components of $T \setminus e$ (the graph formed from $T$ by deleting the edge $e$) by $T_1(e)$ and $T_2(e)$. Let $v(e)$ be the vector in $\mathbb{R}^n$ given by

$$v(e)_j = \begin{cases} \frac{|\beta_j(e)|}{n}, & \text{if } j \in T_1(e) \\ -\frac{|\beta_j(e)|}{n}, & \text{if } j \in T_2(e), \end{cases} \quad j = 1, \ldots, n.$$

Theorem 5.2. If $L$ is the Laplacian matrix of a weighted tree, then $L# = \sum_{e \in E} \frac{1}{w(e)} v(e)v(e)^\top$.

Proof. For each $k = 1, \ldots, n$, note that

$$l^#_{k,k} = \frac{1}{n^2} \sum_{e \in E} \frac{|\beta_k(e)|^2}{w(e)} = \sum_{e \in E} \frac{1}{w(e)} (e_k^\top v(e))^2,$$

since $e_k^\top v(e) = \pm \frac{|\beta_k(e)|}{n}$.

Next suppose that we have indices $i,j$ with $i \neq j$. Fix an edge $e$ of $T$, and suppose that $e \notin P_{i,j}$. Then we have $i,j \in T_1(e)$ or $i,j \in T_2(e)$ and in either case, $e_i^\top v(e)v(e)^\top e_j = \frac{|\beta_i(e)||\beta_j(e)|}{n^2} = \frac{|\beta_i(e)|^2}{n^2}$, since $\beta_i(e) = \beta_j(e)$ in this case. Next, we suppose that $e \in P_{i,j}$, so that $i \in T_1(e), j \in T_2(e)$, or vice-versa. In this case we have $e_i^\top v(e)v(e)^\top e_j = -\frac{|\beta_i(e)||\beta_j(e)|}{n^2} = -\frac{(n-|\beta_i(e)||\beta_j(e)|)}{n^2} = \frac{|\beta_i(e)|^2 - |\beta_j(e)|^2}{n^2}$. By summing over the edges in $T$, it now follows that $l^#_{i,j} = \sum_{e \in E} \frac{1}{w(e)} e_i^\top v(e)v(e)^\top e_j$. □

Corollary 5.2.1. Let $T$ be a weighted tree on vertices $1, \ldots, n$.

a) Fix any vertex $k$ between 1 and n. Then

$$\text{trace}(L#) = \frac{1}{n} \sum_{e \in T} \frac{|\beta_k(e)|(n - |\beta_k(e)|)}{w(e)}.$$

b) For any pair of vertices $i,j$, let $\delta(i,j) = \sum_{e \in P_{i,j}} \frac{1}{w(e)}$. Then

$$\text{trace}(L#) = \frac{1}{n} \sum_{1 \leq i < j \leq n} \delta(i,j).$$

Proof. a) Observe that

$$\text{trace}(L#) = \sum_{e \in E} \frac{1}{w(e)} \text{trace}(v(e)v(e)^\top) = \sum_{e \in E} \frac{1}{w(e)} v(e)^\top v(e).$$

Noting that for any vertex $k$ of $T$, $v(e)^\top v(e) = \frac{1}{n} |\beta_k(e)|(n - |\beta_k(e)|)$, the conclusion follows.

b) Observe that $\sum_{1 \leq i < j \leq n} \delta(i,j) = \sum_{1 \leq i < j \leq n} \sum_{e \in P_{i,j}} \frac{1}{w(e)}$. Since $e \in P_{i,j}$ precisely when $j \in \beta_i(e)$, we find, exchanging the order of summation, that $\sum_{1 \leq i < j \leq n} \delta(i,j) = \sum_{e \in T} \sum_{1 \leq i < j \leq n} \sum_{e \in P_{i,j}} \frac{1}{w(e)} = \sum_{e \in T} \frac{1}{w(e)} |\beta_i(e)|(n - |\beta_i(e)|)$ for some (indeed, any) index $k$ between 1 and $n$. The conclusion now follows from a). □
Example 5.1. Consider the unweighted path $P_n$ on $n$ vertices, with vertex 1 adjacent to vertex 2, vertex $j$ adjacent to vertices $j - 1, j + 1, j = 2, \ldots, n - 1$, and vertex $n$ adjacent to vertex $n - 1$. For each $k = 1, \ldots, n - 1$, let $e(k)$ denote the edge between vertices $k$ and $k + 1$. Then

$$v(e(k))v(e(k))^\top = \begin{bmatrix} \frac{(n-k)^2}{n^2} J_k & -\frac{k(n-k)}{n^2} J_{k,n-k} \\ -\frac{k(n-k)}{n^2} J_{n-k,k} & \frac{k^2}{n^2} J_{n-k} \end{bmatrix}.$$ 

It now follows that for each $j = 1, \ldots, n - 1, e_j^\top v(e(k))v(e(k))^\top e_j = \frac{(n-k)^2}{n^2}$ if $j \leq k$ while $e_j^\top v(e(k))v(e(k))^\top e_j = \frac{k^2}{n^2}$ if $j \geq k + 1$. Next suppose that $i < j$. Then

$$e_i^\top v(e(k))v(e(k))^\top e_j = \begin{cases} \frac{(n-k)^2}{n^2} & \text{if } i < j \leq k \\ -\frac{k(n-k)}{n^2} & \text{if } i \leq k < j \\ \frac{k^2}{n^2} & \text{if } k + 1 \leq i < j. \end{cases}$$

Evidently analogous relations hold for the case that $i > j$. A couple of computations now show that if $L$ is the Laplacian matrix for $P_n$, then

$$t^\#_{i,j} = \begin{cases} \frac{j(j-1)(2j-1) + (n-j)(n-j+1)(2n-2j+1)}{6n^2} - \frac{|j-i|(|j-i-1|}{2n} & \text{if } i \leq j \\ \frac{i(i-1)(2i-1) + (n-i)(n-i+1)(2n-2i+1)}{6n^2} - \frac{|j-i|(|j-i-1|}{2n} & \text{if } i \geq j + 1. \end{cases}$$

6. Algebraic connectivity

Throughout this section, we continue to denote the algebraic connectivity of a weighted graph $G$ by $\alpha(G)$. Our goal is to provide bounds on $\alpha(G)$ in terms of the group inverse of the corresponding Laplacian matrix. For any $n \times n$ real matrix $M$ whose row sums are constant, we define the function $\tau(M)$ by

$$\tau(M) = \frac{1}{2} \max_{i,j = 1, \ldots, n} ||(e_i - e_j)^\top M||_1.$$ 

The following result shows how we can use $\tau$ to bound Laplacian eigenvalues.

Lemma 6.1. Let $G$ be a connected weighted graph on $n$ vertices with Laplacian matrix $L$. Then

a) $\alpha(G) \geq \frac{1}{\tau(L^\#)}$ and

b) $\alpha(G) \leq \frac{n^{-1}}{\max_{j = 1, \ldots, n} t^\#_{i,j}}.$

Proof. a) Suppose that $M$ is a symmetric matrix of order $n$ with constant row sums, say with $M\mathbf{1} = \tau\mathbf{1}$. Let $\lambda \neq r$ be an eigenvalue of $M$; we claim that $\lambda \leq \tau(M)$. To see the claim, let $z$ be a real eigenvector of $M$ such that $||z||_1 = 1$. Observe that $z^\top \mathbf{1} = 0$. It follows (by induction on $n$ – see section 2.5 of [9]) that there are scalars $a(i, j), 1 \leq i < j \leq n$ such that $\sum_{1 \leq i < j \leq n} |a(i, j)| = ||z||_1$
and \( z = \sum_{1 \leq i < j \leq n} a(i, j) \left( \frac{e_i - e_j}{2} \right) \). Hence we have

\[
|\lambda| = |\lambda||z||_1 = ||z^TM||_1 = \left\| \sum_{1 \leq i < j \leq n} a(i, j) \left( \frac{e_i - e_j}{2} \right)^\top M \right\|_1 \\
\leq \sum_{1 \leq i < j \leq n} |a(i, j)||\left( \frac{e_i - e_j}{2} \right)^\top M|_1 \\
\leq \sum_{1 \leq i < j \leq n} |a(i, j)|\tau(M) = ||z||_1 \tau(M),
\]

as claimed.

Next, we consider \( L^\# \), which has constant row sums (equal to 0) and \( \frac{1}{\alpha(G)} \) as a nonzero eigenvalue. From the claim, \( \frac{1}{\alpha(G)} \leq \tau(L^\#) \), and the desired inequality follows.

b) Denote the nonzero eigenvalues of \( L \) by \( \alpha(G) \equiv \lambda_2 \leq \lambda_3 \leq \cdots \leq \lambda_n \), and let \( v_2, \ldots, v_n \) denote an orthonormal collection of corresponding eigenvectors. Then by Theorem 3.1, \( L^\# = \sum_{k=2}^n \frac{1}{\lambda_k} v_k v_k^\top \). Note that \( \sum_{k=2}^n v_k v_k^\top = I - \frac{1}{n} J \). Fix an index \( j \) between 1 and \( n \). Then

\[
b_{jj}^\# = \sum_{k=2}^n \frac{1}{\lambda_k} e_j^\top v_k v_k^\top e_j \leq \frac{1}{\alpha(G)} \sum_{k=2}^n (e_j^\top v_k)^2 = \frac{n-1}{n\alpha(G)}.\]

The conclusion now follows. \( \square \)

Next we apply Lemma 6.1 to weighted trees. For any weighted tree, we let \( \mathcal{P}(T) \) denote the set of pendent vertices of \( T \) – i.e., the set of vertices of degree 1.

**Theorem 6.1.** Let \( T \) be a weighted tree on \( n \) vertices. Then

\[
\max \left\{ \frac{1}{\sum_{e \in \mathcal{P}(T)}} |\beta_i(e)(n-|\beta_i(e)|)| \left| e \in \mathcal{P}(T) \right| \right\} \leq \alpha(T) \]

\[
\leq \min \left\{ \frac{n(n-1)}{\sum_{e \in T} \frac{|\beta_i(e)|^2}{w(e)}}, \left| e \in \mathcal{P}(T) \right| \right\}.
\]

**Proof.** First we consider the lower bound on \( \alpha(T) \) in (3). In view of Lemma 6.1 a), it suffices to show that \( \tau(L^\#) \leq \frac{1}{n} \max \left\{ \sum_{e \in \mathcal{P}(T)} \frac{|\beta_i(e)(n-|\beta_i(e)|)|}{w(e)} \left| e \in \mathcal{P}(T) \right| \}. \)

Applying Theorem 5.2, we have \( L^\# = \sum_{e \in T} \frac{1}{w(e)} v(e)v(e)^\top \), where \( v(e) \) is as defined in (7.1). Observing that for any edge \( e \) and indices \( i, j \),

\[
(e_i - e_j)^\top v(e) = \begin{cases} 
1 & \text{if } e \in P_{i,j} \\
0 & \text{if } e \notin P_{i,j}
\end{cases},
\]

we conclude that \( \alpha(T) \) is determined by the \( n \)-

\[
\frac{1}{n} \max \left\{ \sum_{e \in \mathcal{P}(T)} \frac{|\beta_i(e)(n-|\beta_i(e)|)|}{w(e)} \left| e \in \mathcal{P}(T) \right| \}.
\]

\( \square \)
Since \( \|v(e)\|_1 = \frac{2}{n} |\beta_i(e)| (n - |\beta_i(e)|) \) whenever \( e \in P_{i,j} \), we find that
\[
\| (e_i - e_j)^T L^\# \|_1 = \left\| \sum_{e \in P_{i,j}} \frac{v(e)}{w(e)} \right\|_1 \leq \sum_{e \in P_{i,j}} \frac{\|v(e)\|_1}{w(e)} = \sum_{e \in P_{i,j}} \frac{2}{nw(e)} |\beta_i(e)| (n - |\beta_i(e)|).
\]

It is straightforward to determine that the rightmost expression above is maximized for some pair of indices \( i, j \in \mathcal{P}(T) \). The lower bound on \( \alpha(T) \) now follows.

Next we consider the upper bound on \( \alpha(T) \) in (3). From Lemma 6.1 b) we have \( \alpha(G) \leq \frac{n-1}{n \max_{j=1,\ldots,n} t_{j,j}^\#} \), and note that for any index \( j \),
\[
t_{j,j}^\# = \frac{(e_j^Tv(e))^2}{w(e)} = \sum_{e \in T} \frac{|\beta_i(e)|^2}{nw(e)}.
\]
Consequently, for any \( j \) we have
\[
\alpha(T) \leq \frac{n(n-1)}{\sum_{e \in T} \frac{|\beta_i(e)|^2}{w(e)}}.
\]

Next, we claim that \( t_{j,j}^\# \) is maximised at some pendent vertex \( j \). (Once the claim is established, the upper bound in (3) follows readily.) To see the claim, we suppose that vertex \( k \) is not pendent, say with \( k \) adjacent to vertices \( m_1 \) and \( m_2 \). Let \( e, \hat{e} \) denote the edges between vertex \( k \) and vertices \( m_1, m_2 \), respectively. Observe that \( t_{j,k}^\# \geq t_{m_1,k}^\# \) if and only if \( |\beta_k(e)| \geq |\beta_{m_1}(e)| = n - |\beta_k(e)| \), i.e., if and only if \( |\beta_k(e)| \geq \frac{n}{2} \). Similarly \( t_{j,k}^\# \geq t_{m_2,k}^\# \) if and only if \( |\beta_k(e)| \geq \frac{n}{2} \). Since \( \beta_k(e) \cap \beta_k(\hat{e}) = \emptyset \) and neither set contains vertex \( k \), it must be the case that \( |\beta_k(e)| + |\beta_k(\hat{e})| \leq n - 1 \). We conclude then that \( t_{j,k}^\# \) must be strictly less than one of \( t_{j,m_1}^\# \) and \( t_{j,m_2}^\# \). It now follows that \( t_{j,j}^\# \) is maximised by some pendent vertex \( j \), as claimed.

**Example 6.1.** Consider the (unweighted) star on \( n \) vertices, \( S \). Fix a pendent vertex \( i \) of \( S \), and note that
\[
|\beta_i(e)| = \begin{cases} n-1 & \text{if } e \text{ is incident with } i \\ 1 & \text{if } e \text{ is not incident with } i \end{cases}
\]
We deduce that \( \sum_{e \in S} |\beta_i(e)|^2 = (n-1)^2 + n - 2 = n^2 - n - 1 \). Thus the upper bound in Theorem 6.1 is \( \alpha(S) \leq \frac{n^2-n-1}{n^2-n-1} \). For the star it is known that \( \alpha(S) = 1 \) when \( n \geq 3 \), so we see that in this case the upper bound in (3) is reasonably accurate for large values of \( n \).

**Example 6.2.** Take \( T \) to be the unweighted path on \( n \) vertices, say with \( 1 \) and \( n \) as the pendent vertices. We have \( \sum_{e \in P_{1,n}} |\beta_1(e)|(n-|\beta_1(e)|) = \sum_{k=1}^{n-1} k(n-k) = \frac{n(n^2-1)}{6} \). Hence the lower bound on \( \alpha(T) \) in (3) is \( \frac{6}{n^2-1} \leq \alpha(T) \). It’s known that the true value of \( \alpha(T) \) is \( 2(1 - \cos(\frac{\pi}{n})) \), which is asymptotic to \( \frac{\pi^2}{6n} \) as \( n \to \infty \). So, for this example we see that for large \( n \), the lower bound of (3) is of the correct order of magnitude as the true value, but is about \( 0.6 \alpha(T) \).
7. Joins

Suppose that we have two unweighted graphs $G_1, G_2$ on $k$ and $l$ vertices, respectively. The join of $G_1$ and $G_2$, denoted $G_1 \vee G_2$, is the graph on $k + l$ vertices formed from $G_1 \cup G_2$ by adding in all possible edges between vertices of $G_1$ and vertices of $G_2$. Figure 2 depicts the join of $K_2 \cup K_1$ and $K_2$.

![Figure 2. (K_2 \cup K_1) \vee K_2](image)

Observe that if the Laplacian matrices for $G_1$ and $G_2$ are $L_1$ and $L_2$ respectively, then the Laplacian matrix of $G_1 \vee G_2$ can be written as

$$L = \begin{bmatrix} L_1 + tlI & -J \\ -J & L_2 + klI \end{bmatrix}.$$

In this setting, we can find $L^\#$ from Corollary 3.1.1 (with $t$ chosen as $k + l$) as follows:

$$L^\# = (L + J)^{-1} - \frac{1}{(k + l)^2}J =
\begin{bmatrix}
L_1 + tlI + J & 0 \\
0 & L_2 + klI + J
\end{bmatrix}^{-1} - \frac{1}{(k + l)^2}J =
\begin{bmatrix}
(L_1 + tlI)^{-1} - \frac{1}{(k + l)^2}J & 0 \\
0 & (L_2 + klI)^{-1} - \frac{1}{(k + l)^2}J
\end{bmatrix}^{-1} - \frac{1}{(k + l)^2}J.$$

It turns out that a characterisation of the equality case in Lemma 6.1 a) is not known. The next result supplies a family of examples for which equality holds in that bound.

**Theorem 7.1.** Suppose that $G$ is an unweighted graph of the form $H \cup K_p$, where $H$ is not connected. Denoting the Laplacian matrix for $G$ by $L$, we have $\alpha(G) = \frac{1}{\tau(L^\#)} = p$.

**Proof.** For concreteness, suppose that $H$ has $q$ vertices. Let $L_1$ denote the Laplacian matrix for $H$, and note that $L$ can be written as

$$L = \begin{bmatrix} L_1 + pI & -J \\ -J & (p + q)I - J \end{bmatrix}.$$

Then

$$L + J = \begin{bmatrix} L_1 + pI + J & 0 \\
0 & (p + q)I \end{bmatrix},$$

$$L^\# = \begin{bmatrix} (L_1 + pI)^{-1} - \frac{1}{(p + q)^2}J & 0 \\
0 & (L_2 + qI)^{-1} - \frac{1}{(p + q)^2}J
\end{bmatrix}^{-1} - \frac{1}{(p + q)^2}J.$$
and it follows that
\[
L^\# = \begin{bmatrix} (L_1 + pI)^{-1} - \frac{1}{p(p+q)} J & 0 \\ 0 & \frac{1}{p+q} I \end{bmatrix} - \frac{1}{(p+q)^2} J.
\]

In particular, observe that \( \tau(L^\#) = \tau(L + J)^{-1} \).

Next we claim that \( \tau(L + J)^{-1} = \frac{1}{p} \). It turns out that \( (L_1 + pI)^{-1} \) is entrywise nonnegative, that its row sums are all equal to \( \frac{1}{p} \), and further that since \( H \) is not connected, in fact \( (L_1 + pI)^{-1} \) is a block diagonal matrix. It now follows that for \( 1 \leq i, j \leq q \), \(||(e_i - e_j)^\top (L + J)^{-1}||_1 \leq \frac{1}{p} + \frac{1}{p+q} < \frac{2}{p} \). Finally if \( q + 1 \leq i, j \leq p + q \), \(||(e_i - e_j)^\top (L + J)^{-1}||_1 = \frac{2}{p+q} \) \( < \frac{2}{p} \).

It now follows that \( \tau(L + J)^{-1} = \frac{1}{p} \), as claimed.

Applying Lemma 6.1 a), we thus find that \( \alpha(G) \geq \frac{1}{\tau(L^\#)} = p \). Next, noting that the vertex connectivity of \( G \) is at most \( p \) and applying Proposition 2.2, we find that \( \alpha(G) \leq p \). The conclusion now follows.

Example 7.1. Set \( S_1 = \{ K_p | p \in \mathbb{N} \} \), and for each \( m \in \mathbb{N} \), define \( S_{m+1} = \{ G^c \lor K_{p} | G \in S_{m}, p \in \mathbb{N} \} \). The collection \( S = \bigcup_{m \in \mathbb{N}} S_{m} \) is the family of connected threshold graphs, about which much is known (see [8]). A straightforward application of Theorem 7.1 shows that for any connected threshold graph, equality holds in the inequality of Lemma 6.1 a).

8. Resistance distance

Let \( G \) be a connected weighted graph on \( n \) vertices with Laplacian matrix \( L \). Fix indices \( i, j \), and define the resistance distance from \( i \) to \( j \), \( r(i, j) \) via
\[
r(i, j) = t^\#_{i,i} + t^\#_{j,j} - 2t^\#_{i,j}.
\]

The first result of this section establishes that \( r(i, j) \) can be interpreted as a distance function.

Theorem 8.1. \quad \( r(i, j) \geq 0 \), with equality if and only if \( i = j \).
b) \( r(i, j) = r(j, i) \) for all \( i, j \).
c) for any \( i, j, k \), \( r(i, j) \leq r(i, k) + r(k, j) \), with equality holding if and only if either \( k \) coincides with one of \( i \) and \( j \), or every path from \( i \) to \( j \) passes through vertex \( k \).

Proof. a) Consider the case that \( i \neq j \), and without loss of generality, suppose that \( j = n \). Observe that \( r(i, n) = (e_i - e_n)^\top L^\# (e_i - e_n) \). From Theorem 4.1, we find that
\[
r(i, n) = (e_i - e_n)^\top \begin{bmatrix} B - \frac{1}{n} BJ - \frac{1}{n} JB & -\frac{1}{n} B1 \\ -\frac{1}{n} 1\top B & 0 \end{bmatrix} (e_i - e_n),
\]

where \( B \) is the bottleneck matrix for \( G \) based at vertex \( n \). We thus deduce that \( r(i, j) = b_{i,i} > 0 \).
b) Obvious from the definition.
c) The desired inequality is equivalent to
\[
0 \leq l^\#_{k,k} + l^\#_{i,j} - l^\#_{i,k} - l^\#_{k,j}.
\]
Evidently both sides of (4) are zero if \( k \) is either \( i \) or \( j \), so henceforth we assume that \( k \neq i, j \). Taking \( k = n \) without loss of generality, and letting \( B \) denote the bottleneck matrix for \( G \) based at vertex \( n \), we find from Theorem 4.1 that (4) holds if and only if
\[
0 \leq b_{i,j} - 1 + \frac{1}{n} e_i^\top B 1 + \frac{1}{n} e_j^\top B 1 + \frac{1}{n} e_i^\top B e_j + \frac{1}{n} e_j^\top B e_i.
\]
Thus (4) is equivalent to the inequality
\[
b_{i,j} \geq 0,
\]
and it now follows that \( r(i,j) \leq r(i,n) + r(n,j) \). Inspecting the argument above, we see that \( r(i,j) = r(i,n) + r(n,j) \) if and only if \( b_{i,j} = 0 \). From Fact 2, the latter holds if and only if \( S^{\{i,j\}}_n = \emptyset \), i.e., if and only if every path from \( i \) to \( j \) goes through vertex \( n \). \( \square \)

In intuitive terms, we can think of low resistance distance between two vertices as indicating that they are ‘close’ in some sense. Note that the resistance distance \( r(i,j) \) is affected not just by the ordinary graph theoretic distance between vertices \( i \) and \( j \), but also by the number of paths between \( i \) and \( j \), as illustrated by Figure 3.

![Figure 3. Resistance distance for two related graphs](image)

Consider a weighted graph, which we associated with a network of electrical resistors; each edge \( e \) has an associated resistance \( \rho(e) \equiv \frac{1}{w(e)} \). Fix a pair of indices \( i, j \) and suppose that we allow current to enter at vertex \( i \) and exit at vertex \( j \). Set the voltage at \( i \) to be 1 and the voltage at \( j \) to be 0. The effective resistance between \( i \) and \( j \) is defined as the reciprocal of the current flowing in at vertex \( i \). Using Kirchhoff’s laws and Ohm’s law, it turns out that this effective resistance is given by the diagonal entry corresponding to vertex \( i \) of the bottleneck matrix based at vertex \( j \) – i.e., it is equal to our resistance distance \( r(i,j) \). Thus, the use of the word ‘resistance’ in describing \( r(i,j) \) is appropriate.

**Lemma 8.1.** Let \( G \) be a weighted graph on \( n \) vertices with Laplacian matrix \( L \), and fix indices \( i, j \), and let \( \theta > 0 \) be given. Form \( \tilde{G} \) from \( G \) by adding \( \theta \) to the weight of the edge between vertices \( i \) and \( j \), so that the Laplacian matrix for \( \tilde{G} \) is \( \tilde{L} = L + \theta(e_i - e_j)(e_i - e_j)^\top \). Then
\[
\tilde{L}^\# = L^\# - \frac{\theta}{L^\# - \theta(e_i - e_j)(e_i - e_j)^\top} L^\# L^\# (e_i - e_j)(e_i - e_j)^\top L^\#.
\]

**Proof.** Use Corollary 3.1.1 and the Sherman–Morrison formula (see section 0.7.4 of [5]). \( \square \)
Let $G$ be a weighted connected graph on $n$ vertices. For any pair of vertices $i, j$, let $P(i, j)$ denote the set of all paths from $i$ to $j$ in $G$, and let $\delta(i, j) = \min \{ \sum_{e \in P} \frac{1}{w(e)} \}$. Note that this definition of $\delta(i, j)$ generalises the earlier definition given in Corollary 5.2.1 b), which only applied to weighted trees.

**Corollary 8.1.1.** Let $G$ be a weighted graph on $n$ vertices. For each $i, j = 1, \ldots, n$, $r(i, j) \leq \delta(i, j)$.

**Proof.** It follows from Lemma 8.1 that if we delete any edge of $G$ (while retaining the connectivity of the resulting graph), then we can only increase the resistance distance between any two vertices. Fix vertices $i$ and $j$, and consider a path $\hat{P}$ that yields the minimum value of $\delta(i, j)$, and let $T$ be a spanning (weighted) tree of $G$ for which the unique path from $i$ to $j$ is $\hat{P}$, and let $\hat{r}(i, j)$ be the resistance distance from $i$ to $j$ in $T$. Evidently $r(i, j) \leq \hat{r}(i, j)$. Recalling that $\hat{r}(i, j)$ is the diagonal entry corresponding to vertex $i$ in the bottleneck matrix for $T$ based at vertex $j$. Referring to Theorem 5.1, we see that $\hat{r}(i, j) = \sum_{e \in P} \frac{1}{w(e)} = \delta(i, j)$.

**Theorem 8.2.** Let $G$ be a weighted graph with Laplacian matrix $L$. Then $\sum_{1 \leq i < j \leq n} r(i, j) = n \text{trace}(L^\#)$.

**Proof.** We have $\sum_{1 \leq i < j \leq n} r(i, j) = \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} r(i, j) = \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} (I_{i,j}^\# + I_{j,i}^\# - 2I_{i,j}^\#)$. Since the row sums of $L^\#$ are all zero, it follows that $\frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} (l_{i,j} + l_{j,i} + l_{j,i} - 2l_{i,j}) = \sum_{i=1}^{n} (nl_{i,i} + \text{trace}(L^\#)) = 2n \text{trace}(L^\#)$. The conclusion follows.

The quantity $\sum_{1 \leq i < j \leq n} r(i, j)$ is known as the Kirchhoff index for the weighted graph $G$, and is denoted $K(G)$. The Kirchhoff index is a global parameter of the weighted graph that can be thought of as a measure of the overall resistance in the network.

**Theorem 8.3.** Let $G$ be a connected weighted graph on vertices $1, \ldots, n$, and for each $j = 1, \ldots, n$, let $d_j$ be the sum of the weights of the edges that are incident with vertex $j$. For any $t > 0$, we have $K(G) \geq n \sum_{j=1}^{n} \frac{1}{d_j + t} - \frac{1}{t}$.

**Proof.** Let $L$ be the Laplacian matrix for $G$, and label its eigenvalues as $0 = \lambda_1 < \lambda_2 \leq \cdots \leq \lambda_n$. Consider the matrix $L + tJ$, which has eigenvalues $nt, \lambda_2, \ldots, \lambda_n$ and diagonal entries $d_j + 1, j = 1, \ldots, n$. From Schur’s theorem, the vectors of eigenvalues of $L + tJ$ majorises the vector of diagonal entries (see section 4.3 of [5]). Using the fact that the function $x \mapsto \frac{1}{x}$ is convex on $\mathbb{R}^+$, it now follows that $\sum_{j=2}^{n} \frac{1}{\lambda_j} + \frac{1}{nt} \geq \sum_{j=1}^{n} \frac{1}{d_j + t}$. The conclusion now follows.

**Corollary 8.3.1.** Let $G$ be a connected weighted graph on $n$ vertices, and suppose that the sum of all edge weights is $m$. Then $K(G) \geq \frac{n(n-1)^2}{2m^2}$.

**Proof.** We adopt the notation of Theorem 8.3. Fix a $t > 0$. It is straightforward to show that $\sum_{j=1}^{n} \frac{1}{d_j + t} \geq \frac{n^2}{\sum_{j=1}^{n} (d_j + t)} = \frac{n^2}{2m + nt}$. Applying Theorem 8.3 and substituting in $t = \frac{2m}{n(n-1)}$ yields the desired inequality.
Suppose that $G$ is a connected unweighted graph on $n$ vertices with $m$ edges. As a variant of the Kirchhoff index for $G$, we next consider the minimum Kirchhoff index for $G$, defined as

$$K(G) = \inf\{K(G)\},$$

where the infimum is taken over all nonnegative weightings of $G$ such that the sum of the edge weights is $m$. In fact it turns out that the infimum is always attained as a minimum, since the eigenvalues of the Laplacian matrix of any connected weighted graph are continuous functions of the edge weights.

**Theorem 8.4.** Suppose that $G$ is a connected graph on $n$ vertices. Then $K(G) \geq n - 1$, with equality holding if and only if $G = K_n$.

**Proof.** Denote the number of edges by $m$. From Corollary 8.3.1 it follows that $K(G) \geq \frac{n(n-1)²}{2m}$, and since $2m \leq n(n-1)$, we find easily that $K(G) \geq n - 1$. If $K(G) = n - 1$, then necessarily $2m = n(n-1)$, i.e., $G = K_n$. Conversely, if $G = K_n$ we find that $K(G) = n - 1 \geq K(G) \geq n - 1$, so that $K(G) = n - 1$. □

We have the following explicit formula for trees.

**Theorem 8.5.** Let $T$ be a tree on vertices $1, \ldots, n$, and fix a vertex $i$. For each edge $e$ of $T$, let $x(e) = |\beta_i(e)|(n - |\beta_i(e)|)$. Then

$$K(T) = \frac{1}{n-1} \left( \sum_{e \in T} \sqrt{x(e)} \right)^2.$$ 

In particular, $K(T) \geq (n - 1)^2$, with equality if and only if $T$ is a star.

**Proof.** For any weighting $w$ of the tree $T$, from Corollary 5.2.1, we find that the corresponding Kirchhoff index is equal to $\sum_{e \in T} \frac{x(e)}{w(e)}$. Thus in order to find $K(T)$, we need to minimise $\sum_{e \in T} \frac{x(e)}{w(e)}$ subject to the constraint that $\sum_{e \in T} w(e) = n - 1$. Applying Lagrange multipliers, we find that for a minimising weighting $w$ of $T$, it must be the case that $\frac{x(e)}{w(e)}$ takes on a common value for every edge. Invoking the constraint that $\sum_{e \in T} w(e) = n - 1$, it now follows that for each edge $e$,

$$w(e) = \frac{(n - 1)\sqrt{x(e)}}{\sum_{e \in T} \sqrt{x(e)}},$$

which yields (5).

From the fact that $|\beta_i(e)|(n - |\beta_i(e)|) = x(e) \geq n - 1$ for any edge $e$ of $T$, we find that $K(T) \geq (n - 1)^2$. Further, equality holds if and only if $|\beta_i(e)|(n - |\beta_i(e)|) = n - 1$ for every edge $e$; the latter is readily seen to hold if and only if $T$ is a star. □

9. Computational considerations

The results in the preceding sections suggest that the group inverse of the Laplacian matrix for a connected graph carries some interesting information about the graph. The question then arises: how might one compute that group inverse? In this section, we discuss that issue. Note that both Corollary 3.1.1
and Theorem 4.1 give closed form formulas for the group inverse of the Laplacian matrix of a connected graph. Both results involve the computation of a matrix inverse – the former expression uses the inverse of \( L + \frac{1}{n} J \) (for a graph on \( n \) vertices with Laplacian \( L \)) and the latter requires the computation of a bottleneck matrix. In either case, for a graph with \( n \) vertices, these can be computed using the LU decomposition in roughly \( \frac{4}{3} n^3 \) floating point operations (additions or multiplications), or flops.

**Remark 9.1.** Observe that the LU approach above does not take advantage of the fact that the Laplacian matrix of a connected graph is positive semidefinite. The following strategy uses some of the extra structure of the Laplacian matrix. Recall that any symmetric positive semidefinite matrix \( S \) has a Cholesky decomposition. That is, there is a lower triangular matrix \( N \) so that \( S = NN^\top \) (see section 4.2.3 of [4]). Referring to Theorem 4.1, observe that for the Laplacian matrix \( L \) of a connected graph on \( n \) vertices, the principal submatrix \( L\{\cdot\}_{\{\cdot\}} \) formed by deleting the last row and column of \( L \) is a positive definite matrix. Computing a Cholesky decomposition of \( L\{\cdot\}_{\{\cdot\}} \) as \( L\{\cdot\}_{\{\cdot\}} = NN^\top \), we can then find the bottleneck matrix \( B = L^{-1}\{\cdot\}_{\{\cdot\}} \) via \( B = N^{-\top}N^{-1} \), and apply Theorem 4.1 to compute \( L^\# \).

The Cholesky factorisation of an \( n \times n \) symmetric positive definite matrix can be computed in roughly \( \frac{n^3}{3} \) flops, while the inversion of the triangular Cholesky factor \( N \) can be computed in another \( \frac{n^3}{3} \) flops. The product \( N^{-\top}N^{-1} \) can also be computed in about \( \frac{n^3}{3} \) flops, and consequently, this approach allows us to compute \( L^\# \) in about \( n^3 \) flops.

**Remark 9.2.** Suppose that we have a weighted tree on \( n \) vertices. A straightforward proof by induction shows that there is a labelling of the vertices of \( T \) with the numbers \( 1, \ldots, n \) and the edges of \( T \) with the labels \( e(1), \ldots, e(n - 1) \) such that a) for each \( j = 1, \ldots, n - 1 \), vertex \( j \) is incident with edge \( e(j) \), and b) for each \( j = 1, \ldots, n - 1 \), the end point of \( e(j) \) distinct from \( j \), say \( k_j \), is such that \( k_j > j \). With this labelling in place, we can construct a square matrix \( N \) of order \( n - 1 \) as follows:

\[
n_{i,j} = \begin{cases} 
\sqrt{w(e(j))} & \text{if } i = j \\
-\sqrt{w(e(j))} & \text{if } i = k_j, \ i, j = 1, \ldots, n - 1. \\
0 & \text{if } i \neq j, k_j
\end{cases}
\]

It is readily seen that if we set

\[
Q = \begin{bmatrix} N \\ -1^\top N \end{bmatrix},
\]

then \( QQ^\top \) is the Laplacian matrix for \( T \). Further, the special labelling of vertices and edges ensures that \( N \) is lower triangular, so that it is in fact the Cholesky factor referred to in Remark 9.1. Thus for the special case of a tree, the Cholesky factor \( N \) can be constructed from the labelling of the vertices and edges; this strategy then allows for the computation of the group inverse of the corresponding Laplacian matrix in roughly \( \frac{2}{3} n^3 \) flops.
Remark 9.3. Note that for connected graphs with not very many edges, say \( m = n - 1 + \text{constant} \), the following strategy may be effective: a) find a spanning tree (standard algorithms do this in order \( n^2 \) steps); b) compute the group inverse of the corresponding Laplacian matrix via Remark 9.2 (at a cost of \( \frac{2}{3} n^3 \) flops); c) update the Laplacian matrix using Lemma 8.1 by adding in the remaining \( m - n + 1 \) weighted edges, one at a time. Observe that each update step costs roughly \( n^2 \) flops.

One issue of concern in numerical linear algebra is the sensitivity of a computation to small changes in the input parameters. If we have two Laplacian matrices \( L \) and \( \tilde{L} \) that we believe are ‘close’, what guarantees do we have that \( L^\# \) and \( \tilde{L}^\# \) are close? The follow result provides some insight.

Theorem 9.1. Suppose that \( G \) and \( \tilde{G} \) are connected weighted graphs on \( n \) vertices, and denote their corresponding Laplacian matrices by \( L \) and \( \tilde{L} \), respectively. Set \( E = L - \tilde{L} \), and suppose that \( \|E\|_2 < \alpha(G) \).

Then

\[
\|\tilde{L}^\# - L^\#\|_2 \leq \frac{\|E\|_2}{\alpha(G)^2 - \alpha(G)} \|E\|_2.
\]

Proof. First we note that since \( \|E\|_2 < \alpha(G) \), we have \( \|EL^\#\|_2 \leq \|E\|_2 \|L^\#\|_2 = \frac{\|E\|_2}{\alpha(G)} < 1 \). Hence \( I - EL^\# \) is invertible. It is straightforward to determine that \( L^\# = L^\#(I - EL^\#)^{-1} \), and hence we find that \( \tilde{L}^\# - L^\# = L^\#EL^\#(I - EL^\#)^{-1} \). Taking norms now yields \( \|\tilde{L}^\# - L^\#\|_2 \leq \|L^\#EL^\#\|_2 \|(I - EL^\#)^{-1}\|_2 \leq \frac{\|L^\#\|_2 \|E\|_2}{1 - \|L^\#\|_2 \|E\|_2} \). Using the fact that \( \|L^\#\|_2 = \frac{1}{\alpha(G)} \) and simplifying now yields the desired inequality. \( \square \)

References

Notation

1_k – The all ones vector in \( \mathbb{R}^k \); the subscript is suppressed when the order is clear from the context.

\( \alpha(G) \) – Algebraic connectivity of the weighted graph \( G \).

diag(x) – For a vector \( x \in \mathbb{R}^n \), diag\( (x) \) is the \( n \times n \) diagonal matrix whose \( j \)-th diagonal entry is \( x_j \), \( j = 1, \ldots, n \).

e_j – The \( j \)-th standard unit basis vector in \( \mathbb{R}^n \) (where \( n \) is clear from the context).

\( G \setminus e \) – The weighted graph formed from \( G \) by deleting the edge \( e \).

\( G \cup H \) – The union of the vertex-disjoint weighted graphs \( G \) and \( H \).

\( G \vee H \) – The join of the vertex-disjoint unweighted graphs \( G \) and \( H \).

\( i \sim j \) – The edge between vertices \( i \) and \( j \).

I_k – The identity matrix of order \( k \); the subscript is suppressed when the order of the matrix is clear from the context.

\( J_{k,l} \) – The \( k \times l \) all ones matrix. If \( k = l \), this is shortened to \( J_k \), and subscripts are suppressed when the order is clear from the context.

\( L_{\{i\}}, L_{\{i,j\}} \) – The submatrix of \( L \) formed by deleting the \( i \)-th row and column, and the submatrix of \( L \) formed by deleting the \( i \)-th and \( j \)-th row and column, respectively.

\( M^T \) – Transpose of the matrix \( M \). A similar notation applies to vectors.

\( ||M||_2 \) – The spectral norm of the square matrix \( M \) (i.e., its largest singular value).

\( ||x||_1 \) – The \( \ell_1 \)-norm of the vector \( x \).
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Spectral radius of graphs
WALK COUNTS AND THE SPECTRAL RADIUS OF GRAPHS

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Abstract. We develop a new and useful method that efficiently uses walk counts for comparing spectral radii of graphs similar in a precisely defined fashion. The method is applied to the cases where a path-like or a star-like structure is coalesced to a graph, in order to prove weak inequality in the conjectured inequality of Belardo, Li Marzi and Simić, and to resolve the Brualdi-Solheid problem for the classes of graphs consisting of rooted products with the same rooted graph.

1. Introduction

Study of the spectral radius of adjacency matrix of graphs has been a central research theme in spectral graph theory since its inception in the 1950s [3] to this day. Numerous results on the spectral radius have been surveyed by Cvetković and Rowlinson [6] in 1990 and in a recent research monograph of the author [14].

Graphs mostly considered in the literature are simple graphs, due to the fact that their adjacency matrix is real and symmetric, so that its eigenvectors can be chosen to provide an orthonormal basis for \( \mathbb{R}^n \) [8]. A simple graph \( G = (V, E) \) consists of the vertex set \( V \) with \( n = |V| \) vertices and the edge set \( E \subseteq \binom{V}{2} \) with \( m = |E| \) edges. The adjacency matrix \( A(G) \) of the simple graph \( G \) is the \( n \times n \) matrix, indexed by \( V \), defined by

\[
A(G)_{uv} = \begin{cases} 
1, & \text{if } uv \in E, \\
0, & \text{if } uv \notin E.
\end{cases}
\]

Let us denote the eigenvalues of \( A(G) \) by

\[
\lambda_1(G) \geq \lambda_2(G) \geq \cdots \geq \lambda_n(G),
\]

and the corresponding orthonormal eigenvectors by

\[
x_1(G), x_2(G), \ldots, x_n(G),
\]

so that

\[
(1) \quad A(G)x_i(G) = \lambda_i(G)x_i(G), \quad i = 1, \ldots, n.
\]

and for \( i, j = 1, \ldots, n, \)

\[
(2) \quad x_i^T(G)x_j(G) = \begin{cases} 
1, & \text{if } i = j, \\
0, & \text{if } i \neq j.
\end{cases}
\]
In the sequel we will drop the parameter \( G \) when the graph is clear from the context.

The eigenvalues and the orthonormality of eigenvectors provide spectral decomposition of the adjacency matrix [14]:

\[
A = \sum_{i=1}^{n} \lambda_i x_i x_i^T.
\]

The eigenvalues of \( A \) are also the roots of its characteristic polynomial

\[
P_G(\lambda) = \det(\lambda I - A).
\]

By the Perron-Frobenius theorem [8, Chap. XIII], when the graph \( G \) is connected, its adjacency matrix \( A \) is irreducible, so that its largest eigenvalue \( \lambda_1 \) is also the spectral radius of \( A \). In addition, \( \lambda_1 \) is a simple eigenvalue with a positive eigenvector \( x_1 \).

Most of the research on the spectral radius of graphs deals with the Brualdi-Solheid’s general question [2] that asks to characterize graphs with extremal values of the spectral radius in a given class of graphs (where extremal usually means maximal). The basic ingredient in tackling such extremal problems is the ability to compare spectral radii of different candidate graphs. Two well-developed techniques are mostly used in the literature for such comparisons.

The first technique relies on the classical characterization of the largest eigenvalue \( \lambda_1 \) in terms of the Rayleigh quotient of \( A \) [8]:

\[
\lambda_1 = \max_{y \neq 0} \frac{y^T A y}{y^T y} = \frac{2 \sum_{uv \in E} y_u y_v}{\sum_{u \in V} y_u^2},
\]

with the maximum attained for and only for \( y = x_1 \). From here it is easy to compare spectral radii of two graphs, where one of them is obtained by a small modification of the other one:

a) If \( pq \notin E \) then

\[
\lambda_1(G + pq) \geq \frac{x_1^T A(G + pq) x_1}{x_1^T x_1} = \frac{x_1^T A x_1 + 2x_1, p x_1, q}{x_1^T x_1} > \lambda_1,
\]
due to positivity of \( x_1 \) (and hence of \( x_1, p x_1, q \)).

b) If \( pq \in E, pr \notin E \) and \( x_{1,q} \leq x_{1,r} \), then [13]

\[
\lambda_1(G - pq + pr) \geq \frac{x_1^T A(G - pq + pr) x_1}{x_1^T x_1} = \frac{x_1^T A x_1 + 2x_1, p(x_{1,r} - x_{1,q})}{x_1^T x_1} > \lambda_1.
\]

The equality cannot hold above as in such case one would have that \( x_1 \) is also the principal eigenvector of \( G - pq + pr \) and that \( x_{1,q} = x_{1,r} \), which would then imply contradictory statement \( x_{1,r} = 0 \), by considering the eigenvalue equation (1) in both \( G \) and \( G - pq + pr \) at the vertex \( s \).
c) If $pq, rs \in E$, $pr, qs \notin S$ and $(x_{1,p} - x_{1,s})(x_{1,r} - x_{1,q}) \geq 0$, then [7]

$$\lambda_1(G - pq - rs + pr + qs) \geq \frac{x_1^T A(G - pq - rs + pr + qs)x_1}{x_1^T x_1} = \frac{(x_{1,p} - x_{1,s})(x_{1,r} - x_{1,q})}{x_1^T x_1} \geq \lambda_1.$$ 

The second technique relies on the fact that the value of the characteristic polynomial $P_G(y)$ is positive whenever $y > \lambda_1$. Thus, if one can show that for two graphs $G$ and $H$ holds

$$(\forall y > \lambda_1(G)) P_G(y) < P_H(y)$$

then $P_H(y)$ cannot have real roots that are greater than or equal to $\lambda_1(G)$, so that it must hold $\lambda_1(G) > \lambda_1(H)$.

Illustrative examples of the use of the first technique may be found in [10], and those of the use of the second technique both in [10] and [1].

Our goal here is to propose yet another technique for comparing spectral radii of two graphs, based on the comparisons of closed walk counts in these graphs. We have used comparisons of closed walk counts earlier to compare the Estrada indices of trees [11]. The technique presented in Section 2 is a comprehensive upgrade of the approach used in [11], applied to the spectral radius instead of the Estrada index. In Section 3 we show that the vertices of a path, in the rooted product of a path and another graph, have unimodal closed walk counts. This result helps to showcase fruitfulness of the walk count technique in Section 4, where we give new proofs of the well-known 1979 lemmas of Li and Feng [12], and prove weak inequality in the conjectured inequality of Belardo, Li Marzi and Simić [1].

2. A WALK COUNT TECHNIQUE

Let $G = (V, E)$ be a simple, connected graph with the adjacency matrix $A$, the eigenvalues $\lambda_1 > \lambda_2 \geq \cdots \geq \lambda_n$ and the orthonormal eigenvectors $x_1, x_2, \ldots, x_n$. We assume that $G$ is nontrivial, i.e., that it contains at least one edge. A sequence $W: u = u_0, u_1, \ldots, u_k = v$ of vertices from $V$ such that $u_i u_{i+1} \in E$ is called a walk between $u$ and $v$ in $G$ of length $k$. A walk $W$ is closed if $u = v$. The following classical result relates the adjacency matrix of a graph to its walk counts:

**Theorem 1** ([14]). The number of walks of length $k$, $k \geq 0$, between the vertices $u$ and $v$ in $G$ is equal to $(A^k)_{u,v}$.

From the spectral decomposition (3) and the orthonormality of eigenvectors (2) we now have

$$A^k = \sum_{i=1}^{n} \lambda_i^k x_i x_i^T.$$
For $k \geq 0$, let $N_k$ denote the number of all walks of length $k$ in $G$, and let $M_k$ denote the number of all closed walks of length $k$ in $G$. From (6) we have

\[
N_k = \sum_{u \in V} \sum_{v \in V} (A^k)_{u,v} = \sum_{i=1}^{n} \lambda_i^k \left( \sum_{u \in V'} x_{i,u} \right)^2,
\]

(7)

\[
M_k = \sum_{u \in V} (A^k)_{u,u} = \sum_{i=1}^{n} \lambda_i^k \left( \sum_{u \in V} x_{i,u}^2 \right) = \sum_{i=1}^{n} \lambda_i^k.
\]

(8)

**Lemma 2.** For a connected graph $G$ we have

\[
\lambda_1 = \lim_{k \to \infty} \sqrt{k} N_k.
\]

(9)

If $G$ is not bipartite, then also

\[
\lambda_1 = \lim_{k \to \infty} \sqrt{k} M_k,
\]

(10)

while if $G$ is bipartite, then

\[
\lambda_1 = \lim_{k \to \infty} 2^{k} \sqrt{M_{2k}}.
\]

(11)

The first equality above is taken from [4].

**Proof.** All three equalities rely on the Perron-Frobenius theorem [8, Chapter XIII], which implies that $\lambda_1 \geq |\lambda_i|$ for each $i = 2, \ldots, n$, and that the entries of $x_1$ in a connected graph $G$ with at least one edge are strictly positive.

The distinction between bipartite and nonbipartite graphs stems from the fact that if $G$ is bipartite, then the spectrum of $G$ is symmetric with respect to zero [4]. In such case, $\lambda_n = -\lambda_1$ is also a simple eigenvalue of $G$, and if $V = V' \cup V''$, $V' \cap V'' = \emptyset$, represents a bipartition of $G$, then the eigenvector corresponding to $\lambda_n$ satisfies

\[
x_{n,u} = \begin{cases} x_{1,u}, & \text{if } u \in V', \\ -x_{1,u}, & \text{if } u \in V''. \end{cases}
\]

Therefore,

\[
\frac{2^{k'} + 1}{\sqrt{N_{2k'+1}}} = \lambda_1 \frac{2^{k'} + 1}{\sqrt{2}} \sqrt{\left( \sum_{u \in V'} x_{1,u} \right)^2 - \left( \sum_{u \in V} x_{n,u} \right)^2 + \sum_{i=2}^{n-1} \left( \frac{\lambda_i}{\lambda_1} \right)^{2k'+1} \left( \sum_{u \in V} x_{i,u} \right)^2}
\]

(12)

\[
= \lambda_1 \frac{2^{k'} + 1}{\sqrt{2}} \sqrt{2 \left( \sum_{u \in V'} x_{1,u} \right)^2 + \sum_{i=2}^{n-1} \left( \frac{\lambda_i}{\lambda_1} \right)^{2k'+1} \left( \sum_{u \in V} x_{i,u} \right)^2},
\]

(13)

\[
\frac{2^{k'}}{\sqrt{2k'}} = \lambda_1 \frac{2^{k'}}{\sqrt{2}} \sqrt{\left( \sum_{u \in V} x_{1,u} \right)^2 + \left( \sum_{u \in V} x_{n,u} \right)^2 + \sum_{i=2}^{n-1} \left( \frac{\lambda_i}{\lambda_1} \right)^{2k'} \left( \sum_{u \in V} x_{i,u} \right)^2}
\]

(14)

\[
= \lambda_1 \frac{2^{k'}}{\sqrt{2}} \sqrt{2 \left( \sum_{u \in V'} x_{1,u} \right)^2 + \sum_{i=2}^{n-1} \left( \frac{\lambda_i}{\lambda_1} \right)^{2k'} \left( \sum_{u \in V} x_{i,u} \right)^2}.
\]
Eq. (9) follows from here, as both
\[
(\sum_{u \in V'} x_{1,u})(\sum_{u \in V''} x_{1,u}) \quad \text{and} \quad (\sum_{u \in V'} x_{1,u})^2 + (\sum_{u \in V''} x_{1,u})^2
\]
are positive constants, and for each \(i = 2, \ldots, n-1\) holds \(\frac{\lambda_i}{\lambda_1} < 1\), while the term \((\sum_{u \in V} x_{i,u})^2\) does not depend on \(k\).

For the closed walks we have \(M_{2k'+1} = 0\) for \(k' \geq 0\), while
\[
2^{k'} \sqrt{M_{2k'}} = \lambda_1 2^{k'} \sqrt{\frac{1}{2 + \sum_{i=2}^{n-1} \left(\frac{\lambda_i}{\lambda_1}\right)^{2k'}}},
\]
from where (11) follows, due to \(\frac{\lambda_i}{\lambda_1} < 1\) for each \(i = 2, \ldots, n-1\).

On the other hand, if \(G\) is not bipartite, then \(\lambda_n > -\lambda_1\), so that
\[
\sqrt{N_k} = \lambda_1 k \left[\left(\sum_{u \in V} x_{1,u}\right)^2 + \sum_{i=2}^{n} \left(\frac{\lambda_i}{\lambda_1}\right)^k \left(\sum_{u \in V} x_{i,u}\right)^2\right],
\]
\[
\sqrt{M_k} = \lambda_1 k \left[1 + \sum_{i=2}^{n} \left(\frac{\lambda_i}{\lambda_1}\right)^k\right].
\]
From here both (9) and (10) follow, since \((\sum_{u \in V} x_{1,u})^2\) is a positive constant and for each \(i = 2, \ldots, n, \left|\frac{\lambda_i}{\lambda_1}\right| < 1\), while the term \((\sum_{u \in V} x_{i,u})^2\) does not depend on \(k\). \(\square\)

Our first new result is a simple lemma stating that a connected graph with more walks of arbitrarily large lengths also has the larger spectral radius.

**Lemma 3.** Let \(G_1\) and \(G_2\) be connected graphs such that for an infinite sequence of indices \(k_0 < k_1 < \cdots\) holds
\[
(\forall i \geq 0) \quad N_{k_i}(G_1) \geq N_{k_i}(G_2).
\]
Then \(\lambda_1(G_1) \geq \lambda_1(G_2)\).

**Proof.** From Lemma 2 we get
\[
\lim_{k \to \infty} \frac{\lambda_1(G_1)^{k} \sqrt{N_k(G_2)}}{\lambda_1(G_2)^{k} \sqrt{N_k(G_1)}} = 1,
\]
which implies
\[
(\forall \varepsilon > 0)(\exists k_0)(\forall k \geq k_0) \quad \frac{\lambda_1(G_1)}{\lambda_1(G_2)} > (1 - \varepsilon) \sqrt{\frac{N_k(G_1)}{N_k(G_2)}}.
\]
The condition (12), with \(i_0\) taken to be the smallest index such that \(k_{i_0} \geq k_0\), now implies
\[
(\forall \varepsilon > 0)(\exists i_0)(\forall i \geq i_0) \quad \frac{\lambda_1(G_1)}{\lambda_1(G_2)} > 1 - \varepsilon.
\]
However, since $\lambda_1(G_1)$ and $\lambda_1(G_2)$ are the constants that do not depend on $i$, the previous expression actually means that
\[
(\forall \varepsilon > 0) \quad \frac{\lambda_1(G_1)}{\lambda_1(G_2)} > 1 - \varepsilon,
\]
which is equivalent to $\lambda_1(G_1) \geq \lambda_1(G_2)$. \qed

Remark 1. In order for previous lemma to imply that $\lambda_1(G_1)$ is strictly larger than $\lambda_1(G_2)$, instead of (12) one would need to prove that
\[
(\exists \varepsilon > 0)(\forall i_0)(\exists i \geq i_0) \quad N_{k_i}(G_1) \geq \frac{1}{1-\varepsilon} N_{k_i}(G_2),
\]
which is not always feasible.

We will, thus, allow our forthcoming results to include equality as a feasible case. When applied to graphs in a certain class, this essentially means that, while these lemmas provide characterization of the extremal value of the spectral radius of graphs in that class, they cannot provide characterization of all graphs with the extremal spectral radius. Instead, the lemmas will provide just one example of such extremal graph. In many classes the extremal graph is unique, so that the lemmas will necessarily pinpoint it, but they cannot be used to prove that there are no other extremal graphs.

It is obvious from Lemma 2 that the previous result can be stated in the terms of closed walk counts as well. We restrict ourselves here to closed walks of even length simply to avoid the trouble of considering whether the graphs in question are bipartite or not.

Lemma 4. Let $G_1$ and $G_2$ be connected graphs such that for an infinite sequence of indices $k_0 < k_1 < \cdots$ holds
\[
(13) \quad (\forall i \geq 0) \quad M_{2k_i}(G_1) \geq M_{2k_i}(G_2).
\]
Then $\lambda_1(G_1) \geq \lambda_1(G_2)$.

Let us now define a graph operation that will be the basis for our comparison technique.

Definition 1. Let $F$ and $G$ be the graphs with disjoint vertex sets $V(F)$ and $V(G)$. For $p \in \mathbb{N}$, let $u_1, \ldots, u_p$ be distinct vertices from $V(F)$, and let $v_1, \ldots, v_p$ be distinct vertices from $V(G)$. Assume, in addition, that there is no pair $(i, j)$, $i \neq j$, such that both $u_i u_j$ is an edge of $F$ and $v_i v_j$ is an edge of $G$. The multiple coalescence of $F$ and $G$ with respect to the vertex lists $u_1, \ldots, u_p$ and $v_1, \ldots, v_p$, denoted by
\[
F(u_1 = v_1, \ldots, u_p = v_p)G,
\]
is the graph obtained from the union of $F$ and $G$ by identifying the vertices $u_i$ and $v_i$ for each $i = 1, \ldots, p$.

The multiple coalescence is a generalization of the standard coalescence of two vertex-disjoint graphs, which is obtained by identifying a single pair of vertices, one from each graph [5]. Fig. 1 shows an example of multiple coalescence of the graphs $F$ and $G$, with respect to the selected vertices $u_1, u_2, u_3$ and $v_1, v_2, v_3$. 
The above assumption that for any $i \neq j$ it is not allowed that both $u_i u_j$ is an edge of $F$ and $v_i v_j$ is an edge of $G$, serves to prevent the creation of multiple edges in the multiple coalescence. This assumption is needed later, as our goal will be to have each walk in the multiple coalescence clearly separated in smaller parts whose all edges will belong to only one of its constituents. In such setting, the vertices $v_1, \ldots, v_p$ may be considered as the entrance points for a walk coming from $F$ to enter $G$ (and vice versa).

Our main tool is the following lemma.

**Lemma 5.** Let $F$ and $G$ be graphs with disjoint vertex sets $V(F)$ and $V(G)$. For $p \in \mathbb{N}$, choose distinct vertices $u_1, \ldots, u_p \in V(F)$, and make two separate choices of distinct vertices $v_1, \ldots, v_p \in V(G)$ and $w_1, \ldots, w_p \in V(G)$. Let $G^v$ and $G^w$ be the multiple coalescences

- $G^v = F(u_1 = v_1, \ldots, u_p = v_p)G$,
- $G^w = F(u_1 = w_1, \ldots, u_p = w_p)G$,

such that both $G^v$ and $G^w$ are connected.

Let $A$ be the adjacency matrix of $G$. If for each $1 \leq i, j \leq p$ (including the case $i = j$) and for each $k \geq 1$ holds

\[(A^k)_{v_i, v_j} \geq (A^k)_{w_i, w_j},\]

then

\[\lambda_1(G^v) \geq \lambda_1(G^w).\]

Note that in the above lemma, while we request that $v_i \neq v_j$ and $w_i \neq w_j$ for all $i \neq j$, the possibility that $v_i = w_j$ for some $i$ and $j$ is allowed.

**Proof.** Let us first count the closed walks of length $2k$ in $G^v$. From the fact that $F$ and $G$, as constituents of $G^v$, do not have common edges, we see that the number of closed walks in $G^v$, whose all edges belong to the same constituent, is equal to $M_{2k}(F) + M_{2k}(G)$.
The remaining closed walks in $G^v$ contain edges from both $F$ and $G$. Any such closed walk $W$ can then be decomposed into a sequence of subwalks

$$W : W_0, W_1, \ldots, W_{2l-1},$$

for some $l \in \mathbb{N}$, such that the edges of the even-indexed subwalks $W_0, \ldots, W_{2l-2}$ all belong to $F$, while the edges of the odd-indexed subwalks $W_1, \ldots, W_{2l-1}$ all belong to $G$. As a walk can enter from $F$ to $G$ only through one of the entrance points, we also see that the endpoints of the even-indexed subwalks belong to $\{u_1, \ldots, u_p\}$, while the endpoints of the odd-indexed subwalks belong to $\{v_1, \ldots, v_p\}$. Thus, let $(i_0, \ldots, i_{2l-1})$ denote the $2l$-tuple of indices such that

- the walk $W_{2j}$ goes from $u_{i_{2j}}$ to $u_{i_{2j}+1} (= v_{i_{2j}+1})$ in $F$, while
- the walk $W_{2j+1}$ goes from $v_{i_{2j}+1}$ to $v_{i_{2j}+2} (= u_{i_{2j}+2})$ in $G$,

for $j = 0, \ldots, l-1$. (The addition above is modulo $2l$, so that $i_{2l} = i_0$.)

In addition, let $k_j$ denote the length of the walk $W_j$ for $j = 0, \ldots, 2l-1$. The $4l$-tuple

$$(i_0, \ldots, i_{2l-1}; k_0, \ldots, k_{2l-1})$$

is called the signature of the closed walk $W$. Due to the fact that the walk $W$ is closed, its signatures are rotationally equivalent in the sense that the above signature is identical to the signature

$$(i_{2p}, \ldots, i_{2l-1}, i_0, \ldots, i_{2p-1}; k_{2p}, \ldots, k_{2l-1}, k_0, \ldots, k_{2p-1})$$

for each $p = 1, \ldots, l-1$. In order to assign a unique signature to $W$, we may assume its signature is chosen to be lexicographically minimal among all rotationally equivalent signatures.

Now, let $B$ be the adjacency matrix of $F$. Then for any feasible signature

$$(i_0, \ldots, i_{2l-1}; k_0, \ldots, k_{2l-1})$$

the number of closed walks in $G^v$ with that signature is equal to

$$\prod_{j=0}^{l-1} (B^{k_{2j}})_{u_{i_{2j}}, u_{i_{2j}+1}} \prod_{j=0}^{l-1} (A^{k_{2j}+1})_{v_{i_{2j}+1}, v_{i_{2j}+2}}.$$

The argument is identical for closed walks of length $2k$ in $G^w$: the number of closed walks, whose all edges belong to the same constituent of $G^w$, is equal to $M_{2k}(F) + M_{2k}(G)$, while the number of closed walks with the feasible signature $(i_0, \ldots, i_{2l-1}; k_0, \ldots, k_{2l-1})$ is equal to

$$\prod_{j=0}^{l-1} (B^{k_{2j}})_{u_{i_{2j}}, u_{i_{2j}+1}} \prod_{j=0}^{l-1} (A^{k_{2j}+1})_{v_{i_{2j}+1}, v_{i_{2j}+2}}.$$

From the condition (14) we now see that for any feasible signature the number of closed walks with that signature in $G^w$ is larger than or equal to the number of such closed walks in $G^v$. Summing over all feasible signatures we obtain that

$$M_{2k}(G^v) \geq M_{2k}(G^w),$$

and, thus, from Lemma 4 we conclude that $\lambda_1(G^v) \geq \lambda_1(G^w)$. \qed
The usefulness of the above lemma is clearly visible: in order to obtain an inequality between the spectral radii of the multiple coalescences $G^v$ and $G^w$ it is enough to count just the walks in the $G$-part of the coalescences—the walk counts in the $F$-part have no influence, since the entrance points to $F$ are the same in both $G^v$ and $G^w$.

*Remark 2.* Let $\lambda_1 > \lambda_2 \geq \cdots \geq \lambda_n$ and $x_1, x_2, \ldots, x_n$ denote the eigenvalues and the corresponding orthonormal eigenvectors of the adjacency matrix $A$ of a connected graph $G$. Recall that

$$(A^k)_{v_i,v_j} = \sum_{p=1}^{n} \lambda_p^k x_p,v_i x_p,v_j,$$

$$(A^k)_{w_i,w_j} = \sum_{p=1}^{n} \lambda_p^k x_p,w_i x_p,w_j.$$ 

Since $\lambda_1$ has the largest absolute value among all eigenvalues and a positive eigenvector, the most important summands in the above expressions, especially for larger values of $k$, become $\lambda_1^k x_{1,v_i} x_{1,v_j}$ and $\lambda_1^k x_{1,w_i} x_{1,w_j}$. It is, thus, tempting to think that the condition (14) in Lemma 5 might be replaced by a simpler condition

$$x_{1,v_i} x_{1,v_j} \geq x_{1,w_i} x_{1,w_j}.$$ 

This, however, cannot be done, as shown by the following example. Let $u$ be an arbitrary vertex of the complete graph $K_{50}$, and let $G$ be the graph shown in Fig. 2. Although

$$0.41712 \approx x_{1,a} < x_{1,b} \approx 0.45699,$$

we still have that

$$49.00123 \approx \lambda_1(K_{50}(u = a)G) > \lambda_1(K_{50}(u = b)G) \approx 49.00083.$$ 

![Figure 2](image)

**Figure 2.** The vertex $a$ has smaller principal eigenvector component than the vertex $b$, but there are more closed walks of even lengths up to 12 that start at $a$ than at $b$.

The reason for such behavior lies simply in the fact that the degree of $a$ is larger than the degree of $b$. Note that the degree of a vertex represents, at the same time, also the number of closed walks of length two starting from that vertex. When coalesced with $K_{50}$, which has substantially more closed walks than $G$, the spectral radius of the coalescence is roughly determined by the spectral radius of the larger $K_{50}$, but tends to be fine tuned by the shorter (i.e., the shortest) closed walks in $G$, of which there are more that start at $a$ than those that start at $b$. 
3. ON CLOSED WALK COUNTS IN ROOTED PRODUCTS OF PATHS AND STARS

In order to be able to apply Lemma 5 we need to exhibit sufficiently many graphs satisfying (14). Paths are among the simplest such graphs. The following lemma appeared in the authors’ earlier paper with Ilić:

**Lemma 6 ([11]).** Let \( A \) be the adjacency matrix of the path \( P_n \) on vertices \( 1, \ldots, n \). Then for every \( k \geq 0 \) holds

\[
(A^k)_{1,1} \leq (A^k)_{2,2} \leq \cdots \leq (A^k)_{[n/2],[n/2]}
\]

and

\[
(A^k)_{1,2} \leq (A^k)_{2,3} \leq \cdots \leq (A^k)_{[n/2],[n/2]+1}.
\]

We reprint here the proof of this lemma from [11], as it serves as the basis for the proof of a more general lemma that follows.

**Proof.** We prove slightly more than stated in (15) and (16): that each diagonal of \( A^k \), parallel to the main diagonal, is unimodal. Due to the automorphism of the path \( P_n \) given by \( \alpha: i \mapsto n + 1 - i \) for \( i = 1, \ldots, n \), it is enough to prove that each of these diagonals is nondecreasing up to its middle entry.

We proceed by induction on \( k \) and prove that for all \( 2 \leq i, j \leq n \) such that \( i + j \leq n + 1 \) holds

\[
(A^k)_{i-1,j-1} \leq (A^k)_{i,j}.
\]

This is trivial for \( k = 0 \) and \( k = 1 \), as each diagonal of \( A^0 = I \) and \( A^1 = A \) is either all-zero or all-one. Suppose now that (17) has been proved for some \( k \geq 1 \). The expression \( A^{k+1} = A^k \cdot A \) then yields

\[
(A^{k+1})_{i-1,j-1} = (A^k)_{i-1,j-2} + (A^k)_{i-1,j},
\]

\[
(A^{k+1})_{i,j} = (A^k)_{i-1,j} + (A^k)_{i,j+1}.
\]

(To avoid dealing separately with the endpoints 1 and \( n \) of the path \( P_n \), we simply assume that \( (A^k)_{i-1,0} = 0 \) and \( (A^k)_{i,n+1} = 0 \) in the above equations.)

We have

\[
(A^k)_{i-1,j-2} \leq (A^k)_{i,j-1}
\]

from the inductive hypothesis (and the nonnegativity of \( (A^k)_{i,j-1} \)). If \( i + j + 1 \leq n + 1 \), then

\[
(A^k)_{i-1,j} \leq (A^k)_{i,j+1}
\]

also follows from the inductive hypothesis. For \( i + j + 1 = n + 2 \), from the automorphism \( \alpha: i \mapsto n + 1 - i \) and the symmetry of \( A^k \) we have

\[
(A^k)_{i-1,j} = (A^k)_{n+1-j,n+2-i} = (A^k)_{i,j+1}.
\]

This proves (17). \( \square \)

We will now extend this lemma to the rooted products of a path by another graph.
Definition 2 ([9]). Let $H$ be a labeled graph on $n$ vertices, and let $G_1, \ldots, G_n$ be a sequence of $n$ rooted graphs. The rooted product of $H$ by $G_1, \ldots, G_n$, denoted as $H[G_1, \ldots, G_n]$, is the graph obtained by identifying the root of $G_i$ with the $i$-th vertex of $H$ for $i = 1, \ldots, n$. In the case when all the rooted graphs $G_i$, $i = 1, \ldots, n$, are isomorphic to a rooted graph $G$, we denote $H[G, \ldots, G]_n$ simply as $H[G, n]$.

Lemma 7. Let $n$ be a positive integer and let $G$ be an arbitrary rooted graph. Denote by $G_1, \ldots, G_n$ the copies of $G$, and for any vertex $u$ of $G$, denote by $u_i$ the corresponding vertex in the copy $G_i$, $i = 1, \ldots, n$. If $A$ is the adjacency matrix of the rooted product $P_n[G, n]$, then for any two (not necessarily different) vertices $u$ and $v$ of $G$ and for every $k \geq 0$ holds
\begin{align}
(A^k)_{u_1, v_1} \leq (A^k)_{u_2, v_2} \leq \cdots \leq (A^k)_{u_{\lceil n/2 \rceil}, v_{\lceil n/2 \rceil}}. \quad (18)
\end{align}
and
\begin{align}
(A^k)_{u_1, v_2} \leq (A^k)_{u_2, v_3} \leq \cdots \leq (A^k)_{u_{\lceil N/2 \rceil}, v_{\lceil N/2 \rceil + 1}}. \quad (19)
\end{align}

Proof. Let $r$ denote the root vertex of $G$, so that $r_1, \ldots, r_n$ then also denote the vertices of $P_n$ in the rooted product $P_n[G, n]$.

The number of $k$-walks between $u_i$ and $v_i$ whose edges fully belong to $G_i$ is, obviously, equal to the number of $k$-walks between $u$ and $v$ in $G$. If a $k$-walk $W$ between $u_i$ and $v_i$ contains other edges of $P_n[G, n]$, then let $W'$ denote longest subwalk of $W$ such that $W'$ is a closed walk that starts and ends at $r_i$: simply, the first edge of $W'$ is the first edge of $W$ that does not belong to $G_i$, and the last edge of $W'$ is the last edge of $W$ that does not belong to $G_i$. It is easy to see then that the number of $k$-walks between $u_i$ and $v_i$ in $P_n[G, n]$ is governed by the numbers of walks between $u$ and $v$ in $G$, and the numbers of closed walks (of lengths $k$ and less) that start and end at $r_i$ in $P_n[G, n]$. In particular, the chain of inequalities (18) follows from
\begin{align}
(A^k)_{r_1, v_1} \leq (A^k)_{r_2, v_2} \leq \cdots \leq (A^k)_{r_{\lceil n/2 \rceil}, v_{\lceil n/2 \rceil}}. \quad (20)
\end{align}

Similarly, the number of $k$-walks between $u_i$ in the copy $G_i$ and $v_{i+1}$ in the copy $G_{i+1}$ is governed by the numbers of walks between $u$ and $r$ in $G$ (that get mapped to walks between $u_i$ and $r_i$ in $G_i$), the numbers of walks between $r$ and $v$ in $G$ (that get mapped to walks between $r_{i+1}$ and $v_{i+1}$ in $G_{i+1}$), and the numbers of walks between $r_i$ and $r_{i+1}$ in $P_n[G, n]$. Thus, the chain of inequalities (19) follows from
\begin{align}
(A^k)_{r_1, r_2} \leq (A^k)_{r_2, r_3} \leq \cdots \leq (A^k)_{r_{\lfloor N/2 \rfloor}, r_{\lfloor N/2 \rfloor + 1}}. \quad (21)
\end{align}

Similarly as in the proof of Lemma 6, (18) and (19) are the special cases of the inequalities
\begin{align}
(A^k)_{u_{i-1}, v_{j-1}} \leq (A^k)_{u_i, v_j}, \quad 2 \leq i, j \leq n, \quad i + j \leq n + 1, \quad (22)
\end{align}
which are, from the argument above, corollaries of the inequalities
\begin{align}
(A^k)_{r_{i-1}, r_{j-1}} \leq (A^k)_{r_i, r_j}, \quad k' \leq k, \quad 2 \leq i, j \leq n, \quad i + j \leq n + 1. \quad (23)
\end{align}

We will now prove (22) by induction on $k$. This is trivial for $k = 0$, as $A^0 = I$. 
Suppose, therefore, that (22) has been proved for all values of \( k' \) up to some \( k \geq 0 \). We will now prove that (23) holds for \( k' = k + 1 \), from which the correctness of (22) for \( k' = k + 1 \) follows as well. (Actually, from the above discussion it is easy to see that the correctness of (22) for \( k' = k + 1 \) follows already from the inductive hypothesis if at least one of \( u, v \) is not \( r \). Therefore, one only needs to prove (23) for \( k' = k + 1 \).)

Let \( N(r) \) denote the set of neighbors of the root \( r \) in the graph \( G \). Then

\[
(A^{k+1})_{r_{i-1},r_{j-1}} = (A^k)_{r_{i-1},r_{j-2}} + (A^k)_{r_{i-1},r_j} + \sum_{u \in N(r)} (A^k)_{r_{i-1},u_{j-1}},
\]

and

\[
(A^{k+1})_{r_i,r_j} = (A^k)_{r_{i-1},r_j} + (A^k)_{r_i,r_{j+1}} + \sum_{u \in N(r)} (A^k)_{r_i,u_j}.
\]

The inequalities

\[
(A^k)_{r_{i-1},r_{j-2}} \leq (A^k)_{r_{i-1},r_{j-1}}
\]

and

\[
(A^k)_{r_{i-1},u_{j-1}} \leq (A^k)_{r_i,u_j}
\]

hold by the inductive hypothesis. (We again assume that \((A^k)_{r_{i-1},r_0} = 0\) and \((A^k)_{r_{i-1},r_{n+1}} = 0\) to avoid dealing separately with the end vertices of the path \( P_n \).) If \( i + j + 1 \leq n + 1 \), then

\[
(A^k)_{r_{i-1},r_j} \leq (A^k)_{r_i,r_{j+1}}
\]

also holds by the inductive hypothesis. For \( i + j + 1 = n + 2 \), from the automorphism \( \beta: r_i \to r_{n+1-i} \) of \( P_n[G,n] \) and the symmetry of \( A^k \) we have

\[
(A^k)_{r_{i-1},r_j} = (A^k)_{r_{n+1-j},r_{n+2-i}} = (A^k)_{r_i,r_{j+1}}.
\]

This proves (23), and consequently (22). \( \square \)

In order to be able to prove the conjecture of Belardo, Li Marzi and Simić [1], we need to consider a slight extension of the previous lemma as well.

**Lemma 8.** Let \( n \) be a positive integer and let \( G \) be an arbitrary rooted graph with the root \( r \). Let \( P_n^+[G,n] \) denote the graph obtained from the rooted product \( P_n[G,n] \) by adding two new pendant vertices \( r_0 \) and \( r_{n+1} \) and the edges \( r_0r_1 \) and \( r_nr_{n+1} \) to it. If \( A \) is the adjacency matrix of \( P_n^+[G,n] \), then for any two (not necessarily different) vertices \( u \) and \( v \) of \( G \) and for every \( k \geq 0 \) holds

\[
(A^k)_{u_1,v_1} \leq (A^k)_{u_2,v_2} \leq \cdots \leq (A^k)_{u_{[n/2]},v_{[n/2]}}
\]

and

\[
(A^k)_{u_1,v_2} \leq (A^k)_{u_2,v_3} \leq \cdots \leq (A^k)_{u_{[N/2]},v_{[N/2]+1}}.
\]

**Proof.** The proof of this lemma is fully analogous to the proof of Lemma 7, with the difference that now the terms \((A^k)_{r_{i-1},r_0}\) and \((A^k)_{r_i,r_{n+1}}\) are no longer considered to be identically equal to 0. We will, therefore, indicate here only the differences that the introduction of the pendant vertices \( r_0 \) and \( r_{n+1} \) produces in the proof.

In the proof of (22) and (23) by induction on \( k \), the basis remains trivial and can be extended to both \( k = 0 \) and \( k = 1 \), as the values \( A_{u_{i-1},v_{j-1}} \) and \( A_{u_i,v_j} \)
are nonzero (and equal to 1) if and only if either \( i = j \) and \( u \) and \( v \) are adjacent in \( G \) or \(|i - j| = 1\) and both \( u \) and \( v \) are equal to \( r \).

Since we assume \( 2 \leq i, j \leq n, i + j \leq n + 1 \) in (22), the only difference in the proof of the inductive step lies in encountering the case \( j = 2 \), where we need to additionally prove that

\[
(A^k)_{r_{i-1}, r_0} \leq (A^k)_{r_i, r_1}.
\]

This, however, follows immediately from the fact that \( r_1 r_0 \) has to be the last edge in any walk from \( r_{i-1} \) to \( r_0 \), so that

\[
(A^k)_{r_{i-1}, r_0} = (A^{k-1})_{r_{i-1}, r_1}
\]

and the inequality

\[
(A^k)_{r_i, r_1} = (A^{k-1})_{r_{i-1}, r_1} + (A^{k-1})_{r_{i+1}, r_1} + \sum_{u \in N(r)} (A^{k-1})_{u, r_1} \geq (A^{k-1})_{r_{i-1}, r_1}.
\]

Hence (23), and consequently (22), holds again, which implies the chains of inequalities (24) and (25).

Stars form another, even simpler class of graphs that satisfy (14). Let \( c \) be the center, and \( l_1, \ldots, l_{n-1} \) the leaves of the star \( S_n \), \( n \geq 2 \). The inequality

\[(A^k)_{l_i, l_i} \leq (A^k)_{c, c}\]

for \( i \in \{1, \ldots, n-1\} \) follows easily by induction on \( k \). For \( k = 0 \) we have \((A^0)_{l_i, l_i} = (A^0)_{c, c} = 1\). Assuming that the inequality (26) has been proved up to some \( k \geq 0 \), we then have

\[
(A^{k+1})_{l_i, l_i} = (A^{k})_{c, l_i} \leq \sum_{j=1}^{n-1} (A^{k})_{c, l_j} = (A^{k+1})_{c, c},
\]

simply by observing that any walk that starts at \( l_i \) must use the edge \( l_i c \) first.

Inequality (26) can also be extended to the rooted products of a star by another graph.

**Lemma 9.** For \( n \geq 2 \), let \( c \) be the center and \( l \) an arbitrary leaf of the star \( S_n \). Let \( G \) be an arbitrary rooted graph. Denote by \( G_c \) the copy of \( G \) in \( S_n[G, n] \) whose root is identified with \( c \), and by \( G_l \) the copy of \( G \) in \( S_n[G, n] \) whose root is identified with \( l \). For any vertex \( u \) of \( G \), let \( u_c \) and \( u_l \) denote the corresponding vertices in \( G_c \) and \( G_l \), respectively. If \( A \) is the adjacency matrix of the rooted product \( S_n[G, n] \), then for any two (not necessarily different) vertices \( u \) and \( v \) of \( G \) and for every \( k \geq 0 \) holds

\[(A^k)_{u_l, v_l} \leq (A^k)_{u_c, v_c}.
\]

**Proof.** Let \( r \) denote the root vertex of \( G \), so that \( r_c \) and \( r_l \) become identified with \( c \) and \( l \), respectively, in \( S_n[G, n] \). Following the argument from the proof of Lemma 7, inequality (27) for arbitrary \( u \) and \( v \) will follow from

\[
(A^k)_{r_l, r_l} \leq (A^k)_{r_c, r_c}.
\]

We prove (27) by induction on \( k \). This is trivial for \( k = 0 \), as \( A^0 = I \).

Suppose, therefore, that (27) has been proved for all values of \( k' \) up to some \( k \geq 0 \). We prove that (28) holds for \( k' = k + 1 \), from which the correctness
of (27) for \( k' = k + 1 \) follows as well. Let \( N(r) \) denote the set of neighbors of the root \( r \) in the graph \( G \). Then
\[
(A^{k+1})_{r_l,r_l} = (A^k)_{r_l,r_l} + \sum_{u \in N(r)} (A^k)_{u,r_l},
\]
\[
(A^{k+1})_{r_c,r_c} \geq (A^k)_{r_c,r_c} + \sum_{u \in N(r)} (A^k)_{u_c,r_c},
\]
where in the second expression we have deliberately disregarded \( k \)-walks between roots of other copies of \( G \) and \( r_c \). From the inductive hypothesis we have
\[
(A^k)_{u_l,r_l} \leq (A^k)_{u_c,r_c}
\]
for any vertex \( u \in N(r) \). Together with the fact that \( A^k \) is symmetric, this proves (28), and consequently (27).

\[ \square \]

4. Spectral radii of certain multiple coalescences

As our simplest examples of the use of Lemma 5 and the walk count lemmas from the previous section, we first provide new proofs for the useful and well-cited 1979 lemmas of Li and Feng [12]. Note, however, that the original lemmas claim the strict inequality between the spectral radii, and that we actually prove the weak inequality here, due to reasons explained in Remark 1 on page 146.

Lemma 10 ([12]). Let \( u \) be a vertex of a connected graph \( G \) and for positive integers \( p \) and \( q \), let \( G^u_{p,q} \) denote the graph obtained from \( G \) by adding two pendants paths of lengths \( p \) and \( q \) at \( u \). If \( p \geq q \geq 1 \), then
\[
\lambda_1(G^u_{p,q}) \geq \lambda_1(G^u_{p+1,q-1}).
\]

Lemma 11 ([12]). Let \( u \) and \( v \) be two adjacent vertices of a connected graph \( G \) and for positive integers \( p \) and \( q \), let \( G^u_{p,q} \) denote the graph obtained from \( G \) by adding pendant paths of length \( p \) at \( u \) and \( q \) at \( v \). If \( p \geq q \geq 1 \), then
\[
\lambda_1(G^u_{p,q}) \geq \lambda_1(G^u_{p+1,q-1}).
\]

The proof of Lemma 10 follows by observing that \( G^u_{p,q} \) is a coalescence of the graph \( G \) and the path \( P_{p+q+1} \) by identifying the vertex \( u \) from \( G \) and the vertex \( q + 1 \) of \( P_{p+q+1} \). (Here the vertices of \( P_{p+q+1} \) are enumerated with \( 1, \ldots, q+1, \ldots, p+q+1 \), starting from the endpoint of \( P_{q+1} \) toward \( u \), and then continuing from \( u \) toward the endpoint of \( P_{p+1} \).) The inequality
\[
\lambda_1(G^u_{p,q}) = \lambda_1(G(u = q + 1)P_{p+q+1}) \geq \lambda_1(G(u = q)P_{p+q+1}) = \lambda_1(G^u_{p+1,q-1})
\]
then follows from (15) and Lemma 5.

The proof of Lemma 11 further follows by observing that the graphs \( G^u_{p,q} \) and \( G^u_{p+1,q-1} \) are multiple coalescences of the edge-deleted graph \( G - uv \) and the path \( P_{p+q+2} \):
\[
G^u_{p,q} \cong G - uv(u = q + 2, v = q + 1)P_{p+q+2};
\]
\[
G^u_{p+1,q-1} \cong G - uv(u = q + 1, v = q)P_{p+q+2}.
\]
Lemma 5 requires that for $k \geq 1$
\[
(A^k)_{q+2,q+2} \geq (A^k)_{q+1,q+1}, \\
(A^k)_{q+1,q+1} \geq (A^k)_{q,q}, \\
(A^k)_{q+2,q+1} \geq (A^k)_{q+1,q}.
\]
which are the special cases of (15) and (16), with $(A^k)_{q+2,q+2} = (A^k)_{q+1,q+1}$ in the case $p = q$ due to the automorphism of the path $P_{2q+2}$.

Next, we improve these lemmas by showing their analogs when, instead of a path, the rooted product of a path gets attached to the basis graph.

**Lemma 12.** Let $G$ be a rooted graph, $H$ a connected graph, and $p$ and $q$ two positive integers. For a vertex $u$ of $H$, suppose that $H$ contains a rooted subgraph $G'$, with $u$ as its root, that is isomorphic to the rooted graph $H$.

Let $H_{u,G}^{p,q}$ denote the graph obtained from $H$ by identifying the rooted subgraph $G'$ with the $(q+1)$-st copy of $G$ in the rooted product $P_{p+q+1}[G, p+q+1]$ (see Fig. 3). If $p \geq q \geq 1$, then
\[
\lambda_1(H_{u,G}^{p,q}) \geq \lambda_1(H_{u,G}^{p+1,q-1}).
\]

**Lemma 13.** Let $G$ be a rooted graph, $H$ a connected graph, and $p$ and $q$ two positive integers. For two adjacent vertices $u$ and $v$ of $H$, suppose that $H$ contains two vertex-disjoint rooted subgraphs $G'$, with a root $u$, and $G''$, with a root $v$, both isomorphic to the rooted graph $G$.

Let $H_{u,v,G}^{p,q}$ denote the graph obtained from $H$ by identifying the rooted subgraph $G'$ with the $(q+2)$-nd copy of $G$ and the rooted subgraph $G''$ with the $(q+1)$-st copy of $G$ in the rooted product $P_{p+q+2}[G, p+q+2]$ (see Fig. 3). If $p \geq q \geq 1$, then
\[
\lambda_1(H_{u,v,G}^{p,q}) \geq \lambda_1(H_{u,v,G}^{p+1,q-1}).
\]
Both of these lemmas follow directly from Lemmas 5 and 7 by observing that both \( H^u_{p,q} \) and \( H^{u,v}_{p,q} \) are multiple coalescences.

If \( H' \) is the graph obtained from \( H \) by deleting the edges of \( G' \), then \( H^{u,v}_{p,q} \) is the multiple coalescence of \( H' \) and \( P_{p+q+1}[G,p+q+1] \), obtained by identifying the corresponding vertices of \( G' \) in \( H' \) and the \((q+1)\)-st copy of \( G \) in \( P_{p+q+1}[G,p+q+1] \).

If \( H'' \) is the graph obtained from \( H \) by deleting the edges of \( G' \) and \( G'' \), then \( H^{u,v}_{p,q} \) is the multiple coalescence of \( H'' \) and \( P_{p+q+2}[G,p+q+2] \), obtained by identifying the corresponding vertices of \( G' \) and the \((q+2)\)-nd copy of \( G \) in \( P_{p+q+2}[G,p+q+2] \), and by identifying the corresponding vertices of \( G'' \) and the \((q+1)\)-st copy of \( G \) in \( P_{p+q+2}[G,p+q+2] \).

In addition, note that the conditions that \( H \) has to contain rooted subgraphs isomorphic to \( G \) can be easily removed from the last two lemmas: if \( H \) does not contain a complete copy of \( G \) rooted at \( u \) as its subgraph, then we can form \( H' \) from \( H \) by adding the necessary number of isolated vertices, and then apply Lemmas 5 and 7 to the multiple coalescence of \( H' \) and \( P_{p+q+1}[G,p+q+1] \), where the new isolated vertices are identified with the vertices of the \((q+1)\)-st copy of \( G \) that do not originally appear in \( H \). Similar argument holds in the case of adjacent vertices \( u \) and \( v \) and the two vertex-disjoint copies of \( G \) needed in \( H \). In the extreme case, we can just identify the vertex \( u \) (or \( u \) and \( v \)) of \( H \) with the root(s) of the copies of \( G \) in the rooted product, and apply Lemmas 5 and 7 to obtain the following two lemmas:

**Lemma 14.** Let \( G \) be a rooted graph with the root \( r \), \( p \) and \( q \) two positive integers, and let \( r_q \) and \( r_{q+1} \) denote the roots of the \( q \)-th and the \((q+1)\)-st copies of \( G \), respectively, in the rooted product \( P_{p+q+1}[G,p+q+1] \).

If \( p \geq q \geq 1 \), then for any connected graph \( H \) and any vertex \( u \) of \( H \) holds

\[
\lambda_1(H(u = r_{q+1})P_{p+q+1}[G,p+q+1]) \geq \lambda_1(H(u = r_q)P_{p+q+1}[G,p+q+1]).
\]

**Lemma 15.** Let \( G \) be a rooted graph with the root \( r \), \( p \) and \( q \) two positive integers, and let \( r_{q-1}, r_q \) and \( r_{q+1} \) denote the roots of the \((q-1)\)-st, \( q \)-th and the \((q+1)\)-st copies of \( G \), respectively, in the rooted product \( P_{p+q+2}[G,p+q+2] \).

If \( p \geq q \geq 1 \), then for any connected graph \( H \) and any two adjacent vertices \( u \) and \( v \) of \( H \) holds

\[
\lambda_1(H(u = r_{q+2}, v = r_{q+1})P_{p+q+2}[G,p+q+2]) \geq \lambda_1(H(u = r_{q+1}, v = r_q)P_{p+q+2}[G,p+q+2]).
\]

The use of Lemma 8 instead of Lemma 7 further allows us to state Lemmas 12-15 in terms of multiple coalescences with \( P^+_{p+q+1}[G,p+q+1] \) and \( P^+_{p+q+2}[G,p+q+2] \) as well. This leads to the observation that the weak inequality in the 2009 conjecture of Belardo, Li Marzi and Simić [1] becomes merely a corollary of Lemmas 5 and 8:

**Conjecture 16 ([1]).** Let \( G \) be a rooted graph having \( r \) as its root, with \( \deg(r) \geq \Delta - 2 \). Denote by \( G_\Delta(l,m) \), with \( l, m \geq 0 \), the graph obtained from \( G \) by
identifying $r$ with two pendant vertices of $P^+[K_{1,\Delta-2},l]$ and $P^+[K_{1,\Delta-2},m]$ (see Fig. 4). If $G$ is not the star $K_{1,\Delta-2}$ and $l \geq m \geq 1$ then

$$\lambda_1(G_{\Delta}(l,m)) > \lambda_1(G_{\Delta}(l+1,m-1)).$$

![Figure 4](image)

The graph $G_{\Delta}(l,m)$ is another instance of a multiple coalescence. Let $s_1, \ldots, s_{\Delta-2}$ be distinct neighbors of $r$ in $G$, and let $G^*$ be the edge-deleted subgraph $G^* = G - rs_1 - \cdots - rs_{\Delta-2}$.

Next, let $u_{m+1}$ be the root of the $(m+1)$-st copy of $K_{1,\Delta-2}$ in the graph $P^+[K_{1,\Delta-2},l+m+1]$ (counting the copies of $K_{1,\Delta-2}$ backwards from the $m$-end in Fig. 4), and let $t_{m+1,1}, \ldots, t_{m+1,\Delta-2}$ denote the leaves adjacent to $u_{m+1}$ in $P^+[K_{1,\Delta-2},l+m+1]$. The graph $G_{\Delta}(l,m)$ from the conjecture above is then a multiple coalescence

$$G_{\Delta}(l,m) \cong G^*(r = u_{m+1}, s_1 = t_{m+1,1}, \ldots, s_{\Delta-2} = t_{m+1,\Delta-2}) H_{\Delta}(m+1+l),$$

for which the application of Lemmas 5 and 8 yields the weak inequality in (29).

The combination of Lemmas 5 and 9 yield the following lemmas on multiple coalescence with rooted products of a star by another graph.

**Lemma 17.** For $n \geq 2$, let $c$ be the center and $l$ an arbitrary leaf of the star $S_n$. Let $G$ be a rooted graph and let $H$ be a connected graph. For a vertex $u$ of $H$, suppose that $H$ contains a rooted subgraph $G'$, with $u$ as its root, that is isomorphic to the rooted graph $G$.

Let $H^L$ be the multiple coalescence of $H$ and $S_n[G,n]$, obtained by identifying the rooted subgraph $G'$ with a copy of $G$ rooted at $l$ in $S_n[G,n]$, and let $H^c$ be the multiple coalescence of $H$ and $S_n[G,n]$, obtained by identifying the rooted subgraph $G'$ with a copy of $G$ rooted at $c$ in $S_n[G,n]$. Then

$$\lambda_1(H^c) \geq \lambda_1(H^L).$$

**Lemma 18.** For $n \geq 2$, let $c$ be the center and $l$ an arbitrary leaf of the star $S_n$. Let $G$ be a rooted graph with the root $r$, and let $r_c$ and $r_l$ denote the roots of
copies of $G$ rooted at $c$ and $l$, respectively, in the rooted product $S_n[G, n]$. Let $H$ be a connected graph and $u$ an arbitrary vertex of $H$. Then

$$
\lambda_1(H(u = r_c)S_n[G, n]) \geq \lambda_1(H(u = r_l)S_n[G, n]).
$$

Lemmas 14 and 18 enable us to solve the Brualdi-Solheid problem for the classes of graphs consisting of rooted products with the same rooted graph $G$.

**Theorem 19.** Let $G$ be an arbitrary rooted graph. If $T$ is a tree on $n$ vertices, then

$$
\lambda_1(P_n[G, n]) \leq \lambda_1(T[G, n]) \leq \lambda_1(S_n[G, n]).
$$

**Proof.** If $T$ is not the path $P_n$, then let $u$ be a vertex of $T$ with $\deg(u) \geq 3$ and the largest eccentricity (= the maximum distance from $u$ to any other vertex of $T$). The vertex $u$ cannot lie on a path between any two vertices of degrees at least three, as then one of them would have eccentricity larger than $u$. This shows all other vertices of $T$ with degree at least three belong to only one of the $\deg(u)$ subtrees of $T - u$. Consequently, the remaining $\deg(u) - 1 \geq 2$ subtrees of $T - u$ represent pendant paths of $T$ attached at $u$. Let $P'$ and $P''$ be two such pendant paths of lengths $p$ and $q$, respectively, and let $T'$ be the tree obtained by deleting the vertices of these paths (other than $u$) from $T$. Let $v_1, \ldots, v_{q+1}$ denote the first $q + 1$ vertices of the path $P_{p+q+1}$ of length $p + q$, counting from one of the endpoints. Tree $T'$ can then be represented as a multiple coalescence

$$
T \cong T'(u = v_{q+1})P_{p+q+1},
$$

and from Lemma 14 we then obtain that

$$
\lambda_1(T'[G, n]) = \lambda_1(T'(u = v_{q+1})P_{p+q+1}[G, n]) \geq \lambda_1(T'(u = v_q)P_{p+q+1}[G, n]) \geq \lambda_1(T'(u = v_1)P_{p+q+1}[G, n]).
$$

The degree of $u$ in tree $T'$ is $\deg(u) = 2$, and the largest eccentricity is $\deg(u) - 1 = 1$. Repeating the above procedure as long as the tree contains vertices of degree at least three, we eventually obtain that $\lambda_1(T'[G, n]) \geq \lambda_1(P_n[G, n])$.

With respect to the right-hand side inequality in (30), let $u$ be a vertex of $T$ with $d = \deg(u) \geq 2$ and the largest eccentricity. Let $v_1, \ldots, v_d$ be the neighbors of $u$ in $T$. The vertex $u$ cannot lie on a path between any two other vertices of degree at least two, as one of them would then have eccentricity larger than $u$. If $T$ is not the star $S_n$, then exactly one neighbor of $u$, say $v_1$, has degree at least two, while the remaining neighbors $v_2, \ldots, v_d$ all have degree one. Let

$$
T' = T - uv_2 - \cdots - uv_d + v_1v_2 + \cdots + v_1v_d.
$$

Further, let $T'$ be the tree obtained from $T$ by deleting vertices $u$, $v_2, \ldots, v_d$. If $c$ and $l$ are the center and an arbitrary leaf of the star $S_{d+1}$, then both $T$ and $T'$ can be represented as multiple coalescences:

$$
T \cong T'(v_1 = l)S_{d+1},
$$

$$
T' \cong T'(v_1 = c)S_{d+1}.
$$
From Lemma 18 we then obtain that
\[ \lambda_1(T^*[G,n]) = \lambda_1(T^* - (v_1 = l))S_{d+1}[G,n] \]
\[ \leq \lambda_1(T^* - (v_1 = c))S_{d+1}[G,n] = \lambda_1(T'[G,n]). \]
The degree of \( u \) in \( T' \) is, however, equal to one. Repeating the above procedure as long as the tree contains at least two vertices of degree at least two, we eventually obtain that \( \lambda_1(T[G,n]) \leq \lambda_1(S_n[G,n]). \)

**Theorem 20.** Let \( G \) be an arbitrary rooted graph. If \( H \) is a connected graph on \( n \) vertices, then
\[ \lambda_1(P_n[G,n]) \leq \lambda_1(H[G,n]) < \lambda_1(K_n[G,n]), \]
where \( K_n \) denotes the complete graph on \( n \) vertices.

**Proof.** From the fact that \( K_n[G,n] \) contains \( H[G,n] \) as a proper subgraph for any \( H \neq K_n \), we immediately see that \( \lambda_1(H[G,n]) < \lambda_1(K_n[G,n]) \), as the spectral radius of a connected graph strictly increases with the addition of edges (see item a) on page 142). From the same reason, if \( T \) is an arbitrary spanning tree of \( H \), then \( \lambda_1(T[G,n]) \leq \lambda_1(H[G,n]) \). From the previous theorem, we then have \( \lambda_1(P_n[G,n]) \leq \lambda_1(T[G,n]) \leq \lambda_1(H[G,n]) \).

**5. Conclusion**

We have developed a new method for comparing spectral radii of adjacency matrices of graphs, that applies to graphs that can be represented as multiple coalescences of the same basis graph with different smaller subgraphs. The method, based on Lemma 5, works by comparing walk counts in the smaller subgraphs in order to imply inequality between spectral radii for the whole graphs. We have further developed a number of walk count lemmas for cases when smaller subgraphs are rooted products of paths or stars by another graph. Most of the results in this manuscript are named lemmas, as we expect them to become useful ingredients in the proofs of further results. Examples of such results here include the proof of weak inequality in the 2009 conjecture of Belardo, Li Marzi and Simić [1], and the solution of the Brualdi-Solheid problem for the classes of graphs consisting of rooted products with the same rooted graph.

**References**

Pauline van den Driessche

Sign pattern matrices
Aims of my lectures

To describe some spectral properties of matrices with a given sign pattern from the perspective of combinatorial matrix theory showing some results, techniques, applications and open problems

Some topics will be chosen from the literature on sign patterns, some of these and other topics can be found in the book by Brualdi and Shader, in the chapter by Hall and Li (from the Handbook ed. L. Hogben), and references therein.

Techniques involve analysis, combinatorics, directed graphs (digraphs), matrix theory, numerical examples, ...

Sign patterns arise naturally in economics, population biology, chemistry, sociology, ...and applications are to systems of differential equations arising in different areas
An $n \times n$ sign pattern (matrix) $S = [s_{ij}]$: a matrix with $s_{ij} \in \{+, -, 0\}$.

Associated sign pattern class:

$$Q(S) = \{ A = [a_{ij}] \in \mathbb{R}^{n \times n} : \text{sign } a_{ij} = s_{ij} \text{ for all } i, j \}$$

If matrix $A \in Q(S)$ then $A$ is a (matrix) realization of $S$.

Example

$$S = \begin{bmatrix} - & + \\ + & - \end{bmatrix} \quad A = \begin{bmatrix} -1 & \pi \\ 0.5 & -3 \end{bmatrix} \in Q(S)$$

Require, allow

For a given property $\mathcal{P}$, a sign pattern $S$

- requires $\mathcal{P}$ if every matrix $A \in Q(S)$ has property $\mathcal{P}$
- allows $\mathcal{P}$ if there exists at least one matrix $A \in Q(S)$ that has property $\mathcal{P}$

Note: $S$ requires $\mathcal{P}$ implies that $S$ allows $\mathcal{P}$

Example

$$S = \begin{bmatrix} - & + \\ + & - \end{bmatrix}$$ requires a negative trace

allows (but does not require) a positive determinant
Signed digraph

The signed digraph $D(S)$ of an $n \times n$ sign pattern $S$:
vertex set $\{1, \ldots, n\}$ and a positive (negative) arc
from $i$ to $j$ if and only if $s_{ij}$ is positive (negative)

A (simple, directed) cycle of length $k$ (a $k$-cycle):
a sequence of $k$ arcs $(i_1, i_2), \ldots, (i_k, i_1)$ such that the
vertices $i_1, \ldots, i_k$ are distinct

A cycle is positive (negative) if there is an even (odd) number of
negative arcs on the cycle

Stability

Matrix $A$ is (negative) stable if each of its eigenvalues has
negative real part

Sign pattern $S$ is potentially stable (PS) if there exists a
stable matrix $A \in Q(S)$, i.e. $S$ allows stability

Sign pattern $S$ is sign stable if every $A \in Q(S)$ is a
stable matrix, i.e. $S$ requires stability
Conditions for potential or sign stability of $S$ are often given in terms of the signed digraph $D(S)$
Of particular importance are tree sign patterns:

$S$ is a **tree sign pattern** if $D(S)$ is strongly connected and has no $k$-cycles for $k \geq 3$
i.e. has 2-cycles and 1-cycles (loops)

Examples are path sign patterns, star sign patterns
An $n \times n$ **star sign pattern** has 1 centre vertex with degree $n - 1$
connected to $n - 1$ leaf vertices

---

### Example

$S = \begin{bmatrix} - & + & 0 \\ + & - & + \\ 0 & - & 0 \end{bmatrix}$

is a potentially stable tree (path, star) sign pattern since

$A = \begin{bmatrix} -1 & 1 & 0 \\ 2 & -2 & 1 \\ 0 & -2 & 0 \end{bmatrix} \in Q(S)$

has eigenvalues approx $-2.52, -0.24 \pm 0.86i$

Not sign stable as changing the (2,2) entry of $A$ to $-1$ gives eigenvalues of the resulting matrix as $-2, \pm i$

Changing the (1,1) entry of $S$ to $+$, the resulting sign pattern requires a positive determinant and so is not PS
A little history

Samuelson (1947) considered qualitative problems in economics involving sign patterns

Maybee and Quirk (1969) studied these from a matrix/digraph point of view and wrote:
"Specification of necessary and sufficient conditions for potential stability remains an unsolved problem"
Apart from a few special cases, this remains true today

By contrast, sign stability was characterized by Jeffries, Klee, vD (1977) and an algorithm given to test whether or not a sign pattern is sign stable

Since the 1970s researchers have derived many results about sign patterns and applied some to dynamical systems, e.g. economics, food webs

Stability of a dynamical system

Assume a dynamical system is at an equilibrium $x^* \in \mathbb{R}^n$
Considering small perturbations and linearizing about $x^*$ the time evolution is governed by

$$\frac{dx(t)}{dt} = Ax(t)$$

for some $n \times n$ community matrix $A$

Solutions are of the form $x(t) = e^{At}x_0$
and if $A$ is a stable matrix then perturbations die out and $x^*$ is an asymptotically stable equilibrium

But often the magnitudes of entries in $A$ are unknown whereas the signs are known (for example in a grass-rabbit-fox system: rabbits eat grass, foxes eat rabbits) so $A$ should be regarded as a sign pattern $S$
Community matrix has the sign pattern $S$

$$S = \begin{bmatrix} 0 & - & 0 \\ + & 0 & - \\ 0 & + & - \end{bmatrix}$$

Question: Is the equilibrium potentially stable?

Answer: Yes, it is in fact sign stable
Jeffries’ 5 × 5 example

Example

\[ S = \begin{bmatrix}
0 & + & 0 & 0 & 0 \\
- & 0 & + & 0 & 0 \\
0 & - & - & + & 0 \\
0 & 0 & - & 0 & + \\
0 & 0 & 0 & - & 0
\end{bmatrix} \]

is a tree (path) sign pattern and satisfies the first 3 conditions for sign stability, so is sign semi-stable, i.e. all eigenvalues have nonpositive real parts.

\( S \) requires a nonzero determinant (from \( s_{12} s_{21} s_{33} s_{45} s_{54} \)).

However, \( S \) fails the last condition: take \( \beta = \{1, 2, 4, 5\} \) each row of \( S[\beta] \) contains a nonzero entry, \( S[\beta|^c\beta] = S[1, 2, 4, 5|3] \) has one + in row 2.

If each ± is ±1 then \( A \in Q(S) \) has eigenvalues ±i.

Basic facts for potential stability

- PS is preserved under transposition, permutation similarity, signature similarity (note: not negation).
  Two sign patterns are equivalent if one is obtained from the other by any combination of these operations. So PS sign patterns are given up to equivalence.
- If \( S \) is PS then by continuity any superpattern is PS (a superpattern is obtained from \( S \) by replacing some 0 by + or −, a pattern is a superpattern of itself).
- \( S \) is minimally potentially stable if it is irreducible, PS and replacing any + or − by 0 gives a sign pattern that is not PS.
  Thus usually minimal PS patterns are considered.
Direct sum $S_1 \oplus S_2$ is PS if and only if $S_1$ and $S_2$ are PS

So we need only consider irreducible PS sign patterns

**Theorem**

If an $n \times n$ sign pattern $S$ is potentially stable, then there exists $A \in Q(S)$ such that the sum of the $k \times k$ principal minors is $(-1)^k$ for $k = 1, 2, \ldots, n$

This result comes from considering the characteristic polynomial of a stable matrix $A$

In particular at least one $s_{ii}$ must be negative

---

**Known results on potential stability for small orders**

- Johnson and Summers (1989) compiled a list of all PS tree sign patterns (up to equivalence) of orders $n = 2, 3, 4$

- For $n = 4$: Johnson, Maybee, Olesky, vdD (1997) gave one more and Pang found three more minimally PS path sign patterns (see Lin, Olesky, vdD (2002))

- For $n = 3$: Miyamichi (1988) lists all minimally PS sign patterns (and gives some constructions for general $n$)

There are five such sign patterns, two of which are trees

Minimally PS tree sign patterns (paths)

Minimally PS sign patterns with a 3-cycle
Let $\det B[\{1,\ldots,k\}]$ denote the minor of $B$ on rows and columns $1,\ldots,k$.

Sign pattern $S$ allows a nested sequence of properly signed principal minors if there exists a matrix $A \in Q(S)$ and a permutation matrix $P$ such that $B = PAP^T$ has

$$\text{sign } \det B[\{1,\ldots,k\}] = (-1)^k \text{ for } k = 1,\ldots,n$$

**Sufficient condition for potential stability**

Johnson, Maybee, Olesky, vdD (1997)

**Theorem**

*If $S$ is an $n \times n$ sign pattern that allows a nested sequence of properly signed principal minors, then $S$ is potentially stable.*

The proof uses a result due to Fisher and Fuller (1958) and Ballantine (1970) stating that if an $n \times n$ matrix $A$ has a nested sequence of properly signed principal minors, then $\exists$ a positive diagonal matrix $D$ such that $DA$ is stable.

Converse of the above theorem is false for $n = 3$ and even false for tree sign patterns with $n = 4$. 
For \( n = 3 \) the PS sign pattern associated with this signed digraph does not have a nested sequence of properly signed principal minors.

\[
\begin{pmatrix}
- & + & 0 \\
0 & 0 & + \\
+ & - & 0 \\
\end{pmatrix}
\]

Careful with nested sequences!

Following is due to [JMOv] (1997)

**Example**

Consider

\[
S = \begin{bmatrix}
- & + & 0 \\
- & + & + \\
0 & + & + \\
\end{bmatrix}
\]

For \( A \in Q(S) \), the conditions

\[ det A[1] < 0, \ det A[12] > 0 \text{ and } det A < 0 \]

are not simultaneously realizable; in fact \( S \) is not PS.
Necessary and sufficient conditions for PS for special classes

[JMOv] gave the following result for a restricted class of tree sign patterns

**Theorem**

Let \( S \) be a tree sign pattern with exactly one nonzero \( s_{ii} \) (which is \(-\)). Then \( S \) is potentially stable if and only if \( S \) allows a nested sequence of properly signed principal minors.

Gao and Li (2001) characterized all \( n \times n \) potentially stable star sign patterns in terms of the number of positive loops at the leaf vertices.

**Surprising example**

Potentially stable \( S \) must have a negative diagonal entry
Any \( S \) with all \( s_{ii} < 0 \) is potentially stable
However positive feedback may promote stability

**Example**

Bone (1983)

\[
S = \begin{bmatrix}
- & + & + & 0 \\
- & 0 & 0 & \\
+ & 0 & 0 & + \\
0 & + & 0 & 0
\end{bmatrix}
\]

is potentially stable if \( s_{22} \) is + but not PS if \( s_{22} \) is – or 0

Proof uses the Routh-Hurwitz conditions.
A construction involving cycles by Miyamichi (1988)

Start with a PS sign pattern:

Relabel vertex 2 as $n - 1$, vertex 3 as $n$; replace the 2-cycle on vertices 1, 2 by an $(n - 1)$-cycle; put negative loops on vertices $2, \ldots, n - 2$. Resulting sign pattern is PS

Resulting sign pattern is PS

- $(n - 1)$-cycle $C_{n-1}$ is negative:
  a nested sequence of properly signed principal minors implies PS

- $(n - 1)$-cycle $C_{n-1}$ is positive:
  characteristic polynomial is
  
  $$(z^2 - C_2)(z - a_{11}) \cdots (z - a_{n-2,n-2}) - C_{n-1}z$$

  Use a result in Gantmacher: a polynomial
  
  $$f(z) = h(z^2) + zg(z^2)$$

  with positive coefficients is stable iff the zeros $\alpha_1, \alpha_2, \ldots$ of $h(u)$ and the zeros $\beta_1, \beta_2, \ldots$ of $g(u)$ are all negative and satisfy $0 > \alpha_1 > \beta_1 > \alpha_2 > \beta_2 > \cdots$

  The magnitudes of $C_2, C_{n-1}$ can be chosen to obtain stability
Kim et al (2009) gave a method to take a stable matrix and produce a higher order stable matrix (and thus a PS sign pattern).

A special case of this is now stated.

**Theorem**

Let $A$ be an $n \times n$ stable matrix, $u$ and $x$ be $n$ vectors so that $x^T u = k$ a positive scalar. Then the $(n+1) \times (n+1)$ matrix $B$ given by

$$B = \begin{bmatrix} I_n & 0 \\ x^T & 1 \end{bmatrix} \begin{bmatrix} A & u \\ 0 & -k \end{bmatrix} \begin{bmatrix} I_n & 0 \\ -x^T & 1 \end{bmatrix} = \begin{bmatrix} A - ux^T & u \\ x^T A & 0 \end{bmatrix}$$

is stable with spectrum $\sigma(B) = \sigma(A) \cup \{-k\}$.

**Example**

$$A = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ -1 & -3 & -3 \end{bmatrix}$$

is a stable matrix giving a minimally PS sign pattern.

Applying the theorem with $u = [0, 0, 1]^T$, $x = [3, -3, 1]^T$, $x^T u = k = 1$ gives

$$B = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ -4 & 0 & -4 & 1 \\ -1 & 0 & -6 & 0 \end{bmatrix}$$

$\sigma(B) = \sigma(A) \cup \{-k\}$, thus $B$ gives a minimally PS sign pattern of order 4 (with no nested sequence of properly signed principal minors).
Grundy, Olesky, vdD (2012) proved that an $n \times n$ irreducible sign pattern with a properly signed nest (so is PS) has at least $2n - 1$ nonzero entries.

But there are examples of PS sign patterns with fewer than this number of nonzero entries.

**Example**

Matrix $A$ gives a PS sign pattern with $6 = 2n - 2$ nonzero entries.

Note that this pattern does not allow a nested sequence of properly signed principal minors.
Grundy, Olesky, vdD (2012) studied the minimum number of nonzero entries in an irreducible minimally PS sign pattern for small orders

- $n = 2$ PS sign pattern allows a properly signed nest so 3 nonzeros
- $n = 3$ PS sign pattern has at least 5 nonzeros (from the list)
- $n = 4$ PS sign pattern has at least $2n - 2 = 6$ nonzeros
- $n = 5$ PS sign pattern has at least $2n - 2 = 8$ nonzeros
- $n = 6$ PS sign pattern has at least $2n - 3 = 9$ nonzeros

Proof for $n = 4$:
- $\mathcal{S}$ has at least one negative diagonal entry
- Since $\mathcal{S}$ is irreducible it must have at least 4 nonzero off-diagonal entries
- If $\mathcal{S}$ has at least 5 then the result holds (6 nonzeros)
- Otherwise if $\mathcal{S}$ has only 4 then $D(\mathcal{S})$ contains a cycle of length 4
- But in order for $\mathcal{S}$ to have a positive principal minor of order 2 there must be at least one more nonzero entry, giving $1 + 4 + 1 = 6$ arcs
Grundy et al. also gave examples of irreducible PS sign patterns:

- $n = 7$ with $2n - 3 = 11$ nonzeros
- $n = 8$ with $2n - 3 = 13$ nonzeros
- $n = 9$ with $2n - 4 = 14$ nonzeros

but it is not known whether there exist any with fewer than these numbers of nonzeros

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**Open problems related to potential stability**

- Give necessary and sufficient conditions for a sign pattern to be minimally potentially stable
  - Currently this is open even for tree sign patterns of order 5 and general sign patterns of order 4
- Give easily verifiable conditions to show that a sign pattern is not potentially stable
  - This would be useful in the context of differential equations
- Find an easy way to determine if a sign pattern allows or requires a properly signed nest
- Find the minimum number of nonzero entries in an irreducible potentially stable sign pattern for $n \geq 7$
References


Y. Gao and J. Li, On the potential stability of star sign pattern matrices, Linear Algebra Appl. 327


Some definitions relating to spectra: Inertia

The \textit{inertia} of a real $n \times n$ matrix $A$:

\text{triple of nonnegative integers summing to $n$}

\[ i(A) = (i_+(A), i_-(A), i_0(A)) \]

in which $i_+(A), i_-(A), i_0(A)$ is the number of eigenvalues of $A$
with positive, negative, zero real parts (counting multiplicities),
resp., so $i_+(A) + i_-(A) + i_0(A) = n$

The \textit{inertia of a sign pattern} $S$ is $i(S) = \{ i(A) : A \in Q(S) \}$

**Example**

\[ S = \begin{bmatrix} - & 0 \\ + & - \end{bmatrix} \]

is a reducible sign pattern with $i(S) = (0, 2, 0)$
Example

\[ S = \begin{bmatrix} - & + \\ + & - \end{bmatrix} \]

What is \(i(S)\)?

Take \(A = \begin{bmatrix} -a & b \\ c & -d \end{bmatrix} \in Q(S)\) with \(a, b, c, d > 0\)

The characteristic polynomial of \(A\) is

\[ z^2 + (a + d)z + ad - bc \]

\[ i(A) = (0, 2, 0) \text{ if } ad > bc \]
\[ i(A) = (0, 1, 1) \text{ if } ad = bc \]
\[ i(A) = (1, 1, 0) \text{ if } ad < bc \]

\(i(S) = \{(0, 2, 0), (0, 1, 1), (1, 1, 0)\}\)

Inertially arbitrary

An \(n \times n\) inertially arbitrary pattern (IAP) \(S\) :

\( (n_1, n_2, n_3) \in i(S) \) for all nonnegative integers \(n_i\) satisfying \(\sum_{i=1}^{3} n_i = n\)

- \(S\) allows all \((n + 1)(n + 2)/2\) possible inertias
  - e.g., if \(n = 2\) there are 6 possible inertias
  - \(n = 3\) there are 10

\(\hat{S}\) is a superpattern of \(S\) (and \(S\) is a subpattern of \(\hat{S}\)) if \(\hat{s}_{ij} = s_{ij}\)
  whenever \(s_{ij} \neq 0\)

minimal IAP:

no proper subpattern of \(S\) is an IAP
\( n \times n \) **spectrally arbitrary pattern** (SAP) \( S \) :
- any self-conjugate multiset of complex numbers is the spectrum of some \( A \in Q(S) \)
- for each real monic polynomial \( r(z) \) with degree \( n \), there exists \( A \in Q(S) \) with characteristic polynomial \( = r(z) \)
- \( S \) allows all possible spectra of a real matrix
  (if \( \alpha + i\beta \) with \( \beta \neq 0 \) is an eigenvalue then \( \alpha - i\beta \) is also an eigenvalue)

If \( S \) is a SAP then \( S \) is an IAP (converse false for \( n \geq 4 \))

**minimal SAP** :
- no proper subpattern of \( S \) is a SAP

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\( \text{Potentially nilpotent} \)

**potentially nilpotent** (PN) pattern \( S \) :
- there exists \( A \in Q(S) \) so that \( A \) is nilpotent
  i.e., \( A^q = 0 \) for some \( q > 0 \), \( A \) has all zero eigenvalues

matrix \( A \) is **nilpotent of index** \( q \) if \( A^q = 0 \) and \( q \) is the smallest such positive integer.

If \( S \) is a SAP, then \( S \) is potentially nilpotent, but it is not in general true that an IAP is potentially nilpotent

Smallest example of an IAP not PN is the \( 5 \times 5 \) sign pattern \( G_5 \) given in Kim, Olesky, vdD (2007), see also Cavers, Garnett, Kim, Olesky, vdD (2013)
Equivalence

IAPs, SAPs and PN patterns are preserved under

- negation
- transposition
- permutation similarity
- signature similarity

Two sign patterns are equivalent if one can be obtained from the other by any combination of these four operations.

Two examples

Example

\[ S = \begin{bmatrix} - & + \\ + & - \end{bmatrix} \]

is not an IAP or SAP since \((2, 0, 0) \notin i(S)\)

\(S\) is not PN as \(S\) requires a negative trace

Example

Let \( \mathcal{T}_2 = \begin{bmatrix} - & + \\ - & + \end{bmatrix} \)

It can be shown directly that any monic quadratic polynomial can be achieved as the characteristic polynomial of a matrix in \( Q(\mathcal{T}_2) \)

\( \mathcal{T}_2 \) is a minimal SAP and, up to equivalence, \( \mathcal{T}_2 \) is the unique \( 2 \times 2 \) SAP, is a minimal IAP and is PN
Spectrally arbitrary sign patterns

An obvious necessary condition for a SAP

**Theorem**

*If* $S$ *is an* $n \times n$ *SAP, then* $S$ *allows a positive and a negative principal minor of each order* $k$, *for* $1 \leq k \leq n$.

Drew, Johnson, Olesky, vdD (2000) introduced SAPs and

$$T_n = \begin{bmatrix}
- & + & 0 \\
- & 0 & + \\
- & \cdot & \cdot & \cdot \\
\cdot & \cdot & 0 & + \\
0 & - & +
\end{bmatrix}$$

They developed the Nilpotent-Jacobian method for proving that a sign pattern is a SAP, used it to show that $T_n$ is a minimal SAP for small values of $n$ and conjectured true for all $n$.

**Nilpotent-Jacobian method**

Method for proving that an $n \times n$ pattern is a SAP (Drew et al. (2000)): its proof uses the Implicit Function Theorem

**Theorem**

*(Nilpotent-Jacobian Method) Let* $S$ *be an* $n \times n$ *sign pattern, and suppose that there exists some nilpotent matrix* $A \in Q(S)$ *with at least* $n$ *nonzero entries, say* $a_{i_1j_1}, \ldots, a_{i_nj_n}$. *Let* $X$ *be the real matrix obtained by replacing these entries in* $A$ *by variables* $x_1, \ldots, x_n$ *and let the characteristic polynomial of* $X$ *be given by

$$p(z) = z^n - p_1 z^{n-1} + p_2 z^{n-2} - \cdots + (-1)^{n-1} p_{n-1} z + (-1)^{n} p_n,$$

*where* $p_i = p_i(x_1, \ldots, x_n)$ *is differentiable in each* $x_j$. *If the* $n \times n$ *Jacobian matrix with* $(i,j)$ *entry equal to* $\frac{\partial p_i}{\partial x_j}$ *is nonsingular at* $(x_1, \ldots, x_n) = (a_{i_1j_1}, \ldots, a_{i_nj_n})$, *then every superpattern of* $S$ *(including* $S$ *itself) is spectrally arbitrary.*
Nilpotent-Jacobian method for $T_3$

$$T_3 = \begin{bmatrix} - & + & 0 \\ - & 0 & + \\ 0 & - & + \end{bmatrix}$$

is PN e.g. $A = \begin{bmatrix} -1 & 1 & 0 \\ -1/2 & 0 & 1 \\ 0 & -1/2 & 1 \end{bmatrix}$ is nilpotent

Let $X = \begin{bmatrix} -1 & 1 & 0 \\ -x_1 & 0 & 1 \\ 0 & -x_2 & x_3 \end{bmatrix}$

The characteristic polynomial of $X$ is

$$z^3 + (1 - x_3)z^2 + (x_1 + x_2 - x_3)z + x_2 - x_1 x_3$$

Jacobian matrix $J = \begin{bmatrix} 0 & 0 & -1 \\ 1 & 1 & -1 \\ -x_3 & 1 & -x_1 \end{bmatrix}$

has determinant $-1(1 + x_3) = -2$ at $x_3 = 1$, so $J$ is nonsingular

By the Nilpotent-Jacobian method $T_3$ is a SAP

$T_n$ is a minimal SAP for all $n$

- Drew et al. (2000) used the Nilpotent-Jacobian method to prove that $T_n$ is a SAP for $n = 2, \ldots, 7$
- Elsner, Olesky, vD (2003) used this method with Maple to extend to $n = 16$
- Garnett and Shader (2012) proved $T_n$ is a SAP for all $n$

They used the nilpotent matrices given in Behn, Driessel, Hentzel, Vander Velden, Wilson (2011) and a way of establishing the nonsingularity of $J$ by their Nilpotent-Centralizer method that relies on a centralizer of the nilpotent matrix realization
Behn et al. (2011) Nilpotent matrix

\[ F_n = \begin{bmatrix}
-f_1 & f_1 & 0 \\
-f_2 & 0 & f_2 \\
& -f_3 & \ddots & \ddots \\
& & \ddots & 0 & f_{n-1} \\
0 & & & -f_n & f_n
\end{bmatrix} \]

with \( f_k = 0.5 \csc \left( \frac{(2k-1)\pi}{2n} \right) \) is a nilpotent matrix in \( Q(I_n) \) for \( n \geq 2 \).

They proved this using Chebyshev polynomials.

Garnett and Shader noted that \( F_n \) is similar to a matrix in a special form.

Since \( F_n \) is a tridiagonal matrix, for \( j = 1, \ldots, n-1 \) the \((j, j+1)\) and \((j+1, j)\) entries always appear as a product in its characteristic polynomial, so can be replaced by \( \sqrt{f_j f_{j+1}} \) and \(-\sqrt{f_j f_{j+1}}\), resp.

This new matrix \( \tilde{F}_n \) is diagonally similar to \( F_n \) and was used by Garnett and Shader as the nilpotent realization of \( I_n \).

Since \( \csc(\theta) = \csc(\pi - \theta) \), the entries in \( \tilde{F}_n \) have \( \tilde{f}_1 = -\tilde{f}_n \) and \( \tilde{f}_{j, j+1} = \tilde{f}_{n-j, n+1-j} \).
Granett and Shader (2013) used their Nilpotent-Centralizer
method to prove that \( T_n \) and all its superpatterns are SAPs
B is in the centralizer of A if \( AB = BA \)

**Theorem**

(\textit{Nilpotent-Centralizer Method}) Let \( S \) be an \( n \times n \) sign pattern
and \( A \in O(S) \) be nilpotent of index \( n \). If the only matrix \( B \) in the
centralizer of \( A \) satisfying the Hadamard product \( B \circ A^T = 0 \) is
the zero matrix then every superpattern of \( S \) is a SAP

**Minimal SAPs**

Chronologically the first \( n \times n \) families of minimal SAPs were
given by Britz, McDonald, Olesky, vD (2004). For example the
Hessenberg sign pattern \( \mathcal{H}_n \) is a SAP

\[
\mathcal{H}_n = \begin{bmatrix}
+ & - & - & 0 \\
+ & - & - & - \\
\vdots & \ddots & \ddots & \ddots \\
+ & 0 & - & - \\
+ & - & - & - \\
\end{bmatrix}
\]

They showed explicitly that the characteristic polynomial can be
any arbitrary polynomial of degree \( n \)
Considering all possible cases for $3 \times 3$ sign patterns, Cavers, Vander Meulen (2005) proved the following result.

**Theorem**

If $S$ is a $3 \times 3$ sign pattern, then the following are equivalent:

1. $S$ is a SAP
2. $S$ is an IAP
3. Up to equivalence, $S$ is a superpattern of one of

$$
\begin{bmatrix}
- & + & 0 \\
0 & - & + \\
0 & 0 & -
\end{bmatrix},
\begin{bmatrix}
+ & - & + \\
+ & 0 & - \\
+ & 0 & -
\end{bmatrix},
\begin{bmatrix}
+ & 0 & - \\
0 & + & - \\
0 & 0 & -
\end{bmatrix},
\begin{bmatrix}
+ & 0 & - \\
+ & 0 & - \\
+ & 0 & -
\end{bmatrix}
$$

Note that the first sign pattern is $T_3$
the second is also a *tree sign pattern*
i.e. $D(S)$ is irreducible and has cycles of length only 1 and 2.

**Number of nonzero entries**

Britz et al. (2004) proved a theorem and stated a conjecture.

**Theorem**

An $n \times n$ irreducible SAP has at least $2n - 1$ nonzero entries.

Proof: $n - 1$ entries of a sign pattern can be set to $\pm 1$ using diagonal similarity, and at least $n$ algebraically independent variables are needed in order to allow any monic characteristic polynomial of order $n$.

**Conjecture**

For $n \geq 2$ an $n \times n$ irreducible sign pattern that is spectrally arbitrary has at least $2n$ nonzero entries.

$2n$–conjecture is true for $n = 2$ ($T_2$), $n = 3$ (Cavers, Vander Meulen), $n = 4$ (Corpuz, McDonald), $n = 5$ (DeAlba et al), and for all tree sign patterns.
Pereira's result

Pereira (2007) showed the relevance of potentially nilpotent sign patterns to the study of SAPs

A full sign pattern $\mathcal{S}$ has all $s_{ij}$ nonzero

**Theorem**

*Any potentially nilpotent full sign pattern is a SAP*

The proof uses a perturbation of the Jordan normal form of a nilpotent $n \times n$ matrix $N$ of index $n$ with a given full sign pattern, combined with a companion matrix argument.

Garnett and Shader (2013) used their Nilpotent-Centralizer method to give another proof that a full sign pattern is a SAP if and only if it is PN, since for a full sign pattern, the only matrix $B$ that satisfies $B \circ N^T = 0$ is the zero matrix.

Potential stability and SAPs

$\mathcal{S}$ is potentially stable if there exists matrix $A \in Q(\mathcal{S})$ so that $A$ is stable, i.e. all eigenvalues of $A$ have negative real parts.

- MacGillivray, Tiefenbach, vdD (2005) considered $n \times n$ star sign patterns (i.e. tree sign patterns with one centre vertex of degree $n-1$ connected to $n-1$ leaf vertices), and proved that if $\mathcal{S}$ is a star sign pattern that is potentially nilpotent and potentially stable, then $\mathcal{S}$ is a SAP.

- By determining which of the $4 \times 4$ potentially stable path sign patterns (tridiagonal) are SAPs, Arav, Hall, Li, Kaphle, Manzagol (2010) showed that if $\mathcal{S}$ is a $4 \times 4$ tree sign pattern that is potentially nilpotent and potentially stable, then $\mathcal{S}$ is a SAP.
DeAlba et al. [2007] noted that the direct sum of sign patterns of which at least two are of odd order is not a SAP (since the pattern requires at least two real eigenvalues)

They also gave the following example:

**Example**

The pattern

\[ M_4 = \begin{bmatrix} + & + & - & 0 \\ - & - & + & 0 \\ 0 & 0 & 0 & - \\ + & + & 0 & 0 \end{bmatrix} \]

is not a SAP, but \( M_4 \oplus T_2 \) is a SAP

They showed that \( M_4 \) is not a SAP by finding exactly which real monic polynomials of degree 4 can be realized by a matrix in \( Q(M_4) \) and showing there are some such polynomials that cannot be realized

They showed that \( M_4 \oplus T_2 \) is a SAP by writing a given monic polynomial \( p(z) \) of degree 6 in quadratic and linear factors and finding a subset of the factors that can be realized as the characteristic polynomial of \( A_1 \in Q(M_4) \)

Since \( T_2 \) is a SAP there is a matrix \( A_2 \in Q(T_2) \) having the product of the remaining factor(s) as its characteristic polynomial

Thus \( A_1 \oplus A_2 \in Q(M_4 \oplus T_2) \) has \( p(z) \) as its characteristic polynomial

Note that the same method of proof shows that \( M_4 \oplus \mathcal{S} \) is a SAP if \( \mathcal{S} \) is any SAP
Some open problems concerning SAPs

- Find new techniques for proving that a sign pattern is a SAP
  Current techniques require the knowledge of a nilpotent realization or explicit calculations with the characteristic polynomial
- Are there other families of sign patterns (besides star sign patterns and $4 \times 4$ tree sign patterns) for which potential nilpotency and potential stability imply that the family is spectrally arbitrary?
- Is it possible that $S_1 \oplus S_2$ is a SAP with neither $S_1$ nor $S_2$ a SAP?
- Prove (or disprove!) the $2n$ conjecture

Some additional results on PN Sign Patterns

- The study of potentially nilpotent sign patterns pre-dates the study of SAPs and IAPs; see Eschenbach and Johnson (1988)
- Eschenbach and Li (1999) characterized $3 \times 3$ patterns that allow nilpotence of index 2
- Gao et al (2007) characterized $3 \times 3$ patterns that allow nilpotence of index 3 and give constructions for $n \times n$ patterns that allow nilpotence of index 3
The minimum number of nonzeros in an irreducible $n \times n$ PN pattern is $n+1$ (Catral et al. 2009).

**Example**

$$S = \begin{bmatrix} 0 & + & 0 & + \\ 0 & 0 & + & 0 \\ + & 0 & 0 & 0 \\ 0 & 0 & - & 0 \end{bmatrix}$$

allows nilpotence of index 4, is irreducible and has 5 nonzeros.

MacGillivray et al. (2005) characterized PN star sign patterns.

Key result concerning PN patterns: result of Pereira (2007)

**Constructing full PN sign patterns and SAPs**

Kim et al. 2009

If $A \in \mathbb{R}^{n \times n}$, $U \in \mathbb{R}^{n \times k}$, $X \in \mathbb{R}^{k \times n}$, $K \in \mathbb{R}^{k \times k}$, then

$$B = \begin{bmatrix} A - UX & U \\ XA - UX - KX & XU + K \end{bmatrix}$$

is similar to $\begin{bmatrix} A & U \\ O & K \end{bmatrix}$, so $\sigma(B) = \sigma(A) \cup \sigma(K)$.

**Theorem**

Let $A, U$ be $n \times n$ full sign patterns, with nilpotent $A \in Q(A)$, $U \in Q(U)$, $K = O_k$, and let $X$ be s.t. $XA$, $XU$ have no zero entries. Then

$$B = \begin{bmatrix} A & U \\ S(XA) & S(XU) \end{bmatrix}$$

($S(XA)$ is the sign pattern of $XA$) is a full PN pattern, and thus is a SAP.
Some open problems concerning PN sign patterns

- Find techniques for identifying PN patterns
- Find techniques for constructing PN patterns: this would be useful in the study of SAPs
- Find necessary and/or sufficient conditions to allow nilpotence of index $\geq 4$

References


Inertia

Recall a definition:

The inertia of matrix $A \in \mathbb{R}^{n \times n}$ is the 3-tuple of nonnegative integers summing to $n$

$$i(A) = (n_+, n_-, n_0)$$

where (counting multiplicities):

$n_+$ is the number of eigenvalues with positive real part

$n_-$ is the number of eigenvalues with negative real part

$n_0$ is the number of zero eigenvalues
Motivated by classes of sign patterns relevant for dynamical systems, Kim et al. (2009) introduced the following definition:

The **refined inertia** of matrix $A \in \mathbb{R}^{n \times n}$ is the 4-tuple of nonnegative integers summing to $n$

$$ri(A) = (n_+, n_-, n_z, 2np)$$

where (counting multiplicities):

- $n_+$ is the number of eigenvalues with positive real part
- $n_-$ is the number of eigenvalues with negative real part
- $n_z$ is the number of zero eigenvalues
- $2np$ is the number of nonzero pure imaginary eigenvalues

Note that the inertia of $A$ is $(n_+, n_-, n_z + 2np)$

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**Refined inertia of a sign pattern**

The inertia of a sign pattern $S$ is $\{i(A) : A \in Q(S)\}$

The **refined inertia of a sign pattern** $S$ is $\{ri(A) : A \in Q(S)\}$

Assume that $S$ is an $n \times n$ sign pattern.
If $S$ allows refined inertia $(0, n, 0, 0)$ then $S$ is potentially stable.

If $S$ requires refined inertia $(0, n, 0, 0)$ then $S$ is sign stable.

If $n_z = 0$ i.e. det($A$) $\neq 0$ for all $A \in Q(S)$ then $S$ is sign nonsingular (SNS). So a SNS pattern has all realizations with determinant the same sign.

For $n \geq 2$ the maximum number of distinct inertias allowed by any $n \times n$ sign pattern is $(n+1)(n+2)/2$.

For $n \geq 2$ what is the maximum number of distinct refined inertias allowed by any $n \times n$ sign pattern?
Theorem

Deaett, Olesky, vdD (2010) The maximum number \( R(n) \) of distinct refined inertias allowed by an \( n \times n \) sign pattern with \( n \geq 2 \) is

- \( R(n) = \frac{(k+1)(k+2)(4k+3)}{6} \) for \( n = 2k \)
- \( R(n) = \frac{(k+1)(k+2)(4k+9)}{6} \) for \( n = 2k + 1 \)

Proof: Use induction starting with \( R(2) = 7 \), \( R(3) = 13 \) (easy!)

Suppose \( n \geq 4 \)

If \( n = 2k \) there are \((2k+1)(2k+2)/2\) possible refined inertias with \( n_p = 0 \) and \( R(2k-2) \) possible refined inertias with \( n_p > 0 \)

\( R(n) \) is the sum of these two numbers

If \( n = 2k + 1 \) a similar argument holds

Recall: Stability of a dynamical system

Assume a dynamical system is at a steady state \( x^* \in \mathbb{R}^n \)

Considering small perturbations and linearizing about \( x^* \)
the time evolution is governed by

\[
\frac{dx(t)}{dt} = Ax(t)
\]

for some \( n \times n \) Jacobian community matrix \( A \)

Solutions are of the form \( x(t) = e^{At}x_0 \)
and if \( ri(A) = (0, n, 0, 0, \ldots) \) then perturbations die out and \( x^* \) is a locally asymptotically stable steady state of the system

The magnitudes of entries in \( A \) may be unknown but the signs known (for example, a grass-rabbit-fox system: rabbits eat grass, foxes eat rabbits) so \( A \) should be regarded as a sign pattern \( S \).
Community matrix has the sign pattern $S$

$$S = \begin{bmatrix} 0 & - & 0 \\ + & 0 & - \\ 0 & + & - \end{bmatrix}$$

$ri(S) = (0, 3, 0, 0)$ so system is locally stable for all magnitudes.

Another community matrix $3 \times 3$ example

Example

$$S = \begin{bmatrix} - & + & 0 \\ + & - & + \\ 0 & - & 0 \end{bmatrix} \text{ with } A = \begin{bmatrix} -1 & 1 & 0 \\ 2 & -2 & 1 \\ 0 & -2 & 0 \end{bmatrix}$$

Sign pattern $S$ is PS as $A \in Q(S)$ has refined inertia $(0, 3, 0, 0)$

If the $(2, 2)$ entry is changed to $-1$ then the resulting matrix has refined inertia $(0, 1, 0, 2)$

If the $(2, 2)$ entry is further changed to $-0.5$ then the resulting matrix has refined inertia $(2, 1, 0, 0)$

A pair of eigenvalues can cross the imaginary axis, and the dynamical system with this linearized sign pattern $S$ can exhibit a Hopf bifurcation giving rise to periodic solutions.
We first investigate some properties of sign patterns that allow or require $H_n$.

Then we apply these to some examples from applications to detect whether or not Hopf bifurcation giving rise to periodic solutions may occur.

**Allow/require** $H_n$

Bodine, Deaett, McDonald, Olesky, vdB (2012)

For $n \geq 2$ let $H_n = \{(0, n, 0, 0), (0, n - 2, 0, 2), (2, n - 2, 0, 0)\}$

An $n \times n$ sign pattern $S$

- requires (refined inertia) $H_n$ if $H_n = \{ri(A) \mid A \in Q(S)\}$
- allows (refined inertia) $H_n$ if $H_n \subseteq \{ri(A) \mid A \in Q(S)\}$

If $S$ requires $H_n$ then

- $S$ allows $H_n$
- $S$ is SNS with sign $(\det(A)) = (-1)^n$ for all $A \in Q(S)$

**General Question:**
Which $n \times n$ irreducible sign patterns allow/require $H_n$?
Theorem

If \( S \) is an irreducible \( 3 \times 3 \) SNS pattern that allows \( H_3 \) then \( S \) requires \( H_3 \)

Proof:
The maximum number of distinct refined inertias for \( n = 3 \) is \( R(3) = 13 \)

Since \( S \) is SNS and allows \( H_3 \), \( \det(A) < 0 \) for all \( A \in Q(S) \) thus \( n_z = 0 \)

Of the six refined inertias that have \( n_z = 0 \), three have positive determinant and the remaining three are \( H_3 \)

Olesky, Rempel, vdD (2013) used an exhaustive search to list all refined inertias of tree sign patterns of order 3, three of which require \( H_3 \)

Bodine et al. listed general \( 3 \times 3 \) sign patterns that require \( H_3 \) and the list was completed by Garnett, Olesky, vdD (2014)
Garnett, Olesky, vdD (2014) proved the characterization:

**Theorem**

Let $S$ be an irreducible $3 \times 3$ sign pattern. TFAE:

- $S$ requires $\mathbb{H}_3$
- $S$ is potentially stable, sign nonsingular but not sign stable
- $S$ requires negative determinant and allows refined inertia $(0,1,0,2)$

In the proof it is shown that no irreducible $3 \times 3$ sign pattern $S$ can have $ri(S) = \{(0,3,0,0),(0,1,0,2)\}$

c.f. Jeffries' $5 \times 5$ example $S$ with $ri(S) = \{(0,5,0,0),(0,3,0,2)\}$

**Sign patterns of order 4 and $\mathbb{H}_4$**

Bodine et al. (2012)

**Theorem**

If $S$ is an irreducible $4 \times 4$ SNS pattern that requires a negative trace and allows $\mathbb{H}_4$ then $S$ requires $\mathbb{H}_4$

Proof:

Since $S$ is SNS and PS, $\text{det}(A) > 0$ for all $A \in Q(S)$

A sign pattern of order 4 can allow at most 22 refined inertias but only those in $\mathbb{H}_4$ are consistent with both a negative trace and a positive determinant
Companion matrix sign pattern

Bodine et al. (2012)

Example

\[ B = \begin{bmatrix} 0 & + & 0 & 0 \\ 0 & 0 & + & 0 \\ 0 & 0 & 0 & + \\ - & - & - & - \end{bmatrix} \text{ with } B = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -d & -c & -b & -a \end{bmatrix} \in Q(\mathcal{B}) \]

Sign pattern \( \mathcal{B} \) is a companion matrix sign pattern that allows all characteristic polynomials with all coefficients positive, in particular the following polynomials:

- \((z + 1)^4 \) giving \((0, 4, 0, 0) \in ri(\mathcal{B})\)
- \((z^2 + 1)(z + 1)^2 \) giving \((0, 2, 0, 2) \in ri(\mathcal{B})\)
- \((z^2 - z + 8)(z + 2)^2 \) giving \((2, 2, 0, 0) \in ri(\mathcal{B})\)

Thus \( \mathcal{B} \) allows \( \mathbb{H}_4 \) and since it is SNS and requires a negative trace it requires \( \mathbb{H}_4 \).

\[ n = 4 \]

For tree sign patterns of order 4 (paths or stars), Garnett, Olesky, vdD (2013) started with the list of potentially stable tree sign patterns in Johnson and Summers (1989) and Lin et al. (2002) to prove the characterization

Theorem

A 4 \times 4 tree sign pattern requires \( \mathbb{H}_4 \) if and only if it is potentially stable, sign nonsingular, not sign stable, and its negative is not potentially stable.

These conditions are not sufficient for a tree sign pattern of order \( n \geq 5 \) to require \( \mathbb{H}_n \).
Sign patterns with a diagonal restriction

Bodine et al. (2012)

Lemma

**Continuity Lemma** Let $S$ be a sign pattern with all its diagonal entries nonzero. If $S$ allows refined inertia $(a, b, c, d)$ then by continuity it allows refined inertias $(a + c + d, b, 0, 0)$ and $(a, b + c + d, 0, 0)$

Corollary

An $n \times n$ sign pattern with all its diagonal entries nonzero allows $\mathbb{H}_n$ if and only if it allows refined inertia $(0, n - 2, 0, 2)$

Superpatterns

Sign pattern $S_n' = [s_{ij}']$ is a superpattern of $S_n = [s_{ij}]$ if $s_{ij}' = s_{ij}$ for all $s_{ij} \neq 0$

Lemma

If $S_n$ has all entries on its diagonal negative and allows $\mathbb{H}_n$ then any superpattern of $S_n$ allows $\mathbb{H}_n$

Let $I_m$ be the sign pattern with each diagonal entry equal to + and all other entries 0

If $S_n$ allows $\mathbb{H}_n$ and has all diagonal entries negative then every superpattern of $S_n \oplus -I_m$ allows $\mathbb{H}_{n+m}$
For \( n \geq 3 \), \( \mathcal{K}_n = -I_n + C_n \)

\( C_n = [c_{ij}] \) is the sign pattern of a negative \( n \)-cycle matrix with \( c_{12}, c_{23}, \cdots, c_{n-1,n} = + \) and \( c_{n1} = - \) with all other entries 0

**Theorem**

\( \mathcal{K}_n = -I_n + C_n \) allows \( \mathbb{H}_n \) for all \( n \geq 3 \)

**Proof:**

Each \( A_n \in Q(C_n) \) has eigenvalues that are a positive scalar multiple of the \( n \)th roots of -1, so there is a unique pair of complex conjugate eigenvalues with maximum real part \( \alpha > 0 \)

Matrix \( -\alpha I_n + A_n \in Q(\mathcal{K}_n) \) has \( ri(-\alpha I_n + A_n) = (0, n-2, 0, 2) \)

Applying Corollary of the Continuity Lemma gives that \( \mathcal{K}_n \) allows \( \mathbb{H}_n \)
Theorem
\[ K_n = -I_n + C_n \text{ requires } \mathbb{H}_n \text{ if and only if } 3 \leq n \leq 6 \]

Sketch of Proof: \( n = 3, 4 \): result follows from previous theorems

\( n = 5 \): \( K_5 \) requires negative trace and determinant so \( ri(K_5) \subseteq \{ \mathbb{H}_5, (4, 1, 0, 0), (2, 1, 0, 2), (0, 1, 0, 4) \} \)

To show that \( K_5 \) does not allow refined inertia \((4, 1, 0, 0)\) take a general matrix \( A_5 \in Q(K_5) \), form its characteristic polynomial, the Routh Hurwitz matrix and its leading principal minors

Counting sign changes \( n_+(A) \leq 2 \)

Continuity Lemma gives that \( K_5 \) also does not allow refined inertias \((2, 1, 0, 2)\) and \((0, 1, 0, 4)\)

\( n = 6 \): similar argument as \( n = 5 \)

\( n \geq 7 \): take \( A \in Q(K_n) \) with magnitude 1 for every nonzero entry on the cycle \( C_n \) and magnitude \( \varepsilon < \cos(3\pi/n) \) on the diagonal

Then \( A = C_n - \varepsilon I_n \) has \( n_+ \geq 4 \), so \( K_n \) does not require \( \mathbb{H}_n \)

Detecting periodic solutions: Culos, Olesky, vdD (preprint)

**Theorem**

Let \( J \) be the \( n \times n \) Jacobian matrix of a differential equation system evaluated at a steady state \( x^* \) and depending on a vector of parameters \( p \), with each entry of \( J \) having fixed sign

- If \( sgn(J) \) (the sign pattern of \( J \)) requires refined inertia \((0, n, 0, 0)\) then \( x^* \) is linearly stable for all \( p \)
- If \( sgn(J) \) does not allow \( \mathbb{H}_n \) then the system does not have periodic solutions around \( x^* \) arising from a Hopf bifurcation
- If the entries of \( J \) have (have no) magnitude restrictions and if the restricted (unrestricted) sign pattern \( sgn(J) \) allows \( \mathbb{H}_n \) then the system gives rise to a Hopf bifurcation at a certain vector \( p \)
Note that if \( sgn(J) \) allows \( H_n \) then an additional condition is needed to determine whether or not these bifurcating periodic solutions about \( x^* \) are linearly stable.

The grass-rabbit-fox system is an example of the first and second cases of this theorem.

We now give some examples of the third case.

---

**Goodwin model**

**Example**

A Goodwin model for a regulatory mechanism in cellular physiology is formulated as a system of 3 ODEs:

\[
\begin{align*}
\frac{dM}{dt} &= \frac{V}{K + P^m} - aM \\
\frac{dE}{dt} &= bM - cE \\
\frac{dP}{dt} &= dE - eP
\end{align*}
\]

\( M, E, P \) represent the concentrations of messenger RNA, the enzyme and the product of the reaction of the enzyme and a substrate, other letters are positive parameters.

Linearizing about a steady state (with \( P \) at its steady state)

\[
J = \begin{bmatrix}
-a & 0 & -\frac{V_m P^{m-1}}{(K + P^m)^2} \\
b & -c & 0 \\
0 & d & -e
\end{bmatrix}
\]
The sign pattern of this matrix is

$$\text{sgn}(J) = \begin{bmatrix} - & 0 & - \\ + & - & 0 \\ 0 & + & - \end{bmatrix}$$

which is equivalent to $\mathcal{A}_3$

Since sign patterns that are equivalent have the same set of refined inertias, this sign pattern requires $\mathbb{H}_3$

Periodic solutions are found numerically to occur for this Goodwin model for certain parameters

Plots of $P$ against time with all parameters except $b$ fixed
Top plot: $b = 0.15$, $P$ approaches the steady state
Bottom plot: $b = 0.5$, $P$ oscillates about the steady state
Lorenz system

Consider an example with some magnitude restrictions. This comes from a 3d differential equation system introduced by Lorenz in 1963 to model the motion of a fluid layer. The equations linearized about one of the nonzero steady states give the Jacobian matrix

\[
Y_3^r = \begin{bmatrix}
-\sigma & \sigma & 0 \\
1 & -1 & -\gamma \\
\gamma & \gamma & -b
\end{bmatrix}
\]

with parameters \(\sigma > 0, b > 0, r > 1, \gamma = (b(r - 1))^{\frac{1}{2}}\)

This sign pattern is equivalent to a superpattern of \(\mathcal{A}_3\) so the sign pattern allows \(\mathbb{H}_3\) but does not require \(\mathbb{H}_3\) (not SNS).

BUT the entries in this sign pattern have some magnitude restrictions.

For \(\sigma > b + 1\) taking \(r\) as the bifurcation parameter and defining \(r_0 = \frac{\sigma(b + \sigma + 3)}{\sigma - b - 1}\), the refined inertia of \(Y_3^r\) has the values:

- \(r < r_0\): \(\text{ri}(Y_3^r) = (0, 3, 0, 0)\)
- \(r = r_0\): \(\text{ri}(Y_3^r) = (0, 1, 0, 2)\)
- \(r > r_0\): \(\text{ri}(Y_3^r) = (2, 1, 0, 0)\)

Thus \(Y_3^r\) allows \(\mathbb{H}_3\) and since \(Y_3^r\) has determinant equal to \(-2\sigma\gamma^2 < 0\) and negative trace it requires \(\mathbb{H}_3\).

As \(r\) increases through \(r_0\) the Lorenz system undergoes a Hopf bifurcation and periodic orbits arise that may be stable or unstable depending on the values of \(\sigma\) and \(b\) and the nonlinear terms.
Infectious disease model

A constant population is divided into 3 disjoint classes with $S(t), I(t), R(t)$ denoting the fractions of the population that are susceptible to, infectious with, recovered from a disease

$\beta, \gamma$ are the constant contact, recovery rate

Assume that the disease confers temporary immunity on recovery (e.g. influenza)
This is modeled by splitting $R(t)$ into a chain of recovered classes $R_1, R_2, \ldots, R_k$ with the waiting time in each subclass assumed exponentially distributed with mean waiting time $1/\varepsilon$

The $S, I, R_1, R_2, \ldots, R_k, S$ model is described schematically by

\[
\begin{align*}
S & \xrightarrow{\beta S I} I \xrightarrow{\gamma I} R_1 \xrightarrow{\varepsilon R_1} R_2 \xrightarrow{\varepsilon R_2} \cdots \xrightarrow{\varepsilon R_{k-1}} R_k \\
& \xrightarrow{\varepsilon R_k} S
\end{align*}
\]
This system has a disease free steady state with \( S = 1 \) and other variables zero

If \( \beta < \gamma \) then this is the only steady state and the disease dies out

If \( \beta > \gamma \) there is also an endemic steady state with

\[
S^* = \frac{\gamma}{\beta}, \quad I^* = \frac{(1 - \frac{\gamma}{\beta})/(1 + \frac{k \gamma}{\epsilon})}{1 + \frac{\gamma}{\epsilon}}, \quad R^*_i = \frac{\gamma_i}{\epsilon}
\]

To find out about stability of this endemic steady state, consider the Jacobian matrix at this steady state

\[
S^T = \begin{bmatrix}
-\beta I^* & -\beta I^* & -\beta I^* & -\beta I^*\\
\gamma & -\epsilon & 0 & 0 \\
0 & \epsilon & -\epsilon & 0 \\
0 & 0 & \epsilon & -\epsilon
\end{bmatrix}
\]

This gives another example with magnitude restrictions in which the sign pattern (a superpattern of \( \mathcal{K}_4 \)) allows \( \mathbb{H}_4 \). The leading principal submatrices of orders 2, 3, 4 give the Jacobian with \( k = 1, 2, 3 \)

\( k = 1 \): \( S, I, R_1, S \): The leading \( 2 \times 2 \) subpattern requires refined inertia \((0, 2, 0, 0)\)

\( k = 2 \): \( S, I, R_1, R_2, S \): The leading \( 3 \times 3 \) subpattern allows \( \mathbb{H}_3 \) but the magnitude structure restricts its refined inertia to \((0, 3, 0, 0)\)

\( k = 3 \): \( S, I, R_1, R_2, R_3, S \): Here \( S^T \) allows refined inertia \( \mathbb{H}_4 \) and this model exhibits periodic solutions for some parameters
A three-species competition model has each species competing in a common patch $X$ and also having its own refuge patch $Y_i$, for species $i = 1, 2, 3$. 

$x_i$ is the population size competing in patch $X$ and $y_i$ is the population size in refuge $Y_i$.

\[
\begin{align*}
\frac{dx_1}{dt} &= x_1 r_1 (1 - x_1 - \alpha_2 x_2 - \beta_3 x_3) + \varepsilon_1 (y_1 - x_1), \\
\frac{dx_2}{dt} &= x_2 r_2 (1 - \beta_1 x_1 - x_2 - \alpha_3 x_3) + \varepsilon_2 (y_2 - x_2), \\
\frac{dx_3}{dt} &= x_3 r_3 (1 - \alpha_1 x_1 - \beta_2 x_2 - x_3) + \varepsilon_3 (y_3 - x_3), \\
\frac{dy_1}{dt} &= y_1 R_1 (1 - y_1) + \varepsilon_1 (x_1 - y_1), \\
\frac{dy_2}{dt} &= y_2 R_2 (1 - y_2) + \varepsilon_2 (x_2 - y_2), \\
\frac{dy_3}{dt} &= y_3 R_3 (1 - y_3) + \varepsilon_3 (x_3 - y_3).
\end{align*}
\]

Positive parameters $\alpha_i$, $\beta_i$ are competition coefficients, $\varepsilon_i$ is the dispersal rate for species $i$ between patch $X$ and patch $Y_i$. 

$R_i$ and $r_i$ are intrinsic growth rates of species $i$ in its refuge patch and competition patch.

Assume there exists a positive steady state $x_i^*, y_i^*$, then the Jacobian matrix around this has sign pattern

\[
S = \begin{bmatrix} \mathcal{N} & I \\ I & -I \end{bmatrix},
\]

where $\mathcal{N}$ is the 3-by-3 sign pattern with every entry negative.

Sign pattern $\mathcal{N}$ allows $\mathbb{H}_3$, so $S$ allows $\mathbb{H}_6$ since $S$ is a superpattern of $\mathcal{N} \oplus I$.

Takeuchi shows numerically that the system has periodic solutions for specific parameter values.
Some open problems concerning $\mathbb{H}_n$

- Characterize sign patterns that require $\mathbb{H}_n$ for $n \geq 4$
- Do there exist irreducible sign patterns that require $\mathbb{H}_n$ for $n \geq 8$?
- How to identify sign patterns with purely imaginary (nonzero) eigenvalues?
- How to identify sign patterns that do not allow $\mathbb{H}_n$
- Develop a theory for sign patterns with some magnitude restrictions

Questions ??? (and Answers!)

Thank you


Recall definitions

Recall the definition of the inertia of a sign pattern:
An $n \times n$ sign pattern $S$ is an \textit{inertially arbitrary pattern (IAP)} if $i(S)$ contains every ordered triple of nonnegative integers $(n_+, n_-, n_0)$ with $n_+ + n_- + n_0 = n$
Thus an IAP achieves every possible inertia

Recall the definition of the refined inertia of a sign pattern:
An $n \times n$ sign pattern $S$ is a \textit{refined inertially arbitrary pattern (rIAP)} if $ri(S)$ contains every ordered 4-tuple of nonnegative integers $(n_+, n_-, n_z, 2n_p)$ with $n_+ + n_- + n_z + 2n_p = n$
Necessary conditions for an IAP

Cavers and Vander Meulen (2005)

Theorem

If sign pattern \( S \) is an IAP then \( D(S) \) has at least one positive and one negative 1-cycle and a negative 2-cycle

Proof for the 2-cycle:
Assume \( A \in Q(S) \) has \( i(A) = (0,0,n) \) giving \( \text{tr}(A) = 0 \)
If \( \pm ib_i \) for \( i = 1, \ldots, m \) are the nonzero eigenvalues of \( A \) then the characteristic polynomial of \( A \) has \( z^{n-2} \) coefficient
\[
E_2 = \sum_{k=1}^{m} b_k^2 \geq 0
\]
But \( E_2 \) is \( \sum_{k<j} (a_{kk}a_{jj} - a_{kj}a_{jk}) \)
Also \( (1,0,n-1) \in i(S) \) so \( S \) has at least one nonzero diagonal entry implying \( \sum a_{kk}^2 > 0 \)
From \( 2\sum_{k<j} a_{kk}a_{jj} = (\text{tr}A)^2 - \sum a_{kk}^2 < 0 \) if \( \text{tr}(A) = 0 \) it follows that \( a_{ij}a_{jk} < 0 \) for some \( k < j \)

Obvious methods to show that sign pattern \( S \) is an IAP

1. explicitly find a realization of \( S \) having each possible inertia
2. show that \( S \) is a rIAP
3. show that \( S \) is an SAP
SAP and IAP

For irreducible sign patterns the set of all SAPs and set of all IAPs (and thus the set of rIAPs) are identical for

- \( n = 2 \) and \( 3 \)
- an \( n \times n \) star sign pattern

but these sets are not identical in general

Example

Cavers and VM (2005), Kim et al. (2009)

\[
\mathcal{N} = \begin{bmatrix}
+ & + & 0 & 0 \\
0 & 0 & + & + \\
- & - & 0 & 0 \\
0 & 0 & - & - \\
\end{bmatrix}
\]

is a minimal IAP but not a SAP or rIAP as \( \mathcal{N} \) does not allow refined inertia \((0, 0, 0, 4)\) but is potentially nilpotent

rIAP, IAP and potential nilpotence

If \( \mathcal{S} \) is a refined inertially arbitrary sign pattern then \( \mathcal{S} \) is potentially nilpotent
If \( \mathcal{S} \) is inertially arbitrary this implication may not be true

Example

Kim et al. (2007)

\[
\mathcal{G}_5 = \begin{bmatrix}
- & - & - & 0 & 0 \\
+ & + & + & 0 & 0 \\
0 & 0 & 0 & - & - \\
0 & - & 0 & 0 & - \\
- & 0 & 0 & 0 & 0 \\
\end{bmatrix}
\]

is an IAP that is not potentially nilpotent

Setting every nonzero entry equal to 1 except the \((2, 1)\) entry set to 2 gives a matrix with refined inertia \((0, 0, 3, 2)\)
Generalization of the Nilpotent-Jacobian method


If the $n \times n$ matrix $A = [a_{ij}]$ satisfies the following conditions then $A$ allows a nonzero Jacobian:

(i) $A$ has $m \geq n$ nonzero entries

(ii) Among these $m$ nonzero entries there are $n$ nonzero entries say $a_{i_1j_1}, \ldots, a_{i_nj_n}$ such that if $X$ is the matrix obtained from $A$ by replacing these entries with $x_1, \ldots, x_n$

$$p_X(z) = z^n + p_1 z^{n-1} + \ldots + p_{n-1} z + p_n$$

is the characteristic polynomial of $X$, then the $n \times n$ Jacobian matrix with $(i,j)$ entry equal to $\frac{\partial p_i}{\partial x_j}(x_1, \ldots, x_n)$ is nonsingular at $(x_1, \ldots, x_n) = (a_{i_1j_1}, \ldots, a_{i_nj_n})$

Restatement of the Nilpotent-Jacobian method

Theorem

Let $A$ be a nilpotent realization of a sign or zero-nonzero pattern $S$ such that $A$ allows a nonzero Jacobian

Then every superpattern of $S$ is spectrally arbitrary

This restatement helps in deriving some results about inertias and refined inertias

We illustrate with some results from Cavers et al. (2013)
Modification of refined inertia

Lemma

Let $S$ be an $n \times n$ sign pattern with superpattern $\hat{S}$. Suppose $A \in Q(S)$ allows a nonzero Jacobian and $\text{ri}(A) = (n_+, n_-, n_z, 2n_p)$

1. If $n_z \geq 1$ then $(n_+ + 1, n_-, n_z - 1, 2n_p)$ and $(n_+, n_- + 1, n_z - 1, 2n_p) \in \text{ri}(\hat{S})$
2. If $n_z \geq 2$ then $(n_+, n_-, n_z - 2, 2(n_p + 1)) \in \text{ri}(\hat{S})$
3. If $n_p \geq 1$ then $(n_+ + 2, n_-, n_z, 2(n_p - 1))$ and $(n_+, n_- + 2, n_z, 2(n_p - 1)) \in \text{ri}(\hat{S})$

For each modified refined inertia there is a realization of $\hat{S}$ with this refined inertia that allows a nonzero Jacobian.

Note that the condition that $A$ allows a nonzero Jacobian is necessary for the statement of this modification Lemma.

Jeffries’ $5 \times 5$ sign pattern has a realization $A$ with $\text{ri}(A) = (0, 3, 0, 2)$ but this does NOT allow a nonzero Jacobian.

The sign pattern is sign semi-stable so allows only this refined inertia and $(0,5,0,0)$, it does NOT allow refined inertia $(2,3,0,0)$.
Refined inertia tells about inertia set

Applying the lemma recursively to an initial refined inertia:

**Corollary**

Let $\mathcal{S}$ be an $n \times n$ sign pattern with superpattern $\hat{\mathcal{S}}$

Suppose $A \in Q(\mathcal{S})$ has $ri(A) = (n_+, n_-, n_z, 2n_p)$ with $n_z \geq 2$

If $A$ allows a nonzero Jacobian then for every

$m_+ \geq n_+, m_- \geq n_-$ and $m_0 \geq 0$ with $m_+ + m_- + m_0 = n$

it follows that $(m_+, m_-, m_0) \in i(\hat{\mathcal{S}})$

For example if $A \in Q(\mathcal{S})$ has $ri(A) = (1, 4, 3, 2)$ and allows a nonzero Jacobian then $(2, 7, 1) \in i(\hat{\mathcal{S}})$

---

Centralizer technique for IAPs

If a nilpotent $n \times n$ matrix has index $n$ then it is **nonderogatory**
i.e. its minimum polynomial is equal to its characteristic polynomial

**Theorem**

Let $\mathcal{S}$ be an $n \times n$ sign pattern, $A \in Q(\mathcal{S})$ having $ri(A) = (0, 0, n_z, 2n_p)$ with $n_z \geq 2$

If $A$ is nonderogatory and the only matrix $B$ in the centralizer of $A$ satisfying $B \circ A^T = 0$ is the zero matrix then every superpattern of $\mathcal{S}$ is an IAP

If $n_z = n$ then $A$ is nilpotent, every superpattern is a SAP
but if $n_z < n$ then this may not be true
e.g. $\mathcal{G}_5$ does not allow $ri(0, 0, 5, 0)$ but allows $ri(0, 0, 3, 2)$
Reducible IAPs

If $S_1$ and $S_2$ are IAPs then clearly $S_1 \oplus S_2$ is an IAP
Can $S_1 \oplus S_2$ be an IAP with neither summand an IAP?

Example

(Cavers 2010)

$B_4 = \begin{bmatrix} + & + & + & 0 \\ - & - & - & 0 \\ + & 0 & 0 & + \\ + & 0 & 0 & 0 \end{bmatrix}$

is not an IAP but $B_4 \oplus T_2$ is an IAP

$B_4 \oplus (-B_4)$ is the smallest example of an IAP with both summands not IAPs
but $B_4 \oplus (-B_4)$ is not PN so not a SAP

A GLIMPSE AT ZERO-NONZERO PATTERNS
Zero-nonzero patterns

A zero-nonzero pattern is a matrix with entries from \( \{0, \ast\} \).

Many previous definitions and ideas for sign patterns carry over to zero-nonzero patterns.

Results have been given for these patterns e.g.:

- \( n = 4 \) IAPs by Cavers, Vander Meulen (2007)
- \( n = 4 \) SAPs by Corpuz, McDonald (2007)

Some inclusions hold e.g. \( ri(S_{\text{signpattern}}) \subseteq ri(S_{\text{zero-nonzeropattern}}) \).

Note that matrices \( A \) and \( -A \) have the same zero-nonzero pattern thus if \( S \) is a zero-nonzero pattern that allows \( ri(n_+, n_-, n_z, 2n_p) \) then it allows its reversal \( ri(n_-, n_+, n_z, 2n_p) \).

Theorem

Deaett, Olesky, vdD (2010) The maximum number \( R^* \) of distinct refined inertias excluding reversals allowed by any \( n \times n \) zero-nonzero pattern with \( n \geq 2 \) is:

- \( R^*(n) = \frac{(n+2)(n+3)(n+4)}{24} \) for \( n \) even
- \( R^*(n) = \frac{(n+1)(n+3)(n+5)}{24} \) for \( n \) odd

Proof: Use induction starting with \( R^*(2) = 5 \), \( R^*(3) = 8 \) and subtract from \( R(n) \) (the total number of refined inertias) the number of refined inertias in which the first two coordinates are both equal.
rIAP implies SAP??

- For $n = 2, 3$ IAP, rIAP and SAP patterns are identical
- For $n \leq 4$ an $n \times n$ zero-nonzero pattern is an rIAP if and only if it is a SAP
- For $n = 4$ there are examples of zero-nonzero patterns that are IAPs but not rIAPs
  e.g. $\mathcal{N}^*$ the zero-nonzero pattern from sign pattern $\mathcal{N}$ that is an IAP but not an rIAP
- For $n = 5$ there exists an irreducible zero-nonzero pattern $\mathcal{L}$ that is an rIAP but not a SAP
  Note that the existence of such an example is unknown for sign patterns

Zero-nonzero pattern $\mathcal{L}$

Example

$$\mathcal{L} = \left[ \begin{array}{cccc} * & * & 0 & 0 * \\ 0 & 0 * & 0 * \\ 0 & 0 0 & * 0 \\ 0 & 0 * & 0 * \\ * & * 0 0 & * \end{array} \right]$$

is an rIAP but not a SAP

Let $p(z) = z^5 + p_1 z^4 + p_2 z^3 + p_3 z^2 + p_4 z + p_5$
Then $\mathcal{L}$ fails to allow characteristic polynomial $p(z)$ if and only if $p_1 = p_3 = 0$ while $p_5 \neq 0$, thus $\mathcal{L}$ is not a SAP

$\mathcal{L}$ allows any $p(z)$ of the form $(z - 1)^k(z + 1)^{5-k}$ for $k \in \{0, 1, \ldots, 5\}$ and also any $p(z)$ with a zero on the imaginary axis, thus $\mathcal{L}$ is an rIAP
The pattern $\mathcal{L}$ and the zero-nonzero pattern $\mathcal{M}$ from the sign pattern of DeAlba et al. (2007)

$$\mathcal{M} = \begin{bmatrix}
* & * & * & 0 \\
* & * & * & 0 \\
0 & 0 & 0 & * \\
* & * & 0 & 0
\end{bmatrix}$$

give a $9 \times 9$ reducible pattern $\mathcal{L} \oplus \mathcal{M}$ that is a SAP with neither summand a SAP.

It is unknown whether such an example exists for sign patterns.
More general patterns

Cavers and Fallat (2012) consider allow problems with a larger set of symbols

\[ S = \{ 0, +, -, +0, -0, *, \# \} \]

where

\(+0, -0\) represents a nonnegative, nonpositive real number

\(*, \#\) represents a nonzero, arbitrary real number

An \(S\)-pattern is a matrix with symbols in \(S\)

Definitions of inertially arbitrary etc. carry over to \(S\)-patterns but the different symbols especially \(\#\) allow more "flexibility"

Companion matrix \(S\)-pattern

Example

\[ C_4 = \begin{bmatrix}
0 & + & 0 & 0 \\
0 & 0 & + & 0 \\
0 & 0 & 0 & + \\
\# & \# & \# & \#
\end{bmatrix} \]

\(C_4\) is a SAP, IAP, rIAP and is PN

\(D(C_4)\) allows a positive loop, allows a negative loop and allows a negative 2-cycle, but does not allow two oppositely signed loops

These same properties hold for an \(n \times n\) companion matrix \(S\)-pattern giving SAPs with \(2n - 1\) nonzero entries
Recall that for a sign or zero-nonzero pattern the implications are

\[
\text{SAP} \rightarrow \text{rIAP} \rightarrow \text{IAP} \rightarrow \text{PS} \rightarrow \text{PN}
\]

If \( S \) is an \( n \times n \{+, -, *, \#\} \)-pattern then

\[
\text{SAP} \iff \text{rIAP} \iff \text{PN}
\]

If \( S \) allows \( ri(0,0,n_z,2n_p) \) where \( n_z \geq 2 \) then \( S \) is an IAP

The proofs are modifications of Pereira’s (2007) proof

If \( +_0 \) belongs to the symbol set then the pattern with every entry \( +_0 \) is PN but not a SAP

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### Some open problems concerning IAPs

- If sign pattern \( S \) is an rIAP then is \( S \) a SAP?
- Determine the minimum number of nonzeros in an \( n \times n \) IAP for sign patterns and for zero-nonzero patterns
- Determine conditions on \( i(S_1) \) and \( i(S_2) \) that ensure that certain inertias are in \( i(S_1 \oplus S_2) \) for sign patterns and for zero-nonzero patterns
- Determine any other families (besides star sign patterns) for which the set of IAPs and SAPs are identical
- Is a \( \{+, -, *, \#\} \)-pattern that is an IAP also PN (and hence a SAP)?


