

Non-chordal patterns associated with the positive definite completion problem

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Abstract

A partial matrix, is a matrix for which some entries are specified and some unspecified. In general completion problems ask whether a given partial matrix, may be completed to a matrix where all the entries are specified, such that this completion admits a specific structure. The positive definite completion problem asks whether a partial Hermitian matrix admits a completion such that the completed matrix is positive semidefinite. The minimum solution criterion, is that every fully specified principal submatrix is non-negative. Then the set of partial Hermitian matrices, which admit a positive semidefinite completion, forms a convex cone, and its dual cone can be identified as the set of positive semidefinite Hermitian matrices with zeros in the entries that correspond to non-edges in the graph G . Furthermore, the set of partial Hermitian matrices, with non-negative fully specified principal minors, also forms a convex cone, and its dual cone can be identified as the set of positive semidefinite Hermitian matrices which can be written as the sum of rank one matrices, with underlying graph G . Consequently, the problem reduces to determining when these cones are equal. Indeed, we find that this happens if and only if the underlying graph is chordal. It then follows that the extreme rays of the cone of positive semidefinite Hermitian matrices with zeros in the entries that correspond to non-edges in the graph G is generated by rank one matrices. The question that arises, is what happens if the underlying graph is not chordal. In particular, what can be said about the extreme rays of the cone of positive semidefinite matrices with some non-chordal pattern. This gives rise to the notion of the sparsity order of a graph G , that is, the maximum rank of matrices lying on extreme rays of the cone of positive semidefinite Hermitian matrices with zeros in the entries that correspond to non-edges in the graph G . We will see that those graphs having sparsity order less than or equal to 2 can be fully characterized. Moreover, one can determine in polynomial time whether a graph has sparsity order less than or equal to 2, using a clique-sum decomposition. We also show that one can determine whether a graph has sparsity order less than or equal to 2, by considering the characteristic polynomial of the adjacency matrix of certain forbidden induced subgraphs and comparing it with the characteristic polynomial of principal submatrices of appropriate size.

Keywords: Positive definite completions, chordal graphs, matrix cones, sparsity order of a graph, spectrum of a graph.

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Introduction

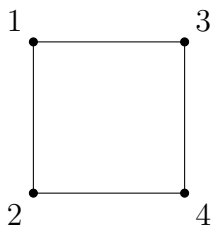
A partial matrix is a matrix where some entries are specified and some are unspecified. A completion of such a matrix allocates specific values to the unspecified entries, thus obtaining a matrix of which all the entries are known. Completion problems try to determine whether there exists completions of a partial matrix with specific properties. In our study we consider the set of all partial Hermitian matrices and determine under which conditions there exists a positive semidefinite completion, i.e., a completion that is a positive semidefinite matrix.

It turns out that the underlying graph G , determined by the unspecified entries of the matrix, is crucial in determining whether a positive semidefinite completion exists. By an underlying graph of a matrix, we mean the graph where the diagonal entries each correspond to a vertex of the graph and the off-diagonal entries correspond to the edges of the graph. Consider the following example:

Let

$$A = \begin{bmatrix} 5 & 3 & 1 & ? \\ 3 & 6 & ? & 1 \\ 1 & ? & 4 & 1 \\ ? & 1 & 1 & 4 \end{bmatrix}$$

Then the underlying graph of the matrix A is as follows:



In [12] it was shown that if this graph is chordal (has no minimal cycle longer than three) and all the fully specified principal minors are positive, there necessarily exists a positive semidefinite completion. It is important to note here that all the partial matrices, with non-negative principal minors, and the same underlying graph, admit a positive semidefinite completion if said graph is chordal. However, more can be said about matrices with underlying graphs being chordal, as we will soon see.

The approach in [12] used entropy maximization via Lagrange multipliers to prove that a positive semidefinite completion exists. More recent approaches rely on convex cone theory. The reason for this is that the set of partial Hermitian matrices, which

admit a positive semidefinite completion, forms a convex cone, and its dual cone can be identified as the set of positive semidefinite Hermitian matrices with zeros in the entries that correspond to non-edges in the graph G . Furthermore, the set of partial Hermitian matrices, with non-negative fully specified principal minors, also forms a convex cone, and its dual cone can be identified as the set of positive semidefinite Hermitian matrices which can be written as the sum of rank one matrices, with underlying graph G . Consequently, the problem reduces to determining when these cones are equal. It turns out that this occurs exactly when the underlying graph is chordal. It then follows that the extreme rays of the cone of positive semidefinite Hermitian matrices with zeros in the entries that correspond to non-edges in the graph G is generated by rank one matrices.

It is interesting to note that this generalizes a well-known result on the extreme rays of the cone of positive semidefinite matrices, since the extreme rays for the cone of positive semidefinite matrices are generated by rank one matrices. This led to the notion of the sparsity order of a graph, introduced in [1]. The sparsity order of a graph G is defined as the maximum rank of a matrix lying on an extreme ray of the cone of positive semidefinite matrices with underlying graph G . It therefore follows that the sparsity order of a chordal graph is 1. In fact it can be shown that the sparsity order is 1 if and only if the graph is chordal.

The question now arises as to what happens when the underlying graph is not chordal? Obviously the maximum rank of extremals (matrices lying on extreme rays) is greater than 1 if the graph is non-chordal, but how can we determine what the maximum rank is? In [1] it is proved that a matrix is extremal, with rank k , if and only if the dimension of the so-called frame space has dimension $\frac{1}{2}(k^2 + k - 2)$, in the real case, and $k^2 - 1$, in the complex case. They also defined the notion of k -blocks, which may be seen as minimal graphs, in terms of induced subgraphs, with sparsity order k . They characterized all the k -blocks, for $k = 1, 2, 3$, in the real case and conjectured that a graph has sparsity order less than or equal to 2 if and only if the graph does not contain, as an induced subgraph, any 3-blocks. In [20] it is shown that this conjecture is in fact true and is extended to characterize graphs having sparsity order less than or equal to 2, in the real and complex case. The main ingredient in the proof of these theorems is a graph decomposition result, which shows that a graph can be decomposed as a clique-sum of graphs, with a specific form, if and only if the graph does not contain certain graphs as induced subgraphs.

It seems that current methods do not rely on the forbidden induced subgraphs, but rather applies clique-sum decompositions to determine whether a graph is an element of a specific set of classes, for which the sparsity order is less than or equal to 2. The approach that we introduce relies on the forbidden induced subgraphs and the fact that they are determined by the spectrum of their adjacency matrices. This means that if the spectrum of a adjacency matrix, of some graph, is equal to the spectrum of one of the forbidden induced subgraphs, it is necessarily isomorphic to the specific forbidden induced subgraph. Therefore, determining whether the sparsity order of a graph is less than or equal to 2, reduces to calculating the characteristic polynomial of principal submatrices of appropriate size, and comparing them to the characteristic polynomials of the forbidden induced subgraphs. If a principal submatrix has the same characteristic polynomials as some forbidden induced subgraphs, it implies that said forbidden induced subgraphs is in our graph.

We organize our study in two parts. The first part is devoted to the positive definite completion problem. In chapter one, we introduce the notion of Hermitian matrices and some properties of Hermitian matrices. We also define what is meant by positive semidefinite matrices and prove some results regarding these matrices. Of particular importance is the notion of Gram matrices, which we will require in our study of the sparsity order of a graph. In chapter two we prove some general results on cones and introduce some cones of Hermitian matrices, related to the positive definite completion problem. It is important to note that these cones rely on the idea of an underlying graph of a matrix, in the sense that elements of these cones are matrices with the same underlying graph. In chapter three we define chordal graphs. We give an algorithmic characterization of chordal graphs in terms of a perfect vertex elimination scheme. Finally, we show that a partial matrix admits a positive definite completion if and only if its underlying graph is chordal. The remarkable thing here, is that any partial matrix, with positive principal minors, admits a positive definite completion if the underlying graph is chordal, regardless of the specific entries of the partial matrix. The argumentation used here can be found in [2]. A different approach, in a C^* -algebra setting, can be found in [24].

The second part of our study is devoted to the sparsity order of a graph. As mentioned earlier, the sparsity order of a graph is 1 if and only if the graph is chordal. This fact is actually already shown to be true in the first part (Proposition 3.2.1). We start by proving the graph decomposition result mentioned earlier. The proof of this result is rather technical and we devote the whole of chapter four to it. In chapter five we formally define what is meant by the sparsity order of a graph and prove some results regarding this notion. In particular, we introduce the notion of k -blocks, which plays a crucial part in determining whether a graph has sparsity order less than or equal to 2. We then prove a theorem of [20] regarding the smallest face of the cone of partial positive semidefinite matrices, which is in fact a generalization of a result found in [1]. In the last section of this chapter we distinguish between the real and complex case, and characterize graphs with sparsity order less than or equal to 2. Our approach to these two chapters relies on work in [20] and [1], where we attempted to optimize some of the argumentation and added more details. In the sixth chapter we introduce the notion of the spectrum of a graph and define what is meant when a graph is determined by its spectrum, as mentioned earlier. We show that all the 3-blocks are determined by their spectrum, and use this fact to determine whether a graph has sparsity order less than or equal to two. In the final section of chapter six we propose an algorithm, where we also make use of eigenvalue interlacing to eliminate some possibilities, to do this. At this stage the algorithm is not very efficient, but it gives a rather simple and nice way to determine whether a graph contains any of the forbidden induced subgraphs of the previous chapter, and we believe there is room for improvement.

Part I

The positive definite completion problem

Chapter 1

Hermitian and positive semidefinite matrices

In this chapter we give an overview of Hermitian matrices and some of their properties. In particular, we focus on positive semidefinite matrices. We will introduce several notions which will later be useful in our study of positive definite completions.

1.1 Hermitian Matrices

Let $\mathcal{M}_{n,m}(\mathbb{F})$ denote the set of all $n \times m$ matrices with entries in \mathbb{F} , where $\mathbb{F} = \mathbb{C}$ or \mathbb{R} . If $m = n$ we simply write $\mathcal{M}_n(\mathbb{F})$. Elements of $\mathcal{M}_n(\mathbb{F})$ are denoted by $A = [a_{ij}]_{i,j=1}^n$, where $a_{ij} \in \mathbb{F}$ is the ij -th entry of A . Since a matrix $A \in \mathcal{M}_{n,m}(\mathbb{R})$ can also be viewed as an element of $\mathcal{M}_{n,m}(\mathbb{C})$, and since most of the results for $\mathbb{F} = \mathbb{R}$ and $\mathbb{F} = \mathbb{C}$ are analogous, in what follows we will mainly refer to the case $\mathbb{F} = \mathbb{C}$, unless stated otherwise. In the case $\mathbb{F} = \mathbb{R}$, A^* is to be understood as A^T , and Hermitian matrices, which we define next, are real symmetric matrices.

Definition 1.1.1 (Hermitian Matrix). A square matrix $A = [a_{ij}]_{i,j=1}^n$ is said to be Hermitian if $A = A^*$, where $A^* = \overline{A}^T = [\overline{a_{ji}}]_{i,j=1}^n$. It is skew-Hermitian if $A = -A^*$.

The linear space $\mathcal{M}_n(\mathbb{C})$ is a Hilbert space over \mathbb{C} , with inner product

$$\langle A, B \rangle = \text{tr}(AB^*),$$

where $A, B \in \mathcal{M}_n(\mathbb{C})$ (Theorem B.1). Similarly, $\mathcal{M}_n(\mathbb{R})$ is the Hilbert space of all $n \times n$ matrices in \mathbb{R} , with inner product

$$\langle A, B \rangle = \text{tr}(AB^T),$$

where $A, B \in \mathcal{M}_n(\mathbb{R})$.

Some observations for $A, B \in \mathcal{M}_n(\mathbb{C})$ [17, p.169]:

1. $A + A^*$, AA^* , and A^*A are Hermitian.

2. If A is Hermitian, then A^k is Hermitian for all $k = 1, 2, 3, \dots$. If A is non-singular as well, then A^{-1} is Hermitian.
3. If A and B are Hermitian, then $\alpha A + \beta B$ is Hermitian for all real scalars α and β .
4. $A - A^*$ is skew-Hermitian for all $A \in \mathcal{M}_n(\mathbb{C})$.
5. If A and B are skew-Hermitian, then $\alpha A + \beta B$ is skew-Hermitian for all real scalars α and β .
6. A is Hermitian if and only if iA is skew-Hermitian.
7. Any $A \in \mathcal{M}_n(\mathbb{C})$ can be written as

$$A = \frac{1}{2}(A + A^*) + \frac{1}{2}(A - A^*) = H(A) + S(A),$$

where $H(A) = \frac{1}{2}(A + A^*)$ is the Hermitian part of A , and $S(A) = \frac{1}{2}(A - A^*)$ is the skew-Hermitian part of A .

8. If A is Hermitian, the main diagonal entries of A are all real.

All of these results are easily verified and we omit a formal proof. The following theorem gives further properties that hold for Hermitian matrices.

Theorem 1.1.2. [17, Theorem 4.1.3] *Let $A \in \mathcal{M}_n(\mathbb{C})$ be Hermitian. Then*

- (i) x^*Ax is real for all $x \in \mathbb{C}^n$;
- (ii) All the eigenvalues of A are real;
- (iii) S^*AS is Hermitian for all $S \in \mathcal{M}_n(\mathbb{C})$.

All of the above is trivially true if $A \in \mathcal{M}_n(\mathbb{R})$.

Since Hermitian matrices are normal ($AA^* = A^*A$) all results regarding normal matrices hold. For more on normal matrices see [17]. One particular result, which we will make repeated use of, is the so called spectral theorem for Hermitian matrices.

Theorem 1.1.3. [17, Theorem 4.1.5] *Let $A \in \mathcal{M}_n(\mathbb{C})$. Then A is Hermitian if and only if there is a unitary matrix $U \in \mathcal{M}_n(\mathbb{C})$, ($U^* = U^{-1}$), and a real diagonal matrix $\Lambda \in \mathcal{M}_n(\mathbb{C})$ such that $A = U\Lambda U^*$. Moreover, A is real and Hermitian (i.e., real symmetric) if and only if there is a real orthogonal matrix $P \in \mathcal{M}_n(\mathbb{C})$, ($P^T = P^{-1}$), and a real diagonal matrix $\Lambda \in \mathcal{M}_n(\mathbb{C})$ such that $A = P\Lambda P^T$. Note that $\Lambda = \text{diag}(\lambda_1, \dots, \lambda_n)$, where $\lambda_1, \dots, \lambda_n$ are the eigenvalues of A and the columns of U are the associated eigenvectors.*

The inner product mentioned earlier naturally gives rise to the so called Frobenius norm of a matrix.

Definition 1.1.4 (Frobenius norm). Let $A \in \mathcal{M}_n(\mathbb{C})$. Then we define the the norm $\|\cdot\|_2$ as follows:

$$\|A\|_2 = \sqrt{\langle A, A \rangle_2} = \sqrt{\text{tr}(AA^*)} = \sqrt{\text{tr}(A^*A)}$$

We will now show that the set of all $n \times n$ Hermitian matrices is a Hilbert space over \mathbb{R} .

Theorem 1.1.5. *The subset $\mathcal{H}_n = \{A \in \mathcal{M}_n(\mathbb{C}) : A = A^*\}$ of $\mathcal{M}_n(\mathbb{C})$ is a Hilbert space over \mathbb{R} , with respect to the inner product*

$$\langle A, B \rangle_2 = \operatorname{tr}(AB^*) = \operatorname{tr}(AB). \quad (1.1)$$

Proof. (i) For all $A, B \in \mathcal{H}_n$ and any $\lambda \in \mathbb{R}$, we have that $\lambda A + B \in \mathcal{H}_n$. Therefore \mathcal{H}_n is closed under linear operations proving that it is a vector space over \mathbb{R} .

(ii) From the proof of Theorem B.1 it is easy to see that \mathcal{H}_n is an inner product space with the inner product defined by (1.1), where the second equality is true since B is Hermitian. However, it is important to note that \mathcal{H}_n is an inner product space over \mathbb{R} and not over \mathbb{C} , since

$$\operatorname{tr}(AB) = \langle A, B \rangle = \overline{\langle B, A \rangle} = \overline{\operatorname{tr}(BA)} = \overline{\operatorname{tr}(AB)},$$

which shows that $\operatorname{tr}(AB)$ is equal to its conjugate and therefore real for all $A, B \in \mathcal{H}_n$.

(iii) To prove the completeness of \mathcal{H}_n we need but note that \mathcal{H}_n is finite dimensional and therefore complete by Theorem A.6. \square

Note that use of the inner product, defined on the space of Hermitian matrices, is compatible with vectors as well, since we have that

$$\langle Ax, x \rangle_{\mathbb{C}}^n = x^*Ax = \operatorname{tr}(x^*Ax) = \operatorname{tr}(Axx^*) = \langle A, xx^* \rangle_2,$$

where $\langle \cdot, \cdot \rangle_{\mathbb{C}}^n$ denotes the standard inner product on \mathbb{C}^n , $x^*Ax = \operatorname{tr}(x^*Ax)$ holds, since x^*Ax is a scalar and $xx^* \in \mathcal{H}_n$. Therefore, we use these inner products interchangeably, as the situation dictates, and in most cases drop the subscript.

It is interesting to note that if $A \in \mathcal{H}_n$, the Frobenius norm, $\|\cdot\|_2$, may be written as $\|A\|_2 = \sqrt{\operatorname{tr}(A^*A)} = \sqrt{\operatorname{tr}(A^2)}$.

We now prove some results regarding rank one matrices. We will see later on that rank one matrices play an important role in our study of the cone of positive semidefinite matrices.

Theorem 1.1.6. *Let $A \in \mathcal{M}_n(\mathbb{C})$. Then A has rank one if and only if there exist two non-zero vectors $u, v \in \mathbb{C}^n$ such that*

$$A = uv^*.$$

*Furthermore, such an A has at most one non-zero eigenvalue (of algebraic multiplicity one), equal to v^*u . Moreover, u is a right and v is a left eigenvector corresponding to this eigenvalue.*

Proof. We start by proving that A does in fact have the form given in the theorem, we then show that it has at most one non-zero eigenvector, of algebraic multiplicity one, and

that this eigenvalue is as stated above. Lastly, we show that u is a right and v is a left eigenvector corresponding to this eigenvalue.

\implies Assume that $A = [a_{ij}]_{i,j=1}^n$ has rank one. Then the dimension of the column space is one, which means that a basis for the column space consists of only one vector, say u . Note that $u \in \mathbb{C}^n$. Therefore, every column vector of A is a linear combination of u , in other words $a_{*j} = \beta_j u$ where a_{*j} denotes the j -th column of A . Now, let $v = [\bar{\beta}_j]_{j=1}^n$, then $A = uv^*$, and $u, v \in \mathbb{C}^n$. Furthermore u and v must be non-zero, else A will be the zero matrix, which has rank 0 and contradicts our assumption that the rank of A is one.

\Leftarrow Let $u, v \in \mathbb{C}^n$ be non-zero vectors such that $A = uv^*$. Say $u = [\alpha_j]_{j=1}^n$ and $v = [\beta_j]_{j=1}^n$. Then

$$A = uv^* = \begin{bmatrix} A_1 \\ \vdots \\ A_n \end{bmatrix} \begin{bmatrix} \bar{\beta}_1 & \cdots & \bar{\beta}_n \end{bmatrix} = \begin{bmatrix} A_1 \bar{\beta}_1 & \cdots & A_1 \bar{\beta}_n \\ \vdots & \ddots & \vdots \\ A_n \bar{\beta}_1 & \cdots & A_n \bar{\beta}_n \end{bmatrix}.$$

From this it is obvious that every column of A is a linear combination of u , therefore $\{u\}$ is a basis for the column space of A . Since the basis of the column space exists of only one vector, it has rank one. Therefore A has rank one if and only if $A = uv^*$ where $u, v \in \mathbb{C}^n$ are non-zero vectors.

Next, assume that A is a $n \times n$ matrix where $n > 1$. Note that since A does not have full rank, $\det(A) = 0$ and thus 0 is an eigenvalue of A . The set of all vectors $x \in \mathbb{C}^n$ satisfying $Ax = \lambda x$ is called the eigenspace of A corresponding to the eigenvalue λ . The dimension of the eigenspace of A , corresponding to the eigenvalue λ , is called the geometric multiplicity of λ . Note that the geometric multiplicity of an eigenvalue is always less than or equal to the algebraic multiplicity of the eigenvalue. Now, the eigenspace of A corresponding to the eigenvalue 0 is the set of all $x \in \mathbb{C}^n$ such that $Ax = 0$, and we see that it is the same as the null space of A . Therefore, to determine the geometric multiplicity of 0 we need but calculate the dimension of the null space, which is called the nullity of A . The following well-known equality gives the relation between the rank and nullity of A :

$$\text{nullity}(A) + \text{rank}(A) = n.$$

Since $\text{rank}(A) = 1$, it follows that $\text{nullity}(A) = n - 1$. Thus, the geometric multiplicity of the eigenvalue 0 is equal to $n - 1$. From this it immediately follows that there exists, at most, one non-zero eigenvalue of A with algebraic multiplicity one.

Now, assume there exists a non-zero eigenvalue of A , say λ . Let x be the associated eigenvector, then

$$Ax = \lambda x.$$

Writing $A = uv^*$, we have the following

$$uv^*x = \lambda x \implies v^*uv^*x = \lambda v^*x \implies (v^*u - \lambda)v^*x = 0.$$

Since $v^*x \neq 0$, $\lambda = v^*u$.

Finally, let $A = uv^*$ with eigenvalue $\lambda = v^*u$. Then $Au = uv^*u = u\lambda = \lambda u$ and $v^*A = v^*uv^* = \lambda v^*$, proving that u is a right and v is a left eigenvector as claimed. \square

1.2 Positive Semidefinite Matrices

The notion of positive semidefinite matrices is central to our question regarding completions of partial Hermitian matrices, as we wish to know when a partial Hermitian matrix admits a positive semidefinite completion.

First of all, we give the condition under which a matrix is said to be positive semidefinite.

Definition 1.2.1 (Positive Semidefinite). Let $A \in \mathcal{H}_n$. A is said to be positive semidefinite if

$$x^*Ax \geq 0, \quad \text{for all non-zero } x \in \mathbb{C}^n.$$

If the inequality is strictly greater than 0, A is said to be positive definite.

Equivalently, we formulate this condition in terms of the inner product defined in the previous section.

Definition 1.2.2. Let $A \in \mathcal{H}_n$. A is said to be positive semidefinite if

$$\langle Ax, x \rangle = \text{tr}(Axx^*) \geq 0, \quad \text{for all non-zero } x \in \mathbb{C}^n.$$

If the inequality is strictly greater than 0, A is said to be positive definite. We write $A \succeq 0$ for a positive semidefinite matrix and $A \succ 0$ for a positive definite matrix. If the inequalities are reversed, we say the matrix is negative (semi)definite. If none of the above is true, we say the matrix is indefinite.

We may now define an ordering on the subset of Hermitian matrices.

Definition 1.2.3 (Partial Ordering of Hermitian Matrices). Let $A, B \in \mathcal{H}_n$. We write $B \succeq A$ if the matrix $B - A$ is positive semidefinite. Similarly, $B \succ A$ means that $B - A$ is positive definite.

Note that if $A \succeq B$ and $B \succeq A$, then $A = B$. It is easy to see that the relation \succeq is transitive and reflexive, say $B \succeq A$ and $C \succeq B$ then $B - A$ and $C - B$ are positive semidefinite and thus $(C - B) + (B - A) = C - A$ is positive semidefinite, and since $A - A = 0$ is positive semidefinite, we have that $A \succeq A$ is always true. However it is not a total order, since there exist $A, B \in \mathcal{H}_n$, such that neither $A \succeq B$ nor $B \succeq A$. All of the above holds for \preceq and \prec . This partial order is known as the Loewner order on matrices.

Positive semidefinite matrices have many useful properties, some of which we now mention.

Lemma 1.2.4. [17, Observation 7.1.2] *The principal submatrices of a positive semidefinite matrix are positive semidefinite. For a positive definite matrix the principal submatrices are positive definite.*

Theorem 1.2.5. [17, Observation 7.1.4] *The eigenvalues of a positive semidefinite matrix are all non-negative numbers. In particular, if A is positive definite, the eigenvalues are positive numbers.*

Corollary 1.2.6. [17, Corollary 7.1.5] *The trace, determinant and all principal minors of a positive semidefinite matrix are non-negative.*

For a positive definite matrix, non-negative becomes positive. From this we see that every positive definite matrix is non-singular, since the determinant is strictly greater than zero. This in turn implies that all positive definite matrices have full rank, i.e., if $A \in \mathcal{M}_n(\mathbb{C})$ is positive definite, then $\text{rank}(A) = n$.

From the following theorem we see that it suffices to calculate the spectrum of a Hermitian matrix when we wish to determine whether the matrix is positive semidefinite.

Theorem 1.2.7. [17, Theorem 7.2.1] *A matrix $A \in \mathcal{H}_n$ is positive semidefinite if and only if all of its eigenvalues are non-negative. It is positive definite if and only if all of its eigenvalues are positive.*

Note that if a Hermitian matrix A is non-singular and positive semidefinite, we may conclude that it is positive definite, since 0 is not an eigenvalue of A and all other eigenvalues are positive.

We now prove a decomposition result for positive semidefinite matrices, with respect to rank one matrices.

Theorem 1.2.8. *Let $A \in \mathcal{H}_n$ be positive semidefinite. Then A has rank one if and only if there exists a non-zero vector $u \in \mathbb{C}^n$ such that*

$$A = uu^*.$$

Proof. Since A is Hermitian, we may apply the spectral theorem for Hermitian matrices (Theorem 1.1.3) and write $A = U\Lambda U^*$. We now prove the theorem.

\implies Assume that $A = [a_{ij}]_{i,j=1}^n$ has rank one. From Theorem 1.1.6 we know that A has, at most, one non-zero eigenvalue, thus we may write $\Lambda = \text{diag}(\lambda_1, 0, \dots, 0)$ as the real diagonal matrix in the spectral decomposition of A . Therefore, $A = U\Lambda U^* = \lambda_1 u_1 u_1^*$, where u_1 denotes the first column of U . Now, the eigenvalues of A are non-negative (Theorem 1.2.5), therefore the square root of λ_1 is real and non-negative and we may define $u = \sqrt{\lambda_1} u_1$. Thus, we have that $A = uu^*$. Note that $u \neq 0$, since $A \neq 0$, from our assumption that A has rank one.

\impliedby Let $u \in \mathbb{C}^n$ be a non-zero vector such that $A = uu^*$. The fact that A has rank one follows from Theorem 1.1.6. \square

Note that, from Theorem 1.1.6, we know that if a matrix A has rank one, it has at most one non-zero eigenvalue. Thus, when A is a rank one positive semidefinite matrix the eigenvalue is equal to u^*u , also u is a right and left eigenvector corresponding to this eigenvalue. We now extend the result of Theorem 1.2.8 to show that any positive semidefinite matrix can be written as the sum of rank one positive semidefinite matrices.

Theorem 1.2.9. [17, Theorem 7.5.2] *Let $A \in \mathcal{H}_n$ be a positive semidefinite matrix, with $\text{rank}(A) = k$, then A may be written in the form*

$$A = v_1 v_1^* + v_2 v_2^* + \dots + v_k v_k^*,$$

where each $v_i \in \mathbb{C}^n$ and the set $\{v_1, \dots, v_k\}$ is an orthogonal set of non-zero vectors.

Proof. Use the spectral theorem, Theorem 1.1.3, to write $A = U\Lambda U^*$ and let v_i be equal to $\lambda_i^{1/2}$ times the i -th column of U , similar to the first part of the proof of Theorem 1.2.8. Then the result follows immediately. \square

Our next goal is to introduce the Cholesky factorization of positive semidefinite matrices. However, we first need the following theorem.

Theorem 1.2.10. [17, Theorem 7.2.7] *A matrix $A \in \mathcal{M}_n(\mathbb{C})$ is positive semidefinite if and only if there is a matrix $C \in \mathcal{M}_n(\mathbb{C})$ such that $A = C^*C$. In particular, A is positive definite if and only if C is non-singular.*

Proof. Assume that A is positive semidefinite. Let $C = A^{1/2}$, where $A^{1/2}$ exists by Theorem B.4 and is positive semidefinite Hermitian. Thus, the wished for factorization does indeed exist. Note that if A is positive definite $A^{1/2}$ is as well (Theorem B.4 (ii)), which implies that C is non-singular.

Conversely, if $A = C^*C$, it is easily seen to be positive semidefinite, since, for all non-zero $x \in \mathbb{C}^n$,

$$\langle Ax, x \rangle = \langle C^*Cx, x \rangle = \langle Cx, Cx \rangle = \|Cx\|^2 \geq 0.$$

Note that equality holds if and only if $Cx = 0$, so if C is non-singular this is impossible and consequently A is positive definite. \square

The factorization $A = C^*C$ of a positive semidefinite matrix can be specialized by applying the QR factorization (Theorem B.3) in the following way:

Every matrix $C \in \mathcal{M}_n(\mathbb{C})$ can be written as $C = QR$, where Q is unitary and R is an upper triangular matrix with the same rank as C . Then we have that

$$A = C^*C = (QR)^*QR = R^*Q^*QR = R^*R,$$

since $Q^*Q = I$. Moreover, if C is non-singular, we may choose R in such a way that all of its diagonal entries are positive and the factorization $C = QR$ is unique. If C is real, Q and R may both be taken to be real. We have therefore established the following corollary, which gives the lower-upper Cholesky factorization of A .

Corollary 1.2.11. [17, Corollary 7.2.9] *A matrix A is positive semidefinite if and only if there exists a lower triangular matrix $L \in \mathcal{M}_n(\mathbb{C})$ with positive diagonal entries such that $A = LL^*$. Moreover, A is positive definite if and only if L is non-singular. If A is real, L may be taken to be real.*

Our final characterization of positive semidefinite matrices is that they may always be seen as, so-called, Gram matrices, which we will now define.

Let $\{u_1, \dots, u_n\}$ be a set of n vectors in an inner product space \mathcal{U} , with some given inner product $\langle \cdot, \cdot \rangle$. The Gram matrix of the vectors $\{u_1, \dots, u_n\}$ is defined as the matrix $G = [g_{ij}]_{i,j}^n \in \mathcal{M}_n(\mathbb{F})$, where $g_{ij} = \langle u_j, u_i \rangle$.

Theorem 1.2.12. [17, Theorem 7.2.10] *Let $G \in \mathcal{M}_n(\mathbb{C})$ be the Gram matrix of the vectors $\{u_1, \dots, u_n\}$, $u_i \in \mathbb{C}^k$, $i = 1, \dots, n$, with respect to a given inner product $\langle \cdot, \cdot \rangle$, and let $U = [u_1 \ \cdots \ u_n] \in \mathcal{M}_{k,n}(\mathbb{C})$. Then*

- (i) G is positive semidefinite;
- (ii) G is non-singular if and only if the vectors u_1, \dots, u_n are linearly independent;
- (iii) There exists a positive definite matrix $A \in \mathcal{M}_k(\mathbb{C})$ such that $G = U^*AU$;
- (iv) $\text{rank}(G) = \text{rank}(U) =$ maximum number of linearly independent vectors in the set $\{u_1, \dots, u_n\}$.

Proof. (i) G is easily seen to be Hermitian, since $g_{ij} = \langle u_j, u_i \rangle = \overline{\langle u_i, u_j \rangle} = \bar{g}_{ji}$. We now show that G is positive semidefinite: Let $x = [x_i]$ be a non-zero vector in \mathbb{C}^n , then

$$\begin{aligned} x^*Gx &= \sum_{i,j=1}^n g_{ij}\bar{x}_i x_j = \sum_{i,j=1}^n \langle u_j, u_i \rangle \bar{x}_i x_j \\ &= \sum_{i,j=1}^n \langle x_j u_j, x_i u_i \rangle = \left\langle \sum_{j=1}^n x_j u_j, \sum_{i=1}^n x_i u_i \right\rangle \\ &= \left\| \sum_{i=1}^n x_i u_i \right\|^2 \geq 0, \end{aligned}$$

where $\|\cdot\|$ is the norm induced by the given inner product. Therefore, G is positive semidefinite.

(ii) Suppose G is singular, then there is some non-zero vector $x = [x_i]$ such that $Gx = 0$. Hence, $\|\sum_{i=1}^n x_i u_i\|^2 = x^*Gx = 0$, which in turn implies that $\sum_{i=1}^n x_i u_i = 0$, since $\|\cdot\|$ is a norm. From this we see that the set $\{u_1, \dots, u_n\}$ must be linearly dependent, because x is a non-zero vector, and, therefore, there exists at least one $x_i \neq 0$.

Conversely, if $\sum_{i=1}^n x_i u_i = 0$, with $x = [x_i] \neq 0$, then $x^*Gx = 0$ so $Gx = 0$, which implies that G is singular, since x is non-zero.

(iii) Let $\{e_1, \dots, e_k\}$ be the standard basis of \mathbb{C}^k , then the matrix $A = [\langle e_j, e_i \rangle]_{i,j=1}^k$ is a non-singular positive semidefinite matrix by (i) and (ii), which implies that it is positive definite (see the remark after Theorem 1.2.7). Now, for any $x, y \in \mathbb{C}^k$ we have

$$\langle y, x \rangle = \left\langle \sum_{j=1}^k y_j e_j, \sum_{i=1}^k x_i e_i \right\rangle = \sum_{i,j=1}^k \langle e_j, e_i \rangle \bar{x}_i y_j = x^*Ay.$$

Thus, $g_{ij} = \langle u_j, u_i \rangle = u_i^* A u_j$, consequently $G = U^*AU$.

(iv) We first show that the null spaces of G and U coincide. Let x be in the null space of G , then $Gx = 0$. Thus,

$$0 = x^*Gx = x^*U^*AUx = (Ux)^*A(Ux),$$

which implies that $Ux = 0$ since A is positive definite, and so x is in the null space of U . Conversely, let x be in the null space of U , then $Ux = 0$. Therefore,

$$Gx = U^*AUx = 0,$$

which shows that x is in the null space of G . Consequently, G and U have the same null space, from which we may conclude that they have the same rank.

Finally, the column rank of U is the maximum number of linearly independent vectors in the set $\{u_1, \dots, u_n\}$. \square

We will now prove that a matrix is positive semidefinite if and only if it is the Gram matrix of some set of linearly independent vectors.

Corollary 1.2.13. *[17, Corollary 7.2.11] Let $A \in \mathcal{M}_n(\mathbb{C})$ be a given matrix. Then A is positive semidefinite with rank $r \leq n$ if and only if there is a set of vectors $S = \{u_1, \dots, u_n\} \subseteq \mathbb{C}^k$ containing exactly r linearly independent vectors such that A is the Gram matrix of S with respect to the standard inner product.*

Proof. We saw in the previous theorem that if A is a Gram matrix, it is positive semidefinite. Conversely, assume that A is positive semidefinite. Then the square root of A exists, namely, $B = A^{1/2}$ and is itself positive semidefinite (Theorem B.4). The rank of B is the same as the rank of A and $A = B^2 = B^*B$ is the Gram matrix of the columns of B with respect to the standard inner product. \square

Chapter 2

Cones of Hermitian matrices

In this chapter we introduce some notions concerning convex cones. We start by proving some results for general convex cones and then focus on cones of Hermitian matrices, in particular, the cone of positive semidefinite matrices.

2.1 Cones and their basic properties

Definition 2.1.1 (Convex Cone). Let \mathcal{H} be a Hilbert space over \mathbb{R} with inner product $\langle \cdot, \cdot \rangle$. A non-empty subset \mathcal{C} of \mathcal{H} is called a convex cone if

- (i) $\mathcal{C} + \mathcal{C} \subseteq \mathcal{C}$
- (ii) $\alpha\mathcal{C} \subseteq \mathcal{C}$, for all $\alpha > 0$.

Thus a subset of \mathcal{H} is called a convex cone if it is closed under addition and multiplication by positive scalars.

If $C_1, C_2 \in \mathcal{C}$ then $sC_1 + (1-s)C_2 \in \mathcal{C}$ for $s \in [0, 1]$. Hence a convex cone is convex. The convex cone \mathcal{C} is closed if $\mathcal{C} = \bar{\mathcal{C}}$, where $\bar{\mathcal{C}}$ denotes the closure of \mathcal{C} . As we will only be using convex cones, we will henceforth refer to them as cones.

We call a cone \mathcal{C} salient if and only if $\mathcal{C} \cap -\mathcal{C} \subseteq \{0\}$, in other words, if X and $-X$ are elements of \mathcal{C} , we have that $X = 0$. \mathcal{C} is pointed if $0 \in \mathcal{C}$. A salient pointed cone \mathcal{C} induces a partial order \leq on \mathcal{H} , defined as follows:

$$X \leq Y \text{ if } Y - X \in \mathcal{C}.$$

If \mathcal{C} is not salient it only induces a preorder.

In the following proposition we see that the intersection and sum of two cones both form a cone.

Proposition 2.1.2. [2, Proposition 1.1.1] Let \mathcal{H} be a Hilbert space and let \mathcal{C}_1 and \mathcal{C}_2 be cones in \mathcal{H} . Then the following are also cones:

(i) $\mathcal{C}_1 \cap \mathcal{C}_2$, and

(ii) $\mathcal{C}_1 + \mathcal{C}_2 = \{C_1 + C_2 : C_1 \in \mathcal{C}_1, C_2 \in \mathcal{C}_2\}$

Next we introduce the notion of a dual cone, which will be of significant importance later on, as the completion process is easily explained through the use of cones and dual cones.

Definition 2.1.3 (Dual of a Cone). Let \mathcal{H} be a Hilbert space and let \mathcal{C} be a cone in \mathcal{H} . The dual \mathcal{C}^* of \mathcal{C} is defined as

$$\mathcal{C}^* = \{L \in \mathcal{H} : \langle L, K \rangle \geq 0 \text{ for all } K \in \mathcal{C}\}.$$

We call a cone \mathcal{C} selfdual if $\mathcal{C} = \mathcal{C}^*$. Not surprisingly, the dual cone is a cone in its own right. Also, it is always closed, regardless of whether the original cone was closed or not.

Lemma 2.1.4. [2, Lemma 1.1.2] *Let \mathcal{H} be a Hilbert space. The dual of a cone is again a cone. Furthermore the dual is always closed, regardless of the original cone.*

Proof. Let \mathcal{C} be a cone and let \mathcal{C}^* be the dual cone of \mathcal{C} . Now let $L_1, L_2 \in \mathcal{C}^*$ and let $\alpha, \beta > 0$ be scalars. Then $\langle L_1, K \rangle \geq 0$ and $\langle L_2, K \rangle \geq 0$ for all $K \in \mathcal{C}$, therefore

$$0 \leq \langle \alpha L_1, K \rangle + \langle \beta L_2, K \rangle = \langle \alpha L_1 + \beta L_2, K \rangle,$$

thus $\alpha L_1 + \beta L_2 \in \mathcal{C}^*$. This proves that \mathcal{C}^* is a cone.

We now prove that \mathcal{C}^* is closed, regardless of whether \mathcal{C} is closed or not. Let $\{L^{(n)}\}_{n \in \mathbb{N}}$ be a Cauchy sequence in \mathcal{H} , such that $L^{(1)}, L^{(2)}, \dots \in \mathcal{C}^*$. Every Cauchy sequence converges in \mathcal{H} , because of the completeness of \mathcal{H} . Now say $\{L^{(n)}\}_{n \in \mathbb{N}}$ converges to L . We need to prove that L is in \mathcal{C}^* . From the continuity of the inner product (Lemma A.5) we have the following

$$0 \leq \langle L^{(n)}, K \rangle \longrightarrow \langle L, K \rangle \text{ for all } K \in \mathcal{C},$$

thus $\langle L, K \rangle \geq 0$, for all $K \in \mathcal{C}$. Therefore $L \in \mathcal{C}^*$, which proves that \mathcal{C}^* is closed. \square

We now consider a subspace of a Hilbert space. This subspace naturally forms a cone, as it is closed under addition and scalar multiplication. However, it is not so obvious that the dual cone of this subspace is equal to its orthogonal complement, which we will prove in the following theorem.

Theorem 2.1.5. [2, Lemma 1.1.2] *Let \mathcal{H} be a Hilbert space and \mathcal{W} a subspace of \mathcal{H} . Then \mathcal{W} is a cone and its dual is equal to its orthogonal complement.*

Proof. We start by showing that \mathcal{W} is a cone and then that its dual is equal to its orthogonal complement.

Let \mathcal{W} be a subspace of \mathcal{H} . Then \mathcal{W} is an inner product space with the same inner product as \mathcal{H} restricted to $\mathcal{W} \times \mathcal{W}$. Now \mathcal{W} is a vector space and therefore closed under addition and multiplication, in particular multiplication by positive scalars. Thus \mathcal{W} is a cone.

We need but prove that $\mathcal{W}^* \subseteq \mathcal{W}^\perp$, since $\mathcal{W}^\perp \subseteq \mathcal{W}^*$ is always true. If $h \in \mathcal{W}^*$ and $w \in \mathcal{W}$, then $\langle h, w \rangle \geq 0$, thus for $-w \in \mathcal{W}$ we have $\langle h, -w \rangle \leq 0$. Since $-w \in \mathcal{W}$, we also have $\langle h, -w \rangle \geq 0$. Hence $\langle h, -w \rangle = 0$. Then also $\langle h, w \rangle = 0$. So if $h \in \mathcal{W}^*$ then $\langle h, w \rangle = 0$ for all $w \in \mathcal{W}$, which shows that $h \in \mathcal{W}^\perp$. Thus $\mathcal{W}^* \subseteq \mathcal{W}^\perp$. \square

In the following theorem we make use of hyperplanes. A hyperplane is a generalization of the two-dimensional plane in \mathbb{R}^3 into a larger number of dimensions. A hyperplane of an n -dimensional space is a flat subset with dimension $n - 1$. By its nature, it separates the space into two half spaces, as we will now see.

Theorem 2.1.6. [10, Theorem 4.4.2] *Let \mathcal{H} be a Hilbert space. Given a closed convex cone $\mathcal{C} \subset \mathcal{H}$ and a point $X \in \mathcal{H} \setminus \mathcal{C}$, there exists a $L \in \mathcal{H}$ such that*

$$\langle X, L \rangle < 0 \text{ and } \langle K, L \rangle \geq 0 \text{ for all } K \in \mathcal{C}.$$

Proof. We start the proof by setting $L = S - X$, with $S \in \mathcal{C}$ the nearest point to X (in terms of the metric induced by the inner product). The existence of S follows from Theorem A.7. Note that $L \neq 0$, since S and X are distinct values.

We first prove that $\langle X, L \rangle < 0$. Observe the following

$$0 < \langle L, L \rangle = \langle S - X, L \rangle = \langle S, L \rangle - \langle X, L \rangle.$$

If we can show that $\langle S, L \rangle = 0$, the wished for result follows.

If $S = 0$ it is clear. For $S \neq 0$, we first assume that $\langle S, L \rangle > 0$, and set $S' = (1 - \alpha)S = L + X - \alpha(L + X)$, for $0 < \alpha < 1$ and $\alpha \in \mathbb{R}$. Note that $S' \in \mathcal{C}$, since \mathcal{C} is a cone. Now,

$$\|S' - X\|^2 = \|L - \alpha S\|^2 = \langle (L - \alpha S), (L - \alpha S) \rangle = \|L\|^2 - 2\alpha \operatorname{Re}(\langle S, L \rangle) + \alpha^2 \|S\|^2.$$

From our assumption that $\langle S, L \rangle > 0$, it follows that $\operatorname{Re}(\langle S, L \rangle) > 0$ which in turn implies that $2\alpha \operatorname{Re}(\langle S, L \rangle) > \alpha^2 \|S\|^2$ for all sufficiently small $\alpha > 0$. Thus $\|S' - X\|^2 < \|L\|^2 = \|S - X\|^2$, which contradicts S being the nearest point to X . This shows that $\langle S, L \rangle > 0$ cannot be true. For the case $\langle S, L \rangle < 0$ a similar argument follows for $S' = (1 + \alpha)S$. This proves that $\langle S, L \rangle = 0$. Therefore $\langle X, L \rangle < 0$.

Next, we prove that $\langle K, L \rangle \geq 0$. Let $K \in \mathcal{C}$, $K \neq S$. The angle $\angle KSX$ has to be at least 90° . Say this were not so, then $\angle KSX < 90^\circ$. We may then take the projection S' , not equal to S , of X , on the line through K and S , such that

$$S' \in \{K + \delta(S - K) : \delta \in [0, 1]\} \subseteq \mathcal{C}.$$

Now,

$$\|X - S'\| \leq \|X - S\| = \inf_{K \in \mathcal{C}} \|X - K\| \leq \|X - S'\|.$$

Hence, $\|X - S'\| = \|X - S\|$, but S is the unique point with smallest distance to X , thus $S' = S$, which contradicts our choice of S' . Therefore, $\angle KSX \geq 90^\circ$. Next, note that the inner product may be written as $\langle x, y \rangle = \|x\| \|y\| \cos \theta$, where θ is the angle between the vectors x and y and $\theta \in [-180^\circ, 180^\circ]$. Now using this form of the inner product we have the following

$$\langle (K - S), (X - S) \rangle = \|K - S\| \|X - S\| \cos \theta \leq 0,$$

since $\theta = \angle K S X \geq 90^\circ$ and $\cos \theta \leq 0$ for $\theta \in [90^\circ, 180^\circ]$. Thus,

$$0 \geq \langle (K - S), (X - S) \rangle = \langle (K - S), -L \rangle = -\langle K, L \rangle + \langle S, L \rangle,$$

and from the first part of the proof we know that $\langle S, L \rangle = 0$. Thus $-\langle K, L \rangle \leq 0$ which implies that $\langle K, L \rangle \geq 0$. \square

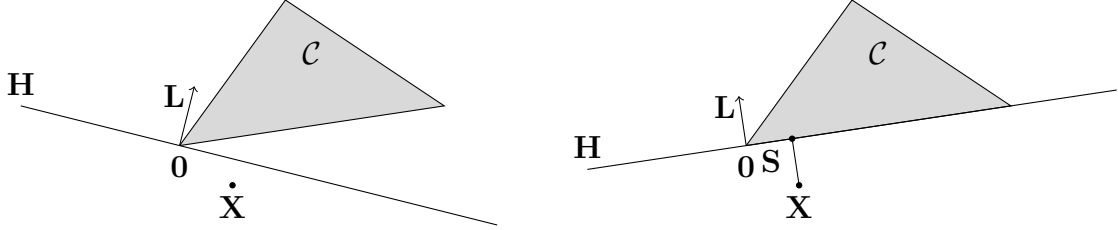


Figure 2.1: In the figure on the left we see a point $X \in \mathbb{R}^2 \setminus \mathcal{C}$ can be separated from \mathcal{C} by a hyperplane $H = \{K \in \mathbb{R}^2 : \langle L, K \rangle = 0\}$ through the origin. The figure on the right shows the separating hyperplane resulting from the proof of Theorem 2.1.6.

We are now ready to prove some properties of cones and their duals.

Lemma 2.1.7. [2, Lemma 1.1.2] For cones \mathcal{C} , \mathcal{C}_1 and \mathcal{C}_2 we have the following statements:

- (i) if $\mathcal{C}_1 \subseteq \mathcal{C}_2$, then $\mathcal{C}_2^* \subseteq \mathcal{C}_1^*$;
- (ii) $(\mathcal{C}^*)^* = \overline{\mathcal{C}}$;
- (iii) $\mathcal{C}_1^* + \mathcal{C}_2^* \subseteq (\mathcal{C}_1 \cap \mathcal{C}_2)^*$;
- (iv) $(\mathcal{C}_1 + \mathcal{C}_2)^* = \mathcal{C}_1^* \cap \mathcal{C}_2^*$.

Proof. (i) Let $L \in \mathcal{C}_2^*$. Then $\langle L, C \rangle \geq 0$, for all $C \in \mathcal{C}_2$. Since $\mathcal{C}_1 \subseteq \mathcal{C}_2$, it follows that $\langle L, C \rangle \geq 0$, for all $C \in \mathcal{C}_1$, thus $L \in \mathcal{C}_1^*$. Therefore $\mathcal{C}_2^* \subseteq \mathcal{C}_1^*$.

(ii) For any $C \in \mathcal{C}$, we have, by the definition of the dual of a cone, that $\langle K, C \rangle \geq 0$, for all $K \in \mathcal{C}^*$. We therefore have that $C \in (\mathcal{C}^*)^*$. Thus, $\overline{\mathcal{C}} \subseteq \overline{(\mathcal{C}^*)^*} = (\mathcal{C}^*)^*$, where the last equality holds, since $(\mathcal{C}^*)^*$ is the dual of a cone and is therefore closed by Lemma 2.1.4. Next we will prove, by contradiction, that $(\mathcal{C}^*)^* \subset \overline{\mathcal{C}}$. Suppose $(\mathcal{C}^*)^* \subset \overline{\mathcal{C}}$ is not true, then there exists a $X \in (\mathcal{C}^*)^* \setminus \overline{\mathcal{C}}$. Now, by Theorem 2.1.6, we have the following,

$$\langle X, L \rangle < 0 \text{ and } \langle K, L \rangle \geq 0 \text{ for all } K \in \overline{\mathcal{C}},$$

for some $L \in \mathcal{H}$. From the second inequality we see that $L \in \mathcal{C}^*$. Therefore, we have a contradiction, since for $X \in (\mathcal{C}^*)^*$ and $L \in \mathcal{C}^*$, we should have that $\langle X, L \rangle \geq 0$, but the first inequality shows that $\langle X, L \rangle < 0$. Thus $(\mathcal{C}^*)^* \subset \overline{\mathcal{C}}$ and so, $(\mathcal{C}^*)^* = \overline{\mathcal{C}}$.

(iii) Let $L = L_1 + L_2 \in \mathcal{C}_1^* + \mathcal{C}_2^*$, where $L_1 \in \mathcal{C}_1^*$ and $L_2 \in \mathcal{C}_2^*$. For any $K \in \mathcal{C}_1 \cap \mathcal{C}_2$ we have, $0 \leq \langle L, K \rangle = \langle L_1, K \rangle + \langle L_2, K \rangle$, and since $L_i \in \mathcal{C}_i^*$, for $i = 1, 2$, it follows that $\langle L_1, K \rangle \geq 0$ for all $K \in \mathcal{C}_1$, and $\langle L_2, K \rangle \geq 0$ for all $K \in \mathcal{C}_2$. Therefore $L \in (\mathcal{C}_1 \cap \mathcal{C}_2)^*$. Thus $\mathcal{C}_1^* + \mathcal{C}_2^* \subseteq (\mathcal{C}_1 \cap \mathcal{C}_2)^*$.

(iv) We prove the two inclusions $(\mathcal{C}_1 + \mathcal{C}_2)^* \subseteq \mathcal{C}_1^* \cap \mathcal{C}_2^*$ and $\mathcal{C}_1^* \cap \mathcal{C}_2^* \subseteq (\mathcal{C}_1 + \mathcal{C}_2)^*$.

For the first inclusion, note that if $0 \in \mathcal{C}_2$, then $\mathcal{C}_1 \subseteq \mathcal{C}_1 + \mathcal{C}_2$, and thus $(\mathcal{C}_1 + \mathcal{C}_2)^* \subseteq \mathcal{C}_1^*$ (by part (i)). Similarly, $0 \in \mathcal{C}_1$ implies $(\mathcal{C}_1 + \mathcal{C}_2)^* \subseteq \mathcal{C}_2^*$. Hence, if $0 \in \mathcal{C}_1 \cap \mathcal{C}_2$, the inclusion follows. If \mathcal{C}_i , $i = 1, 2$, is not closed, 0 need not be in \mathcal{C}_i . However, we can get arbitrarily close to 0 with elements from \mathcal{C}_i . Recall that $\alpha\mathcal{C} \subseteq \mathcal{C}$ for $\alpha > 0$. Let $L \in (\mathcal{C}_1 + \mathcal{C}_2)^*$ then $\langle L, C \rangle \geq 0$, for all $C \in \mathcal{C}_1 + \mathcal{C}_2$. Now, say $C = C_1 + \alpha C_2$, where $C_1 \in \mathcal{C}_1, C_2 \in \mathcal{C}_2$ and $\alpha > 0$, then

$$0 \leq \langle L, C \rangle = \langle L, C_1 + \alpha C_2 \rangle = \langle L, C_1 \rangle + \langle L, \alpha C_2 \rangle.$$

Let $\alpha \rightarrow 0$, then we have that $L \in \mathcal{C}_1^*$. We use a similar argument to show that $L \in \mathcal{C}_2^*$. Therefore, $(\mathcal{C}_1 + \mathcal{C}_2)^* \subseteq \mathcal{C}_1^* \cap \mathcal{C}_2^*$.

Next, let $L \in \mathcal{C}_1^* \cap \mathcal{C}_2^*$. Then $L \in \mathcal{C}_1^*$ and $L \in \mathcal{C}_2^*$. Thus, $\langle L, C_1 \rangle \geq 0$ for all $C_1 \in \mathcal{C}_1$ and $\langle L, C_2 \rangle \geq 0$ for all $C_2 \in \mathcal{C}_2$. Now, we have $0 \leq \langle L, C_1 \rangle + \langle L, C_2 \rangle = \langle L, C_1 + C_2 \rangle$. Therefore, $L \in (\mathcal{C}_1 + \mathcal{C}_2)^*$, proving that $\mathcal{C}_1^* \cap \mathcal{C}_2^* \subseteq (\mathcal{C}_1 + \mathcal{C}_2)^*$. Thus, $\mathcal{C}_1^* \cap \mathcal{C}_2^* = (\mathcal{C}_1 + \mathcal{C}_2)^*$. \square

Note that if \mathcal{C} is a closed cone, we have that $(\mathcal{C}^*)^* = \overline{\mathcal{C}} = \mathcal{C}$, by (ii) of the preceding lemma. Now, if we have a $X \notin \mathcal{C}$, it follows that $X \notin (\mathcal{C}^*)^*$. This in turn implies that there exists a $L \in \mathcal{C}^*$ such that $\langle X, L \rangle < 0$, and $\langle K, L \rangle \geq 0$ for any $K \in \mathcal{C}$, because $L \in \mathcal{C}^*$. Therefore, we may say that Lemma 2.1.7 (ii) is equivalent to the separation theorem (Theorem 2.1.6), stated before the lemma.

Lemma 2.1.7 now has the following interesting corollary.

Corollary 2.1.8. *Let \mathcal{C}_1 and \mathcal{C}_2 be closed cones. Then*

$$\overline{\mathcal{C}_1^* + \mathcal{C}_2^*} = (\mathcal{C}_1 \cap \mathcal{C}_2)^*.$$

Proof. Applying property (iv) of Lemma 2.1.7 with \mathcal{C}_1 and \mathcal{C}_2 replaced by \mathcal{C}_1^* and \mathcal{C}_2^* , respectively, and keeping in mind that both cones are closed, we obtain $(\mathcal{C}_1^* + \mathcal{C}_2^*)^* = (\mathcal{C}_1^*)^* \cap (\mathcal{C}_2^*)^* = \mathcal{C}_1 \cap \mathcal{C}_2$. Consequently we have that

$$(\mathcal{C}_1 \cap \mathcal{C}_2)^* = ((\mathcal{C}_1^* + \mathcal{C}_2^*)^*)^* = \overline{\mathcal{C}_1^* + \mathcal{C}_2^*}. \quad \square$$

Applying this corollary we may give an alternative proof for property (iii) of Lemma 2.1.7. We need but note that $\mathcal{C}_1^* + \mathcal{C}_2^* \subseteq \overline{\mathcal{C}_1^* + \mathcal{C}_2^*}$, and the result follows immediately.

We end this section by defining faces and extreme rays of a cone.

Definition 2.1.9 (Face of a cone). Let \mathcal{C} be a cone. A subset $\mathcal{F} \subseteq \mathcal{C}$ is called a face of \mathcal{C} if it is a subcone of \mathcal{C} such that $X = Y + Z$, with $X \in \mathcal{F}$ and $Y, Z \in \mathcal{C}$, implies that $Y, Z \in \mathcal{F}$.

Equivalently, \mathcal{F} is a face of \mathcal{C} if $0 \leq Y \leq X$ with $X \in \mathcal{F}$, implies that $Y \in \mathcal{F}$, where \leq is the order induced by \mathcal{C} . We define the dimension of the face \mathcal{F} as the dimension of its span, that is,

$$\dim(\mathcal{F}) := \dim(\text{span}(\mathcal{F})).$$

Note that since a face \mathcal{F} is also a cone, we have that $\text{span}(\mathcal{F}) = \mathcal{F} - \mathcal{F}$.

Definition 2.1.10 (Extreme ray). An extreme ray of a cone \mathcal{C} is a subset of $\mathcal{C} \cup \{0\}$ of the form $\{\alpha K : \alpha \geq 0\}$, where $0 \neq K \in \mathcal{C}$ is such that

$$K = A + B, \text{ for } A, B \in \mathcal{C} \Rightarrow A = \alpha K \text{ for some } \alpha \in [0, \infty).$$

Equivalently, $\{\alpha K : \alpha \geq 0\}$ is an extreme ray of \mathcal{C} if $0 \leq A \leq K$ implies that $A = \alpha K$, for some $\alpha \in [0, \infty)$, where \leq is the order induced by \mathcal{C} . Note that the extreme rays of a cone \mathcal{C} , are its faces of dimension 1.

2.2 The cone of positive semidefinite matrices

In this section we prove that the set of positive semidefinite matrices is in fact a selfdual cone. We then give a nice characterization of the smallest face containing a positive semidefinite matrix. Finally, we show that the extreme rays, of the cone of positive semidefinite matrices, are generated by rank one positive semidefinite matrices.

The following corollary of Theorem 1.2.9, besides being interesting, is necessary to show that the cone of positive semidefinite matrices is selfdual.

Corollary 2.2.1. *Let $A \in \mathcal{H}_n$. Then A is positive semidefinite if and only if $\langle A, B \rangle \geq 0$, for all positive semidefinite $B \in \mathcal{H}_n$. Furthermore, if A and B are positive semidefinite and $\langle A, B \rangle = 0$, it follows that $AB = 0$.*

Proof. \implies Since A and B are positive semidefinite, the square root of each exists (Theorem B.4), such that $A = A^{\frac{1}{2}}A^{\frac{1}{2}}$ and $B = B^{\frac{1}{2}}B^{\frac{1}{2}}$. Thus

$$\begin{aligned} \langle A, B \rangle &= \text{tr}(AB) = \text{tr}(A^{\frac{1}{2}}A^{\frac{1}{2}}B^{\frac{1}{2}}B^{\frac{1}{2}}) = \text{tr}(A^{\frac{1}{2}}B^{\frac{1}{2}}B^{\frac{1}{2}}A^{\frac{1}{2}}) \\ &= \text{tr}(A^{\frac{1}{2}}B^{\frac{1}{2}}(A^{\frac{1}{2}}B^{\frac{1}{2}})^*) = \langle A^{\frac{1}{2}}B^{\frac{1}{2}}, A^{\frac{1}{2}}B^{\frac{1}{2}} \rangle = \|A^{\frac{1}{2}}B^{\frac{1}{2}}\|^2. \end{aligned}$$

Thus, $\langle A, B \rangle \geq 0$.

\Leftarrow Let $u \in \mathbb{C}^n$, $u \neq 0$. Then $B = uu^*$ is positive semidefinite, by Theorem 1.2.8. We then have the following,

$$\langle Au, u \rangle = u^*Au = \text{tr}(u^*Au) = \text{tr}(Auu^*) = \text{tr}(AB) = \langle A, B \rangle \geq 0.$$

Therefore, A is positive semidefinite.

Next, let $\langle A, B \rangle = 0$. Since $\langle A, B \rangle = 0$, it follows that $\|A^{\frac{1}{2}}B^{\frac{1}{2}}\| = 0$. So $A^{\frac{1}{2}}B^{\frac{1}{2}} = 0$, which implies that $AB = A^{\frac{1}{2}}A^{\frac{1}{2}}B^{\frac{1}{2}}B^{\frac{1}{2}} = 0$. \square

Theorem 2.2.2 (The cone PSD_n). [2, Lemma 1.1.3] *The set of all $n \times n$ positive semidefinite matrices forms a salient pointed cone, which we will call PSD_n . Furthermore, this set is a self-dual cone ($\text{PSD}_n = (\text{PSD}_n)^*$) in the Hilbert space \mathcal{H}_n .*

Proof. We start by proving that the set of all $n \times n$ positive semidefinite matrices forms a cone. Let $A, B \in \text{PSD}_n$ and let $\alpha, \beta > 0$. Now consider

$$x^*(\alpha A + \beta B)x = \alpha x^*Ax + \beta x^*Bx \geq 0,$$

this shows that $\alpha A + \beta B$ is an element of PSD_n and therefore, per definition, PSD_n is a cone.

Next, we prove that (i) $\text{PSD}_n \subseteq (\text{PSD}_n)^*$ and (ii) $(\text{PSD}_n)^* \subseteq \text{PSD}_n$, to show that it is self-dual.

(i) Let $A \in \text{PSD}_n$. Then, from Corollary 2.2.1, it follows that $\langle A, B \rangle \geq 0$, for all $B \in \text{PSD}_n$. Thus $A \in (\text{PSD}_n)^*$, proving that $\text{PSD}_n \subseteq (\text{PSD}_n)^*$.

(ii) The second inclusion, also follows from Corollary 2.2.1. Let $A \in (\text{PSD}_n)^*$, then we have that $\langle A, B \rangle \geq 0$ for every positive semidefinite matrix B . Thus, A is positive semidefinite. Therefore, $(\text{PSD}_n)^* \subseteq \text{PSD}_n$.

Finally, it is easy to see that PSD_n is salient, since $X \in \text{PSD}_n$ and $-X \in \text{PSD}_n$ implies that $X = 0$ and it is pointed since the zero matrix is positive semidefinite. \square

Note that since PSD_n is selfdual, it immediately follows that it is a closed subset of \mathcal{H}_n , by Lemma 2.1.4.

Let $X \in \text{PSD}_n$ and denote by $\mathcal{F}_{\text{PSD}_n}(X)$ the smallest (with respect to inclusion) face of PSD_n that contains X . We now have the following proposition regarding the structure of $\mathcal{F}_{\text{PSD}_n}(X)$.

Proposition 2.2.3. [3, Lemma 4] *Let $X \in \text{PSD}_n$. Then*

$$\mathcal{F}_{\text{PSD}_n}(X) = \{Y \in \text{PSD}_n : \ker(X) \subseteq \ker(Y)\}.$$

Proof. We show that $Y \in \mathcal{F}_{\text{PSD}_n}(X)$ if and only if $\ker(X) \subseteq \ker(Y)$.

Assume that $Y \in \mathcal{F}_{\text{PSD}_n}(X)$, then $X - Y$ is positive semidefinite. If $k \in \ker(X)$, we have

$$0 \leq \langle (X - Y)k, k \rangle = \langle Xk, k \rangle - \langle Yk, k \rangle = -\langle Yk, k \rangle \leq 0.$$

which implies that $k \in \ker(Y)$.

Conversely, assume that $\ker(X) \subseteq \ker(Y)$. Let

$$H = \{h \in \mathbb{C}^n : h \in \text{ran}(X) \text{ and } \|h\| = 1\},$$

where $\text{ran}(X)$ denotes the range of X . Note that $\text{ran}(X) = (\ker(X))^\perp$, since $\text{ran}(X)$ is finite dimensional and, hence, closed. H is compact and $\langle Xh, h \rangle > 0$ for all $h \in H$. Hence,

$$0 \leq \lambda = \sup_{h \in H} \left(\frac{\langle Yh, h \rangle}{\langle Xh, h \rangle} \right) < \infty.$$

Now, for all $t \in \mathbb{C}^n$, there exist $h \in \text{ran}(X)$ and $k \in \ker(X)$ such that $t = h + k$. Then, $\langle Xt, t \rangle = \langle Xh, h \rangle$ and $\langle Yt, t \rangle = \langle Yh, h \rangle$, since $k \in \ker(X) \subseteq \ker(Y)$. Moreover, Y is non-zero, so there exists some $t \in \mathbb{C}^n$ such that $0 < \langle Yt, t \rangle = \langle Yh, h \rangle$, which implies that $\lambda > 0$. Therefore, for all $t \in \mathbb{C}^n$, we have that

$$\langle Xt, t \rangle = \langle Xh, h \rangle \geq \frac{1}{\lambda} \langle Yh, h \rangle = \frac{1}{\lambda} \langle Yt, t \rangle,$$

which shows that $\lambda X \geq Y$. Since $X \in \mathcal{F}_{\text{PSD}_n}(X)$ we have that $\lambda X \in \mathcal{F}_{\text{PSD}_n}(X)$ and so we may conclude that $Y \in \mathcal{F}_{\text{PSD}_n}(X)$. \square

In the next proposition we will see that the extreme rays of the cone PSD_n are generated by rank one positive semidefinite matrices.

Proposition 2.2.4. [2, Proposition 1.1.4] *The extreme rays of PSD_n are given by*

$$\{\alpha vv^* : \alpha \geq 0\},$$

where v is a non-zero vector in \mathbb{C}^n . In other words, all extreme rays of PSD_n are generated by rank one positive semidefinite matrices.

Proof. We prove this proposition in two parts. In part (i) we show that rank one matrices generate extreme rays of PSD_n , and in part (ii) we show that if a matrix is not of rank one, it does not generate an extreme ray of PSD_n .

(i) Let $v \in \mathbb{C}^n$ and suppose that $vv^* = A + B$ with A and B positive semidefinite. If $w \in \mathbb{C}^n$ is orthogonal to v , we have that $0 = w^*vv^*w = w^*(A + B)w = w^*Aw + w^*Bw$, and as both A and B are positive semidefinite, we have that $w^*Aw = 0 = w^*Bw$. Thus $0 = \text{tr}(w^*Aw) = \text{tr}(w^*A^{\frac{1}{2}}A^{\frac{1}{2}}w) = \text{tr}(A^{\frac{1}{2}}ww^*A^{\frac{1}{2}}) = \text{tr}(A^{1/2}w(A^{\frac{1}{2}}w)^*) = \langle A^{\frac{1}{2}}w, A^{\frac{1}{2}}w \rangle$, where $A^{\frac{1}{2}}$ represents the unique positive semidefinite matrix the square of which is A . The same argument holds for w^*Bw . Thus $\langle A^{\frac{1}{2}}w, A^{\frac{1}{2}}w \rangle = 0 = \langle B^{\frac{1}{2}}w, B^{\frac{1}{2}}w \rangle$. Then, per definition of the inner product, $A^{\frac{1}{2}}w = 0 = B^{\frac{1}{2}}w$. Therefore $A^{\frac{1}{2}}A^{\frac{1}{2}}w = Aw = 0 = Bw = B^{\frac{1}{2}}B^{\frac{1}{2}}w$. Thus, w is in the null space of A and B . Now, the orthogonal complement of the span of v has dimension $n - 1$, since vv^* has rank one (follows from Theorem 1.2.9). Therefore, A and B have at most rank one, since the nullity of A and B is, at least, $n - 1$. If they have rank one, the eigenvector corresponding to the single non-zero eigenvalue must be a multiple of v , as seen in the comments after Theorem 1.2.8, and this implies that both A and B are multiples of vv^* . Therefore, we have an extreme ray generated by rank one positive semidefinite matrices.

(ii) Let $K \in \text{PSD}_n$ be a matrix of rank $k \geq 2$, then, by Theorem 1.2.9, we may write K as the sum of rank one matrices, $K = v_1v_1^* + \dots + v_kv_k^*$, where v_1, \dots, v_k are non-zero vectors in \mathbb{C}^n . Hence for $k \geq 2$ we can write $K = A + B$ with $A = v_1v_1^*$ and $B = v_2v_2^* + \dots + v_kv_k^*$. Now, if $\alpha = 0$, we have that $\text{rank}(\alpha K) = 0$, else, $\text{rank}(\alpha K) = \text{rank}(K)$, since rank is invariant under scalar multiplication. Thus, $v_1v_1^* = \alpha K$ cannot hold for $k \geq 2$, since they do not have the same rank. Therefore K is not an extreme ray. \square

2.3 Matrix cones related to a symmetric pattern

In this section we show a connection between graph theory and matrices by associating the vertices and edges of a graph with the entries of a matrix. This will allow us to determine when a positive semidefinite completion exists, by looking at the underlying graph of the matrix. See Appendix C for some basic definitions regarding graph theory.

We start by defining a symmetric pattern and then associating it with the vertices and edges of a graph $G = (V, E)$. Note that throughout all graphs mentioned are simple undirected graphs.

Definition 2.3.1 (Symmetric Pattern). A subset $P \subseteq \{1, \dots, n\} \times \{1, \dots, n\}$ with the properties

- (i) $(i, i) \in P$ for $i = 1, \dots, n$;
- (ii) $(i, j) \in P \iff (j, i) \in P$.

is called an $n \times n$ symmetric pattern. Such a pattern is said to be a sparsity pattern for a matrix $A \in \mathcal{H}_n$ (recall that \mathcal{H}_n is the set of all Hermitian matrices in $\mathcal{M}_n(\mathbb{C})$), if for every $1 \leq i, j \leq n$, such that $(i, j) \notin P$, it follows that the (i, j) entry of A is 0.

With an $n \times n$ symmetric pattern, P , we associate the graph $G = (V, E)$, with $V = \{1, \dots, n\}$ and $(i, j) \in E$ if and only if $(i, j) \in P$ and $i \neq j$. From this it is clear that G is a simple undirected graph. Conversely, a simple undirected graph $G = (V, E)$, with $V = \{1, \dots, n\}$, defines a symmetric pattern in the sense that $(i, j) \in P$ if and only if $(i, j) \in E$ and $(i, i) \in P$, for all $i = 1, \dots, n$. Note that G being simple, implies that $(i, i) \notin E$, for $i = 1, \dots, n$. Thus, it is necessary to specify that $(i, i) \in P$, for all $i = 1, \dots, n$, else P is not a symmetric pattern. In what follows we will usually start with a simple undirected graph $G = (V, E)$. Hence, from now on, each graph will be assumed to be simple and undirected.

For a pattern with associated graph $G = (V, E)$, we introduce the following subspace of \mathcal{H}_n :

$$\mathcal{H}_G = \{A \in \mathcal{H}_n : a_{ij} = 0 \text{ for all } (i, j) \notin P\},$$

that is, the set of all $n \times n$ Hermitian matrices with sparsity pattern P . Of course, since \mathcal{H}_G is a subspace, its dual, as a cone, is equal to its orthogonal complement (Theorem 2.1.5). Furthermore, since \mathcal{H}_G is a closed subspace of the Hilbert space \mathcal{H}_n , we have that $\mathcal{H}_n = \mathcal{H}_G \oplus \mathcal{H}_G^\perp$ (Theorem A.8). From this it is immediately clear that

$$\mathcal{H}_G^\perp = \{A \in \mathcal{H}_n : a_{ij} = 0 \text{ for all } (i, j) \in P\}.$$

Recall, when $A = [a_{ij}]_{i,j=1}^n$ is an $n \times n$ matrix and $K \subseteq \{1, \dots, n\}$, then $A[K]$ denotes the $\text{card } K \times \text{card } K$ principal submatrix

$$A[K] = [a_{ij}]_{i,j \in K} = [a_{ij}]_{(i,j) \in K \times K}.$$

We are now ready to define four new cones that stand central to the whole problem of when a positive semidefinite completion of a matrix exists.

Proposition 2.3.2. [2, p.7] *Let $G = (V, E)$ be a graph. The following sets are cones in \mathcal{H}_G ,*

- (i) $\text{PPSD}_G = \{A \in \mathcal{H}_G : A[K] \succcurlyeq 0 \text{ for all cliques } K \text{ of } G\}$;
(PPSD - Partial Positive Semidefinite)
- (ii) $\text{PSD}_G = \{X \in \mathcal{H}_G : X \succcurlyeq 0\}$;
- (iii) $\mathcal{A}_G = \{Y \in \mathcal{H}_G : Y + W \succcurlyeq 0, \text{ for some } W \in \mathcal{H}_G^\perp\}$;
- (iv) $\mathcal{B}_G = \{B \in \mathcal{H}_G : B = \sum_{i=1}^{n_B} B_i, \text{ where } B_1, \dots, B_{n_B} \in \text{PSD}_G \text{ are of rank } 1\}$.

Proof. (i) Let $A, B \in \text{PPSD}_G$ and $\alpha > 0$. Then $A[K] \succcurlyeq 0$ and $B[K] \succcurlyeq 0$ for all cliques K of G , therefore $\alpha A[K] + B[K] \succcurlyeq 0$ for all cliques K of G . Thus $\alpha A + B \in \text{PPSD}_G$.

(ii) The sum of two positive semidefinite matrices is positive semidefinite, and multiplication of a positive scalar with a positive semidefinite matrix yields a positive semidefinite matrix. Thus PSD_G is a cone.

(iii) Let $X, Y \in \mathcal{A}_G$ and $\alpha > 0$. Then there exist $W, Z \in \mathcal{H}_G^\perp$ such that $X + W \succcurlyeq 0$ and $Y + Z \succcurlyeq 0$. Note that if $W, Z \in \mathcal{H}_G^\perp$, then $\alpha W + Z \in \mathcal{H}_G^\perp$. Therefore

$$\alpha(X + W) + (Y + Z) = (\alpha X + Y) + (\alpha W + Z) \succcurlyeq 0,$$

and this proves that $\alpha X + Y \in \mathcal{A}_G$.

(iv) Let $\alpha > 0$ and $A, B \in \mathcal{B}_G$, then $A = \sum_{i=1}^{n_A} A_i$ ($A_i \in \text{PSD}_G$, and $\text{rank}(A_i) = 1$, for $i = 1, \dots, n_A$) and $B = \sum_{i=1}^{n_B} B_i$ ($B_i \in \text{PSD}_G$ and $\text{rank}(B_i) = 1$, for $i = 1, \dots, n_B$). Then

$$\alpha A + B = \alpha \sum_{i=1}^{n_A} A_i + \sum_{i=1}^{n_B} B_i = \sum_{i=1}^{n_A} \alpha A_i + \sum_{i=1}^{n_B} B_i.$$

Thus $\alpha A + B$ is equal to the sum of positive semidefinite rank 1 matrices. This proves $\alpha A + B \in \mathcal{B}_G$. \square

Note that $\text{PSD}_G = \text{PSD}_n \cap \mathcal{H}_G$, that is, the set of all positive semidefinite matrices with underlying graph G . Furthermore, PPSD_G is the set of all matrices whose fully specified principal submatrices are positive semidefinite. This is a necessary solution criterion for a partial Hermitian matrix to admit a positive semidefinite completion (Lemma 1.2.4). In other words the only matrices that may have a positive semidefinite completion are those that are elements of PPSD_G . The cone \mathcal{A}_G is the set of all matrices in \mathcal{H}_G for which a positive semidefinite completion exists. We therefore see that it must be true that $\mathcal{A}_G \subseteq \text{PPSD}_G$. We will confirm this fact in the next theorem and also show the connection between the four cones in the previous proposition, for an arbitrary graph G .

Theorem 2.3.3. [2, Proposition 1.2.1] *Let $G = (V, E)$ be a graph. The cones PPSD_G , PSD_G , \mathcal{A}_G , and \mathcal{B}_G are closed, and their duals, in \mathcal{H}_G , are*

$$(\text{PSD}_G)^* = \mathcal{A}_G, \text{ and } (\text{PPSD}_G)^* = \mathcal{B}_G.$$

Moreover

$$(\text{PPSD}_G)^* \subseteq \text{PSD}_G \subseteq (\text{PSD}_G)^* \subseteq \text{PPSD}_G.$$

Before we prove this theorem we need the following lemma regarding rank one matrices and the maximal cliques of a graph G .

Lemma 2.3.4. *Let $G = (V, E)$ be a graph and $B \in \mathcal{B}_G$, i.e., $B = \sum_{k=1}^{n_B} B_k$, with $B_k \in \text{PSD}_G$ of rank 1, for each k . Write J_1, \dots, J_p for the maximal cliques of G . Then all the non-zero entries of B_k lie in $J_k \times J_k$, for $k = 1, \dots, p$.*

Proof. We complete the proof in three parts. In part (i) we show that if $(i, j) \notin E$ and $b_{ii} \neq 0$, for $i \neq j$, then $b_{jj} = 0$. In part (ii) we define the set $J = \{i \in \{1, \dots, n\} : b_{ii} \neq 0\}$ and prove that it is a clique in G . Finally, in part (iii) we conclude that J is contained in a maximal clique of G and prove the result of the lemma.

(i) Fix a $k \in \{1, \dots, n\}$, and say $B_k = [b_{ij}]_{i,j=1}^n$. The fact that B_k has rank one, implies $B_k \neq 0$. Thus, B_k has a non-zero entry on its diagonal (because $B_k \in \text{PSD}_G$), say on the (i, i) -th position. Let $j \in \{1, \dots, p\}$ such that $j \neq i$ and $(i, j) \notin E$. Since $B_k \succcurlyeq 0$ and $\text{rank}(B_k) = 1$, we may write $B_k = vv^*$ for some $v \in \mathbb{C}^n$, $v \neq 0$ (Theorem 1.2.8). Then $b_{ij} = v_i \bar{v}_j = 0$, since (i, j) is not in the sparsity pattern of B_k . Furthermore $b_{ii} = |v_i|^2 \neq 0$ implies that $v_i \neq 0$, and it must be true that $v_j = 0$. Now, $b_{jj} = v_j \bar{v}_j = |v_j|^2$, therefore $b_{jj} = 0$.

(ii) Define the set $J = \{i \in \{1, \dots, n\} : b_{ii} \neq 0\}$. To prove that J is a clique we need to show that any pair of distinct vertices in J are connected by an edge in E . Let $i, j \in J$, then $b_{ii} \neq 0$ and $b_{jj} \neq 0$. The proof is by contradiction. Assume $(i, j) \notin E$. Then from part (i) and the fact that $b_{ii} \neq 0$, we have that $b_{jj} = 0$. But this contradicts our choice of j , therefore, $(i, j) \in E$. Since this holds for any pair of distinct vertices in J , it follows that J is a clique.

(iii) Since J is a clique it must be contained in some maximal clique of G , say J_k , for some $q \in \{1, \dots, p\}$. Let $(i, j) \notin J_k \times J_k$, then we have that $i \notin J_k$, or $j \notin J_k$, which implies that $i \notin J$ or $j \notin J$. Therefore, either $b_{ii} = 0$ or $b_{jj} = 0$. We may assume, without loss of generality, that $j \notin J_k$. Since $b_{jj} = |v_j|^2$ (see part (i) of the proof), it follows that $v_j = 0$. Finally, since $b_{ij} = v_i \bar{v}_j$, we have that $b_{ij} = 0$, and the same holds for b_{ji} . Thus, if $(i, j) \notin J_k \times J_k$, we have that $b_{ij} = b_{ji} = 0$. Hence, all the non-zero entries of B_k lie in $J_k \times J_k$, for some $q \in \{1, \dots, p\}$. \square

Proof of Theorem 2.3.3. We start the proof by showing that all the cones, in the proposition, are in fact closed. We then prove that all the equalities stated hold, namely $(\text{PSD}_G)^* = \mathcal{A}_G$, and $(\text{PPSD}_G)^* = \mathcal{B}_G$. Finally, we prove the inclusions $(\text{PPSD}_G)^* \subseteq \text{PSD}_G \subseteq (\text{PSD}_G)^* \subseteq \text{PPSD}_G$.

The fact that PPSD_G and PSD_G are closed is trivial, since the limit of a sequence of positive semidefinite matrices is again positive semidefinite.

We now prove that \mathcal{A}_G is closed. Let $Y_k \in \mathcal{A}_G$ and say $Y_k \rightarrow Y$. Since $Y_k \in \mathcal{A}_G$ there exists a $W_k \in \mathcal{H}_G^\perp$, such that $Y_k + W_k \succcurlyeq 0$. The fact that $Y_k + W_k$ is positive semidefinite implies, by use of Gerschgorin circles, that the diagonal elements are a bound for the elements in each row, since all the eigenvalues are non-negative. Now say $Y_k + W_k = [y_{ij} + w_{ij}]_{i,j=1}^n$, and let $\rho = \sup\{y_{pp} : p = 1, \dots, n\}$ then it follows that $|y_{ij} + w_{ij}| \leq \rho < \infty$, for each $i, j = 1, \dots, n$ and $i \neq j$ ($\rho < \infty$ follows from the fact that Y_k is convergent and therefore bounded). In particular, we have that $|w_{ij}| \leq \rho$, for all $i, j = 1, \dots, n$. Therefore, each element of W_k is bounded; equivalently $\sup \|W_k\|_2 < \infty$. Hence, there exists a convergent subsequence, $\{W_{k_l}\}_{l \in \mathbb{N}}$, with limit, say W . Note that $W \in \mathcal{H}_G^\perp$, since \mathcal{H}_G^\perp is closed. The fact that Y_k converges implies that there exists a convergent subsequence $\{Y_{k_l}\}_{l \in \mathbb{N}}$, with the same limit as Y_k . Thus $0 \preceq Y_{k_l} + W_{k_l} \rightarrow Y + W$, and it follows that $Y \in \mathcal{A}_G$, since $W \in \mathcal{H}_G^\perp$. This proves that \mathcal{A}_G is closed.

Now, to prove that \mathcal{B}_G is closed, we first observe that if J_1, \dots, J_p are all the maximal

cliques of the graph G , then any $B \in \mathcal{B}_G$ can be written as $B = B_1 + \cdots + B_p$, where $B_k \succcurlyeq 0$ and we may conclude from the preceding lemma (Lemma 2.3.4) that all the non-zero entries of B_k lie in $J_k \times J_k$, for some $q \in \{1, \dots, p\}$. Note that $B \succcurlyeq B_k$, for $k = 1, \dots, p$. We now let $A^{(s)} = \sum_{k=1}^p A_k^{(s)} \in \mathcal{B}_G$, such that the non-zero entries of $A_k^{(s)}$ lie in $J_k \times J_k$, and assume that $A^{(s)}$ converges to A as $s \rightarrow \infty$. Then $A_1^{(s)}$ is a bounded sequence of matrices, and thus there is a convergent subsequence $\{A_1^{(s_{k_1})}\}_{k \in \mathbb{N}}$ with limit, say A_1 . Note that A_1 is positive semidefinite and has non-zero entries only in $J_1 \times J_1$. Next take a subsequence $\{A_2^{(s_{k_l})}\}_{l \in \mathbb{N}}$, of $\{A_2^{(s_k)}\}_{k \in \mathbb{N}}$ that converges to a limit, say A_2 . Note that A_2 is also positive semidefinite and has non-zero entries only in $J_2 \times J_2$. Repeating this argument, we ultimately obtain $m_1 < m_2 < \dots$ so that $\lim_{j \rightarrow \infty} A_k^{(m_j)} = A_k \succcurlyeq 0$ with A_k having non-zero entries only in $J_k \times J_k$. Then we have the following

$$A = \lim_{s \rightarrow \infty} A^{(s)} = \sum_{k=1}^p \lim_{j \rightarrow \infty} A_k^{(m_j)} = \sum_{k=1}^p A_k \in \mathcal{B}_G.$$

Therefore $A \in \mathcal{B}_G$, proving that \mathcal{B}_G is closed.

We start by proving the duality of PSD_G and \mathcal{A}_G . Note that $\text{PSD}_G = \text{PSD}_n \cap \mathcal{H}_G$. Applying Corollary 2.1.8, recalling that PSD_n is self-dual and using the fact that the dual of a subspace is its orthogonal complement, we have that

$$(\text{PSD}_G)^* = (\text{PSD}_n \cap \mathcal{H}_G)^* = \overline{(\text{PSD}_n)^* + (\mathcal{H}_G)^*} = \overline{\text{PSD}_n + \mathcal{H}_G^\perp}.$$

Now $\mathcal{A}_G = \text{PSD}_n + \mathcal{H}_G^\perp$, therefore $(\text{PSD}_G)^* = \overline{\mathcal{A}_G}$. However, \mathcal{A}_G is closed, thus $(\text{PSD}_G)^* = \mathcal{A}_G$.

We now prove the duality of PPSD_G and \mathcal{B}_G . To do this we prove the two inclusions (i) $\text{PPSD}_G \subseteq \mathcal{B}_G^*$ and (ii) $\mathcal{B}_G^* \subseteq \text{PPSD}_G$.

(i) Let $B_1 \in \text{PSD}_G$ and $\text{rank}(B_1) = 1$, then $B_1 = ww^*$ (Theorem 1.2.8), where w is a vector with support in a clique K of G . Now form a new vector, say w' , where all the entries of w whose index is not in K , are deleted. Let $L \in \text{PPSD}_G$, then

$$\begin{aligned} \langle L, B_1 \rangle &= \langle L, ww^* \rangle = \text{tr}(Lww^*) \\ &= \text{tr}(w^*Lw) = \text{tr}((w')^*L[K]w') \\ &= \text{tr}(L[K]w'(w')^*) = \langle L[K]w', w' \rangle \\ &\geq 0, \end{aligned}$$

since $L[K]$ is positive semidefinite. Therefore, $L \in \mathcal{B}_G^*$, since every element of \mathcal{B}_G is the sum of rank one matrices. Thus $\text{PPSD}_G \subseteq \mathcal{B}_G^*$.

(ii) Now, if $A \notin \text{PPSD}_G$ there is a clique K such that $A[K]$ is not positive semidefinite. Thus there is a vector v such that $\langle A[K]v, v \rangle = \text{tr}(A[K]vv^*) < 0$. Therefore, there exists a positive semidefinite rank one matrix $B = vv^*$ with all its non-zero entries in K (Lemma 2.3.4), so that $\langle A, B \rangle = \text{tr}(A[K]B) = \text{tr}(A[K]vv^*) < 0$. As $B \in \mathcal{B}_G$, this shows that A is not in the dual of \mathcal{B}_G . We have thus shown that $A \notin \text{PPSD}_G$ implies that $A \notin \mathcal{B}_G^*$. Therefore, $A \in \mathcal{B}_G^*$ implies that $A \in \text{PPSD}_G$, and so, $\mathcal{B}_G^* \subseteq \text{PPSD}_G$.

Combining (i) and (ii) we have that $\text{PPSD}_G = \mathcal{B}_G^*$. Thus, $(\text{PPSD}_G)^* = (\mathcal{B}_G^*)^* = \mathcal{B}_G$, where the last inequality follows from Lemma 2.1.7 (ii) and the fact that \mathcal{B}_G is closed.

We now prove the inclusions stated in the proposition: It suffices to prove the inclusions $\text{PSD}_G \subseteq (\text{PSD}_G)^*$ and $(\text{PPSD}_G)^* \subseteq \text{PSD}_G$. This follows from the fact that all of the cones are closed, which implies that $(\text{PPSD}_G)^{**} = \text{PPSD}_G$, $(\text{PSD}_G)^{**} = \text{PSD}_G$ and the fact that $(\text{PPSD}_G)^* \subseteq \text{PSD}_G$ implies that $(\text{PSD}_G)^* \subseteq \text{PPSD}_G$ (Lemma 2.1.7 (i), (ii)).

$(\text{PPSD}_G)^* \subseteq \text{PSD}_G$: Let $A \in \mathcal{B}_G$, then $A \in \text{PSD}_G$, by our definition of \mathcal{B}_G , since the sum of positive semidefinite matrices is again positive semidefinite.

$\text{PSD}_G \subseteq (\text{PSD}_G)^*$: Let $A \in \text{PSD}_G$, then it is also an element of \mathcal{H}_G , and there exists a $W \in \mathcal{H}_G^\perp$ ($W = 0$), such that $A + W \succcurlyeq 0$, which shows that $A \in \mathcal{A}_G = (\text{PSD}_G)^*$.

Therefore, $(\text{PPSD}_G)^* \subseteq \text{PSD}_G \subseteq (\text{PSD}_G)^* \subseteq \text{PPSD}_G$. □

2.4 Notes

The proof of Proposition 2.3.2 is our own. With regards to Theorem 2.3.3, the only part of the proof that is the same as the one found in [2], is the proof of the closedness of \mathcal{B}_G , the rest is our own work.

Chapter 3

Positive semidefinite matrix completion problem

In this chapter we consider the positive semidefinite matrix completion problem. We wish to determine under which conditions every element, with the same sparsity pattern, admits a positive definite completion. In other words, we want to know when does there exist a positive definite completion, for every element satisfying the necessary solution criterion, regardless of the specific entries of each element. We will see that the structure of the underlying graph is crucial. In the first section we introduce the notion of chordal graphs and prove some results regarding graphs with this property. In the second section we will see that if the underlying graph is chordal, there necessarily exists a positive semidefinite completion for every element.

3.1 Chordal graphs

Definition 3.1.1 (Chordal Graph). A graph G is called chordal if every cycle of length longer than 3 possesses a chord, that is, an edge joining two non-consecutive vertices of the cycle.



Figure 3.1: Chordal vs. Non-Chordal

Definition 3.1.2 (Minimum fill-in of a graph). Let $G = (V, E)$ be a graph. Then the minimum fill-in of G is the minimum number of edges which need to be added to G to obtain a chordal graph. We will denote the minimum fill-in of G by $\text{fill}(G)$.

The minimum fill-in of a graph is sometimes called the minimum triangulation.

Definition 3.1.3 (Perfect Vertex Elimination Scheme). Let $G = (V, E)$ be a graph, where $V = \{v_1, \dots, v_n\}$. The ordering $\sigma = (v_1, \dots, v_n)$ of the vertices is called a perfect vertex elimination scheme (or perfect scheme) if each set

$$S_i = \{v_j \in \text{Adj}(v_i) : j > i\}$$

is a clique, where $\text{Adj}(v) = \{u \in V : (u, v) \in E\}$ is the adjacency set of the vertex v .

Definition 3.1.4 (Simplicial vertex). Let $G = (V, E)$ be a graph. A vertex $v \in V$ is said to be simplicial if $\text{Adj}(v)$ is a clique.

Thus, $\sigma = \{v_1, \dots, v_n\}$ is a perfect scheme if each v_i is simplicial in the induced graph $G[\{v_i, \dots, v_n\}]$.

Perfect vertex elimination schemes go hand in hand with chordal graphs, as we will see in Theorem 3.1.9.

We now introduce the notion of connected components and cutsets, both of which play an important role in the characterization of chordal graphs.

Definition 3.1.5 (Connected Components). Let $G = (V, E)$ be a graph. A subgraph H of G is called a connected component if it is a connected graph and the vertices in H are not connected to any other vertices of G .

Definition 3.1.6 (Cutset, ab -cutset). Let $G = (V, E)$ be a connected graph. A subset Q of V is called a cutset if $G[V \setminus Q]$ is not connected. For vertices $a, b \in V$, an ab -cutset is a subset Q of $V \setminus \{a, b\}$ such that $G[V \setminus Q]$ has, at least, two distinct connected components $G[A] = (A, E[A])$ and $G[B] = (B, E[B])$, containing a and b , respectively. We also say that such a subset Q separates a and b . If no proper subset of Q is a cutset, then Q is called a minimal cutset.

We now have an important property regarding minimal cutsets of a chordal graph.

Proposition 3.1.7. [2, Proposition 1.2.2] *Every minimal cutset of a chordal graph induces a clique.*

Proof. Let S be a minimal ab -cutset in a chordal graph $G = (V, E)$, and let $G[A] = (A, E[A])$ and $G[B] = (B, E[B])$ be the connected components in $G[V \setminus S]$ containing a and b , respectively. Let $x, y \in S$ be arbitrary. Each vertex in S must be connected to at least one vertex in A and at least one in B . We can choose minimal length paths, $[x, a_1, \dots, a_r, y]$ and $[y, b_1, \dots, b_s, x]$, such that $a_i \in A$ for $i = 1, \dots, r$ and $b_j \in B$ for $j = 1, \dots, s$. Then $[x, a_1, \dots, a_r, y, b_1, \dots, b_s, x]$ is a cycle in G of length greater than 3 (if it has length 3 there is nothing to prove) and because G is a chordal graph it must

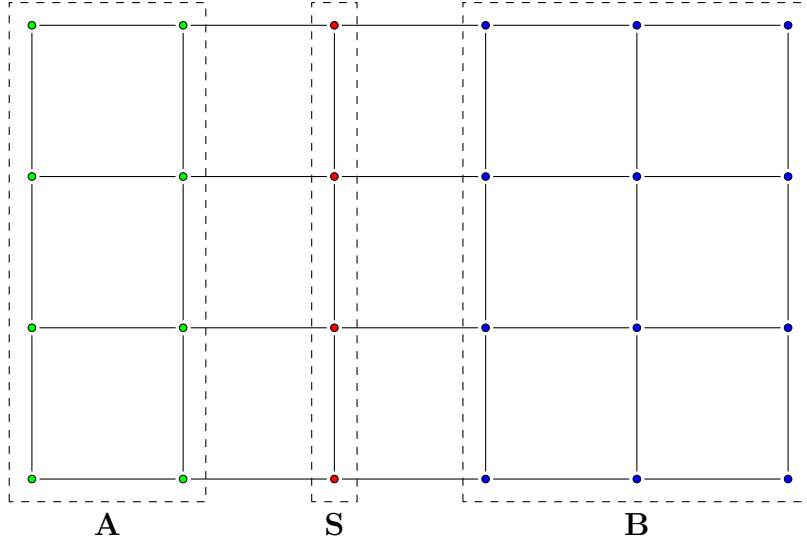


Figure 3.2: An example of a cutset Q , separating the vertex sets A and B . Here A and B are the vertex sets of the connected components $G[A] = (A, E[A])$ and $G[B] = (B, E[B])$, respectively.

have a chord in this cycle. Now it holds that $(a_i, b_j) \notin E$, by the definition of a cutset and, $(a_i, a_j), (b_i, b_j) \notin E$, for $i < j, j \neq i + 1$, by the minimality of r and s . Therefore the only possible chord is (x, y) . Hence, every pair of distinct vertices in S is connected by an edge in E . Thus S is a clique. \square

The next result is known as Dirac's Lemma, which gives a characterization of chordal graphs.

Lemma 3.1.8 (Dirac's Lemma). *[2, Lemma 1.2.3] Every chordal graph G has a simplicial vertex. Moreover, if G is not complete, it has two non-adjacent simplicial vertices.*

Proof. Proof by induction on n , where n is the number of vertices of G . When $n < 4$, the result is trivial (since every chordal graph with 3 or less vertices is complete). Let $n \geq 4$ and assume that the result is true for graphs with fewer than n vertices. Now say $G = (V, E)$ has n vertices. If G is complete, the result holds. Therefore say G is not complete, and let S be a minimal ab -cutset for two non-adjacent vertices a and b . Let $G[A] = (A, E[A])$ and $G[B] = (B, E[B])$ be the connected components in $G[V \setminus S]$ containing a and b , respectively. By our assumption, either the subgraph $G[A \cup S]$ has two non-adjacent simplicial vertices, one of which must be in $G[A]$ (since, by Proposition 3.1.7, $G[S]$ is complete and therefore all its simplicial vertices are adjacent), or $G[A \cup S]$ is complete and any vertex in A is simplicial in $G[A \cup S]$. Since $\text{Adj}(a) \subseteq A \cup S$, for any $a \in A$, a simplicial vertex of $G[A \cup S]$ in A , is simplicial in G . Similarly, B contains a simplicial vertex of G , and therefore if G is not complete it has two non-adjacent simplicial vertices, and this proves the lemma. \square

The following is an algorithmic characterization of chordal graphs, and the main result of this section.

Theorem 3.1.9. [2, Theorem 1.2.4] *A graph is chordal if and only if it has a perfect scheme. Moreover, any simplicial vertex can start a perfect scheme.*

Proof. \implies Let $G = (V, E)$ be a chordal graph with n vertices. We use an induction argument. For $n = 1$ the result is trivial and we may therefore assume that every chordal graph with fewer than n vertices has a perfect scheme. Now from Dirac's Lemma (Lemma 3.1.8) we know that G has a simplicial vertex, say u . Let $\{v_1, \dots, v_{n-1}\}$ be a perfect scheme for $G[V \setminus \{u\}]$ (the existence follows from our induction argument). Then $\{u, v_1, \dots, v_{n-1}\}$ is a perfect scheme for G .

\impliedby Let $G = (V, E)$ be a graph with a perfect scheme, say, $\sigma = \{v_1, \dots, v_n\}$. If there are no cycles greater than 3 in G , then G is automatically chordal and there is nothing to prove, therefore assume that C is a cycle of length greater than 3 in G . Let u be the vertex in C with the smallest index in σ . By definition of a perfect scheme, the two vertices in C adjacent to u must be connected by an edge ($\text{Adj}(u)$ is a clique), so C has a chord. Since our choice of C was arbitrary, G is chordal. \square

3.2 Matrix cones with chordal patterns

We start this section by showing that Theorem 1.2.9 holds, for matrices in \mathcal{H}_G , if the underlying graph is chordal, i.e., PSD_G is equal to $(\text{PPSD}_G)^*$ when the graph G is chordal. In other words, any positive semidefinite matrix with underlying graph G may be written as the sum of rank one positive semidefinite matrices (also with underlying graph G), if the graph G is chordal.

Proposition 3.2.1. [2, Proposition 1.2.6] *Let $A \in \text{PSD}_G$, where G is a chordal graph with n vertices. Then A can be written as $A = \sum_{i=1}^r w_i w_i^*$, where $r = \text{rank}(A)$ and $w_i \in \mathbb{C}^n$ are non-zero vectors such that $w_i w_i^* \in \text{PSD}_G$ for $i = 1, \dots, r$. In other words, we have $\text{PSD}_G = (\text{PPSD}_G)^*$.*

Proof. Proof by induction on n . For $n = 1$ the result is trivial. Now assume $n \geq 2$, such that it holds for $n - 1$. Let $A \in \text{PSD}_G$, where $G = (V, E)$ is a chordal graph with $V = \{1, \dots, n\}$ and let $r = \text{rank}(A)$. We may assume, without loss of generality, that the vertex 1 is simplicial (otherwise we reorder the rows and columns of A in an order that starts with a simplicial vertex). If $a_{11} = 0$, the first row and column of A are necessarily zero, else A would not be positive semidefinite, and the result follows from our assumption for $n - 1$. Now say $a_{11} \neq 0$, and let $w_1 \in \mathbb{C}^n$ be the first column of A multiplied by $\frac{1}{\sqrt{a_{11}}}$. An entry (k, l) , $2 \leq k, l \leq n$ of $w_1 w_1^*$ is zero if $(1, k), (1, l) \notin E$. Since the vertex 1 is simplicial, we have $(k, l) \in E$. Then by Lemma B.5, $A - w_1 w_1^*$ is a positive semidefinite matrix of rank $r - 1$, and has its first row and column equal to zero. From this it follows that all the principal submatrices of $A - w_1 w_1^*$ are positive semidefinite (Lemma 1.2.4).

We now show that if $(i, j) \notin E$, where $i, j > 1$ and $i \neq j$, the (i, j) -th entry of $w_1 w_1^*$ is equal to zero. Let $i, j > 1$, with $i \neq j$, such that $(i, j) \notin E$. Then it follows that at least one of $(1, i)$ and $(1, j)$ is not in E , since 1 is simplicial. Assume, without loss of generality, that $(1, i) \notin E$, then the $(1, i)$ -th entry of w_1 is zero (i.e., $a_{1i} = 0$). Now, the (i, j) -th

entry of $w_1 w_1^*$ is equal to $a_{1i} a_{1j} / a_{11}$, and consequently, equal to zero. We also note that the (i, j) -th entry of A is equal to zero, since $A \in \text{PSD}_G$ and $(i, j) \notin E$.

Therefore, if $(i, j) \notin E$, where $i, j > 1$ and $i \neq j$, the (i, j) -th entry of $A - w_1 w_1^*$ is equal to zero. This, combined with the fact that every principal submatrix of $A - w_1 w_1^*$ is positive semidefinite, ensures that $(A - w_1 w_1^*)[\{2, \dots, n\}] \in \text{PSD}_{G[\{2, \dots, n\}]}$.

Since $G[\{2, \dots, n\}]$ is also chordal, by our assumption for $n - 1$, we have that $A - w_1 w_1^* = \sum_{i=2}^r w_i w_i^*$, where each $w_i \in \mathbb{C}^n$ is a non-zero vector with its first component equal to zero. Thus

$$A = w_1 w_1^* + \sum_{i=2}^r w_i w_i^* = \sum_{i=1}^r w_i w_i^*.$$

We have therefore shown that every $A \in \text{PSD}_G$ can be written as the sum of rank one positive semidefinite matrices. \square

Proposition 3.2.1 has the following two corollaries.

Corollary 3.2.2. [2, Corollary 1.2.7] *Let P be a symmetric pattern with associated graph $G = (V, E)$. Then Gaussian elimination can be carried out on every $A \in \text{PSD}_G$ such that in the process no entry corresponding to $(i, j) \notin P$ is changed even temporarily to a non-zero, if and only if $\sigma = \{1, 2, \dots, n\}$ is a perfect scheme for G .*

Corollary 3.2.3. [2, Corollary 1.2.8] *Let $G = (V, E)$ be a graph. Then the lower-upper Cholesky factorization $A = LL^*$, of every $A \in \text{PSD}_G$ satisfies $l_{ij} = 0$ for $1 \leq j < i \leq n$ such that $(i, j) \notin E$, if and only if $\sigma = \{1, 2, \dots, n\}$ is a perfect scheme for G .*

Proof. Follows immediately from the fact that $L = [w_1 \ w_2 \ \dots \ w_n]$ where w_1, \dots, w_n are obtained recursively as in the proof of Proposition 3.2.1. \square

We now show that if G is not chordal, there exist matrices, whose principal submatrices are all positive semidefinite, which do not admit a positive semidefinite completion.

Proposition 3.2.4. [2, Proposition 1.2.9] *Let $G = (V, E)$ be a non-chordal graph. Then $(\text{PSD}_G)^*$ is a proper subset of PPSD_G .*

Proof. From Proposition 2.3.3, we know that $(\text{PSD}_G)^* \subseteq \text{PPSD}_G$. Now, for $m \geq 4$ define the $m \times m$ Toeplitz matrix

$$A_m = \begin{pmatrix} 1 & 1 & 0 & 0 & \dots & -1 \\ 1 & 1 & 1 & 0 & \dots & 0 \\ 0 & 1 & 1 & 1 & \dots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ -1 & 0 & 0 & 0 & \dots & 1 \end{pmatrix}, \quad (1.5.1)$$

the graph of which is the chordless cycle $(1, \dots, m)$. For each $m \geq 4$, we have $A_m \in \text{PPSD}_G$, since both matrices $\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$ and $\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}$ are positive semidefinite. We cannot modify the zeros of A_m in any way to obtain a positive semidefinite matrix, since the

only positive semidefinite matrix with the three middle diagonals equal to 1, is the matrix with all entries equal to 1 (see [12, Lemma 6]).

Let $G = (V, E)$, $V = \{1, \dots, n\}$, be a non-chordal graph and assume, without loss of generality, that it contains the chordless cycle $(1, \dots, m)$, $4 \geq m \geq n$. Let A be the matrix, with underlying graph G , having 1 on its main diagonal, the matrix A_m in (1.5.1) as its $m \times m$ upper-left corner, and 0 on any other position. Then $A \in \text{PPSD}_G$, but $A \notin (\text{PSD}_G)^*$, since the zeros in its upper left $m \times m$ corner cannot be modified such that this corner becomes a positive semidefinite matrix. Therefore $(\text{PSD}_G)^* \subsetneq \text{PPSD}_G$. \square

The following and final result of this section, summarizes all the important results in the preceding sections and shows that equality between $(\text{PPSD})^*$ and PSD_G (or equivalently, between $(\text{PSD}_G)^*$ and PPSD_G) occurs exactly when G is chordal.

Theorem 3.2.5. [2, Theorem 1.2.10] *Let $G = (V, E)$ be a graph. Then the following are equivalent:*

- (i) G is chordal.
- (ii) $\text{PPSD}_G = (\text{PSD}_G)^*$.
- (iii) $(\text{PPSD}_G)^* = \text{PSD}_G$.
- (iv) *There exists a permutation σ of $(1, \dots, n)$ such that after reordering the rows and columns of every $A \in \text{PSD}_G$ by the order σ , A has the lower-upper Cholesky factorization $A = LL^*$ with $l_{ij} = 0$ for every $1 \leq j < i \leq n$ such that $(i, j) \notin E$.*

Proof. (i) \implies (iv) follows from the fact that a graph is chordal if and only if it has a perfect scheme (Theorem 3.1.9) and Corollary 3.2.3.

(iv) \implies (iii) from Corollary 3.2.3 and Proposition 3.2.1, since (iv) is true if and only if $\sigma = (1, 2, \dots, n)$ is a perfect scheme for G , but then G is chordal (Theorem 3.1.9) and therefore we may apply Proposition 3.2.1.

(iii) \implies (ii) from property (ii) of Lemma 2.1.7 and the fact that the cones are closed.

(ii) \implies (i) follows from Proposition 3.2.4 and Proposition 3.2.1, since $\text{PPSD}_G \subsetneq (\text{PSD}_G)^*$ implies that G is non-chordal, therefore, if $\text{PPSD}_G = (\text{PSD}_G)^*$ then G is chordal. \square

Thus, we see that every element of PPSD_G admits a positive definite completion if and only if G is chordal. This is remarkable, since the specific entries of each matrix are, in a sense, irrelevant, all that is required, is that the fully specified principal submatrices are positive semidefinite. We also see that Theorem 1.2.9 holds for positive semidefinite matrices in \mathcal{H}_G , that is, every element of PSD_G can be written as the sum of rank 1 positive semidefinite matrices if and only if G is chordal. We will explore this relationship further in Part II.

3.3 Notes

Proposition 3.2.1 has been written out in more detail and the part where we prove that the (i, j) -th entry of $w_1 w_1^*$ is equal to zero if $(i, j) \notin E$, is our own work.

Part II

The sparsity order of a graph

Chapter 4

Graph decomposition theorem

4.1 Introduction

The main theorem of this section states that a graph may be decomposed as a clique-sum of a set of graphs belonging to four basic classes if and only if the graph does not contain certain graphs as induced subgraphs. The whole chapter will be devoted to proving this rather technical result.

We start by defining what is meant by a clique-sum and the related notion of clique-cutsets. Recall that a cutset of a connected graph $G = (V, E)$, is a subset Q of V such that $G[V \setminus Q]$ is not connected.

Definition 4.1.1 (Clique-sum, Clique-cutset). Let $G = (V, E)$ be a connected graph and let K be a cutset of G . If the connected components of G are $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ and K is a clique, we call G the clique-sum of G_1 and G_2 and K the clique-cutset of G . Equivalently,

$$G = (V_1 \cup V_2, E_1 \cup E_2)$$

$K = V_1 \cap V_2$ is a clique in G_1 and G_2 and there are no edges between the sets $V_1 \setminus V_2$ and $V_2 \setminus V_1$.

It now follows that a graph containing a clique-cutset may be decomposed into the clique-sum of a set of smaller graphs. Note that if a graph contains more than one clique-cutset, we decompose it as the clique-sum of graphs containing no clique-cutsets. This process of decomposition by clique-cutsets can be done in $\mathcal{O}(nm)$ time, where n is the number of vertices of the graph and m the number of edges [27]. Furthermore, it was shown in [21] that this decomposition can be made unique if the clique-cutsets are also minimal. This decomposition can obviously be reversed, in the following way: Let $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ be two distinct connected graphs. If they contain cliques of equal size the the clique-sum of G_1 and G_2 is formed from their disjoint union of vertices by identifying pairs of vertices in these two cliques to form a single shared clique. We can also form a clique-sum of several graphs by repeated use of the process described here for two graphs. For more on decomposing a graph as a clique-sum see [4].

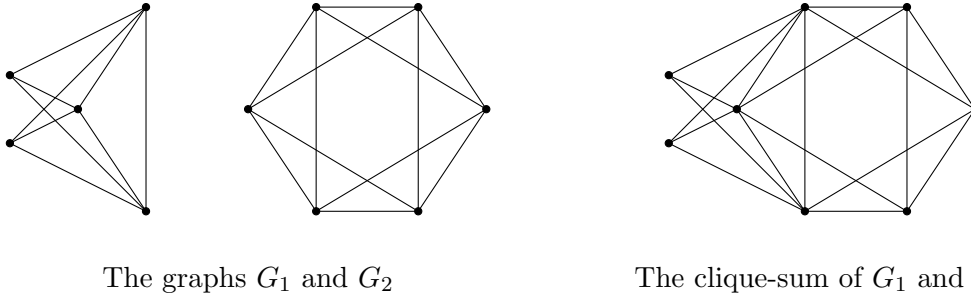


Figure 4.1: An example of two distinct connected graphs and the clique-sum of these graphs

We now introduce the four basic classes mentioned in the previous paragraph. We will denote these graphs and their induced subgraphs by \mathcal{G}_i , for $i = 1, 2, 3, 4$, and use the following convention, as seen in [20, p.550]:

A small dark dot indicates a vertex, a big dark circle indicates a clique, while a big white circle indicates a stable set; edges are indicated by lines, while a thick line between two spheres or between two sets of vertices shows that every vertex in one set is adjacent to every vertex in the other set.

The form of the four classes \mathcal{G}_i , $i = 1, 2, 3, 4$ can be seen in Figure 4.2. Note that these classes include all graphs of this form and their induced subgraphs, for example, a chordal graph is an element of \mathcal{G}_1 , since it is an induced subgraph of a graph with the form seen in \mathcal{G}_1 . We also give the form of the complementary classes of \mathcal{G}_i , for $i = 2, 3, 4$, which we will denote by $\overline{\mathcal{G}}_2, \overline{\mathcal{G}}_3, \overline{\mathcal{G}}_4$.

We will call the forbidden induced subgraphs mentioned earlier $A_1 - A_{10}, B_1 - B_6$. The form of the complements of these graphs can be seen in Figure 4.3. Note that we give the complements, since they have a very simple form.

Our main goal in this chapter is to prove the following theorem:

Theorem 4.1.2. [20, Theorem 8] *The following statements are equivalent for a graph G :*

- (i) *G does not contain, as an induced subgraph, a cycle C_n , $n \geq 5$, nor any of the graphs $A_2 - A_{10}$ and $B_1 - B_6$.*
- (ii) *G is a clique-sum of a set of graphs belonging to $\bigcup_{i=1}^4 \mathcal{G}_i$.*

We may assume, without loss of generality, that G is connected. Indeed, if G were disconnected, we need but prove the result for each of its connected components and we are done. This follows from the fact that a disconnected graph is a clique-sum of its connected components and the null graph.

As a starting point we will show that the vertex set of a graph can be partitioned in the following way:

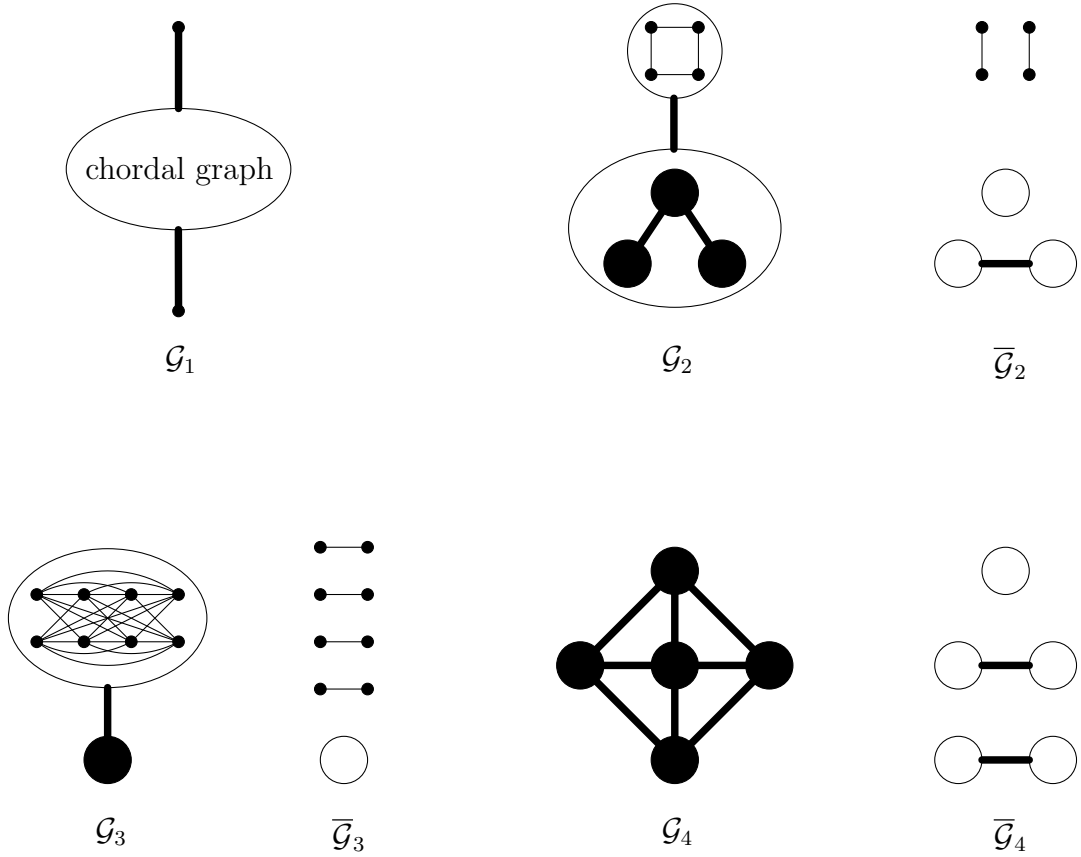


Figure 4.2: The classes $\mathcal{G}_1, \mathcal{G}_2, \mathcal{G}_3, \mathcal{G}_4$ and the complementary classes $\bar{\mathcal{G}}_2, \bar{\mathcal{G}}_3, \bar{\mathcal{G}}_4$

Let $G = (V, E)$ be a graph. For $S \subseteq V$ define

$$N = \{i \in V \setminus S : i \text{ is adjacent to some vertex in } S\},$$

$$\bar{N} = V \setminus (S \cup N).$$

Then S, N and \bar{N} are mutually disjoint and

$$V = S \cup N \cup \bar{N}.$$

If G is a clique, we have that $N = V \setminus S$, which implies that $\bar{N} = \emptyset$. Now, if G is not a clique, we may refine the partitioning of the vertex set V even further. We first note that since G is not a clique, there exists a vertex $u \in V$, which is not adjacent to all the other vertices in V . Define $S \subseteq V$ to be the maximal subset which contains u such that $G[S]$ is connected and $V \neq S \cup N$. Note that if $S = \{u\}$, both of these conditions are satisfied, hence the maximal subset does indeed exist and is non-empty. Furthermore, $\bar{N} \neq \emptyset$, since $V \neq S \cup N$. Since N and \bar{N} are disjoint, it follows that there are no edges between the sets S and \bar{N} . Finally, we observe that every vertex in N is adjacent to every vertex in \bar{N} . Indeed, if this were not so, there exists a vertex i in N which is not adjacent to all the vertices of \bar{N} . Then, we could increase S by i , contradicting the maximality assumption on S .

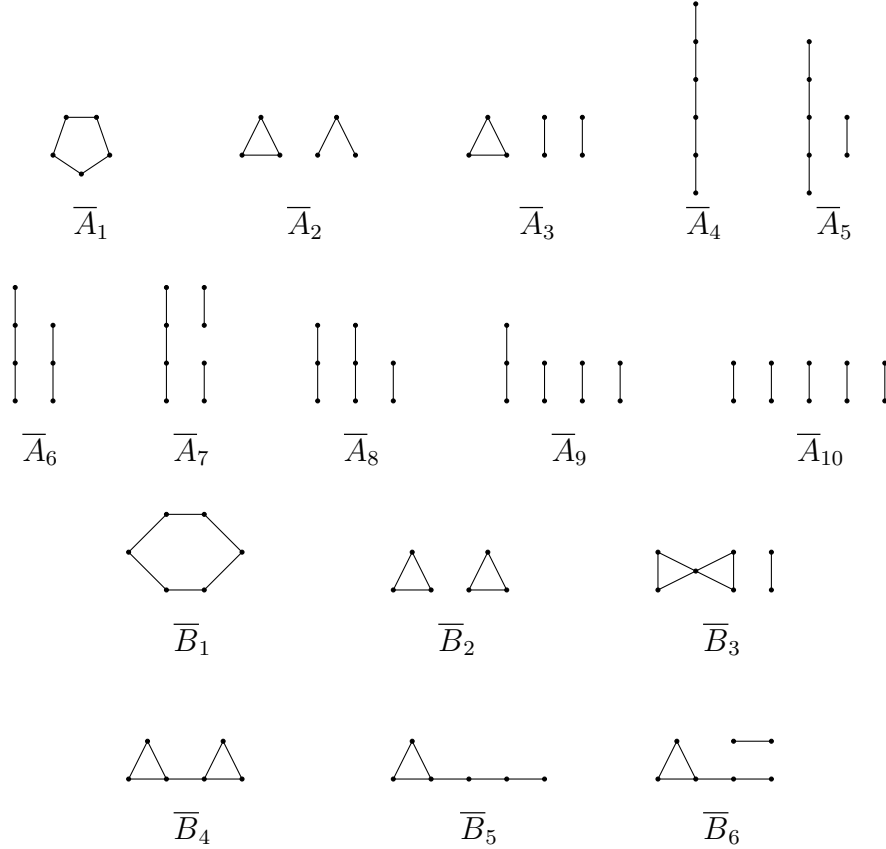


Figure 4.3: Complements of the graphs $A_1 - A_{10}, B_1 - B_6$.

Proposition 4.1.3. *If G is chordal, then N is a clique.*

Proof. Suppose G is chordal, but N is not a clique, then there exist non-adjacent vertices i and j in N . Choose $\bar{n} \in \bar{N}$ and let $P = [a_1, \dots, a_p]$, $p \geq 1$, be a shortest path in $S \cup N$ connecting i and j . Then, $(\bar{n}, i, a_1, \dots, a_p, j)$ is a cycle of length at least 4, a contradiction. \square

We now return to the proof of Theorem 4.1.2. For the implication (ii) \implies (i) we note that the graphs C_n , $n \geq 5$, $A_2 - A_{10}$, $B_1 - B_6$ contain no clique-cutsets (apply the algorithm described in [28]) and cannot occur as induced subgraphs of a graph in $\bigcup_{i=1}^4 \mathcal{G}_i$. Therefore, if G is a clique-sum of a set of graphs belonging to $\bigcup_{i=1}^4 \mathcal{G}_i$, it does not contain, as an induced subgraph, a cycle C_n , $n \geq 5$, nor any of the graphs $A_2 - A_{10}$ and $B_1 - B_6$.

For the proof of the reverse implication (i) \implies (ii) we start with the following corollary. Note that this corollary and Lemma 3.1.8 are essentially the same, although the proofs differ. In this case we rely on the partitioning of the vertex set V , discussed earlier, to prove the result.

Corollary 4.1.4. [25, Theorem 7.9] *Every chordal graph $G = (V, E)$ which is not a clique, has a clique-cutset. In particular, every chordal graph is the clique-sum of cliques.*

Proof. Let $G = (V, E)$ be a chordal graph which is not a clique. Then V admits the following partitioning, as seen above,

$$V = S \cup N \cup \overline{N},$$

where $G[S]$ is connected, $\overline{N} \neq \emptyset$ and there are no edges between the sets \overline{N} and S . Thus, N is a clique-cutset in G (Proposition 4.1.3). \square

Assume that G has clique-cutsets. This implies that G can be decomposed as the clique-sum of a finite number of subgraphs (since G is finite) which contain no clique-cutset, say G_1, G_2, \dots, G_p . Since we wish to show that a graph satisfying Theorem 4.1.2 (i), is the clique-sum of a set of graphs belonging to $\bigcup_{i=1}^4 \mathcal{G}_i$, it suffices to show that $G_1, G_2, \dots, G_p \in \bigcup_{i=1}^4 \mathcal{G}_i$, to prove the result. Thus, there is no loss of generality if we assume that G has no clique-cutset. Furthermore, as mentioned earlier, $C_n, n \geq 5, A_1 - A_{10}, B_1 - B_6$ contain no clique-cutsets. This is an important fact, since it then follows that if G_1, G_2, \dots, G_p all satisfy Theorem 4.1.2 (i), G does as well.

If G is a clique, it is an induced subgraph of a graph belonging to $\bigcup_{i=1}^4 \mathcal{G}_i$. Therefore, if G is a clique, there is nothing to prove; consequently it makes sense to assume that G is not a clique.

In summary, the assumptions on the graph G are as follows:

Assumption. Let $G = (V, E)$ be a graph. We assume the following:

- (i) G does not contain, as an induced subgraph, a cycle $C_n, n \geq 5$, nor any of the graphs $A_2 - A_{10}$ and $B_1 - B_6$;
- (ii) G is connected;
- (iii) G has no clique-cutset;
- (iv) G is not a clique.

In the rest of the chapter $G = (V, E)$ is a graph which satisfies these assumptions. We now apply the partitioning discussed earlier to the vertex set V . Hence, V will be partitioned as

$$V = S \cup N \cup \overline{N},$$

where $S \neq \emptyset, G[S]$ is connected, $\overline{N} \neq \emptyset$, there is no edge between the sets S and \overline{N} , every vertex in N is adjacent to every vertex in \overline{N} , and N is not a clique (else it would be a clique-cutset in G).

4.2 Preliminary results

We group here a number of preliminary results on the structure of G which will lead to two distinct cases that we have to consider.

Proposition 4.2.1. [20, Claim 3, 5 and 7] Let I and J be distinct stable sets in N , then:

- (i) *There exists an $s \in S$ adjacent to all the vertices in I . Moreover, if $|I| \geq 3$, this vertex s is unique.*
- (ii) *If $|I| \geq 2, |J| \geq 2, I \cap J \neq \emptyset$ and $s \in S$ is adjacent to all the vertices in I , then s is adjacent to all the vertices in J .*

Proof. (i) If $|I| = 0$ or $|I| = 1$, the statement is trivial. We proceed by induction on $|I|$. Throughout, \bar{n} will denote a vertex in \bar{N} .

Assume that $|I| = 2$. Let $i, j \in N$ be non-adjacent and assume that no vertex in S is adjacent to both i and j . There exist $s, t \in S$ such that $(s, i), (t, j) \in E$, per definition of N , and $(s, j), (t, i) \notin E$, by our assumption. Let P be a shortest path in S from s to t , which exists since $G[S]$ is connected. Then this path P , together with the edges $(s, i), (i, \bar{n}), (\bar{n}, j), (j, t)$ forms a cycle of length greater than 4 in G , a contradiction. Note that we may have that i or j is adjacent to some vertex in P ; if this should be the case, we merely take this vertex to be our new s or t , depending on whether i or j is adjacent to said vertex. Regardless of the number of times we may need to do this, we still find a cycle of length greater than 4 in G .

Assume that $|I| = 3$. Let $I = \{i, j, k\}$. Assume there exists no vertex in S adjacent to i, j, k . Then, from the case $|I| = 2$, we know there exist vertices $r, s, t \in S$ such that $(r, i), (r, j), (s, i), (s, k), (t, j), (t, k) \in E$. By our assumption $(r, k), (s, j), (t, i) \notin E$. Now, assume that r and s are adjacent, then we find an induced cycle C_5 in G on $\{\bar{n}, j, r, s, k\}$, a contradiction. Similarly, if $(r, t) \in E$ or $(s, t) \in E$. Therefore, r, s and t are pairwise non-adjacent. However, we then find an induced cycle C_6 in G on $\{r, i, s, k, t, j\}$, a contradiction. Thus, there exists a vertex in S adjacent to all the vertices in I .

Now assume that $|I| > 3$ and that the claim is valid for any stable subset of N of cardinality $|I| - 1$. Say $I = \{i_1, \dots, i_p\}$, $p \geq 4$ and that no vertex in S is adjacent to all the vertices in I . By the induction hypothesis, we may assume that for every $j = 1, \dots, p$, there exists an $s_j \in S$ adjacent to all vertices in $I \setminus \{i_j\}$. However, we then find B_4 , as an induced subgraph, on the vertices $\{\bar{n}, s_1, s_p, i_{p-2}, i_{p-1}, i_p\}$ (see Figure 4.4). Hence, there exists an $s \in S$ adjacent to all the vertices in I .

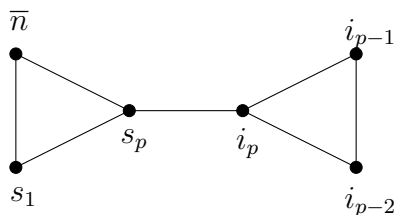


Figure 4.4: The complementary graph on the vertex set $\{\bar{n}, s_1, s_p, i_{p-2}, i_{p-1}, i_p\}$

Next we prove the uniqueness claim. First, assume that $|I| = 3$. Assume $s, t \in S$ are distinct vertices, adjacent to i, j and k . Then i, j and k form a C_3 in \bar{G} , non-adjacent to s, t and \bar{n} , while \bar{n} is adjacent to s and t . Thus we find B_2 or A_2 , as induced subgraphs, on the vertices $\{i, j, k, s, t, \bar{n}\}$ (see Figure 4.5), depending on whether $(s, t) \in E$ or not, a contradiction. Hence the result holds when $|I| = 3$.

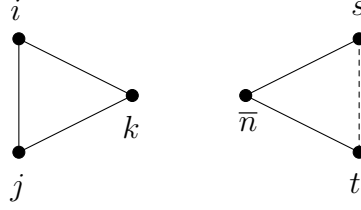


Figure 4.5: The complementary graph on the vertex set $\{i, j, k, s, t, \bar{n}\}$

Assume that $|I| > 3$. For any subset of I consisting of three vertices there can be only one $s \in S$ adjacent to all the vertices of the subset, by the preceding paragraph. Therefore, there can be only one $s \in S$ adjacent to all the vertices of I .

(ii) Let $i \in I$, $j \in J$ and let $s \in S$ be adjacent to all the vertices in I . Let $k \in I \cap J$, which exists since $|I| \geq 2$, $|J| \geq 2$, and $I \cap J$ is assumed to be non-empty. Then $(i, k), (j, k) \notin E$.

Our proof is by contradiction. Assume that j is non-adjacent to s . If i and j are non-adjacent there exists, by the first part of the proposition, a vertex $t \in S$ adjacent to i, j and k . However, we then find B_4 or B_5 , as an induced subgraph, on the on the vertex set $\{\bar{n}, s, t, i, j, k\}$ (see Figure 4.6) depending on whether $(s, t) \in E$ or not. Thus, i and j are adjacent.

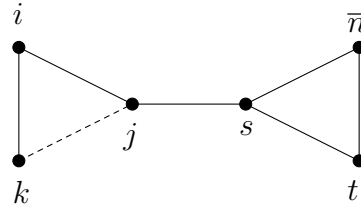


Figure 4.6: The complementary graph on the vertex set $\{\bar{n}, s, t, i, j, k\}$

Now, there exists a $u \in S$ adjacent to i, j and k . Indeed, if this were not so, there exists, by the first part of the proposition, vertices $u_1, u_2 \in S$ such that u_1 is adjacent to i and j but not k , and u_2 is adjacent to j and k but not i . Then u_1 and u_2 are adjacent, else we find an induced cycle of length 5 on the vertices $\{u_1, u_2, i, j, k\}$. However, u_1 and u_2 adjacent, leads to another contradiction, since $(\bar{n}, u_1, k, j, i, u_2)$ is an induced C_6 in \bar{G} , which implies that B_1 is an induced subgraph on the vertices $\{\bar{n}, u_1, u_2, i, j, k\}$. Therefore, there necessarily exists a vertex $u \in S$ adjacent to i, j and k .

Now we find A_4 or B_5 , as an induced subgraph, on the vertex set $\{\bar{n}, s, u, i, j, k\}$ (see Figure 4.7) depending on whether $(s, u) \in E$ or not. This contradiction shows that s must be adjacent to all the vertices of J .

□

Corollary 4.2.2. [20, p.559] $G[\bar{N}]$ is chordal.

Proof. The proof is by contradiction. Assume that $G[\bar{N}]$ is not chordal. By our assumption G , and hence $G[\bar{N}]$, does not contain a cycle of length greater than or equal to 5. So we assume that $G[\bar{N}]$ contains C_4 , as an induced subgraph. Let $i, j \in N$ be non-adjacent.

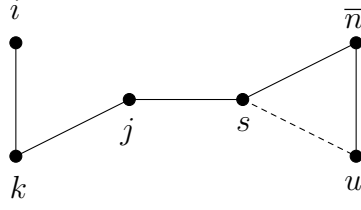


Figure 4.7: The complementary graph on the vertex set $\{\bar{n}, s, u, i, j, k\}$

Then both i and j are adjacent to all the vertices in the induced C_4 in $G[\bar{N}]$, since every vertex in N is adjacent to every vertex in \bar{N} . Moreover, by Proposition 4.2.1 (i), there exists an $s \in S$ adjacent to both i and j , but not to any vertex in the induced C_4 in $G[\bar{N}]$, since there are no edges between the sets S and \bar{N} . Then we find B_3 , as an induced subgraph, on the vertices of C_4 and i, j, s , a contradiction. \square

Proposition 4.2.3. [20, Claim 8] *Let (i, h, j, k) be an induced C_4 in $G[N]$. Then we have the following:*

- (i) *Any vertex $s \in S$ adjacent to i and j is adjacent to h and k .*
- (ii) *Every vertex $x \in N \setminus \{i, j, h, k\}$ is adjacent to at least three vertices in $\{i, j, h, k\}$.*

Proof. (i) By Proposition 4.2.1 (i) there exists vertices $s, t \in S$ such that s is adjacent to i and j , and t is adjacent to h and k . Assume that s is not adjacent to both h and k . We will show that this leads to a contradiction. Let $\bar{n} \in \bar{N}$. Now, the complementary graph induced by the vertex set $\{i, j, h, k, s, t, \bar{n}\}$ has the form shown in Figure 4.8. The solid lines indicate edges in the complementary graph and dotted lines indicate possible edges in the complementary graph.

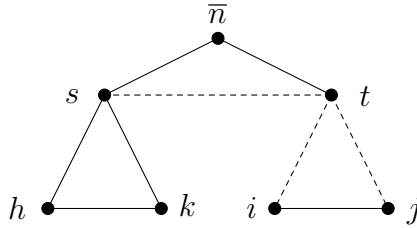


Figure 4.8: The complementary graph on the vertex set $\{\bar{n}, s, t, i, j, h, k\}$

We list all the possibilities in the table below, along with the vertex set and forbidden induced subgraph which arises in each case. A check in the appropriate column indicates that the edge is present in the graph G , which of course implies that it is not an edge in the complementary graph \bar{G} , i.e., not an edge in Figure 4.8.

(s, t)	(s, h)	(s, k)	(t, i)	(t, j)	Vertex set	Induced subgraph
✓			✓	✓	$\{\bar{n}, s, t, i, j, h, k\}$	B_6
✓			✓		$\{s, t, i, j, h, k\}$	A_2
✓				✓	$\{s, t, i, j, h, k\}$	A_2
✓					$\{s, t, i, j, h, k\}$	B_2
			✓	✓	$\{\bar{n}, s, t, i, j, h, k\}$	B_3
			✓		$\{s, t, i, j, h, k\}$	B_5
				✓	$\{s, t, i, j, h, k\}$	B_5
					$\{s, t, i, j, h, k\}$	B_4

Therefore, we may assume, without loss of generality, that $(s, h) \in E$ and, similarly, $(t, i) \in E$. The graph in Figure 4.9 gives the form of the complementary graph under the new assumptions. Again we list all the possibilities in the table below.

(s, t)	(s, h)	(s, k)	(t, i)	(t, j)	Vertex set	Induced subgraph
✓	✓		✓	✓	$\{\bar{n}, s, t, i, j, h, k\}$	A_5
✓	✓		✓		$\{\bar{n}, s, t, i, j, k\}$	A_4
	✓		✓	✓	$\{s, t, i, j, h, k\}$	B_6
	✓		✓		$\{s, t, i, j, h, k\}$	A_4

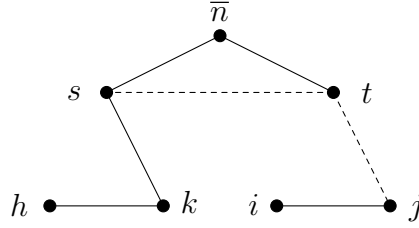


Figure 4.9: The complementary graph on the vertex set $\{\bar{n}, s, t, i, j, h, k\}$

We may therefore conclude that $(s, k) \in E$. Hence, s is adjacent to h and k .

(ii) Let $x \in N \setminus \{i, j, h, k\}$ and assume that $(x, i) \notin E$. We show, by contradiction, that x is adjacent to j, h and k . Thus, assume that x is not adjacent to each of j, h and k . Let $\bar{n} \in \bar{N}$. We start by proving that there exists a vertex $s \in S$ adjacent to i, j, h, k and x . We need but consider two cases: (a) $(x, j) \notin E$; and (b) $(x, h) \in E, (x, k) \notin E$.

(a) Assume that $(x, j) \notin E$. Then $\{x, i, j\}$ is a stable set in N and, by Proposition 4.2.1 (i) there exists a $s \in S$ adjacent to x, i and j . Now, by (i) of the current lemma, it follows that s is adjacent to h and k .

(b) Assume that $(x, h) \in E, (x, k) \notin E$. Then $\{h, k\}$ and $\{x, k\}$ are two intersecting stable sets. Thus, by Proposition 4.2.1 (i) and (ii), there exists a vertex $s \in S$ adjacent to x, h and k . Therefore, by (i) of the current lemma, it follows that s is adjacent to i and j .

Thus, there exists a vertex $s \in S$ adjacent to i, j, h, k and x . The complementary graph induced by the vertex set $\{i, j, h, k, x, s, \bar{n}\}$ has the form shown in Figure 4.10. In the

table below we list all the possibilities. Note that in all of the cases the relevant vertex set is $\{\bar{n}, s, i, j, h, k, x\}$.

(x, j)	(x, h)	(x, k)	Induced subgraph
✓	✓		A_5
✓		✓	A_5
	✓	✓	A_3
✓			B_6
	✓		B_6
		✓	B_6
			B_3

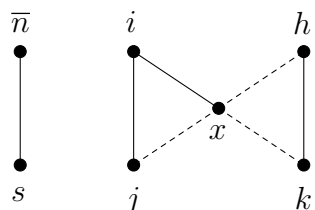


Figure 4.10: The complementary graph on the vertex set $\{\bar{n}, s, i, j, h, k, x\}$

We may therefore conclude that $(x, j), (x, h), (x, k) \in E$. □

Corollary 4.2.4. [20, Corollary 9] *If \bar{N} is not a clique, then $G[N]$ is chordal and there are at least two edges among any three vertices in N .*

Proof. Assume \bar{n}_1 and \bar{n}_2 are two non-adjacent vertices in \bar{N} and that $G[N]$ is not chordal. Note that all cycles C_n , $n \geq 5$, are forbidden by assumption. Hence, $G[N]$ contains an induced C_4 . Let (i, h, j, k) be an induced C_4 in N . By Proposition 4.2.1 (i) and Proposition 4.2.3 (i) there exists a vertex $s \in S$ adjacent to i, j, h and k , then we find A_3 , as an induced subgraph, on $\{\bar{n}_1, \bar{n}_2, s, i, j, h, k\}$, a contradiction (see Figure 4.11). Thus, $G[N]$ is chordal.

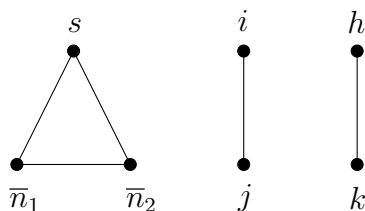


Figure 4.11: The complementary graph on the vertex set $\{\bar{n}_1, \bar{n}_2, s, i, j, h, k\}$,

Next, let i, j and k be distinct vertices in N and assume that there are less than two edges among them. Our proof is by contradiction. We start by showing that there exists a vertex $s \in S$ adjacent to i, j and k . There are two cases: either there are no edges between i, j and k ; or there is one edge, say $(i, j) \in E$. In the first case, there exists a vertex $s \in S$ adjacent to i, j and k , by Proposition 4.2.1 (i), and in the second case,

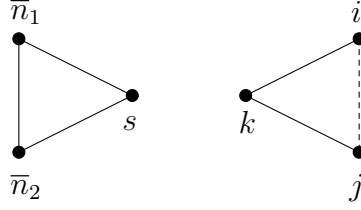


Figure 4.12: The complementary graph on the vertex set $\{\bar{n}_1, \bar{n}_2, s, i, j, k\}$

$\{i, k\}$ and $\{j, k\}$ are two intersecting stable sets, which implies that there exists a vertex $s \in S$ adjacent to i, j and k , by Proposition 4.2.1 (i) and (ii). The complementary graph, induced by the vertex set $\{\bar{n}_1, \bar{n}_2, s, i, j, k\}$, is shown in Figure 4.12. Again the solid lines indicate edges in the complementary graph and dotted lines indicate possible edges in the complementary graph.

It is now clear that if there are no edges between the vertices i, j and k we find B_2 as an induced subgraph, and if there is only one edge we find A_2 , as an induced subgraph. \square

From this corollary we see that if $G[N]$ is not chordal, or if there are fewer than two edges among any three vertices in N , it must be true that \bar{N} is a clique.

We will now show that the proof of Theorem 4.1.2 (i) \implies (ii) may be split into two disjoint cases, but first we need to introduce the notion of a matching and prove some results regarding this notion.

Definition 4.2.5 (Matching). Let $G = (V, E)$ be a graph. A subset $F \subseteq E$ is called a matching in G if no two edges of F have a common end-vertex.

We say that F is an induced matching if it is a matching together with any vertices that are the endpoints of edges in the matching. Now, let ν denote the largest cardinality of an induced matching in $\bar{G}[N]$. The following proposition gives bounds for ν .

Proposition 4.2.6. [20, p.561] Let ν denote the largest cardinality of an induced matching in $\bar{G}[N]$. Then

$$1 \leq \nu \leq 3.$$

Proof. We first observe that $\nu \geq 1$, since N is not a clique. Now, assume that $\nu \geq 4$ and let $\{(i_a, j_a) : a = 1, 2, 3, 4\}$ be an induced matching in $\bar{G}[N]$. By Proposition 4.2.1 (i) there exists a vertex $s \in S$ such that $(s, i_1), (s, j_1) \in E$. Then, by Proposition 4.2.3 (i), it follows that $(s, i_2), (s, j_2), (s, i_3), (s, j_3), (s, i_4), (s, j_4) \in E$, since $(i_1, i_2, j_1, j_2), (i_2, i_3, j_2, j_3)$ and (i_3, i_4, j_3, j_4) are all induced C_4 's in N . We then find A_{10} , as an induced subgraph, in G on $\{\bar{n}, s, i_1, i_2, i_3, i_4, j_1, j_2, j_3, j_4\}$, where $\bar{n} \in \bar{N}$. Therefore, $\nu \leq 3$ and the proof is complete. \square

Using the parameter ν we split the rest of the proof into two disjoint cases:

Case I: $\nu = 1$.

Case II: $\nu \in \{2, 3\}$.

For Case I we show that $G \in \mathcal{G}_1 \cup \mathcal{G}_4$, and for Case II that $G \in \mathcal{G}_\nu$, $\nu \in \{2, 3\}$.

4.3 Case I

We assume here that $\nu = 1$. This easily implies that $G[N]$ is chordal. Furthermore, under the assumption that G contains no clique-cutsets, it follows that N can not be a clique. Therefore, by Corollary 4.1.4, N contains a clique-cutset K . Consequently, we may partition N as

$$N = N_1 \cup K \cup N_2,$$

with $K \neq \emptyset$ a clique and N_1, N_2 both non-empty sets, such that there are no edges between N_1 and N_2 .

Our first goal in this section, is to prove the following proposition:

Proposition 4.3.1. *Every vertex in S is adjacent to every vertex in $N \setminus K_0$, where K_0 is defined as*

$$K_0 := \{k \in K : (i, k) \in E \text{ for all } i \in N_1 \cup N_2\}.$$

We start by defining the following set

$$S_{12} := \{s \in S : s \text{ adjacent to a vertex in } N_1 \text{ and a vertex in } N_2\}.$$

It is not hard to see that $S_{12} \neq \emptyset$. Indeed, let $i_1 \in N_1$ and $i_2 \in N_2$. Then, by Proposition 4.2.1 (i), there exists a vertex $s \in S$ adjacent to i_1 and i_2 , since $(i_1, i_2) \notin E$. Thus, $s \in S_{12}$. In the next proposition we will see that every vertex in S_{12} is adjacent to every vertex in $N \setminus K_0$.

Proposition 4.3.2. *[20, p.562] Every vertex in S_{12} is adjacent to every vertex in $N \setminus K_0$.*

Proof. Let $s \in S_{12}$ and let $i_1 \in N_1, i_2 \in N_2$ be adjacent to s . Then s , by Proposition 4.2.1 (ii), is adjacent to every other vertex in $j_1 \in N_1$, since $\{i_1, i_2\}$ and $\{j_1, i_2\}$ are two intersecting stable sets in N . A similar argument shows that s is adjacent to every vertex in N_2 . Now, let $k \in K \setminus K_0$, then k must be non-adjacent to some element in $N_1 \cup N_2$. We may assume, without loss of generality, that k and i_1 are non-adjacent. Then $\{k, i_1\}$ and $\{i_2, i_1\}$ are two intersecting stable sets in N , so applying Proposition 4.2.1 (ii) again, we have that s is adjacent to k . Thus, every vertex in S_{12} is adjacent to every vertex in $N \setminus K_0$. \square

If we can show that $S = S_{12}$ it immediately follows that every vertex in S is adjacent to every vertex in $N \setminus K_0$. However, some more work needs to be done before we can show that this is in fact true. For the sake of brevity we define the following sets:

$$S_1 := \{s \in S : s \text{ is adjacent to a vertex in } N_1 \text{ but not to a vertex in } N_2\},$$

$$S_2 := \{s \in S : s \text{ is adjacent to a vertex in } N_2 \text{ but not to a vertex in } N_1\},$$

$$S_0 = S \setminus (S_1 \cup S_2 \cup S_{12}),$$

and, for $a = 1, 2$

$$K_a := \{k \in K : (i, k) \notin E \text{ for some } i \in N_a\}.$$

Thus, $S = S_0 \cup S_1 \cup S_2 \cup S_{12}$ and $K = K_0 \cup K_1 \cup K_2$. Setting $T := S_0 \cup S_1 \cup S_2$, we see that $S = S_{12}$ is equivalent to $T = \emptyset$. Therefore, in what follows we will prove that $T = \emptyset$. For $s \in T$, set

$$X_s := \{x \in S_{12} \cup N : (s, x) \in E\}.$$

Note that the set X_s is, in essence, the adjacency set of s , minus possible neighbours in T , i.e., $X_s = \text{Adj}(s) \setminus T$.

Lemma 4.3.3. [20, Claim 14] *Let $s, t \in T$. Then*

- (i) X_s is a clique.
- (ii) $X_s \cup X_t$ is a clique for every $(s, t) \in E$.

Proof. (i) Assume that X_s is not a clique, for some $s \in T$. Then there are two non-adjacent vertices $x, y \in X_s$. Thus, $x, y \in S_{12} \cup N$ and s is adjacent to x and y . Let $i_1 \in N_1$, $i_2 \in N_2$ and $\bar{n} \in \bar{N}$. Note that the following combinations are impossible:

- $x \in S_{12}, y \in N \setminus K_0$: Since every vertex in S_{12} is adjacent to every vertex in $N \setminus K_0$ (Proposition 4.3.2).
- $x, y \in K$: Since K is a clique.
- $x \in N_1 \cup N_2, y \in K_0$: Follows from the definition of K_0 .
- $x \in N_1, y \in N_2$: Since $s \in T$ implies that s is in one of S_0, S_1, S_2 and s is adjacent to x and y .
- $x \in K_1, y \in N_1$ or $x \in K_2, y \in N_2$: Assume $x \in K_1, y \in N_1$. The fact that $y \in N_1$ implies that $s \in S_1$. Then, $\{x, y\}$ and $\{i_2, y\}$ are two intersecting stable sets, which implies, by Proposition 4.2.1 (ii), that s is adjacent to i_2 . However, this contradicts the fact that $s \in S_1$. A similar argument shows that $x \in K_2, y \in N_2$ is impossible.
- $x \in N_1, y \in K_2$ or $x \in N_2, y \in K_1$: Assume that $x \in N_1, y \in K_2$. Then $s \in S_1$ and we may assume, without loss of generality, that $(y, i_2) \notin E$. Then, $\{x, y\}$ and $\{i_2, y\}$ are two intersecting stable sets, which implies, by Proposition 4.2.1 (ii), that s is adjacent to i_2 . However, this contradicts the fact that $s \in S_1$. A similar argument shows that $x \in K_2, y \in N_2$ is impossible.

Thus, the only remaining combinations are:

- $x, y \in S_{12}$ or $x \in S_{12}, y \in K_0$.
- $x, y \in N_1$ or $x, y \in N_2$.

We treat each case separately. Assume that $x, y \in S_{12}$ or $x \in S_{12}, y \in K_0$. In the table below we list all the possibilities. The first three columns of the table indicate in which sets s, x and y are and the last column indicates which forbidden induced subgraph occurs in each case. The relevant vertex set is $\{\bar{n}, x, y, s, i_1, i_2\}$. In Figure 4.13

we illustrate the complementary graph, induced by the vertex set $\{\bar{n}, s, i, j, k\}$. The solid lines indicate edges in the complementary graph and dotted lines indicate possible edges in the complementary graph.

s	x	y	Induced subgraph
S_0	S_{12}	S_{12}	B_4
S_0	S_{12}	K_0	B_5
$S_1 \cup S_2$	S_{12}	S_{12}	B_5
$S_1 \cup S_2$	S_{12}	K_0	A_4

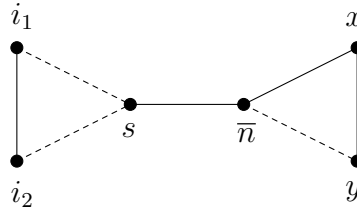


Figure 4.13: The complementary graph on the vertex set $\{\bar{n}, s, x, y, i_1, i_2\}$.

We may therefore conclude that the combinations $x, y \in S_{12}$ and $x \in S_{12}, y \in K_0$ are impossible.

Assume that $x, y \in N_1$ or $x, y \in N_2$. The two cases are symmetric, therefore, there is no loss of generality in assuming that $x, y \in N_1$. Consequently, $s \in S_1$. Furthermore, $\{x, y, i_2\}$ is a stable set in N . Thus, by Proposition 4.2.1 (i), there exists a unique vertex $s_1 \in S$ adjacent to x, y and i_2 . There now arises four distinct cases, depending on whether s is adjacent to i_2 and s_1 , or not. We list these four possibilities in the table below. The first two columns of the table indicate whether s and is adjacent to i_2 and s_1 , or not, and the last column indicates which forbidden induced subgraph occurs. Note that the relevant vertex set is $\{\bar{n}, s_1, s, i_2, x, y\}$. The graph in Figure 4.14 gives the form of the complementary graph on the vertex set $\{\bar{n}, s_1, s, i_2, x, y\}$.

(s, i_2)	(s, s_1)	Induced subgraph
✓	✓	A_2
✓		B_2
	✓	B_5
		B_4

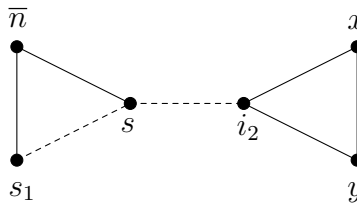


Figure 4.14: The complementary graph on the vertex set $\{\bar{n}, s_1, s, i_2, x, y\}$.

We may therefore conclude that the combinations $x, y \in N_1$ or $x, y \in N_2$ are impossible.

Now, since we have exhausted all the possibilities, we may conclude that X_s is a clique for every $s \in T$.

(ii) Assume that $X_s \cup X_t$ is not a clique, for some $(s, t) \in E$, $s, t \in T$. Then there are two non-adjacent vertices $x, y \in X_s \cup X_t$. We show that this leads to a contradiction. Let $\bar{n} \in \bar{N}$, $i_1 \in N_1$ and $i_2 \in N_2$.

By (i) of the current lemma X_s is a clique for every $s \in T$. Therefore, we necessarily have that $x \in X_s \setminus X_t$ and $y \in X_t \setminus X_s$. Thus, $x, y \in S_{12} \cup N$ with s adjacent to x , but not y , and t adjacent to y , but not x . We immediately have that $x, y \in N$ is impossible, else (\bar{n}, x, s, t, y) is an induced cycle of length 5. The only remaining possibility is $x \in S_{12}$, $y \in S_{12} \cup K_0$. In these cases we have that x and y are adjacent to both i_1 and i_2 .

Now, $s, t \in S_0 \cup S_1$ or $s, t \in S_0 \cup S_2$. Indeed, assume that $s \in S_1$ and $t \in S_2$. Then $(\bar{n}, i_1, s, t, i_2)$ is an induced C_5 , a contradiction. We may therefore assume, without loss of generality, that $s, t \in S_0 \cup S_1$.

Thus, assume that $x \in S_{12}$, $y \in S_{12} \cup K_0$ and $s, t \in S_0 \cup S_1$. Then (i_2, x, s, t, y) is an induced C_5 . Consequently, $x \in S_{12}$, $y \in S_{12} \cup K_0$ is impossible.

We have again exhausted all possibilities and may thus conclude that $X_s \cup X_t$ is a clique for every $(s, t) \in E$, $s, t \in T$. \square

Assume that $T \neq \emptyset$. Let A denote a maximal subset of T such that

- $G[A]$ is connected;
- $X(A) = \bigcup_{a \in A} X_a$ is a clique.

Lemma 4.3.4. [20, Claim 15] *There are no edges between the sets A and $T \setminus A$.*

Proof. The proof is by contradiction. Assume that $a \in A$ and $b \in T \setminus A$ are adjacent. The maximality of A implies that $X(A) \cup X_b$ is not a clique. Indeed, $G[A \cup \{b\}]$ is connected, since $(a, b) \in E$. Thus, if $X(A) \cup X_b$ is a clique, A is not maximal. Hence, there exist two non-adjacent vertices $x \in X(A)$ and $y \in X_b$. Let $\bar{n} \in \bar{N}$, $i_1 \in N_1$ and $i_2 \in N_2$.

Now, since $x \in X(A)$ there exists a vertex $a_0 \in A$, such that $(x, a_0) \in E$. Then $a_0 \neq a$. Indeed, if $a_0 = a$, we have that $X_{a_0} \cup X_b$ is a clique, by Lemma 4.3.3 (ii), which implies that $(x, y) \in E$, a contradiction. A similar argument, and application of Lemma 4.3.3 (i) and (ii), shows that $(a, y), (a_0, b), (a_0, y), (x, b) \notin E$.

Observe that there exists no path from S_1 to S_2 , with all internal vertices in S_0 . Indeed, assume that $s_1 \in S_1$, $s_2 \in S_2$ and that $[s_1, u_1, \dots, u_p, s_2]$, $p \geq 0$, is a path with $u_i \in S_0$, for $i = 1, \dots, p$. Without loss of generality, assume that $(i_1, s_1), (i_2, s_2) \in E$. Then, $(\bar{n}, i_1, s_1, u_1, \dots, u_p, s_2, i_2)$ is an induced cycle of length greater than or equal to 5, a contradiction. This implies that any induced path contained in T , is necessarily contained in either $S_0 \cup S_1$ or $S_0 \cup S_2$. We will use this fact in what follows.

The fact that $G[A]$ is connected, implies there exists a shortest path $[a_0, a_1, \dots, a_p, a]$, $p \geq 0$, from a_0 to a . Then, $P = [x, a_0, a_1, \dots, a_p, a, b, y]$ is an induced path of length

greater than 3, from x to y , with internal vertices in T . By the preceding paragraph we may assume, without loss of generality, that the internal vertices of P are contained in $S_0 \cup S_1$.

We now have two cases: either $x, y \in N$ or $x \in S_{12}, y \in S_{12} \cup K_0$. (Note that $x, y \in K_0$ is impossible, since K_0 is a clique.) However, both of these cases lead to contradictions. Indeed, if $x, y \in N$, then $(\bar{n}, x, a_0, a_1, \dots, a_p, a, b, y)$ is an induced C_n , $n \geq 6$; if $x \in S_{12}, y \in S_{12} \cup K_0$, then $(i_2, x, a_0, a_1, \dots, a_p, a, b, y)$ is an induced C_n , $n \geq 6$.

Thus, we may conclude that there exist no edges between the sets A and $T \setminus A$. \square

Proof of Proposition 4.3.1. We prove that the set T is empty. Indeed, if $T \neq \emptyset$ implies that $A \neq \emptyset$. Moreover, there are no edges between A and the sets $T \setminus A$, $(S_{12} \cup N) \setminus X(A)$ and \bar{N} . Hence, if we delete the clique $X(A)$, the graph G is disconnected, which shows that $X(A)$ is a clique-cutset, contradicting our assumption that G contains no clique-cutsets. Consequently, $T = \emptyset$, which implies that $S = S_{12}$. In other words, every vertex in S is adjacent to every vertex in $N \setminus K_0$. \square

We are now ready to show that $G \in \mathcal{G}_1 \cup \mathcal{G}_4$. We do this in the form of several propositions.

Proposition 4.3.5. [20, Corollary 16] *If $|N_a| = 1$ and $K_a = \emptyset$, for $a = 1, 2$, then $G \in \mathcal{G}_1$.*

Proof. Assume that $|N_a| = 1$, for $a = 1, 2$. Then $N_1 = \{i_1\}$ and $N_2 = \{i_2\}$. Moreover, $K = K_0$, since $K_1 = K_2 = \emptyset$. Thus, i_1 and i_2 are adjacent to all the vertices in $S \cup K \cup \bar{N}$. All that remains is to show that $G[S \cup K \cup \bar{N}]$ is chordal.

We prove this by contradiction. By our assumption G , and hence $G[S \cup K \cup \bar{N}]$, does not contain a cycle of length greater than or equal to 5. Thus, assume that $G[S \cup K \cup \bar{N}]$ contains a C_4 , as an induced subgraph. Note that $G[K \cup \bar{N}]$ is chordal, since K is a clique, every vertex in K is adjacent to every vertex in \bar{N} and $G[\bar{N}]$ is chordal (Corollary 4.2.2). Hence a possible C_4 is necessarily in $G[S \cup K]$, with at least two vertices in S , since K is a clique. We now have three possibilities:

- (a) (i, j, s, t) is an induced C_4 , with $i, j \in K$ and $s, t \in S$.
- (b) (i, r, s, t) is an induced C_4 , with $i \in K$ and $r, s, t \in S$.
- (c) (r, s, t, u) is an induced C_4 , with $r, s, t, u \in S$.

The complementary graphs of all three possibilities can be seen in Figure 4.15.

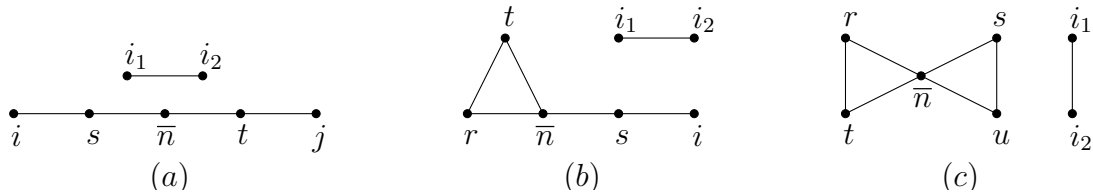


Figure 4.15: The complementary graphs of the three possibilities (a) – (c)

It is now easy to see that the forbidden induced subgraphs which occur are: (a) A_5 ; (b) B_6 ; and (c) B_3 . We may therefore conclude that $G[S \cup K \cup \overline{N}]$ is chordal. Consequently, $G \in \mathcal{G}_1$. \square

Henceforth, we assume that $|N_1 \cup K_1| \geq 2$ or $|N_2 \cup K_2| \geq 2$. Note that the two cases are symmetric. Thus, there is no loss of generality if we assume that $|N_1 \cup K_1| \geq 2$.

Lemma 4.3.6. [20, p.564] *If $|N_1 \cup K_1| \geq 2$, we have that \overline{N} and S are cliques. Moreover, every vertex in S is adjacent to every vertex in N .*

Proof. Since $|N_1 \cup K_1| \geq 2$ we either have that $i_1, j_1 \in N_1$ or $i_1 \in N_1, k \in K_1$. For the case $i_1 \in N_1, k \in K_1$ we may assume, without loss of generality, that $(i_1, k) \notin E$. Let $\overline{n} \in \overline{N}$ and $i_2 \in N_2$.

Now, \overline{N} is a clique. Indeed, observe that in both cases there is, at most, one edge among the two vertices and the vertex i_2 . We may therefore conclude, by Corollary 4.2.4, that \overline{N} is a clique.

Next, we show that S is a clique. We prove this by contradiction. Assume that S is not a clique, then there exist two non-adjacent vertices $s, t \in S$. Now, if $i_1, j_1 \in N_1$ there are two possibilities, depending on whether i_1 and j_1 are adjacent. The graph in Figure 4.16 is the complementary graph induced by the vertex set $\{\overline{n}, s, t, i_2, i_1, j_1\}$. The solid lines indicate edges in the complementary graph and dotted lines indicate possible edges in the complementary graph. It is therefore clear that we find A_2 , as an induced subgraph, if i_1 and j_1 are adjacent, and B_2 , as an induced subgraph, if i_1 and j_1 are not adjacent. A similar argument holds for $i_1 \in N_1, k \in K_1$. Thus, S is a clique.

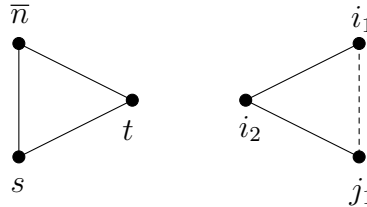


Figure 4.16: The complementary graph on the vertex set $\{\overline{n}, s, t, i_2, i_1, j_1\}$

Finally, we show that every vertex in S is adjacent to every vertex in N . We again prove this by contradiction. Assume that $s \in S$ is not adjacent to some vertex $h \in N$. Now, by Proposition 4.3.2, s is adjacent to every vertex in $N \setminus K_0$. Thus, $h \in K_0$. Moreover, h is adjacent to some vertex $t \in S$, by the definition of N . Note that s and t are adjacent, since S is a clique. Assume that $i_1, j_1 \in N_1$. Note that h is adjacent to i_1, j_1 and i_2 . Consequently, there are two possibilities, depending on whether i_1 and j_1 are adjacent. The graph in Figure 4.17 is the complementary graph induced by the vertex set $\{\overline{n}, s, t, h, i_2, i_1, j_1\}$. Clearly we find A_6 , as an induced subgraph, if i_1 and j_1 are adjacent, and A_2 , as an induced subgraph, if i_1 and j_1 are not adjacent. A similar argument holds for $i_1 \in N_1, k \in K_1$. Therefore, every vertex in S is adjacent to every vertex in N . \square

Proposition 4.3.7. [20, Corollary 18] *If $|S| = |\overline{N}| = 1$, then $G \in \mathcal{G}_1$.*

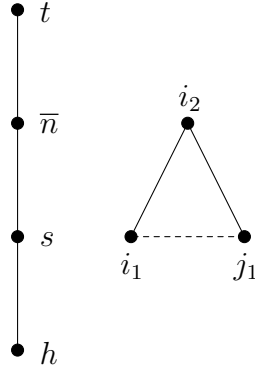


Figure 4.17: The complementary graph on the vertex set $\{\bar{n}, s, t, h, i_2, i_1, j_1\}$

Proof. If $|S| = |\bar{N}| = 1$, we have that $S = \{s\}$ and $\bar{N} = \{\bar{n}\}$. Recall that $|N_1 \cup K_1| \geq 2$. Thus, by Lemma 4.3.6, s and \bar{n} are adjacent to every vertex in N . Moreover, $G[N]$ is chordal. Therefore, $G \in \mathcal{G}_1$. \square

In what follows we assume that $|S \cup \bar{N}| \geq 3$.

Lemma 4.3.8. [20, p.564] *If $|N_1 \cup K_1| \geq 2$ and $|S \cup \bar{N}| \geq 3$, then*

- (i) $G[N]$ does not contain an induced path of length 3;
- (ii) N does not contain a stable set of cardinality greater than or equal to 3. That is, $\alpha(G[N]) = 2$, where $\alpha(H)$ denotes the stability number of the graph H .

Proof. By Lemma 4.3.6, \bar{N} and S are cliques and every vertex in S is adjacent to every vertex in N . Now, since $|S \cup \bar{N}| \geq 3$, we either have that $s_1, s_2 \in S$, $\bar{n} \in \bar{N}$ or $s \in S$, $\bar{n}_1, \bar{n}_2 \in \bar{N}$.

(i) Our proof is by contradiction. Assume that $G[N]$ contains a path $[i, j, k, l]$ of length 3. Now, if $s_1, s_2 \in S$, $\bar{n} \in \bar{N}$, we find A_6 , as an induced subgraph, on the vertex set $\{\bar{n}, s_1, s_2, i, j, h, k\}$. This can be seen in Figure 4.18 where the graph is the complementary graph on the vertex set $\{\bar{n}, s_1, s_2, i, j, h, k\}$. A similar argument holds for $s \in S$, $\bar{n}_1, \bar{n}_2 \in \bar{N}$. Thus, $G[N]$ does not contain an induced path of length 3.

(ii) Note that $\alpha(G[N]) \geq 2$, since N is not a clique. We again prove the result by contradiction. Assume that $\{i, j, k\}$ is a stable set in N . Now, if $s_1, s_2 \in S$, $\bar{n} \in \bar{N}$, we find A_2 , as an induced subgraph, on the vertex set $\{\bar{n}, s_1, s_2, i, j, k\}$. This is depicted in Figure 4.19 where the graph is the complementary graph on the vertex set $\{\bar{n}, s_1, s_2, i, j, k\}$. A similar argument holds for $s \in S$, $\bar{n}_1, \bar{n}_2 \in \bar{N}$. \square

Lemma 4.3.9. [20, Lemma 12] *If $H = (V_H, E_H)$ is a chordal graph, containing no induced path of length 3 and with $\alpha(H) = 2$, its vertex set V_H may be partitioned as follows:*

$$V_H = V_0 \cup V_1 \cup V_2,$$

where $V_0 \cup V_1$ and $V_0 \cup V_2$ are cliques and there are no edges between the sets V_1 and V_2 .

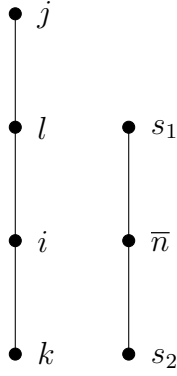


Figure 4.18: The complementary graph on the vertex set $\{\bar{n}, s_1, s_2, i, j, h, k\}$

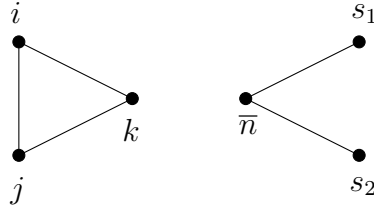


Figure 4.19: The complementary graph on the vertex set $\{\bar{n}, s_1, s_2, i, j, k\}$.

Proof. Note that $\alpha(H) = 2$ implies that H is not a clique. Thus, by Corollary 4.1.4, H contains a clique-cutset K . Consequently, the vertex set V_H may be partitioned as

$$V_H = N_1 \cup K \cup N_2,$$

where N_1, N_2 are both non-empty sets, such that there are no edges between N_1 and N_2 . Moreover, N_1 and N_2 are both cliques. Indeed, assume that there exist two non-adjacent vertices $i_1, j_1 \in N_1$ and let $i_2 \in N_2$. Then $\{i_1, j_1, i_2\}$ is a stable set of cardinality 3, contradicting $\alpha(H) = 2$.

Recall that K_a , for $a = 1, 2$, is defined as

$$K_a := \{k \in K : (i, k) \notin E \text{ for some } i \in N_a\}.$$

and

$$K_0 := \{k \in K : (i, k) \in E \text{ for all } i \in N_1 \cup N_2\}.$$

Thus, $K = K_0 \cup K_1 \cup K_2$. Moreover, $K_2 \cup N_1$ and $K_1 \cup N_2$ are cliques. Indeed, assume that $K_1 \cup N_2$ is not a clique. Then, there exist two non-adjacent vertices $i_2 \in N_2, k \in K_1$. Take $i_1 \in N_1$ non-adjacent to k , then, $\{i_1, i_2, k\}$ is a stable set of cardinality 3, contradicting $\alpha(H) = 2$.

Now, assume that K_1 is non-empty. Let $k \in K_1$, then there exists a vertex $i_1 \in N_1$ such that $(i_1, k) \notin E$. Consequently, k is not adjacent to any other vertex in N_1 . Indeed, assume that $j_1 \in N_1$ is adjacent to k and let $i_2 \in N_2$. Then, $[i_1, j_1, k, i_2]$ is an induced path of length 3, since N_1 and $K_1 \cup N_2$ are cliques. We may therefore conclude that there

are no edges between the sets K_1 and N_1 . Moreover, we have that $K_2 = \emptyset$. To see this, assume that $k_2 \in K_2$ exists and let $i_1 \in N_1$, $i_2 \in N_2$ and $k_1 \in K_1$. Then, $[i_1, k_2, k_1, i_2]$ is an induced path of length 2, since $K_2 \cup N_1$, $K_1 \cup N_2$ and K are cliques.

Thus, we may partition the vertex set V_H as follows:

$$V_H = N_1 \cup K_0 \cup (K_1 \cup N_2),$$

where the sets $N_1 \cup K_0$ and $K_0 \cup (K_1 \cup N_2)$ are cliques and there are no edges between the sets N_1 and $K_1 \cup N_2$. Thus, setting $V_0 = K_0$, $V_1 = N_1$ and $V_2 = K_1 \cup N_2$ completes the proof. \square

Proposition 4.3.10. [20, p.565] *If $|N_1 \cup K_1| \geq 2$ and $|S \cup \overline{N}| \geq 3$, then $G \in \mathcal{G}_4$.*

Proof. By Lemma 4.3.6, \overline{N} and S are cliques and every vertex in S is adjacent to every vertex in N . Furthermore $|S \cup \overline{N}| \geq 3$ implies, by Lemma 4.3.8, that $G[N]$ does not contain an induced path of length 3 and $\alpha(G[N]) = 2$. Now, since $G[N]$ is chordal, it follows, by Lemma 4.3.9, that N may be partitioned as

$$N = N_1 \cup K_0 \cup (K_1 \cup N_2),$$

where $N_1 \cup K_0$ and $K_0 \cup (K_1 \cup N_2)$ are cliques and there are no edges between the sets N_1 and $K_1 \cup N_2$.

In summary we have the following:

- \overline{N} , S , K_0 , $N_1 \cup K_0$ and $K_0 \cup (K_1 \cup N_2)$ are all cliques.
- Every vertex in the set K_0 is adjacent to every vertex in the sets \overline{N} , S , $N_1 \cup K_0$ and $K_0 \cup (K_1 \cup N_2)$.
- Every vertex in the sets \overline{N} and S is adjacent to every vertex in the sets $N_1 \cup K_0$ and $K_0 \cup (K_1 \cup N_2)$.
- There are no edges between the sets \overline{N} and S .
- There are no edges between the sets $N_1 \cup K_0$ and $K_0 \cup (K_1 \cup N_2)$.

We may therefore conclude that $G \in \mathcal{G}_4$. \square

This completes the proof for Case I.

4.4 Case II

We assume here that $\nu \in \{2, 3\}$. Thus $G[N]$ is non-chordal, since the existence of an induced matching of cardinality 2 in $\overline{G}[N]$ implies the existence of an induced C_4 in $G[N]$. We may therefore conclude that \overline{N} is a clique, by Corollary 4.2.4.

Let $\{(i_a, j_a) : a = 1, \dots, \nu\}$ be an induced matching of maximum cardinality in $\overline{G}[N]$. Now, by Proposition 4.2.3 (ii), we have that every vertex in N is non-adjacent to, at most, one of the i_a 's or j_a 's. Consequently, it makes sense to define the following pairwise disjoint sets:

$$I_a := \{i \in N : i \neq j_a, (i, j_a) \notin E\}, \quad J_a := \{j \in N : j \neq i_a, (j, i_a) \notin E\}$$

for $a = 1, \dots, \nu$. Thus, $i_a \in I_a$ and $j_a \in J_a$ for $a \leq \nu$. Set

$$I := \bigcup_{a=1}^{\nu} I_a \cup J_a, \quad N_0 := N \setminus I.$$

Lemma 4.4.1. [20, p.567] *Every vertex in N_0 is adjacent to every vertex in I .*

Proof. We start by noting $x \in N_0$ implies that x is adjacent to i_a, j_a, i_b and j_b , else $x \in I$.

Now, the proof is by contradiction. Assume that $x \in N_0$ and $y \in I$ is non-adjacent and let $\bar{n} \in \overline{N}$. We may assume, without loss of generality, that $y \in I_a$ and $y \neq i_a$. We now have that y is adjacent to i_a, i_b and j_b , by Proposition 4.2.3 (ii). Next, by Proposition 4.2.1 (i) there exists a vertex $s \in S$ adjacent to i_a and j_a . Then, by Proposition 4.2.3 (i), s is adjacent to i_b, j_b, x and y , since (j_b, i_a, i_b, j_a) and (x, i_b, y, j_b) are both induced C_4 's in $G[N]$. Thus, we find A_7 , as an induced subgraph, on the vertex set $\{i_a, j_a, i_b, j_b, x, y, s, \bar{n}\}$ (see Figure 4.20).

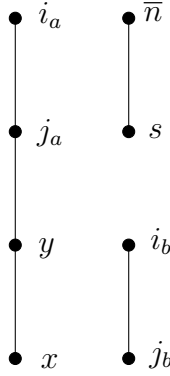


Figure 4.20: The complementary graph on the vertex set $\{i_a, j_a, i_b, j_b, x, y, s, \bar{n}\}$

Therefore, every vertex in N_0 is adjacent to every vertex in I . □

Proposition 4.4.2. [20, p.567] *The sets N_0, I_a and $J_a, a = 1, \dots, \nu$, are pairwise disjoint cliques with the following properties:*

- (i) *Every vertex in $I_a \cup J_a$ is adjacent to every vertex in $I_b \cup J_b$, for $a, b \in \{1, \dots, \nu\}, a \neq b$. Moreover, if $x \in I_a \cup J_a$ and $y \in I_b \cup J_b$ are adjacent, either $x \in \{i_a, j_a\}$ or $y \in \{i_b, j_b\}$.*

(ii) *There are no edges between the sets I_a and J_a , for $a = 1, \dots, \nu$.*

Proof. From the preceding lemma it is not hard to see that N_0 is a clique. Indeed, assume that this is not the case. Then there exist two non-adjacent vertices $n_1, n_2 \in N_0$. Thus, we find an induced matching in $\overline{G}[N]$ on the vertices n_1 and n_2 . However, we then have an induced matching of cardinality $\nu + 1$ in $\overline{G}[N]$, since every vertex in N_0 is adjacent to every vertex in I , by Lemma 4.4.1. Therefore, N_0 is a clique.

We now show that I_a and J_a , $a = 1, \dots, \nu$, are cliques. We prove this by contradiction. Assume that I_a is not a clique. Then there exist two non-adjacent vertices $x, y \in I_a$. Furthermore, x and y are both non-adjacent to j_a . Thus, by Proposition 4.2.3 (ii), x and y are both adjacent to i_b , and j_b . By Proposition 4.2.1 (i) there exists a vertex s adjacent to i_a and j_a . Therefore, by Proposition 4.2.3 (i) s is adjacent to i_b, j_b, x and y , since (j_b, i_a, i_b, j_a) and (x, i_a, y, j_a) are both induced C_4 's in $G[N]$. Thus, we find A_3 , as an induced subgraph, on the vertex set $\{j_a, i_b, j_b, x, y, s, \bar{n}\}$ (see Figure 4.21). A similar argument holds for J_a .

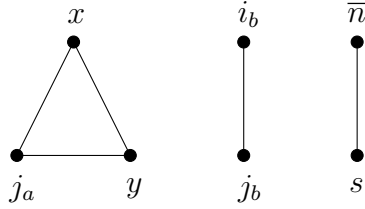


Figure 4.21: The complementary graph on the vertex set $\{j_a, i_b, j_b, x, y, s, \bar{n}\}$

Therefore, I_a and J_a , $a = 1, \dots, \nu$, are cliques.

(i) We need to show that the following holds:

- every vertex in I_a is adjacent to every vertex in I_b ;
- every vertex in J_a is adjacent to every vertex in J_b ;
- every vertex in I_a is adjacent to every vertex in J_b ;
- every vertex in I_b is adjacent to every vertex in J_a .

However, it suffices to prove one of the above, since all four cases are symmetric.

Our proof is by contradiction. Assume that $x \in I_a$ and $y \in I_b$ are non-adjacent. Thus, $(x, j_a), (y, j_b) \notin E$. Note that the case $x = i_a, y = i_b$ is impossible, by the definition of an induced matching. Also, the cases $x = i_a, y \neq i_b$ and $x \neq i_a, y = i_b$ are impossible, by Proposition 4.2.3 (ii). Furthermore, if $x \neq i_a$ and $y \neq i_b$ we find A_4 , as an induced subgraph, on the vertex set $\{i_a, j_a, i_b, j_b, x, y\}$ (see Figure 4.22). Thus, x and y must be adjacent.

Consequently, every vertex in $I_a \cup J_a$ is adjacent to every vertex in $I_b \cup J_b$.

Now, let $\bar{n} \in \overline{N}$ and assume that $x \in I_a \cup J_a$ and $y \in I_b \cup J_b$ are adjacent, such that $x \notin \{i_a, j_a\}$ and $y \notin \{i_b, j_b\}$. We may assume, without loss of generality, that $x \in I_a$ and



Figure 4.22: The complementary graph on the vertex set $\{i_a, j_a, i_b, j_b, x, y\}$

$y \in I_b$. Thus, $(x, j_a), (y, j_b) \notin E$. By Proposition 4.2.1 (i), there exists a $s \in S$ adjacent to i_a and j_a . Therefore, by Proposition 4.2.3 (i), s is adjacent to i_b and j_b . We now have several possibilities, which we list in the table below. A check mark indicates whether the edge is in the graph. We also provide the relevant vertex set and indicate which forbidden induced subgraph occurs in each case. In Figure 4.23 we illustrate the complementary graph, induced by the vertex set $\{\bar{n}, s, i_a, j_a, i_b, j_b, x, y\}$. The solid lines indicate edges in the complementary graph and dotted lines indicate possible edges in the complementary graph.

(s, x)	(s, y)	Vertex set	Induced subgraph
✓	✓	$\{\bar{n}, s, i_a, j_a, i_b, j_b, x, y\}$	A_8
✓		$\{s, i_a, j_a, i_b, j_b, x, y\}$	A_6
	✓	$\{s, i_a, j_a, i_b, j_b, x, y\}$	A_6
		$\{s, j_a, i_b, j_b, x, y\}$	A_4

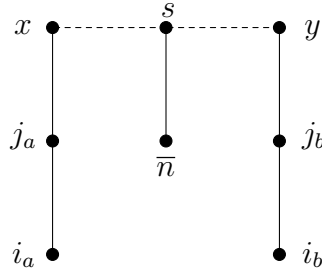


Figure 4.23: The complementary graph on the vertex set $\{\bar{n}, s, i_a, j_a, i_b, j_b, x, y\}$

We may therefore conclude that, if $x \in I_a \cup J_a$ and $y \in I_b \cup J_b$ are adjacent, either $x \in \{i_a, j_a\}$ or $y \in \{i_b, j_b\}$.

(ii) If $x = i_a$ or $y = j_a$, the result is immediate. Thus, assume that $x \neq i_a$ and $y \neq j_a$. Our proof is by contradiction. Assume that x and y are adjacent and let $\bar{n} \in \bar{N}$. Note that $(x, j_a), (y, i_a) \notin E$. Consequently, x is adjacent to i_a, i_b, j_b and y is adjacent to j_a, i_b, j_b , by Proposition 4.2.3 (ii). Next, by Proposition 4.2.1 (i), there exists a vertex $s \in S$ adjacent to i_a and j_a . Therefore, by Proposition 4.2.3 (i), s is adjacent to i_b and j_b , since (i_a, j_b, j_a, i_b) is an induced C_4 in $G[N]$. Furthermore, s is adjacent to x and y . Indeed, if this were not the case, we either have that s is adjacent to neither of x, y or s is adjacent to only one of x, y . In the first case, (s, j_a, y, x, i_a) is an induced C_5 , a contradiction; and in the second case, we may assume, without loss of generality, that s and x are not adjacent. Then we find A_5 , as an induced subgraph, on the vertex set $\{s, i_a, j_a, i_b, j_b, x, y\}$ (see Figure 4.24).

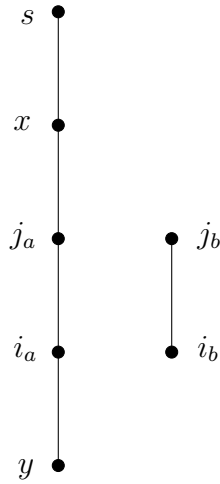


Figure 4.24: The complementary graph on the vertex set $\{s, i_a, j_a, i_b, j_b, x, y\}$

Now, we find A_7 , as an induced subgraph, on the vertex set $\{\bar{n}, s, i_a, j_a, i_b, j_b, x, y\}$ (see Figure 4.25).

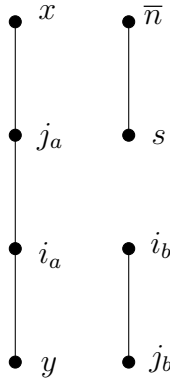


Figure 4.25: The complementary graph on the vertex set $\{\bar{n}, s, i_a, j_a, i_b, j_b, x, y\}$

Therefore, x and y are not adjacent. □

It now follows that the set N has the form shown in Figure 4.26, for $\nu \in \{2, 3\}$.

Thus, the structure of N is well-understood. Also, the structure of \bar{N} and its interaction with the sets N and S is clear. Our next objective is to understand the structure of S and its interaction with the set N . To that end, we define the set S_I as

$$S_I := \{s \in S : s \text{ is adjacent to all the vertices of } I\}$$

and set $T := S \setminus S_I$.

Proposition 4.4.3. [20, p.567] *The set S_I is non-empty and the following holds:*

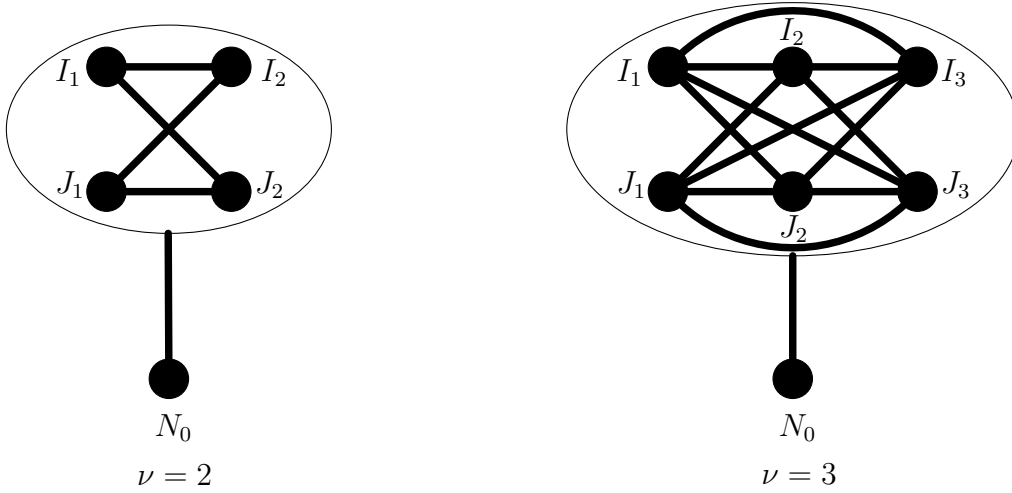


Figure 4.26: The form of the set N for $\nu \in \{2, 3\}$

- (i) S_I is a clique.
- (ii) A vertex $s \in S$ belongs to S_I if and only if s is adjacent to i_a and j_a for some $a = 1, \dots, \nu$.
- (iii) If $s \in T$ and $x, y \in I_a \cup J_a$ are non-adjacent, then s is adjacent to, at most, one of x and y .

Proof. By Proposition 4.2.1 (i) there exists a vertex s adjacent to i_a and j_a . Then, by Proposition 4.2.3 (i) s is adjacent to i_b and j_b . Now, assume that $x \in I$, such that x is not equal to i_a or j_a , for $a = 1, \dots, \nu$. Since $x \in I$ it follows that x is non-adjacent to, at least, one of the vertices i_a, j_a, i_b and j_b . Moreover, by Proposition 4.2.3 (ii), x is adjacent to at least three of the vertices i_a, j_a, i_b and j_b . Consequently, x is non-adjacent to exactly one of these vertices. We may therefore assume, without loss of generality, that x is non-adjacent to i_a , then (i_b, x, j_b, j_a) is an induced C_4 in $G[N]$. Thus, s is adjacent to x , by Proposition 4.2.3 (i). Therefore, s is adjacent to all the vertices in I , which shows that $s \in S_I$; so, S_I is non-empty.

(i) We prove this by contradiction. Assume that S_I is not a clique and let $\bar{n} \in \bar{N}$. Then there exist two non-adjacent vertices $s, t \in S_I$. We then find A_3 , as an induced subgraph, on the vertex set $\{\bar{n}, s, t, i_a, j_a, i_b, j_b\}$ (see Figure 4.27).

Thus, S_I is a clique.

(ii) If $s \in S_I$ it follows that s is adjacent to every vertex in I . Conversely, assume that $s \in S$ is adjacent to i_a and j_a , for some $a = 1, \dots, \nu$. A similar argument as the one used to show that $S_I \neq \emptyset$ proves that s is adjacent to all the vertices of I ; thus, $s \in S_I$.

(iii) Assume that $s \in T$ and $x, y \in I_a \cup J_a$, such that x and y are non-adjacent. The proof is by contradiction. Assume that s is adjacent to x and y . Then, by Proposition

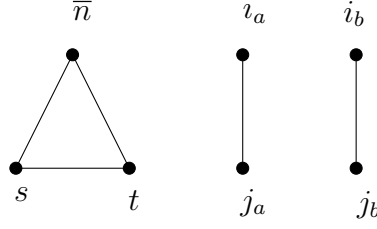


Figure 4.27: The complementary graph on the vertex set $\{\bar{n}, s, t, i_a, j_a, i_b, j_b\}$

4.2.3 (i), s is adjacent to i_b and j_b , since (i_b, x, j_b, y) is an induced C_4 in $G[N]$. By the same proposition s is adjacent to i_a and j_a , since (i_b, i_a, j_b, j_a) is an induced C_4 in $G[N]$. Continuing in this fashion, we have that s is adjacent to all the vertices of I ; thus $s \in S_I$. However, this contradicts our choice of $s \in T = S \setminus S_I$. Therefore, s is adjacent to, at most, one of x and y . \square

Similar to Case I, we wish to show that $T = \emptyset$, which is equivalent to $S = S_I$. We start by defining, for $s \in T$, the set

$$Y_s := \{x \in S_I \cup N : (s, x) \in E\}.$$

Lemma 4.4.4. [20, Claim 28] *Let $s, t \in T$. Then*

- (i) Y_s is a clique.
- (ii) $Y_s \cup Y_t$ is a clique for every $(s, t) \in E$.

Proof. (i) Assume that Y_s is not a clique, for some $s \in T$. Then there are two non-adjacent vertices $x, y \in Y_s$. Thus, $x, y \in S_I \cup N$ and s is adjacent to x and y . Note that the following combinations are impossible:

- $x \in N_0, y \in I$: Since every vertex in N_0 is adjacent to every vertex in I (Lemma 4.4.1).
- $x, y \in N_0$: Since N_0 is a clique (Proposition 4.4.2).
- $x \in I_a \cup J_a$ and $y \in I_b \cup J_b$, for $a, b \in \{1, \dots, \nu\}, a \neq b$: Since every vertex in $I_a \cup J_a$ is adjacent to every vertex in $I_b \cup J_b$ (Proposition 4.4.2 (i)).
- $x \in S_I$ and $y \in I$: By the definition of S_I .
- $x, y \in S_I$: Since S_I is a clique (Proposition 4.4.3 (i)).
- $x, y \in I_a \cup J_a$, for $a = 1, \dots, \nu$: Since $(x, y) \notin E$ implies, by Proposition 4.4.3 (iii), that s is adjacent to, at most, one of x and y , contradicting the fact that $x, y \in Y_s$.

Thus, the only combination that remains, is $x \in S_I$ and $y \in N_0$. Note that x and y are both adjacent to all the vertices in I . Also, since $s \in T$ it is non-adjacent to at least one of the vertices i_a, j_a, i_b and j_b . Thus, assume that s is non-adjacent to i_a . Consequently,

by Proposition 4.4.3 (iii), s can not be adjacent to i_b and j_b . In the table below we list all of the possibilities. A check in the appropriate column indicates that the edge is present in the graph, which implies that it is not an edge in the complementary graph shown in Figure 4.28. Note that in each case the relevant vertex set is $\{i_a, i_a, i_b, j_b, x, y, s\}$.

(s, j_a)	(s, i_b)	(s, j_b)	Induced subgraph
✓	✓		A_5
✓		✓	A_5
	✓	✓	A_3
✓			B_6
	✓		B_6
		✓	B_6
			B_3

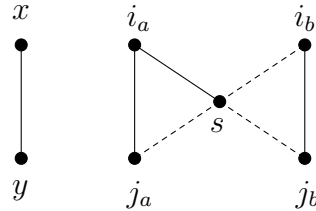


Figure 4.28: The complementary graph on the vertex set $\{i_a, i_a, i_b, j_b, x, y, s\}$.

Now, since we have exhausted all the possibilities, we may conclude that Y_s is a clique for every $s \in T$.

(ii) Assume that $Y_s \cup Y_t$ is a not clique, for $(s, t) \in E$, $s, t \in T$ and Let \bar{n} . Then there are two non-adjacent vertices $x, y \in Y_s \cup Y_t$. We show that this leads to a contradiction.

By (i) of the current lemma Y_s is a clique for every $s \in T$. Therefore, we necessarily have that $x \in Y_s \setminus Y_t$ and $y \in Y_t \setminus Y_s$. Thus, $x, y \in S_I \cup N$ with s adjacent to x , but not y , and t adjacent to y , but not x . We immediately have that $x, y \in N$ is impossible, else (\bar{n}, x, s, t, y) is an induced C_5 .

Hence, $x \in S_I$ and $y \in N_0$. Now, by Proposition 4.4.3 (iii), s and t are adjacent to, at most, one of i_a and j_a . In fact, s and t are both adjacent to exactly one of i_a and j_a . Indeed, assume that s is not adjacent to i_a or j_a , then (j_a, x, s, t, y) and (i_a, x, s, t, y) are both induced C_5 's. A similar argument shows that t must also be adjacent to exactly one of i_a and j_a .

Now, assume that $(s, j_a), (t, i_a) \in E$. Then (t, j_a, i_a, s, y, x) is an induced C_6 in \overline{G} , which implies that B_1 is an induced subgraph, on the vertex set $\{i_a, j_a, x, y, s, t\}$.

We have again exhausted all possibilities and may thus conclude that $Y_s \cup Y_t$ is a clique for every $(s, t) \in E$, $s, t \in T$. \square

Assume that $T \neq \emptyset$. Let A denote a maximal subset of T such that

- $G[A]$ is connected;

- $Y(A) = \bigcup_{a \in A} Y_a$ is a clique.

Lemma 4.4.5. [20, Claim 29] *There are no edges between the sets A and $T \setminus A$.*

Proof. The proof is by contradiction. Assume that $a \in A$ and $b \in T \setminus A$ are adjacent. The maximality of A implies that $Y(A) \cup Y_b$ is not a clique. Indeed, $G[A \cup \{b\}]$ is connected, since $(a, b) \in E$. Thus, if $Y(A) \cup Y_b$ is a clique, A is not maximal. Hence, there exist two non-adjacent vertices $x \in Y(A)$ and $y \in Y_b$. Let $\bar{n} \in \bar{N}$.

Now, since $x \in Y(A)$ there exists a vertex $a_0 \in A$, such that $(x, a_0) \in E$. Then $a_0 \neq a$. Indeed, if $a_0 = a$, we have that $Y_{a_0} \cup Y_b$ is a clique, by Lemma 4.4.4 (ii), which implies that $(x, y) \in E$, a contradiction. A similar argument, and application of Lemma 4.4.4 (i) and (ii), shows that $(a, y), (a_0, b), (a_0, y), (x, b) \notin E$.

The fact that $G[A]$ is connected, implies there exists a shortest path P from a_0 to a . We may therefore conclude that a path from x to y , with internal vertices in T , is of length at least equal to 3, since $(x, a_0), (a, b), (b, y) \in E$ and P has length at least 1. Denote this path from x to y by $[x, a_1, \dots, a_p, y]$, $p \geq 3$, and $a_i \in T$, for $i = 1, \dots, p$.

The case $x, y \in N$ is impossible, else $(x, a_1, \dots, a_p, y, \bar{n})$ is an induced C_n , $n \geq 6$, a contradiction. The only possibility that remains, is $x \in S_I$ and $y \in N_0$.

Now, i_a is adjacent to one of a_1, a_2 . Indeed, i_a is adjacent to some a_l , else we have that $(i_a, x, a_1, \dots, a_p, y)$ is an induced cycle C_n , $n \geq 6$ in G . Let $k \geq 1$ be the smallest index such that $(i_a, a_k) \in E$, then $(i_a, x, a_1, \dots, a_k)$ is an induced cycle, which implies that $k \leq 2$. Similarly, j_a is adjacent to one of a_1, a_2 . Hence, we can assume that $(i_a, a_1) \in E$ and $(j_a, a_2) \in E$. Then, Proposition 4.4.3 (iii), implies that $(i_a, a_2), (j_a, a_1) \notin E$. However, we then have that $(i_a, a_1, \dots, a_p, y)$ is an induced C_n , $n \geq 5$.

Thus, we may conclude that there exist no edges between the sets A and $T \setminus A$. \square

Now, $T \neq \emptyset$ implies that $A \neq \emptyset$. Moreover, there are no edges between A and the sets $T \setminus A$, $(S_I \cup N) \setminus Y(A)$ and \bar{N} . Hence, if we delete the clique $Y(A)$, the graph G is disconnected, which shows that $Y(A)$ is a clique-cutset, contradicting our assumption that G contains no clique-cutsets. Consequently, $T = \emptyset$, which implies that $S = S_I$. In other words, every vertex in S is adjacent to every vertex in I .

Lemma 4.4.6. *Every vertex in S is adjacent to every vertex in N .*

Proof. We already know that every vertex in S is adjacent to every vertex in I . Thus, it suffices to show that every vertex in S is adjacent to every vertex in N_0 .

The proof is by contradiction. Assume there exist two non-adjacent vertices $s \in S$, $n_0 \in N_0$ and let $\bar{n} \in \bar{N}$. Then there exists some vertex $t \in S$ adjacent to n_0 , per definition of N . Note that t is adjacent to s and to every vertex in I . We then find A_7 , as an induced subgraph, on the vertex set $\{\bar{n}, s, t, n_0, i_a, j_a, i_b, j_b\}$ (see Figure 4.29).

Thus, every vertex in S is adjacent to every vertex in N_0 . \square

Thus, the structure of S and its interaction with N is now clear. Consequently, the vertex set V has the form depicted in Figure 4.30, for $\nu \in \{2, 3\}$.

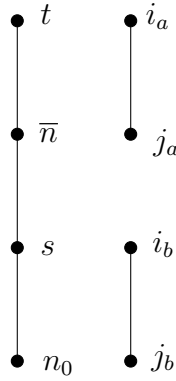


Figure 4.29: The complementary graph on the vertex set $\{\bar{n}, s, i_a, j_a, i_b, j_b, x, y\}$

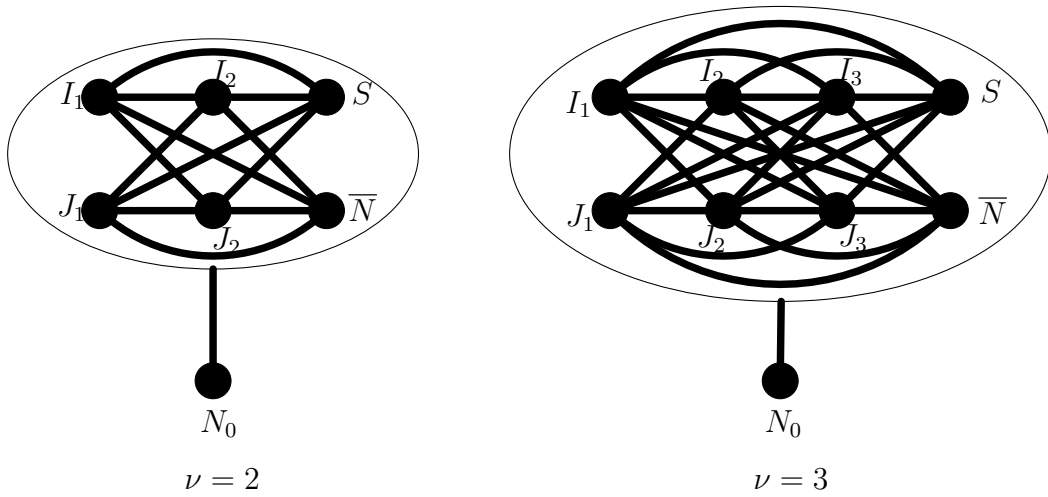


Figure 4.30: The form of the set N for $\nu \in \{2, 3\}$

We are now ready to show that $G \in \mathcal{G}_\nu$, for $\nu \in \{2, 3\}$.

Proposition 4.4.7. [20, Corollary 30]

- (i) If $\nu = 2$, then $G \in \mathcal{G}_2$.
- (ii) If $\nu = 3$, then $G \in \mathcal{G}_3$.

Proof. (i) Assume that $\nu = 2$. If $|S| = |\bar{N}| = |I_a| = |J_a| = 1$, for $a = 1, 2$, then we are done (see Figure 4.30).

Now, assume, without loss of generality, that $|S \cup \bar{N}| \geq 3$. It then follows that $|I_a| = |J_a| = 1$, for $a = 1, 2$. Indeed, assume that $|I_a| = 2$. It is then clear from Figure 4.30, that we find A_8 , as an induced subgraph.

Therefore, $G \in \mathcal{G}_2$.

(ii) Assume that $\nu = 3$. Then $|S| = |\overline{N}| = |I_a| = |J_a| = 1$, for $a = 1, 2$. Indeed, assume, without loss of generality, that $|\overline{N}| = 2$. It is then clear from Figure 4.30, that we find A_9 , as an induced subgraph.

Therefore, $G \in \mathcal{G}_3$. □

This completes the proof for Case II, and indeed, for Theorem 4.1.2.

4.5 Notes

Although the argumentation followed in this chapter relies on the work done in [20], there are some significant changes. One of the main changes, which allowed us to organize the proof in a more optimal way, is the relaxation of the assumption that I and J are maximal stable sets in Proposition 4.2.1 (ii). This allowed us to drop all assumptions made regarding the existence of a stable set of some predetermined cardinality in $G[N]$. Consequently, we could combine the two Cases A and B, found in [20], into one case, which we called Case I. Case II is similar to Case C, found in [20], since the starting assumptions are the same for both cases. However, we focused on describing the structure of the sets N , S and \overline{N} and the interaction between these three sets, as can be seen in Figures 4.26 and 4.30. Consequently, proving that $G \in \mathcal{G}_\nu$, for $\nu \in \{2, 3\}$ followed almost immediately. We also included graphs for all of the results shown here, which allows one to easily follow the argumentation in each case.

Chapter 5

The sparsity order of a graph

In this chapter we introduce the notion of the sparsity order of a graph and show that a graph is chordal if and only if it has sparsity order less than or equal to 1. The sparsity order of a graph has some interesting properties, as we will see in the first section. If a graph has sparsity order equal to k and all induced subgraphs have order less than k , even more can be said about the specific graph. Graphs having this property are called k -blocks. We will see in the second section that knowledge of the k -blocks contained in a graph is central in determining the sparsity order of a graph.

5.1 Extremal matrices and the sparsity order of a graph

Definition 5.1.1 (Extremal matrices). A matrix $A \in \text{PSD}_G$ is called extremal if $A = A_1 + A_2$, where $A_1, A_2 \in \text{PSD}_G$ implies that $A_j = \alpha_j A$, for some $\alpha_j \geq 0$, and for $j = 1, 2$. Denote by EXT_G the set of all extremal matrices in PSD_G .

Note that the extremal matrices of PSD_G are exactly the matrices which lie on the extreme rays of PSD_G . Furthermore, every element of PSD_G can be written in terms of the extremals of PSD_G , as we will see in the next theorem.

Theorem 5.1.2. [1, p.107] *Let $A \in \text{PSD}_G$. Then A can be written as a linear combination, with positive coefficients, of elements from EXT_G .*

Proof. We first note that, if $A = 0$, the result follows immediately, since $0 \in \text{EXT}_G$. Hence, we assume that $A \neq 0$. To prove this theorem, we will make use of the Krein-Milman theorem (Theorem A.9).

Observe that $K = \{Y \in \text{PSD}_G : \text{tr}(Y) = 1\}$ is a compact, convex subset of PSD_G . Therefore, by Krein-Milman, $K = \overline{\text{conv}(\text{ext}(K))}$. Thus, A can be written as a linear combination, with positive coefficients, of elements from EXT_G , since a non-zero $X \in \text{PSD}_G$ is extremal if and only if $\text{tr}(X)^{-1}X$ is extremal in K . \square

Definition 5.1.3 (Sparsity order of a graph). Let G be a graph. Then, the sparsity order of G is defined as the maximum rank of an extremal matrix of the cone PSD_G . We will refer to the sparsity order of a graph as its order and denote it by $\text{ord}_{\mathbb{F}}(G)$, where $\mathbb{F} = \mathbb{R}$ or \mathbb{C} .

Theorem 5.1.4. [1, Theorem 4.1] Let G be a graph and let H be an induced subgraph of G . Then

$$\text{ord}_{\mathbb{F}}(H) \leq \text{ord}_{\mathbb{F}}(G).$$

Proof. Let $\text{ord}_{\mathbb{F}}(H) = k$ and $\text{ord}_{\mathbb{F}}(G) = \tilde{k}$. Let A be extremal in PSD_H with $\text{rank}(A) = k$. Define $\tilde{A} \in \text{PSD}_G$ as follows:

$$\tilde{A} = \begin{bmatrix} A & 0 \\ 0 & 0 \end{bmatrix}.$$

Then, \tilde{A} is extremal in PSD_G . To see this, consider $\tilde{A} = \tilde{A}_1 + \tilde{A}_2$, with $\tilde{A}_j \in \text{PSD}_G$, $j = 1, 2$. Let

$$\tilde{A}_j = \begin{bmatrix} A_j & B_j \\ B_j^* & C_j \end{bmatrix},$$

where $A_j, C_j \in \text{PSD}_G$. Then, $C_1 + C_2 = 0$ and since C_j , $j = 1, 2$, is positive semidefinite, it follows that $C_1 = C_2 = 0$. This implies that $B_j = 0$, for $j = 1, 2$. Thus, \tilde{A}_j has the form

$$\tilde{A}_j = \begin{bmatrix} A_j & 0 \\ 0 & 0 \end{bmatrix}.$$

Consequently,

$$\tilde{A} = \begin{bmatrix} A & 0 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} A_1 & 0 \\ 0 & 0 \end{bmatrix} + \begin{bmatrix} A_2 & 0 \\ 0 & 0 \end{bmatrix}.$$

Since A is extremal, it follows that $A = \alpha_j A_j$, for some $\alpha_j \geq 0$, $j = 1, 2$. Thus, $\tilde{A} = \alpha_j \tilde{A}_j$, $j = 1, 2$. Moreover, $\text{rank}(\tilde{A}) = \text{rank}(A) = k$, since the zero rows and columns of \tilde{A} have no effect on the rank. We may therefore conclude that $k = \text{rank}(\tilde{A}) \leq \tilde{k}$, since \tilde{A} is an extremal matrix of PSD_G and \tilde{k} is the maximum rank of an extremal matrix of PSD_G . \square

The next theorem is a slight variant on a result found in [16] regarding the order of a clique-sum of graphs.

Theorem 5.1.5. [16, Theorem 3.1] Let G be a graph. If G is the clique-sum of the graphs G_1, \dots, G_p , then

$$\text{ord}_{\mathbb{F}}(G) = \max_{1 \leq i \leq p} (\text{ord}_{\mathbb{F}}(G_i)).$$

Proof. Note that since each G_i is an induced subgraph of G , we have $\text{ord}_{\mathbb{F}}(G_i) \leq \text{ord}_{\mathbb{F}}(G)$, for $i = 1, \dots, p$, by Theorem 5.1.4. In particular, $\max_{1 \leq i \leq p} (\text{ord}_{\mathbb{F}}(G_i)) \leq \text{ord}_{\mathbb{F}}(G)$.

We will now show that $\text{ord}_{\mathbb{F}}(G) \leq \max_{1 \leq i \leq p} (\text{ord}_{\mathbb{F}}(G_i))$. Without loss of generality we may assume that there is only one clique-cutset in G (otherwise, use an induction argument). Let K denote a clique-cutset in G . Then every non-zero element $X \in \text{PSD}_G$ has

the form

$$X = \begin{bmatrix} Y_1 & 0 & \cdots & 0 & Q_1 \\ 0 & Y_2 & \cdots & 0 & Q_2 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & Y_p & Q_p \\ Q_1^* & Q_2^* & \cdots & Q_p^* & Q \end{bmatrix}.$$

Now, since X is positive semidefinite, it follows that $\text{ran}(Q_i) \subseteq \text{ran}(Y_i)$, for $i = 1, \dots, p$. Therefore, for some matrix W_i , we have $Q_i = Y_i W_i$. Thus, X can be factorized as follows:

$$\begin{aligned} X &= \begin{bmatrix} I & 0 & \cdots & 0 & 0 \\ 0 & I & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & I & 0 \\ W_1^* & W_2^* & \cdots & W_p^* & I \end{bmatrix} \begin{bmatrix} Y_1 & 0 & \cdots & 0 & 0 \\ 0 & Y_2 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & Y_p & 0 \\ 0 & 0 & \cdots & 0 & \tilde{Q} \end{bmatrix} \begin{bmatrix} I & 0 & \cdots & 0 & W_1 \\ 0 & I & \cdots & 0 & W_2 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & I & W_p \\ 0 & 0 & \cdots & 0 & I \end{bmatrix} \\ &= \begin{bmatrix} I \\ 0 \\ \vdots \\ 0 \\ W_1^* \end{bmatrix} Y_1 \begin{bmatrix} I & 0 & \cdots & 0 & W_1 \end{bmatrix} + \begin{bmatrix} 0 \\ I \\ \vdots \\ 0 \\ W_2^* \end{bmatrix} Y_2 \begin{bmatrix} 0 & I & \cdots & 0 & W_2 \end{bmatrix} + \cdots + \\ &\quad \begin{bmatrix} 0 \\ 0 \\ \vdots \\ I \\ W_p^* \end{bmatrix} Y_p \begin{bmatrix} 0 & 0 & \cdots & I & W_p \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ I \end{bmatrix} \tilde{Q} \begin{bmatrix} 0 & 0 & \cdots & 0 & I \end{bmatrix}, \end{aligned}$$

where $\tilde{Q} = Q - \sum_{i=1}^p W_i^* Y_i W_i$. Note that $Y_i \in \text{PSD}_{G_i}$ and $\tilde{Q} \in \text{PSD}_K$, since X is positive semidefinite. Now, if X is extremal, the Y_i 's and \tilde{Q} are all extremal. Moreover, it follows that Y_i , for $i = 1, \dots, p$, and \tilde{Q} is a linear combination of X . This implies that only one of the Y_i 's or \tilde{Q} is non-zero.

Now, assume that \tilde{Q} is non-zero. Then the rank of \tilde{Q} is equal to 1, since K is a clique (Theorem 5.2.2). Next we assume, without loss of generality, that Y_1 is non-zero. Since $\begin{bmatrix} I & 0 & \cdots & 0 & W_1 \end{bmatrix}$ has full row rank, we may conclude that the rank of X is equal to the rank of Y_1 .

Finally, since

$$\text{rank}(X) = \text{rank}(Y_1) \leq \text{ord}_{\mathbb{F}}(G_1) \leq \max_{1 \leq i \leq p} (\text{ord}_{\mathbb{F}}(G_i)),$$

it follows that $\text{ord}_{\mathbb{F}}(G) \leq \max_{1 \leq i \leq p} (\text{ord}_{\mathbb{F}}(G_i))$. \square

From this theorem it follows that there is no loss of generality if we assume that G has no clique-cutset.

We now introduce the notion of k -blocks. These are in a sense the minimal graphs of sparsity order k , since any induced subgraph of a k -block, has sparsity order strictly less than k .

Definition 5.1.6 (*k*-block). Let G be a graph. Then G is called a k -block if $\text{ord}_{\mathbb{F}}(G) = k$ and $\text{ord}_{\mathbb{F}}(H) < k$ for every proper induced subgraph H of G .

Theorem 5.1.7. [1, Theorem 4.2] Let G be a graph. If $\text{ord}_{\mathbb{F}}(G) = k$, then G contains, as an induced subgraph, a k -block. Conversely, if G has an induced subgraph which is a k -block, then $\text{ord}_{\mathbb{F}}(G) \geq k$.

Proof. To see that the first statement holds let H be the minimal induced subgraph of G with order k . The second statement is an easy consequence of Theorem 5.1.4. \square

It is clear from the preceding theorem that the sparsity order of a graph G is equal to

$$\inf\{k : G \text{ has no induced } p\text{-block with } p > k\}.$$

In the next proposition we see that all cycles with more than 4 vertices are k -blocks.

Proposition 5.1.8. [1, Theorem 6.5] Let C_{k+2} be a cycle on $k + 2$ vertices, with $k > 1$, then C_{k+2} is a k -block, in the real and complex case.

5.2 The dimension theorem

We start this section with the following result on the sparsity order of chordal graphs. This result leads to a list of equivalent conditions under which a graph has sparsity order less than or equal to 1.

Theorem 5.2.1. Let $G = (V, E)$ be a graph. G is chordal if and only if $\text{ord}_{\mathbb{F}}(G) = 1$.

The equivalence of these two statements follows from Proposition 3.2.1 and Theorem 5.1.2 (see also the proof of Proposition 2.2.4).

Theorem 5.2.2. [20, p.552] The following assertions are equivalent for a graph G :

- (i) $\text{ord}_{\mathbb{F}}(G) \leq 1$.
- (ii) G does not contain, as an induced subgraph, a cycle C_n , $n \geq 4$, i.e. G is chordal.
- (iii) G can be decomposed as a clique-sum of cliques.

Proof. (i) \implies (ii) An immediate consequence of Theorem 5.2.1.

(ii) \implies (iii) If G contains no cycles of length greater than or equal to 4 it is chordal. Furthermore, by Corollary 4.1.4, a chordal graph is the clique-sum of cliques.

(iii) \implies (i) Follows from Theorem 5.1.5 and the fact that cliques are also chordal graphs and therefore have sparsity order 1, by Theorem 5.2.1. \square

Our goal for the remainder of this chapter is to generalize this result to graphs of sparsity order less than or equal to 2.

Recall that a subset $\mathcal{F} \subseteq \text{PSD}_G$ is called a face of PSD_G if $X = Y + Z$ with $X \in \mathcal{F}$, $Y, Z \in \text{PSD}_G$ implies that $Y, Z \in \mathcal{F}$. The extreme rays of PSD_G are its faces of dimension 1, where the dimension of \mathcal{F} is defined as the dimension of its span,

$$\dim(\mathcal{F}) := \dim(\text{span}(\mathcal{F})).$$

Since a face \mathcal{F} is a cone itself, we have $\text{span}(\mathcal{F}) = \mathcal{F} - \mathcal{F}$.

Proposition 2.2.3 gives a characterization of the facial structure of the smallest face of PSD_n containing some element $X \in \text{PSD}_n$. In this case the underlying graph is K_n , the complete graph on n vertices. In the next proposition we extend this result to arbitrary graphs G . We omit the proof of this result, since it is similar to the proof of Proposition 2.2.3, where the underlying graph is now arbitrary.

Proposition 5.2.3. [3, Lemma 4] *Let $X \in \text{PSD}_G$. Then*

$$\mathcal{F}_{\text{PSD}_G}(X) = \{Y \in \text{PSD}_G : \ker(X) \subseteq \ker(Y)\}.$$

We will now define what is meant by a perturbation of X and show that the set of perturbations of X is equal to the span of its smallest face, $\mathcal{F}_{\text{PSD}_G}(X)$.

Definition 5.2.4 (Perturbation of X). Let $X \in \text{PSD}_G$. Then, $B \in \mathcal{H}_G$ is called a perturbation of X if $X \pm \lambda B \in \text{PSD}_G$, for some $\lambda > 0$. Denote the set of perturbations of X by $\text{Pert}(X)$.

Lemma 5.2.5. *Let $X \in \text{PSD}_G$. Then,*

$$\text{Pert}(X) = \text{span}(\mathcal{F}_{\text{PSD}_G}(X)).$$

Proof. We will prove that the two inclusions (i) $\text{Pert}(X) \subseteq \text{span}(\mathcal{F}_{\text{PSD}_G}(X))$ and (ii) $\text{span}(\mathcal{F}_{\text{PSD}_G}(X)) \subseteq \text{Pert}(X)$ hold.

(i) Let $B \in \text{Pert}(X)$, then $X \pm \lambda B \in \text{PSD}_G$, for some $\lambda > 0$. Now,

$$X = \frac{X + \lambda B}{2} + \frac{X - \lambda B}{2},$$

which implies that $\frac{X \pm \lambda B}{2} \in \mathcal{F}_{\text{PSD}_G}(X)$, since $X \in \mathcal{F}_{\text{PSD}_G}(X)$ and $\mathcal{F}_{\text{PSD}_G}(X)$ is a face. Next,

$$\lambda B = \frac{X + \lambda B}{2} - \frac{X - \lambda B}{2},$$

which implies that $\lambda B \in \text{span}(\mathcal{F}_{\text{PSD}_G}(X))$. Therefore, $B \in \text{span}(\mathcal{F}_{\text{PSD}_G}(X))$, which proves the first inclusion.

(ii) Let $Y \in \text{span}(\mathcal{F}_{\text{PSD}_G}(X))$, then $Y = Y_1 - Y_2$ for $Y_1, Y_2 \in \mathcal{F}_{\text{PSD}_G}(X)$. Since $\ker(X) \subseteq \ker(Y_i)$, for $i = 1, 2$, it follows that $\ker(X) \subseteq \ker(Y)$.

If $h \in \ker(Y)$, we have that

$$\langle (X \pm \lambda Y)h, h \rangle = \langle Xh, h \rangle \geq 0 \text{ for any } \lambda > 0.$$

Now, let $h \in \text{ran}(Y) = (\ker(Y))^\perp$, then $h \in \text{ran}(X) = (\ker(X))^\perp$. It is immediate that $\langle (X + \lambda Y)h, h \rangle \geq 0$, since $X, Y \in \text{PSD}_G$ and $\lambda > 0$. To show that $\langle (X - \lambda Y)h, h \rangle \geq 0$, we first need to define

$$\tilde{X} := P_{(\ker(Y))^\perp} X,$$

the projection of X onto $(\ker(Y))^\perp$. Then, \tilde{X} is invertible, which implies that 0 is not in its spectrum. Thus, there exists a $\delta > 0$, such that

$$\langle \tilde{X}h, h \rangle \geq \delta \langle h, h \rangle.$$

Therefore, for $\lambda = \delta/\|Y\| > 0$, we have that

$$\begin{aligned} \langle (X - \lambda Y)h, h \rangle &= \langle Xh, h \rangle - \lambda \langle Yh, h \rangle \\ &= \langle \tilde{X}h, h \rangle - \lambda \langle Yh, h \rangle \\ &\geq \delta \|h\|^2 - \lambda \|Y\| \|h\|^2 \\ &= \delta \|h\|^2 - \delta \|h\|^2 \\ &= 0, \end{aligned}$$

where the first inequality follows from the fact that $\langle h, h \rangle = \|h\|^2$ and the Cauchy-Schwartz inequality.

Thus, $\langle (X \pm \lambda Y)h, h \rangle \geq 0$ for all h , which implies that $Y \in \text{Pert}(X)$, and proves the second inclusion. \square

We now apply the notion of Gram matrices (see Section 1.2) to study the extremals in PSD_G . To that end, let $G = (V, E)$ be a graph with $V = \{1, \dots, n\}$. Recall that a matrix is positive semidefinite if and only if it is the Gram matrix of some set of vectors (see Corollary 1.2.13). So the $n \times n$ positive semidefinite matrix X is the Gram matrix of a set of vectors, which we will denote by $\{u_1, \dots, u_n\}$. It is clear that $X \in \text{PSD}_G$ if and only if the vectors u_1, \dots, u_n satisfy

$$\langle u_j, u_i \rangle = 0 \text{ for all } (i, j) \notin E.$$

We will call a set of vectors which satisfies this condition an orthogonal representation of G . Let $\bar{G} = (V, \bar{E})$ be the complement of G . For a given subset $A \subseteq E \cup \bar{E}$, define the following subspace of $\mathcal{M}_n(\mathbb{F})$:

$$\mathcal{U}_A = \text{span}\{u_i u_j^* : (i, j) \in A\}$$

\mathcal{U}_A is easily seen to be closed, since it is a finite dimensional subspace.

If $X \in \text{PSD}_G$, then all the matrices in $\mathcal{U}_{\bar{E}}$ are orthogonal to the identity matrix. Indeed, for $U = u_i u_j^*$, $(i, j) \in \bar{E}$, we have

$$\langle U, I \rangle = \text{tr}(UI) = \text{tr}(u_i u_j^*) = \text{tr}(u_j^* u_i) = u_j^* u_i = \langle u_i, u_j \rangle = 0.$$

Also, it is obvious that $U \in \mathcal{U}_{\bar{E}}$ implies that $U^* \in \mathcal{U}_{\bar{E}}$.

In the next lemma we show that the perturbations of X can always be written in terms of the Gram representation of X and some Hermitian matrix, which respects the structure imposed by G .

Lemma 5.2.6. [8, Theorem 31.5.3] Let $X \in \text{PSD}_G$ with rank k and Gram representation (u_1, \dots, u_n) in \mathbb{F}^k . Let U denote the $k \times n$ matrix whose columns are the vectors u_1, \dots, u_n . Then, B is a perturbation of X if and only if $B = U^*RU$ for some $k \times k$ Hermitian matrix R satisfying

$$\langle R, u_i u_j^* \rangle = \langle R, u_j u_i^* \rangle = 0 \text{ for all } (i, j) \in \overline{E}.$$

Thus,

$$\text{Pert}(X) = \{U^*RU : R \in \mathcal{H}_k, \langle R, u_i u_j^* \rangle = \langle R, u_j u_i^* \rangle = 0 \text{ for all } (i, j) \in \overline{E}\}.$$

Proof. Assume that B is a perturbation of X . Then, $X \pm \lambda B \in \text{PSD}_G$, and $b_{ij} = 0$ for all $(i, j) \in \overline{E}$. Define the $n \times n$ matrix V as follows:

$$V = \begin{bmatrix} U \\ x_1^* \\ \vdots \\ x_{n-k}^* \end{bmatrix},$$

where $x_i \in \mathbb{F}^n$, for $i = 1, \dots, n-k$ such that all the columns of V are linearly independent. Consequently, V is non-singular. Now, set $Q = (V^{-1})^*BV^{-1}$, so, $B = V^*QV$. Then,

$$X \pm \lambda B = V^* \begin{bmatrix} I_k & 0 \\ 0 & 0 \end{bmatrix} V \pm \lambda V^*QV = V^* \left(\begin{bmatrix} I_k & 0 \\ 0 & 0 \end{bmatrix} \pm \lambda \begin{bmatrix} R & S \\ S^* & T \end{bmatrix} \right) V,$$

setting $Q = \begin{bmatrix} R & S \\ S^* & T \end{bmatrix}$, where R is a $k \times k$ Hermitian matrix. Hence, $\begin{bmatrix} I_k & 0 \\ 0 & 0 \end{bmatrix} \pm \lambda \begin{bmatrix} R & S \\ S^* & T \end{bmatrix}$ are positive semidefinite, which implies that S and T are zero matrices, so $B = U^*RU$. Furthermore, $b_{ij} = u_i^* R u_j = \langle R, u_i u_j^* \rangle$, and so

$$\langle R, u_i u_j^* \rangle = \langle R, u_j u_i^* \rangle = 0$$

for all $(i, j) \in \overline{E}$, since $b_{ij} = 0$ if $(i, j) \in \overline{E}$.

Conversely, say $B = U^*RU$ for some R satisfying the required conditions. Then,

$$X \pm \lambda B = U^*(I \pm \lambda R)U$$

is positive semidefinite for λ sufficiently small. Moreover, $\langle R, u_i u_j^* \rangle = \langle R, u_j u_i^* \rangle = 0$ for all $(i, j) \in \overline{E}$, implies that $b_{ij} = 0$ for all $(i, j) \in \overline{E}$ and so $X \pm \lambda B \in \text{PSD}_G$. \square

It is not hard to see that the mapping $R \mapsto U^*RU$ is a linear bijection between the subspaces $\text{Pert}(X)$ and $\{R \in \mathcal{H}_k : \langle R, u_i u_j^* \rangle = \langle R, u_j u_i^* \rangle = 0 \text{ for all } (i, j) \in \overline{E}\}$, since U has full row rank, which implies that it is surjective. We may therefore conclude that they have the same dimension. Furthermore, the latter subspace is equal to $\mathcal{H}_k \cap \mathcal{U}_{\overline{E}}^\perp$, the orthogonal complement of $\mathcal{U}_{\overline{E}}$, in the space $\mathcal{M}_k(\mathbb{F})$, intersected with the subspace of $k \times k$ Hermitian matrices. We have therefore shown that the following theorem holds.

Theorem 5.2.7. [20, Theorem 6] Let $X \in \text{PSD}_G$. Then,

$$\dim_{\mathbb{R}}(\mathcal{F}_{\text{PSD}_G}(X)) = \dim_{\mathbb{R}}(\mathcal{H}_k \cap \mathcal{U}_{\overline{E}}^\perp).$$

In what follows we will distinguish between the real and complex case.

5.2.1 The real case

It is assumed throughout this subsection that $\mathbb{F} = \mathbb{R}$. In this case $\mathcal{H}_k = \mathcal{S}_k(\mathbb{R})$, the set of $k \times k$ real symmetric matrices.

For the real case we need to define a new set. For a given subset $A \subseteq E \cup \bar{E}$ let:

$$\tilde{\mathcal{U}}_A = \text{span}\{u_i u_j^T + u_j u_i^T : (i, j) \in A\}.$$

Clearly $\tilde{\mathcal{U}}_A$ is also closed.

If $X \in \text{PSD}_G$, then all the matrices in $\tilde{\mathcal{U}}_{\bar{E}}$ are orthogonal to the identity matrix (see the proof for $\mathcal{U}_{\bar{E}}$).

Observe that the following is in general true for a $k \times k$ real symmetric matrix Q

$$\langle Q, A \rangle = 0 \iff \langle Q, A + A^T \rangle = 0, \text{ for every } A \in \mathcal{M}_k(\mathbb{R}).$$

We start by showing that

$$\langle M, N \rangle = \langle M^T, N^T \rangle, \text{ for } M, N \in \mathcal{M}_k(\mathbb{R}).$$

Note that $\langle M, N \rangle = \text{tr}(MN^T)$. Then

$$\langle M, N \rangle = \text{tr}(MN^T) = \text{tr}((MN^T)^T) = \text{tr}(NM^T) = \text{tr}(M^T N) = \langle M^T, N^T \rangle,$$

where we have exploited the cyclic property of the trace and the fact that $\text{tr}(B) = \text{tr}(B^T)$, for all $B \in \mathcal{M}_k(\mathbb{R})$.

Now, for $Q = Q^T$ and $A \in \mathcal{M}_k(\mathbb{R})$, we have

$$\langle Q, A \rangle = \langle Q, A^T \rangle.$$

Thus, $\langle Q, A \rangle = 0$ implies that $\langle Q, A^T \rangle = 0$. Therefore, $\langle Q, A + A^T \rangle = 0$. Conversely, if $\langle Q, A + A^T \rangle = 0$ it follows that $\langle Q, A \rangle = -\langle Q, A^T \rangle$. However, by the first part, we know that $\langle Q, A \rangle = \langle Q, A^T \rangle$. Consequently, $\langle Q, A \rangle = \langle Q, A^T \rangle = 0$.

Thus,

$$\langle R, u_i u_j^T \rangle = \langle R, u_j u_i^T \rangle = 0 \text{ for all } (i, j) \in \bar{E}$$

implies that $\langle R, u_i u_j^T + u_j u_i^T \rangle = 0$ and the converse also holds. Therefore,

$$\dim_{\mathbb{R}}(\mathcal{H}_k \cap \mathcal{U}_{\bar{E}}^{\perp}) = \dim_{\mathbb{R}}(\mathcal{S}_k(\mathbb{R}) \cap \tilde{\mathcal{U}}_{\bar{E}}^{\perp}) = \dim_{\mathbb{R}}(\tilde{\mathcal{U}}_{\bar{E}}^{\perp}),$$

since $\tilde{\mathcal{U}}_{\bar{E}}^{\perp} \subseteq \mathcal{S}_k(\mathbb{R})$, where $\tilde{\mathcal{U}}_{\bar{E}}^{\perp}$ is understood to be the orthogonal complement of $\tilde{\mathcal{U}}_{\bar{E}}$ in $\mathcal{S}_k(\mathbb{R})$.

Theorem 5.2.8. [20, Theorem 6] *Let $X \in \text{PSD}_G$ with rank k and Gram representation (u_1, \dots, u_n) in \mathbb{R}^k , and let $\tilde{\mathcal{U}}_{\bar{E}}$ be defined as before. Then,*

$$\dim_{\mathbb{R}}(\mathcal{F}_{\text{PSD}_G}(X)) = \binom{k+1}{2} - \dim_{\mathbb{R}}(\tilde{\mathcal{U}}_{\bar{E}})$$

Proof. By the preceding discussion and Theorem 5.2.7 it suffices to find the dimension of $\widetilde{\mathcal{U}}_{\overline{E}}^\perp$ to prove the result.

Note that $\mathcal{S}_k(\mathbb{R}) = \mathcal{U}_{\overline{E}} \oplus \mathcal{U}_{\overline{E}}^\perp$. Therefore, by Theorem B.2, we may conclude that

$$\dim_{\mathbb{R}}(\mathcal{U}_{\overline{E}}^\perp) = \dim_{\mathbb{R}}(\mathcal{S}_k(\mathbb{R})) - \dim_{\mathbb{R}}(\mathcal{U}_{\overline{E}}).$$

Now, the dimension of $\mathcal{S}_k(\mathbb{R})$ is equal to $\binom{k+1}{2}$. To see this let S_{ij} be the matrix with ij -th and ji -th entries equal to 1 and all other entries equal to 0, in particular S_{ii} is the matrix with ii -th entry equal to 1 and all other entries equal to 0. Then the S_{ij} 's form a basis for $\mathcal{S}_k(\mathbb{R})$ and $\dim_{\mathbb{R}}(\mathcal{S}_k(\mathbb{R})) = \frac{k^2-k}{2} + k = \binom{k+1}{2}$. Thus,

$$\dim_{\mathbb{R}}(\mathcal{F}_{\text{PSD}_G}(X)) = \dim_{\mathbb{R}}(\mathcal{U}_{\overline{E}}^\perp) = \binom{k+1}{2} - \dim_{\mathbb{R}}(\mathcal{U}_{\overline{E}}). \quad \square$$

Recall that the extreme rays of a cone are the faces of dimension 1. This gives rise to the following corollary of Theorem 5.2.8. See [1] for two examples illustrating the use of this corollary.

Corollary 5.2.9. [20, Proposition 5] *Let $X \in \text{PSD}_G$. Then X is extremal if and only if*

$$\dim_{\mathbb{R}}(\widetilde{\mathcal{U}}_{\overline{E}}) = \binom{k+1}{2} - 1 = \frac{1}{2}(k^2 + k - 2).$$

Theorem 5.2.10. [1, Theorem 4.3] *Let $G = (V, E)$ be a graph. If G is a k -block, then*

$$|V| \leq k^2 + k - 2.$$

Therefore, the number of k -blocks is finite for every k .

The next corollary gives an upper bound for the sparsity order of a graph in terms of its non-edges.

Corollary 5.2.11. [1, Theorem 4.6] *If $\text{ord}_{\mathbb{R}}(G) = k$, then*

$$|\overline{E}| \geq \frac{1}{2}(k^2 + k - 2).$$

In particular,

$$k \leq \frac{-1 + \sqrt{8|\overline{E}| + 9}}{2}.$$

Proof. If $\text{ord}_{\mathbb{R}}(G) = k$, then $\dim_{\mathbb{R}}(\mathcal{U}_{\overline{E}}) = \frac{1}{2}(k^2 + k - 2)$. From this it follows that there are exactly $\frac{1}{2}(k^2 + k - 2)$ elements in a basis for $\mathcal{U}_{\overline{E}}$ which is only possible if there are at least $\frac{1}{2}(k^2 + k - 2)$ edges in \overline{G} . The second assertion is merely a reformulation of the first. \square

If the set of vectors $\{u_1, \dots, u_n\}$ in \mathbb{R}^k is an orthogonal representation of G , $\text{rank}(U) = k$, where $U = [u_1 \ \dots \ u_n]$ and they satisfy $\dim_{\mathbb{R}}(\tilde{\mathcal{U}}_{\overline{E}}) = \frac{1}{2}(k^2 + k - 2)$, we call this set of vectors a k -dimensional extremal orthogonal representation of G . Hence, the sparsity order of G is equal to the largest k for which there exists a k -dimensional extremal orthogonal representation of G .

Recall that the minimum fill-in of a graph G is the minimum number of edges required to make G chordal, denoted by $\text{fill}(G)$.

In the next theorem we show that there exists a connection between the minimum fill-in and the sparsity order of a graph. We will show how this inequality may be derived from Theorem 5.2.8. For an alternative approach see [26, Theorem B].

Theorem 5.2.12. [20, Proposition 3] *Let $G = (V, E)$ be a graph, then*

$$\text{ord}_{\mathbb{R}}(G) \leq \text{fill}(G) + 1$$

Proof. Let $G = (V, E)$ be a graph on n vertices. Set $k = \text{ord}_{\mathbb{R}}(G)$ and $p = \text{fill}(G)$. Then, there exists a subset F of \overline{E} of cardinality p such that the graph $H = (V, E \cup F)$ is chordal. Now, let X be an extremal matrix in PSD_G of rank k with Gram representation $\{u_1, \dots, u_n\}$ in \mathbb{R}^k . Clearly, $X \in \text{PSD}_H$. By Corollary 5.2.9, we have that

$$\dim_{\mathbb{R}}(\tilde{\mathcal{U}}_{\overline{E}}) = \binom{k+1}{2} - 1 \tag{5.1}$$

and by Theorem 5.2.8

$$\dim_{\mathbb{R}}(\tilde{\mathcal{U}}_{\overline{E \cup F}}) = \binom{k+1}{2} - \dim_{\mathbb{R}}(\mathcal{F}_{\text{PSD}_H}(X)). \tag{5.2}$$

On the other hand we have that

$$\dim_{\mathbb{R}}(\tilde{\mathcal{U}}_{\overline{E}}) \leq \dim_{\mathbb{R}}(\tilde{\mathcal{U}}_{\overline{E \cup F}}) + \dim_{\mathbb{R}}(\tilde{\mathcal{U}}_F) \leq \dim_{\mathbb{R}}(\tilde{\mathcal{U}}_{\overline{E \cup F}}) + |F|, \tag{5.3}$$

where the first inequality follows from Theorem B.2, and the second inequality from Corollary 5.2.11. Substituting (5.1) and (5.2) into (5.3) gives

$$\binom{k+1}{2} - 1 \leq \binom{k+1}{2} - \dim_{\mathbb{R}}(\mathcal{F}_{\text{PSD}_H}(X)) + |F|,$$

which implies that

$$\dim_{\mathbb{R}}(\mathcal{F}_{\text{PSD}_H}(X)) \leq |F| + 1 = p + 1.$$

Next, observe that there exists $d \leq \dim_{\mathbb{R}}(\mathcal{F}_{\text{PSD}_H}(X))$ extremal matrices $X_1, \dots, X_d \in \text{PSD}_H$ such that $X = X_1 + \dots + X_d$ (Theorem 5.1.2). This implies that $\text{rank}(X) \leq \text{rank}(X_1) + \dots + \text{rank}(X_d)$. Moreover, $\text{rank}(X_i) = 1$, for $i = 1, \dots, d$, since H is chordal (Theorem 5.2.1). Thus, $\text{rank}(X) \leq d$. All that remains is to note that $\text{rank}(X) = k$ and $d \leq p + 1$, therefore $k \leq p + 1$. That is, $\text{ord}_{\mathbb{R}}(G) \leq \text{fill}(G) + 1$. \square

Now, applying our new found knowledge we may further characterize the k -blocks over \mathbb{R} . A graph has order less than or equal to 1 if and only if it is chordal (Theorem 5.2.1). We may therefore conclude that the only 1-block is the graph K_1 , the graph with a single vertex, since chordality is a hereditary property.

By Proposition 5.1.8 we know that C_4 is a 2-block. In the next proposition we will show that it is in fact the only 2-block.

Proposition 5.2.13. [1, Theorem 7.1] C_4 is the only 2-block over \mathbb{R} .

Proof. Let $G = (V, E)$ be a 2-block over \mathbb{R} . By Theorem 5.2.10 G can have at most 4 vertices. Furthermore, G must have at least 4 edges, else it would be chordal and have sparsity order equal to 1 (Theorem 5.2.1). This implies that $|\overline{E}| \leq 2$, since the maximum number of edges a graph on 4 vertices can have, is 6. Now, Corollary 5.2.11 implies that $|\overline{E}| \geq 2$. Thus, $|\overline{E}| = 2$ and G has exactly 4 edges. Consequently, there are only two possibilities, shown in Figure 5.1. The graph on the right is clearly chordal, therefore, $G = C_4$ and we are done. \square

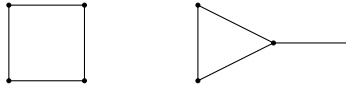


Figure 5.1: The graphs with 4 vertices and 4 edges

It was shown in [1] that the graphs $A_1 - A_{10}$, $B_1 - B_6$ (Figure 4.3) all have sparsity order 3 and are in fact 3-blocks. We record this fact in the next proposition.

Proposition 5.2.14. [1, Section 8] The graphs $A_1 - A_{10}$, $B_1 - B_6$ (Figure 4.3) are 3-blocks over \mathbb{R} .

We give a sketch of the proof: It is easily verified by Corollary 5.2.11 that all of the graphs here can have sparsity order at most 3. It is then a routine exercise to find 3-dimensional orthogonal representations for each graph, which proves that the sparsity order of each graph is in fact equal to 3. All that remains is to verify that no proper induced subgraph has sparsity order 3. For $A_1 - A_{10}$ this follows from Corollary 5.2.11, since the number of non-edges of any proper induced subgraph of these graphs is at most 4. The same holds for B_1, B_2 and B_4 . Finally, for the graphs B_3, B_5 and B_6 note that any proper induced subgraph has minimum fill-in at most 1, that is, $\text{fill}(G) \leq 1$. Therefore, by Theorem 5.2.12, the sparsity order of any proper induced subgraph is at most 2.

Later on we will show that these graphs are indeed the only 3-blocks over \mathbb{R} . However, some work still needs to be done. The main tool which we will need is a theorem which gives two equivalent conditions under which a graph has sparsity order less than or equal to 2. These two conditions are exactly the two equivalent assertions of Theorem 4.1.2 in the previous chapter. Recall that the following statements are equivalent for a graph G :

- (i) G does not contain, as an induced subgraph, a cycle C_n , $n \geq 5$, nor any of the graphs $A_2 - A_{10}$ and $B_1 - B_6$ (Figure 4.3).

(ii) G is a clique-sum of a set of graphs belonging to $\bigcup_{i=1}^4 \mathcal{G}_i$ (Figure 4.2).

It is easy to see that a graph in any of the classes \mathcal{G}_i , with $i = 1, 2, 3$, has a minimum fill-in of at most i , while graphs in \mathcal{G}_4 may have an arbitrarily large minimum fill-in. We need but consider the number of induced matchings of cardinality 2 in the complement of each graph. Indeed, an induced matching of cardinality 2 in the complement, implies that the graph contains C_4 , as an induced subgraph.

We now show that the sparsity order of a graph in $\bigcup_{i=1}^4 \mathcal{G}_i$ is less than or equal to 2.

Proposition 5.2.15. [20, Proposition 7] *If $G \in \bigcup_{i=1}^4 \mathcal{G}_i$, then $\text{ord}_{\mathbb{R}}(G) \leq 2$.*

Proof. If $G \in \mathcal{G}_1$, then $\text{ord}_{\mathbb{R}}(G) \leq 2$, by Proposition 5.2.12, since $\text{fill}(G) \leq 1$.

Assume that $G \in \mathcal{G}_i$ for $i = 2, 3, 4$. Let X be an extremal matrix in the cone PSD_G with rank $k = \text{ord}_{\mathbb{R}}(G)$ and with Gram representation $\{u_1, \dots, u_n\}$ in \mathbb{R}^k . Then, by Corollary 5.2.9,

$$\dim_{\mathbb{R}}(\tilde{\mathcal{U}}_{\bar{E}}) = \frac{1}{2}(k^2 + k - 2).$$

Using this fact, we compute in each case the dimension of the subspace $\tilde{\mathcal{U}}_{\bar{E}}$.

If $G \in \mathcal{G}_2$, let A and B denote the vertex sets of the two connected stable sets in \bar{G} and set $U_A := \text{span}\{u_i : i \in A\}$ and $U_B := \text{span}\{u_j : j \in B\}$. Let a and b denote the dimension of U_A and U_B , respectively. Now, a basis for elements of the form $u_i u_j^T + u_j u_i^T$, where $u_i \in U_A$ and $u_j \in U_B$, has dimension ab . Indeed, any element $u_i u_j^T + u_j u_i^T$, is a linear combination of the basis elements of U_A and U_B , which shows that the only elements which forms a basis for $u_i u_j^T + u_j u_i^T$, are the different combinations of linearly independent elements in U_A and U_B . We may therefore conclude that,

$$\dim_{\mathbb{R}}(\tilde{\mathcal{U}}_{\bar{E}}) \leq 2 + ab,$$

where the 2 on the right hand side is obtained from the two edges in the complement of a graph in \mathcal{G}_2 . Since every $u_i \in U_A$ is orthogonal to every $u_j \in U_B$, we have that $a + b \leq k$ (Theorem 1.2.12 (iv)), and so

$$k^2 \geq (a + b)^2 = a^2 + 2ab + b^2 \geq 2ab + 2ab = 4ab,$$

consequently $ab \leq \frac{1}{4}k^2$. Therefore,

$$\frac{1}{2}(k^2 + k - 2) \leq 2 + \frac{1}{4}k^2,$$

and so $-1 - \sqrt{13} \leq k \leq -1 + \sqrt{13}$, which implies that $k \leq 2$.

If $G \in \mathcal{G}_3$, then $|\bar{E}| \leq 4$. Thus, by Corollary 5.2.11,

$$\frac{1}{2}(k^2 + k - 2) \leq 4,$$

implying again that $k \leq 2$.

Finally, if $G \in \mathcal{G}_4$, we obtain, in a similar way as in the case when $G \in \mathcal{G}_2$, that

$$\frac{1}{2}(k^2 + k - 2) \leq \frac{1}{4}k^2 + \frac{1}{4}k^2,$$

which also implies that $k \leq 2$. □

We are now ready to characterize the graphs, in the real case, which have order less than or equal to 2. This result is clearly a generalization of Theorem 5.2.2.

Theorem 5.2.16. [20, Theorem 9] *The following assertions are equivalent for a graph G :*

- (i) $\text{ord}_{\mathbb{R}}(G) \leq 2$.
- (ii) G does not contain, as an induced subgraph, a cycle C_n , $n \geq 5$, nor any of the graphs $A_2 - A_{10}$ and $B_1 - B_6$.
- (iii) G is a clique-sum of a set of graphs belonging to $\bigcup_{i=1}^4 \mathcal{G}_i$.

Proof. (i) \implies (ii) Note that the graphs C_n , $n \geq 5$, all have sparsity order greater than or equal to 3 over \mathbb{R} (Proposition 5.1.8). Moreover, $A_1 - A_{10}, B_1 - B_6$ are all 3-blocks (Proposition 5.2.14). Therefore, by Theorem 5.1.4, a graph with sparsity order less than or equal to 2 over \mathbb{R} , can not contain, as an induced subgraph, any of the graphs C_n , $n \geq 5$, $A_1 - A_{10}, B_1 - B_6$.

(ii) \implies (iii) Holds by Theorem 4.1.2.

(iii) \implies (i) Follows from Theorem 5.1.5 and Proposition 5.2.15. □

We will now consider two applications of Theorem 5.2.16. As a first application we may determine whether a graph has sparsity order less than or equal to 2 in polynomial time, by making a clique-sum decomposition (see [27]) and checking whether the graph is contained in one of the classes $\mathcal{G}_1 - \mathcal{G}_4$. In the next chapter we will show that checking whether a graph has sparsity order less than or equal to 2, can also be done by means of the forbidden induced subgraphs C_n , $n \geq 5$, $A_2 - A_{10}$ and $B_1 - B_6$.

The second application is the classification of the 3-blocks over \mathbb{R} , which was obtained by [1]. By Proposition 5.2.14 we know that $A_1 - A_{10}, B_1 - B_6$ are 3-blocks, but using Theorem 5.2.16 we see that these are indeed the only 3-blocks over \mathbb{R} . Indeed, if G is a 3-block it necessarily contains one of the graphs $A_1 - A_{10}, B_1 - B_6$, as an induced subgraph, by Theorem 5.2.16. Thus, G is equal to it (by the definition of a block).

Theorem 5.2.17. [20, Theorem 10] *In the real case, the only 3-blocks are the graphs $A_1 - A_{10}$ and $B_1 - B_6$.*

5.2.2 The complex case

The complex case is in a sense more direct than the real case, since we do not need to define a new set and use $\mathcal{U}_{\overline{E}}$ as defined before.

Theorem 5.2.18. [20, Theorem 6] Let $X \in \text{PSD}_G$ with rank k and Gram representation (u_1, \dots, u_n) in \mathbb{F}^k , and let $\mathcal{U}_{\bar{E}}$ be defined as before. Then,

$$\dim_{\mathbb{R}}(\mathcal{F}_{\text{PSD}_G}(X)) = k^2 - \dim_{\mathbb{C}}(\mathcal{U}_{\bar{E}}).$$

Proof. By Theorem 5.2.7 it suffices to find the dimension of $\mathcal{H}_k \cap \mathcal{U}_{\bar{E}}^{\perp}$ over \mathbb{R} to prove the result.

The real dimension of the set $\mathcal{H}_k \cap \mathcal{U}_{\bar{E}}^{\perp}$ is equal to the complex dimension of its superset $\mathcal{M}_k(\mathbb{C}) \cap \mathcal{U}_{\bar{E}}^{\perp}$. To prove that this is indeed true, we start by showing that

$$R_1, R_2 \in \mathcal{H}_k \cap \mathcal{U}_{\bar{E}}^{\perp} \iff R := R_1 + iR_2 \in \mathcal{M}_k(\mathbb{C}) \cap \mathcal{U}_{\bar{E}}^{\perp}.$$

If $R_1, R_2 \in \mathcal{H}_k \cap \mathcal{U}_{\bar{E}}^{\perp}$ it is clear that $R := R_1 + iR_2 \in \mathcal{M}_k(\mathbb{C}) \cap \mathcal{U}_{\bar{E}}^{\perp}$. For the converse, observe that $T \in \mathcal{U}_{\bar{E}}^{\perp}$ if and only if $T^* \in \mathcal{U}_{\bar{E}}$, for $T \in \mathcal{M}_n(\mathbb{C})$. Indeed, if $U \in \mathcal{U}_{\bar{E}}$ and $T \in \mathcal{U}_{\bar{E}}^{\perp}$, we have that

$$0 = \langle T, U \rangle = \text{tr}(TU^*) = \text{tr}(U^*T) = \langle U^*, T^* \rangle,$$

which implies that $T^* \in \mathcal{U}_{\bar{E}}$, since $U^* \in \mathcal{U}_{\bar{E}}$. Now, assume that $R \in \mathcal{M}_k(\mathbb{C}) \cap \mathcal{U}_{\bar{E}}^{\perp}$, and define R_1 and R_2 as follows:

$$R_1 = \frac{R + R^*}{2} \quad \text{and} \quad R_2 = \frac{R - R^*}{2i}.$$

Then $R = R_1 + iR_2$ and since $R \in \mathcal{U}_{\bar{E}}^{\perp}$ it follows that $R^* \in \mathcal{U}_{\bar{E}}$. Consequently, $R_1, R_2 \in \mathcal{H}_k \cap \mathcal{U}_{\bar{E}}^{\perp}$.

We may now define a mapping $(X, Y) \mapsto X + iY$ from $(\mathcal{H}_k \cap \mathcal{U}_{\bar{E}}^{\perp}) \times (\mathcal{H}_k \cap \mathcal{U}_{\bar{E}}^{\perp})$ to $\mathcal{M}_k(\mathbb{C}) \cap \mathcal{U}_{\bar{E}}^{\perp}$. It is clear that this mapping is indeed a linear bijection, therefore the dimension of these two subspaces is equal. Thus,

$$\dim_{\mathbb{R}}((\mathcal{H}_k \cap \mathcal{U}_{\bar{E}}^{\perp}) \times (\mathcal{H}_k \cap \mathcal{U}_{\bar{E}}^{\perp})) = \dim_{\mathbb{R}}(\mathcal{M}_k(\mathbb{C}) \cap \mathcal{U}_{\bar{E}}^{\perp})$$

We may therefore conclude that the real dimension of $(\mathcal{H}_k \cap \mathcal{U}_{\bar{E}}^{\perp})$ is equal to the complex dimension of $\mathcal{M}_k(\mathbb{C}) \cap \mathcal{U}_{\bar{E}}^{\perp}$, since the real dimension of $(\mathcal{H}_k \cap \mathcal{U}_{\bar{E}}^{\perp}) \times (\mathcal{H}_k \cap \mathcal{U}_{\bar{E}}^{\perp})$ is twice the real dimension of $(\mathcal{H}_k \cap \mathcal{U}_{\bar{E}}^{\perp})$ and the complex dimension of $\mathcal{M}_k(\mathbb{C}) \cap \mathcal{U}_{\bar{E}}^{\perp}$ is twice the real dimension of $\mathcal{M}_k(\mathbb{C}) \cap \mathcal{U}_{\bar{E}}^{\perp}$.

Note that $\mathcal{M}_k(\mathbb{C}) \cap \mathcal{U}_{\bar{E}}^{\perp} = \mathcal{U}_{\bar{E}}^{\perp}$, since $\mathcal{U}_{\bar{E}}^{\perp} \subseteq \mathcal{M}_k(\mathbb{C})$. Now, $\mathcal{M}_k(\mathbb{C}) = \mathcal{U}_{\bar{E}} \oplus \mathcal{U}_{\bar{E}}^{\perp}$. Thus, by Theorem B.2, we have that

$$\dim_{\mathbb{C}}(\mathcal{M}_k(\mathbb{C})) = \dim_{\mathbb{C}}(\mathcal{U}_{\bar{E}}) + \dim_{\mathbb{C}}(\mathcal{U}_{\bar{E}}^{\perp}).$$

It is easy to see that $\dim_{\mathbb{C}}(\mathcal{M}_k(\mathbb{C})) = k^2$, thus,

$$\dim_{\mathbb{R}}(\mathcal{F}_{\text{PSD}_G}(X)) = \dim_{\mathbb{R}}(\mathcal{U}_{\bar{E}}^{\perp}) = k^2 - \dim_{\mathbb{C}}(\mathcal{U}_{\bar{E}}). \quad \square$$

The next corollary is the complex analogue of Corollary 5.2.9 and follows easily from Theorem 5.2.18.

Corollary 5.2.19. [20, Proposition 5] Let $X \in \text{PSD}_G$. Then X is extremal if and only if

$$\dim_{\mathbb{C}}(\mathcal{U}_{\overline{E}}) = k^2 - 1$$

Theorem 5.2.20. [1, Theorem 4.3] Let $G = (V, E)$ be a graph. If G is a k -block, then

$$|V| \leq 2(k^2 - 1).$$

It therefore follows that the number of k -blocks in the complex case, is also finite.

In the next corollary we again obtain an upper bound for the sparsity order of a graph in terms of its non-edges.

Corollary 5.2.21. [1, Theorem 4.6] If $\text{ord}_{\mathbb{C}}(G) = k$, then

$$|\overline{E}| \geq \frac{1}{2}(k^2 - 1).$$

In particular,

$$k \leq \sqrt{2|\overline{E}| + 1}.$$

Proof. If $\text{ord}_{\mathbb{C}}(G) = k$, then $\dim_{\mathbb{C}}(\mathcal{U}_{\overline{E}}) = k^2 - 1$. Thus, there are $k^2 - 1$ elements in a basis for $\mathcal{U}_{\overline{E}}$. However, it is important to note that if $u_i u_j^*$ is in $\mathcal{U}_{\overline{E}}$ we have that $u_j u_i^*$ is also in $\mathcal{U}_{\overline{E}}$ which gives the same edge in \overline{G} . Therefore, there must be at least $\frac{1}{2}(k^2 - 1)$ edges in \overline{G} to give a basis of $k^2 - 1$ elements. The second assertion is merely a reformulation of the first. \square

Similar to the real case, if the set of vectors $\{u_1, \dots, u_n\}$ in \mathbb{C}^k is an orthogonal representation of G , $\text{rank}(U) = k$, where $U = [u_1 \ \dots \ u_n]$ and they satisfy $\dim_{\mathbb{C}}(\mathcal{U}_{\overline{E}}) = k^2 - 1$, we call this set of vectors a k -dimensional extremal orthogonal representation of G . Consequently, the sparsity order of G is equal to the largest k for which there exists a k -dimensional extremal orthogonal representation of G . So we see that while the details differ for the real and complex case, the two cases are in many ways analogous.

We know that in the real case the only 2-block is C_4 (Proposition 5.2.13). This remains true for the complex case, as we will now see.

Proposition 5.2.22. [1, Theorem 7.1] C_4 is the only 2-block over \mathbb{C} .

Proof. Let $G = (V, E)$ be a 2-block over \mathbb{C} . By Theorem 5.2.10 G can have at most 6 vertices. Furthermore, since G is a 2-block it has sparsity order 2, which implies, by Theorem 5.2.2, that it contains a cycle of length greater than 3. Consequently, G has at least 4 vertices. Therefore, G can have 4, 5 or 6 vertices. We will treat each case separately. If G has 4 vertices we can show in a similar way as the real case (Proposition 5.2.13) that $G = C_4$. Now, if G has 5 vertices it can not contain C_4 , as an induced subgraph, since C_4 has sparsity order 2. Thus, $G = C_5$, but by Theorem 5.1.8, we know that C_5 has sparsity order 3, a contradiction. This shows that G can not have 5 vertices and in a similar fashion we can show that if G has 6 vertices, it leads to a contradiction. We can thus conclude that $G = C_4$, which completes the proof. \square

The next result is the complex analogue of Theorem 5.2.12. We will omit the proof, since it is almost exactly the same as the real case.

Theorem 5.2.23. [20, Proposition 3] *Let $G = (V, E)$ be a graph, then*

$$\text{ord}_{\mathbb{C}}(G) \leq 2 \cdot \text{fill}(G) + 1.$$

We will again characterize the graphs having sparsity order less than or equal to 2, by giving two equivalent conditions under which this is true. These two conditions are also in terms of forbidden induced subgraphs and a decomposition into a clique-sum, similar to the real case. However, the forbidden induced subgraphs are different from those in the real case and we will need an additional class of graphs for our decomposition. We start by introducing this new class of graphs, which we will denote by \mathcal{G}_5 . A graph in this class can be obtained from a complete graph by deleting a matching of cardinality at most 3. The form of the class \mathcal{G}_5 and its complementary class $\bar{\mathcal{G}}_5$ are depicted in Figure 5.2. As was the case for $\mathcal{G}_1 - \mathcal{G}_4$, we use the following convention:

A small dark dot indicates a vertex, a big dark circle indicates a clique, while a big white circle indicates a stable set; edges are indicated by lines, while a thick line between two spheres or between two sets of vertices shows that every vertex in one set is adjacent to every vertex in the other set.

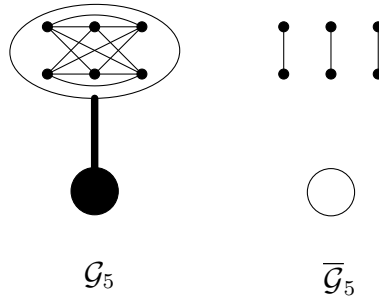


Figure 5.2: The class \mathcal{G}_5 and its complementary class $\bar{\mathcal{G}}_5$

The following proposition shows that the sparsity order of a graph in either of the classes \mathcal{G}_4 or \mathcal{G}_5 is less than or equal to 2 over \mathbb{C} .

Proposition 5.2.24. [20, p.555] *If $G \in \mathcal{G}_4 \cup \mathcal{G}_5$, then $\text{ord}_{\mathbb{C}}(G) \leq 2$.*

The proof for the case when $G \in \mathcal{G}_4$ is rather involved and can be found in [22, Proposition 2.6]. The case when $G \in \mathcal{G}_5$ easily follows from Corollary 5.2.21, since $|\bar{E}| \leq 3$, for any graph in \mathcal{G}_5 .

We will also need four new graphs, which we denote by $D_1 - D_4$. The form of the complements of these four graphs can be seen in Figure 5.3.

Proposition 5.2.25. [22, Lemma 2.8] [20, p.556] *The graphs $A_1, A_4, B_1, D_1 - D_4$ (Figures 4.3 and 5.3) are 3-blocks over \mathbb{C} .*

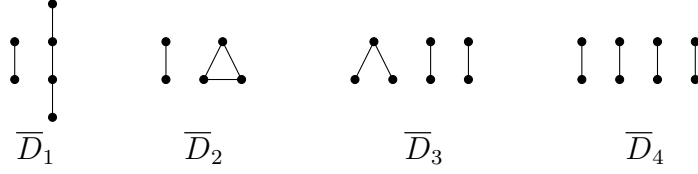


Figure 5.3: Complements of the graphs $D_1 - D_4$

As in the real case we only give a sketch of the proof: By Corollary 5.2.21 we may conclude that all of these graphs have sparsity order at most 3. Again, finding 3-dimensional orthogonal representations for each graph is routine (see [22, Lemma 2.8] and [20, p.556]). All that remains, is to show that no proper induced subgraph of any of these graphs has sparsity order equal to 3. For the graphs $A_1, D_1 - D_4$ this follows from Corollary 5.2.21, since any proper induced subgraphs has at most 3 non-edges. Finally, for the graphs A_4 and B_1 the only possible subgraph with sparsity order equal to 3, is the graph with complement isomorphic to a path of length five. However, this graph is the clique-sum of a C_3 and C_4 , therefore it has sparsity order equal to two, since C_4 is a 2-block and the sparsity order of a clique-sum is equal to the maximum sparsity order of its components (Theorem 5.1.5).

Lemma 5.2.26. [20, Lemma 12, p.556]

- (i) If $G \in \mathcal{G}_1$ is non-chordal and contains neither D_1 nor D_2 , as an induced subgraph, then $G \in \mathcal{G}_4$.
- (ii) If $G \in \mathcal{G}_2$ does not contain D_3 , as an induced subgraph, then $G \in \mathcal{G}_5$.
- (iii) If $G \in \mathcal{G}_3$ does not contain D_4 , as an induced subgraph, then $G \in \mathcal{G}_5$.

Proof. (i) Let $G \in \mathcal{G}_1$ and let H denote the chordal part in G . Assume that H is not a clique, else we are done. If G is non-chordal, it follows that G has two non-adjacent vertices (see Figure 4.2), adjacent to every element in H . Thus, if G contains neither D_1 nor D_2 , as induced subgraphs, then H does not contain an induced path of length 3 and $\alpha(H) = 2$. Therefore, by Lemma 4.3.9, the vertex set of H may be partitioned in such a way that G is indeed in \mathcal{G}_4 .

(ii) Let $G \in \mathcal{G}_2$. If G does not contain D_3 , then the two non-adjacent cliques each have only one vertex. Indeed, if one considers the complement of G we see that if one of the adjacent stable sets contain more than one vertex, we find \overline{D}_3 , as an induced subgraph. Thus, $G \in \mathcal{G}_5$.

(iii) Let $G \in \mathcal{G}_3$. If G does not contain D_4 , its complement may contain a matching of cardinality at most 3, which is exactly the form of a graph in \mathcal{G}_5 . \square

The next theorem is the complex variant of Theorem 5.2.16, and the proof of this result again relies on a decomposition result, which follows from Theorem 4.1.2.

Theorem 5.2.27. [20, Theorem 13] *The following assertions are equivalent for a graph G :*

(i) $\text{ord}_{\mathbb{C}}(G) \leq 2$.

(ii) G does not contain, as an induced subgraph, any of the graphs C_n , $n \geq 5$, A_4 , B_1 , $D_1 - D_4$ (Figures 4.3 and 5.3).

(iii) G is a clique-sum of set of graphs belonging to $\mathcal{G}_4 \cup \mathcal{G}_5$ (Figures 4.2 and 5.2).

Proof. (i) \implies (ii) Note that the graphs C_n , $n \geq 5$, all have sparsity order greater than or equal to 3 over \mathbb{C} (Proposition 5.1.8). Moreover, $A_1, A_4, B_1, D_1 - D_4$ are all 3-blocks over \mathbb{C} (Proposition 5.2.25). Therefore, by Theorem 5.1.4, a graph with sparsity order less than or equal to 2 over \mathbb{C} can not contain, as an induced subgraph, any of the graphs C_n , $n \geq 5$, A_4 , B_1 , $D_1 - D_4$.

(ii) \implies (iii) Let G be a graph satisfying Theorem 5.2.27 (ii). Then, G satisfies Theorem 5.2.16 (ii), since the graphs $A_2, A_3, B_2 - B_6$ all contain D_2 , while $A_5 - A_7$ contain D_1 , A_8, A_9 contain D_3 , and finally A_{10} contains D_4 . Therefore, G is a clique-sum of a set of graphs belonging to $\bigcup_{i=1}^4 \mathcal{G}_i$. If $G \in \mathcal{G}_1$ is a chordal graph, it can be decomposed as a clique-sum of cliques (Corollary 4.1.4), from which it follows that it is a clique-sum of graphs belonging to $\mathcal{G}_4 \cup \mathcal{G}_5$. If $G \in \mathcal{G}_1$ is a non-chordal graph satisfying Theorem 5.2.27 (ii), it belongs to \mathcal{G}_4 , by Lemma 5.2.26. Finally, by the same lemma, a graph belonging to $\mathcal{G}_2 \cup \mathcal{G}_3$ and satisfying Theorem 5.2.27 (ii) necessarily belongs to \mathcal{G}_5 .

(iii) \implies (i) Follows from Theorem 5.1.5, Proposition 5.2.24 and Theorem 5.2.2. \square

Again we consider two applications of Theorem 5.2.27. A first obvious application is that we may determine whether a graph has sparsity order less than or equal to 2 over \mathbb{C} in polynomial time, in a similar fashion as the real case.

The second application of Theorem 5.2.27 is the classification of the 3-blocks over \mathbb{C} . The proof of this corollary is similar to the proof of Corollary 5.2.17.

Theorem 5.2.28. [20, Corollary 14] *In the complex case, the only 3-blocks are the graphs $A_1, A_4, B_1, D_1 - D_4$.*

5.3 Notes

In [1, Theorem 7.1] it is shown that C_4 is the only 2-block, in the real and complex case. In the proof of this theorem, they apply the notion of k -superblocks. We were able to provide a new proof of this result, which, essentially, only relies on the fact that a 2-block necessarily contains a cycle of length at least equal to 4 and Corollary 5.2.9, in the real case, and Corollary 5.2.19 and Theorem 5.2.20, in the complex case. In the real case, we prove that $A_1 - A_{10}$ and $B_1 - B_6$ contain no induced subgraphs of sparsity order 3, by applying Corollary 5.2.9 and Theorem 5.2.12. Since each of these graphs have sparsity order 3, this shows that they are 3-blocks over \mathbb{R} . In this way we have applied more recent work to prove known results. In the complex case, we have also shown that $A_1, A_4, B_1, D_1 - D_4$ contain no induced graphs of sparsity order 3, by applying Corollary 5.2.21 and Theorem 5.1.5. This, then implies that all of these graphs are 3-blocks over \mathbb{C} . Although

this fact is used in [20], it is not immediately clear that these graphs are, indeed, 3-blocks. All that seems to be shown, is that they each have sparsity order equal to 3. Finally, Lemma 12 (ii) in [20], seems to be only partially correct, since it requires that both of the non-adjacent vertices, adjacent to all the vertices in the chordal part, be present in the class \mathcal{G}_1 . However, this obviously need not always be the case, since any chordal graph is an induced subgraph of \mathcal{G}_1 . It should be noted though that the main result, Theorem 5.2.27, remains unaffected, since a chordal graph can be decomposed as the clique-sum of cliques and a non-chordal graph in \mathcal{G}_1 , containing neither D_1 nor D_2 , as an induced subgraph, is in fact in \mathcal{G}_4 .

Chapter 6

Relating the sparsity order of a graph and its spectrum

6.1 Spectrum of a graph and cospectral mates

In this final chapter, we will show how one can determine whether a graph has sparsity order less than or equal to 2 by means of the forbidden induced subgraphs mentioned in the previous chapter. We introduce the notion of the spectrum of a graph and provide a novel way to find induced subgraphs by calculating the characteristic polynomial of principal submatrices. In this way we move from a graph theoretic setting to a linear algebra setting to determine whether the sparsity order of a graph is less than or equal to 2.

Note that when we refer to the spectrum of a graph, we also refer to the characteristic polynomial of the graph. So in some cases when we say that a certain property of a graph is determined by its spectrum, it may actually mean that it is determined by its characteristic polynomial, in particular, the coefficients of the characteristic polynomial. The context in which it is used should make the distinction clear. The reason why we distinguish between these two notions, which may seem like the same thing, is that numerically the characteristic polynomial is easy to compute, while the spectrum is usually only an approximation.

We start with some preliminary results on the spectrum of a graph and introduce some more graph theoretic notions which will be relevant in our study.

Definition 6.1.1 (Walk, Closed Walk). A walk $[v_1, \dots, v_k]$ in a graph $G = (V, E)$ is a sequence of vertices (not necessarily distinct) such that $(v_j, v_{j+1}) \in E$ for $j = 1, \dots, k-1$. The walk $[v_1, \dots, v_k]$ is referred to as a walk between v_1 and v_k . Furthermore, if $v_1 = v_k$ we say the walk is closed.

Note that the main difference between a walk and a path is that a walk is permitted to use vertices more than once. The closed walks of a graph can easily be obtained by calculating powers of the adjacency matrix, which we define next.

Definition 6.1.2 (Adjacency matrix of a graph). Let $G = (V, E)$ be a graph on n

vertices. Define the $n \times n$ adjacency matrix of G as follows:

$$A_G = [a_{ij}]_{i,j=1}^n, \text{ where } a_{ij} = \begin{cases} 1, & \text{if } (i, j) \in E \\ 0, & \text{if } (i, j) \notin E. \end{cases}$$

If the underlying graph is clear, we will drop the subscript and simply write A .

The following proposition shows that the number of closed walks, of any length, between two vertices can be obtained by calculating the powers of the adjacency matrix.

Proposition 6.1.3. [11, Lemma 8.1.2] *Let G be a graph with adjacency matrix A . The number of walks from the vertex i to the vertex j in G with length r is equal to the ij -th entry of the matrix A^r .*

The proof of this result follows by induction on r . From this proposition it follows that the number of closed walks of length r in G is equal to $\text{tr}(A^r)$, hence we have the following corollary.

Corollary 6.1.4. [11, Corollary 8.1.3] *Let G be a graph with e edges and t triangles. If A is the adjacency matrix of G , then*

$$(i) \quad \text{tr}(A) = 2e, \quad (ii) \quad \text{tr}(A^2) = 2e, \quad (iii) \quad \text{tr}(A^3) = 6t.$$

Since the trace of a square matrix is also equal to the sum of its eigenvalues, and the eigenvalues of A^r are the r -th powers of the eigenvalues of A , we see that $\text{tr}(A^r)$ is determined by the spectrum of A . Therefore, it makes sense to define the spectrum of a graph G as the spectrum of its adjacency matrix, as we do now.

Definition 6.1.5 (Spectrum of a graph). Let G be a graph. Then, the spectrum of G is defined as the spectrum of the adjacency matrix of G .

More will be said on the relationship between the spectrum of a graph and its structural properties, such as number of vertices, edges and triangles, later on.

To illustrate the notion of the spectrum of a graph, we give some examples of graphs and their spectrum.

Example 6.1.6. Let $G = K_n$, the complete graph on n vertices. Then the adjacency matrix of G is given by $A_G = J_n - I_n$, where J_n is the $n \times n$ matrix with all entries equal to 1, and I_n is the $n \times n$ identity matrix. The spectrum of G is given by $\{-1^{(n-1)}, n-1\}$ where the exponent indicates the multiplicity of the eigenvalue -1.

Let $G = K_4$, the complete graph on 4 vertices. Then the adjacency matrix of G is given by

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

The characteristic polynomial of A_G is given by $p(t) = t^4 - 6t^2 - 8t - 3$ and so the spectrum of A_G is $\{-1^{(3)}, 3\}$ where the exponent indicates the multiplicity of the eigenvalue -1.

Example 6.1.7. Let $G = C_n$, the cycle on n vertices. Then the spectrum of G is given by

$$2 \cos \left(\frac{2\pi j}{n} \right),$$

for $j = 0, \dots, n-1$.

Let $G = C_4$ with edges $\{(1, 2), (2, 3), (3, 4), (4, 1)\}$. Then the adjacency matrix of G is given by

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

The characteristic polynomial of A_G is given by $p(t) = t^4 - 4t^2$, and so the spectrum of A_G is $\{-2, 0^{(2)}, 2\}$ where the exponent indicates the multiplicity of the eigenvalue 0.

Note that since the adjacency matrix is always symmetric when G is a simple undirected graph (as is the case here), the eigenvalues are always real (Theorem 1.1.2).

Definition 6.1.8 (Bipartite Graph). A graph G is bipartite if its vertex set can be partitioned into two subsets X and Y so that every edge has one end in X and one end in Y . Such a partition (X, Y) is called a bipartition of the graph, and X and Y its parts. We denote a bipartite graph G with bipartition (X, Y) by $G[X, Y]$.

If the bipartite graph $G[X, Y]$ is complete in the sense that every vertex in X is adjacent to every vertex in Y we denote G by $K_{n,m}$ where n and m are the number of vertices in X and Y , respectively.

Recall that the adjacency set of a vertex v is defined as the set

$$\text{Adj}(v) = \{u \in V : (u, v) \in E\}.$$

Definition 6.1.9 (Degree of a vertex). Let $G = (V, E)$ be a graph on n vertices. The degree of a vertex v in a graph G , denoted by $d_G(v)$, is equal to the cardinality of its adjacency set. We denote by $\delta(G)$ and $\Delta(G)$ the minimum and maximum degrees of the vertices of G , and by $d(G)$ their average degree, $\frac{1}{n} \sum_{v \in V} d(v)$.

It is not hard to see that the sum of all the degrees of the vertices of a graph is equal to twice the number of edges of the graph. We now introduce a special class of graphs where all the vertices have the same degree.

Definition 6.1.10 (Regular Graph). A graph $G = (V, E)$ is k -regular if $d(v) = k$ for all $v \in V$. In particular, we call a graph regular if it is k -regular for some k .

An easy example of a regular graph is the complete graph on n vertices, K_n , which is $(n-1)$ -regular. Another example is the cycle on n vertices, C_n , which is 2-regular.

Definition 6.1.11 (Circumference and Girth of a graph). Let G be a graph which contains at least one cycle. Then, the circumference of G is the length of a longest cycle in the graph and the girth of G is the length of a shortest cycle in the graph.

The spectrum of a graph is a very useful thing, since some structural properties of a graph can be determined by calculating the spectrum. We list these properties in the next lemma.

Lemma 6.1.12. [14, Lemma 4] *The following can be deduced from the spectrum of a graph:*

- (i) *The number of vertices.*
- (ii) *The number of edges.*
- (iii) *Whether G is regular.*
- (iv) *Whether G is regular with any fixed girth.*
- (v) *The number of closed walks of any fixed length.*
- (vi) *Whether G is bipartite.*

We will now show how the characteristic polynomial can be used to obtain the number of closed walks, of any length, of a graph G . Let $p(t) = t^n + a_{n-1}t^{n-1} + a_{n-2}t^{n-2} + a_{n-3}t^{n-3} + \dots + a_1t + a_0$ be the characteristic polynomial of the adjacency matrix A of a graph G . Then, using Newton's identities (see Appendix D), we have the following

$$\operatorname{tr}(A^k) + a_{n-1} \operatorname{tr}(A^{k-1}) + \dots + a_{n-k+1} \operatorname{tr}(A) = -ka_{n-k} \quad \text{if } 1 \leq k \leq n.$$

Now, working recursively for $k = 1, \dots, n$ we obtain the following equations:

$$\begin{aligned} a_{n-1} &= -\operatorname{tr}(A), \\ a_{n-2} &= -\frac{1}{2}(\operatorname{tr}(A^2) + a_{n-1} \operatorname{tr}(A)), \\ a_{n-3} &= -\frac{1}{3}(\operatorname{tr}(A^3) + a_{n-1} \operatorname{tr}(A^2) + a_{n-2} \operatorname{tr}(A)), \\ a_{n-4} &= -\frac{1}{4}(\operatorname{tr}(A^4) + a_{n-1} \operatorname{tr}(A^3) + a_{n-2} \operatorname{tr}(A^2) + a_{n-3} \operatorname{tr}(A)), \\ &\dots \end{aligned}$$

Note that for the adjacency matrix of a graph, the trace is equal to zero, so we have that

$$a_{n-1} = 0, \quad a_{n-2} = -\frac{1}{2} \operatorname{tr}(A^2), \quad a_{n-3} = -\frac{1}{3} \operatorname{tr}(A^3), \quad a_{n-4} = \frac{1}{8} \operatorname{tr}(A^2)^2 - \frac{1}{4} \operatorname{tr}(A^4), \dots,$$

where A is the adjacency matrix of G . From this we see that the number of closed walks of the graph G can be calculated simply by using the coefficients of the characteristic polynomial. In particular, $|a_{n-2}|$ and $|a_{n-3}|$ are the number of edges and twice the number of triangles of G , respectively.

Two graphs G and H are said to be isomorphic if there exists a bijection between the vertex sets of G and H

$$f : V_G \rightarrow V_H$$

such that $(u, v) \in E_G$ if and only if $(f(u), f(v)) \in E_H$. In other words, G and H are the same after a relabelling of the vertices of one of these graphs. This is, in essence, what is done in the next theorem.

Theorem 6.1.13. *Two simple graphs, $G = (V_G, E_G)$ and $H = (V_H, E_H)$, with finite vertex sets are isomorphic if and only if their adjacency matrices are permutation similar, that is,*

$$A_G = P^{-1}A_HP,$$

where P is a permutation matrix.

Proof. Assume that G and H are isomorphic. Then there exists a bijection between the vertex sets of G and H

$$f : V_G \rightarrow V_H$$

such that $(u, v) \in E_G$ if and only if $(f(u), f(v)) \in E_H$. Let A_G and A_H denote the adjacency matrices of G and H , respectively. Let $V_G = \{1, \dots, n\}$ and $V_H = \{1, \dots, n\}$; this holds since both vertex sets are finite and have the same dimension. Then

$$f : \{1, \dots, n\} \rightarrow \{1, \dots, n\}$$

is a permutation of these n elements. We can represent this permutation in matrix form as follows:

$$\begin{pmatrix} 1 & 2 & \cdots & n \\ f(1) & f(2) & \cdots & f(n) \end{pmatrix}.$$

Now, let

$$P = \begin{pmatrix} \mathbf{e}_{f(1)} \\ \mathbf{e}_{f(2)} \\ \vdots \\ \mathbf{e}_{f(n)} \end{pmatrix},$$

where \mathbf{e}_i denotes a row vector of length n with 1 in the i -th position and 0 in every other position. Clearly P is a permutation matrix, furthermore $A_G = P^{-1}A_HP$ (where $P^{-1} = P^T$). Therefore, A_H and A_G are permutation similar.

Conversely, assume that A_G and A_H are permutation similar. Then, there exists a $n \times n$ permutation matrix P such that $A_G = P^{-1}A_HP$. Since P simply reorders the rows and columns of A_H to give A_G , it is clear that the only difference between G and H is the labelling of their vertices; therefore the graphs must be isomorphic. \square

From this theorem, it easily follows that the spectrum of two isomorphic graphs is always equal. However, the converse need not be true, that is, if two graphs have the same spectrum they are not necessarily isomorphic, as can be seen in the next example. We will call non-isomorphic graphs with the same spectrum cospectral.

Example 6.1.14. Let G and H be the graphs given in Figure 6.1. Then the adjacency matrices of G and H are as follows:

$$A_G = \begin{bmatrix} 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}, \quad A_H = \begin{bmatrix} 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 \\ 1 & 1 & 1 & 1 & 0 \end{bmatrix}$$

The characteristic polynomial for both of these matrices is $p(t) = t^5 - 4t^3$, and consequently G and H have the same spectrum, namely $\{-2, 0^{(3)}, 2\}$. However, they are clearly not isomorphic.

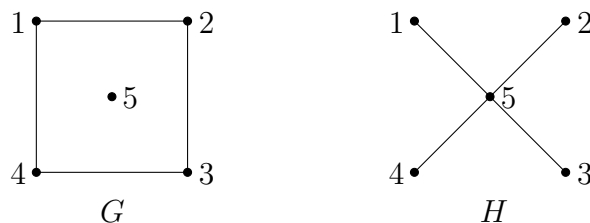


Figure 6.1: The graphs G and H of Example 6.1.14

We say that a graph G is determined by its spectrum if any other graph with the same spectrum is isomorphic to G , in other words, G has no cospectral mates. In the previous example we saw that not all graphs with the same spectrum are isomorphic. Consequently, calculating the spectrum of two graphs to see whether they are isomorphic is sufficient if and only if one of the graphs is determined by its spectrum. Some classes of graphs are known to be determined by their spectrum (as we will soon see), however, in general it is not known which graphs are determined by their spectrum. In [13] it is conjectured that almost no graphs have cospectral mates (graphs with the same spectrum), as the number of vertices tends to infinity. The problem though in showing that a graph is determined by its spectrum, is that to do this, the graph must exhibit some specific structure, which is of course not the case for most arbitrary graphs. In the next proposition, we list some graphs which are determined by their spectrum; note that all these graphs have a specific structure.

Proposition 6.1.15. [14, Proposition 4] *The following graphs and their complements are determined by their spectrum:*

- (i) *The complete graph K_n .*
- (ii) *The regular complete bipartite graph $K_{m,m}$.*
- (iii) *The path P_n .*
- (iv) *The cycle C_n .*

The proofs of (i) – (iii) can be found in Proposition 4 [14, p.16] and the proof of (iv) in Proposition 1 [14, p.3] and [9].

6.2 The forbidden induced subgraphs have no cospectral mates

In this section, we show that all the forbidden induced subgraphs ($A_1 - A_{10}, B_1 - B_6, D_1 - D_4$) of the previous chapter are determined by their spectrum. We will use this fact in an algorithm to determine whether a graph has sparsity order less than or equal to 2. Unfortunately, these graphs exhibit no obvious structural property which we can use to show that they are determined by their spectrum. Therefore, we will have to rely on computer results. Note that, by Proposition 6.1.15, the cycles $C_n, n \geq 5$, are determined by their spectrum, with spectrum given by

$$2 \cos \left(\frac{2\pi j}{n} \right),$$

for $j = 0, \dots, n - 1$.

We start with the following table, where the characteristic polynomial of each graph is given:

Graph	Characteristic polynomial
A_1	$p(t) = t^5 - 5t^3 + 5t - 2$
A_2	$p(t) = t^6 - 10t^4 - 6t^3 + 3t^2$
A_3	$p(t) = t^7 - 16t^5 - 24t^4$
A_4	$p(t) = t^6 - 10t^4 - 8t^3 + 9t^2 + 4t - 1$
A_5	$p(t) = t^7 - 16t^5 - 26t^4 + 4t^3 + 16t^2$
A_6	$p(t) = t^7 - 16t^5 - 26t^4 + 2t^3 + 16t^2 + t - 2$
A_7	$p(t) = t^8 - 23t^6 - 56t^5 - 27t^4 + 24t^3 + 12t^2$
A_8	$p(t) = t^8 - 23t^6 - 56t^5 - 29t^4 + 20t^3 + 11t^2 - 4t$
A_9	$p(t) = t^9 - 31t^7 - 100t^6 - 102t^5 - 8t^4 + 24t^3$
A_{10}	$p(t) = t^{10} - 40t^8 - 160t^7 - 240t^6 - 128t^5$
B_1	$p(t) = t^6 - 9t^4 - 4t^3 + 12t^2$
B_2	$p(t) = t^6 - 9t^4$
B_3	$p(t) = t^7 - 14t^5 - 16t^4 + 8t^3$
B_4	$p(t) = t^6 - 8t^4 + 4t^2$
B_5	$p(t) = t^6 - 9t^4 - 4t^3 + 7t^2$
B_6	$p(t) = t^7 - 15t^5 - 20t^4 + 8t^3 + 8t^2$
D_1	$p(t) = t^6 - 11t^4 - 12t^3 + 5t^2 + 4t$
D_2	$p(t) = t^5 - 6t^3$
D_3	$p(t) = t^7 - 17t^5 - 32t^4 - 8t^3 + 8t^2$
D_4	$p(t) = t^8 - 24t^6 - 64t^5 - 48t^4$

We will make use of the computer results of [5] and [6] to show that all of the graphs here are determined by their spectrum. Let n be the number of vertices, e the number

of edges and t be the number of triangles. The results from [6] show that there are no cospectral graphs on:

n	e
5	5,6
6	8,9,10,11,12
7	17
8	23,24
9	31
10	40

Therefore, the graphs $A_1, A_2, A_4, A_7 - A_{10}, B_1, B_2, B_4, B_5, D_1 - D_4$ are all determined by their spectrum. All that remains is to show that A_3, A_5, A_6, B_3, B_6 are also all determined by their spectrum. Note that $n = 7$ for all of these graphs. In the following table we list e and t , for the remaining graphs.

Graph	e	t
A_3	16	12
A_5	16	13
A_6	16	13
B_3	14	8
B_6	15	10

Recall that the number of triangles is determined by the spectrum of a graph, therefore, for two graphs to be cospectral they must have the same number of triangles. Now, according to [5] we have the following for $n = 7$:

- There is only one graph with $e = 16$ and $t = 12$.
- There are three graphs with $e = 16$ and $t = 13$ (Figure 6.2).
- There are 12 graphs with $e = 14$ and $t = 8$ (Figure 6.3).
- There are six graphs with $e = 15$ and $t = 10$. (Figure 6.4)

We may therefore conclude that the graph A_3 is determined by its spectrum. For the remaining four graphs, it suffices to calculate the characteristic polynomial of all the graphs given in Figures 6.2-6.4 to see that the spectrum of all of these graphs are different. One easily verifies that this is the case, therefore, each is determined by their spectrum. In particular, note that the first two graphs of Figure 6.2 are A_5 and A_6 , the first graph of Figure 6.3 is B_3 and the first graph of Figure 6.3 is B_6 .

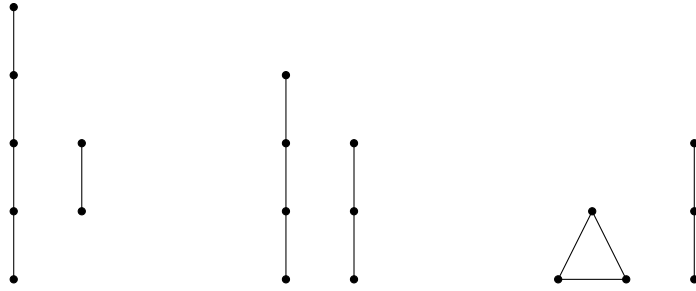


Figure 6.2: The complements of the graphs on 7 vertices with 16 edges and 13 triangles

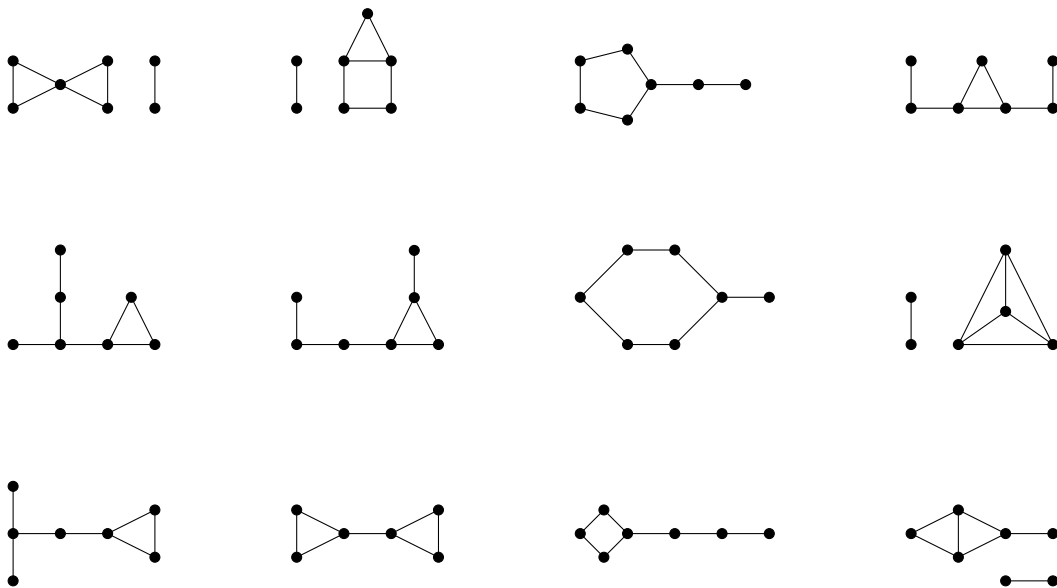


Figure 6.3: The complements of the graphs on 7 vertices with 14 edges and 8 triangles

6.3 Sparsity order algorithm

To determine whether a graph G has sparsity order less than or equal to 2, it suffices to calculate the spectrum of the principal submatrices, of the adjacency matrix of G , of appropriate size. If the spectrum of one of these principal submatrices is equal to that of one of the forbidden induced subgraphs, we know that the forbidden induced subgraph is in fact a subgraph of G , since these graphs are determined by their spectrum. Therefore, G must have sparsity order greater than 2. Unfortunately, calculating all the principal submatrices of appropriate size can be very expensive if the number of vertices of G is large. To partially overcome this problem we introduce the notion of eigenvalue interlacing, which will greatly simplify matters.

Theorem 6.3.1. [17, Theorem 4.3.15] *Let $A \in \mathcal{M}_n(\mathbb{C})$ be a Hermitian matrix, let $A[K]$ be a principal submatrix of A , where $K \subseteq \{1, \dots, n\}$ and $\text{card}(K) = k$. Let $\lambda_i, i =$*

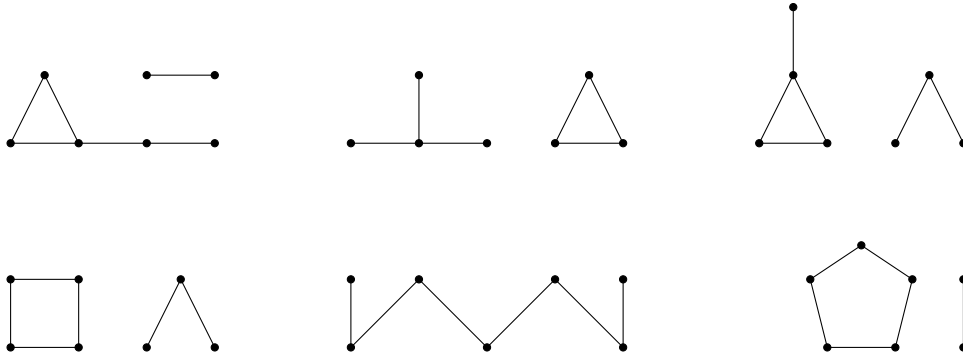


Figure 6.4: The complements of the graphs on 7 vertices with 15 edges and 10 triangles

$1, \dots, n$, and μ_j , $j = 1, \dots, k$ denote the eigenvalues of A and $A[K]$, respectively, and assume that they have been arranged in increasing order, i.e., $\lambda_1 \leq \dots \leq \lambda_n$ and $\mu_1 \leq \dots \leq \mu_k$. Then, for each integer r such that $1 \leq r \leq k$, we have

$$\lambda_r \leq \mu_r \leq \lambda_{r+n-k}.$$

If we consider principal submatrices of size $(n-1) \times (n-1)$, the inequality of Theorem 6.3.1 gives the following

$$\lambda_1 \leq \mu_1 \leq \lambda_2 \leq \dots \leq \lambda_{n-1} \leq \mu_{n-1} \leq \lambda_n,$$

which makes it clear why we refer to eigenvalue interlacing.

Turning back to the problem at hand we may now describe an algorithm to determine whether a graph has sparsity order less than or equal to 2, where we will also incorporate the notion of eigenvalue interlacing:

Sparsity order algorithm

Let G be a graph on n vertices. Let λ_i , $i = 1, \dots, n$, be the eigenvalues of G arranged in increasing order, i.e., $\lambda_1 \leq \dots \leq \lambda_n$. To determine whether G has sparsity order less than or equal to 2, we will apply the following procedure:

Step 1

- Calculate the spectrum of the graph G and arrange the eigenvalues of G in increasing order.
- If the spectrum of a forbidden induced subgraph does not interlace the spectrum of G , as described in Theorem 6.3.1, it is not an induced subgraph of G .

Step 2

- Calculate the characteristic polynomial of each principal submatrix, of appropriate size w.r.t. the remaining forbidden induced subgraphs.

- If the characteristic polynomial of one of these principal submatrices is equal to the characteristic polynomial of one of the forbidden induced subgraphs, G has sparsity order greater than 2, if not, it has sparsity order less than 2 (Theorem 5.2.16 and 5.2.27).

We will illustrate the use of this algorithm in the next example.

Example 6.3.2. Let G be the graph with adjacency matrix

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

The characteristic polynomial of A_G is $p(t) = t^7 - 14t^5 - 18t^4 + 15t^3 + 30t^2 + 6t - 4$ and the spectrum is $\{-2.4397, -1.191, -1, -1, 0.2706, 1.2326, 4.1275\}$. The only forbidden induced subgraphs we need to check for are those on 7 vertices or less.

Clearly none of the forbidden induced subgraphs on 7 has the same characteristic polynomial as G , so all that remains is to check for $C_6, A_1, A_2, A_4, B_1, B_2, B_4, B_5$ in the real case; and A_4, B_1, D_1, D_2 in the complex case.

We now have to check for induced subgraphs on 5 and 6 vertices. Thus, applying eigenvalue interlacing, we obtain the following:

Let H be a graph on 5 vertices, with eigenvalues $\lambda_i, i = 1, 2, 3, 4, 5$, arranged in increasing order. Then,

- $\lambda_1 \in [-2.4397, -1]$,
- $\lambda_2 \in [-1.191, -1]$,
- $\lambda_3 \in [-1, 0.2706]$,
- $\lambda_4 \in [-1, 1.2326]$,
- $\lambda_5 \in [0.2706, 4.1275]$.

Let F be a graph on 6 vertices, with eigenvalues $\mu_i, i = 1, 2, 3, 4, 5, 6$, arranged in increasing order. Then,

- $\mu_1 \in [-2.4397, -1.191]$,
- $\mu_2 \in [-1.191, -1]$,
- $\mu_3 \in [-1, -1]$,

- $\mu_4 \in [-1, 0.2706]$,
- $\mu_5 \in [0.2706, 1.2326]$,
- $\mu_6 \in [1.2326, 4.1275]$.

Next, calculating the spectrum of the forbidden induced subgraphs gives:

$$\begin{aligned}\sigma(C_6) &= \{-2, -1, -1, 1, 1, 2\}, \\ \sigma(A_1) &= \{-1.618, -1.6180, 0.618, 0.618, 2\}, \\ \sigma(A_2) &= \{-2.7177, -1, 0, 0, 0.3254, 3.3923\}, \\ \sigma(A_4) &= \{-2.247, -1.5758, -0.555, 0.1873, 0.8019, 3.3885\}, \\ \sigma(B_1) &= \{-2, -2, 0, 0, 1, 3\}, \\ \sigma(B_2) &= \{-3, 0, 0, 0, 0, 3\}, \\ \sigma(B_4) &= \{-2.7321, -0.7321, 0, 0, 0.7321, 2.7321\}, \\ \sigma(B_5) &= \{-2.5086, -1.2855, 0, 0, 0.702, 3.0922\}, \\ \sigma(D_1) &= \{-2.2307, -1.618, -0.4829, 0, 0.6180, 3.7136\}, \\ \sigma(D_2) &= \{-2, -2, 0, 0, 0, 4\},\end{aligned}$$

It is not hard to verify that none of the graphs here satisfy the required eigenvalue interlacing. Therefore, the sparsity order of G is less than or equal to 2, in the real and complex case.

We saw in this example that it was sufficient to check for eigenvalue interlacing to verify that the graph has sparsity order less than or equal to 2. Thus, all that was required of the sparsity order algorithm, was Step 1. In the next example we will see that Step 1 is not sufficient and will have to apply Step 2 of the algorithm, that is, calculate the characteristic polynomial of the principal submatrices of appropriate size and compare with the characteristic polynomials of the forbidden induced subgraphs.

Example 6.3.3. Let G be the graph with adjacency matrix

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

The characteristic polynomial of A_G is $p(t) = t^7 - 12t^5 - 10t^4 + 23t^3 + 20t^2 - 9t - 6$ and the spectrum is $\{-2.2083, -1.7053, -1.1268, -0.4663, 0.6585, 1.2968, 3.5515\}$. The only forbidden induced subgraphs we need to check for are those on 7 vertices or less.

Again the only graphs we need to check for are $C_6, A_1, A_2, A_4, B_1, B_2, B_4, B_5$ in the real case; and A_4, B_1, D_1, D_2 in the complex case.

Let H be a graph on 5 vertices, with eigenvalues $\lambda_i, i = 1, 2, 3, 4, 5$, arranged in increasing order. Then,

- $\lambda_1 \in [-2.2083, -1.1268]$,
- $\lambda_2 \in [-1.7053, -0.4663]$,
- $\lambda_3 \in [-0.4663, 1.2968]$,
- $\lambda_4 \in [-1, 1.2326]$,
- $\lambda_5 \in [0.6585, 3.5515]$.

Let F be a graph on 6 vertices, with eigenvalues μ_i , $i = 1, 2, 3, 4, 5, 6$, arranged in increasing order. Then,

- $\mu_1 \in [-2.2083, -1.7053]$,
- $\mu_2 \in [-1.7053, -1.1268]$,
- $\mu_3 \in [-1.1268, -0.4663]$,
- $\mu_4 \in [-0.4663, 0.6585]$,
- $\mu_5 \in [0.6585, 1.2968]$,
- $\mu_6 \in [1.2968, 3.5515]$.

From the previous example we know the spectrum of the forbidden induced subgraphs are:

$$\begin{aligned} \sigma(C_6) &= \{-2, -1, -1, 1, 1, 2\}, \\ \sigma(A_1) &= \{-1.618, -1.6180, 0.618, 0.618, 2\}, \\ \sigma(A_2) &= \{-2.7177, -1, 0, 0, 0.3254, 3.3923\}, \\ \sigma(A_4) &= \{-2.247, -1.5758, -0.555, 0.1873, 0.8019, 3.3885\}, \\ \sigma(B_1) &= \{-2, -2, 0, 0, 1, 3\}, \\ \sigma(B_2) &= \{-3, 0, 0, 0, 0, 3\}, \\ \sigma(B_4) &= \{-2.7321, -0.7321, 0, 0, 0.7321, 2.7321\}, \\ \sigma(B_5) &= \{-2.5086, -1.2855, 0, 0, 0.702, 3.0922\}, \\ \sigma(D_1) &= \{-2.2307, -1.618, -0.4829, 0, 0.6180, 3.7136\}, \\ \sigma(D_2) &= \{-2, -2, 0, 0, 0, 4\}, \end{aligned}$$

We can now easily verify that the only possibility which remains is A_5 . Therefore, we need to consider all possible 5×5 principal submatrices and calculate their characteristic polynomials. Using the following Matlab script we see that one of the principal submatrices does indeed have the same characteristic polynomial as A_1 .

```

function [t,x]=sparse2(G) %if t=1 G contains A1, else G does not contain
%A1.

n=length(G);
v=nchoosek(1:n,5); %gives all the possible permutations of 7 elements
%into groups of 5 elements

[c,d]=size(v);
y=zeros(c,1);
x=zeros(c,d);
p=zeros(c,d+1);

for i=1:c
    p(i,:)=charpoly(G(v(i,:),v(i,:))); %calculate the characteristic
    %polynomial of each 5x5 principal submatrix
    if(p(i,:)==charpoly(A1)) %test whether the characteristic
    %polynomial of A1 is equal to one of the characteristic
    %polynomials of the principal submatrices
        y(i,1)=1;
        x(i,:)=v(i,:); %store the permutation for which the
        %characteristic polynomials are equal
    else
        y(i,1)=0;
    end
end

x=x(any(x,2),:); %delete all zero rows of x

if(norm(y)==0)
    t=0;
else
    t=1;
end
end

```

```

>> [t,x]=sparse2(A-G)

t =

    1

x =

    2     4     5     6     7

```

Thus, A_1 is a induced subgraph of G on the vertex set $\{2, 4, 5, 6, 7\}$ and so G has sparsity order greater than 2, in the real and complex case.

Note that the algorithm proposed here is expensive, since calculating all possible permutations can be very time consuming. A possible solution would be to use a kind of divide-and-conquer approach, in the sense that we delete only one row and column of the

adjacency matrix at a time and apply eigenvalue interlacing on the resulting principal submatrix to determine whether or not it contains a possible forbidden induced subgraph. If it does not contain a possible forbidden induced subgraph, we need not consider the particular principal submatrix further. However, if it does contain a possible forbidden induced subgraph we apply the same method described here to form smaller principal submatrices and repeat this process until all possibilities are exhausted. The rationale behind this method is that we repeatedly consider induced subgraphs of the graph by deleting a single vertex at a time, to determine which vertices can possibly induce a forbidden subgraph.

The algorithm proposed here runs in polynomial time when we wish to determine whether a graph contains a 3-block, as an induced subgraph, since the 3-blocks have a fixed number of vertices, which implies that the number of principal submatrices is bounded by a polynomial function, i.e., the number of $k \times k$ principal submatrices in a $n \times n$ matrix is equal to $\binom{n}{k}$, which is bounded by n^k . Unfortunately a problem arises in determining whether the sparsity order is less than or equal to 2, since the graph may not contain any induced cycle of length 5 or greater. Consequently, we need to check every $k \times k$ principal submatrix, for $k = 5, \dots, n$, to determine whether there is a cycle present, as an induced subgraph, which could turn out to be a very expensive exercise. Consequently, a different method needs to be applied to determine whether the graph contains any induced cycles C_n , $n \geq 5$. One way of doing this can be found in [23], who showed that one can determine in polynomial time whether the graph contains a cycle C_n , $n \geq 5$. Therefore, combining these two algorithms, one can determine in polynomial time whether a graph has sparsity order less than or equal to 2.

In conclusion the connection between the sparsity order of a graph and its spectrum is not at all obvious. However, it is interesting that all graphs with sparsity order less than or equal to 2, can also be characterized in terms of forbidden characteristic polynomials of principal submatrices.

Appendices

Appendix A

Inner product and Hilbert spaces

In the following two definitions, we define the concept of an inner product, an inner product space and a Hilbert space.

Definition A.1 (Inner product). Let \mathcal{U} be a vector space over the field \mathbb{F} (\mathbb{R} or \mathbb{C}). A function, $\langle \cdot, \cdot \rangle: \mathcal{U} \times \mathcal{U} \rightarrow \mathbb{F}$ is an inner product if, for all $x, y, z \in \mathcal{U}$:

$$\langle x, x \rangle \geq 0 \quad \text{and} \quad \langle x, x \rangle = 0 \iff x = 0 \tag{A.1}$$

$$\langle x + y, z \rangle = \langle x, z \rangle + \langle y, z \rangle \tag{A.2}$$

$$\langle \alpha x, y \rangle = \alpha \langle x, y \rangle, \quad \forall \alpha \in \mathbb{F} \tag{A.3}$$

$$\langle x, y \rangle = \overline{\langle y, x \rangle} \tag{A.4}$$

An inner product on \mathcal{U} defines a norm on \mathcal{U} given by

$$\|x\| = \sqrt{\langle x, x \rangle},$$

and a metric on \mathcal{U} given by

$$d(x, y) = \|x - y\| = \sqrt{\langle x - y, x - y \rangle}.$$

Definition A.2 (Inner product space, Hilbert space). An inner product space is a vector space \mathcal{U} with an inner product defined on \mathcal{U} . A Hilbert space is a complete inner product space (complete in the metric $d(x, y) = \|x - y\| = \sqrt{\langle x - y, x - y \rangle}$).

Hence inner product spaces are normed spaces, and Hilbert spaces are Banach spaces, with norm $\|x\| = \sqrt{\langle x, x \rangle}$. The converse is not necessarily true.

Inner product spaces retain many useful features of Euclidean space, and may be considered to be a natural generalization of Euclidean space. One such feature that will be of particular interest in our study, is that of orthogonality, which we define next.

Definition A.3 (Orthogonality). An element x of an inner product space \mathcal{X} is said to be orthogonal to an element $y \in \mathcal{X}$ if

$$\langle x, y \rangle = 0.$$

We also say that x and y are orthogonal, and write $x \perp y$. Similarly, for subsets $\mathcal{U}, \mathcal{V} \subset \mathcal{X}$ we write $x \perp \mathcal{U}$ if $x \perp u$ for all $u \in \mathcal{U}$, and $\mathcal{U} \perp \mathcal{V}$ if $u \perp v$ for all $u \in \mathcal{U}$ and all $v \in \mathcal{V}$.

Definition A.4 (Orthogonal Complement). The orthogonal complement of a set $\mathcal{U} \subseteq \mathcal{H}$ is the set

$$\mathcal{U}^\perp = \{h \in \mathcal{H}: \langle h, u \rangle = 0, \text{ for all } u \in \mathcal{U}\}.$$

Another property of the inner product is its continuity, which will be especially useful to prove the closedness of a set.

Lemma A.5. [19, Lemma 3.2.2] *If in an inner product space, $x_n \rightarrow x$ and $y_n \rightarrow y$, then $\langle x_n, y_n \rangle \rightarrow \langle x, y \rangle$.*

In the next theorem, we see that a subspace of a Hilbert space is itself a Hilbert space if it is closed or finite dimensional. In particular, every finite dimensional subspace of a Hilbert space is closed.

Theorem A.6. [19, Theorem 3.2,4] *Let \mathcal{Y} be a subspace of a Hilbert space \mathcal{H} . Then*

- (i) \mathcal{Y} is complete if and only if \mathcal{Y} is closed in \mathcal{H} .
- (ii) If \mathcal{Y} is finite dimensional, then \mathcal{Y} is complete.

The next result ensures that there exists a unique vector, in a convex subset of an inner product space, that minimizes the metric on the inner product space for every element of the inner product space.

Theorem A.7. [19, Theorem 3.3.1] *Let \mathcal{X} be an inner product space and $\mathcal{Y} \neq \emptyset$ a convex set which is complete (in the metric induced by the inner product). Then, for every given $x \in \mathcal{X}$, there exists a unique $y \in \mathcal{Y}$ such that*

$$\delta = \inf_{\tilde{y} \in \mathcal{Y}} \|x - \tilde{y}\| = \|x - y\|.$$

In other words, there exists a vector $y \in \mathcal{Y}$ nearest to x , for every $x \in \mathcal{X}$, which is unique.

Theorem A.8. *Let \mathcal{Y} be any closed subspace of a Hilbert space \mathcal{H} . Then*

$$\mathcal{H} = \mathcal{Y} \oplus \mathcal{Y}^\perp.$$

The following result is true for much more general spaces than Hilbert spaces. We only state it at the generality required in this thesis.

Theorem A.9. [7, Theorem V.7.4] *If K is a non-empty compact convex subset of a Hilbert space \mathcal{H} , then $\text{ext}(K) \neq \emptyset$ and $K = \overline{\text{conv}(\text{ext}(K))}$, where $\text{ext}(K)$ is the set of extreme points of K and $\text{conv}(S)$ is the closure of the convex hull of the set S .*

Appendix B

Linear algebra preliminaries

We will start by showing that the set of all $n \times n$ complex matrices, denoted by $\mathcal{M}_n(\mathbb{C})$, is a Hilbert space over \mathbb{C} . A proof is added since some of the argumentation reappears in Chapter 1.

Theorem B.1. *Let $\mathcal{M}_n(\mathbb{C})$ be the vector space of all $n \times n$ matrices in \mathbb{C} . Then $\mathcal{M}_n(\mathbb{C})$ is a Hilbert space over \mathbb{C} , with respect to the inner product*

$$\langle A, B \rangle_2 = \text{tr}(AB^*),$$

where $\text{tr}(M)$ denotes the trace of the square matrix M and B^* denotes the complex conjugate transpose of the matrix B .

Proof. We start by showing that $\mathcal{M}_n(\mathbb{C})$ is an inner product space. First of all we state some properties of the trace of a matrix. Let A and B be matrices in $\mathcal{M}_n(\mathbb{C})$ and $c \in \mathbb{C}$. Then:

- (i) $\text{tr}(A + B) = \text{tr}(A) + \text{tr}(B)$;
- (ii) $\text{tr}(cA) = c \text{tr}(A)$;
- (iii) $\text{tr}(AB) = \text{tr}(BA)$.

Now for all $A, B, C \in \mathcal{M}_n(\mathbb{C})$ and $c \in \mathbb{C}$ we have:

(A.1) $\langle A, A \rangle_2 = \text{tr}(AA^*) = \sum_{i=1}^n \sum_{j=1}^n a_{ij} \bar{a}_{ij} = \sum_{i=1}^n \sum_{j=1}^n |a_{ij}|^2$, which is of course always greater than or equal to zero. Furthermore it is exactly zero if and only if $a_{ij} = 0$ for all i, j , which in turn means that $A = 0$.

(A.2) $\langle A + B, C \rangle_2 = \text{tr}((A + B)C^*) = \text{tr}(AC^* + BC^*) = \text{tr}(AC^*) + \text{tr}(BC^*) = \langle A, C \rangle_2 + \langle B, C \rangle_2$.

(A.3) $\langle cA, B \rangle_2 = \text{tr}(cAB^*) = c \text{tr}(AB^*) = c \langle A, B \rangle_2$.

(A.4) $\overline{\langle B, A \rangle_2} = \overline{\text{tr}(AB^*)} = \sum_{i=1}^n \sum_{j=1}^n \overline{b_{ij} \bar{a}_{ij}} = \sum_{i=1}^n \sum_{j=1}^n \bar{b}_{ij} a_{ij} = \text{tr}(B^*A) = \text{tr}(AB^*) = \langle A, B \rangle_2$.

This proves that $\langle A, B \rangle_2 = \text{tr}(AB^*)$ is an inner product and therefore $\mathcal{M}_n(\mathbb{C})$ is an inner product space.

Moreover, $\mathcal{M}_n(\mathbb{C})$ is finite dimensional and so, by Theorem A.6, it is complete. We have therefore shown that $\mathcal{M}_n(\mathbb{C})$ is a Hilbert space over \mathbb{C} . \square

Next we mention a few results from linear algebra.

Theorem B.2. [29, Theorem 1.1] *Let V be a finite dimensional vector space, and let V_1 and V_2 be subspaces of V . Then*

$$\dim(V_1) + \dim(V_2) = \dim(V_1 + V_2) + \dim(V_1 \cap V_2).$$

In particular, if $V = V_1 \oplus V_2$, i.e., V is the direct sum of V_1 and V_2 , we have that

$$\dim(V) = \dim(V_1 + V_2) = \dim(V_1) + \dim(V_2).$$

Theorem B.3 (QR factorization). [17, Theorem 2.6.1] *If $A \in \mathcal{M}_{n,m}(\mathbb{C})$ and $n \geq m$, there is a matrix $Q \in \mathcal{M}_{n,m}(\mathbb{C})$ with orthonormal columns and an upper triangular matrix $R \in \mathcal{M}_m(\mathbb{C})$ such that $A = QR$. If $m = n$, Q is unitary. Moreover, if A is non-singular, we may choose R in such a way that all of its diagonal entries are positive, and in this case, the factors Q and R are both unique. If $A \in \mathcal{M}_{n,m}(\mathbb{R})$, then both Q and R may be taken to be real.*

See Section 1.2 for the definition of positive (semi)definite matrices.

Theorem B.4. [17, Theorem 7.2.6] *Let $A \in \mathcal{M}_n(\mathbb{C})$ be positive semidefinite and let $k \geq 1$ be a given integer. Then there exists a unique positive semidefinite Hermitian matrix B such that $B^k = A$. We also have*

- (i) $BA = AB$ and there is a polynomial $p(t)$ such that $B = p(A)$;
- (ii) $\text{rank}(B) = \text{rank}(A)$, so B is positive definite if A is;
- (iii) B is real if A is real.

The matrix $C - B^*A^{-1}B$ is known as the Schur complement of M with respect to the matrix A .

Lemma B.5. [2, Lemma 1.2.5] *Let $A \in \mathcal{M}_n(\mathbb{C})$ be positive definite. Then*

$$M = \begin{bmatrix} A & B \\ B^* & C \end{bmatrix} \in \mathcal{M}_{n+m}(\mathbb{C})$$

*is positive (semi)definite if and only if $C - B^*A^{-1}B$ is positive (semi)definite.*

Appendix C

Graph theory preliminaries

We collect here various basic graph theory definitions that will be used throughout the thesis.

Definition C.1 (Undirected Graph). A simple undirected graph is a pair $G = (V, E)$ in which V , the vertex set, is finite and the edge set $E \subseteq V \times V = \{(u, v) : u, v \in V\}$ is a symmetric binary relation on V such that $(v, v) \notin E$ for all $v \in V$.

In what follows all graphs are assumed to be simple and undirected.

Definition C.2 (Complement of a graph). Let $G = (V, E)$ be a graph. The complement of G is the graph which has the same vertices as G and its edges coincide with non-edges of G . We denote the complement of G by $\overline{G} = (V, \overline{E})$, where $(i, j) \in \overline{E}$ if and only if $(i, j) \notin E$.

Definition C.3 (Induced subgraph). Given a subset $A \subset V$, the subgraph of G induced by A is $G[A] = (A, E[A])$, where $E[A] = \{(u, v) \in E : u, v \in A\}$.

Definition C.4 (Complete Graph). We call a graph $G = (V, E)$ complete if every pair of distinct vertices in V is connected by an edge in E . We will denote complete graphs on n vertices by K_n .

Definition C.5 (Clique, Stable set). A subset $S \subseteq V$ is called a clique if $(i, j) \in E$ for all $i \neq j \in S$ and a stable set if $(i, j) \notin E$ for all $i \neq j \in S$. The clique number of a graph G is the maximum cardinality of a clique in G and is denoted by $\omega(G)$. Similarly, the stability number of a graph G is defined as the maximum cardinality of a stable set in G and is denoted by $\alpha(G)$.

It is easy to see that the clique and stability number are related in the following way

$$\omega(G) = \alpha(\overline{G}),$$

with \overline{G} the complement of the graph G .

Definition C.6 (Adjacency Set). The adjacency set of a vertex $v \in V$ is the set of all vertices $u \in V$ such that $(u, v) \in E$. It is denoted by $\text{Adj}(v)$. In other words

$$\text{Adj}(v) = \{u \in V : (u, v) \in E\}.$$

If the adjacency set of a vertex v is empty, i.e., there are no other vertices adjacent to v , we call v an isolated vertex.

Definition C.7 (Path). A path $[v_1, \dots, v_k]$ in a graph $G = (V, E)$ is a sequence of distinct vertices such that $(v_j, v_{j+1}) \in E$ for $j = 1, \dots, k - 1$. The path $[v_1, \dots, v_k]$ is referred to as a path between v_1 and v_k . We denote a path on n vertices by P_n .

Definition C.8 (Connected and Disconnected Graphs). A graph is called connected if there exists a path between any two different vertices in the graph. If this is not the case we say the graph is disconnected.

Definition C.9 (Cycle). A cycle of length $k > 2$ is a path $[v_1, \dots, v_k, v_1]$ in which v_1, \dots, v_k are distinct. We will use the notation (v_1, \dots, v_k) to indicate that a set of vertices form a cycle and denote arbitrary cycles of length k by C_k .

Definition C.10 (Null graph). The null graph is the graph with no vertices.

The null graph may be seen as a graph theoretic analogue of the empty set. Note that the null graph is vacuously a clique and a stable set, since it has no vertices nor edges. This can be seen in the same light as the empty set being both open and closed. The usefulness of the null graph is discussed in [15].

Appendix D

Newton's identities

Newton's identities relate sums of powers of roots of a polynomial with the coefficients of the polynomial.

Theorem D.1 (Newton's identities). [18] *Let $p(x) = x^n + a_{n-1}x^{n-1} + \cdots + a_0$ be a polynomial in \mathbb{C} of degree n , with roots r_j , $j = 1, \dots, n$. Define $s_k = \sum_{j=1}^n r_j^k$. Then*

$$s_k + a_{n-1}s_{k-1} + \cdots + a_0s_{k-n} = 0 \quad \text{if } k > n$$

and

$$s_k + a_{n-1}s_{k-1} + \cdots + a_{n-k+1}s_1 = -ka_{n-k} \quad \text{if } 1 \leq k \leq n.$$

Before we prove the theorem, we translate these identities to a matrix algebra setting. To start with, let C be as follows:

$$C = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 1 \\ -a_0 & -a_1 & -a_2 & \cdots & -a_{n-1} \end{bmatrix}.$$

Then the characteristic polynomial of C is given by p , since C is the companion matrix of p . So the roots of p are exactly the eigenvalues of C . From this, it follows that the k -th powers of the roots of p are the eigenvalues of C^k . Note that the sum of the eigenvalues of C^k is equal to the trace of C^k . Consequently, we have that $s_k = \sum_{j=1}^n r_j^k = \sum_{j=1}^n \lambda_j^k = \text{tr}(C^k)$, where λ_j , $j = 1, \dots, n$ are the eigenvalues of C . We are now ready to prove the theorem.

Proof of Theorem D.1. Let $k > n$. Since the trace is a linear function and $p(C) = C^n + a_{n-1}C^{n-1} + \cdots + a_0$, we have that

$$\begin{aligned} \text{tr}(C^k) + a_{n-1}\text{tr}(C^{k-1}) + \cdots + a_0\text{tr}(C^{k-n}) &= \text{tr}(C^k + a_{n-1}C^{k-1} + \cdots + a_0C^{k-n}) \\ &= \text{tr}(C^{k-n}(C^n + a_{n-1}C^{n-1} + \cdots + a_0)) \\ &= \text{tr}(C^{k-n}p(C)) \end{aligned}$$

By the Cayley-Hamilton theorem, $p(C) = 0$, therefore $\text{tr}(C^{k-n}p(C)) = 0$ which completes the proof for the case $k > n$.

Let $1 \leq k \leq n$. Our approach here is a bit different from the previous case and will become clear as we go along. Let $X = xI$, $x \in \mathbb{C}$. Note that, since $p(C) = 0$, we have the following factorization

$$p(X) = (X - C)[X^{n-1} + (C + a_{n-1}I)X^{n-2} + (C^2 + a_{n-1}C + a_{n-2}I)X^{n-3} + \dots + (C^{n-1} + a_{n-1}C^{n-2} + \dots + a_1I)I].$$

To confirm that this factorization indeed holds it suffices to multiply the $(X - C)$ factor into the brackets.

Now, we wish to introduce the trace operation, however, the factor $(X - C)$ complicates matters. Fortunately, we know that $X - C = xI - C$ is non-singular, if we choose x such that it is not an eigenvalue of C . Then, for such an x , we have

$$(X - C)^{-1}p(X) = X^{n-1} + (C + a_{n-1}I)X^{n-2} + (C^2 + a_{n-1}C + a_{n-2}I)X^{n-3} + \dots + (C^{n-1} + a_{n-1}C^{n-2} + \dots + a_1I)I.$$

We now take the trace on both sides and obtain

$$\begin{aligned} \text{tr}[(X - C)^{-1}p(X)] &= nx^{n-1} + \text{tr}(C + a_{n-1}I)x^{n-2} + \dots \\ &\quad + \text{tr}(C^{n-1} + a_{n-1}C^{n-2} + \dots + a_1I), \end{aligned} \tag{D.1}$$

since $\text{tr}(I) = n$ and $\text{tr}(X^k A) = \text{tr}(x^k I A) = x^k \text{tr}(A)$ for any matrix A .

Our next goal is to show that $p'(x) = \text{tr}[(X - C)^{-1}p(X)]$. To that end, let $A = (X - C)^{-1}p(X)$. Observe that $p(X) = p(xI) = p(x)I$, hence $A = p(x)(xI - C)^{-1}$. Therefore,

$$\text{tr}(A) = p(x) \text{tr}[(xI - C)^{-1}].$$

Since the trace is equal to the sum of the eigenvalues and the eigenvalues of $(xI - C)^{-1}$ are $1/(x - \lambda_1), 1/(x - \lambda_2), \dots, 1/(x - \lambda_n)$, we have that

$$\text{tr}(A) = p(x) \left(\frac{1}{x - \lambda_1} + \frac{1}{x - \lambda_2} + \dots + \frac{1}{x - \lambda_n} \right).$$

Using the fact that $p(x) = (x - \lambda_1)(x - \lambda_2) \dots (x - \lambda_n)$, it is immediately clear that $\text{tr}[(X - C)^{-1}p(X)]$ is in fact equal to $p'(x)$, as we wished to show.

Finally, comparing the coefficients of $p'(x)$ with the corresponding coefficients of the right-hand side of (D.1) completes the proof. Indeed, equating the coefficient of x^{n-k-1} in $p'(x)$ with the corresponding coefficient on the right-hand side of (D.1) gives

$$(n - k)a_{n-k} = \text{tr}(C^k + a_{n-1}C^{k-1} + \dots + a_{n-k+1}C + a_{n-k}I)$$

or

$$\text{tr}(C^k + a_{n-1}C^{k-1} + \dots + a_{n-k+1}C) = -ka_{n-k},$$

since $\text{tr}(a_{n-k}I) = na_{n-k}$. This completes the proof for the case $1 \leq k \leq n$, and we are done. \square

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