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Sandwich Theorem and Calculation of the Theta Function for Several Graphs

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SANDWICH THEOREM AND CALCULATION OF THE THETA FUNCTION FOR SEVERAL GRAPHS

by

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of a thesis submitted by

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ABSTRACT

SANDWICH THEOREM AND CALCULATION OF THE
THETA FUNCTION FOR SEVERAL GRAPHS

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This paper includes some basic ideas about the computation of a function $\vartheta(G)$, the theta number of a graph G, which is known as the Lovász number of G. $\vartheta(G^c)$ lies between two hard-to-compute graph numbers $\omega(G)$, the size of the largest clique in a graph G, and $\chi(G)$, the minimum number of colors need to properly color the vertices of G. Lovász and Grötschel called this the "Sandwich Theorem". Donald E. Knuth gives four additional definitions of ϑ, ϑ_1, ϑ_2, ϑ_3, ϑ_4 and proves that they are all equal.

First I am going to describe the proof of the equality of ϑ, ϑ_1 and ϑ_2 and then I will show the calculation of the ϑ function for some specific graphs: K_n, graphs related to K_n, and C_n. This will help us understand the ϑ function, an important function for graph theory. Some of the results are calculated in different ways. This will benefit students who have a basic knowledge of graph theory and want to learn more about the theta function.

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Contents

Terminology

Graph: Given a nonempty finite set V, let $V^{(2)}$ be the set of all 2-element subsets of V. A graph $G = (V, E)$ consists of two things, a nonempty finite set V called the vertices of G and a (possibly empty) subset E of $V^{(2)}$ called the edges of G. Let $n = |V|$ be the number of vertices of G.

When more than one graph is under consideration, it may be useful to write $V(G)$ and $E(G)$ for the vertex and edge sets of G, respectively. We will use the notation of ab instead of $\{a, b\}$ to represent an edge. For example, let C_4 be the graph with 4 vertices, $V = \{1, 2, 3, 4\}$ and $E = \{12, 13, 24, 34\}$, shown in Figure 1.

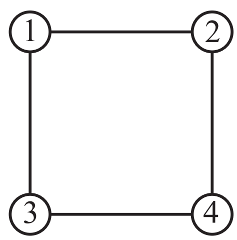


Figure 1: Graph of C_4

Subgraph: A subgraph of a graph G is a graph H such that $V(H) \subseteq V(G)$ and $E(H) \subseteq E(G)$.

Induced subgraph: An induced subgraph of G is a subgraph H such that every edge of G whose vertices are contained in $V(H)$ belongs to $E(H)$.

Complement G^c of G: the graph which has $V(G)$ as its vertex set, and in which two vertices are adjacent if and only if they are *not* adjacent in G. If G has n vertices, then G^c can be constructed by removing from K_n all the edges of G. Note that the complement of a complete graph is a empty graph. An example of a graph and its complement is seen in Figure 2.

Positive definite (positive semidefinite) matrix: a real $n \times n$ symmetric matrix A which satisfies $x^T Ax > 0$ for all $x \in \mathbb{R}^n \setminus \{0\}$ ($x^T Ax \geq 0$ for all $x \in \mathbb{R}^n$).

Negative definite (negative semidefinite) matrix: a real $n \times n$ symmetric matrix A

Figure 2: A graph and its complement

is negative definite if $-A$ is positive definite and is negative semidefinite if $-A$ is positive demidefinite.

Clique: a nonempty set of pairwise adjacent vertices. Some cliques in the graph G in Figure 3 are $\{1, 2\}$, $\{3, 4, 5\}$, and $\{6, 7\}$.

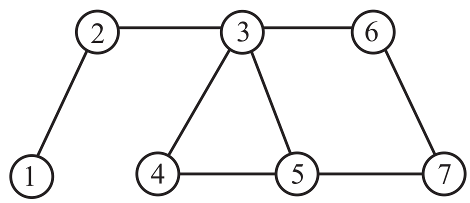


Figure 3: A graph with three large cliques

Clique number: the maximum number of vertices of a clique in a graph. It is denoted by $\omega(G)$. The clique number of G in Figure 3 is 3.

Independent set: a set of pairwise nonadjacent vertices of G. This is also called a *stable set*. Some independent sets of the graph G in Figure 3 are: $V_1 = \{1, 3, 7\}$, $V_2 = \{2, 5, 6\}$, $V_3 = \{1, 4, 6\}$. So, $S \subset V(G)$ is an independent set if and only if no two of its vertices are adjacent, or if and only if S is a clique in G^c.

Independence number, $\alpha(G) = \omega(G^c)$: the maximum number of vertices in an independent set of G.

Chromatic number $\chi(G)$: the minimum number of independent sets that partition $V(G)$. A graph G is m-partite if $V(G)$ can be partitioned into m or fewer independent sets. The independent sets in a specified partition are partite sets. The graph G in Figure 3 has chromatic number 3 and is 3-partite.

Clique cover number: the smallest number of cliques that cover the vertices of G.

It is denoted by $\overline{\chi}(G)$. For example, $\overline{\chi}(G) = 3$ for G in Figure 3. We can also think of it as the minimum number of independent sets that partition $V(G^c)$. It is clear that $\overline{\chi}(G) = \chi(G^c)$.

Perfect graph: a graph G such that each induced subgraph G' of G satisfies $\omega(G') = \chi(G')$. The graph G in Figure 3 is perfect.

Imperfect graph: a graph that is not perfect. The graph C_5 (shown in Figure 4) is an imperfect graph because the clique number is $\omega(G) = 2$ but the chromatic number is $\chi(G) = 3$. It is the only imperfect graph for $n \leq 5$ vertices.

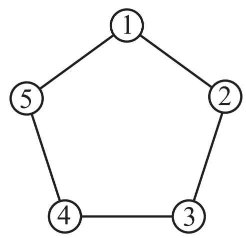


Figure 4: C_5

Dot product: The dot product of (column) vectors a and b is $a \cdot b = a^T b$.

Orthogonal vectors: the vectors $a, b \in \mathbb{R}^n$ are orthogonal if $a \cdot b = 0$.

Orthogonal matrix: a square matrix Q such that $Q^T Q$ is the identity matrix I. In other words, Q is orthogonal if and only if its columns are unit vectors perpendicular to each other.

Symmetric matrix: A matrix A is symmetric if $A = A^T$. For any symmetric matrix A we have that $A = QDQ^T$ where Q is orthogonal and D is a diagonal matrix.

Orthogonal labeling: an assignment of vectors $a_v \in \mathbb{R}^d$ to each vertex v of a graph G such that $a_u \cdot a_v = 0$ for each pair of nonadjacent vertices u and v. In other words, whenever a_u is not perpendicular to a_v in the labeling, we will have u and v adjacent in the graph G.

Convex set: A set in Euclidean space $\mathbb{R}^d$ is a convex set if it contains all the line segments connecting any pair of its points.

Convex hull: Given a set of vectors $S \in \mathbb{R}^n$, the convex hull of S is the smallest convex set containing S.

STAB(G), TH(G) and QSTAB(G)

Definition 1. The *incidence vector* X^S of a set S of vertices of a graph G is defined by

$$X_i^S = \begin{cases} 1 & \text{if } i \in S \\ 0 & \text{if } i \notin S \end{cases}.$$

Typically, S will be a clique or independent set.

Definition 2. Given a graph G, $STAB(G)$ is the convex hull of incidence vectors of all stable sets of G.

Example 1. Consider K_3 (a clique with 3 vertices): the independent sets are $\emptyset$, $\{1\}$, $\{2\}$, $\{3\}$ and the corresponding incidence vectors are

$$\begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}.$$

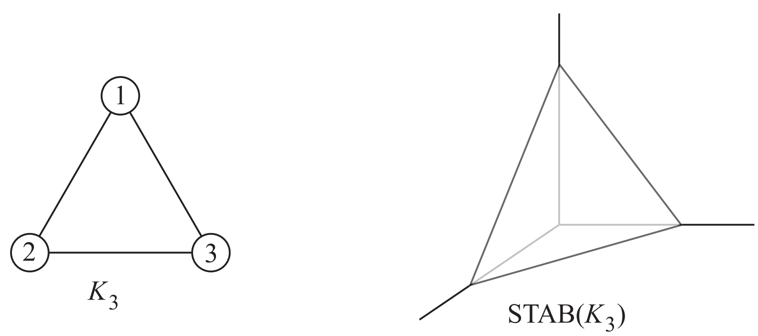


Figure 5: K_3 and STAB(K_3)

Definition 3. QSTAB(G) is the set in $\mathbb{R}^n$ defined by

$$x_i \geq 0 \text{ for each } i \in V, \qquad \sum_{i \in K} x_i \leq 1 \text{ for each clique } K \text{ of } G.$$

It suffices to consider the maximal cliques of G. In the example of K_3, these become $x_1 \geq 0$, $x_2 \geq 0$ and $x_3 \geq 0$, $x_1+x_2+x_3 \leq 1$. It is clear that the last inequality implies $x_1 + x_2 \leq 1$, corresponding to the nonmaximal clique $\{1, 2\}$. For K_3, STAB(K_3)=QSTAB(K_3). These can be seen in Figure 5.

Definition 4. The cost $c(u_i)$ of a vector u_i in an orthogonal labeling of G is defined to be 0 if $u_i = 0$, otherwise

$$c(u_i) = \frac{u_{1i}^2}{\|u_i\|^2} = \frac{u_{1i}^2}{u_{1i}^2 + \ldots + u_{di}^2}.$$

Because $c(u)$ is a homogenous function, we may whenever convenient take all nonzero vectors in an orthogonal labeling to be unit vectors.

Definition 5. Given a graph $G = (V, E)$ on n vertices,

$$\text{TH}(G) = \{x \geq 0 \mid \sum_{i \in V} c(u_i)x_i \leq 1 \text{ for all orthogonal labelings } u \text{ of } G\}.$$

Notice that TH(G) is the intersection of infinitely many halfspaces, so TH(G) is a convex set.

Lemma 1. If S is a stable set in G and u is an orthogonal labeling of G, then $\sum_{i \in S} c(u_i) \leq 1$.

Proof. Let $S = \{i_1, i_2, \ldots, i_k\}$. It suffices to consider the case when $\{u_{i_1}, u_{i_2}, \ldots, u_{i_k}\}$ is a set of k orthonormal vectors. There exists a $d \times d$ orthogonal matrix Q such that the first k columns are $u_{i_1}, u_{i_2}, \ldots, u_{i_k}$. Since the length of the first row of Q is 1,

$$1 \geq u_{1i_1}^2 + u_{1i_2}^2 + \cdots + u_{1i_k}^2 = c(u_{i_1}) + c(u_{i_2}) + \cdots + c(u_{i_k}) = \sum_{i \in S} c(u_i).$$

Hence, $\sum_{i \in S} c(u_i) \leq 1$. □

Lemma 2. STAB(G) ⊆ TH(G) ⊆ QSTAB(G).

Proof. If S is a stable set, X^S is its incidence vector and $\{u_1, u_2, \ldots, u_n\}$ is an orthogonal labeling of G, by the previous lemma,

$$\sum_{i \in V} c(u_i) \cdot X_i^S = \sum_{i \in S} c(u_i) \cdot 1 + \sum_{i \notin S} c(u_i) \cdot 0 \leq 1.$$

Since TH(G) contains each incidence vector, TH(G) contains the convex hull of incidence vectors of stable sets. Therefore, TH(G) ⊇ STAB(G).

For each clique K of G, define the map from V to $\mathbb{R}^1$ by $i \to X_i^K$. If $ij \notin E$, either $i \notin K$ or $j \notin K$. So we know that $X_i^K X_j^K = 0$. So this map is an orthogonal labeling. Therefore, if $x \in \mathrm{TH}(G)$,

$$1 \geq \sum_{i \in V} c(X_i^K) x_i = \sum_{i \in V} X_i^K \cdot x_i = \sum_{i \in K} 1 \cdot x_i + \sum_{i \notin K} 0 \cdot x_i = \sum_{i \in K} x_i,$$

so $x \in$ QSTAB(G). Hence TH(G) $\subseteq$ QSTAB(G). □

1 The Theta Function

Definition 6. Given a graph G, we define

$$\vartheta(G) = \max\{\sum_{i \in V} x_i \mid x \in \mathrm{TH}(G)\}.$$

Similar definitions can be given for STAB and QSTAB:

$$\begin{aligned} \alpha(G) &= \max\{\sum_{i \in V} x_i \mid x \in \mathrm{STAB}(G)\}, \\ \kappa(G) &= \max\{\sum_{i \in V} x_i \mid x \in \mathrm{QSTAB}(G)\}. \end{aligned}$$

First, we need to show that this definition of $\alpha(G)$ is in fact the size of the largest stable set in G.

Let G be a graph with $\alpha(G) = m$. Let S be an independent set of size m and let $X^S = [x_1, x_2, \cdots, x_n]$ be the incidence vector of S. Then,

$$\sum_{i=1}^{n} x_i = m.$$

So,

$$\alpha(G) = m \leq \max\{\sum x_i \mid x \in \mathrm{STAB}(G)\}.$$

For example consider the graph G' shown in Figure 6. For this graph we have, $\alpha(G') = 2$. The incidence vector of the stable set $\{1, 4\}$ is $x = [1, 0, 0, 1]^T \in \mathrm{STAB}(G')$, so we have $\sum_{i=1}^{4} x_i = 2$. It is clear that $2 \leq \max\{\Sigma x_i \mid x \in \mathrm{STAB}(G')\}$. So

$$\alpha(G') \leq \max\{\sum x_i \mid x \in \mathrm{STAB}(G')\}.$$

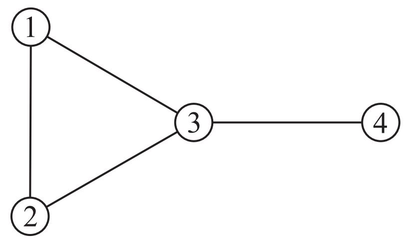


Figure 6: G'

We now prove the reverse inequality.

We know that STAB(G) is convex set. Let $\{X^{S_1}, X^{S_2}, \cdots, X^{S_m}\}$ be the set of incidence vectors of the stable sets of G. Then any vector $x \in \text{STAB}(G)$ is a convex combination of $X^{S_1}, X^{S_2}, \cdots, X^{S_m}$, so

$$x = \sum_{i=1}^{m} a_i X^{S_i}, \text{ where } \sum_{i=1}^{m} a_i = 1 \text{ and } a_i \geq 0 \text{ for } i = 1, 2, \ldots, m.$$

Since $\alpha(G)$ is the maximum number of vertices in an independent set of G, for each vector X^{S_i}, $\alpha(G) \geq \sum_{j=1}^{n} X_j^{S_i}$, so we have,

$$\sum_{j=1}^{n} x_j = \sum_{j=1}^{n} (\sum_{i=1}^{m} a_i X_j^{S_i}) = \sum_{i=1}^{m} a_i \sum_{j=1}^{n} X_j^{S_i} \leq \sum_{i=1}^{m} a_i \cdot \alpha(G) = \alpha(G) \cdot \sum_{i=1}^{m} a_i = \alpha(G),$$

so

$$\alpha(G) \geq \max\{\sum_{i \in V} x_i \mid x \in \text{STAB}(G)\}.$$

Therefore,

$$\alpha(G) = \max\{\sum_{i \in V} x_i \mid x \in \text{STAB}(G)\}.$$

This shows that our two different definitions of $\alpha(G)$ are consistent.

We want to prove the sandwich theorem that we have mentioned at the beginning of the paper which is that for any graph G, $\vartheta(G^c)$ lies between the clique number $\omega(G)$ and the chromatic number $\chi(G)$.

Theorem 1 (Sandwich Theorem). $\omega(G) \leq \vartheta(G^c) \leq \chi(G)$.

Proof. Since $\alpha(G^c) = \omega(G)$ and $\bar{\chi}(G^c) = \chi(G)$, this is equivalent to proving that $\alpha(G^c) \leq \vartheta(G^c) \leq \bar{\chi}(G^c)$ or $\alpha(G) \leq \vartheta(G) \leq \bar{\chi}(G)$.

Since $\vartheta(G) = \max\{\sum_{i\in V} x_i \mid x \in \mathrm{TH}(G)\}$, $\alpha(G) = \max\{\sum_{x\in V} x_i \mid x \in \mathrm{STAB}(G)\}$, and $\mathrm{STAB}(G) \subseteq \mathrm{TH}(G)$, we have $\alpha(G) \leq \vartheta(G)$.

Similarly, since $\mathrm{TH}(G) \subseteq \mathrm{QSTAB}(G)$, we have $\vartheta(G) \leq \kappa(G)$.

Now, we need to show that $\kappa(G) \leq \overline{\chi}(G)$.

Suppose $K_1, \cdots, K_p$ is a smallest set of cliques that cover the vertices of G, and let $x \in \mathrm{QSTAB}(G)$. Then

$$\sum_{i=1}^{n} x_i = \sum_{j=1}^{p} \sum_{i\in K_j} x_i \leq \sum_{j=1}^{p} 1 = p = \overline{\chi}(G).$$

Therefore,

$$\kappa(G) = \max\{\sum_{i\in V} x_i \mid x \in \mathrm{QSTAB}(G)\} \leq \overline{\chi}(G).$$

Combining, we have $\alpha(G) \leq \vartheta(G) \leq \kappa(G) \leq \overline{\chi}(G)$, which completes the proof. $\square$

For example, consider the cyclic graph C_5 in Figure 4 with vertices $\{1, 2, 3, 4, 5\}$. For $x \in \mathrm{QSTAB}(G)$, $x_1 + x_2 \leq 1$, $x_2 + x_3 \leq 1$, $x_3 + x_4 \leq 1$, $x_4 + x_5 \leq 1$, $x_5 + x_1 \leq 1$. Then $2(x_1+x_2+x_3+x_4+x_5) \leq 5$. Hence $\kappa(C_5) \leq \frac{5}{2}$. Since $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}) \in \mathrm{QSTAB}(C_5), \kappa(C_5) = \frac{5}{2}$. But $\overline{\chi}(C_5) = 3 > \kappa(C_5)$.

Corollary 1. If G is a perfect graph, then $\vartheta(G) = \alpha(G)$.

Proof. By the Perfect Graph Theorem, G^c is a perfect graph. Therefore, we have $\omega(G^c) = \chi(G^c)$.

By the Sandwich Theorem, $\omega(G^c) \leq \vartheta(G) \leq \chi(G^c)$, so $\vartheta(G) = \omega(G^c)$. Since $\alpha(G) = \omega(G^c)$, therefore $\vartheta(G) = \alpha(G)$. $\square$

2 Two Additional Functions $\vartheta_1(G)$ and $\vartheta_2(G)$

We have just shown that $\vartheta(G)$ lies between $\overline{\chi}(G)$ and $\alpha(G)$. In this part, we are going to introduce the other two functions $\vartheta_1(G)$ and $\vartheta_2(G)$. They are different ways of defining $\vartheta(G)$. This will not only help us to understand $\vartheta(G)$ but also help us to compute $\vartheta(G)$. We will prove that $\vartheta(G) \leq \vartheta_1(G) \leq \vartheta_2(G)$. In [3], Donald Knuth introduced two additional functions ϑ_3, ϑ_4 in order to prove $\vartheta_2 \leq \vartheta$. Therefore $\vartheta, \vartheta_1, \vartheta_2$ are all equivalent.

2.1 The $\vartheta_1(G)$ function

If G is a graph,

$$\vartheta_1(G) = \min_a \left(\max_v (1/c(a_v)) \right), \text{ over all orthogonal labelings } a.$$

The max is ∞ if there is some v such that $c(a_v) = 0$.

Lemma 3. $\vartheta(G) \leq \vartheta_1(G)$.

Proof. If G is a graph, suppose $x \in \mathrm{TH}(G)$ and a is an orthogonal labeling of G. Then

$$\begin{aligned}
\vartheta(G) &= \max\{\sum_v x_v \mid x \in \mathrm{TH}(G)\} \\
&= \max\{\sum_v \frac{1}{c(a_v)} \cdot c(a_v) \cdot x_v \mid x \in \mathrm{TH}(G)\} \\
&\leq \max_v \frac{1}{c(a_v)} \max\{\sum_v c(a_v) \cdot x_v \mid x \in \mathrm{TH}(G)\}.
\end{aligned}$$

By the definition of $\mathrm{TH}(G)$, $\sum_v c(a_v) x_v \leq 1$. Therefore,

$$\vartheta(G) \leq \max_v \frac{1}{c(a_v)} \cdot 1.$$

Since this inequality holds for each orthogonal labeling,

$$\vartheta(G) \leq \min_a \left(\max_v \frac{1}{c(a_v)} \right) = \vartheta_1(G).$$

□

2.2 The $\vartheta_2(G)$ function

Definition 7. Matrix A is a *feasible matrix* for the graph G if A is indexed by the vertices of G and

(i) A is real and symmetric,

(ii) $a_{ii} = 1$, for all $i \in V$,

(iii) $a_{ij} = 1$, whenever i and j are nonadjacent in G.

The rank 1 matrix

$$A_0 = [1, 1, \cdots, 1]^T [1, 1, \cdots, 1] \text{ is feasible for any graph } G$$

and has one nonzero eigenvalue

$$\lambda_1(A_0) = \mathrm{tr}(A) = \sum_{i=1}^{n} 1 = n.$$

If A is any real symmetric matrix which has eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$, by the Spectral Theorem, $A = QDQ^T$ for some orthogonal matrix Q and diagonal matrix D where $D = \mathrm{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$. Since all the eigenvalues of A are real, by the Rayleigh-Ritz Theorem, A has the maximum eigenvalue,

$$\lambda_1(A) = \max\{x^T A x \mid \|x\|_2 = 1,\ x \in \mathbb{R}^n\}$$

Lemma 4. The set of feasible A with $\lambda_1(A) \leq n$ is compact.

Proof. Starting with

$$\lambda_1(A) + \lambda_2(A) + \cdots + \lambda_n(A) = n,$$

we use what we know about the ordering to get

$$(n-1)\lambda_1(A) + \lambda_n(A) \geq n \quad \text{so} \quad (n-1)n + \lambda_n(A) \geq n.$$

In particular, we have that

$$\lambda_n(A) \geq -(n-2)n \quad \text{so that} \quad -(n-2)n \leq \lambda_i(A) \leq n \quad \text{for} \quad i = 1, \cdots, n.$$

This shows that $\lambda_i^2(A) \leq n^2(n-2)^2$ and so

$$\sum_{i,j=1}^{n} |a_{ij}|^2 = \sum_{i=1}^{n} \lambda_i^2(A) \leq n^3(n-2)^2.$$

Therefore, the set is bounded. The set is clearly closed, so it is compact. $\square$

From Lemma 4 and the fact that $\lambda_1(A)$ is a continuous function of the entries of A, we know that the minimum value of $\lambda_1(A)$ exists.

Definition 8. Given a graph G, then

$$\vartheta_2(G) = \min\{\lambda_1(A) \mid A \text{ is a feasible matrix for } G\}.$$

Lemma 5. $\vartheta_1(G) \leq \vartheta_2(G)$.

Proof. Let A be a feasible matrix such that $\vartheta_2(G) = \lambda_1 \geq 0$ and let $B = \lambda_1 I - A$. Let $\lambda_2 \geq \lambda_3 \geq \cdots \geq \lambda_n$ be the remaining eigenvalues of A.

The eigenvalues of B are $\lambda_1 - \lambda_i$. It is clear that all the eigenvalues of B are nonnegative, so B is positive semidefinite.

If

$$A = Q \begin{bmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_n \end{bmatrix} Q^T$$

then

$$\begin{aligned} B &= Q \begin{bmatrix} \lambda_1 - \lambda_1 & & & \\ & \lambda_1 - \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_1 - \lambda_n \end{bmatrix} Q^T \\ &= Q \begin{bmatrix} (\sqrt{\lambda_1 - \lambda_1})^2 & & & \\ & (\sqrt{\lambda_1 - \lambda_2})^2 & & \\ & & \ddots & \\ & & & (\sqrt{\lambda_1 - \lambda_n})^2 \end{bmatrix} Q^T \\ &= X^T X, \end{aligned}$$

where

$$X = Q \begin{bmatrix} \sqrt{\lambda_1 - \lambda_1} & & & \\ & \sqrt{\lambda_1 - \lambda_2} & & \\ & & \ddots & \\ & & & \sqrt{\lambda_1 - \lambda_n} \end{bmatrix} Q^T.$$

Let $X = [x_1, x_2, \cdots, x_n]$ (i.e., the x_i are the columns of X), so that we have $b_{ij} = x_i^T x_j$.

Let $u_i = \begin{bmatrix} 1 \\ x_i \end{bmatrix} \in \mathbb{R}^{n+1}, \ x_i \in \mathbb{R}^n$.

If $i \neq j$ and ij is not in E,

$$u_i \cdot u_j = 1 + x_i^T x_j = 1 + b_{ij} = a_{ij} + b_{ij}.$$

Since $B = \lambda_1 I - A$, we have $b_{ij} = -a_{ij}$, so $u_i \cdot u_j = a_{ij} - a_{ij} = 0$.

Therefore,

$$u_1, u_2, \cdots, u_n \text{ is an orthogonal labeling of } G.$$

Note that appealing to the definition of cost that

$$c(u_i) = \frac{1}{1 + \|x_i\|^2}.$$

So for each $i = 1, 2, \cdots, n$,

$$\frac{1}{c(u_i)} = 1 + \|x_i\|^2 = 1 + x_i \cdot x_i = 1 + b_{ii} = a_{ii} + \lambda_1 - a_{ii} = \lambda_1.$$

This implies

$$\lambda_1 = \max_{i \in v} \frac{1}{c(u_i)}.$$

Hence,

$$\vartheta_1(G) = \min_a \max_i \left(\frac{1}{c(a_i)} \right) \leq \max_i \frac{1}{c(u_i)} = \lambda_1 = \vartheta_2(G).$$

This completes the proof. □

In [3], Donald E. Knuth has proved that $\vartheta_2(G) \leq \vartheta(G)$ by proving $\vartheta_2(G) \leq \vartheta_3(G) \leq \vartheta_4(G) \leq \vartheta(G)$. So, we can conclude that $\vartheta(G) = \vartheta_2(G)$.

3 $\vartheta_2(G)$ and K_n

Now we are going to use $\vartheta_2(G)$ to calculate $\vartheta(G)$ for the two simplest graphs, K_n and K_n^c.

3.1 $\vartheta_2(K_n)$ and $\vartheta_2(K_n^c)$

Lemma 6. $\vartheta(K_n) = \vartheta_2(K_n) = 1$.

Consider the graph K_n. We know that K_n is a perfect graph. By the Sandwich Theorem, $\vartheta(K_n) = \alpha(K_n) = 1$.

We also obtain this conclusion in two different ways.

There are no missing edges in the graph K_n, so any set of n vectors is an orthogonal labeling. Let $u_i = [\sqrt{a}, \sqrt{b}]^T$ for $i = 1, 2, \ldots, n$, then $c(u_i) = a/(a+b)$. Now consider the following,

$$\sum c(u_i) \cdot x_i = \sum \frac{a}{a+b} \cdot x_i \leq 1, \quad \text{rearranging we get} \quad \sum x_i \leq 1 + \frac{b}{a}.$$

From this last statement, it is clear that if we let $b = 0$ then $\sum x_i \leq 1$. It follows that

$$\mathrm{TH}(K_n) = \{x \geq 0 \,|\, \sum x_i \leq 1\}.$$

Therefore,

$$\vartheta(K_n) = \max\{\sum_{i \in V} x_i \,|\, x \in \mathrm{TH}(K_n)\} = \max\{\sum_{i \in V} x_i \,|\, \sum x_i \leq 1, \forall x \geq 0\} = 1.$$

We should get the same result if we look at $\vartheta_2(K_n)$.

Let A_n be the feasible matrix of K_n, and let λ_1 be the maximum eigenvalue of A_n, then the matrix A_n has the form

$$A_n = \begin{bmatrix} 1 & x_{12} & \cdots & x_{1(n-1)} & x_{1n} \\ x_{12} & 1 & \cdots & x_{2(n-1)} & x_{2n} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ x_{1(n-1)} & x_{2(n-1)} & \cdots & 1 & x_{(n-1)n} \\ x_{1n} & x_{2n} & \cdots & x_{(n-1)n} & 1 \end{bmatrix}.$$

Since for any graph G

$$n\lambda_1 = \lambda_1 + \lambda_1 + \cdots + \lambda_1 \geq \lambda_1 + \lambda_2 + \cdots + \lambda_n = \mathrm{tr}A_n = n,$$

we have that $\lambda_1 \geq 1$. On the other hand, A_n becomes I when $x_{ij} = 0$ for any $i \neq j$, and in that case $\lambda_1 = 1$.

So $\vartheta_2(K_n) = \min \lambda_1 = 1$.

Lemma 7. $\vartheta_2(K_n^c) = n$.

The graph of K_n^c is very simple. It just contains n vertices without any edges, which means there are no pairwise adjacent vertices. Since K_n^c is a perfect graph, by the Sandwich Theorem, $\vartheta(K_n^c) = \alpha(K_n^c) = n$.

We can also see this result very easily from the definition of the ϑ_2 function. Since the feasible matrix A_n of K_n^c is a $n \times n$ matrix with all the entries equal to 1, the rank of A_n is 1. Therefore, there is only one nonzero eigenvalue and it equals $\mathrm{tr}(A_n)$ which is n. Hence $\vartheta(K_n^c) = \vartheta_2(K_n^c) = n$.

3.2 $\vartheta_2(G)$ for complete multipartite graphs

Definition 9. The *union* of graphs G and H with $V(G) \cap V(H) = \emptyset$, written $G \cup H$, has vertex set $V(G) \cup V(H)$ and edge set $E(G) \cup E(H)$.

Similarly, the *join* of graphs G and H with $V(G) \cap V(H) = \emptyset$, written $G \vee H$, is obtained from $G \cup H$ by adding the edges $\{xy : x \in V(G), y \in V(H)\}$.

Let $G = K_{n_1,n_2,\ldots,n_k}$ be a complete multipartite graph, then

$$\begin{aligned} K_{n_1,n_2,\cdots,n_k} &= (K_{n_1} \cup K_{n_2} \cup \cdots \cup K_{n_k})^c \\ &= K_{n_1}^c \vee K_{n_2}^c \vee \cdots \vee K_{n_k}^c. \end{aligned}$$

For example, in Figure 7 we have the union and the join of the two graphs P_3 and K_3. The bold edge in the join indicates that we join all vertices between these two sets.

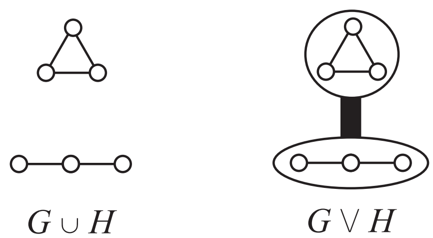


Figure 7:

Lemma 8. $\vartheta(K_{n_1,n_2,\cdots,n_k}) = \max\{n_1, n_2, \cdots, n_k\}$.

We will prove this lemma in two different ways.

Proof. For our first proof, consider the following.

First, let $G = K_{n_1,n_2,\cdots,n_k}$. We show that G is a perfect graph. This follows since,

$$\omega(K_{n_1} \cup K_{n_2} \cup \cdots \cup K_{n_k}) = \max\{n_1, n_2, \cdots, n_k\} = \chi(K_{n_1} \cup K_{n_2} \cup \cdots \cup K_{n_k}),$$

with a similar equality for each induced subgraph. So $K_{n_1} \cup K_{n_2} \cup \cdots \cup K_{n_k}$ is a perfect graph. By the Perfect Graph Theorem, a graph is perfect if and only if its complement is perfect. Therefore, $K_{n_1,n_2,\cdots,n_k} = (K_{n_1} \cup K_{n_2} \cup \cdots \cup K_{n_n})^c$ is perfect. So by Corollary 1,

$$\vartheta(K_{n_1,n_2,\cdots,n_k}) = \alpha(K_{n_1,n_2,\cdots,n_k}) = \omega(K_{n_1} \cup K_{n_2} \cup \cdots \cup K_{n_k}) = \max\{n_1, n_2, \cdots, n_k\}.$$

$\square$

Before we use the second method of proving the lemma, we need to state a useful result.

Theorem 2 (Interlacing Inequalities). *Let $A \in M_n$ be Hermitian and for any $i \in N$, let $A(i)$ be the principal submatrix obtained from A by deleting the i^{th} row and column. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ be the eigenvalues of A and $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_{n-1}$ be the eigenvalues of $A(i)$, then*

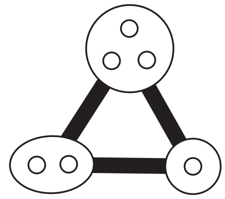
$$\lambda_1 \geq \mu_1 \geq \lambda_2 \geq \mu_2 \geq \lambda_3 \geq \mu_3 \cdots \geq \lambda_{n-1} \geq \mu_{n-1} \geq \lambda_n.$$

Corollary 2. Let $A \in M_n$ be a Hermitian matrix and $B \in M_m$ be any principal submatrix of A, then $\lambda_k(A) \geq \lambda_k(B),\ k = 1, 2, \cdots, m.$

Now we are ready prove Lemma 8 by using the definition of the ϑ_2 function. First, consider an example, namely let $G = K_{3,2,1} = (K_3 \cup K_2 \cup K_1)^c$. This graph is shown in Figure 8.

Let A be a feasible matrix of $K_{3,2,1}$. Then A has the form

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



$K_{3,2,1} = (K_3 \cup K_2 \cup K_1)^c$

Figure 8:

where the remaining entries are any real numbers for which A is symmetric. There are three blocks in A, they are A_3, A_2, A_1, the feasible matrices for K_3^c, K_2^c and K_1^c. The eigenvalues for these matrices are:

$$\lambda(A_3) = 3, 0, 0; \qquad \lambda(A_2) = 2, 0; \qquad \lambda(A_1) = 1.$$

Let λ_1 be the maximum eigenvalue of A. Then by Corollary 2,

$$\vartheta_2(K_{3,2,1}) = \lambda_1 \geq \max\{\lambda_1(A_3), \lambda_1(A_2), \lambda_1(A_1)\} = 3.$$

However if we set all remaining entries in A equal to 0, $A = A_3 \oplus A_2 \oplus A_1$ which has eigenvalues $3, 0, 0, 2, 0, 1$ and so $\lambda_1 = 3$. Therefore $\vartheta_2(K_{3,2,1}) = 3$.

We are now ready to generalize this for the proof of Lemma 8.

Proof. For our second proof, consider the following.

Consider the feasible matrix A_n of the graph $G = K_{n_1,n_2,\cdots,n_k}$. Then

$$A_n = \begin{bmatrix} J_{n_1} & & & \\ & J_{n_2} & & \\ & & \ddots & \\ & & & J_{n_k} \end{bmatrix},$$

where all the off diagonal entries are some real numbers which preserve symmetry and J_{n_i} are the feasible matrices for $K_{n_i}^c$, so all the entries equal 1. Let λ_1 be the maximum eigenvalue. By Corollary 2, $\lambda_1(A_n) \geq \lambda_1(J_{n_i})$ for $i = 1, 2, \cdots, k$. Since the eigenvalues of the matrix J_{n_i} are n_i and 0, $\lambda_1(J_{n_i}) = n_i$. Therefore $\lambda_1(K_{n_1,n_2,\cdots,n_k}) \geq \max\{n_1, n_2, \cdots, n_k\}$. Equality holds when all the off diagonal entries of A_n equal 0 which reaches the minimum value of λ_1. Hence $\vartheta_2(K_{n_1,n_2,\cdots,n_k}) = \max\{n_1, n_2, \cdots, n_k\}$. $\square$

3.3 $\vartheta_2(G)$ for the union of two complete graphs

We have proved earlier that $\vartheta(K_n) = 1$ (Lemma 6). Now we want to show the calculation of the ϑ function for the union of two complete graphs.

Lemma 9. $\vartheta(K_n \cup K_m) = 2$.

Proof. Let $G = K_m \cup K_n$, and A, A_m and A_n be feasible matrices of G, K_m, and K_n respectively. Let $\lambda_1(A), \lambda_1(A_m), \lambda_1(A_n)$ represent the maximum eigenvalues of each matrix. Then A_m is a $m \times m$ symmetric matrix with all the diagonal entries equal 1 and all the off diagonal entries are real numbers. Similarly, A_n is a $n \times n$ symmetric matrix with all the diagonal entries equal 1 and all the off diagonal entries are real numbers. So A has the form

$$A = \begin{bmatrix} A_n & 1 \\ 1 & A_m \end{bmatrix}.$$

Now suppose each off diagonal entry in A_n and A_m equals x and define

$$B = A + (x-1)I.$$

Then we will obtain an $(m+n) \times (m+n)$ symmetric matrix

$$\left[\begin{array}{c|c} x & 1 \\ \hline 1 & x \end{array}\right].$$

Since the rank of B is at most two, we have at most two nonzero eigenvalues. So, at least $(m+n-2)$ eigenvalues are zero. The characteristic polynomial for B is

$$t^{m+n} - (m+n)xt^{m+n-1} + mn(x^2-1)t^{m+n-2}.$$

Using the quadratic formula to solve for the possible nonzero eigenvalues we find they are

$$t = \frac{(m+n)x \pm \sqrt{(m-n)^2x^2 + 4mn}}{2}.$$

Hence the eigenvalues of B are:

$$\frac{(m+n)x \pm \sqrt{(m-n)^2x^2 + 4mn}}{2}, \text{ and } 0 \text{ with multiplicity } m+n-2.$$

It follows that the eigenvalues of A are $\lambda(B) - (x-1)$:

$$\frac{(m+n)x \pm \sqrt{(m-n)^2x^2 + 4mn}}{2} - (x-1), \text{ and } -(x-1) \text{ with multiplicity } m+n-2.$$

When $x = -1$ the eigenvalues are 0, $-(m+n)$ and 2. We have the largest eigenvalue $\lambda_1 = 2$. This shows $\vartheta_2(K_n \cup K_m) \leq 2$. By the Sandwich Theorem, $\vartheta(K_n \cup K_m) \geq \alpha(K_n \cup K_m) = 2$, therefore, $\vartheta(K_n \cup K_m) = 2$. $\square$

4 $\vartheta_2(G)$ and C_n

In this part, we are going to utilize the $\vartheta_2(G)$ function to find $\vartheta(G)$ for the n-cycle, C_n, which is an imperfect graph for each odd integer greater than three.

First we will illustrate how to use ϑ_2 to calculate $\vartheta(C_5)$.

We first need to prove one important fact. Given a symmetric matrix A, let $\lambda_1(A)$ denote the maximum eigenvalue of A.

Lemma 10. Let $A_i, i = 1, 2, \cdots, k$ be symmetric matrices. Then

$$\lambda_1\left(\sum_{i=1}^{k} A_i\right) \leq \sum_{i=1}^{k} \lambda_1(A_i).$$

Proof. Let A and B be symmetric matrices.

By the Rayleigh-Ritz theorem

$$\lambda_1(A) = \max_{x \neq 0} \frac{x^TAx}{x^Tx}, \ \lambda_1(B) = \max_{x \neq 0} \frac{x^TBx}{x^Tx}.$$

Since

$$\frac{x^T(A+B)x}{x^Tx} = \frac{x^TAx}{x^Tx} + \frac{x^TBx}{x^Tx} \leq \max_{x \neq 0} \frac{x^TAx}{x^Tx} + \max_{x \neq 0} \frac{x^TBx}{x^Tx} = \lambda_1(A) + \lambda_1(B),$$

we have

$$\lambda_1(A+B) = \max_{x \neq 0} \frac{x^T(A+B)x}{x^Tx} \leq \lambda_1(A) + \lambda_1(B).$$

The result follows by mathematical induction. $\square$

Notice that the Lemma is false if A is not a symmetric matrix. For example, if $A = \begin{bmatrix} 0 & \frac{1}{m} \\ m & 0 \end{bmatrix}$ and $B = \begin{bmatrix} 0 & m \\ \frac{1}{m} & 0 \end{bmatrix}$, then the eigenvalues of A and B are 1 and -1. Then $\lambda_1(A) + \lambda_1(B) = 2$, but $A + B = \begin{bmatrix} 0 & m + \frac{1}{m} \\ m + \frac{1}{m} & 0 \end{bmatrix}$, and the eigenvalues of $A + B$ are $m + \frac{1}{m}, -(m + \frac{1}{m})$. It is clear that $m + \frac{1}{m} > 2$ for any $m > 0$ but $m \neq 1$.

Now we compute $\vartheta_2(C_5)$. Consider the graph $G = C_5$ with $V = \{1, 2, 3, 4, 5\}$, $E = \{x_1, x_2, x_3, x_4, x_5\}$. The relationship of the vertices with the edges is shown in Figure 9.

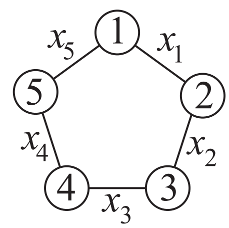


Figure 9:

The feasible matrix for C_5 is:

$$A_1 = \begin{bmatrix} 1 & x_1 & 1 & 1 & x_5 \\ x_1 & 1 & x_2 & 1 & 1 \\ 1 & x_2 & 1 & x_3 & 1 \\ 1 & 1 & x_3 & 1 & x_4 \\ x_5 & 1 & 1 & x_4 & 1 \end{bmatrix}$$

where now x_1, x_2, x_3, x_4, x_5 represent real numbers. We want to show that the minimum value of λ_1 occurs when $x_1 = x_2 = x_3 = x_4 = x_5$. To do this consider the matrix P where,

$$P = \begin{bmatrix} 0 & 1 & & & \\ & 0 & 1 & & \\ & & 0 & 1 & \\ & & & 0 & 1 \\ 1 & & & & 0 \end{bmatrix},$$

i.e., P is a permutation matrix. Now define

$$A_2 = P^T A P = \begin{bmatrix} 1 & x_5 & 1 & 1 & x_4 \\ x_5 & 1 & x_1 & 1 & 1 \\ 1 & x_1 & 1 & x_2 & 1 \\ 1 & 1 & x_2 & 1 & x_3 \\ x_4 & 1 & 1 & x_3 & 1 \end{bmatrix}.$$

We may view the action of P as rotating each vertex of the graph C_5 one position counterclockwise, or equivalently, each edge one position clockwise. This is seen in Figure 10.

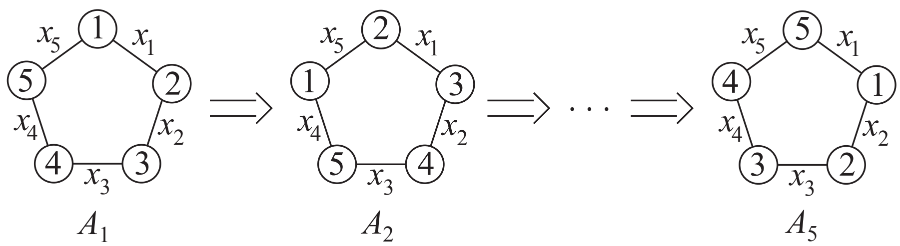


Figure 10:

We similarly define $A_3 = (P^2)^T AP^2$, $A_4 = (P^3)^T AP^3$ and $A_5 = (P^5)^T AP^5$,

$$A_3 = \begin{bmatrix} 1 & x_4 & 1 & 1 & x_3 \\ x_4 & 1 & x_5 & 1 & 1 \\ 1 & x_5 & 1 & x_1 & 1 \\ 1 & 1 & x_1 & 1 & x_2 \\ x_3 & 1 & 1 & x_2 & 1 \end{bmatrix}, \qquad A_4 = \begin{bmatrix} 1 & x_3 & 1 & 1 & x_2 \\ x_3 & 1 & x_4 & 1 & 1 \\ 1 & x_4 & 1 & x_5 & 1 \\ 1 & 1 & x_5 & 1 & x_1 \\ x_2 & 1 & 1 & x_1 & 1 \end{bmatrix}$$

$$A_5 = \begin{bmatrix} 1 & x_2 & 1 & 1 & x_1 \\ x_2 & 1 & x_3 & 1 & 1 \\ 1 & x_3 & 1 & x_4 & 1 \\ 1 & 1 & x_4 & 1 & x_5 \\ x_1 & 1 & 1 & x_5 & 1 \end{bmatrix}.$$

Since A_1, A_2, A_3, A_4 and A_5 are similar, they have the same eigenvalues. Now let

$$A_0 = \frac{1}{5}(A_1 + A_2 + A_3 + A_4 + A_5) = \begin{bmatrix} 1 & x & 1 & 1 & x \\ x & 1 & x & 1 & 1 \\ 1 & x & 1 & x & 1 \\ 1 & 1 & x & 1 & x \\ x & 1 & 1 & x & 1 \end{bmatrix}$$

where $x = \frac{1}{5}(x_1 + x_2 + x_3 + x_4 + x_5)$. By Lemma 10 we have

$$\begin{aligned} \lambda_1(A_0) &= \lambda_1[\frac{1}{5}(A_1 + A_2 + A_3 + A_4 + A_5)] \\ &\le \lambda_1(\frac{1}{5}A_1) + \lambda_1(\frac{1}{5}A_2) + \lambda_1(\frac{1}{5}A_3) + \lambda_1(\frac{1}{5}A_4) + \lambda_1(\frac{1}{5}A_5) \\ &= \frac{1}{5}[\lambda_1(A_1) + \lambda_1(A_2) + \lambda_1(A_3) + \lambda_1(A_4) + \lambda_1(A_5)] \\ &= \lambda_1(A_1). \end{aligned}$$

Therefore, the minimum eigenvalue λ_1 occurs at A_0, which means when $x_1 = x_2 = x_3 = x_4 = x_5$.

I used Maple to compute the eigenvalues of A_0 as follows:

$$3 + 2x, \quad (-\tfrac{1}{2} + \tfrac{1}{2}\sqrt{5})(-1 + x), \quad (-\tfrac{1}{2} - \tfrac{1}{2}\sqrt{5})(-1 + x),$$
$$(-\tfrac{1}{2} + \tfrac{1}{2}\sqrt{5})(-1 + x), \quad (-\tfrac{1}{2} - \tfrac{1}{2}\sqrt{5})(-1 + x).$$

Notice that there are only three distinct eigenvalues, namely,

$$\lambda_{11} = 3 + 2x,\ \ \lambda_{12} = (-\frac{1}{2} + \frac{1}{2}\sqrt{5})(-1 + x),\ \ \lambda_{13} = (-\frac{1}{2} - \frac{1}{2}\sqrt{5})(-1 + x).$$

We know that $\vartheta_2(C_5) = \min \lambda_1$ over all feasible matrices. Figure 11 shows plots of the lines λ_{11}, λ_{12}, λ_{13} as functions of x.

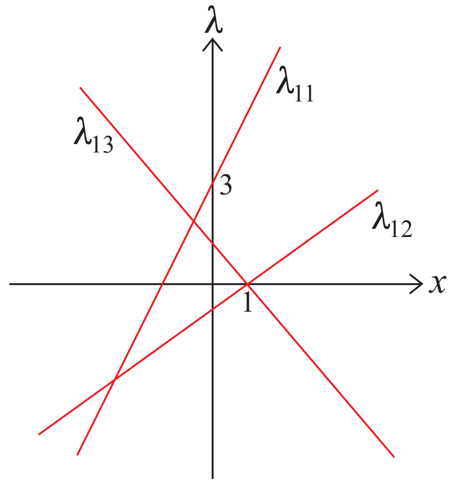


Figure 11:

From the graph (Figure 11) we see that the minimum λ_1 occurs at the intersection of λ_{11} and λ_{13}, which occurs at $x = (-3 + \sqrt{5})/2$, and gives $\lambda_1 = \sqrt{5}$.

Therefore, $\vartheta_2(C_5) = \min \lambda_1(A) = \sqrt{5}$. Since $C_5^c = C_5$, the Sandwich Theorem says that $\omega(C_5) \leq \vartheta(C_5) \leq \chi(C_5)$ which is $2 < \sqrt{5} < 3$. This is our first example of the sandwich theorem in which the inequalities are strict.

Now, we will look at another important property of the ϑ_2 function which enables us to compute $\vartheta_2(C_n)$.

First, we need to introduce some related definitions and prove one lemma.

Definition 10. Let $G = (V, E)$ be a graph with vertex set $V = \{1, 2, 3, \cdots, n\}$. The n-by-n *adjacency matrix* $A_n(G) = (a_{ij})$ is defined by

$$a_{ij} = \begin{cases} 1 & \text{if } ij \in E. \\ 0 & \text{otherwise.} \end{cases}$$

Definition 11. The *eigenvalues* of a graph are the eigenvalues of its adjacency matrix.

Lemma 11. Let A_n be the adjacency matrix of C_n. Then the eigenvalues for A_n are

$$\lambda_j = 2\cos\frac{2\pi j}{n}, \quad j = 0, 1, \ldots, n-1.$$

Proof. Assume the vertices of C_n are labeled 1 through n. Then the adjacency matrix A_n of C_n is

$$A_n = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 & 1 \\ 1 & 0 & 1 & \cdots & 0 & 0 \\ 0 & 1 & 0 & \ddots & 0 & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & \ddots & 0 & 1 \\ 1 & 0 & 0 & \cdots & 1 & 0 \end{bmatrix}.$$

Assume λ is an eigenvalue of A_n and $x = [x_1, x_2, \ldots, x_n]^T$ is a corresponding eigenvector. The equation $Ax = \lambda x$ written in components is

$$x_n + x_2 = \lambda x_1$$

$$x_1 + x_3 = \lambda x_2$$

$$x_2 + x_4 = \lambda x_3$$

$$\vdots$$

$$x_{n-1} + x_1 = \lambda x_n$$

We can rewrite this as a single equation

$$x_{k-1} + x_{k+1} = \lambda x_k \tag{1}$$

with boundary conditions $x_1 = x_{n+1}$ and $x_0 = x_n$.

This is a second degree linear difference equation with constant coefficients. For a difference equation, the fundamental solutions have the form r^k, $r \neq 0$.

Let $x_k = r^k$ in equation (1). Then we have $r^{k-1} + r^{k+1} = \lambda r^k$. Dividing by r^{k-1}, we have $r^2 - \lambda r + 1 = 0$. Let r_1, r_2 be the two roots of this equation. Then

$$r_1 + r_2 = \lambda, \qquad r_1 \cdot r_2 = 1.$$

First assume that $r_1 = r_2$. So $r_1 = r_2 = 1$ or $r_1 = r_2 = -1$.

Consider $r_1 = r_2 = 1$, then $\lambda = 2$. The solution for equation (1) is $x_k = 1^k = 1$. Also $x_k = k \cdot 1^k = k$ is a solution since

$$x_{k-1} + x_{k+1} - \lambda x_k = (k-1) + (k+1) - 2k = 0.$$

So if $r_1 = r_2 = 1$, the general solution for equation (1) is $x_k = c_1 + c_2 \cdot k$. From the boundary conditions we have

$$c_1 = c_1 + nc_2 \qquad \text{and} \qquad c_1 + c_2 = c_1 + (n+1)c_2.$$

Therefore $c_2 = 0$. Hence $x_1 = x_2 = \cdots = x_n = c_1$, i.e., $c_1[1, 1, \ldots, 1]^T$ is an eigenvector corresponding to $\lambda = 2$.

Similarly, if $r_1 = r_2 = -1$, $\lambda = -2$, the solutions for the equation (1) are $x_k = (-1)^k$ and $x_k = k \cdot (-1)^k$. The general solution for equation (1) is also

$$x_k = c_1(-1)^k + c_2 \cdot k(-1)^k.$$

From the boundary conditions we have

$$x = c_1[-1, 1, -1, 1, \cdots, 1]^T \text{ if } n \text{ is even, and } x = 0 \text{ if } n \text{ is odd.}$$

So $\lambda = -2$ is an eigenvalue if n is even.

Now we assume that $r_1 \neq r_2$. Then the general solution for equation (1) is

$$x_k = c_1 r_1^k + c_2 r_2^k.$$

From the boundary conditions we have

$$c_1 + c_2 = c_1 r_1^n + c_2 r_2^n \quad \text{and} \quad c_1 r_1 + c_2 r_2 = c_1 r_1^{n+1} + c_2 r_2^{n+1}.$$

Equivalently,

$$c_1(1 - r_1^n) + c_2(1 - r_2^n) = 0 \quad \text{and} \quad c_1 r_1(1 - r_1^n) + c_2 r_2(1 - r_2^n) = 0. \tag{2}$$

From equation (2) we have

$$\begin{bmatrix} 1-r_1^n & 1-r_2^n \\ r_1(1-r_1^n) & r_2(1-r_2^n) \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = 0.$$

Since $[c_1, c_2]^T$ is nonzero, therefore $B = \begin{bmatrix} 1-r_1^n & 1-r_2^n \\ r_1(1-r_1^n) & r_2(1-r_2^n) \end{bmatrix}$ is a singular matrix, which means $\det(B) = 0$. That is,

$$(1-r_1^n)r_2(1-r_2^n) - (1-r_2^n)r_1(1-r_1^n) = 0,$$

so,

$$(1-r_1^n)(1-r_2^n)(r_2-r_1) = 0.$$

For $r_1^n = 1$, $r_1 = e^{\frac{2\pi i j}{n}}$, $j = 0, 1, \ldots, n-1$. Then $r_2 = \frac{1}{r_1} = e^{\frac{-2\pi i j}{n}}$ which gives possible eigenvalues

$$\begin{aligned} \lambda_j &= r_1 + r_2 \\ &= e^{\frac{2\pi i j}{n}} + e^{\frac{-2\pi i j}{n}} \\ &= 2\cos\frac{2\pi j}{n},\ j = 0, 1, \ldots, n-1. \end{aligned}$$

For $r_2^n = 1$, we obtain the same result.

Now we see the only solutions are

$$\lambda_j = 2\cos\frac{2\pi j}{n},\ \text{for } j = 0, 1, \ldots, n-1.$$

Note that $j = 0$ gives the solution for the case $r_1 = r_2 = 1$ and when n is even, $j = n/2$ gives the solution for $r_1 = r_2 = -1$, Therefore, these two previous cases can be combined with this case.

Next, we need to show that the eigenvalues of A and the λ_j are in one-to-one correspondence.

Consider the matrix

$$B = A - \lambda I = \begin{bmatrix} -\lambda & 1 & 0 & \cdots & 0 & 1 \\ 1 & -\lambda & 1 & \cdots & 0 & 0 \\ 0 & 1 & -\lambda & \ddots & 0 & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & \ddots & -\lambda & 1 \\ 1 & 0 & 0 & \cdots & 1 & -\lambda \end{bmatrix}$$

If we delete the first and last rows and first two columns, we obtain an upper triangular matrix, which is invertible. Therefore $\operatorname{rank}(B) \geq n-2$, so $\operatorname{nullity}(B) \leq 2$. So

$$\text{geometric multiplicity}(\lambda) \leq 2,$$

$$\text{algebraic multiplicity}(\lambda) \leq 2.$$

For $\lambda_0 = 2$, we consider the matrix $B_1 = A - 2I$,

$$B_1 = \begin{bmatrix} -2 & 1 & & & 1 \\ 1 & -2 & 1 & & \\ & 1 & -2 & & \\ & & & \ddots & 1 \\ 1 & & & 1 & -2 \end{bmatrix}.$$

If we delete the first row and first column, we obtain the matrix

$$B_{11} = \begin{bmatrix} -2 & 1 & & \\ 1 & -2 & & \\ & & \ddots & 1 \\ & & 1 & -2 \end{bmatrix}.$$

For any $x \in \mathbb{R}^{n-1}$,

$$\begin{aligned} x^T B_{11} x &= -2x_1^2 + 2x_1x_2 - 2x_2^2 + 2x_2x_3 - 2x_3^2 + \cdots + 2x_{n-2}x_{n-1} - 2x_{n-1}^2 \\ &= -x_1^2 - (x_1 - x_2)^2 - (x_2 - x_3)^2 - \cdots - (x_{n-2} - x_{n-1})^2 - x_{n-1}^2 \leq 0. \end{aligned}$$

So, B_{11} is negative semidefinite.

If $x^T B_{11} x = 0$, then $x_1 = 0, x_1 - x_2 = 0, x_2 - x_3 = 0, \ldots, x_{n-2} - x_{n-1} = 0$. Therefore $x_1 = x_2 = \cdots = x_{n-1} = 0$. So if $x \neq 0$, then $x^T B_{11} x < 0$ and B_{11} is negative definite. We know that $-B_{11}$ is invertible because it is positive definite. Therefore B_{11} is also invertible.

So the rank of B_1 is at least $n-1$. Also, since B_1 is a singular matrix, we have

$$n - 1 \geq \operatorname{rank}(B_1) \geq n - 1.$$

Therefore $\operatorname{rank}(B_1) = n-1$ and $\operatorname{nullity}(B_1) = 1$. Therefore,

$$\text{geometric multiplicity}(2) = 1, \quad \text{and} \quad \text{algebraic multiplicity}(2) = 1.$$

If n is an odd number there are $(n+1)/2$ distinct values in $\lambda_j = 2\cos(2\pi j/n)$. We let $\lambda^{(2)}$ be the number of eigenvalues with algebraic multiplicity equal 2, and $\lambda^{(1)}$ be the number of eigenvalues with algebraic multiplicity equal 1. Since B has n eigenvalues

$$\begin{aligned} n &= \lambda^{(2)} + \lambda^{(1)} \\ &\leq 2\left(\frac{n+1}{2} - 1\right) + 1 \\ &= n. \end{aligned}$$

So each eigenvalue $2\cos(2\pi j/n)$, $j = 1, \ldots, \frac{n-1}{2}$ has multiplicity 2.

If n is an even number, $\lambda = -2$ is also one of the eigenvalues of matrix A since for eigenvector $x = [-1, 1, -1, 1, \ldots, 1]^T$

$$\begin{bmatrix} 0 & 1 & 0 & \cdots & 0 & 1 \\ 1 & 0 & 1 & \cdots & 0 & 0 \\ 0 & 1 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots & \\ 0 & 0 & \cdots & 1 & 0 & 1 \\ 1 & 0 & \cdots & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} -1 \\ 1 \\ -1 \\ 1 \\ \vdots \\ 1 \end{bmatrix} = (-2) \begin{bmatrix} -1 \\ 1 \\ -1 \\ 1 \\ \vdots \\ 1 \end{bmatrix}.$$

Consider the matrix $B_2 = A - \lambda I$

$$B_2 = \begin{bmatrix} 2 & 1 & & & 1 \\ 1 & 2 & 1 & & \\ & 1 & 2 & & \\ & & & \ddots & \\ 1 & & & 1 & 2 \end{bmatrix}.$$

If we delete the first row and the first column, we obtain the matrix

$$B_{21} = \begin{bmatrix} 2 & 1 & & \\ 1 & 2 & & \\ & & \ddots & 1 \\ & & 1 & 2 \end{bmatrix}.$$

For any $x \in \mathbb{R}^{n-1}$, by an argument similar to the case when $\lambda_0 = 2$, B_{21} is positive definite. Therefore B_{21} is invertible.

So the rank of B_2 is at least $n-1$. On the other hand, B_2 is a singular matrix because -2 is an eigenvalue. So

$$n - 1 \geq \text{rank}(B_2) \geq n - 1.$$

Therefore $\text{rank}(B_2) = n - 1$ and $\text{nullity}(B_2) = 1$. So we have

$$\text{geometric multiplicity}(-2) = 1, \quad \text{and} \quad \text{algebraic multiplicity}(-2) = 1.$$

So the dimension of the eigenspace of B_2 corresponding to the eigenvalue -2 is one. By a similar argument as for when n is odd, we see that 2 and -2 are eigenvalues of multiplicity one and $2\cos(2\pi j/n), j = 1, 2 \cdots, (n/2) - 1$ are eigenvalues of multiplicity two.

Equivalently, the eigenvalues of A in all cases are

$$\lambda_j = 2\cos\frac{2\pi j}{n}, \quad j = 0, 1, \ldots, n-1.$$

$\square$

Theorem 3. *For any odd number n*

$$\vartheta(C_n) = \begin{cases} \frac{n\cos(\pi/n)}{1+\cos(\pi/n)} & \text{if } n \text{ is odd.} \\ \frac{n}{2} & \text{if } n \text{ is even.} \end{cases}$$

Proof. Let A_n be the adjacency matrix of C_n and J_n be a n-by-n matrix with all entries equal to 1. As in the case $n = 5$, it is sufficient to consider a feasible matrix for C_n to be $J_n - (1-x)A_n$. We have just proved that the eigenvalues of the graph C_n are

$$2\cos\frac{2\pi j}{n}, \text{ for } j = 0, 1, \ldots, n-1.$$

Let u_j be the corresponding eigenvector. Note that $u_0 = [1, 1, \ldots, 1]^T$ is an eigenvector corresponding to $\lambda_0 = 2$. Then we have

$$\begin{aligned} [J_n - (1-x)A_n]u_0 &= [n - (1-x)2]u_0 \\ &= (n - 2 + 2x)u_0. \end{aligned}$$

Since all the eigenvectors corresponding to distinct eigenvalues of a symmetric matrix are orthogonal, then for $j > 0$ we have,

$$J_n u_j = \begin{bmatrix} u_0^T \\ \vdots \\ u_0^T \end{bmatrix} u_j = \begin{bmatrix} u_0^T u_j \\ \vdots \\ u_0^T u_j \end{bmatrix} = 0,$$

so then,

$$\begin{aligned}[J_n - (1-x)A_n]u_j &= 0u_j - (1-x)A_n u_j \\ &= -(1-x)2\cos\frac{2\pi j}{n}u_j.\end{aligned}$$

So the eigenvalues of $J_n - (1-x)A_n$ are

$$\begin{aligned}&\mu_0 = n - 2 + 2x \\ &\mu_j = -2(1-x)\cos\frac{2\pi j}{n}, \ j = 1, 2, \cdots, n-1.\end{aligned}$$

Let λ_1 be the maximum eigenvalue.

If n is even, we consider the graph of μ_0 and μ_i, and consider the intersection of these lines. We know that all the lines of the form $\mu_i = -2(1-x)\cos(2\pi j/n)$ for $j = 1, 2, \ldots, n-1$ pass through the point $(1, 0)$. Since line $\mu_0 = n - 2 + 2x$ has biggest positive slope and biggest y intercept, it crosses each of the lines $\mu_1, \mu_2, \ldots, \mu_{n-1}$ to the left of the vertical axis. The line $\mu_{n/2} = -2(1-x)\cos(\pi) = 2 - 2x$ has the most negative slope so is the first to meet μ_0.

It is easy to see this result if we consider the example of $n = 6$, which is illustrated in Figure 12. The distinct eigenvalues are

$$\begin{aligned}&\mu_0 = 4 + 2x \\ &\mu_1 = -2(1-x)\cos\frac{\pi}{3} \\ &\mu_2 = -2(1-x)\cos\frac{2\pi}{3} \\ &\mu_3 = -2(1-x)\cos\pi.\end{aligned}$$

By graphing these eigenvalues, we can see that the maximum eigenvalue occurs at the intersection of μ_0 and μ_3 which occurs at $(-1/2, 3)$ and gives $\lambda_1 = 3 = n/2$.

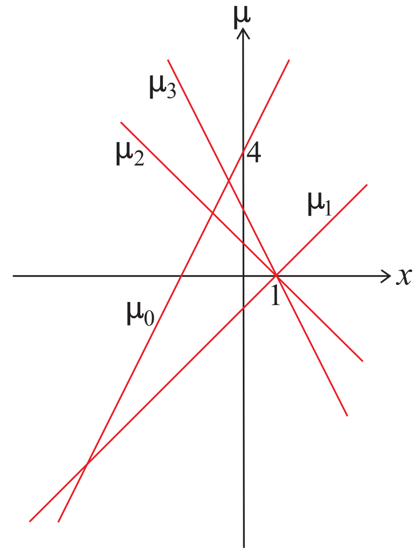


Figure 12:

So, for any even n, we consider the intersection of the lines $2-2x$ and $n-2+2x$, which occurs when $x = 1-(n/4)$. Then

$$\lambda_1 = n-2+2\left(1-\frac{n}{4}\right) = \frac{n}{2} = \alpha(C_n).$$

If n is odd and $j = (n-1)/2$,

$$\mu_j = -2(1-x)\cos\left(\frac{2\pi(\frac{n-1}{2})}{n}\right) = -2(1-x)\cos\left(\pi - \frac{\pi}{n}\right) = 2(1-x)\cos\frac{\pi}{n}.$$

Similarly, we can find the maximum eigenvalue λ_1 by finding the intersection of μ_0 and μ_j. This occurs when

$$n-2+2x = 2\cos\frac{\pi}{n} - 2x\cos\frac{\pi}{n}.$$

Rearranging we get,

$$2\left((1+\cos\frac{\pi}{n}\right))x = 2\cos\frac{\pi}{n} - n + 2,$$

so that the intersection will occur when

$$x = \frac{2\cos(\pi/n)+2-n}{2(1+\cos(\pi/n))} = 1 - \frac{n}{2(1+\cos(\pi/n))}.$$

Therefore

$$\begin{aligned}\lambda_1 &= n-2+2x = n-2+2\left(1-\frac{n}{2(1+\cos(\pi/n))}\right)\\ &= n-2+2-\frac{2n}{2(1+\cos(\pi/n))} = n-\frac{n}{1+\cos(\pi/n)}\\ &= \frac{n\cos(\pi/n)}{1+\cos(\pi/n)}.\end{aligned}$$

Hence

$$\vartheta_2(C_n) = \frac{n\cos(\pi/n)}{1+\cos(\pi/n)}, \text{ for any odd } n.$$

$\square$

References

[1] Barrett, Wayne W., "Introduction to Spectral Graph Theory," unpublished notes.

[2] Horn, Roger A. and Charles R. Johnson, *Matrix Analysis*, Cambridge University Press, 1985.

[3] Knuth, Donald E., "The Sandwich Theorem," *The Electronic Journal of Combinatorics* I (1994) $\sharp A1$.

[4] Lovasz, Laszlo, "On the Shannon Capacity of a Graph," *IEEE Transactions on Information Theory*, Vol. IT-25, No. 1, January 1979.

[5] Merris, Russell, *Graph Theory*, John Wiley & Sons, Inc., New York, 2001.

[6] West, Douglas B., *Introduction to Graph Theory*, Prentice Hall, Upper Saddle River, NY, 1996.