國立臺灣大學理學院應用數學科學研究所

碩士論文

Institute of Applied Mathematical Sciences

College of Science

National Taiwan University

Master Thesis

圖上的曲率及相關問題

On Curvature of Graphs and Related Problems

陳威嘉

Wei-Chia Chen

指導教授: 崔茂培 博士

Advisor: Mao-Pei Tsui, Ph.D.

中華民國 112 年 7 月

July, 2023

doi:10.6342/NTU202301030

Acknowledgements

可以完成這篇論文，我要感謝我的指導老師崔茂培教授，老師給我很充分的自由與時間，讓我摸索與學習。感謝 Shagnik Das 教授，帶領我進入組合和圖論的世界，並且為這篇論文提供建議。此外，我要感謝朋友祁安和智皓，在我碩士的路上與我閒聊、關心我，帶來許多歡樂與支持。感謝葉芳萍老師，教我學術英文寫作的架構。最後，我想感謝我的父母經濟上的支持，讓我能夠順利完成這個碩士學位。

doi:10.6342/NTU202301030

中文摘要

2022 年，Steinerberger 在圖上定義了一個曲率的概念，這個定義和圖的距離矩陣有關。在這篇論文，我們介紹 Steinerberger 曲率 [27]、探討另一個他的相關研究 [26]，並提供新的結果。我們刻畫在經過圖操作後的距離矩陣，這些操作包括在兩個圖加入一條邊連接、在兩個圖在一個點合併，和在一個圖移除一個橋。我們證明了如果一個圖有正曲率，在這些操作下，新的圖除了至多兩個點外會有正曲率。若 D 是圖的距離矩陣，我們提供了一個方法來建構圖使得 $Dx = \mathbf{1}$ 無解。最後，若 v 是一個樹的距離矩陣最大特徵值的特徵向量，且其元都為正，我們提供了一個和葉子個數有關的 $\langle v, \mathbf{1} \rangle$ 的下界估計。

關鍵字：距離矩陣、圖、Perron-Frobenius、曲率

doi:10.6342/NTU202301030

Abstract

In 2022, Steinerberger proposed a notion of curvature on graphs involving the graph distance matrix. In this thesis, we give a survey of his works [26, 27] and extend further results. We characterize the distance matrices when certain graph operations are applied, such as adding an edge between two graphs, merging two graphs at a vertex, or removing a bridge from a graph. We show that positive curvatures are preserved except for one or two vertices under these graph operations. Let D be the distance matrix of a graph. We provide a method to construct graphs with the property that $Dx = \mathbf{1}$ has no solution. Finally, let v be the first eigenvector of the distance matrix of a tree with positive entries, as guaranteed by the Perron-Frobienius theorem. We provide a lower bound of $\langle v, \mathbf{1} \rangle$ involving the number of leaves.

Keywords: Distance Matrix, Graph, Perron-Frobenius, Curvature

doi:10.6342/NTU202301030

Contents

		Page
Acknowledgements		**i**
中文摘要		**ii**
Abstract		**iii**
Contents		**iv**
List of Figures		**vi**
Chapter 1	**Introduction**	**1**
Chapter 2	**Background**	**3**
2.1	Graph Theory	3
2.2	Operations on Graphs	6
2.3	Duality Theorems	8
2.4	Von Neumann's Minimax Theorem	11
Chapter 3	**Curvature on Graphs**	**15**
3.1	Definition and Examples	15
3.2	Properties of Curvature	18
3.3	Geometric Implications	23
3.4	Existence of Curvature: A Sufficient Condition	30
Chapter 4	**Behavior of Curvature under Graph Operations**	**34**
4.1	Bridging, Merging and Cutting Graphs	34
4.2	The Null Space of Graph Distance Matrix	43
4.3	New Proof of Invariance of Total Curvature	46
4.4	Nonexistence of Curvature	46
4.5	Further Remarks	48

doi:10.6342/NTU202301030

Chapter 5 The Perron Eigenvector of Graph Distance Matrix **50**

5.1 Background: The Perron-Frobenius Theorem 50

5.2 The Perron Eigenvector and the Constant Vector 53

5.3 Special Cases: Trees and Antipodal Graphs 55

5.4 Minimum Entries of the Perron eigenvector 59

5.5 Further Remarks 60

References **62**

doi:10.6342/NTU202301030

List of Figures

2.1 K_5: complete graph with 5 vertices 4
2.2 A path and a cycle. 4
2.3 An example of a tree. 5

3.1 Examples of graphs that have a constant curvature. 17
3.2 Path admits a nonnegative curvature 18
3.3 A graph that has constant curvature but not vertex-transitive. 20
3.4 The prism graph $C_5 \square P_2$. 21
3.5 Four graphs that $Dx = \mathbf{1}$ does not have a solution. 30

4.1 Add an edge between K_4 and C_5. 36
4.2 The 5-barbell graph. 38
4.3 Merging K_4 and C_6 at one vertex. 39
4.4 Four graphs that $Dx = \mathbf{1}$ has no solution. 48
4.5 Merging $K_{1,1,1,4}$ and Quartic-$(11, 18)$ at a vertex, the resulting graph has no solution to $Dx = \mathbf{1}$. 49

5.1 The star graph with 8 vertices 57
5.2 The minimum entry of the Perron eigenvector of the graph distance matrix does not occur at the vertex with maximum degree. 60

doi:10.6342/NTU202301030

Chapter 1 Introduction

Over the past two decades, curvature, a crucial concept in differential geometry, has been introduced to the edges of graphs, [19, 22, 25]. In his paper [27], Steinerberger proposed a potential notion of curvature on the vertices of graphs. He showed that the proposed notion of curvature on graphs satisfies several properties that a curvature on a manifold would satisfy. These include a Bonnet-Myers theorem, a Cheng theorem, and a Lichnerowicz theorem. However, there has been little discussion on the behavior of curvature when we make operations on graphs, such as adding an edge between two graphs, merging two graphs at a vertex, or removing an edge from a graph. Let D be the distance matrix of a graph. With his definition, a necessary condition for a graph to have a curvature with these geometric properties is that the linear system $Dx = \mathbf{1}$ has a solution. He investigated the graphs in Mathematica with fewer than 500 vertices and reported that there are only 5 graphs that $Dx = \mathbf{1}$ do not have a solution. This phenomenon leads to the intriguing question: why does the linear system of equations $Dx = \mathbf{1}$ tend to have a solution for most graphs?

In his subsequent work [26], Steinerberger gave a sufficient condition for the linear system $Dx = \mathbf{1}$ to have a solution, in terms of the Perron-root λ_1 (the largest positive eigenvalue) and the Perron-eigenvector v (the eigenvector corresponding to λ_1 whose entries are positive) of D. A problem of this condition is that it degenerates to whether the matrix D is singular or not. However, this condition motivates the investigation of the lower bound of $\langle v, \mathbf{1} \rangle$ in [26].

The purpose of this thesis is to extend the results in [27] and [26]. The main contributions are as follows.

1. We prove that positive curvatures are preserved except for one or two vertices when

doi:10.6342/NTU202301030

we add an edge between two graphs, merge two graphs at a vertex, or remove a bridge from a graph.

2. We prove that if two graphs have the property that $Dx = \mathbf{1}$ does not have a solution, then after merging them at a vertex, the resulting graph has the same property.
3. We provide an elementary linear algebraic proof of Proposition 3 in [27] (the invariance of total curvature) without invoking von Neumann's Minimax theorem.
4. We provide a lower bound of $\langle v, \mathbf{1} \rangle$ involving the number of leaves when the graph is a tree.
5. We show that if a graph has a universal vertex, then the minimum of the Perron-eigenvector of the distance matrix occurs at that vertex.

This thesis consists of five chapters. Chapter 2 gives the preliminary background to graph theory and von Neumann's Minimax Theorem. The latter theorem is used for the geometric implications of the graph curvature. In Chapter 3, we introduce the curvature on graphs and establish its properties. In Chapter 4, we provide new results on how the curvature and distance matrices behave under certain graph operations. Finally, Chapter 5 focuses on the Perron-eigenvector of graph distance matrices and lower bounds of $\langle v, \mathbf{1} \rangle$.

doi:10.6342/NTU202301030

Chapter 2 Background

In the first and second sections of this chapter, we give an overview of graph theory and certain graph operations. These operations will be used in Chapters 3 and 4 when establishing properties of curvature on graphs. The third section introduces duality theorems, which are used in proving von Neumann's Minimax Theorem in the fourth section. The minimax theorem is the foundation of geometric properties of curvature on graphs in Chapter 3.

2.1 Graph Theory

A graph $G = (V, E)$ consists of vertices V and edges E. A vertex u is adjacent to v if $\{u, v\} \in E$. We denote it as $u \sim v$ or $uv \in E$, and call v a neighbor of u. The degree of a vertex u is the number of neighbors of u. This is denoted as deg(u). We call a graph k-regular if every vertex has degree k. We call a graph complete if there is an edge between any pair of vertices.

A graph of the form $V = \{v_1, ..., v_n\}, E = \{\{v_i, v_{i+1}\} : 1 \leq i \leq n-1\}$ is called a path of length $n-1$. This is denoted as P_n. If the first vertex and the last vertex are the same, the graph is called a cycle and denoted as C_n.

A graph is connected if for every two vertices u and v, there is a path starting at u and ending at v. A graph is disconnected if it is not connected. An edge e in a connected graph is a bridge if the removal of e disconnects the graph.

A tree T is a connected graph without cycles. A vertex $v \in T$ is called a leaf if it has only one neighbor, i.e., deg$(v) = 1$. The following properties of trees can be easily proved.

Lemma 2.1. *[10, p. 14] If T is a tree with n vertices, then it has $n-1$ edges. Furthermore,*

doi:10.6342/NTU202301030

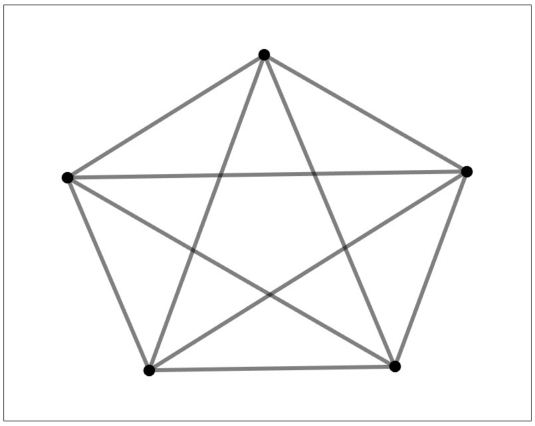


Figure 2.1: K_5: complete graph with 5 vertices

Figure 2.2: A path and a cycle.

doi:10.6342/NTU202301030

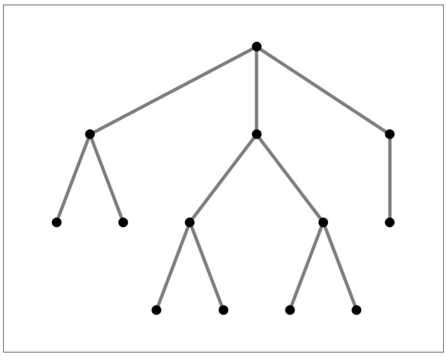


Figure 2.3: An example of a tree.

for any $u, v \in V(T)$, there is a unique path from u to v.

The distance between any two vertices u and v, denoted as $d(u, v)$, is the length of a shortest path from u to v. The diameter of G is the maximum distance between any two vertices. Namely,

$$\text{diam}(G) = \max_{u,v \in V} d(u, v).$$

The distance matrix D is defined as $D_{ij} = d(v_i, v_j)$ for all i, j. Note that D is integral and symmetric, with diagonal entries being 0. Since v_i is adjacent to v_j if and only if $D_{ij} = 1$, we can infer the adjacency of G by looking at the entries of D. We often denote $d(v_i, v_j)$ by d_{ij} or D_{ij}.

The adjacency matrix A of a graph is defined as $A_{ij} = 1$ if v_i is adjacent to v_j, and $A_{ij} = 0$, otherwise. The matrix A is integral and symmetric, with diagonal entries being 0.

The Laplacian matrix L is defined as

$$L_{ij} = \begin{cases} \deg(v_i) & \text{if } i = j \\ -1 & \text{if } i \neq j \text{ and } v_i \sim v_j \\ 0 & \text{otherwise.} \end{cases}$$

It is a well-known fact that all eigenvalues of L are non-negative. Let $\lambda_1(G)$ be the smallest positive eigenvalue of L. Equivalently, following the arguments in [6], we have

$$\lambda_1(G) = \inf_{\substack{f: V \to \mathbb{R} \\ \sum_{v \in V} f(v) = 0}} \frac{\sum_{\{u,v\} \in E} (f(u) - f(v))^2}{\sum_{v \in V} f(v)^2}.$$

doi:10.6342/NTU202301030

Given a graph G, an automorphism $\phi : G \to G$ is a bijection so that $u \sim v \iff \phi(u) \sim \phi(v)$, i.e., ϕ preserves the adjacency of the vertices. A graph G is vertex-transitive if for any two vertices $u, v \in V(G)$, there is an automorphism $\phi : G \to G$ so that $\phi(u) = v$. Informally, this means that each vertex is indistinguishable from another.

Example. The complete graph and the cycle graph are vertex-transitive.

All vertex-transitive graphs are regular. To see this, let u, v be two vertices of a graph G and let $\phi : G \to G$ be an automorphism with $\phi(u) = v$. Since the automorphism preserves adjacency, we have $\deg(u) = \deg(v)$. However, not all k-regular graphs are vertex-transitive. Examples are given in [12] and Figure 3.3.

Define the interval $[u, v]$ from u to v to be the vertices lying on the shortest paths from u to v. Namely,

$$[u, v] = \{z \in V : d(u, z) + d(z, v) = d(u, v)\}.$$

A graph is called antipodal, as in [8], if for every vertex u there is another vertex $\bar{u}$ so that $[u, \bar{u}] = V$.

Example. The cycle graph C_{2n} on $2n$ vertices with $n \geq 3$ is an antipodal graph.

The following lemma can be proved by using the definition and the triangular inequality. Its proof can be found in [28].

Lemma 2.2. *Let G be an antipodal graph. The function $\bar{\cdot} : G \to G$ is an automorphism and* $\operatorname{diam}(G) = d(u, \bar{u})$ *for every vertex u.*

2.2 Operations on Graphs

Let G_1 and G_2 be two connected graphs. We can *bridge* them by adding an edge between a vertex v of G_1 and a vertex u of G_2. We *merge* G_1 and G_2 at v and at u so that v and u are viewed as identical vertex in the new graph. Equivalently, this new graph can be obtained by bridging G_1 and G_2 by an edge $\{v, u\}$, and performing an edge contraction on the edge $\{v, u\}$.

Let G and H be two graphs. The Cartesian product graph $G \square H$ is the graph whose vertex set is $V(G) \times V(H)$, and two vertices $gh, g'h'$ form an edge if either $g = g'$ and

doi:10.6342/NTU202301030

$hh' \in E(H)$, or $gg' \in E(G)$ and $h = h'$.

The projection map $p_G : E(G\Box H) \to G$ is defined as

$$p_G(gh, g'h') = \begin{cases} g & \text{if } g = g' \text{ and } hh' \in E(H) \\ gg' & \text{if } gg' \in E(G) \text{ and } h = h'. \end{cases}$$

The projection map $p_H : E(G\Box H) \to H$ can be defined in a similar way.

Lemma 2.3 (Proposition 5.1, [15])**.** *Let G and H be connected graphs. We have*

$$d_{G\Box H}((gh, g'h')) = d_G(g, g') + d_H(h, h').$$

Proof. Let $\{g =: a_1, a_2, ..., a_{k+1} := g'\}$ be a shortest path from g to g' in G, and let $\{h =: b_1, b_2, ..., b_{k'+1} := h'\}$ be a shortest path from h to h' in H. Then

$$P := \{a_1b_1, a_2b_1, ..., a_{k+1}b_1, a_{k+1}b_2, ..., a_{k+1}b_{k'+1}\}$$

is a path in $G\Box H$ from gh to $g'h'$, with length $k + k' = d_G(g, g') + d_H(h, h')$. Thus,

$$d_{G\Box H}(gh, g'h') \leq d_G(g, g') + d_H(h, h').$$

Conversely, suppose R is a shortest path from gh to $g'h'$. If $e = \{g_ih_i, g_i'h_i'\}$ is an edge in R, then one of $\{p_G(e), p_H(e)\}$ is an edge and the other is a vertex. Furthermore, the edges $E(p_G(R))$ forms a path from g to g' in G, and the edges $E(p_H(R))$ forms a path from h to h' in H. This implies that

$$\begin{aligned} d_{G\Box H}(gg', hh') &= |E(R)| \\ &= |E(p_G(R))| + |E(p_H(R))| \\ &\geq d_G(g, g') + d_H(h, h') \end{aligned}$$

□

The following corollary is stated in [5].

Corollary 2.4. $\mathrm{diam}(G\Box H) = \mathrm{diam}(G) + \mathrm{diam}(H)$.

doi:10.6342/NTU202301030

Proof. Let gh and $g'h'$ be two vertices of $G\Box H$ so that $d_{G\Box H}(gh, g'h') = \text{diam}(G\Box H)$. Then

$$\text{diam}(G\Box H) = d_{G\Box H}(gh, g'h') = d_G(g, g') + d_H(h, h') \leq \text{diam}(G) + \text{diam}(H).$$

Conversely, now assume $g, g' \in V(G)$ with $d_G(g, g') = \text{diam}(G)$ and $h, h' \in V(H)$ with $d_H(h, h') = \text{diam}(H)$. Then

$$\text{diam}(G) + \text{diam}(H) = d_G(g, g') + d_H(h, h') = d_{G\Box H}(gg', hh') \leq \text{diam}(G\Box H).$$

□

Throughout this thesis, we assume G is connected and $|V|$ is finite.

2.3 Duality Theorems

We introduce linear programming and duality theorems in this section. The main references are [4] and [20].

We consider the problem

$$\begin{aligned} \text{maximize } & 2x_1 - 3x_2 \\ \text{subject to } & 3x_1 + 5x_2 \leq 10 \\ & 2x_1 - 2x_2 \leq 7 \\ & x_1, x_2 \geq 0. \end{aligned}$$

Let $f : \mathbb{R}^2 \to \mathbb{R}$ be the objective function $f(x_1, x_2) = 2x_1 - 3x_2$. Let $F \subset \mathbb{R}^2$ be the region of the constraint. A feasible solution is a point $x \in F$ so that $f(x)$ is finite. For example, $(2, 0)$ is a feasible solution. A feasible solution where the objective function achieves a maximum is called an optimal solution. Note that any feasible solution gives a lower bound of f. To find an upper bound of f, assume $y_1, y_2 \geq 0$. By multiplying the first constraint by y_1 and the second constraint by y_2, we get

$$y_1(3x_1 + 5x_2) + y_2(2x_1 - 2x_2) \leq 10y_1 + 7y_2,$$

doi:10.6342/NTU202301030

that is,

$$(3y_1 + 2y_2)x_1 + (5y_1 - 2y_2)x_2 \le 10y_1 + 7y_2.$$

If we further require that $2 \le 3y_1 + 2y_2$ and $-3 \le 5y_1 - 2y_2$ then we get

$$2x_1 - 3x_2 \le 10y_1 + 7y_2.$$

Thus, $10y_1 + 7y_2$ is an upper bound for $f(x_1, x_2)$, where $(x_1, x_2) \in F$. We want to minimize this upper bound. Therefore we get the following problem:

$$\begin{aligned} \text{minimize } & 10y_1 + 7y_2 \\ \text{subject to } & 2 \le 3y_1 + 2y_2 \\ & -3 \le 5y_1 - 2y_2 \\ & y_1, y_2 \ge 0. \end{aligned}$$

The original problem is called the $primal$ problem and the latter problem is called the $dual$ problem.

In general, we consider the primal problem:

$$\begin{aligned} \text{maximize } & c_1x_1 + c_2x_2 + \cdots + c_nx_n \\ \text{subject to } & a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n \le b_1 \\ & a_{21}x_1 + a_{22}x_2 + \cdots + a_{2n}x_n \le b_2 \\ & \vdots \\ & a_{n1}x_1 + a_{n2}x_2 + \cdots + a_{nn}x_n \le b_n \\ & x_1, ..., x_n \ge 0. \end{aligned}$$

doi:10.6342/NTU202301030

By similar arguments as above, the dual problem is:

$$
\begin{aligned}
\text{minimize } & b_1y_1 + b_2y_2 + \cdots + b_ny_n \\
\text{subject to } & a_{11}y_1 + a_{21}y_2 + \cdots + a_{n1}y_n \geq c_1 \\
& a_{12}y_1 + a_{22}y_2 + \cdots + a_{n2}y_n \geq c_2 \\
& \vdots \\
& a_{1n}y_1 + a_{2n}y_2 + \cdots + a_{nn}y_n \geq c_n \\
& y_1, ..., y_n \geq 0.
\end{aligned}
$$

In matrix form, let $b, c \in \mathbb{R}^n$ and $A \in \mathbb{R}^{n\times n}$ be given. The dual of the primal problem

$$
\begin{aligned}
\text{maximize } & c \cdot x \\
\text{subject to } & Ax \leq b \\
& x \geq \mathbf{0}, x \in \mathbb{R}^n
\end{aligned}
$$

is

$$
\begin{aligned}
\text{minimize } & b \cdot y \\
\text{subject to } & A^T y \geq c \\
& y \geq \mathbf{0}, y \in \mathbb{R}^n,
\end{aligned}
$$

where for $w, u \in \mathbb{R}^n, w \geq u \iff \forall i, w_i \geq u_i$. Since the objective function and the constraint are linear, the primal problem is called the primal linear program, and the dual problem is called the dual linear program.

John von Neumann first conjectured the following duality theorems. These theorems were later proved by Gale, Kuhn, and Tucker. They give a relation between the primal and the dual.

Theorem 2.5 (Weak Duality Theorem, [4, 20]). *Let $x, y \in \mathbb{R}^n$ be feasible solutions to the primal and the dual, respectively. Then $c \cdot x \leq b \cdot y$. If the equality holds, then x, y are optimal solutions to the primal and the dual, respectively.*

Theorem 2.6 (Strong Duality Theorem, [20]). *If both the primal and the dual have a feasible solution, then both problems have an optimal solution. Furthermore, the optimal*

doi:10.6342/NTU202301030

values of the objective functions are identical.

The proof of the weak duality theorem is straightforward and the strong duality theorem can be proved by the simplex method. We omit the proofs here. The strong duality theorem is used in proving von Neumann's Minimax theorem.

2.4 Von Neumann's Minimax Theorem

In this section, we present von Neumann's Minimax theorem and its variants. This theorem will be used to prove the geometric theorems in Chapter 3. The main reference is [14].

Player 1 and Player 2 are playing a game. Each player has n strategies to use, one at a time. Let $A \in \mathbb{R}^{n\times n}$ be a matrix, which represents the payoff matrix. Whenever Player 1 uses strategy i and Player 2 uses strategy j, Player 2 gives A_{ij} dollars to Player 1. We say that Player 1 gains A_{ij} dollars and Player 2 loses A_{ij} dollars (even if A_{ij} is negative). The objective of Player 1 is to maximize the payoffs, while Player 2 aims to minimize the payoffs.

Suppose that Player 1 uses strategy i with probability x_i and Player 2 uses strategy j with probability y_j, where $x_i, y_j \geq 0$ for $1 \leq i, j \leq n$ and $\sum_{i=1}^n x_i = \sum_{j=1}^n y_j = 1$. The vectors x and y are called mixed strategies. The expected payoff is

$$\sum_{1\leq i,j\leq n} x_i A_{ij} y_j = \langle x, Ay\rangle.$$

Let

$$X = \{z \in \mathbb{R}^n : \sum_{i=1}^n z_i = 1 \text{ and } z_i \geq 0 \text{ for all } i\} = Y$$

be the space of mixed strategy for Player 1 and Player 2. In this thesis, we consider the special case that A is symmetric.

John von Neumann introduced the Minimax theorem in [29]. We prove this theorem by using the strong duality theorem.

Theorem 2.7 (von Neumann's Minimax theorem, [29]). *Let $A \in \mathbb{R}^{n\times n}$ be a symmetric matrix and X, Y denoted the space of mixed strategy as defined above. Then there is a*

doi:10.6342/NTU202301030

unique $\alpha \in \mathbb{R}$ *so that*

$$\max_{x\in X}\min_{y\in Y}\langle x, Ay\rangle = \alpha = \min_{y\in Y}\max_{x\in X}\langle x, Ay\rangle.$$

Proof. We follow the proof in [14]. Intuitively, for any given strategy of Player 2, Player 1 will select the strategy with the largest payoff. Mathematically, for any $y \in Y$, we have

$$\max_{x\in X}\langle x, Ay\rangle = \max_{1\le i\le n}(Ay)_i.$$

To see this, let $x \in X$ be given. Then

$$\langle x, Ay\rangle = \sum_{i=1}^{n} x_i(Ay)_i \le \max_i (Ay)_i \sum_i x_i = \max_i (Ay)_i.$$

Taking the maximum over $x \in X$, we get

$$\max_{x\in X}\langle x, Ay\rangle \le \max_{1\le i\le n}(Ay)_i.$$

The other direction of the inequality is easy by considering the Euclidean coordinate vectors.

Thus,

$$\min_{y\in Y}\max_{x\in X}\langle x, Ay\rangle = \min_{y\in Y}\max_{1\le i\le n}(Ay)_i.$$

Similarly, given a strategy $x \in X$ of Player 1, Player 2 will choose a strategy that minimizes the payoff. Thus, by the symmetry of A,

$$\min_{y\in Y}\langle x, Ay\rangle = \min_{y\in Y}\langle y, Ax\rangle = \min_{1\le i\le n}(Ax)_i.$$

We get

$$\max_{x\in X}\min_{y\in Y}\langle x, Ay\rangle = \max_{x\in X}\min_{1\le i\le n}(Ax)_i.$$

Let $v_1 = \max_{x\in X}\min_{1\le i\le n}(Ax)_i$ and $v_2 = \min_{y\in Y}\max_{1\le i\le n}(Ay)_i$. We aim to show that $v_1 = v_2$ by using the strong duality theorem.

Case 1. $A_{ij} > 0$ for all i, j. Fix $x \in X$. Note that $\min_{1\le i\le n}(Ax)_i$ is the maximum value

doi:10.6342/NTU202301030

w so that $(Ax)_i \geq w$ for all i. Thus finding v_1 is equivalent to the problem

$$\max w \text{ subject to } \begin{cases} (Ax)_i \geq w \text{ for } 1 \leq i \leq n, \\ \sum_i x_i = 1, \\ x_i \geq 0 \text{ for } 1 \leq i \leq n. \end{cases}$$

Since $A_{ij} > 0$ for all i, j, we can only consider the case when $w > 0$. Put $x'_i = \frac{x_i}{w}$. The problem is equivalent to

$$\max w \text{ subject to } \begin{cases} (Ax')_i \geq 1 \text{ for } 1 \leq i \leq n, \\ \sum_i x'_i = \frac{1}{w}, \\ x'_i \geq 0 \text{ for } 1 \leq i \leq n. \end{cases}$$

Since $\max w = \min \frac{1}{w}$, we can use the second constraint and the problem is equivalent to

$$\min \mathbf{1} \cdot x' \text{ subject to } Ax' \geq \mathbf{1}, x' \geq \mathbf{0} \tag{2.4.1}$$

where $\mathbf{1} \in \mathbb{R}^n$ is the all-one vector and $\mathbf{0} \in \mathbb{R}^n$ is the all-zero vector.

Similarly, finding v_2 is equivalent to the problem

$$\max \mathbf{1} \cdot y' \text{ subject to } Ay' \leq \mathbf{1}, y' \geq \mathbf{0}. \tag{2.4.2}$$

We identify Problem 2.4.2 as the primal problem and Problem 2.4.1 as the dual problem. Note that $\mathbf{0}$ is a feasible solution to the primal. In addition, $a_{ij} > 0$ for all i, j implies that the dual is feasible (for example, take x' to be very far from the origin). By the strong duality theorem, both the primal and the dual have optimal solutions and the optimal value coincides. Thus, $v_1 = v_2$.

Case 2. General case. Find $r > 0$ so that $A_{ij} + r > 0$ for all i, j. Let E be the matrix whose entries are 1. Consider the game with the payoff matrix $A' = A + rE$. Given $x \in X, y \in Y$, the expected payoff of this game is $\langle x, A'y \rangle = \langle x, Ay \rangle + r$. By the first

doi:10.6342/NTU202301030

case, we get

$$\begin{aligned}\max_{x\in X}\min_{y\in Y}\langle x, Ay\rangle &= \max_{x\in X}\min_{y\in Y}\langle x, A'y\rangle - r\\ &= \min_{y\in Y}\max_{x\in X}\langle x, A'y\rangle - r\\ &= \min_{y\in Y}\max_{x\in X}\langle x, Ay\rangle,\end{aligned}$$

as desired. □

We have the following corollary.

Corollary 2.8. *[27, p. 428] Let $A \in \mathbb{R}^{n\times n}$ be a symmetric matrix. There is a unique $\alpha \in \mathbb{R}$ so that for all $(z_1, \cdots, z_n) \in \mathbb{R}^n_{\geq 0}$ with $\sum_i z_i = 1$,*

$$\min_{1\leq i\leq n}(Az)_i \leq \alpha \leq \max_{1\leq i\leq n}(Az)_i.$$

Proof. By the Minimax theorem above, the first paragraph of its proof, and $X = Y$, there exists $\alpha \in \mathbb{R}$ so that

$$\max_{x\in X}\min_{1\leq i\leq n}(Ax)_i = \alpha = \min_{y\in Y}\max_{1\leq i\leq n}(Ay)_i = \min_{x\in X}\max_{1\leq i\leq n}(Ax)_i.$$

Fix $z \in \mathbb{R}^n$ so that $z_i \geq 0$ and $\sum_i z_i = 1$, i.e., fix $z \in X$. Since

$$\min_{1\leq i\leq n}(Az)_i \leq \max_{x\in X}\min_{1\leq i\leq n}(Ax)_i$$
$$\min_{x\in X}\max_{1\leq i\leq n}(Ax)_i \leq \max_{1\leq i\leq n}(Az)_i$$

we get the desired result. □

doi:10.6342/NTU202301030

Chapter 3 Curvature on Graphs

In this chapter, we introduce the Steinerberger curvature on graphs. In the first two sections, we compute the curvature for certain graphs, show that vertex-transitive graphs have constant curvature, and discuss the curvature of Cartesian product graphs. As shown in the third section, the curvature satisfies three theorems that a curvature would satisfy in differential geometry. In the last section, we discuss a sufficient condition for the graphs to have a curvature and point out its limitation. The materials of this chapter are based on [26, 27]. In this and the remaining chapters, $G = (V, E)$ represents a connected graph.

3.1 Definition and Examples

Following the definition in [27], we define a *curvature* of G as a measure $\mu : V \to \mathbb{R}$ so that

$$\forall v \in V, \sum_{u \in V} d(v, u)\mu(u) = |V|.$$

We view $\mu(v)$ as the curvature of v. Denote the vertices by $V = \{v_1, \ldots, v_n\}$. Equivalently, if we put $w = (\mu(v_1), \ldots, \mu(v_n))$ and consider the graph distance matrix D, then the curvature of G is a vector $w \in \mathbb{R}^n$ satisfying

$$Dw = n \cdot \mathbf{1},$$

where $\mathbf{1} \in \mathbb{R}^n$ is the all-one vector. We interpret $||w||_{l^1} = \sum_i |w_i|$ as the total curvature of the graph. We say the graph admits a nonnegative curvature if $w \in \mathbb{R}^n_{\geq 0}$. We say G admits a constant curvature if w is a constant vector.

doi:10.6342/NTU202301030

Complete graph K_n. The complete graph K_n admits constant curvature

$$K = \frac{n}{n-1},$$

since for every vertex $v \in V(K_n)$, we have $n = \sum_{j=1}^{n} d(v, v_j)K = K(n-1)$.

Remark. The distance matrix of K_n is $D = J_n - I_n$, where J_n is the all-one n by n matrix and I_n is the identity matrix. Note that $D\mathbf{1} = (n-1) \cdot \mathbf{1}$ implies $D(\frac{n}{n-1})\mathbf{1} = n \cdot \mathbf{1}$.

In fact, as long as the sums of each row of the distance matrix are equal, the graph admits a constant curvature. This is true for vertex-transitive graphs. See Theorem 3.1 for more details.

Cycle graph C_n. The cycle graph C_n admits constant curvature

$$K = \frac{n}{\lfloor \frac{n^2}{4} \rfloor}.$$

To see this, let $v_i \in V$ be arbitrary. Assume n is even. Then

$$\sum_{v_j \in V} d(v_i, v_j) = 2\sum_{i=1}^{n/2-1} i + \frac{n}{2} = \frac{n^2}{4}.$$

If n is odd then

$$\sum_{v_j \in V} d(v_i, v_j) = 2\sum_{i=1}^{(n-1)/2} i = \frac{n^2-1}{4}.$$

Cocktail Party graph CP_n. The cocktail party graph CP_n has vertices $\{v_1, ..., v_n, u_1, ..., u_n\}$ and edges $\{(v_i, u_j) : i \neq j\}$. For any vertex $v \in V$, we have

$$\sum_{u \in V} d(v, u) = (2n-2) \cdot 1 + 2 \cdot 1 = 2n = |V|.$$

Thus, it has constant curvature 1.

Remark. The only eigenvalues of the distance matrix of CP_n are $2n, 0,$ and -2, ([1]). Therefore, it is possible for a graph to admit a constant curvature even if $\det(D) = 0$.

Path graph P_n. We have the fact that for all i,

$$\frac{n}{n-1}(i-1) + \frac{n}{n-1}(n-i) = n.$$

doi:10.6342/NTU202301030

Define the curvature w as $w(v_1) = w(v_n) = n/(n-1)$ and $w(v_i) = 0$ for $2 \leq i \leq n-1$. Therefore, the curvature of a path is $n/(n-1)$ on the two endpoints and 0, otherwise.

Trees T_n. Let T be a tree with n vertices. Set $\tau = \mathbf{2} - (\deg(v_1), \cdots, \deg(v_n))^t$. We claim that $D\tau = (n-1)\mathbf{1}$. Thus, T admits a curvature.

Proof of claim, [3]. We prove this by induction. When $n = 1$, there is nothing to prove. If $n = 2$, then

$$D = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

and $\tau = (1, 1)^t$. Then $D\tau = \mathbf{1}$. Assume $n \geq 3$ and the claim holds for all smaller n. Without loss of generality, assume that v_n is a leaf in T and adjacent to v_{n-1}. Let $T' = T \setminus \{v_n\}$. Then T' is a tree with $n-1$ vertices. Let D' be the distance matrix of T'. Write $\tau = (\tau_1, ..., \tau_n)^t$ and put $\tau' = (\tau_1, ..., \tau_{n-1})^t + e_{n-1}^t$, where $e_{n-1} = (0, ..., 0, 1) \in \mathbb{R}^{n-1}$. Note that

$$\begin{aligned} \deg_{T'}(v_i) &= \deg_T(v_i), \text{ for } 1 \leq i \leq n-2 \\ \deg_{T'}(v_{n-1}) &= \deg_T(v_{n-1}) - 1. \end{aligned}$$

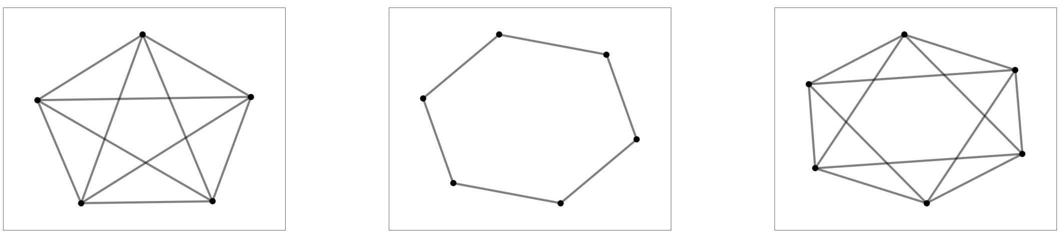
Thus,

$$\tau' = \mathbf{2} - (\deg_{T'}(v_1), ..., \deg_{T'}(v_{n-1}))^t.$$

By the induction hypothesis, $D'\tau' = (n-2)\mathbf{1}$. Let y be the last column of D'. Write

$$D = \begin{bmatrix} D' & x \\ x^t & 0 \end{bmatrix}.$$

Since $d(v_i, v_n) = d(v_i, v_{n-1}) + 1$ for $1 \leq i \leq n-1$ in T, we have $x = y + \mathbf{1}$. Note the



(a) The complete graph K_5. (b) The cycle graph C_6 (c) A cocktail party graph.

Figure 3.1: Examples of graphs that have a constant curvature.

doi:10.6342/NTU202301030

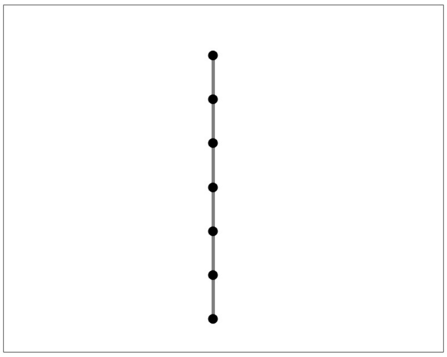


Figure 3.2: Path admits a nonnegative curvature

last entry of y is $d(v_{n-1}, v_{n-1}) = 0$. Then

$$D\tau = \begin{bmatrix} D' & y + \mathbf{1} \\ y^t + \mathbf{1}^t & 0 \end{bmatrix} \begin{bmatrix} \tau' - e_{n-1} \\ 1 \end{bmatrix} = \begin{bmatrix} D'\tau' - y + y + \mathbf{1} \\ y^t\tau' + \mathbf{1}^t\tau' - 1 \end{bmatrix} = \begin{bmatrix} (n-1)\mathbf{1} \\ n - 3 + \mathbf{1}^t\tau' \end{bmatrix}$$

since $y^t\tau' = n - 2$. Note that

$$\mathbf{1}^t\tau' = 2(n-1) - \sum_{i=1}^{n-1} \deg_{T'}(v_i) = 2,$$

since the sum of all degrees is equal to twice the number of edges, which is $n - 2$. Thus, we get $D\tau = (n-1)\mathbf{1}$, as desired. $\square$

Remark. Since the curvature at the vertex v_i is proportional to $2 - \deg(v_i)$, every leaf has positive curvature. In addition, every non-leaf has non-positive curvature, and all non-leaves have zero curvature if and only if the tree is a path.

Remark. Graham and Pollack showed that the distance matrix of a tree with n vertices has determinant $(-1)^{n-1}(n-1)2^{n-2}$ in [13]. Therefore, the distance matrix of a tree is invertible if $n > 1$. This also implies a tree admits a curvature.

3.2 Properties of Curvature

In this section, we establish several properties of the curvature. The first theorem states that vertex-transitive graphs, such as complete graphs and cycles, admit constant curvature.

doi:10.6342/NTU202301030

Theorem 3.1 (Proposition 2, [27]). *Let G be a vertex-transitive graph. Then G has constant curvature $K > 0$ and*

$$K = \left(\frac{1}{n}\sum_{i=1}^{n} d(v, v_i)\right)^{-1}$$

for every $v \in V$. If H is any graph with constant curvature K_H then

$$K_H = 1/(\frac{1}{n^2}\sum_{i,j=1}^{n} d_H(v_i, v_j)).$$

Informally, G is vertex-transitive means each vertex is indistinguishable from another. Therefore, if we ask how curved a vertex is in a vertex-transitive graph, it is natural that each vertex has the same curvature.

Proof, [27]. The idea is to show that the sums of each row of the distance matrix are the same. Let $u \in V$ be a vertex and k be an integer. Let

$$S_u^k = \{v \in V : d(u, v) = k\}$$

be the sphere centered at u with radius k. We claim that the size of S_u^k depends only on k and is independent of the choice of u. To see this, let $w \in V$. Since G is vertex-transitive, there is an automorphism $\phi : G \to G$ so that $\phi(u) = w$. Thus,

$$\begin{aligned} |S_w^k| &= |\{v \in V : d(\phi(u), v) = k\}| \\ &= |\{v \in V : d(u, \phi^{-1}(v)) = k\}| \\ &= |\{v' \in V : d(u, v') = k\}| \\ &= |S_u^k|. \end{aligned}$$

This implies that each row of the distance matrix D is a permutation of another. Thus, for every i, the sum

$$R := \sum_{j=1}^{n} d(v_i, v_j)$$

is constant. Therefore, $K = n/R$ is a constant positive curvature of G. For the second

doi:10.6342/NTU202301030

part of the theorem, assume that H has constant curvature K_H. Then

$$\sum_{j=1}^{n} d_H(v_i, v_j) K_H = n$$

for all i. Summing over i, we obtain

$$K_H \sum_{i,j=1}^{n} d_H(v_i, v_j) = n^2$$

as desired. $\square$

Remark. The converse of this theorem is not true. The graph in Figure 3.3 is 4-regular and has constant curvature $K = 7/8$. However, it is not vertex-transitive ([17]).

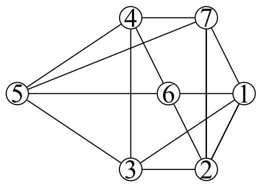


Figure 3.3: A graph that has constant curvature but not vertex-transitive.

Proof. The vertex 2 is contained in three triangles: $123, 127$, and 126. The vertex 3 is contained in two triangles only: 123 and 345. Thus, there is no automorphism ϕ so that $\phi(2) = 3$. For if there is one, then ϕ will preserve adjacency. Thus, it preserves the number of cycles of length 3, which leads to a contradiction. $\square$

The next theorem states that the Cartesian product graphs preserve nonnegative curvatures. In particular, when the graphs have constant curvature, we can easily compute the curvature of their Cartesian product graph.

Theorem 3.2 (Proposition 1, [27])**.** *Suppose G and H are two graphs nonnegatively curved. Then the Cartesian product graph $G \square H$ is nonnegatively curved. Suppose G and H have constant curvatures $K_1, K_2 > 0$. Then the curvature of $G \square H$ is constant $K > 0$ with*

$$\frac{1}{K} = \frac{1}{K_1} + \frac{1}{K_2}.$$

Furthermore, $G^n = G \square \cdots \square G$ has constant curvature K/n.

Example. The prism graph, defined as $C_n \square P_2$, has constant curvature.

doi:10.6342/NTU202301030

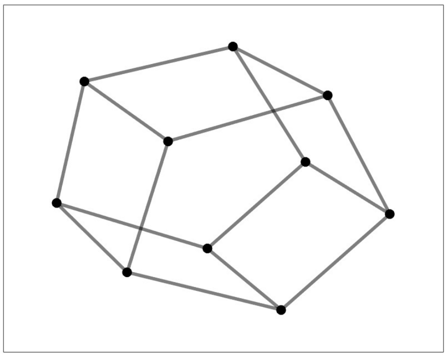


Figure 3.4: The prism graph $C_5 \Box P_2$.

Proof, [27]. Assume D_1 and D_2 are the distance matrices of G and H, respectively. Assume $|V(G)| = n_1, |V(H)| = n_2$. There exists $w_i \in \mathbf{R}^{n_i}_{\geq 0}$ so that $D_i w_i = n_i \cdot \mathbf{1}$. Put $K_i = \min_j (w_i)_j$ for $i = 1, 2$. Consider the function $\mu : V(G) \times V(H) \to \mathbb{R}_{\geq 0}$ defined as

$$\mu(g, h) = w_1(g) w_2(h)$$

for $(g, h) \in V(G) \times V(H)$. Let $(g_1, h_1) \in V(G \Box H)$ be arbitrary. Then we get

$$\begin{aligned} X :=& \sum_{(g_2,h_2) \in V(G \Box H)} d((g_1, h_1), (g_2, h_2)) \mu((g_2, h_2)) \\ =& \sum_{(g_2,h_2) \in V(G \Box H)} (d(g_1, g_2) + d(h_1, h_2)) w_1(g_2) w_2(h_2) \\ =& \sum_{(g_2,h_2) \in V(G \Box H)} d(g_1, g_2) w_1(g_2) w_2(h_2) \\ +& \sum_{(g_2,h_2) \in V(G \Box H)} d(h_1, h_2) w_1(g_2) w_2(h_2) \end{aligned}$$

The first term is equal to

$$\sum_{h_2 \in V(H)} w_2(h_2) \sum_{g_2 \in V(G)} d(g_1, g_2) w_1(g_2) = ||w_2||_{l^1} \cdot n_1.$$

Similarly, the second term is equal to $||w_1||_{l^1} \cdot n_2$. Thus,

$$X = ||w_2||_{l^1} \cdot n_1 + ||w_1||_{l^1} \cdot n_2 > 0$$

doi:10.6342/NTU202301030

is constant for any $(g_1, h_1) \in V(G \square H)$. Define

$$\begin{aligned} w &= \frac{n_1 n_2}{||w_2||_{l^1} \cdot n_1 + ||w_1||_{l^1} \cdot n_2} \mu \\ &= (\frac{||w_1||_{l^1}}{n_1} + \frac{||w_2||_{l^1}}{n_2})^{-1} \mu. \end{aligned}$$

Then we get $D_{G \square H} w = n_1 n_2 \cdot \mathbf{1} = |V(G \square H)| \cdot \mathbf{1}$, that is, $G \square H$ admits a nonnegative curvature w. Suppose that G and H have constant curvatures K_1, K_2. Then

$$K := \min w = (K_1 + K_2)^{-1} K_1 K_2,$$

i.e.,

$$\frac{1}{K} = \frac{1}{K_1} + \frac{1}{K_2}.$$

The curvature of the graph G^n can be proved easily by induction. □

The curvature satisfies a special version of von Neumann's Minimax Theorem. The following theorem will be used to prove geometric properties in Section 3.3.

Theorem 3.3 (Minimax Theorem, [27]). *If G admits a nonnegative curvature with total curvature $||w||_{l^1}$ and ν is a probability measure on V, then*

$$\min_{a \in V} \sum_{v \in V} d(a, v) \nu(v) \leq \frac{n}{||w||_{l^1}} \leq \max_{b \in V} \sum_{v \in V} d(b, v) \nu(v).$$

Proof. We follow the proof in [27]. The idea is to apply von Neumann's Minimax Theorem 2.8 to the distance matrix D. Let ν be a probability measure on V. We can view ν as a vector in $\mathbb{R}^n$. By the Minimax Theorem 2.8, there is a unique $\alpha \in \mathbb{R}$ independent of ν so that

$$\min_{1 \leq i \leq n} (D\nu)_i \leq \alpha \leq \max_{1 \leq i \leq n} (D\nu)_i.$$

This is equivalent to

$$\min_{a \in V} \sum_{v \in V} d(a, v) \nu(v) \leq \alpha \leq \max_{b \in V} \sum_{v \in V} d(b, v) \nu(v).$$

To determine the value of α, recall that $Dw = n \cdot \mathbf{1}$ and $w \in \mathbb{R}^n_{\geq 0}$. Let

$$\nu = \frac{w}{||w||_{l^1}}$$

doi:10.6342/NTU202301030

be a probability measure. For every $u \in V$,

$$\sum_{v \in V} d(u,v)\nu(v) = \frac{1}{||w||_{l^1}} \sum_{v \in V} d(u,v) w_v = \frac{(Dw)_u}{||w||_{l^1}} = \frac{n}{||w||_{l^1}}.$$

Taking the maximum and minimum for all $u \in V$, we get

$$\alpha = \frac{n}{||w||_{l^1}}.$$

□

It is possible that a graph admits two curvatures w_1 and w_2, that is, $Dw_1 = n \cdot \mathbf{1} = Dw_2$. This does not imply $w_1 = w_2$ in general. However, the total curvatures are equal provided the graph is nonnegatively curved.

Theorem 3.4 (Invariance of total curvature, [27]). *Suppose G is a connected graph and there are $w_1, w_2 \in \mathbb{R}^n_{\geq 0}$ such that $Dw_1 = Dw_2 = n \cdot \mathbf{1}$. Then $||w_1||_{l^1} = ||w_2||_{l^1}$.*

The following is the original proof in [27] involving von Neumann's Minimax theorem. We will provide an elementary linear algebraic proof in Section 4.3.

Proof. Consider the probability measure

$$\nu_i = \frac{w_i}{||w_i||_{l^1}}.$$

By the argument in the proof of Theorem 3.3 above, we have for every vertex u,

$$\sum_{v \in V} d(u,v)\nu_i(v) = \frac{1}{||w_i||_{l^1}} \sum_{v \in V} d(u,v)(w_i)_v = \frac{n}{||w_i||_{l^1}} = \alpha$$

for $i = 1, 2$. Thus, $||w_1||_{l^1} = ||w_2||_{l^1}$. □

3.3 Geometric Implications

The discrete Bonnet-Myers theorem asserts that if a graph admits a nonnegative curvature, then it cannot be too large, since its diameter is bounded. This theorem also provides an upper bound to the total curvature.

doi:10.6342/NTU202301030

Theorem 3.5 (Discrete Bonnet-Myers, [27]). *Suppose G has nonnegative curvature, namely, $Dw = n \cdot \mathbf{1}$ for some $w \in \mathbb{R}^n_{\geq 0}$. Let $K = \min_i w_i \geq 0$. We have*

$$\operatorname{diam}(G) \leq \frac{2n}{||w||_{l^1}} \leq \frac{2}{K}$$

and $\operatorname{diam}(G) \cdot K = 2$ implies G admits constant curvature.

Proof, [27]. The second inequality follows by $||w||_{l^1} = \sum_i |w_i| \geq \sum_i K = nK$.

To show the first inequality, let $a, b \in V$ with $d(a,b) = \operatorname{diam}(G)$. Define a probability measure $\nu : V \in [0,1]$ such that $\nu(a) = \nu(b) = 1/2$ and $\nu(v) = 0$ if $v \notin \{a, b\}$. By Theorem 3.3, there is $c \in V$ so that

$$\sum_{v \in V} d(c,v)\nu(v) = \frac{1}{2}(d(a,c) + d(b,c)) \leq \frac{n}{||w||_{l^1}}.$$

On the other hand, we have

$$\frac{1}{2}(d(a,c) + d(b,c)) \geq \frac{1}{2} d(a,b) = \frac{1}{2}\operatorname{diam}(G).$$

Combining the two equations above, we get the desired result.

If $\operatorname{diam}(G)K = 2$, then the equality $||w||_{l^1} = nK$ implies $w_i = K$ for all i, that is, G has constant curvature. $\square$

Examples of Bonnet-Myers sharpness. The cycle graph C_{2n} with $2n$ vertices has constant curvature $2/n$ and diameter n. The cocktail party graph CP_n has constant curvature 1 and diameter 2.

The Cartesian product graphs preserves the discrete Bonnet-Myers sharpness.

Corollary 3.6. *Let G, H be connected graphs that are discrete Bonnet-Myers sharp, i.e., they satisfy the assumptions in Theorem 3.5 and $\operatorname{diam}(G)K_G = \operatorname{diam}(H)K_H = 2$. Then the product graph $G \square H$ is discrete Bonnet-Myers sharp, that is, $\operatorname{diam}(G \square H)K_{G \square H} = 2$.*

Proof. By Theorem 3.2, $G \square H$ has a positive constant curvature and

$$K_{G \square H} = \left(\frac{1}{K_G} + \frac{1}{K_H}\right)^{-1} = \frac{K_G K_H}{K_G + K_H}.$$

doi:10.6342/NTU202301030

By Corollary 2.4, we have $\text{diam}(G\square H) = \text{diam}(G) + \text{diam}(H)$. Thus,

$$\text{diam}(G\square H)K_{G\square H} = 2.$$

$\square$

The next theorem provides a lower bound to the total curvature.

Theorem 3.7 (Reverse Bonnet-Myers, [27])**.** *Suppose G is nonnegatively curved, namely, $Dw = n \cdot \mathbf{1}$ for some $w \in \mathbb{R}^n_{\geq 0}$. We have*

$$||w||_{l^1} \geq \frac{n^2}{n-1}\frac{1}{\text{diam}\, G},$$

where equality holds if and only if G is the complete graph.

Proof, [27]. Consider the uniform probability measure $\nu : V \to [0,1]$ defined as $\nu(v) = \frac{1}{n}$ for every vertex v. By the Minimax Theorem 3.3, there is a vertex b so that

$$\begin{aligned}
\frac{n}{||w||_{l^1}} &\leq \sum_{v\in V} d(b,v)\nu(v) \\
&= \frac{1}{n}\sum_{v\in V} d(b,v) \\
&= \frac{1}{n}\sum_{v\in V, v\neq b} d(b,v) \\
&\leq \frac{1}{n}\sum_{v\in V, v\neq b} \text{diam}(G) \\
&= \frac{n-1}{n}\text{diam}(G).
\end{aligned}$$

This gives the desired lower bound to $||w||_{l_1}$.

The equality holds if and only if $d(b,v) = \text{diam}(G)$ for all $v \neq b$. If $G = K_n$ is complete then $d(b,v) = 1 = \text{diam}(G)$ for all $v \neq b$. Conversely, suppose that $d(b,v) = \text{diam}(G)$ for all $v \neq b$. Let v be a neighbor of b, we get $1 = d(b,v) = \text{diam}(G)$. Thus, $G = K_n$. $\square$

The above theorems imply the following.

Corollary 3.8 ([27])**.** *If G admits a constant curvature $K > 0$, then*

$$\frac{1}{K} \leq \text{diam}(G) \leq \frac{2}{K}.$$

doi:10.6342/NTU202301030

The following theorem gives a bound on the smallest nontrivial eigenvalue $\lambda_1(G)$ of the Laplacian matrix L, in terms of total curvature.

Theorem 3.9 (Discrete Lichnerowicz, [27])**.** *Suppose G is positively curved, namely, $Dw = n \cdot \mathbf{1}$ for some $w \in \mathbb{R}^n_{>0}$. Let $K = \min_i w_i > 0$ and λ_1 be the smallest positive eigenvalue of the Laplacian matrix. Then*

$$\lambda_1 \geq \frac{||w||_{l^1}}{2n^2} \geq \frac{K}{2n}.$$

Proof, [27]. The second inequality follows by $||w||_{l^1} \geq nK$. We will show that

$$\lambda_1 \geq \frac{1}{n}\frac{1}{\text{diam}(G)}.$$

Then by the Discrete Bonnet-Myers theorem, we get

$$\lambda_1 \geq \frac{1}{n}\frac{1}{\text{diam}(G)} \geq \frac{||w||_{l^1}}{2n^2}.$$

Recall that

$$\lambda_1(G) = \inf_{\substack{f:V\to\mathbb{R} \\ \sum_{v\in V} f(v)=0}} \frac{\sum_{(u,v)\in E} (f(u)-f(v))^2}{\sum_{v\in V} f(v)^2}.$$

Let $f : V \to \mathbb{R}$ be a l^2-normalized function achieving the minimum, so f satisfies $\sum_{v\in V} f(v) = 0$, and $\sum_{v\in V} f(v)^2 = 1$. The first equality implies f will change sign somewhere. The second equality implies

$$1 = \sum_{v\in V} f(v)^2 \leq \sum_{v\in V} ||f||^2_{l^\infty} = n||f||^2_{l^\infty}.$$

Therefore,

$$\frac{1}{\sqrt{n}} \leq ||f||_{l^\infty} = \max_{v\in V} |f(v)| \leq \max_{v\in V} f(v) - \min_{w\in V} f(w).$$

Let $a, b \in V$ be vertices where f achieves the maximum and the minimum, respectively. Let P be a path from a to b of length at most $\text{diam}(G)$. Denote

$$P = \{u_1, u_2, ..., u_k, u_{k+1}\},$$

doi:10.6342/NTU202301030

where $u_1 = a, u_{k+1} = b$. Then

$$\begin{aligned}
\frac{1}{\sqrt{n}} &\le f(a) - f(b) \\
&= |f(a) - f(b)| \\
&= |\sum_{i=1}^{k} f(u_i) - f(u_{i+1})| \\
&\le \sum_{i=1}^{k} |f(u_i) - f(u_{i+1})| \\
&\le k^{1/2} \left(\sum_{i=1}^{k} |f(u_i) - f(u_{i+1})|^2 \right)^{1/2} \\
&\le \sqrt{\text{diam}(G)} \left(\sum_{i=1}^{k} |f(u_i) - f(u_{i+1})|^2 \right)^{1/2},
\end{aligned}$$

where we used the Cauchy-Schwarz inequality. Thus,

$$\lambda_1 = \sum_{(u,v)\in E} (f(u) - f(v))^2 \ge \sum_{(u,v)\in P} (f(u) - f(v))^2 \ge \frac{1}{n} \frac{1}{\text{diam}(G)}$$

□

The linear system of equations $Dx = n \cdot \mathbf{1}$ does not always have a solution. (See Sections 3.4 and 4.4 for more on the solvability of $Dx = \mathbf{1}$.) In this case, we consider the pseudo-inverse $w = D^{\dagger}(n \cdot \mathbf{1})$ as the curvature, which is the vector z that minimizes $||Dz - n \cdot \mathbf{1}||_{l^2}$. If there are multiple such vectors, we consider the one with the smallest l^2 norm. The following theorem applies to such cases when w has positive entries.

Theorem 3.10 (Theorem 5, [27])**.** *Suppose G is connected and $w \in \mathbb{R}^n_{>0}$ is any vector with positive entries. Let $K = \min_i w_i > 0$. Then*

$$\text{diam}(G) \le \frac{||Dw||_{l^\infty}}{n} \frac{8}{K}$$

and

$$\lambda_1(G) \ge \frac{1}{8||Dw||_{l^\infty}} K.$$

doi:10.6342/NTU202301030

Proof, [27]. Define the average distance between any two vertices by

$$\text{avdiam}(G) := \frac{1}{n^2}\sum_{i,j} d(v_i, v_j).$$

We first show that

$$\text{avdiam}(G) \le \frac{||Dw||_{l^\infty}}{n}\frac{1}{K}.$$

Note that there is i so that

$$\text{avdiam}(G) \le \frac{1}{n}\sum_{j} d(v_i, v_j).$$

Otherwise, there will be a contradiction. Looking at the i-th row of Dw, we have

$$\begin{aligned} ||Dw||_{l^\infty} &= \max_k (Dw)_k \\ &\ge \sum_j d(v_i, v_j) w_j \\ &\ge K \sum_j d(v_i, v_j) \\ &\ge Kn\, \text{avdiam}(G), \end{aligned}$$

as desired.

Choose $0 < \delta < 1$ so that $\delta\, \text{diam}(G) = \text{avdiam}(G)$. We have

$$\text{diam}(G) = \frac{1}{\delta}\,\text{avdiam}(G) \le \frac{1}{\delta}\frac{||Dw||_{l^\infty}}{n}\frac{1}{K}.$$

Case 1. $\delta \ge \frac{1}{8}$. We get the desired result.

Case 2. $0 < \delta \le \frac{1}{8}$. By the definition of avdiam(G) and a contradiction argument, there is i_0 so that

$$\frac{1}{n}\sum_{j=1}^{n} d(v_{i_0}, v_j) \le \text{avdiam}(G) = \delta\, \text{diam}(G).$$

Put

$$A = \{j : d(v_{i_0}, v_j) \le 2\delta\, \text{diam}(G)\}$$

which represents the indices of the vertices close to v_{i_0}. We show that $|A|$ is large. Note

doi:10.6342/NTU202301030

that

$$\begin{aligned}
\delta \operatorname{diam}(G) &\geq \frac{1}{n}\sum_{j=1}^{n} d(v_{i_0}, v_j) \\
&\geq \frac{1}{n}\sum_{j\notin A} d(v_{i_0}, v_j) > \frac{|A^c|}{n} 2\delta \operatorname{diam}(G) \\
&= \frac{n-|A|}{n} 2\delta \operatorname{diam}(G).
\end{aligned}$$

Therefore, $|A| \geq \frac{n}{2}$.

Pick two vertices $a, b \in V$ so that $d(a,b) = \operatorname{diam}(G)$. Without loss of generality, assume that $d(a, v_{i_0}) \leq d(b, v_{i_0})$. Then $\operatorname{diam}(G) = d(a,b) \leq d(a, v_{i_0}) + d(b, v_{i_0}) \leq 2d(b, v_{i_0})$. For any $j \in A$, we have

$$d(v_j, b) \geq d(v_{i_0}, b) - d(v_{i_0}, v_j) \geq (\frac{1}{2} - 2\delta) \operatorname{diam}(G).$$

Thus,

$$\begin{aligned}
||Dw||_{l^\infty} &\geq \sum_{j=1}^{n} d(b, v_j) w_j \\
&\geq K \sum_{j=1}^{n} d(b, v_j) \\
&\geq K \sum_{j\in A} d(b, v_j) \\
&\geq K \sum_{j\in A} (\frac{1}{2} - 2\delta) \operatorname{diam}(G) \\
&= K|A|(\frac{1}{2} - 2\delta) \operatorname{diam}(G) \\
&\geq K\frac{n}{2}(\frac{1}{2} - 2\delta) \operatorname{diam}(G).
\end{aligned}$$

This implies that

$$\operatorname{diam}(G) \leq \frac{2}{(\frac{1}{2} - 2\delta)n} \frac{||Dw||_{l^\infty}}{K} \leq \frac{||Dw||_{l^\infty}}{n} \frac{8}{K},$$

as desired.

doi:10.6342/NTU202301030

The eigenvalue estimate $\lambda_1(G) \geq \frac{1}{n}\frac{1}{\text{diam}(G)}$ proved in Theorem 3.9 implies

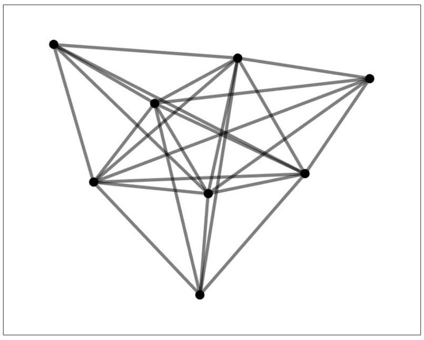
$$\lambda_1(G) \geq \frac{1}{8||Dw||_{l^\infty}} K.$$

□

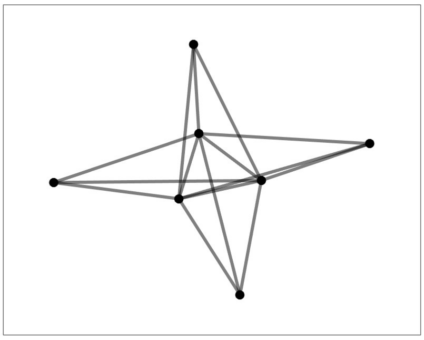
3.4 Existence of Curvature: A Sufficient Condition

In his paper [27], Steinerberger examined all graphs with $1 \leq n \leq 500$ in Mathematica 12 and reported there are only 5 graphs that $Dx = n \cdot \mathbf{1}$ does not have a solution. Figure 3.5 illustrates four of them. He raised the following problem.

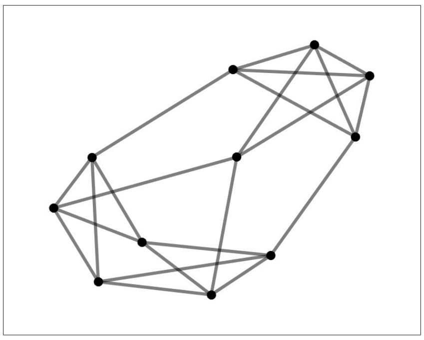
Problem. It seems that for most graphs, the linear system of equation $Dx = \mathbf{1}$ tends to have a solution. Why?



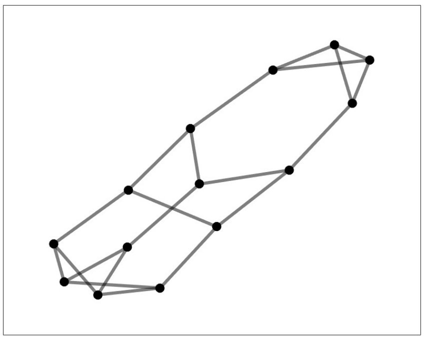
(a) The multipartite graph $K_{1,1,1,1,3}$.



(b) The multipartite graph $K_{1,1,1,4}$.



(c) The Quartic-$(11, 18)$ graph.



(d) The Cubic-$(14, 52)$ graph.

Figure 3.5: Four graphs that $Dx = \mathbf{1}$ does not have a solution.

doi:10.6342/NTU202301030

The following proposition is a sufficient condition for $Dx = \mathbf{1}$ to have a solution.

Proposition 3.11 (Proposition 1, [26]). *Suppose that $D \in \mathbb{R}^{n\times n}_{\geq 0}$ has eigenvalues $\lambda_1 > 0 \geq \lambda_2 \geq \cdots \geq \lambda_n$ and the first eigenvector $Dv = \lambda_1 v$. If*

$$1 - \left\langle v, \frac{\mathbf{1}}{\sqrt{n}} \right\rangle^2 < \frac{|\lambda_2|}{\lambda_1 - \lambda_2},$$

then $Dx = \mathbf{1}$ has a solution.

Proof, [26]. Define $Q : \mathbb{R}^n \to \mathbb{R}$ by

$$Q(v) = \langle v, Dv \rangle .$$

We aim to maximize the function Q subject to the constraint

$$\langle v, \mathbf{1} \rangle = 1.$$

By the Perron-Frobenius Theorem, the eigenvector associated with the largest eigenvalue $\lambda_1 > 0$ of D can be chosen to have nonnegative entries. Thus, $\sup_{\langle v, \mathbf{1}\rangle = 1} Q(v) > 0$. By the Spectral Theorem,

$$v = \langle v, v_1 \rangle v_1 + \sum_{i=2}^{n} \langle v, v_i \rangle v_i.$$

Namely, we decompose the vector v into the eigenvectors of D. We now give an upper bound for $Q(v)$ and show that the maximum is attained. Note that

$$\begin{aligned} Q(v) &= \langle v, v_1 \rangle^2 \lambda_1 + \sum_{i=2}^{n} \lambda_i \langle v, v_i \rangle^2 \\ &\leq \langle v, v_1 \rangle^2 \lambda_1 + \lambda_2 \sum_{i=2}^{n} \langle v, v_i \rangle^2 \\ &= \langle v, v_1 \rangle^2 \lambda_1 + \lambda_2 \left(\|v\|^2 - \langle v, v_1 \rangle^2 \right) \\ &= (\lambda_1 - \lambda_2) \langle v, v_1 \rangle^2 + \lambda_2 \|v\|^2. \end{aligned}$$

Note that

$$v_1 = \left\langle v_1, \frac{\mathbf{1}}{\sqrt{n}} \right\rangle \frac{\mathbf{1}}{\sqrt{n}} + v_1^*,$$

doi:10.6342/NTU202301030

where v_1^* is defined as the remainder. Then

$$\begin{aligned}\langle v, v_1\rangle^2 &= \left(\left\langle v_1, \frac{\mathbf{1}}{\sqrt{n}}\right\rangle \left\langle v, \frac{\mathbf{1}}{\sqrt{n}}\right\rangle + \langle v, v_1^*\rangle\right)^2 \\ &= \left(\left\langle v_1, \frac{\mathbf{1}}{\sqrt{n}}\right\rangle \frac{1}{\sqrt{n}} + \langle v, v_1^*\rangle\right)^2 \text{ since } \langle v, \mathbf{1}\rangle = 1. \\ &\leq \langle v, v_1^*\rangle^2 + \mathcal{O}(\|v\|) \text{ since the first term is a constant} \\ &\leq \|v\|^2\|v_1^*\|^2 + \mathcal{O}(\|v\|),\end{aligned}$$

by the Cauchy-Schwarz inequality. Thus,

$$Q(v) \leq \left[(\lambda_1 - \lambda_2)\|v_1^*\|^2 + \lambda_2\right] \cdot \|v\|^2 + \mathcal{O}(\|v\|).$$

Note that

$$1 = \|v_1\|^2 = \left\langle v_1, \frac{\mathbf{1}}{\sqrt{n}}\right\rangle^2 + \|v_1^*\|^2$$

by the Pythagorean theorem. This and the assumption imply

$$(\lambda_1 - \lambda_2)\,\|v_1^*\|^2 + \lambda_2 < 0.$$

Thus, $Q(v) \to -\infty$ as $\|v\| \to \infty$ in all directions of $\langle v, \mathbf{1}\rangle = 0$.

Consider the problem of maximizing Q subject to the constraint $\langle v, \mathbf{1}\rangle = 0$ and $||v|| \leq M$ for some $M > 0$. By compactness, Q achieves a maximum by some vector, denoted by v_m. On the other hand, by the Lagrange multiplier theorem, there is $\lambda \in \mathbb{R}$ such that

$$\nabla Q(v_m) = 2Dv_m = \lambda \cdot \mathbf{1}.$$

Note that $\langle Dv_m, v_m\rangle = Q(v_m) > 0$ implies $Dv_m \neq 0$ and $\lambda \neq 0$. Therefore, the equation $D(\frac{2}{\lambda}v_m) = \mathbf{1}$ implies that the linear system of equation $Dx = \mathbf{1}$ has a solution. □

Limitation.

When D is a graph distance matrix, this proposition implies that if there is a spectral gap and $\langle v, \frac{\mathbf{1}}{\sqrt{n}}\rangle$ is close to 1, then the graph admits a curvature. However, this condition degenerates to whether D is singular or not. Since if $\lambda_1 > 0 > \lambda_2 \geq \cdots \lambda_n$, then the determinant of D is not zero, which implies that $Dx = \mathbf{1}$ has a unique solution. On the other hand, if $\lambda_1 > 0 = \lambda_2 \geq \cdots \lambda_n$, then $\frac{|\lambda_2|}{\lambda_1 - \lambda_2} = 0$, and the required inequality will

doi:10.6342/NTU202301030

never satisfy. This condition still motivates the study of $\langle v, \mathbf{1} \rangle$ in Chapter 5.

doi:10.6342/NTU202301030

Chapter 4 Behavior of Curvature under Graph Operations

This chapter constitutes the main contribution of this thesis. We characterize distance matrix after certain graph operations, such as adding an edge between two graphs, merging two graphs at a vertex, or removing a bridge from a graph. This characterization enables us to prove that non-negative curvature stays preserved except for at most two vertices under these operations. In Sections 2 and 3, we characterize the null space of the distance matrix when we add an edge between two graphs and provide an elementary proof of Theorem 3.4 (invariance of total curvature) that does not rely on von Neumann's Minimax theorem. In Section 4, we provide a method for constructing graphs so that the equation $Dx = \mathbf{1}$ does not have a solution.

4.1 Bridging, Merging and Cutting Graphs

In this section, we investigate the behavior of the curvature after adding an edge between two graphs and after cutting a graph by an edge.

Given graphs admitting nonnegative curvatures, we can create a larger graph so that it admits a curvature nonnegative everywhere except at one or two vertices.

Proposition 4.1 (Appending a pendant vertex)**.** *Assume G admits a nonnegative curvature so that $Dw = n \cdot \mathbf{1}$ for some $w \in \mathbb{R}^n_{\geq 0}$. Let $v \in V(G)$ and let G' be the graph obtained by adding an edge between v and an additional vertex v'. In other words, $V(G') = V(G) \cup \{v'\}$ and $E(G') = E(G) \cup \{(v, v')\}$. Then G' admits a curvature nonnegative on every vertex except at the vertex v.*

doi:10.6342/NTU202301030

Proof. Without loss of generality, assume $v_n = v$ and let $v_{n+1} = v'$. Let D' be the distance matrix of G'. To show that $D'x = \mathbf{1}$ has a solution, write

$$D' = \begin{bmatrix} D & u \\ u^t & 0 \end{bmatrix},$$

where $u \in \mathbb{R}^n$. Let y be the last column of D, i.e.,

$$y = [d_G(v_1, v_n), ..., d_G(v_n, v_n)]^t.$$

Since $d_G(v_i, v_n) + 1 = d_{G'}(v_i, v_{n+1})$ for $1 \leq i \leq n$, we have $u = y + \mathbf{1}$. Let $e_n = (0, ..., 0, 1)^t \in \mathbb{R}^n$. Let $\tilde{w} = w - se_n$, where $s \in \mathbb{R}$ is to be chosen. Then

$$D' \begin{bmatrix} \tilde{w} \\ s \end{bmatrix} = \begin{bmatrix} Dw - sy + su \\ u^t\tilde{w} \end{bmatrix} = \begin{bmatrix} n\mathbf{1} + s\mathbf{1} \\ u^t\tilde{w} \end{bmatrix}.$$

Note that

$$u^t\tilde{w} = (y + \mathbf{1})^t(w - se_n) = y^t w + \mathbf{1}^t w - s = n - s + \mathbf{1}^t w,$$

by looking at the last row of $Dw = n \cdot \mathbf{1}$ and $y_n = 0$. If we set $s = \frac{1}{2}\mathbf{1}^t w > 0$ then $n + s = n - s + \mathbf{1}^t w$. Consequently,

$$D' \begin{bmatrix} \tilde{w} \\ s \end{bmatrix} = (n + s)\mathbf{1}.$$

Define

$$w' = \frac{n+1}{n+s} \begin{bmatrix} \tilde{w} \\ s \end{bmatrix}.$$

We obtain $D'w' = (n + 1) \cdot \mathbf{1}$.

Since $w \in \mathbb{R}^n_{\geq 0}$, and $s > 0$, w' is nonnegative at every vertex except at v_n. $\square$

Remark. From the above computations, the curvature at v_n is proportional to

$$w_n - \frac{1}{2}||w||_1.$$

Similarly, we have a general result for adding an edge between two graphs. See Figure 4.1 for an illustration.

doi:10.6342/NTU202301030

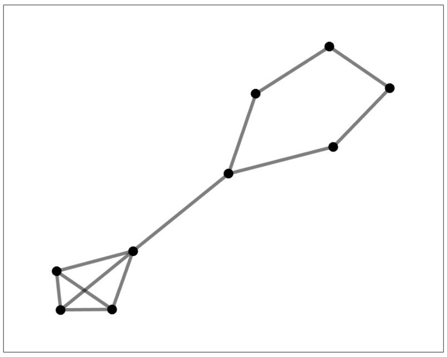


Figure 4.1: Add an edge between K_4 and C_5.

Theorem 4.2 (Bridging two graphs)**.** *Assume G_1, G_2 are two connected graphs admitting nonnegative curvatures w_1 and w_2, respectively. Let $v \in V(G_1), u \in V(G_2)$ be two vertices, and let G be the graph obtained by adding an edge between v and u. Then G admits a curvature nonnegative everywhere except at the two vertices u, v.*

Proof. Let D_1, D_2, D be the distance matrices of G_1, G_2 and G, respectively, so that $D_i w_i = n_i \cdot \mathbf{1}$ for $i = 1, 2$. Write $V(G_1) = \{v_1, ..., v_{n_1}\}$ and $V(G_2) = \{u_1, ..., u_{n_2}\}$. Without loss of generality, assume $v = v_{n_1}$ and $u = u_1$. Let y be the last column of D_1 and x be the first row of D_2. Namely,

$$y = \begin{bmatrix} d_{G_1}(v_1, v_{n_1}) \\ \vdots \\ d_{G_1}(v_{n_1}, v_{n_1}) \end{bmatrix}, x = [d_{G_2}(u_1, u_1) \cdots d_{G_2}(u_1, u_{n_2})].$$

Note that

$$d_G(v_i, u_j) = d_{G_1}(v_i, v_{n_1}) + 1 + d_{G_2}(u_1, u_j) \text{ for } 1 \le i \le n_1, 1 \le j \le n_2.$$

Namely,

$$d_G(v_i, u_j) = y_i + 1 + x_j \text{ for all } i, j.$$

Thus, we can write

$$D = \begin{bmatrix} D_1 & y\mathbf{1}^t + \mathbf{1}\mathbf{1}^t + \mathbf{1}x \\ \mathbf{1}y^t + \mathbf{1}\mathbf{1}^t + x^t\mathbf{1}^t & D_2 \end{bmatrix}.$$

Let $\alpha, s \in \mathbb{R}$ to be chosen later. Let $e_{n_1} = (0, ..., 0, 1)^t \in \mathbb{R}^{n_1}$ and $e_1 = (1, 0, ..., 0)^t \in \mathbb{R}^{n_2}$.

doi:10.6342/NTU202301030

Put

$$w = \begin{bmatrix} \alpha w_1 + s e_{n_1} \\ w_2 + s e_1 \end{bmatrix}.$$

Then

$$Dw = \begin{bmatrix} \alpha n_1 \mathbf{1} + y \mathbf{1}^t w_2 + \mathbf{1}\mathbf{1}^t w_2 + \mathbf{1} x w_2 \\ \alpha \mathbf{1} y^t w_1 + \alpha \mathbf{1}\mathbf{1}^t w_1 + \alpha x^t \mathbf{1}^t w_1 + n_2 \mathbf{1} \end{bmatrix} + \begin{bmatrix} sy \\ s(x^t + \mathbf{1}) \end{bmatrix} + \begin{bmatrix} s(y+\mathbf{1}) \\ s x^t \end{bmatrix},$$

since $x_1 = y_{n_1} = 0$. Note that $y^t w_1 = n_1$ and $x w_2 = n_2$ by looking at the corresponding rows of $D_i w_i = n_i \cdot \mathbf{1}$. Thus,

$$Dw = \begin{bmatrix} (\alpha n_1 + \mathbf{1}^t w_2 + n_2 + s)\mathbf{1} + (2s + \mathbf{1}^t w_2) y \\ (\alpha n_1 + n_2 + \alpha \mathbf{1}^t w_1 + s)\mathbf{1} + (2s + \alpha \mathbf{1}^t w_1) x^t. \end{bmatrix}.$$

Put

$$s = \frac{-\mathbf{1}^t w_2}{2}, \alpha = \frac{\mathbf{1}^t w_2}{\mathbf{1}^t w_1} > 0.$$

Since $\mathbf{1}^t w_1 > 0$, α is well defined. Then $2s = -\mathbf{1}^t w_2 = -\alpha \mathbf{1}^t w_1$. Then we get

$$Dw = (\alpha n_1 + \mathbf{1}^t w_2 + n_2 + s)\mathbf{1} = (\alpha n_1 + n_2 + \frac{\mathbf{1}^t w_2}{2})\mathbf{1},$$

which implies that G admits a curvature by scaling. We have

$$\alpha n_1 + n_2 + \frac{\mathbf{1}^t w_2}{2} > 0.$$

Therefore, G admits a curvature being nonnegative at every vertex except for at v_{n_1} and u_1. □

We have a similar statement when the graph admits a positive curvature. The proof is the same as above.

Proposition 4.3. *Let G_1 and G_2 be two graphs admitting positive curvatures. Let G be the graph obtained by adding an edge between G_1 and G_2. Then G admits a curvature that is positive at every vertex except at the vertices belonging to the edge.*

Remark. By the above computations, the curvature at v_{n_1} and u_1 are

$$\frac{||w_2||_1(n_1+n_2)}{n_1||w_2||_1 + n_2||w_1||_1 + \frac{1}{2}||w_1||_1||w_2||_1} \cdot ((w_1)_{n_1} - \frac{1}{2}||w_1||_1)$$

doi:10.6342/NTU202301030

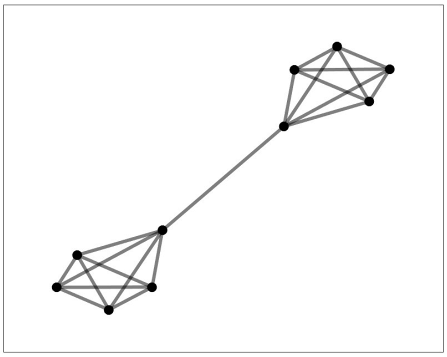


Figure 4.2: The 5-barbell graph.

and

$$\frac{||w_1||_1(n_1+n_2)}{n_1||w_2||_1+n_2||w_1||_1+\frac{1}{2}||w_1||_1||w_2||_1}\cdot((w_2)_1-\frac{1}{2}||w_2||_1),$$

respectively.

It is possible for the vertices being bridged to have negative curvatures. Consider two copies of the 3-cycle C_3, and connect them by an edge. It has a unique curvature

$$w=(\frac{12}{11},\frac{12}{11},\frac{-6}{11},\frac{-6}{11},\frac{12}{11},\frac{12}{11}).$$

It remains unclear whether the two vertices belonging to the bridge always have negative curvatures. We do not know if there are graphs with positive curvature w such that $w_i > \frac{1}{2}||w||_1$ for some i.

Remark. Following the proof in the above theorem, as long as G_1, G_2 admit curvatures and $\mathbf{1}^t w_2 \neq 0$ (so that α is well-defined), then the resulting graph G admits a curvature. It is unclear whether a graph that admits a curvature w implies $\mathbf{1}^t w \neq 0$.

Example. By adding an edge between two copies of K_n, we get the *n-barbell graph*. See Figure 4.2. Since K_n has a constant curvature $K=\frac{n}{n-1}>0$, and $\alpha=1$, the n-barbell graph admits a curvature that is constant and positive everywhere except at the vertices belonging to the bridge.

We have the following corollary by following the proof in the above theorem.

Corollary 4.4. *Assume G admits a constant curvature $K>0$, and let G' be two copies of G with an edge connecting them. Then G' admits a curvature whose value is $\frac{(2-n)2K}{4+K}<0$*

doi:10.6342/NTU202301030

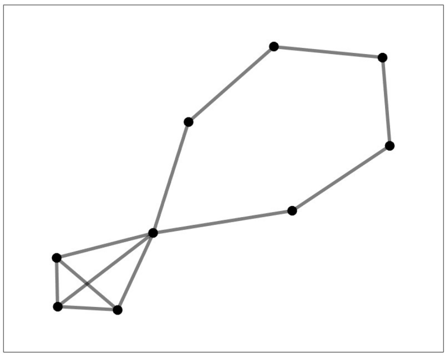


Figure 4.3: Merging K_4 and C_6 at one vertex.

at the vertices belonging to the edge and $\frac{4K}{4+K} > 0$ *at all the other vertices.*

We next show that non-negative curvature stays preserved when we merge two graphs at a vertex, that is, add an edge between two graphs then perform an edge contraction on this edge. See Figure 4.3.

Theorem 4.5 (Merging two graphs at a vertex)**.** *Let G_1, G_2 be graphs admitting nonnegative curvatures. Let G be the graph obtained by merging a vertex v in G_1 and a vertex u in G_2. Then G admits a curvature nonnegative everywhere except at the vertex that is merged.*

Proof. Write $V(G_1) = \{v_1, ..., v_{n_1}\}$ and $V(G_2) = \{u_1, ..., u_{n_2}\}$. Without loss of generality, assume that the vertices that are merged are v_{n_1} and u_1. Let D_i be the distance matrix of G_i with $D_1 w = n_1 \cdot \mathbf{1}$ and $D_2 g = n_2 \cdot \mathbf{1}$. Let D be the distance matrix of G. Let $y \in \mathbb{R}^{n_1}$ be the last column of D_1 and $x \in \mathbb{R}^{n_2 - 1}$ be the first row of D_2 without the first entry. Namely,

$$y = \begin{bmatrix} d_{G_1}(v_1, v_{n_1}) \\ \vdots \\ d_{G_2}(v_{n_1}, v_{n_1}) \end{bmatrix}, x = [d_{G_2}(u_1, u_2) \cdots d_{G_2}(u_1, u_{n_2})].$$

Let $\bar{g} = (g_2, ..., g_{n_2})$, and $\bar{D_2}$ be the matrix obtained by removing the first column and the first row of D_2. Thus,

$$D_2 = \begin{bmatrix} 0 & x \\ x^t & \bar{D_2} \end{bmatrix}.$$

doi:10.6342/NTU202301030

The equation $D_2 g = n_2 \cdot \mathbf{1}$ gives $\bar{D}_2 \bar{g} = n_2 \mathbf{1} - g_1 x^t$ and $x\bar{g} = n_2$. Note that

$$d_G(v_i, u_j) = d_{G_1}(v_i, v_{n_1}) + d_{G_2}(u_1, u_j) = y_i + x_{j-1}$$

for all $1 \leq i \leq n_1$ and $2 \leq j \leq n_2$. Also, we have

$$d_G(v_i, v_j) = d_{G_1}(v_i, v_j)$$

$$d_G(u_i, u_j) = d_{G_2}(u_i, u_j)$$

for all i, j. Thus, we can write

$$D = \begin{bmatrix} D_1 & y\mathbf{1}^t + \mathbf{1}x \\ \mathbf{1}y^t + x^t\mathbf{1}^t & \bar{D}_2 \end{bmatrix} \in \mathbb{R}^{(n_1+n_2-1)\times(n_1+n_2-1)}$$

Let $\alpha, s \in \mathbb{R}$ be chosen later. Define

$$w' = \begin{bmatrix} \alpha w \\ \mathbf{0}_{n_2-1} \end{bmatrix} + \begin{bmatrix} \mathbf{0}_{n_1} \\ \bar{g} \end{bmatrix} + (s + g_1)e_{n_1} \in \mathbb{R}^{n_1+n_2-1},$$

where $e_{n_1} \in \mathbb{R}^{n_1+n_2-1}$ is the n_1-th coordinate vector. Then

$$\begin{aligned} Dw' &= \begin{bmatrix} \alpha n_1 \mathbf{1} \\ \alpha \mathbf{1} y^t w + \alpha x^t \mathbf{1}^t w \end{bmatrix} + \begin{bmatrix} y\mathbf{1}^t\bar{g} + \mathbf{1}x\bar{g} \\ n_2\mathbf{1} - g_1 x^t \end{bmatrix} + (s + g_1)\begin{bmatrix} y \\ x^t \end{bmatrix} \\ &= \begin{bmatrix} (\alpha n_1 + x\bar{g})\mathbf{1} \\ (\alpha y^t w + n_2)\mathbf{1} \end{bmatrix} + \begin{bmatrix} (\mathbf{1}^t\bar{g} + s + g_1)y \\ (\alpha\mathbf{1}^t w + s)x^t \end{bmatrix}. \end{aligned}$$

Note that $x\bar{g} = n_2$ and $y^t w = n_1$. Also, G_1 admits a nonnegative curvature implies $\mathbf{1}^t w > 0$. Set

$$\begin{aligned} s &= -g_1 - \mathbf{1}^t\bar{g} = -\mathbf{1}^t g \\ \alpha &= \frac{-s}{\mathbf{1}^t w} = \frac{\mathbf{1}^t g}{\mathbf{1}^t w}. \end{aligned}$$

Then $Dw' = (\alpha n_1 + n_2)\mathbf{1}$. Thus, we have

$$D\left(\frac{n_1 + n_2 - 1}{\alpha n_1 + n_2} w'\right) = (n_1 + n_2 - 1)\mathbf{1},$$

and G admits a curvature. Since $w \in \mathbb{R}^{n_1}_{\geq 0}$ and $g \in \mathbb{R}^{n_2}_{\geq 0}$, we have $\alpha > 0$. Thus, by the

doi:10.6342/NTU202301030

construction, G admits a curvature that is nonnegative everywhere except at the vertex v_{n_1}. $\square$

Remark. By the computations above, the curvature at v_{n_1} is

$$\frac{||g||_1(w)_{n_1} - ||w||_1||\bar{g}||_1}{||g||_1 n_1 + ||w||_1 n_2} \cdot (n_1 + n_2 - 1).$$

We have a version when the graph admits a positive curvature. The proof is same as above.

Proposition 4.6. *Let G_1, G_2 be two graphs admitting positive curvatures. Let G be the graph obtained by merging G_1 and G_2 at a vertex. Then G admits a curvature positive everywhere except at this vertex.*

If a graph contains a bridge that admits a nonnegative curvature, then after removing the bridge from the graph, the two connected components also have nonnegative curvatures. To give an intuition of the proof, we first consider the simple case when there is a pendant vertex.

Proposition 4.7 (Removing a pendant vertex.)**.** *Let G be a connected graph and suppose there is a vertex v with degree 1. Let $G' = G \setminus \{v\}$. If G admits a nonnegative curvature then G' admits a nonnegative curvature. If G admits a constant curvature then G' admits a constant curvature except at one vertex.*

Proof. Assume $v = v_n$. Let D be the distance matrix of G, and w be its curvature. Thus, $Dw = n \cdot \mathbf{1}$. Let D' be the distance matrix of G'. Then D' is the matrix obtained by removing the last row and the last column of D. Write

$$D = \begin{bmatrix} D' & u \\ u^t & 0 \end{bmatrix}.$$

Let y be the last column of D', i.e.,

$$y = [d(v_1, v_{n-1}), ..., d(v_{n-1}, v_{n-1})]^t.$$

Then $u = y + \mathbf{1}$. Let

$$\bar{w} = (w_1, ..., w_{n-1})^t,$$

doi:10.6342/NTU202301030

$$e_{n-1} = (0, ..., 0, 1)^t \in \mathbb{R}^{n-1},$$

$$\tilde{w} = \bar{w} + w_n e_{n-1},$$

where w_i is the ith entry of w. Then $Dw = n \cdot \mathbf{1}$ implies $D'\bar{w} + w_n u = n \cdot \mathbf{1}$ and $u^t \bar{w} = n$. Thus,

$$D'\tilde{w} = D'\bar{w} + D'(w_n e_{n-1}) = n\mathbf{1} - w_n u + w_n y = (n - w_n)\mathbf{1}.$$

Note that $Dw = n\mathbf{1}$ and $w \in \mathbb{R}^n$ implies $w_n < n$. Put

$$w' = \frac{\tilde{w}(n-1)}{n - w_n}.$$

We get $D'w' = (n-1)\mathbf{1}$ and $w' \in \mathbb{R}^{n-1}_{\geq 0}$.

If $w \equiv K > 0$, then w' is constant everywhere except possibly at vertex v_{n-1}. $\square$

We now consider the general case when we remove a bridge from a graph.

Proposition 4.8 (Removing a bridge from a graph)**.** *Let G be a connected graph containing a bridge e. Let G_1, G_2 be the two connected components obtained by removing e from G. If G admits a nonnegative curvature, then G_i admits a nonnegative curvature for $i = 1, 2$. If G admits a constant curvature, then G_i admits a constant curvature for $i = 1, 2$ except at the vertices belonging to e.*

Proof. Let D_i be the distance matrix of G_i for $i = 1, 2$ and $V(G_1) = \{v_1, ..., v_{n_1}\}$, $V(G_2) = \{u_1, ..., u_{n_2}\}$. Assume that $e = \{v_{n_1}, u_1\}$ without loss of generality. Write

$$Dw = (n_1 + n_2)\mathbf{1}, w = \begin{bmatrix} w_1 \\ w_2 \end{bmatrix}$$

where $w_i \in \mathbb{R}^{n_i}_{\geq 0}$. Let y be the last column of D_1 and let x be the first row of D_2, as in the proof of Theorem 4.2. Then

$$D = \begin{bmatrix} D_1 & y\mathbf{1}^t + \mathbf{1}\mathbf{1}^t + \mathbf{1}x \\ \mathbf{1}y^t + \mathbf{1}\mathbf{1}^t + x^t\mathbf{1}^t & D_2 \end{bmatrix}.$$

Since $Dw = (n_1 + n_2)\mathbf{1}$, we get

$$D_1 w_1 + y\mathbf{1}^t w_2 + \mathbf{1}\mathbf{1}^t w_2 + \mathbf{1}x w_2 = (n_1 + n_2)\mathbf{1}$$

doi:10.6342/NTU202301030

$$\mathbf{1}y^t w_1 + \mathbf{1}\mathbf{1}^t w_1 + x^t \mathbf{1}^t w_1 + D_2 w_2 = (n_1 + n_2)\mathbf{1}.$$

Furthermore, by looking at the n_1-th and the $n_1 + 1$-th rows of $Dw = (n_1 + n_2)\mathbf{1}$, we have

$$y^t w_1 + (x + \mathbf{1}^t) w_2 = n_1 + n_2$$

$$(\mathbf{1} + y)^t w_1 + x w_2 = n_1 + n_2$$

Define

$$\bar{w_1} = w_1 + \mathbf{1}^t w_2 e_{n_1}$$

$$\bar{w_2} = w_2 + \mathbf{1}^t w_1 e_1.$$

Then

$$D_1 \bar{w_1} = D_1 w_1 + \mathbf{1}^t w_2 y = (n_1 + n_2 - \mathbf{1}^t w_2 - x w_2)\mathbf{1} = y^t w_1 \mathbf{1}$$

$$D_2 \bar{w_2} = D_2 w_2 + \mathbf{1}^t w_1 x^t = (n_1 + n_2 - y^t w_1 - \mathbf{1}^t w_1)\mathbf{1} = (x w_2)\mathbf{1}.$$

Since $w_i \in \mathbb{R}^{n_i}_{\geq 0}$ are nonnegative curvatures for $i = 1, 2$, we have $y^t w_1, x w_2 > 0$. Consider

$$w_1' = \frac{\bar{w_1}}{y^t w_1} n_1$$

$$w_2' = \frac{\bar{w_2}}{x w_2} n_2,$$

then $D_i w_i' = n_i$ for $i = 1, 2$. Thus, G_i admits a nonnegative curvature for $i = 1, 2$.

If both w_1, w_2 are constant, then by construction, w_1' is constant everywhere except at vertex v_{n_1} and w_2' is constant everywhere except at vertex u_1. □

4.2 The Null Space of Graph Distance Matrix

In this section, we study the null space of the graph distance matrix after we connect two nonnegatively curved graphs via an edge. We first need a lemma.

Lemma 4.9. *If G admits a nonnegative curvature $w \in \mathbb{R}^n_{\geq 0}$ and $Dg = \mathbf{1}$, then $\mathbf{1}^t g > 0$.*

Proof. Since G admits a nonnegative curvature, $Dw = n \cdot \mathbf{1}$. If the null space of D is empty, then $g = \frac{1}{n} w \in \mathbb{R}^n_{\geq 0}$. Therefore, $\mathbf{1}^t g > 0$. Otherwise, let $z_1, ..., z_k \in$ null(D). Then

doi:10.6342/NTU202301030

we can write $g = \frac{w}{n} + c_1 z_1 + \cdots + c_k z_k$ for some coefficients c_i. Thus,

$$\mathbf{1}^t g = \mathbf{1}^t \frac{w}{n} + c_1 \mathbf{1}^t z_1 + \cdots + c_k \mathbf{1}^t z_k = \mathbf{1}^t \frac{w}{n} > 0,$$

where we used the fact that $\mathbf{1} \in Im(D) = \text{null}(D)^{\perp}$. $\square$

Proposition 4.10. *Let G_1, G_2 be two nonnegatively curved graphs, and let G be the graph obtained by adding an edge between a vertex in G_1 and another vertex in G_2. Let D, D_1, D_2 be the distance matrices of G, G_1, G_2, respectively. Then we have*

$$\text{null}(D) = \text{null}(D_1) \oplus \text{null}(D_2)$$

and

$$\dim(\text{null}(D)) = \dim(\text{null}(D_1)) + \dim(\text{null}(D_2)),$$

where we canonically embed $\text{null}(D_i) \subset \mathbb{R}^{n_i}$ *into* $\mathbb{R}^{n_1+n_2}$. *Note this implies*

$$\text{rank}(D) = \text{rank}(D_1) + \text{rank}(D_2).$$

Proof. As in the proof of Theorem 4.2, we write

$$D = \begin{bmatrix} D_1 & y\mathbf{1}^t + \mathbf{1}\mathbf{1}^t + \mathbf{1}x \\ \mathbf{1}y^t + \mathbf{1}\mathbf{1}^t + x^t\mathbf{1}^t & D_2 \end{bmatrix},$$

where y is the last column of D_1, and x is the first row of D_2. Since G_1 and G_2 are nonnegatively curved, $\mathbf{1} \in Im(D_i) = \text{null}(D_i)^{\perp}$. This implies $\mathbf{1}$ is perpendicular to $\text{null}(D_i)$. In addition, by Theorem 4.2, G admits a curvature. This implies $\mathbf{1} \in Im(D) = \text{null}(D)^{\perp}$. If $D_1 u = \mathbf{0}$ then we have $D \begin{bmatrix} u \\ \mathbf{0}_{n_2} \end{bmatrix} = \mathbf{0}$, since $y^t u = \mathbf{1}^t u = 0$. If $D_2 v = \mathbf{0}$, then $D \begin{bmatrix} \mathbf{0}_{n_1} \\ v \end{bmatrix} = \mathbf{0}$, since $\mathbf{1}^t v = xv = 0$. Therefore if $u_1, ...u_{k_1}$ is a basis of $\text{null}(D_1)$ and $v_1, ..., v_{k_2}$ is a basis of $\text{null}(D_2)$, then

$$\begin{bmatrix} u_1 \\ \mathbf{0}_{n_2} \end{bmatrix}, ..., \begin{bmatrix} u_{k_1} \\ \mathbf{0}_{n_2} \end{bmatrix}, \begin{bmatrix} \mathbf{0}_{n_1} \\ v_1 \end{bmatrix}, ..., \begin{bmatrix} \mathbf{0}_{n_1} \\ v_{k_2} \end{bmatrix}$$

is linearly independent in $\text{null}(D)$. Thus, $\dim \text{null}(D) \geq k_1 + k_2 = \dim \text{null}(D_1) +$

doi:10.6342/NTU202301030

$\dim \operatorname{null}(D_2)$. On the other hand, if $\begin{bmatrix} u \\ v \end{bmatrix} \in \operatorname{null} D$, then we have

$$\begin{aligned} \mathbf{0}_{n_1} &= D_1 u + y\mathbf{1}^t v + \mathbf{1}xv + \mathbf{1}\mathbf{1}^t v \\ \mathbf{0}_{n_2} &= \mathbf{1}y^t u + x^t \mathbf{1}^t u + \mathbf{1}\mathbf{1}^t u + D_2 v \\ 0 &= \mathbf{1}^t \begin{bmatrix} u \\ v \end{bmatrix} \end{aligned}$$

By looking at the n_1-th row of the first equation and using $y_{n_1} = 0$, we get

$$0 = y^t u + xv + \mathbf{1}^t v.$$

The first row of the second equation and $x_1 = 0$ give

$$0 = y^t u + \mathbf{1}^t u + xv.$$

Combining these with the third equation, we conclude that

$$\mathbf{1}^t u = \mathbf{1}^t v = 0.$$

Therefore, we get

$$\begin{aligned} D_1 u &= -xv\mathbf{1} \\ D_2 v &= -y^t u\mathbf{1}. \end{aligned}$$

Suppose that $xv \neq 0$. Since G_1 admits a nonnegative curvature, by Lemma 4.9, we have $0 < \mathbf{1}^t \frac{u}{-xv} = 0$, a contradiction. Thus, $xv = 0$ and $D_1 u = \mathbf{0}$. Similarly, we have $D_2 v = \mathbf{0}$. Therefore, $u \in \operatorname{null} D_1$ and $v \in \operatorname{null} D_2$. We can thus write $u = c_1 u_1 + \cdots + c_k u_{k_1}$ and $v = d_1 v_1 + \cdots + d_{k_2} v_{k_2}$ where c_i and d_j are not all zeroes. This means that

$$\begin{bmatrix} u \\ v \end{bmatrix} = c_1 \begin{bmatrix} u_1 \\ \mathbf{0}_{n_2} \end{bmatrix} + \cdots + c_{k_1} \begin{bmatrix} u_{k_1} \\ \mathbf{0}_{n_2} \end{bmatrix} + d_1 \begin{bmatrix} \mathbf{0}_{n_1} \\ v_1 \end{bmatrix} + \cdots + d_{k_2} \begin{bmatrix} \mathbf{0}_{n_1} \\ v_{k_2} \end{bmatrix}.$$

Thus, the vectors

$$\begin{bmatrix} u_1 \\ \mathbf{0}_{n_2} \end{bmatrix}, \ldots, \begin{bmatrix} u_{k_1} \\ \mathbf{0}_{n_2} \end{bmatrix}, \begin{bmatrix} \mathbf{0}_{n_1} \\ v_1 \end{bmatrix}, \ldots, \begin{bmatrix} \mathbf{0}_{n_1} \\ v_{k_2} \end{bmatrix}$$

doi:10.6342/NTU202301030

form a basis of null D. This implies $\dim(\text{null } D) = \dim \text{null } D_1 + \dim \text{null } D_2$, as desired. $\square$

4.3 New Proof of Invariance of Total Curvature

In this section, we provide an elementary linear algebraic proof of Theorem 3.4, without using von Neumann's Minimax Theorem.

Theorem 4.11 (Invariance of Total Curvature, [27])**.** *Suppose G is a connected graph and there are $w_1, w_2 \in \mathbb{R}^n_{\geq 0}$ so that $Dw_1 = Dw_2 = n \cdot \mathbf{1}$. Then $||w_1||_{l^1} = ||w_2||_{l^1}$.*

New Proof. Since $Dw_1 = n \cdot \mathbf{1}$, we have $\mathbf{1} \in Im(D) = (\text{null}(D^t))^\perp = (\text{null}(D))^\perp$. Since $D(w_1 - w_2) = 0$, we have $\langle w_1 - w_2, \mathbf{1}\rangle = 0$. Thus, $||w_1||_{l^1} = \langle w_1, \mathbf{1}\rangle = \langle w_2, \mathbf{1}\rangle = ||w_2||_{l^1}$. $\square$

Remark. Suppose we only know the graph admits curvature, that is, $Dw_1 = Dw_2 = n \cdot \mathbf{1}$ for $w_1, w_2 \in \mathbb{R}^n$ that possibly have negative entries. The above proof implies that $\mathbf{1}^t w_1 = \mathbf{1}^t w_2$.

4.4 Nonexistence of Curvature

Recall that in Section 3.4, there seem to be much fewer graphs that the equation $Dx = \mathbf{1}$ does not have a solution. Figure 4.4 are four such graphs. In these cases, the curvature is defined as $D^\dagger(n \cdot \mathbf{1})$, where $D^\dagger$ is the pseudo-inverse of D. We discover the following theorem, which provides a way to create infinitely many graphs that $Dx = \mathbf{1}$ does not have a solution.

Theorem 4.12. *Let G_1 and G_2 be two connected graphs so that for $D_i x = \mathbf{1}$ does not have a solution for $i = 1, 2$, where D_i is the distance matrix of G_i. Let G be the graph obtained by adding an edge between G_1 and G_2 then perform an edge contraction on this edge. Then $Dx = \mathbf{1}$ does not have a solution, where D is the distance matrix of G.*

Proof. As in the proof of Theorem 4.5, without loss of generality, we assume that the last vertex of G_1 is merged with the first vertex of G_2 in G.

doi:10.6342/NTU202301030

Note that $D_1 x = n_1 \cdot \mathbf{1}$ has no solution is equivalent to $\mathbf{1} \notin (\text{null}(D_1))^\perp = Im(D_1)$, which is equivalent to the condition that there is $u \in \text{null}(D_1)$ with $\langle u, \mathbf{1}\rangle \neq 0$. Similarly, we can find a vector $v \in \text{null}(D_2)$ with $\langle v, \mathbf{1}\rangle \neq 0$. Our goal is to find a vector $z \in \text{null}(D)$ so that $\langle z, \mathbf{1}\rangle \neq 0$.

Consider the vector

$$z = \alpha \begin{bmatrix} u \\ \mathbf{0}_{n_2-1} \end{bmatrix} + \begin{bmatrix} \mathbf{0}_{n_1} \\ \bar{v} \end{bmatrix} + (s + v_1) e_{n_1},$$

where $\bar{v} = (v_2, ..., v_{n_2})$, e_{n_1} is the n_1-th coordinate vector, and $s \in \mathbb{R}$ is to be chosen. As in the proof of Theorem 4.5, let $y \in \mathbb{R}^{n_1}$ be the last column of D_1 and $\eta \in \mathbb{R}^{n_2-1}$ be the first row of D_2 without the first entry. Write

$$D = \begin{bmatrix} D_1 & y\mathbf{1}^t + \mathbf{1}\eta \\ \mathbf{1}y^t + \eta^t\mathbf{1}^t & \bar{D}_2 \end{bmatrix} \in \mathbb{R}^{(n_1+n_2-1)\times(n_1+n_2-1)},$$

where

$$D_2 = \begin{bmatrix} 0 & \eta \\ \eta^t & \bar{D}_2 \end{bmatrix}.$$

Then $D_2 v = \mathbf{0}$ implies $\eta\bar{v} = 0$ and $\bar{D}_2\bar{v} + \eta^t v_1 = \mathbf{0}_{n_2-1}$. Therefore,

$$Dz = \begin{bmatrix} \mathbf{0}_{n_1} \\ \alpha\mathbf{1}y^t u + \alpha\eta^t\mathbf{1}^t u \end{bmatrix} + \begin{bmatrix} y\mathbf{1}^t\bar{v} \\ -v_1\eta^t \end{bmatrix} + (s + v_1) \begin{bmatrix} y \\ \eta^t \end{bmatrix}.$$

Note that $D_1 u = \mathbf{0}_{n_1}$ gives $y^t u = 0$. Thus,

$$Dz = \begin{bmatrix} (\mathbf{1}^t v + s)y \\ (\mathbf{1}^t u\alpha + s)\eta^t \end{bmatrix}.$$

Set $s = -\mathbf{1}^t v$ and $\alpha = \frac{\mathbf{1}^t v}{\mathbf{1}^t u}$. Note that α is well defined since $\mathbf{1}^t u \neq 0$. Then

$$Dz = \mathbf{0}_{n_1+n_2-1}.$$

In addition, we have

$$\langle z, \mathbf{1}\rangle = \alpha\mathbf{1}^t u + \mathbf{1}^t v + s = \mathbf{1}^t v \neq 0.$$

Therefore,

$$\mathbf{1} \notin (\text{null}(D))^\perp = Im(D)$$

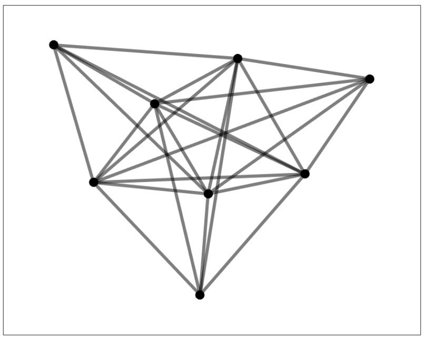
doi:10.6342/NTU202301030

implies that $Dx = \mathbf{1}$ does not have a solution. □

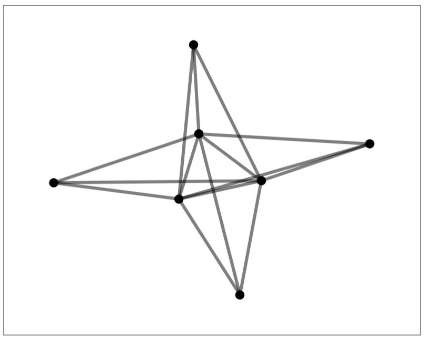
Example. The graph obtained by merging $K_{1,1,1,4}$ and the Quartic-$(11, 18)$ graph at a vertex has no solution to $Dx = \mathbf{1}$. See Figure 4.5.

4.5 Further Remarks

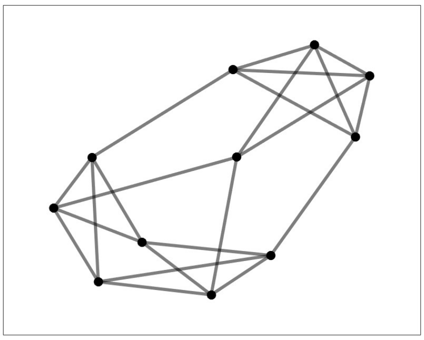
To explain why for most graphs, the linear system of equations $Dx = n \cdot \mathbf{1}$ tends to have a solution, we consider the Erdös-Rényi random graph. The Erdös-Rényi random graph $G(n, p)$ on n vertices is the graph that the vertices v_i and v_j are adjacent with probability p. If p is a constant, then with high probability, the random graph $G(n, p)$ has diameter 2, [31, Theorem 8.5.18]. Note that if a graph G has diameter 2, then its distance matrix has entries $d_{ij} = 1$ if v_i is adjacent to v_j, and $d_{ij} = 2$ otherwise. Thus, there is a connection



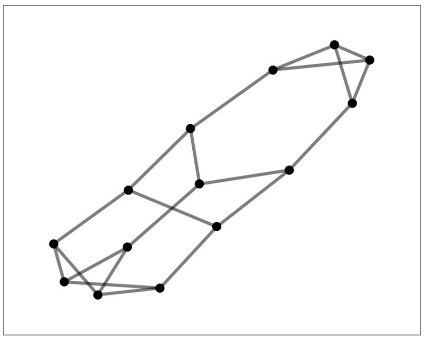
(a) The multipartite graph $K_{1,1,1,1,3}$.



(b) The multipartite graph $K_{1,1,1,4}$.



(c) The Quartic-$(11, 18)$ graph.



(d) The Cubic-$(14, 52)$ graph.

Figure 4.4: Four graphs that $Dx = \mathbf{1}$ has no solution.

doi:10.6342/NTU202301030

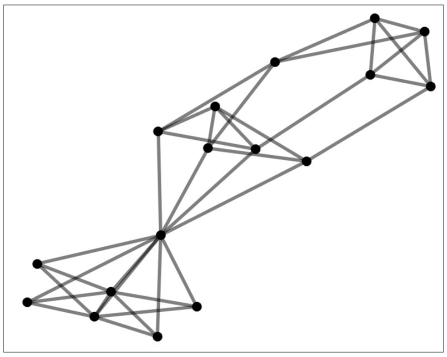


Figure 4.5: Merging $K_{1,1,1,4}$ and Quartic-$(11, 18)$ at a vertex, the resulting graph has no solution to $Dx = \mathbf{1}$.

between the distance matrix D and the adjacency matrix A, that is,

$$D = 2J_n - A - 2I_n \tag{4.5.1}$$

where J_n is the all-one matrix, and I_n is the identity matrix.

We use Matlab to generate Erdös-Rényi random graphs $G(n, p)$, with $n = 50$ and $p = 1/2$. We generate 10000 random graphs and find that for every graph we generate, both the adjacency matrix and the distance matrix have full rank. This suggests the following conjecture.

Conjecture. If p is constant, then with high probability, the distance matrix of $G(n, p)$ is nonsingular.

If this is true, then it can be used to explain why for most graphs, $Dx = \mathbf{1}$ tends to have a solution.

Let Q_n be a random symmetric matrix of size n whose upper triangular entries $q_{ij}(1 \leq i \leq j \leq n)$ are independent Bernoulli random variables. We can view Q_n as the adjacency matrix of $G(n, 1/2)$ if self-loops are allowed. Costello, Tao, and Vu showed the probability that Q_n is singular is $O(n^{-1/8+\delta})$ for any constant $\delta > 0$ in [7]. In other words, with probability 1, the matrix Q_n is invertible as $n \to \infty$. Can we use this result and equation 4.5.1 to show that with probability 1, the distance matrix D of $G(n, 1/2)$ is invertible as $n \to \infty$?

doi:10.6342/NTU202301030

Chapter 5 The Perron Eigenvector of Graph Distance Matrix

Recall in Section 3.4, we presented a sufficient condition for the equation $Dx = n \cdot \mathbf{1}$ to have a solution. This condition requires $\langle v, \mathbf{1} \rangle$ to be close to $\sqrt{n}$, where v denotes the normalized Perron eigenvector of the distance matrix. In this chapter, we further explore the term $\langle v, \mathbf{1} \rangle$ by providing its lower bound. The first section gives an introduction to the Perron-Frobenius theorem, which states that the first eigenvector of graph distance matrices can be chosen to have positive entries. In the second section, a lower bound of $\langle v, \mathbf{1} \rangle$ given in [26] is introduced. The third and fourth sections are original results. We provide lower bounds for $\langle v, \mathbf{1} \rangle$ when the graph is a tree or antipodal and explore the minimum entry of v when the graph has a universal vertex. Further remarks are provided in the final section.

5.1 Background: The Perron-Frobenius Theorem

The Perron-Frobenius theorem was proved by Oskar Perron in 1907 [23]. This theorem guarantees the existence of a positive eigenvalue of a positive matrix and guarantees that the corresponding eigenvector has positive entries. Georg Frobenius generalized this theorem for nonnegative matrices in 1912 [11].

Recall that the distance matrix of a graph is a real, nonnegative, and symmetric matrix. Therefore, its eigenvalues are real numbers. The following theorem is a special version of the Perron-Frobenius theorem for distance matrices. Readers interested in the Perron-Frobenius theory can consult [16, Chapter 8].

Theorem 5.1 (Perron-Frobenius Theorem for Graph Distance Matrix)**.** *Let $D = (d_{ij})$ be*

doi:10.6342/NTU202301030

a graph distance matrix so that $d_{ij} > 0$ for $i \neq j$ and $d_{ii} = 0$ for all i. Let λ be its largest eigenvalue. Then $\lambda > 0$, and there is an eigenvector (x_i) corresponding to λ with positive entries.

The largest eigenvalue $\lambda > 0$ of D is called the *Perron root*, and the corresponding eigenvector x with positive entries is called the *Perron eigenvector*.

We modify the proof in [21], in which Ninio proves a version of this theorem for positive symmetric matrices.

Proof. By the spectral theorem, we can diagonalize $D = Q\Lambda Q^t$, where Λ is a real diagonal matrix and Q is an orthogonal matrix. Since the trace of D is 0 and $D \neq 0$, there is a largest positive eigenvalue. Thus $\lambda > 0$. Suppose $Du = \lambda u$ and $||u||_2 = 1$. Then

$$\lambda u_i = \sum_j d_{ij} u_j \text{ for } i = 1, ..., n.$$

Set $x_j = |u_j| \geq 0$. Then $||x||_2 = 1$. Recall that $\lambda = \sup_{||v||=1} \langle Dv, v\rangle$. Then

$$0 < \lambda = \sum_{i,j} d_{ij} u_i u_j = |\sum_{i,j} d_{ij} u_i u_j| \leq \sum_{ij} d_{ij} x_i x_j \leq \lambda.$$

Since the equality holds, we have $\lambda = \langle Dx, x\rangle$ with $||x||_2 = 1$. Note that we have $Dx = \lambda x$. Indeed, consider the problem of maximizing $R(v) = \langle Dv, v\rangle$ subject to the constraint $||v|| = 1$. Then x is an extremum. Let $\mathcal{L}(v, \eta) = \langle Dv, v\rangle - \eta(||v||^2 - 1)$ be a Lagrange multiplier. We have

$$0 = \nabla_v \mathcal{L}(v, \eta)|_{v=x} = 2(Dx - \eta x)$$

implies $Dx = \eta x$. Therefore, $\lambda = \langle Dx, x\rangle = \eta\langle x, x\rangle = \eta$ implies $Dx = \lambda x$. Thus,

$$\lambda x_i = \sum_j d_{ij} x_j$$

for all i. Suppose that there is some i with $x_i = 0$. We have

$$0 = \sum_{j \neq i} d_{ij} x_j$$

Since $d_{ij} > 0$ and $x_j \geq 0$ for all $j \neq i$, we get $x_j = 0$ for all $j \neq i$. This implies $x = \mathbf{0}$, a contradiction.

doi:10.6342/NTU202301030

Thus, all entries in x are positive. $\square$

Remark. We can also use Perron's theorem to show the above special case. Perron's theorem states that if M is a positive matrix then its largest eigenvalue is positive (in fact, equal to its spectral radius) and the corresponding eigenvector can be chosen to have positive entries ([16, Theorem 8.2.8]). Let λ be the largest eigenvalue of D. Note that $D+I$ is a positive matrix whose largest eigenvalue is $\lambda+1$. By Perron's Theorem, there is a positive eigenvector x so that $(D+I)x=(\lambda+1)x$. Then $Dx=\lambda x$ implies x is a positive eigenvector of D corresponding to λ.

We have a bound for the Perron root of graph distance matrices.

Lemma 5.2 ([9, 33]). *Let D be the distance matrix of a graph G and λ be its largest positive eigenvalue. Let D_{min}, D_{max} be the smallest and largest row sum of D, respectively. Then*

$$D_{max} \geq \lambda \geq \frac{\sum_{i,j} D_{ij}}{n} \geq D_{min} \geq n-1.$$

Proof. We have

$$\lambda = \max \frac{x^t D x}{x^t x} \geq \frac{\mathbf{1}^t D \mathbf{1}}{\mathbf{1}^t \mathbf{1}} = \frac{\sum_{i,j} D_{ij}}{n} \geq D_{min} \geq n-1.$$

On the other hand, let x be the eigenvector with positive entries corresponding to λ, as guaranteed in the Perron-Frobenius theorem. Let i be the index of the maximum entries of x, that is, $x_i \geq x_j$ for every j. Then

$$\lambda x_i = \sum_{j=1}^{n} D_{ij} x_j \leq x_i \sum_{j=1}^{n} D_{ij}.$$

Since $x_i > 0$, we can eliminate it and get

$$\lambda \leq \sum_{j=1}^{n} D_{ij} \leq D_{max}.$$

$\square$

doi:10.6342/NTU202301030

5.2 The Perron Eigenvector and the Constant Vector

In his paper [26], Steinerberger found that for most graphs in the Mathematica 12 database, the Perron eigenvector v of the distance matrix seems to be parallel to the constant vector, in the sense that $\langle v, \frac{\mathbf{1}}{\sqrt{n}}\rangle^2$ is close to 1. He raised the following problem.

Problem. Let G be a connected graph with n vertices. Let D be its distance matrix and v be the Perron eigenvector of D. It seems that $|\langle v, \frac{\mathbf{1}}{\sqrt{n}}\rangle|$ is close to 1 for most graphs. Can we quantify this or make this precise?

The following theorem provides a lower bound of $\langle v, \mathbf{1}\rangle^2$.

Theorem 5.3 (Proposition 2, [26])**.** *Let $D \in \mathbb{R}^{n\times n}$ be the distance matrix of a graph G. Let λ be the Perron root of D and let $v \in \mathbb{R}^n_{>0}$ be the Perron eigenvector of D with $||v||_{l^2} = 1$. Then*

$$\min_{1\leq i\leq n} v_i \geq \frac{1}{2\sqrt{n}}$$

and

$$n \geq \langle v, \mathbf{1}\rangle^2 \geq \frac{n}{2}.$$

Proof. Fix k. Then

$$\begin{aligned}\lambda = \langle Dv, v\rangle = \sum_{i,j=1}^{n} d_{ij}v_iv_j &\leq \sum_{i,j=1}^{n}(d_{ik}+d_{kj})v_iv_j \\ &= 2\left(\sum_{j=1}^{n} v_j\right)\sum_{i=1}^{n} d_{ki}v_i.\end{aligned}$$

We have

$$\sum_{i=1}^{n} d_{ki}v_i = \lambda v_k$$

by looking at the k-th row of $Dv = \lambda v$. Thus,

$$0 < \lambda \leq 2\lambda v_k \cdot \langle v, \mathbf{1}\rangle .$$

Therefore,

$$v_k \geq \frac{1}{2\langle v, \mathbf{1}\rangle} \tag{5.2.1}$$

doi:10.6342/NTU202301030

By the Cauchy-Schwarz inequality, we get

$$v_k \geq \frac{1}{2\|v\| \cdot \|\mathbf{1}\|} = \frac{1}{2\sqrt{n}}.$$

By taking the minimum overall k, we get the first bound. On the other hand, if we sum over $1 \leq k \leq n$ in equation 5.2.1 we obtain

$$\langle v, \mathbf{1} \rangle \geq \frac{n}{2 \langle v, \mathbf{1} \rangle},$$

which implies $\langle v, \mathbf{1}\rangle^2 \geq n/2$. The bound $\langle v, \mathbf{1}\rangle^2 \leq n$ follows by the Cauchy-Schwarz inequality. □

Remark. By more careful and similar arguments, the second bound can be slightly improved:

$$\langle v, \mathbf{1}\rangle^2 \geq \frac{n}{2} + \frac{n-1}{\lambda}.$$

Proof. Fix k. Then

$$\begin{aligned}
\lambda &= \sum_{i,j=1}^{n} d_{ij} v_i v_j \\
&= \sum_{i \neq j} d_{ij} v_i v_j \\
&\leq \sum_{i \neq j} (d_{ik} + d_{kj}) v_i v_j \\
&= \sum_{i,j} (d_{ik} + d_{kj}) v_i v_j - \sum_{i=1}^{n} d_{ik} 2 v_i^2.
\end{aligned}$$

Thus,

$$\lambda + 2 \sum_{i=1}^{n} d_{ik} v_i^2 \leq 2 \langle v, \mathbf{1} \rangle \lambda v_k.$$

Note that

$$\sum_{i=1}^{n} d_{ik} v_i^2 = \sum_{i \neq k} d_{ik} v_i^2 \geq \sum_{i \neq k} v_i^2 = ||v||^2 - v_k^2 = 1 - v_k^2.$$

Thus, we get

$$\lambda + 2 - 2v_k^2 \leq 2\langle v, \mathbf{1}\rangle \lambda v_k. \tag{5.2.2}$$

Sum over k and use the fact that $||v||_2^2 = 1$ we get

$$n\lambda + 2n - 2 \leq 2\langle v, \mathbf{1}\rangle^2 \lambda$$

doi:10.6342/NTU202301030

and thus,

$$\langle v, \mathbf{1}\rangle^2 \geq \frac{n}{2} + \frac{n-1}{\lambda}.$$

Vertex-transitive graphs. Recall from the proof of Theorem 3.1, a vertex-transitive graph, such as the cycle, has the property that the sums of each row of its distance matrix are equal. Therefore, together with the bound in Lemma 5.2, we have $D\mathbf{1} = \lambda\mathbf{1}$, that is, $v := \mathbf{1}$ is a Perron eigenvector, and λ is the Perron root of D. Then $\langle \frac{v}{||v||_2}, \mathbf{1}\rangle^2 = n$.

5.3 Special Cases: Trees and Antipodal Graphs

We consider the special case when the graph is a tree. We provide a lower bound of $\langle v, \mathbf{1}\rangle^2$ involving the number of leaves.

Proposition 5.4. *Let T be a tree with n vertices and l leaves. Let D be its distance matrix, λ be its Perron root, and v be its Perron eigenvector with $||v||_{l^2} = 1$. Then*

$$\langle v, \mathbf{1}\rangle^2 > \frac{n}{2}(\frac{\lambda}{\lambda - l + 2}) + \frac{n-l-1}{\lambda - l + 2}.$$

Proof. Let $V = \{u_1, ..., u_n\}$ be the vertices of T. Let $L \subset V$ be the leaves of T. Fix k. Let $u_k \in L$ be a leaf. Note that if $i, j \neq k$ then

$$d_{ij} \leq d_{ik} + d_{kj} - 2.$$

To see this, assume that u_k is adjacent to $u_{k'}$. Then $d_{ik} = d_{ik'} + 1, d_{jk} = d_{jk'} + 1$. Thus, $d_{ij} \leq d_{ik'} + d_{jk'} = d_{ik} + d_{jk} - 2$. Then we have

$$\begin{aligned}
\lambda &= \sum_{i,j} v_i v_j d_{ij} \\
&\leq \sum_{i,j\neq k} v_i v_j (d_{ik} + d_{kj} - 2) + 2\sum_{i\neq k} v_i v_k d_{ik} + v_k^2 d_{kk} \\
&= 2(\langle v, \mathbf{1}\rangle - v_k)\lambda v_k - 2(\langle v, \mathbf{1}\rangle - v_k)^2 + 2\lambda v_k^2 \\
&= (2\lambda + 4)v_k\langle v, \mathbf{1}\rangle - 2\langle v, \mathbf{1}\rangle^2 - 2v_k^2.
\end{aligned}$$

doi:10.6342/NTU202301030

By summing k over all leaves, we get

$$\lambda l \leq (2\lambda + 4)\langle v, \mathbf{1}\rangle \sum_{k:u_k \in L} v_k - 2\langle v, \mathbf{1}\rangle^2 l - 2 \sum_{k:u_k \in L} v_k^2. \tag{5.3.3}$$

If u_k is not a leaf then $d_{ij} \leq d_{ik} + d_{kj}$. By equation 5.2.2, we get

$$\lambda \leq 2\langle v, \mathbf{1}\rangle \lambda v_k + 2v_k^2 - 2.$$

Summing k over all non-leaves we get,

$$\lambda(n - l) \leq 2\langle v, \mathbf{1}\rangle \lambda \sum_{k:u_k \notin L} v_k + 2 \sum_{k:u_k \notin L} v_k^2 - 2(n - l). \tag{5.3.4}$$

Thus, adding equations 5.3.3 and 5.3.4, we get

$$\lambda n \leq (2\lambda - 2l)\langle v, \mathbf{1}\rangle^2 + 4\langle v, \mathbf{1}\rangle \sum_{k:u_k \in L} v_k + 2\Big(\sum_{k:u_k \notin L} v_k^2 - \sum_{k:u_k \in L} v_k^2\Big) - 2(n - l).$$

Since

$$\sum_{k:u_k \notin L} v_k^2 - \sum_{k:u_k \in L} v_k^2 < \sum_{k:u_k \notin L} v_k^2 + \sum_{k:u_k \in L} v_k^2 = 1$$
$$\sum_{k:u_k \in L} v_k < \langle v, \mathbf{1}\rangle,$$

we get

$$\lambda n < (2\lambda - 2l + 4)\langle v, \mathbf{1}\rangle^2 + 2 - 2(n - l).$$

By Lemma 5.2, we have $\lambda \geq n - 1$. Note that $l \leq n - 1$ since T is a tree. Therefore, the term $\lambda - l + 2$ is positive. Thus,

$$\langle v, \mathbf{1}\rangle^2 > \frac{n}{2}\Big(\frac{\lambda}{\lambda - l + 2}\Big) + \frac{n - l - 1}{\lambda - l + 2}.$$

□

Example. The star graph with n vertices is the graph $S_n = (V, E)$, where $V = \{u_1, ..., u_n\}$, $E = \{(u_i, u_n) : 1 \leq i \leq n - 1\}$. By Lemma 5.2,

$$2n - 2 \geq \lambda \geq \frac{\sum_{i,j} d_{ij}}{n} = \frac{2(n - 1)^2}{n}.$$

doi:10.6342/NTU202301030

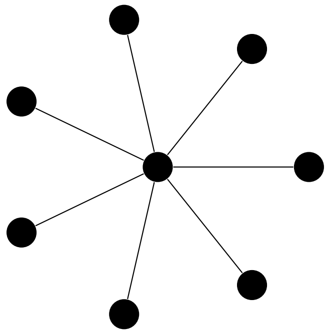


Figure 5.1: The star graph with 8 vertices

There are $l = n - 1$ leaves in S_n. Thus, the bound above gives

$$\langle v, \mathbf{1} \rangle^2 > \frac{(n-1)^2}{n+1} \approx n$$

when n is sufficiently large.

We have the following lower bound of $\langle v, \mathbf{1} \rangle$ in terms of the diameter of the graph and the Perron root of the distance matrix.

Proposition 5.5. *Let G be a connected graph, $\lambda > 0$ be the Perron root of the distance matrix D, and v be the Perron eigenvector. Then*

$$\frac{\lambda}{\text{diam}(G)} \leq \langle v, \mathbf{1} \rangle^2.$$

Proof. The idea is similar to the arguments above. However, we will bound d_{ij} by $\text{diam}(G)$ this time. We have

$$\begin{aligned} \lambda &= \sum_{i,j} d_{ij} v_i v_j \\ &\leq \text{diam}(G) \sum_{i,j} v_i v_j \\ &= \text{diam}(G) \langle v, \mathbf{1} \rangle^2. \end{aligned}$$

Thus, we have

$$\langle v, \mathbf{1} \rangle^2 \geq \frac{\lambda}{\text{diam}(G)}.$$

$\square$

We consider the case when the graph is antipodal. See Chapter 2 for its definition and

doi:10.6342/NTU202301030

properties. Though the following bounds of $\langle v, \mathbf{1}\rangle^2$ is not better than the bound above, its proof may be helpful for future improvements.

Proposition 5.6. *Let G be a connected antipodal graph. Let λ be the largest eigenvalue of the distance matrix D and v be the Perron eigenvector with $||v||_2 = 1$. Then*

$$\frac{\lambda}{\operatorname{diam} G} < \langle v, \mathbf{1}\rangle^2 \leq \frac{2\lambda}{\operatorname{diam} G}.$$

Proof. Since the graph is antipodal, for each $v_i \in V$, we have $d(v_i, v_j) = d(v_i, \bar{v}_i) - d(v_j, \bar{v}_i)$. Thus,

$$\begin{aligned}
\lambda &= \sum_{i,j} d_{ij} v_i v_j \\
&= \sum_{i=1}^{n} v_i \sum_{j=1}^{n} (d_{i\bar{i}} - d_{j\bar{i}}) v_j \\
&= \sum_{i=1}^{n} v_i d_{i\bar{i}} \langle v, \mathbf{1}\rangle - \sum_{i=1}^{n} v_i \sum_{j=1}^{n} d_{j\bar{i}} v_j \\
&= \sum_{i=1}^{n} v_i \operatorname{diam} G \langle v, \mathbf{1}\rangle - \sum_{i=1}^{n} v_i \lambda v_{\bar{i}} \\
&= \operatorname{diam} G \langle v, \mathbf{1}\rangle^2 - \lambda \sum_{i=1}^{n} v_i v_{\bar{i}},
\end{aligned}$$

where we use the fact that $d_{i\bar{i}} = \operatorname{diam}(G)$ from Lemma 2.2. Denote $\bar{v} = (v_{\bar{1}}, \ldots, v_{\bar{n}})$. Since $\bar{\cdot}$ is an automorphism (Lemma 2.2), we get $||\bar{v}|| = ||v|| = 1$. Applying the bounds

$$0 < \sum_{i} v_i v_{\bar{i}} \leq ||v||_2^{\frac{1}{2}} ||\bar{v}||_2^{\frac{1}{2}} = 1,$$

we get the desired result. $\square$

Example. The cycle graph C_{2n} with $2n$ vertices has diameter n and the Perron root of its distance matrix is n^2. Thus, we get

$$\frac{|V|}{2} = n \leq \langle v, \mathbf{1}\rangle^2 \leq 2n = |V|.$$

doi:10.6342/NTU202301030

5.4 Minimum Entries of the Perron eigenvector

We next study the entries of the Perron eigenvector of graph distance matrices. Ruzieh and Powers showed that for a tree, the minimum value among the entries of the Perron eigenvector cannot occur at a leaf [24]. Inspired by the techniques in their proof, we have the following proposition.

Proposition 5.7. *Suppose that the graph G has a vertex v_n with degree $n-1$. Let D be the distance matrix, λ be its Perron root, and x be the Perron eigenvector with all positive entries. Then $x_n = \min\{x_i : 1 \leq i \leq n\}$.*

In other words, if a graph has a universal vertex, then the minimum among all entries of the Perron eigenvector occurs at this vertex.

Proof. Note that $d_{in} = 1$ for $i \neq n$. Then $Dx = \lambda x$ gives

$$\lambda x_n = \sum_{j=1}^{n-1} x_j = \sum_{j \neq i}^{n-1} x_j + x_i.$$

and

$$\lambda x_i = \sum_{j \neq i}^{n} d_{ij} x_j = \sum_{j \neq i}^{n-1} d_{ij} x_j + x_n$$

for $i = 1, ..., n-1$. Thus, for $i \neq n$, we have

$$\lambda(x_i - x_n) = x_n - x_i + \sum_{j \neq i}^{n-1} (d_{ij} - 1) x_j$$

which implies

$$(\lambda + 1)(x_i - x_n) = \sum_{j \neq i}^{n-1} (d_{ij} - 1) x_j \geq 0.$$

Thus, $x_i \geq x_n$ for all i. □

Remark. If $\deg(v_i) < n-1$, then there is a vertex v_j nonadjacent to v_i. This indicates $d_{ij} > 1$. Therefore, by the last inequality in the proof above, $x_i > x_n$. On the other hand, if $\deg(v_i) = n-1$, then $d_{ij} = 1$ for all j implies that $x_i = x_n$.

Remark. It is in general not true that the minimum among the entries of the Perron eigenvector occurs at the vertex with the maximum degree. Figure 5.2 is a counterexample.

doi:10.6342/NTU202301030

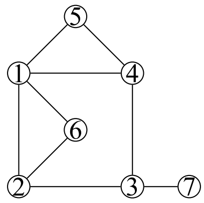


Figure 5.2: The minimum entry of the Perron eigenvector of the graph distance matrix does not occur at the vertex with maximum degree.

Vertex 1 has the maximum degree. However, a numerical computation shows that the minimum entry of the Perron eigenvector occurs at vertex 3.

5.5 Further Remarks

The Davis-Kahan theorem may be helpful in improving the lower bound of $\langle v, \mathbf{1} \rangle$.

Theorem 5.8 (Corollary 3, [32])**.** *Let $D, T \in \mathbb{R}^{n \times n}$ be symmetric. Let λ_1, λ_2 be the largest and the second largest eigenvalues of D. Let η_1 be the largest eigenvalue of T. Assume that $\lambda_1 > \lambda_2$. If $Dv = \lambda_1 v$ and $Tu = \eta_1 u$. Then*

$$\sin\theta(v, u) \leq \frac{2||D - T||_{op}}{\lambda_2 - \lambda_1}.$$

Let D be the distance matrix of a graph and v be its Perron eigenvector with $||v||_2 = 1$. To show that $\langle v, \frac{\mathbf{1}}{\sqrt{n}} \rangle$ is close to 1, that is, the angle between v and $\frac{\mathbf{1}}{\sqrt{n}}$ is small, we shall find a symmetric matrix T to approximate D, so that $\mathbf{1}$ is the first eigenvector of T and the operator norm of $D - T$ is as small as possible.

For example, let $a_i = \sum_{j=1}^{n} D_{ij}$ be the sum of the i-th row of D, and let $\mu = \frac{\sum_i a_i}{n}$ be the average of the sums of rows. Take $T_{ij} = D_{ij}$ if $i \neq j$, and $T_{ii} = \mu - a_i$. We have

$$T\mathbf{1} = \mu\mathbf{1}.$$

By [16, Theorem 8.3.4], μ is the Perron root of T and $\mathbf{1}$ is a Perron eigenvector. Therefore, we get

$$\sin\theta(v, \mathbf{1}) \leq \frac{2\max_i |a_i - \mu|}{\lambda_2 - \lambda_1}.$$

Another question is how the Perron root and the Perron eigenvector behave when we add

doi:10.6342/NTU202301030

an edge between two graphs.

doi:10.6342/NTU202301030

References

[1] G. Aalipour, A. Abiad, Z. Berikkyzy, J. Cummings, J. De Silva, W. Gao, K. Heysse, L. Hogben, F. H. J. Kenter, J. C. H. Lin, and M. Tait. On the distance spectra of graphs, 2015.

[2] J. Azarija. A short note on a short remark of graham and lovász. *Discrete Mathematics*, 315-316:65–68, 2014.

[3] R. B. Bapat. *Distance Matrix of a Tree*, pages 95–109. Springer London, London, 2010.

[4] O. A. Camarena. Math 340: Linear programming. https://www.matem.unam.mx/~omar/math340/math340notes.pdf, September 2018. [Online; accessed 6-February-2023].

[5] M. Chithra and A. Vijayakumar. The diameter variability of the cartesian product of graphs. *Discrete Mathematics, Algorithms and Applications*, 06, 02 2014.

[6] F. Chung and C. B. of the Mathematical Sciences. *Spectral Graph Theory*, pages 1–6. Conference Board of Mathematical Sciences. American Mathematical Society, 1997.

[7] K. Costello, T. Tao, and V. Vu. Random symmetric matrices are almost surely non-singular, 2005.

[8] D. Cushing, S. Kamtue, J. Koolen, S. Liu, F. Münch, and N. Peyerimhoff. Rigidity of the bonnet-myers inequality for graphs with respect to ollivier ricci curvature, 2018.

[9] N. Denny. Bounds on the largest eigenvalue of the distance matrix of connected graphs. Master thesis project., Portland State University, 2020.

doi:10.6342/NTU202301030

[10] R. Diestel. *Graph Theory*. Springer Publishing Company, Incorporated, 5th edition, 2017.

[11] G. Frobenius. *Über Matrizen aus nicht negativen Elementen*. Preussische Akademie der Wissenschaften Berlin: Sitzungsberichte der Preußischen Akademie der Wissenschaften zu Berlin. Reichsdr., 1912.

[12] D. Gagliardi, M. Gargano, and L. Quintas. Neighborhood regular graphs. *Congressus Numerantium*, page 3, Jan 2007.

[13] R. L. Graham and H. O. Pollak. On the addressing problem for loop switching. *The Bell System Technical Journal*, 50(8):2495–2519, 1971.

[14] M. Hall. Game theory and von neumann' s minimax theorem. Honors student work. 5., Bethel University, 2011.

[15] R. Hammack, W. Imrich, and S. Klavzar. *Handbook of Product Graphs, Second Edition*, pages 49–51. CRC Press, Inc., USA, 2nd edition, 2011.

[16] R. Horn and C. Johnson. *Matrix Analysis*. Cambridge University Press, 2012.

[17] S. C. (https://math.stackexchange.com/users/180309/samuel coskey). What is the smallest example of a connected regular graph which is not vertex-transitive? Mathematics Stack Exchange. URL:https://math.stackexchange.com/q/2126259 (version: 2017-04-13).

[18] J. Koolen, V. Moulton, and D. Stevanović. The structure of spherical graphs. *European Journal of Combinatorics*, 25(2):299–310, 2004. In memory of Jaap Seidel.

[19] Y. Lin, L. Lu, and S.-T. Yau. Ricci curvature of graphs. *Tohoku Mathematical Journal*, 63(4):605 – 627, 2011.

[20] J. Matousek and B. Gärtner. *Understanding and Using Linear Programming*, pages 80–104. Universitext. Springer Berlin Heidelberg, 2006.

[21] F. Ninio. A simple proof of the perron-frobenius theorem for positive symmetric matrices. *Journal of Physics A: Mathematical and General*, 9(8):1281, Aug 1976.

[22] Y. Ollivier. A survey of ricci curvature for metric spaces and markov chains. 2010.

doi:10.6342/NTU202301030

[23] O. Perron. Zur theorie der matrices. *Mathematische Annalen*, 64(2):248–263, Jun 1907.

[24] S. N. Ruzieh and D. L. Powers. The distance spectrum of the path pn and the first distance eigenvector of connected graphs. *Linear and multilinear algebra*, 28(1-2):75–81, 1990.

[25] R. P. Sreejith, K. Mohanraj, J. Jost, E. Saucan, and A. Samal. Forman curvature for complex networks. *Journal of Statistical Mechanics: Theory and Experiment*, 2016(6):063206, Jun 2016.

[26] S. Steinerberger. The first eigenvector of a distance matrix is nearly constant, 2022.

[27] S. Steinerberger. Curvature on graphs via equilibrium measures. *Journal of Graph Theory*, 103(3):415–436, 2023.

[28] D. Stevanović. Antipodal graphs of small diameter. *Filomat*, 15:79–83, 2001.

[29] J. von Neumann. Zur theorie der gesellschaftsspiele. *Mathematische Annalen*, 100:295–320, 1928.

[30] V. Vu. Recent progress in combinatorial random matrix theory, 2020.

[31] D. West. *Introduction to Graph Theory*. Featured Titles for Graph Theory. Prentice Hall, 2001.

[32] Y. Yu, T. Wang, and R. J. Samworth. A useful variant of the davis–kahan theorem for statisticians, 2014.

[33] B. Zhou and N. Trinajstić. On the largest eigenvalue of the distance matrix of a connected graph. *Chemical Physics Letters*, 447(4):384–387, 2007.

doi:10.6342/NTU202301030