Characterization of Trivalent Graphs with Minimal Eigenvalue Gap*

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Among all trivalent graphs on \( n \) vertices, let \( G_n \) be one with the smallest possible eigenvalue gap. (The eigenvalue gap is the difference between the two largest eigenvalues of the adjacency matrix; for regular graphs, it equals the second smallest eigenvalue of the Laplacian matrix.) We show that \( G_n \) is unique for each \( n \) and has maximum diameter. This extends work of Guiduli and solves a conjecture implicit in a paper of Bussemaker, Čobaljić, Cvetković and Seidel. Depending on \( n \), the graph \( G_n \) may not be the only one with maximum diameter. We thus also determine all cubic graphs with maximum diameter for a given number \( n \) of vertices.

Keywords
trivalent graphs
eigenvalue gap
Laplacian matrix

NOMENCLATURE

Graphs in this paper are undirected, connected, trivalent (also called cubic) graphs on \( n \) vertices, without loops or multiple edges. For such a graph \( G \), we denote the edge set by \( E \) or \( E(G) \) if we have to emphasize its dependence on \( G \). Similarly, we write the vertex set as \( V = V(G) = \{1, 2, ..., n\} \). The Laplacian matrix \( L \) or \( L(G) \) is defined as \( L(G) = D(G) - A(G) \), where \( A \) denotes the adjacency matrix. Spectral theory originally defines the spectrum of \( G \) as the spectrum of \( A \). This paper, however, prefers to deal with the Laplacian spectrum of \( G \), that is, the spectrum of \( L \). Obviously, these spectra are in a linear relationship with each other. (Therefore, the choice of \( L \) instead of \( A \) is mathematically irrelevant for regular graphs; however, there are applications where \( L \) arises more naturally than \( A \), cf. Ref. 1.) The matrix \( L \) is positive semidefinite, with an eigenvector \( j = (1, 1, ..., 1)^T \) corresponding to the eigenvalue 0. As \( G \) is connected, this eigenvalue has multiplicity 1.

INTRODUCTION

Let \( 0 = \lambda_1 < \lambda_2 \leq ... \leq \lambda_n \), be the eigenvalues of \( L \). The eigenvalue \( \lambda = \lambda_2 \) is called the eigenvalue gap (for connected regular graphs, this is the difference between the two largest eigenvalues of the adjacency matrix). The eigenvalue gap was first investigated by Fiedler in 1973, who called it the algebraic connectivity of a graph (see Ref. 2). The intuition is that the gap is large if and only if the graph has large »connectivity«. Fiedler bounded the gap above and below by functions of the edge connectivity of the graph. This was extended by Alon and Milman3 and Alon4, who bounded the isoperimetric ratio (a more
global measure of connectivity) above and below, respectively, by functions of the eigenvalue gap (see their respective papers). The difference between two consecutive eigenvalues of various matrices has applications in chemistry or biology, see e.g. Refs. 5 and 6.

We show that the trivalent graph on \( n \) vertices with minimal second-largest eigenvalue is uniquely determined.

Guiduli\(^7\) already proved that such a graph must look like a path; more precisely, he showed that the graph must be reduced path-like. A trivalent graph is said to be reduced path-like if it is built from non-trivial blocks with bridges in-between:

\[
\begin{array}{c}
\text{At the left end we have one of the blocks:} \\
\text{The block at the right end is the mirror image of one of these blocks. Each interior block is of the type:}
\end{array}
\]

We will refer to these four types of blocks as small or big blocks, at the end or in the interior, respectively. Note that in our figures we draw the bridges (which in the sense of the usual definition are blocks, too) as outgoing edges of non-trivial blocks. Speaking of blocks we thus always mean the non-trivial ones.

The main result of this paper, Theorem 1, states that the trivalent graph with minimum eigenvalue gap is the one specified explicitly in the next definition.

**Definition 1.** – Let \( G_n \) be the reduced path-like graph on \( n \) vertices with small interior blocks and one small end block. The other end block is then forced by the value of \( n \). (Notice that trivalent graphs only exist for even \( n \) and that, so far, \( G_n \) only makes sense for \( n \geq 10 \).) If \( n \equiv 2 \) (mod 4), then \( G_n \) is the graph:

\[
\begin{array}{c}
\text{If } n \equiv 0 \text{ (mod 4), then } G_n \text{ is the graph:}
\end{array}
\]

\( G_4, G_6 \) and \( G_8 \) are:

\[
\begin{array}{c}
\text{Numerical values of the eigenvalue gap for some } n \text{ are}
\end{array}
\]

\[
\begin{array}{c|c|c|c|c}
\hline
n & \lambda_2(G_n) & n & \lambda_2(G_n) & n & \lambda_2(G_n) \\
\hline
4 & 4 & 12 & 0.167742 & 20 & 0.0515873 \\
6 & 2 & 14 & 0.104893 & 50 & 0.00789634 \\
8 & 0.763932 & 16 & 0.0840222 & 100 & 0.0019742 \\
10 & 0.221543 & 18 & 0.0620222 & 200 & 0.000493469 \\
\hline
\end{array}
\]

The values for \( n = 50, 100, 200 \) indicate the asymptotic behaviour: Doubling \( n \) reduces \( \lambda_2 \) by about a factor 4. Indeed, asymptotically \( \lambda_2(G_n) = 2n^2 / n^2 + O(n^{-3}) \). (The proof of this result will be the subject of a separate note.)

We prove the following theorem, conjectured by Bussemaker, Čobelić, Cvetković and Seidel:\(^8\)

**Theorem 1.** – The graph \( G_n \) is the unique trivalent graph on \( n \) vertices with minimum eigenvalue gap.

**Proof:** Guiduli\(^7\) showed that the graph with minimum eigenvalue gap must be reduced path-like, built from big and small blocks as specified in (1) and (2). Starting from there, the proof distinguishes several cases. The next three sections deal with technical details, cast into several lemmas and corollaries.

Let us summarize the main course of the arguments: Lemma 4 rules out big interior blocks. Thus, only the type of blocks at the end has to be determined. For \( n \equiv 0 \) (mod 4), Corollary 1 settles the affair. For \( n \equiv 2 \) (mod 4), two graphs remain to consider: \( G_n \) and the graph \( H_n \) with big blocks at both ends. Lemma 5 will rule out the second possibility.

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**EIGENSYSTEMS OF PATH-LIKE TRIVALENT GRAPHS**

For path-like graphs built from the four blocks specified in (1) and (2), we need some properties of their Laplacian eigensystems and, specifically, the eigenvalue gap \( \lambda_2 \).

Let \( L \) be the Laplacian matrix of a connected graph \( G \) on \( n \) vertices, and let \( x \in \mathbb{R}^n \) be an \( n \)-vector. The value

\[
x^T L x / \|x\|^2
\]

is called the Rayleigh quotient. Let \( j = (1, 1, ..., 1)^T \in \mathbb{R}^n \), \( \alpha \in \mathbb{R} \); it is well known, cf. e.g. Refs. 1 and 9, that:

\[
\lambda_2 = \min_{x \neq 0, x \perp j} \frac{x^T L x}{\|x\|^2} = \min_{x \neq 0, x \perp j} \frac{\sum_{i \neq j} (x_i - x_j)^2}{\|x\|^2} = n \min_{x \neq 0, x \perp j} \frac{\sum_{i \neq j} (x_i - x_j)^2}{\|x\|^2}
\]

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The Rayleigh quotient will be our main tool. Right now, we use it for a rough estimate of the eigenvalue gap $\lambda_2$.

**Lemma 1.** – Let $G$ be a connected trivalent graph on $n$ vertices ($n \geq 10$), built from big and small blocks as specified in (1) and (2). Then,

$$\lambda_2 < \frac{12}{n}.$$

**Proof:** Define $x$ with $x_1, \ldots, x_{n/2} = -1$ for all vertices in the left half of $G$, $x_1 = 1$ for the remaining $n/2$ vertices in the right half of $G$. Clearly, $x \perp f$, and at most three edges will contribute to the sum for the Rayleigh quotient. □

This estimate is far from optimal and easy to improve, but it tells us that we definitely do not have to search for the minimal $\lambda_2$ at values greater than 2.

**Definition 2.** – Let $G$ be a connected trivalent graph on $n$ vertices, built from big and small blocks as specified in (1) and (2). We define a partition $\Pi(G) = (C_1, \ldots, C_m)$, where the cells $C_i$ are disjoint subsets, each containing exactly one or two vertices from $V = \{1, \ldots, n\}$, their union being $V$. We specify that vertices drawn vertically above each other in our figures shall belong to the same cell, and we will number cells consecutively from left to right.

To illustrate this principle, a graph starting with a small block (1) at the left end will have two vertices in cell $C_1$, two in $C_2$, one in both $C_3$ and $C_4$, and so on.

This partition is equitable. That means: for all $i$ and $j$, the number of neighbors which a vertex in $C_i$ has in the cell $C_j$ is independent of the choice of vertex in $C_j$. We will amply exploit the relations between equitable partitions and eigensystems, see, e.g., Ref. 10 and only sketch the proof of the following result.

**Lemma 2.** – Let $G$ be a connected trivalent graph on $n$ vertices, built from big and small blocks as specified in (1) and (2). Let there be $m$ cells in the partition $\Pi$ as defined just before. Then, there are $m$ orthogonal eigenvectors, each constant on the cells of $\Pi$. The remaining $n-m$ orthogonal eigenvectors belong to eigenvalues $> 2$ and can be chosen so that each of them is nonzero in one block only.

For us, only $\lambda_2$ is of interest, and we need to make sure that the corresponding eigenvector is in the first group. Therefore, we list for the $n-m$ eigenvectors from the second group the values they can take in each type of block, and the associated eigenvalues. The simple estimate from Lemma 1 then ensures that $\lambda_2$ is well below these values.

For a small block at the end with cells $C_1$, $C_2$, and $C_3$, nonzero components may occur either in $C_1$ or $C_2$.

<table>
<thead>
<tr>
<th>$C_1$</th>
<th>$C_2$</th>
<th>$C_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>$\lambda = 4$, or 0</td>
</tr>
<tr>
<td>-1</td>
<td>0</td>
<td>$\lambda = 3$.</td>
</tr>
</tbody>
</table>

For a big block at the end, there are three eigenvectors with nonzero values in cells $C_1$, $C_2$, and $C_3$ only. Let $\phi = (1 + \sqrt{5}) / 2$ (the golden ratio). Then

<table>
<thead>
<tr>
<th>$C_1$</th>
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<td>$\lambda = 4$, or 0</td>
</tr>
<tr>
<td>-1</td>
<td>0</td>
<td>$\lambda = 4 - \phi$.</td>
</tr>
</tbody>
</table>

For a small interior block, the eigenvalue $\lambda = 4$ corresponds to components $\pm 1$ in the middle cell. For a big interior block, components $\pm 1, \pm 1$ in the two central cells give $\lambda = 3$, the pattern $\pm 1, \mp 1$ gives $\lambda = 5$.

It is easily checked that in this way $n-m$ orthogonal eigenvectors of a path-like trivalent graph on $n$ vertices can be constructed. Each of the other $m$ eigenvectors belongs to the subspace of vectors that are constant on the cells $C_1, \ldots, C_m$ of $\Pi$.

**Definition 3.** – There is an obvious one-to-one correspondence between an $n$-vector that is constant on the cells $C_1, \ldots, C_m$ of $\Pi$ and an $m$-vector $x$ with components $(x_1, \ldots, x_m)$, so that the values at vertices in cell $C_i$ are $x_i$. Therefore, from now on we will identify the corresponding $m$- and $n$-vectors. The context should make it clear whether a vector $x$ has $m$ or $n$ components.

**Lemma 3.** – Let $G$ be a connected trivalent graph on $n$ vertices, built from big and small blocks as specified in (1) and (2). Consider an eigenvector to $\lambda_2$ and the partition $\Pi = (C_1, \ldots, C_m)$. Let $x = (x_1, \ldots, x_m)$ so that $x_i$ is the value of the eigenvector at vertices in cell $C_i$, cells numbered consecutively from left to right. Then, the $x_i$ form a strictly monotone sequence changing sign once.

This follows from Fiedler, 9 Theorem (3,12). □

**NO BIG BLOCKS IN THE MIDDLE**

In this section, we show that big blocks cannot occur in the interior of the graph $G_n$ with minimal eigenvalue gap $\lambda_2$. The idea here is that if there were a big block, pushing this block towards one end (by local switching of edges) would reduce $\lambda_2$. Figure 1 illustrates the principle, assuming that the block is to be pushed to the left, away from the center. (We consider the position where the
Lemma 4. Let $G$ be a connected trivalent graph on $n \geq 10$ vertices, built from big and small blocks as specified in (1) and (2). In the cells $C_k$, $C_{k+1}, C_{k+2}$ of the partition $\Pi$, let $x_k, x_{k+1}, x_{k+2}$ be the components of the eigenvector associated with $\lambda_2$. Assume an edge between cells $C_k$ and $C_{k+1}$ and a big interior block to the right of this edge, as diagrammed in the upper part of Figure 1. We may select the orientation of the graph and the sign of the eigenvector so that, by Lemma 3, $x_k$ is orthogonal to $j$ in the inner product with $x$, and make it orthogonal to $j$ as diagrammed in the upper part of Figure 1. We may assume $|x_k|$ is orthogonal to $j$, and $x_k$ changes sign as the »center« in some intuitive sense.

$$\lambda_2 = \sum_{E(G)} (x_i - x_j)^2,$$

where the sum counts all edges in $G$. We define a vector $y$ with values $(y_1, ..., y_m)$ in the cells $C_1, ..., C_m$ of $\Pi(G)$. Note that $x$ is orthogonal to $j = (1, ..., 1)$; we will assume $||x|| = 1$. Then

$$y_i = \begin{cases} x_k + x_{k+2} - x_{k+1} - \delta & \text{if } i = k+1, \\ x_j - \delta & \text{else}, \end{cases}$$

where $\delta = 2(x_k - x_{k+1})/n$ ensures orthogonality to $j$. (Note that for the graph $H$ the value $y_j$ in cell $C_j$ counts twice in the inner product with $j$, the value in cell $C_{k+2}$ counts only once. For $x$ and $G$, it is the other way round!)

From the definition of $y$,

$$\sum_{E(G)} (x_i - x_j)^2 = \sum_{E(H)} (y_i - y_j)^2.$$

We will show that $||y|| > 1$, which means that the Rayleigh quotient for $y$ on $H$ is smaller than $\lambda_2$ of $G$.

$$||y||^2 = \sum_{V(G)} y_j^2 = \sum_{V(G)} (x_i - \delta)^2 - (x_{i+1} - \delta)^2 - (x_{i+2} - \delta)^2 +$$

$$\sum_{V(G)} x_i^2 - 2\delta \sum_{V(G)} x_j + n\delta^2 + 2(x_k - x_{k+1})(x_k + x_{k+2} - 2\delta) =$$

$$1 + n\delta^2 + 2(x_k - x_{k+1})(x_k(1 - 4/n) + 4x_{k+1}/n + x_{k+2}).$$

The sum is $> 1$, since we assumed that $x_k > x_{k+1} > x_{k+2} \geq 0$ and $n \geq 10$. □

Corollary 1. For $n \geq 12$ and $n \equiv 0 \pmod{4}$, the graph $G_n$ from Definition 1 is the unique trivalent graph on $n$ vertices with minimal eigenvalue gap.

Proof: Guiduli showed that only blocks as specified in (1) and (2) can build a graph with minimal eigenvalue gap. Lemma 4 rules out big interior blocks. Thus, only the blocks at the end are to be determined. For $n \equiv 0 \pmod{4}$, the only possibility is one big and one small block. □

TWO CANDIDATES FOR THE MINIMUM

If $G$ is reduced path-like with no big blocks in the middle, and $n \equiv 2 \pmod{4}$, then there are two alternatives: either the graph has a big block at each end, or it has small blocks only. The graphs are drawn below.

![Graphs G_n and H_n](image)

The graph $G_n$ has diameter $(3n - 10)/4$, while $H_n$ has diameter $(3n - 14)/4$. Intuitively, we would expect the graph with a larger diameter to have the smaller eigenvalue $\lambda$. The calculations in this section will confirm that this is true indeed.

![Graphs G_n and H_n](image)

Lemma 5. For $n \geq 10$ and $n \equiv 2 \pmod{4}$, the graph $G_n$ from Definition 1 is the unique trivalent graph on $n$ vertices with minimal eigenvalue gap.

Proof: Because of Lemma 4, solely $H_n$ competes against $G_n$. For $n = 10$, note that $G_n$ wins by being the only

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candidate; the definition of $H_n$ starts with $n \geq 14$. Thus, let now $n \geq 14$. The idea of the proof is simple: We modify an eigenvector $x$ of $H_n$ to get a new vector $y$, still perpendicular to $j$. We then show that the Rayleigh quotient for $G_n$ with the newly defined vector is less than the eigenvalue of $H_n$. There are two different cases, though similar: when the diameter of $G_n$ is even and when it is odd. Section Even Diameter of $G_n$: Case $n \equiv 6 \pmod{8}$ demonstrates the even case in detail, and for the odd case, Section Odd Diameter of $G_n$: Case $n \equiv 2 \pmod{8}$ shows where the evaluation differs.

Even Diameter of $G_n$: Case $n \equiv 6 \pmod{8}$

Definition of $x$ and $y$. — We will exploit the symmetry of $H_n$ and $G_n$ to define the vectors $x$ and $y$. We will use the convention of Definition 3. For both graphs, the reflection about the central vertical axis is an automorphism. Vertices interchanged by this reflection have components with opposite sign. Figure 2 shows the right half of each graph and establishes the nomenclature. For convenience, we start counting cells and vector components at the center.

Let the vector $x$ be an eigenvector to the second-smallest eigenvalue $\lambda = \lambda_2$ of the Laplacian $L(H_n)$ (no other eigenvalue than $\lambda_2$ will be of importance here, so let us drop the subscript from now on). From $x$, we define a vector $y$, which we will use to calculate the Rayleigh quotient of $G_n$.

$$y_0 = 0, \quad y_1 = x_1, \quad (5)$$

$$y_2 = x_3, \quad y_3 = \frac{x_3 + x_4}{2 - \lambda}, \quad y_4 = x_4,$$

$$y_5 = x_6, \quad y_6 = \frac{x_6 + x_7}{2 - \lambda}, \quad y_7 = x_7, \quad \ldots, \quad (6)$$

$$y_{k-5} = x_{k-4}, \quad y_{k-4} = \frac{x_{k-4} + x_{k-3}}{2 - \lambda}, \quad y_{k-3} = x_{k-3},$$

$$y_{k-2} = x_{k-1}, \quad y_{k-1} = 2x_{k-1} - x_k - y_{k-2} = y_k = x_k + x_{k-1} - x_{k-2}.$$ Symmetry and Lemma 3 allow us to assume $x_{-1} < 0 < x_1 < x_2 < \ldots < x_k$. Correspondingly, $0 = y_0 < y_1 < y_2 < \ldots < y_k$, and $y$ is orthogonal to $j$.

Establishing Certain Relationships among the Coordinates. — First, we establish a few relationships among the components of $x$, using the eigenvalue equations $L(H_n)x = \lambda x$.

We can write $x_2$ in terms of $x_1$, $x_3$, and $\lambda$ from the equation $-x_1 + 2x_2 - x_3 = \lambda x_2$. We do the same for $x_5$, ..., $x_{k-2}$.

$$x_2 = \frac{x_1 + x_3}{2 - \lambda}, \quad x_5 = \frac{x_4 + x_6}{2 - \lambda}, \quad \ldots,$$

$$x_{k-2} = \frac{x_{k-1} + x_{k-3}}{2 - \lambda}. \quad (7)$$

From the eigenvalue equations:

$$-x_{-1} + 3x_1 - 2x_2 = \lambda x_1 \quad \text{and} \quad -x_1 + 2x_2 - x_3 = \lambda x_2 \quad (8)$$

we may express $x_1$ in terms of $x_{-1}$ and $x_3$,

$$x_1 = \frac{(2 - \lambda)x_{-1} + 2x_3}{4 - \lambda(1 - \lambda)}. \quad (9)$$

As long as $0 < \lambda < 1$, an upper bound for $x_1$ follows; corresponding inequalities hold for $x_3$, $x_7$, ..., $x_{k-3}$.

$$x_1 < \frac{2(x_{-1} + x_3)}{(4 - \lambda)(1 - \lambda)}, \quad x_4 < \frac{2(x_3 + x_6)}{(4 - \lambda)(1 - \lambda)}, \quad \ldots,$$

$$x_{k-3} < \frac{2(x_{k-4} + x_{k-1})}{(4 - \lambda)(1 - \lambda)}. \quad (9)$$

We can write the values at the ends of both graphs in terms of $\lambda$ and $y_{k-1}$. Consider the eigenvalue equations:

$$-x_{k-2} + 3x_{k-1} - 2x_k = \lambda y_{k-1} \quad \text{and} \quad -2x_{k-1} + 2x_k = \lambda y_k.$$ Solving these as well as substituting in the definitions of $y_{k-1}$ and $y_k$ gives:

$$x_{k-2} = \frac{2 - 5\lambda + \lambda^2}{2 - \lambda} x_{k-1}, \quad x_k = \frac{2}{2 - \lambda} x_{k-1},$$

$$y_{k-1} = \frac{2 + 3\lambda - \lambda^2}{2 - \lambda} x_{k-1}, \quad y_k = \frac{2 + 4\lambda - \lambda^2}{2 - \lambda} x_{k-1}. \quad (10)$$

Estimating the Norm. — We will bound from below the difference $\|y\|^2 - \|x\|^2$ in terms of $x_{k-1}$ and $\lambda$. The squared norms of $x$ and $y$ are:

$$\|x\|^2 = 2(x_1^2 + x_2^2 + x_3^2 + 2x_4^2 + \ldots + x_{k-1}^2 + 2x_{k-2}^2 + 2x_k^2),$$

$$\|y\|^2 = 2(y_1^2 + y_2^2 + y_3^2 + 2y_4^2 + y_5^2 + \ldots + y_{k-1}^2 + y_{k-2}^2 + 2y_k^2).$$

Their difference is:

$$\|y\|^2 - \|x\|^2 = 4(-x_2^2 + y_2^2 - x_5^2 + y_5^2 - \ldots - y_{k-4}^2 + x_{k-2}^2) - 2x_{k-1}^2 + 4(y_{k-1}^2 + y_k^2 - x_k^2). \quad (11)$$

Substituting the definitions (5) of $y_3$, $y_6$, ..., $y_{k-4}$, the expressions (7) for $x_2$, ..., $x_{k-2}$ and adding a term $0 = (x_{-1} + x_1)$ transforms the first part. Expansion cancels most of the squares and yields an intermediate result $S_1$. 

4(−x_3^2 + y_3^2 − x_6^2 − y_6^2 + ... + y_{k-3}^2 + x_{k-3}^2) =

\[ \frac{4}{(2-\lambda)^2} \left( (x_{k-1} + x_1)^2 - (x_1 + x_3)^2 + (x_3 + x_4)^2 - ... +
\right.

\left. (x_{k-4} + x_{k-3})^2 - (x_{k-3} + x_{k-1})^2 \right) =

\[ \frac{4}{(2-\lambda)^2} \left( x_7^2 - 2x_1 (x_3 - x_{k-1}) - 2x_4 (x_6 - x_3) - ... - 2x_{k-3} (x_{k-1} - x_{k-4}) - x_{k-1}^2 \right) = S_1

The inequalities (9) for x_1, x_2, ..., x_{k-1} in terms of x_{k-1}, x_3, x_4, ..., x_{k-4} bound the sum from below and form a telescopic sum. We neglect positive contributions from x_3 and arrive at the final result, a bound in terms of \( \lambda \) and x_{k-1}.

\[ S_1 > \frac{4}{(2-\lambda)^2} \left( x_1^2 - \frac{4}{(4-\lambda)(1-\lambda)} (x_3 + x_{k-1})(x_3 - x_{k-1}) + (x_6 + x_3)(x_6 - x_3) + ... + (x_{k-1} + x_{k-4})(x_{k-1} - x_{k-4}) \right) - \]

\[ \frac{4}{(2-\lambda)^2} \left[ x_1^2 - \frac{4}{(4-\lambda)(1-\lambda)} (x_2^2 + x_{k-1}^2) - x_{k-1}^2 \right] > \]

\[ -4\lambda x_{k-1}^2 \left( \frac{4}{(4-\lambda)(1-\lambda)} + 1 \right) = \frac{4(8 - 5\lambda^2 + \lambda^4) x_{k-1}}{(2-\lambda)^2 (4-\lambda)(1-\lambda)}. \]

(12)

The remaining terms in equation (11) become with equations (10):

\[ -2x_{k-1}^2 + 4(y_{k-1}^2 + y_k^2 - x_k^2) = \]

\[ \frac{2(4 + 6\lambda + 33\lambda^2 - 28\lambda^3 + 4\lambda^4)}{(2-\lambda)^2} x_{k-1}^2. \]

For 0 < \( \lambda < 1 \), certainly

\[ 33\lambda^2 - 28\lambda^3 + 4\lambda^4 = \lambda^2(3 - 2\lambda)(11 - 2\lambda) > 0. \]

Thus, dropping these terms gives a lower bound,

\[ -2x_{k-1}^2 + 4(y_{k-1}^2 + y_k^2 - x_k^2) > \frac{8(1 + 15\lambda)}{(2-\lambda)^2} x_{k-1}^2. \]

Together with inequality (12), the bound now is:

\[ ||y||^2 - ||x||^2 > \frac{4\lambda(115 - 149\lambda + 30\lambda^2)}{(2-\lambda)^2 (4-\lambda)(1-\lambda)} x_{k-1}^2 > \]

\[ \lambda(115 - 149\lambda) \]

\[ \frac{(2-\lambda)^2}{(2-\lambda)^2} x_{k-1}^2. \]

(13)

\[ y^T L(G_x) y - x^T L(H_y) x = \sum_{\{i,j\in E(G_x)\}} (y_j - y_i)^2 - \]

\[ \sum_{\{i,j\in E(H_y)\}} (y_j - y_i)^2. \]

In these sums, the contribution of the edge between x_1 and x_3 in H_y is equal to the contributions from the four edges between y_1 and y_3 in G_x. Between x_1 and x_3, using expression (7) for x_2,

\[ 2\alpha (x_1 - x_3)^2 + 2(\alpha - x_3)^2 = \]

\[ (x_1 - x_3)^2 \left( 1 + \frac{\lambda^2}{(2-\lambda)^2} \right) > (y_1 - y_2)^2; \]

that is, the edges in H_y contribute more than the corresponding edges in G_x. The same holds for the edges between x_3 and x_6 in H_y and the edges from y_2 to y_5 in G_x. The difference \( \delta \) of their contributions is

\[ \delta = (x_3 - x_4)^2 + (x_4 - x_5)^2 + 2(x_5 - x_6)^2 - 2(y_2 - y_3)^2 - 2(y_3 - y_4)^2 - (y_4 - y_5)^2. \]

Inserting from equations (5) and (7) establishes:

\[ \delta = \frac{\lambda^2}{(2-\lambda)^2} (x_6 - x_3)(x_3 + 2x_4 + x_6) > 0. \]

(14)

In the same way, all other edges between x_6 and x_{k-1} contribute more than the corresponding edges in G_x. Edges between x_{k-1} and x_k contribute as much as edges between y_k and y_{k+1}. The only exception are the edges between y_{k-2} and y_{k-1} and their mirror images at the other end of G_x, which are not counterbalanced by any edges in H_y. Their contribution is

\[ 4(y_{k-2} - y_{k-1})^2 = \frac{4\lambda^2 (4 - \lambda)^2}{(2-\lambda)^2} x_{k-1}^2. \]

Thus,

\[ y^T L(G_x) y - x^T L(H_y) x < \frac{4\lambda^2 (4 - \lambda)^2}{(2-\lambda)^2} x_{k-1}^2 < \]

\[ \frac{64\lambda^2}{(2-\lambda)^2} x_{k-1}^2. \]

(15)

\[ \begin{array}{cccccc}
- y_1 & y_1 & y_2 & y_3 & y_4 & y_5 & y_6 & y_{k-1} & y_k & y_{k+1} \\
H_y & G_x & ... & \end{array} \]

Figure 3. Graphs H and G for n = 2 (mod 8).
The Rayleigh Quotient. – Now comes the easy part. We combine the inequalities (13) and (15).

\[
y^T L(G_n) y \leq \frac{x^T L(H_n) x + 64\lambda^2}{2(\lambda^2 - 1)} x_k^2 - 1 = \frac{\lambda(115 - 149\lambda)}{2(\lambda^2 - 1)} x_k^2 - 1
\]

The last inequality holds as long as \(115 - 149\lambda > 64\) and \(\lambda > 0\). For the smallest possible graph \(H_n\) with \(n = 14\), already \(\lambda = 0.12709\), and for larger \(n\) the eigenvalues will be smaller.

\begin{align*}
\text{Odd Diameter of } G_n: \text{ Case } n \equiv 2 \pmod{8} \\
\text{The arguments in this case follow closely those presented in the previous section. The essential difference is that now } H_n \text{ has two vertices labeled by } x_0 \text{ at its center; there are no components } y_0 \text{ in } G_n \text{, but additional vertices } y_{2(k+1)}. \text{ Figure 3 illustrates the situation. Equations and estimates differ mainly in the subscripts. The equivalents of equations (5), (7), (9) and (10) are, respectively,}
\end{align*}

\begin{align*}
y_1 &= x_1, \quad y_2 = \frac{x_1 + x_2}{2 - \lambda}, \quad y_3 = x_2, \\
y_4 &= x_4, \quad y_5 = \frac{x_4 + x_5}{2 - \lambda}, \quad y_6 = x_5, \ldots, \ y_{k-1} = x_{k-1} \quad (17) \\
y_k &= 2x_{k-1} - x_{k-2}, \quad y_{k+1} = x_k + x_{k-1} - x_{k-2}. \\
x_3 &= \frac{x_2 + x_4}{2 - \lambda}, \quad x_6 = \frac{x_5 + x_7}{2 - \lambda}, \ldots, \ x_{k-2} = \frac{2x_{k-3} + x_{k-1} - x_{k-2}}{2 - \lambda}, \\
x_2 &< \frac{2(x_1 - x_4)}{(4 - \lambda)(1 - \lambda)}, \quad x_5 < \frac{2(x_4 + x_7)}{(4 - \lambda)(1 - \lambda)}, \ldots, \\
x_{k-3} &< \frac{2(x_{k-4} + x_{k-1})}{(4 - \lambda)(1 - \lambda)} \quad (19) \\
x_{k-2} &= \frac{2 - 5\lambda + \lambda^2}{2 - \lambda} x_{k-1}, \quad x_k = \frac{2}{2 - \lambda} x_{k-1}, \\
y_k &= \frac{2 + 3\lambda - \lambda^2}{2 - \lambda} x_{k-1}, \quad y_{k+1} = \frac{2 + \lambda - \lambda^2}{2 - \lambda} x_{k-1} \quad (20)
\end{align*}

The difference between the squares of \(x\) and \(y\) is:

\[
||y||^2 - ||x||^2 = 4(y_2^2 - x_2^2) + 4(y_3^2 - x_3^2) + \ldots + 4(y_{k-3}^2 - x_{k-3}^2) - 2x_{k-1}^2 + 4(y_k^2 + y_{k+1}^2 - x_k^2).
\]

Using equations (17), (18), (19) and (20), we get:

\[
||y||^2 - ||x||^2 > \frac{\lambda(115 - 149\lambda)}{2(\lambda^2 - 1)} x_k^2 - 1,
\]

which is exactly an inequality (13).

To bound \(y^T L(G_n) y\), we compare the contributions of edges between \(x_1\) and \(x_4\) with those from \(y_1\) to \(y_4\).

\[
\delta = 2(y_1 - y_2)^2 + 2(y_2 - y_3)^2 + (y_3 - y_4)^2 - (x_1 - x_2)^2 - 2(x_2 - x_3)^2 - 2(x_3 - x_4)^2.
\]

Inserting from equations (17) and (18) brings:

\[
\delta = \frac{-\lambda^2}{2(\lambda^2 - 1)} (x_4 - x_1)(x_1 + 2x_2 + x_4) < 0.
\]

an expression analogous to equation (14). In the same way, all other edges between \(x_4\) and \(x_{k-1}\) may be compared. Edges between \(x_{k-1}\) and \(x_k\) contribute as much as edges between \(y_k\) and \(y_{k+1}\). The only exception are the edges between \(y_{k-1}\) and \(y_k\) and their mirror images at the other end of \(G_n\), which are not counterbalanced by edges in \(H_n\). Their contribution is

\[
4(y_{k-1} - y_k)^2 = \frac{4\lambda^2(4 - \lambda)^2}{2(\lambda^2 - 1)} x_k^2 - 1.
\]

The resulting inequality is identical with equation (15). Consequently, the final estimate (16) also holds.

With due relief, we pronounce the concluding quod erat demonstrandum for Lemma 5, and thus for Theorem 1 as well.\[\]

TRIVALENT GRAPHS WITH MAXIMUM DIAMETER

The following theorem characterizes the cubic graphs with maximum diameter for a given number \(n\) of vertices.

\begin{center}
\textit{Theorem 2. – The graph } G_n \text{ from Definition 1 is the graph of maximum diameter among all trivalent graphs on } n \text{ vertices.}
\end{center}

\begin{center}
For \(n = 4\) (trivially), and for \(n \geq 10\) and \(n \equiv 2 \pmod{4}\), the graph \(G_n\) is the unique graph of maximum diameter. For \(n = 6\) and \(n = 8\), the other extremal graphs are:
\end{center}

\begin{center}
\begin{itemize}
\item For \(n \geq 12\) and \(n \equiv 0 \pmod{4}\), the graph \(G_n\) shares its extremal position with graphs built from small blocks as specified in (1) and (2), and exactly one big block, either
\end{itemize}
\end{center}
at the end or in the interior, taken also from (1) and (2) or from:

\begin{align*}
\text{Proof: The proof starts with reformulating the question: instead of maximizing the diameter } d \text{ for a given } n, \text{ let us find among all cubic graphs with fixed } d \text{ a graph with minimal number } n \text{ of vertices. These two formulations are almost equivalent; but inspection reveals for } d = 4 \text{ a minimum } n = 10, \text{ while the maximum diameter for } n = 10 \text{ vertices is } d = 5. \text{ Except for } n = 10, \text{ however, the correspondence between diameter } d \text{ and minimal } n \text{ will turn out to be a bijective mapping. Consequently, we may prove the second formulation.}

\text{For } n \leq 8, \text{ enumeration solves the problem (see, e.g., the tables in Ref. 11). For } n \geq 10, \text{ we derive a lower bound (23) for } n \text{ in terms of the given } d, \text{ and we show that this bound is sharp for exactly those graphs specified in this theorem. The following lemmas cover the technical details.} \quad \square

\text{In the case of the minimal eigenvalue gap, the first observation was that the graphs in question must be reduced path-like. Not surprisingly, a graph with the minimum number of vertices for a given diameter will be of similar structure. This is the topic of the next lemmas. In the following, a block is defined, as usual, as a maximal connected subgraph without a point of articulation. In this sense, a block is either a maximal 2-connected subgraph or a K}_2, \text{ its edge being a bridge.}

\text{Lemma 6. -- Let G be a cubic graph with minimal number of vertices for a given, fixed diameter } d. \text{ Then, the block graph of G is a path, i.e., the blocks of G are single edges (with two vertices of degree one), or blocks with one or two vertices of degree two.}

\text{Proof: We observe first that of any two blocks that have a vertex in common exactly one must be a K}_2, \text{ because every vertex has degree 3. Consider a diameter } P \text{ in G and denote the subgraph formed by all the blocks it meets in at least two vertices by } G_P. \text{ Clearly (since block graphs are trees), the block graph of } G_P \text{ is a path. If the assertion of the proposition is not true, there must be a block } B \text{ that is connected to } G_P \text{ by an edge } e \text{ where the endpoint } a \text{ of } e \text{ in } G_P \text{ has two neighbors } a_1 \text{ and } a_2 \text{ in } G_P. \text{ We now delete } e \text{ and } B \text{ as well as all edges incident with them from } G \text{ and connect } a_1 \text{ and } a_2 \text{ by a small interior block (2). This decreases the number of vertices in } G \text{ by at least 2 and does not decrease the diameter.} \quad \square

\text{Lemma 7. -- Let } B \text{ be a block of diameter } d \geq 2, i \in \{0, 1, 2\} \text{ and suppose that } B \text{ has } |B| - i \text{ vertices of degree 3 and } i \text{ of degree 2. Then:

\[ |B| \geq 2d + 2 - i. \]

\text{Proof: Let } B \text{ have diameter } d \text{ and let } P, Q \text{ be two disjoint paths connecting vertices } a, b \text{ of distance } d \text{ in } B. \text{ Choose } P, Q \text{ so that no shorter disjoint path exists. Let } a_i \text{ and } b_j, j \in \{0, 1\}, \text{ be the neighbors of } a \text{ and } b \text{ in } P \cup Q. \text{ If } a \text{ has degree 3, there exists another neighbor } a_2 \text{ of } a \text{ and, similarly, there exists another neighbor } b_2 \text{ of } b \text{ if } b \text{ has degree 3. For } d > 2 \text{ all these vertices must be distinct, for } d = 2 \text{ it could be that } a_2 = b_2. \text{ We distinguish two cases:

\text{CASE 1. } i = 0. \text{ Neither } a_2 \text{ nor } b_2 \text{ are on } P \text{ or } Q \text{ (otherwise a shorter path would exist). Thus, even if } a_2 = b_2, \text{ the number of vertices of } B \text{ is at least

\[ |P \cup Q| + 1 \geq 2d + 1. \]

\text{Since a cubic graph must have an even number of vertices, } |B| \geq 2d + 2.

\text{CASE 2. } i > 0. \text{ If } a \text{ or } b \text{ or both have degree three, by the same argument as above,

\[ |B| \geq |P \cup Q| + 1 \geq 2d + 1. \]

\text{If both of them are of degree 2, then neither } a_2 \text{ nor } b_2 \text{ exist and the bound has to be lowered by one.} \quad \square

\text{Furthermore, we note that graphs of diameter one are complete. Thus, there is only one cubic block of diameter 1, the complete graph K}_4.

\text{As we shall see, only minimal blocks of diameter } \leq 3 \text{ will be of importance for the characterization of cubic graphs with a given diameter and minimal number of vertices. These minimal blocks are:

\text{For diameter 1, the complete graph } K}_4.

\text{For diameter 2 and } i = 0, \text{ the two cubic graphs on 6 vertices; for } i = 1 \text{ a } K_4 \text{ in which one edge is subdivided by an additional vertex (of degree 2), i.e., the small end block (1); and for } i = 2 \text{ a } K_4 \text{ from which an edge has been deleted, i.e., the small interior block (2).}

\text{For diameter 3 and } i = 0, \text{ we have the three cubic graphs on 8 vertices with diameter 3; for } i = 1 \text{ just two graphs, the large end block (1) and the one depicted in Theorem 2; and for } i = 2 \text{ three graphs, only two of which are interesting to us, because in one of them the vertices of degree 2 have distance 2. These two are the big interior block (2) and the one depicted in Theorem 2.

\text{Lemma 8. -- Let } G \text{ be a cubic graph on } n \text{ vertices, with diameter } d. \text{ Then, its number } k \text{ of bridges satisfies the inequality:

\[ n \geq 2d - 2k + 2 \quad (22) \]}

Proof: Let $B_0, e_1, B_1, e_2, \ldots, e_{k-1}, B_{k-1}, e_k, B_k$ be the succession of blocks on a diameter $P$ of $G$, the notation being chosen such that the $e_i$ are trivial blocks, i.e., their edges are bridges. Furthermore, let $d_i, i = 0, 1, \ldots, k$, denote the diameter of the $B_i$; or, more precisely, the distance between vertices of degree 2 in $B_i$ for $i = 1, \ldots, k-1$, respectively, the maximal distance from the vertex of degree two in $B_i$ for $i = 0, k$. Then:

$$ n \geq 2d_0 + 1 + 2 \sum_{i=1}^{k-1} d_i + 2d_k + 1. $$

Since

$$ d_0 + \sum_{i=1}^{k-1} d_i + d_k = d - k $$

we infer the validity of the assertion of the proposition. \hfill \Box

Thus, for a given $d$, the lower bound (22) for the number of vertices will be minimal for maximal $k$. For $d \leq 4$, no bridge is possible, so let us assume $d \geq 5$. We then maximize $k$ by taking blocks of the smallest possible diameter. Consequently, either there are $k+1$ blocks with diameter 2, or just one block has diameter three. Then,

$$ d = k + 2(k + 1), \quad \text{or} \quad d = k + 2k + 3. $$

The lower bound (22) in these cases becomes:

$$ n \geq \begin{cases} \frac{2}{3} (5 + 2d) & \text{if } d \equiv 2 \pmod{3}, \\ 4d & \text{if } d \equiv 0 \pmod{3}, \end{cases} $$

(23)

which is valid if $d \geq 5$

In the first case, when $d \equiv 2 \pmod{3}$, the bound is sharp if and only if the blocks are small blocks as specified in (1) and (2). That means that both endblocks have five vertices and the interior blocks have four, or $n \equiv 2 \pmod{4}$.

In the second case, when $d \equiv 0 \pmod{3}$, possible combinations are both endblocks with five vertices, one middle block with six and all other middle blocks with four vertices; or one endblock with five, one with seven vertices and all middle blocks with four. Then, $n \equiv 0 \pmod{4}$.

Theorem 2 lists all these types of blocks; the number of possible extremal graphs can easily be computed.

Note that the mapping from the set of possible diameters $D = \{5, 6, 8, 9, 11, 12, \ldots\}$ to the set of minimal vertex numbers $N = \{10, 12, 14, 16, \ldots\}$, defined by requiring equality in equations (23), is one-to-one. We need this fact in Theorem 2.

REFERENCES


SAŽETAK

Karakterizacija trivalentnih grafova najmanjim procjepom vlastitih vrijednosti

Clemens Brand, Barry Guiduli i Wilfried Imrich

Neka je $G_n$ graf s najmanjim mogućim procjepom vlastitih vrijednosti među svima trivalentnim grafovima s $n$ čvorova. (Procjep vlastitih vrijednosti je razlika između dvije najveće vlastite vrijednosti matrice susjedstva grafa; za regularne grafove procjep je jednak drugoj najmanjoj vlastitoj vrijednosti Laplaceove matrice grafa.) Pokazano je da je $G_n$ jedinstven za svaki $n$ i da ima najveći mogući promjer, čime su prošireni raniji Guidulijevi rezultati i rješena implicitna pretpostavka iz rada Bussemakera, Čobeliša, Cvetkovića i Seidelara. Ovisno o $n$, graf $G_n$ ne mora biti jedini graf s maksimalnim dijametrom. Stoga također određujemo sve kubične grafove s maksimalnim dijametrom za zadani broj $n$ vrhova.