The characterization of trivalent graphs with minimal eigenvalue gap

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Abstract

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, Čobeljić, 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.

1 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 the dependence on G. Similarly, we write the vertex set as $V = V(G) = \{1, 2, \dots, n\}$. The Laplacian matrix L or $L(G)$ is defined as $L(G) = 3I - A(G)$, where A

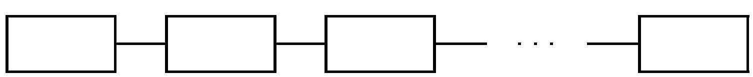
*Barry Guiduli now works for an investment bank in New York, NY denotes the adjacency matrix. Spectral theory originally defines the spectrum of G as the spectrum of A. This paper, however, prefers to deal with the Laplacian spectrum of G, that is, the spectrum of L. Obviously, these spectra are in a 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. [10].) The matrix L is positive semidefinite, with an eigenvector $\mathbf{j} = (1, 1, \ldots, 1)^T$ corresponding to the eigenavalue 0. As G is connected, this eigenvalue has multiplicity 1.

2 Introduction

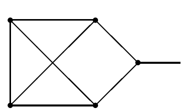
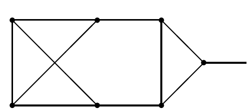
Let $0 = \lambda_1 < \lambda_2 \leq \cdots \leq \lambda_n$, be the eigenvalues of L. The eigenvalue $\lambda = \lambda_2$ is called the *eigenvalue gap* (for connected regular graphs, this is the difference between the two largest eigenvalues of the adjacency matrix). The eigenvalue gap was first investigated by Fiedler in 1973, who called it the *algebraic connectivity* of a graph (see [5]). 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 Milman [2] and Alon [1] 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. [9, 11]

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

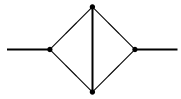
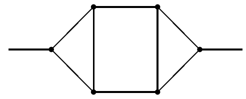
Guiduli [8] already proved that such a graph must look like a path; more precisely, he showed that the graph must be *reduced path-like*. A trivalent graph is said to be *reduced path-like* if it is built from non-trivial blocks with bridges in between:



The block at the left end is either

 or  . (1)

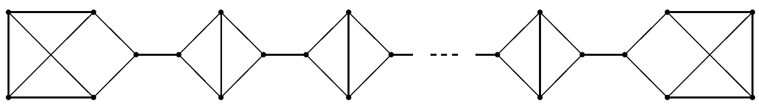
The block at the right end is the mirror image of one of these blocks. Each interior block is either

 or  . (2)

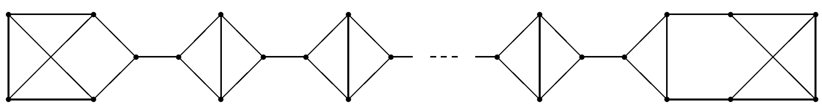
We will refer to these four types of blocks as small or big blocks, at the end or in the interior, respectively. Note that in our figures we draw the bridges (which in the sense of the usual definition are blocks, too) as outgoing edges of non-trivial blocks. Speaking of blocks we thus always mean non-trivial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

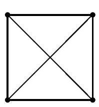
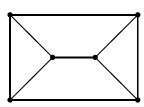
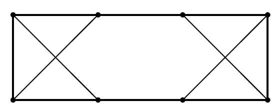
Definition 1 *Let G_n be the reduced path-like graph on n vertices with small interior blocks and one small end block. The other end block is then forced by the value of n. (Notice that trivalent graphs only exist for even n and that, so far, G_n only makes sense for $n \geq 10$.) If $n \equiv 2 \pmod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



If $n \equiv 0 \pmod 4$, then G_n is the graph:



For $n = 4, 6$ and 8, we define

$G_4 =$  , $G_6 =$  , $G_8 =$ 

Numerical values of the eigenvalue gap for some n are

n	$\lambda_2(G_n)$	n	$\lambda_2(G_n)$	n	$\lambda_2(G_n)$
4	4	12	0.167742	20	0.0515873
6	2	14	0.104893	50	0.00789634
8	0.763932	16	0.0840422	100	0.0019742
10	0.221543	18	0.0620222	200	0.000493469

The values for $n = 50, 100, 200$ indicate the asympyotic behaviour: Doubling n reduces λ_2 by about a factor 4. Indeed, asymptotically $\lambda_2(G_n) = 2\pi^2/n^2 + \mathcal{O}(n^{-3})$. (The proof of this result will be subject of a separate note.)

We prove the following theorem, conjectured by Bussemaker, Čobeljić, Cvetković, and Seidel [3].

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

Proof: Guiduli [8] 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 $n \equiv 0 \pmod 4$, Corollary 1 settles the affair. For $n \equiv 2 \pmod 4$, there remain two graphs to consider: G_n and the graph H_n with big blocks at both ends. Lemma 5 will rule out the second possibility. □

3 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 λ_2.

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

$$\frac{\mathbf{x}^T L \mathbf{x}}{\|\mathbf{x}\|^2}$$

is called the Rayleigh quotient. Let $\mathbf{j} = (1, 1, \ldots, 1)^T \in \mathbf{R}^n, \alpha \in \mathbf{R}$; it is well known, cf. e.g. [6, 10], that

$$\begin{aligned}\lambda_2 &= \min_{\mathbf{x}\neq 0, \mathbf{x}\perp\mathbf{j}} \frac{\mathbf{x}^T L \mathbf{x}}{\|\mathbf{x}\|^2} = \min_{\mathbf{x}\neq 0, \mathbf{x}\perp\mathbf{j}} \frac{\sum_{i\sim j}(x_i - x_j)^2}{\|\mathbf{x}\|^2} = \\ &= n \min_{\mathbf{x}\neq\alpha\mathbf{j}} \frac{\sum_{i\sim j}(x_i - x_j)^2}{\sum_{(i,j), i<j}(x_i - x_j)^2} \qquad (3)\end{aligned}$$

The Rayleigh quotient will be our main tool. Right now, we use it for a crude estimate of the eigenvalue gap λ_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 $\mathbf{x}$ with $x_1, \ldots, x_{n/2} = -1$ for all vertices in the left half of G, $x_i = 1$ for the remaining $n/2$ vertices in the right half of G. Clearly, $\mathbf{x} \perp \mathbf{j}$, and at most three edges will contribute in 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 λ_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_i. We will amply exploit the relations between equitable partitions and eigensystems, see, e.g., [7] 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 Π as defined just before. Then, there are m orthogonal eigenvectors, each constant on the cells of Π. 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 λ_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 λ_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.

$$\left.\begin{array}{rr} C_1 & C_2 \\ 1 & 0 \\ -1 & 0 \end{array}\right\} \lambda = 4, \quad \text{or} \quad \left.\begin{array}{rr} C_1 & C_2 \\ 0 & 1 \\ 0 & -1 \end{array}\right\} \lambda = 3$$

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

$$\left.\begin{array}{rrr} C_1 & C_2 & C_3 \\ 1 & 0 & 0 \\ -1 & 0 & 0 \end{array}\right\} \lambda = 4, \quad \left.\begin{array}{rrr} C_1 & C_2 & C_3 \\ 0 & \phi & 1 \\ 0 & -\phi & -1 \end{array}\right\} \lambda = 4-\phi, \quad \left.\begin{array}{rrr} C_1 & C_2 & C_3 \\ 0 & \phi & -1 \\ 0 & -\phi & 1 \end{array}\right\} \lambda = 4-\frac{1}{\phi}.$$

For a small interior block, the eigenvalue $\lambda = 4$ corresponds to components ± 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 Π.

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 Π and an m-vector $\mathbf{x}$ with components $(x_1, \ldots, x_m)$, so that the values at vertices in cell C_i are x_i. Therefore, we will identify from now on corresponding m- and n-vectors. The context should make it clear whether a vector $\mathbf{x}$ 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 λ_2 and the partition $\Pi = (C_1, \ldots, C_m)$. Let $\mathbf{x} = (x_1, \ldots, x_m)$ 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 [6], Theorem (3,12).□

4 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 λ_2. The idea here is that if there were a big block, pushing this block towards one end (by a local switching of edges) would reduce λ_2. Figure 1 illustrates the principle, assuming that

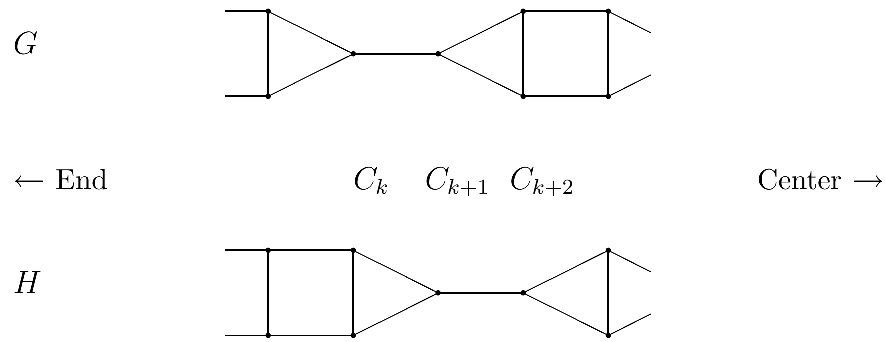


Figure 1: Pushing a block outwards

the block is to be pushed to the left, away from the center. (We consider the position where the eigenvector changes sign as the "center" in some intuitive sense.)

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 Π, let x_k, x_{k+1}, x_{k+2} be the components of the eigenvector associated with λ_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, $x_k > x_{k+1} > x_{k+2} \geq 0$. Then the graph H obtained by local switching of edges as shown in the lower part of Figure 1 has a smaller eigenvalue gap than G.*

Proof: Let $\mathbf{x}$ be the eigenvector associated with λ_2 on G, and let $(x_1, \ldots, x_m)$ be the values of $\mathbf{x}$ in the cells $C_1, \ldots, C_m$ of $\Pi(G)$. Note that $\mathbf{x}$ is orthogonal to $\mathbf{j} = (1, \ldots, 1)$; we will assume $\|\mathbf{x}\| = 1$. Then

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

where the sum counts all edges in G. We define a vector $\mathbf{y}$ with values $(y_1, \ldots, y_m)$ in the cells $C_1, \ldots, C_m$ of $\Pi(H)$ and make it orthogonal to $\mathbf{j}$.

$$y_i = \begin{cases} x_k + x_{k+2} - x_{k+1} - \delta & \text{if } i = k+1, \\ x_i - \delta & \text{else,} \end{cases} \tag{4}$$

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

From the definition of $\mathbf{y}$,

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

We will show that $\|\mathbf{y}\| > 1$, which means that the Rayleigh quotient for $\mathbf{y}$ on H is smaller than λ_2 of G.

$$\begin{aligned}
\|\mathbf{y}\| &= \sum_{V(H)} y_i^2 = \sum_{V(G)} (x_i - \delta)^2 - (x_{k+1} - \delta)^2 - (x_{k+2} - \delta)^2 \\
&\quad + (x_k - \delta)^2 + (x_k + x_{k+2} - x_{k+1} - \delta)^2 \\
&= \sum_{V(G)} x_i^2 - 2\delta \sum_{V(G)} x_i + n\delta^2 + 2(x_k - x_{k+1})(x_k + x_{k+2} - 2\delta) \\
&= 1 + n\delta^2 + 2(x_k - x_{k+1})(x_k(1 - 4/n) + 4x_{k+1}/n + x_{k+2})
\end{aligned}$$

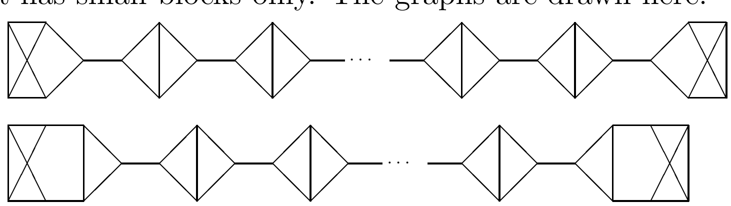
The sum is > 1, since we assumed that $x_k > x_{k+1} > x_{k+2} \geq 0$ and $n \geq 10$. $\square$

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 [8] showed that only blocks as specified in (1) and (2) can build the 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. $\square$

5 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 here.



G_n

H_n

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

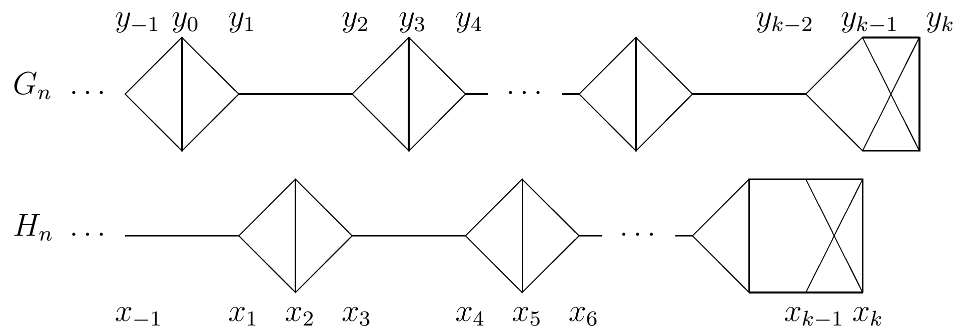


Figure 2: Graphs G_n and H_n for $n \equiv 6 \pmod 8$

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 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 $\mathbf{x}$ of H_n, to get a new vector $\mathbf{y}$, still perpendicular to $\mathbf{j}$. 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, for when the diameter of G_n is even and when it is odd. Section 5.1 demonstrates the even case in detail, and for the odd case, Section 5.2 shows where the evaluation differs. $\square$

5.1 Even diameter of G_n: Case $n \equiv 6 \pmod 8$

Definiton of x and y. We will exploit the symmetry of H_n and G_n to define the vectors $\mathbf{x}$ and $\mathbf{y}$. 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 $\mathbf{x}$ be an eigenvector to the second-smallest eigenvalue $\lambda = \lambda_2$ of the Laplacian $L(H_n)$ (no other eigenvalue than λ_2 will be of importance here, so let us drop the subscript from now on). From $\mathbf{x}$, we define a vector

$\mathbf{y}$, which we will use to calculate the Rayleigh quotient of G_n.

$$y_0 = 0, \qquad y_1 = x_1, \tag{5}$$

$$\begin{aligned} &y_2 = x_3, && y_3 = \frac{x_3 + x_4}{2-\lambda}, && y_4 = x_4, \\ &y_5 = x_6, && y_6 = \frac{x_6 + x_7}{2-\lambda}, && y_7 = x_7, \qquad \dots, \\ &y_{k-5} = x_{k-4}, && y_{k-4} = \frac{x_{k-4} + x_{k-3}}{2-\lambda}, && y_{k-3} = x_{k-3}, \\ &y_{k-2} = x_{k-1}, && y_{k-1} = 2x_{k-1} - x_{k-2}, && y_k = x_k + x_{k-1} - x_{k-2}. \end{aligned} \tag{6}$$

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

Establishing certain relationships among the coordinates. First we establish a few relationships among the components of $\mathbf{x}$, using the eigenvalue equations $L(H_n)\mathbf{x} = \lambda\mathbf{x}$.

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

$$x_2 = \frac{x_1 + x_3}{2-\lambda}, \quad x_5 = \frac{x_4 + x_6}{2-\lambda}, \quad \dots, \quad x_{k-2} = \frac{x_{k-3} + x_{k-1}}{2-\lambda}. \tag{7}$$

From the eigenvalue equations

$$-x_{-1} + 3x_1 - 2x_2 = \lambda x_1 \qquad \text{and} \qquad -x_1 + 2x_2 - x_3 = \lambda x_2 \tag{8}$$

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

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

As long as $0 < \lambda < 1$, an upper bound for x_1 follows; corresponding inequalities hold for $x_4, x_7, \dots, x_{k-3}$.

$$x_1 < \frac{2(x_{-1} + x_3)}{(4-\lambda)(1-\lambda)}, \; x_4 < \frac{2(x_3 + x_6)}{(4-\lambda)(1-\lambda)}, \dots, \; x_{k-3} < \frac{2(x_{k-4} + x_{k-1})}{(4-\lambda)(1-\lambda)}. \tag{9}$$

We can write the values on the ends of both graphs in terms of λ and x_{k-1}. Consider the eigenvalue equations:

$$-x_{k-2} + 3x_{k-1} - 2x_k = \lambda x_{k-1} \qquad \text{and} \qquad -2x_{k-1} + 2x_k = \lambda x_k.$$

Solving these as well as substituting in the definitions of y_{k-1} and y_k gives

$$\begin{aligned} x_{k-2} &= \frac{2 - 5\lambda + \lambda^2}{2-\lambda} x_{k-1}, & x_k &= \frac{2}{2-\lambda} x_{k-1}, \\ y_{k-1} &= \frac{2 + 3\lambda - \lambda^2}{2-\lambda} x_{k-1}, & y_k &= \frac{2 + 4\lambda - \lambda^2}{2-\lambda} x_{k-1}. \end{aligned} \tag{10}$$

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

$$\|\mathbf{x}\|^2 = 2(x_1^2 + 2x_2^2 + x_3^2 + x_4^2 + 2x_5^2 + \cdots + x_{k-3}^2 + 2x_{k-2}^2 + 2x_{k-1}^2 + 2x_k^2),$$
$$\|\mathbf{y}\|^2 = 2(y_1^2 + y_2^2 + 2y_3^2 + y_4^2 + y_5^2 + \cdots + y_{k-3}^2 + y_{k-2}^2 + 2y_{k-1}^2 + 2y_k^2).$$

Their difference is

$$\begin{aligned} \|\mathbf{y}\|^2 - \|\mathbf{x}\|^2 \;\; &= \;\; 4(-x_2^2 + y_3^2 - x_5^2 + y_6^2 - \cdots + y_{k-4}^2 - x_{k-2}^2) \\ &\quad - 2x_{k-1}^2 + 4(y_{k-1}^2 + y_k^2 - x_k^2). \end{aligned} \tag{11}$$

Substituting the definitions (5) of $y_3, y_6, \ldots, y_{k-4}$, the expressions (7) for $x_2, \ldots, x_{k-2}$ 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.

$$\begin{aligned} &4(-x_2^2 + y_3^2 - x_5^2 + y_6^2 - \cdots + y_{k-4}^2 - x_{k-2}^2) \\ &= \frac{4}{(2-\lambda)^2}\big((x_{-1}+x_1)^2 - (x_1+x_3)^2 + (x_3+x_4)^2 - \cdots \\ &\qquad + (x_{k-4}+x_{k-3})^2 - (x_{k-3}+x_{k-1})^2\big) \\ &= \frac{4}{(2-\lambda)^2}\big(x_1^2 - 2x_1(x_3 - x_{-1}) - 2x_4(x_6 - x_3) - \cdots \\ &\qquad - 2x_{k-3}(x_{k-1} - x_{k-4}) - x_{k-1}^2\big) = S_1 \end{aligned}$$

The inequalities (9) for $x_1, x_4, \ldots, x_{k-3}$ in terms of $x_{-1}, x_3, x_6, \ldots, x_{k-1}$ bound the sum from below and form a telescopic sum. We neglect positive contributions from x_{-1} and arrive at the final result, a bound in terms of λ and x_{k-1}.

$$\begin{aligned} S_1 &> \frac{4}{(2-\lambda)^2}\Big[x_1^2 - \frac{4}{(4-\lambda)(1-\lambda)}\big((x_3+x_{-1})(x_3-x_{-1}) \\ &\quad + (x_6+x_3)(x_6-x_3) + \cdots + (x_{k-1}+x_{k-4})(x_{k-1}-x_{k-4})\big) - x_{k-1}^2\Big] \\ &= \frac{4}{(2-\lambda)^2}\Big[x_1^2 - \frac{4}{(4-\lambda)(1-\lambda)}\big(-x_{-1}^2 + x_{k-1}^2\big) - x_{k-1}^2\Big] \\ &> -\frac{4x_{k-1}^2}{(2-\lambda)^2}\Big[\frac{4}{(4-\lambda)(1-\lambda)} + 1\Big] = -\frac{4(8-5\lambda+\lambda^2)x_{k-1}}{(2-\lambda)^2(4-\lambda)(1-\lambda)} \end{aligned} \tag{12}$$

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

$$-2x_{k-1}^2 + 4(y_{k-1}^2 + y_k^2 - x_k^2) = \frac{2(4 + 60\lambda + 33\lambda^2 - 28\lambda^3 + 4\lambda^4)}{(2-\lambda)^2} x_{k-1}^2.$$

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

$$\|\mathbf{y}\|^2 - \|\mathbf{x}\|^2 > \frac{4\lambda(115-149\lambda+30\lambda^2)}{(2-\lambda)^2(4-\lambda)(1-\lambda)}x_{k-1}^2 > \frac{\lambda(115-149\lambda)}{(2-\lambda)^2}x_{k-1}^2. \qquad (13)$$

A Bound for $\mathbf{y}^T L\mathbf{y}$. Here we wish to find an upper bound for $\mathbf{y}^T L(G_n)\mathbf{y} - \mathbf{x}^T L(H_n)\mathbf{x}$ in terms of x_{k-1} and λ. From equation (3),

$$\mathbf{y}^T L(G_n)\mathbf{y} - \mathbf{x}^T L(H_n)\mathbf{x} = \sum_{\{i,j\}\in E(G_n)}(y_i - y_j)^2 - \sum_{\{i,j\}\in E(H_n)}(x_i - x_j)^2.$$

In these sums, the contribution of the edge between x_{-1} and x_1 in H_n is equal to the contributions from the four edges between y_{-1} and y_1 in G_n. Between x_1 and x_3, using the expression (7) for x_2,

$$2(x_1-x_2)^2 + 2(x_2-x_3)^2 = (x_1-x_3)^2\left(1+\frac{\lambda^2}{(2-\lambda)^2}\right) > (y_1-y_2)^2;$$

that is, the edges in H_n contribute more than the corresponding edge in G_n. The same holds for the edges between x_3 and x_6 in H_n and the edges from y_2 to y_5 in G_n. The difference δ of their contributions is

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

Inserting from equations (5) and (7) establishes

$$\delta = \frac{\lambda^2}{(2-\lambda)^2}(x_6-x_3)(x_3+2x_4+x_6) > 0. \qquad (14)$$

In the same way, all other edges between x_6 and x_{k-1} contribute more than the corresponding edges in G_n. 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 on the other end of G_n, which are not counterbalanced by any edges in H_n. 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,

$$\mathbf{y}^T L(G_n)\mathbf{y} - \mathbf{x}^T L(H_n)\mathbf{x} < \frac{4\lambda^2(4-\lambda)^2}{(2-\lambda)^2}x_{k-1}^2 < \frac{64\lambda^2}{(2-\lambda)^2}x_{k-1}^2 \qquad (15)$$

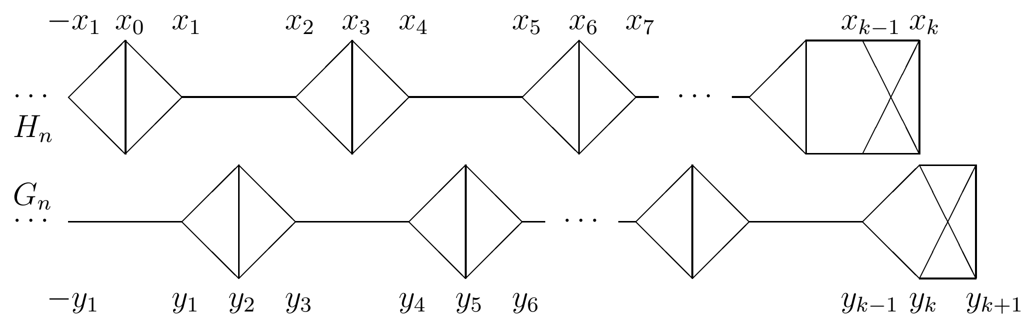


Figure 3: Graphs H_n and G_n for $n \equiv 2 \pmod 8$

The Rayleigh Quotient. Now comes the easy part. We combine the inequalities (13) and (15).

$$\begin{aligned}\frac{\mathbf{y}^T L(G_n)\mathbf{y}}{\|\mathbf{y}\|^2} &< \frac{\mathbf{x}^T L(H_n)\mathbf{x} + \frac{64\lambda^2}{(2-\lambda)^2}x_{k-1}^2}{\|\mathbf{x}\|^2 + \frac{\lambda(115-149\lambda)}{(2-\lambda)^2}x_{k-1}^2} \\ &= \lambda\frac{(2-\lambda)^2\|\mathbf{x}\|^2 + 64\lambda x_{k-1}^2}{(2-\lambda)^2\|\mathbf{x}\|^2 + \lambda(115-149\lambda)x_{k-1}^2} < \lambda. \qquad (16)\end{aligned}$$

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 $\lambda \approx 0.12709$, and for larger n the eigenvalues will be smaller.

5.2 Odd diameter of G_n: Case $n \equiv 2 \pmod 8$

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

$$\begin{aligned}&y_1 = x_1,\ y_2 = \frac{x_1+x_2}{2-\lambda},\ y_3 = x_2,\\ &y_4 = x_4,\ y_5 = \frac{x_4+x_5}{2-\lambda},\ y_6 = x_5,\ \ldots,\ y_{k-1} = x_{k-1} \qquad (17)\\ &y_k = 2x_{k-1} - x_{k-2},\ y_{k+1} = x_k + x_{k-1} - x_{k-2}.\end{aligned}$$

$$x_3 = \frac{x_2+x_4}{2-\lambda},\ x_6 = \frac{x_5+x_7}{2-\lambda},\ \cdots,\ x_{k-2} = \frac{x_{k-3}+x_{k-1}}{2-\lambda}. \qquad (18)$$

$$x_2 < \frac{2(x_1+x_4)}{(4-\lambda)(1-\lambda)},\ x_5 < \frac{2(x_4+x_7)}{(4-\lambda)(1-\lambda)}, \ldots,\ x_{k-3} < \frac{2(x_{k-4}+x_{k-1})}{(4-\lambda)(1-\lambda)}. \qquad (19)$$

$$x_{k-2} = \frac{2-5\lambda+\lambda^2}{2-\lambda}x_{k-1}, \qquad x_k = \frac{2}{2-\lambda}x_{k-1},$$
$$y_k = \frac{2+3\lambda-\lambda^2}{2-\lambda}x_{k-1}, \qquad y_{k+1} = \frac{2+4\lambda-\lambda^2}{2-\lambda}x_{k-1}. \tag{20}$$

The difference of the squares of $\mathbf{x}$ and $\mathbf{y}$ is

$$\begin{aligned} \|\mathbf{y}\|^2 - \|\mathbf{x}\|^2 &= 4(y_2^2 - x_3^2 + y_5^2 - x_6^2 + \cdots + y_{k-3}^2 - x_{k-2}^2) \\ &\quad - 2x_{k-1}^2 + 4(y_k^2 + y_{k+1}^2 - x_k^2). \end{aligned} \tag{21}$$

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

$$\|\mathbf{y}\|^2 - \|\mathbf{x}\|^2 > \frac{\lambda(115-149\lambda)}{(2-\lambda)^2}x_{k-1}^2,$$

which is exactly inequality (13).

To bound $\mathbf{y}^T L(G_n)\mathbf{y}$, we compare the contributions 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

$$\delta = \frac{-\lambda^2}{(2-\lambda)^2}(x_4-x_1)(x_1+2x_2+x_4) < 0,$$

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 on the other end of G_n, which are not counterbalanced by edges in H_n. Their contribution is

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

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

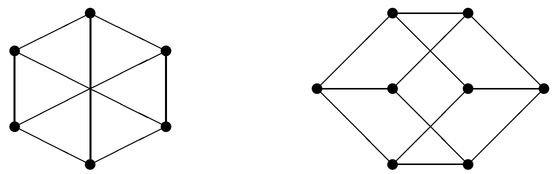
With due relief, we pronounce the concluding *quod erat demonstrandum* for Lemma 5, and thus for Theorem 1 as well. □

6 Trivalent graphs with maximum diameter

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

Theorem 2 *The graph G_n from Definition 1 is a graph of maximum diameter among all trivalent graphs on n vertices.*

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:



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 at the end or in the interior, taken also from (1) and (2) or from:

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

For $n \leq 8$, enumeration solves the problem (see, e.g., the tables in Cvetković et al.[4]). For $n \geq 10, d \geq 5$, we derive a lower bound (23) for n in terms of given d, and we show that this bound is sharp for exactly those graphs specified in this theorem. The following lemmas cover the technical details. $\square$

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 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, its edge being a bridge.

Lemma 6 *Let G be a cubic graph with minimal number of vertices for a given, fixed diameter d. 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.*

Proof: We observe first that of any two blocks that have a vertex in common exactly one must be a K_2, because every vertex has degree 3.

Consider a diameter P in G and denote the subgraph formed by all the blocks it meets in at least two vertices by G_P. Clearly (since block graphs are trees), the block graph of G_P is a path. If the assertion of the proposition is not true there must be a block B which is connected to G_P by an edge e where the endpoint a of e in G_P has two neighbors a_1 and a_2 in G_P. We now delete e and B as well as all edges incident with them from G and connect a_1 and a_2 by a small interior block (2). This decreases the number of vertices in G by at least 2 and does not decrease the diameter. $\Box$

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

$$|B| \geq 2d + 2 - i.$$

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

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

$$|P \cup Q| + 1 \geq 2d + 1.$$

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

Case 2. $i > 0$. If a or b or both have degree three, by the same argument as above,

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

If both of them are of degree 2, then neither a_2 nor b_2 exist and the bound has to be lowered by one. $\Box$

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.

As we shall see, only minimal blocks of diameter ≤ 3 will be of importance for the charcterization of cubic graphs with given diameter and minimal number of vertices. These minimal blocks are:

For diameter 1 the complete graph K_4.

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

For diameter 3 and $i = 0$ we have the three cubic graphs on 8 vertices with diameter 3; for $i = 1$ just two graphs, the large end block (1) and the one depicted in Theorem 2; and for $i = 2$ three graphs, only two of which are interesting for 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.

Lemma 8 *Let G be a cubic graph on n vertices, with diameter d. Then its number k of bridges satisfies the inequality*

$$n \geq 2d - 2k + 2. \tag{22}$$

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. □

Thus, for 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 smallest possible diameter.

Consequently, either there are $k+1$ blocks with diameter 2, or just one block has diameter three. Then,

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

The lower bound (22) in these cases becomes

$$\begin{aligned} n &\geq \frac{2}{3}(5+2d) \quad \text{if } d \equiv 2 \pmod 3, \quad \text{or} \\ n &\geq 4 + \frac{4}{3}d \quad \text{if } d \equiv 0 \pmod 3, \end{aligned} \tag{23}$$

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, both endblocks have five vertices and the interior blocks 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

[1] N. Alon, Eigenvalues and expanders, *Combinatorica* **6** (1986), 83–96.

[2] N. Alon and V. D. Milman, Eigenvalues, expanders, and superconcentrators, *Proc. 25th IEEE FOCS,* (Singer Island, Florida, 1984), pp. 320–322.

[3] F. C. Bussemaker, S. Čobeljić, D. M. Cvetković, and J. J. Seidel, Computer investigation of cubic graphs. Technological University Eindhoven, 1976. (Report 76-WSK-01).

[4] D. M. Cvetković, M. Doob and H. Sachs, *Spectra of Graphs*, Academic Press, New York 1980

[5] M. Fiedler, Algebraic connectivity of graphs, *Czech. Math. J.* **23** (1973), pp. 298–305.

[6] M. Fiedler, A property of eigenvectors of nonnegative symmetric matrices and its application to graph theory, *Czech. Math. J.* **25** (1975), pp. 619–633.

[7] C. D. Godsil, *Algebraic Combinatorics*, Chapman & Hall, New York, 1993.

[8] B. Guiduli, The structure of trivalent graphs with minimal eigenvalue gap, *Journal of Algebraic Combinatorics* **6** (1997), pp. 321–329

[9] G. Jaklič, T. Pisanski, M. Randić, Characterization of complex biological systems by matrix invariants. *Journal of Computational Biology*, **13** (2006), pp. 1558–1564

[10] B. Mohar, Laplace eigenvalues of graphs—a survey, *Dics. Math.*, **109** (1992), pp. 171–183.

[11] F. Zhang, A. Chang, Acyclic molecules with greatest HOMO-LUMO separation. *Discrete Appl. Math.*, **98** (1999), no. 1-2, 165–171.