

# The Structure of Trivalent Graphs with Minimal Eigenvalue Gap\*

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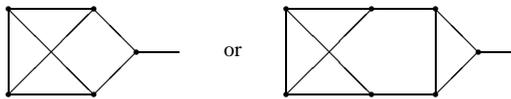
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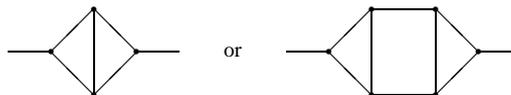
**Abstract.** Let  $G$  be a connected trivalent graph on  $n$  vertices ( $n \geq 10$ ) such that among all connected trivalent graphs on  $n$  vertices,  $G$  has the largest possible second eigenvalue. We show that  $G$  must be *reduced path-like*, i.e.  $G$  must be of the form:



where the ends are one of the following:



(the right-hand end block is the mirror image of one of the blocks shown) and the middle blocks are one of the following:



This partially solves a conjecture implicit in a paper of Bussemaker, Čobeljčić, Cvetković, and Seidel [3].

**Keywords:** trivalent graph, eigenvalue

## 1. Introduction

We let  $G$  be a connected  $k$ -regular graph on  $n$  vertices, and  $A$  its adjacency matrix. Let  $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$ , be the eigenvalues of  $A$ , also called the eigenvalues of  $G$ . They are real,  $\lambda_1 = k$  and  $\lambda_2 < k$ . The difference between  $\lambda_1$  and  $\lambda_2$  is called the *eigenvalue gap*. The eigenvalue gap was first investigated by Fiedler in 1973, who called it the *algebraic connectivity* (see [5]). He bounded this gap above and below by functions of the edge connectivity of  $G$ . Later, Alon and Milman [2] and Alon [1] bounded the isoperimetric ratio of  $G$  (a more global measure of connectivity) above and below, respectively, by functions of the eigenvalue gap.

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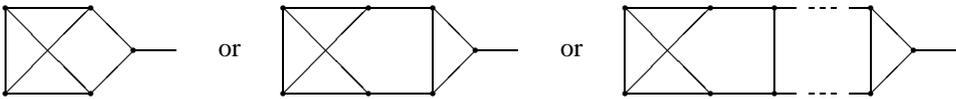
In 1976, Bussemaker, Čobeljčić, Cvetković, and Seidel ([3], see also [4]) enumerated all connected trivalent graphs with up to 14 vertices. (We note that trivalent graphs must have an even number of vertices.) They ordered the graphs lexicographically by their eigenvalues. The ordering is interesting in that certain combinatorial properties change gradually (e.g. diameter, connectivity, girth). Graphs whose second largest eigenvalue is large, tend to be very long, path-like; they have cut edges, large diameter, and small girth. Moving down the list, as the second eigenvalue decreases, diameter decreases and both connectivity and girth increase. Those for which the second eigenvalue is smallest are very compact, they have small diameter, large girth, and high connectivity.

We show that the trivalent graph on  $n$  vertices with maximal second eigenvalue must look like a path. We formalize this with the following definitions.

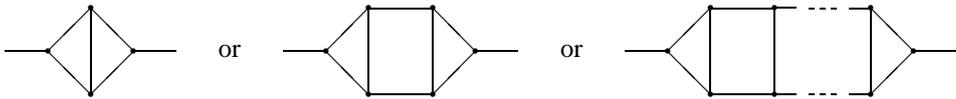
**Definition** A trivalent graph is said to be *path-like* if it has the form:



where each end block is one of the following:



(the right-hand end block is the mirror image of one of the blocks shown) and each middle block is one of the following:



**Definition** We define a trivalent graph to be *reduced path-like* if it is path-like, the end blocks are of the first two types, and the middle blocks are of the first two types.

Let  $H_n$  be the reduced path-like graph on  $n$  vertices with middle blocks of the first type and one end block of the first type. The other end block is then forced by the value of  $n$ .

The graph  $H_n$  only makes sense for  $n \geq 10$ , and the enumeration of Bussemaker et al. shows that for  $n = 10, 12, 14$ ,  $H_n$  is the unique connected trivalent graph with maximal second eigenvalue. L. Babai proposed the following conjecture, implicit in the results of Bussemaker et al.:

**Conjecture.** For  $n \geq 10$ , the graph  $H_n$  is the unique connected trivalent graph with maximum second eigenvalue.

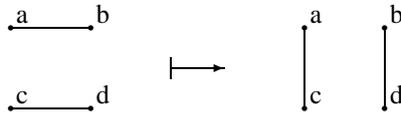
We do not prove the conjecture, instead we prove the following result which supports the conjecture.

**Theorem 1** *Let  $G$  be a connected trivalent graph on  $n$  vertices ( $n \geq 10$ ), such that among all connected trivalent graphs on  $n$  vertices,  $G$  has maximal possible second eigenvalue. Then  $G$  is reduced path-like.*

(Note: for the exact graphs achieving the maximum second eigenvalue for  $n < 10$ , see the paper of Bussemaker et al. [3])

We make one more elementary definition and then outline the proof of the theorem.

**Definition** An *elementary move* in a graph is a switching of parallel edges: let  $a \sim b$  and  $c \sim d$  in  $G$ ,  $a \not\sim c$ ,  $b \not\sim d$  (here  $\sim$  and  $\not\sim$  denote adjacency and non-adjacency in  $G$ ), then the elementary move  $\text{SWITCH}(a, b, c, d)$  removes the edges  $\{a, b\}$  and  $\{c, d\}$  and replaces them with the edges  $\{a, c\}$  and  $\{b, d\}$ .



We prove the theorem in two parts. First we show that if  $G$  is not already minimal path-like, we may transform it into such a graph by elementary moves, never decreasing the second eigenvalue (and assuming it is maximal, never increasing it). Throughout the transformation, we maintain connectivity. We then show that the eigenvector for the second eigenvalue is strictly decreasing from left to right (when the graph is drawn path-like, as above). It then follows that any elementary move will decrease the second eigenvalue, thus showing that  $G$  must have been minimal path-like to begin with.

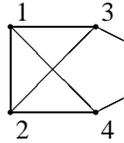
**2. General set-up**

Let  $G$  be a connected trivalent graph on  $n$  vertices. Let  $A$  be the adjacency matrix of  $G$ . The largest eigenvalue of  $G$  is 3 with eigenvector  $\mathbf{j}$ , the all one's vector. The second eigenvalue,  $\lambda_2$ , is given by the maximum of the Rayleigh quotient:

$$\lambda_2 = \max_{\mathbf{x} \perp \mathbf{j}} \frac{\mathbf{x}^t A \mathbf{x}}{\|\mathbf{x}\|^2}.$$

Let  $\mu : V \rightarrow \mathbb{R}$  be an eigenvector for the second eigenvalue, considered as a weighting on the vertices; for  $v \in V$  we write  $\mu_v = \mu(v)$ . For convenience, we may assume the vertex set is  $[n] = \{1, 2, \dots, n\}$  and that the vertices are numbered so that  $\mu_1 \geq \mu_2 \geq \dots \geq \mu_n$ . We call this a *proper labeling* of the vertices (with respect to the eigenvector for the second eigenvalue).

We can now clarify the reconnecting. With respect to a proper labeling, we show that we can reconnect to get vertex 1 adjacent to vertices 2, 3, and 4. We can then reconnect to get 2 adjacent to 3 and 4. This now looks like:



We show that we can continue in this way, getting a path-like graph, with the labels increasing from left to right. The trick is not to disconnect the graph while we are reconnecting, and not to lower the second eigenvalue. We ensure that the eigenvalue does not decrease by choosing our switch carefully.

**Lemma 1** *Let  $G$  be a connected trivalent graph with maximal  $\lambda_2$ . Let  $\mu : V \rightarrow \mathbb{R}$  be an eigenvector for  $\lambda_2$ . If there are vertices  $a, b, c, d$  in  $G$  such that  $a \sim b, c \sim d, a \not\sim c, b \not\sim d, \mu_a \geq \mu_d$ , and  $\mu_c \geq \mu_b$ , then  $\text{SWITCH}(a, b, c, d)$  does not decrease the second eigenvalue.*

**Proof:** We may assume that  $\|\mu\| = 1$ , then  $\lambda_2 = \mu^t A \mu$ , where  $A$  is the adjacency matrix of  $G$ . Let  $A'$  be the adjacency matrix of the graph after the reconnection. In light of the Rayleigh quotient, it suffices to show that

$$\mu^t A' \mu \geq \mu^t A \mu.$$

This follows immediately from

$$\begin{aligned} \mu^t A' \mu - \mu^t A \mu &= \mu^t (A' - A) \mu = 2\mu_a \mu_c + 2\mu_b \mu_d - 2\mu_a \mu_b - 2\mu_c \mu_d = \\ &= 2(\mu_a - \mu_d)(\mu_c - \mu_b) \geq 0. \end{aligned} \quad \square$$

We have the following lemma to help with keeping the graph connected during reconnecting:

**Lemma 2** *Let  $G$  be a connected trivalent graph on  $[n]$  with maximal  $\lambda_2$ , properly labeled with respect to an eigenvector  $\mu$ . Assume that  $G \setminus [r]$  is disconnected and that each of its components has an edge which is not a cut edge. Then we may reconnect the graph using elementary moves to connect  $G \setminus [r]$ , not changing  $\lambda_2$ .*

**Proof:** It suffices to prove the lemma when  $G \setminus [r]$  has two connected components  $H$  and  $K$ . We will prove the lemma by contradiction. Assume that we cannot reconnect the graph to accomplish our goal. Let  $\{u_1, u_2\}$  be a non-cut edge in  $H$  and  $\{v_1, v_2\}$  a non-cut edge in a cycle in  $K$ . Because these edges are not cut edges, both  $\text{SWITCH}(u_1, u_2, v_1, v_2)$  and  $\text{SWITCH}(u_1, u_2, v_2, v_1)$  would leave  $G$  and  $G \setminus [r]$  connected, so it must be the case that these switches decrease  $\lambda_2$ . Based on the previous lemma, this only happens if the weights of one pair are strictly greater than those of the other pair. We may assume that  $\mu_{u_1}, \mu_{u_2} > \mu_{v_1}, \mu_{v_2}$ . Let  $x$  be an element in  $[r]$  adjacent to  $K$  and let  $(v_1, v_2, v_3, \dots, v_t)$  be a shortest path in  $G$ ,  $v_t = x$  (we may possibly need to switch the roles of  $v_1$  and  $v_2$ ). For  $1 \leq i < t$ ,  $\text{SWITCH}(u_1, u_2, v_i, v_{i+1})$  and  $\text{SWITCH}(u_1, u_2, v_{i+1}, v_i)$  would connect  $H$  and  $K$ , leaving the graph connected, so by induction,  $\mu_{u_1}, \mu_{u_2} > \mu_{v_1}, \mu_{v_2}, \dots, \mu_{v_t}$ , but this is a contradiction, as  $\mu_x \geq \mu_v$  for all  $v \in H$ . □

### 3. Reconnecting to get reduced path-like

Assume that  $G$  is a connected trivalent graph on  $n$  vertices,  $n \geq 10$ . We further assume that among all connected trivalent graphs on  $n$  vertices,  $G$  has maximal second eigenvalue, and that  $G$  is properly labeled. During the reconnecting, we will denote  $G$  by  $G_k$  to indicate that the first  $k$  vertices are in path-like form.

#### 3.1. Getting $G_4$

##### 3.1.1. Connecting 1 to 2.

If  $1 \not\sim 2$  then there is a shortest path  $(1, i_1, \dots, i_r, 2)$  from 1 to 2. Let  $x$  be a neighbor of 1 such that  $x \neq i_1$  and  $x \not\sim i_r$ , then we may apply SWITCH(1,  $x$ , 2,  $i_r$ ), not decreasing the second eigenvalue and leaving 1 adjacent to 2 and  $G$  connected.

##### 3.1.2. Connecting 1 to 3.

If  $1 \not\sim 3$  then let  $x \neq 2$  be a neighbor of 1. By a simple counting argument, each connected component of  $G \setminus \{1\}$  contains a cycle. We may therefore use Lemma 2 to assume that  $G \setminus \{1\}$  is connected. Let  $(x, i_1, \dots, i_r, 3)$  be a shortest path from  $x$  to 3 not passing through 1. Let  $y$  be a neighbor of 3 so that  $y \neq i_r$  and  $y \not\sim i_r$ , then SWITCH(1,  $x$ , 3,  $y$ ).

##### 3.1.3. Connecting 1 to 4.

(This is identical to the previous reconnection.) If  $1 \not\sim 4$  then let  $x$  be the third neighbor of 1. We may assume (by Lemma 2), that  $G \setminus \{1\}$  is connected. Let  $(x, i_1, \dots, i_r, 4)$  be a shortest path from  $x$  to 4 not passing through 1. Let  $y$  be a neighbor of 4 so that  $y \neq i_r$  and  $y \not\sim i_r$ , then SWITCH(1,  $x$ , 4,  $y$ ).

##### 3.1.4. Connecting 2 to 3.

We may assume that  $G \setminus \{1\}$  is connected. Let  $(2, i_1, \dots, i_r, 3)$  be a shortest path in  $G \setminus \{1\}$ . Let  $x$  be the third neighbor of 2 and  $y$  the third neighbor of 3. If  $r = 2$ ,  $x \sim i_2$ , and  $i_1 \sim y$ , then  $x$  cannot be adjacent to  $y$  because  $G \setminus \{1\}$  is connected, so SWITCH(2,  $x$ , 3,  $y$ ) connects 2 to 3, as required. Otherwise, either  $x \not\sim i_r$  and SWITCH(2,  $x$ , 3,  $i_r$ ), or  $i_1 \not\sim y$  and SWITCH(2,  $i_1$ , 3,  $y$ ).

##### 3.1.5. Connecting 2 to 4.

If there is a vertex  $x$  adjacent to 2, 3, and 4, let  $y$  be the third neighbor of 4, then  $x \not\sim y$  and SWITCH(2,  $x$ , 4,  $y$ ). Otherwise, we may assume by Lemma 2 that  $G \setminus [4]$  is connected.

Let  $x$  be the third neighbor of 2,  $y$  the third neighbor of 3, and let  $u$  and  $v$  be the two other neighbors of 4. If  $3 \sim 4$  then SWITCH(2,  $x$ , 4, 3). Otherwise, if  $x \neq u$  and  $x \not\sim u$ , then apply SWITCH(2,  $x$ , 4,  $u$ ). If one of these relations does not hold, try the same for  $v$  instead of  $u$ . If the same relations hold for  $v$ , try to get  $3 \sim 4$  by considering 3 instead of 2 and looking at  $u$  and  $v$ ; then SWITCH(2,  $x$ , 4, 3) will work. If none of these are allowed, then  $G \setminus [4]$  has a connected component consisting of just  $\{x, y, u, v\}$ , this set having 2 or 4 points depending on the equalities, and being disconnected from the rest of the graph. This contradicts the fact that  $G \setminus [4]$  is connected (in fact, in this case  $G$  has a connected component with 6 or 8 vertices, contradicting the fact that  $G$  is connected with at least 10 vertices).

### 3.2. General Steps

We now introduce general steps that deal with the remaining vertices. We assume at this point that the graph  $G$  has the desired connections among the vertices  $[r]$ , i.e. we have  $G_r$ . The next three sets of general steps show how to reconnect  $G_r$  to get either  $G_{r+1}$  or  $G_{r+2}$ .

#### 3.2.1. $r$ is odd.

Based on our construction, we only arrive at this case when  $r \sim r-2$  and  $r \sim r-1$ , so there is only one edge leaving the first  $r$  vertices, and it leaves from  $r$ . We need to connect  $r$  to  $r + 1$ . Let  $x$  be the third neighbor of  $r$  and  $y$  be a neighbor of  $r + 1$  the furthest possible from  $r$  and SWITCH( $r$ ,  $x$ ,  $r + 1$ ,  $y$ ). This gives us  $G_{r+1}$ .

#### 3.2.2. $r$ is even and the two edges leaving the first $r$ vertices both come from $r$ .

**Step 1.** Connect  $r$  to  $r + 1$ . Let  $x$  be the neighbor of  $r$  closest to  $r + 1$  and let  $y$  be the neighbor of  $r + 1$  furthest from  $r$ . SWITCH( $r$ ,  $x$ ,  $r + 1$ ,  $y$ ).

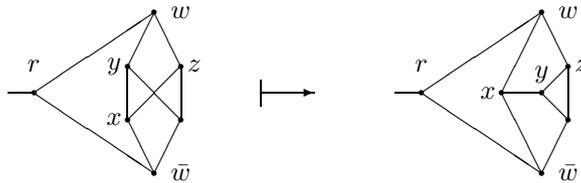
**Step 2.** Connect  $r$  to  $r + 2$ . We may assume that  $G \setminus [r + 1]$  is connected. Let  $x$  be the third neighbor of  $r$ . Let  $y$  be the neighbor of  $r + 2$  furthest from  $x$  in  $G \setminus [r]$ . SWITCH( $r$ ,  $x$ ,  $r + 2$ ,  $y$ ). This does not disconnect because there is a path from  $x$  to one of the other neighbors of  $r + 2$  not using the two removed edges.

**Step 3.** Connect  $r + 1$  to  $r + 2$ . We may assume that  $G \setminus [r + 2]$  is connected. There are some cases to consider:

CASE I:  $r + 1$  and  $r + 2$  share two neighbors. Call the neighbors  $x$  and  $y$ . If  $x \sim y$ , then  $n = r + 4$  and we are done as this is  $G_n$ . Otherwise, SWITCH( $r + 1$ ,  $x$ ,  $r + 2$ ,  $y$ ). This leaves  $G_{r+2}$ .



CASE II:  $\text{dist}_{G \setminus [r]}(r + 1, r + 2) = 3$  and both neighbors of  $r + 1$  and  $r + 2$  are adjacent to each other (then  $n = r + 6$ ). Let  $x$  be the smallest among the remaining vertices (i.e.  $x = r + 3$ ), so  $\mu_x$  is largest among the remaining vertices. Let  $y, z$  be the two neighbors of  $x$  and let  $w = r + 1$  or  $r + 2$ , whichever is adjacent to  $y$  and  $z$ , and call the other  $\bar{w}$ . Then  $\text{SWITCH}(w, y, x, z)$  reduces the graph to CASE III.



CASE III:  $\text{dist}_{G \setminus [r]}(r + 1, r + 2) = 2$ . If we arrive at this case then  $r + 1$  and  $r + 2$  share one neighbor (because of CASE I). Call this neighbor  $x$  and let  $y$  and  $z$  be the other neighbors of  $r + 1$  and  $r + 2$  respectively. Then either  $x \not\sim y$  and  $\text{SWITCH}(r + 1, y, r + 2, x)$ , or  $x \not\sim z$  and  $\text{SWITCH}(r + 1, x, r + 2, z)$ . This leaves  $G_{r+2}$ .

CASE IV: Let  $x$  and  $y$  be neighbors of  $r + 1$  and  $r + 2$  respectively, such that  $x \not\sim y$  and one is on a path from  $r + 1$  to  $r + 2$ .  $\text{SWITCH}(r + 1, x, r + 2, y)$ .

3.2.3.  $r$  is even and the two edges leaving the first  $r$  vertices come from  $r$  and  $r - 1$ .

We note that if we arrive at this case, then  $r \sim r - 1$ .

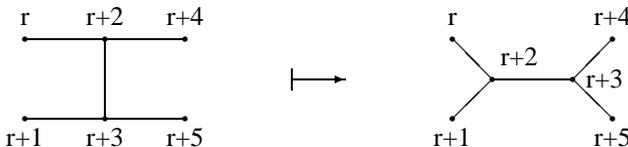
**Step 1.** Connect  $r - 1$  to  $r + 1$ . We may assume that  $G \setminus [r]$  is connected and hence there is a path from  $r - 1$  to  $r + 1$  not passing through  $r$ . Let  $x$  be the third neighbor of  $r - 1$  and let  $y$  be the neighbor of  $r + 1$  furthest from  $r - 1$  in  $G_r \setminus \{r\}$ .  $\text{SWITCH}(r - 1, x, r + 1, y)$ . If  $r \sim r + 1$  too, then this is  $G_{r+1}$  and skip the following steps.

**Step 2.** Connect  $r$  to  $r + 2$ . This is the same as step 2 above.

**Step 3.** Connect  $r + 1$  to  $r + 2$ . This is the same as for step 3 above.

3.3. Putting  $G$  in reduced path-like form

We may now assume that  $G$  is path-like with labels increasing from left to right in a proper labeling (this is what we have achieved in the previous reconnecting). By applying  $\text{SWITCH}(r + 1, r + 3, r + 2, r + 4)$  as often as possible to  $G$ , we put  $G$  in minimal path-like form without decreasing  $\lambda_2$ .



**4. The eigenvector coordinates are strictly decreasing**

In the previous section we reconnected the graph to put it in reduced path-like form with the weights given by  $\mu$  non-increasing from left to right. Assume that the graph is drawn horizontally like the original example in the definition of path-like, with the vertices numbered 1 to  $n$ , increasing from left to right. Further, assume that the weights of the vertices given by an eigenvector  $\mu$  of  $\lambda_2$  are non-increasing from left to right. We will show that these weights are in fact strictly decreasing. We may assume that vertices with the same vertical position (a set of points are in the said to have the same *vertical position* if they lie on the same vertical line) have the same weight (we may assume this by noticing that there is a graph automorphism interchanging any two vertices in the same vertical position, and then averaging the eigenvector). Assume that there are two adjacent vertices in a different vertical position with the same weight. If this is the case, then we can find two such ones  $c$  and  $d$  ( $c$  to the left of  $d$ ) so that the left-most neighbor of  $c$ , call it  $a$ , has greater weight than the right-most neighbor of  $d$ , call this  $f$ . Let  $b$  and  $e$  be the other neighbors of  $c$  and  $d$ , respectively. It is possible that some of these coincide, but here are some important observations:  $a$  cannot be to the right or  $c$ ,  $f$  cannot be to the left of  $d$ ,  $b$  cannot be to the right of  $d$ , and  $e$  cannot be to the left of  $c$ . Summarizing what we know about the weights, we have  $\mu_a > \mu_f$  and  $\mu_a \geq \mu_b \geq \mu_c = \mu_d \geq \mu_e \geq \mu_f$ . We show that there exists some  $\epsilon > 0$  such that we may increase  $\mu_c$  by  $\epsilon$  and decrease  $\mu_d$  by  $\epsilon$  (keeping the vector perpendicular to  $j$ ) to increase the Rayleigh quotient, thus showing that the second eigenvalue was not maximal, and hence arriving at a contradiction. We assume that  $\|\mu\| = 1$ , then for the new vector, the Rayleigh quotient is

$$\frac{\lambda_2 + 2\epsilon(\mu_a + \mu_b + \mu_d - \mu_c - \mu_e - \mu_f - \epsilon)}{1 + 2\epsilon(\mu_c - \mu_d + \epsilon)},$$

which is greater than  $\lambda_2$  if

$$\mu_a + \mu_b - \mu_e - \mu_f > (\lambda_2 + 1)\epsilon.$$

This is possible, as the left hand side is greater than zero, and taking an appropriate  $\epsilon$ , we arrive at a contradiction.

**5. QED**

We need to show that any elementary move will now decrease the Rayleigh quotient, so that  $G$  must have been in this shape all along. If we apply SWITCH( $a, b, c, d$ ) to reconnect without decreasing the Rayleigh quotient, we must find four vertices  $a, b, c, d$  such that  $a \sim b$ ,  $c \sim d$ ,  $a \not\sim c$ ,  $b \not\sim d$ , SWITCH( $a, b, c, d$ ) does not disconnect  $G$ , and  $\mu_a \geq \mu_d$ ,  $\mu_c \geq \mu_b$ . In a path-like graph with  $\mu$  strictly decreasing from left to right, these four vertices only exist when  $a$  and  $b$  are in the same vertical position,  $c$  and  $d$  are in the same vertical position,  $a \sim d$ , and  $b \sim c$ . In this case, reconnecting leaves a graph isomorphic to the original. This completes the proof of Theorem 1.

□

## 6. Addendum

We Note that the full conjecture has recently been proved by Brand, Guiduli, and Imrich [6].

## Acknowledgments

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