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# An improved upper bound for the order of mixed graphs

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## Abstract

A mixed graph  $G$  can contain both (undirected) edges and arcs (directed edges). Here we derive an improved Moore-like bound for the maximum number of vertices of a mixed graph with diameter at least three. Moreover, a complete enumeration of all optimal  $(1, 1)$ -regular mixed graphs with diameter three is presented, so proving that, in general, the proposed bound cannot be improved.

*Keywords:* Mixed graph, Moore bound, network design, degree/diameter problem

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## 1. Introduction

A *mixed* (or *partially directed*) graph  $G = (V, E, A)$  consists of a set  $V$  of vertices, a set  $E$  of edges, or unordered pairs of vertices, and a set  $A$  of arcs, or ordered pairs of vertices. Thus,  $G$  can also be seen as a digraph having *digons*, or pairs of opposite arcs between some pairs of vertices. If there is an edge between vertices  $u, v \in V$ , we denote it by  $u \sim v$ , whereas if there is an arc from  $u$  to  $v$ , we write  $u \rightarrow v$ . We denote by  $r(u)$  the *undirected degree* of  $u$ , or the number of edges incident to  $u$ . Moreover, the *out-degree* [respectively, *in-degree*] of  $u$ , denoted by  $z^+(u)$  [respectively,  $z^-(u)$ ], is the number of arcs emanating from [respectively, to]  $u$ . If  $z^+(u) = z^-(u) = z$  and  $r(u) = r$ , for all  $u \in V$ , then  $G$  is said to be *totally regular* of degrees  $(r, z)$ , with  $r + z = d$  (or simply  $(r, z)$ -*regular*). The length of a shortest path from  $u$  to  $v$  is the *distance* from  $u$  to  $v$ , and it is denoted by  $\text{dist}(u, v)$ . Note that  $\text{dist}(u, v)$  may be different from  $\text{dist}(v, u)$  when the shortest paths between  $u$  and  $v$  involve arcs. The maximum distance between any pair of vertices is the *diameter*  $k$  of  $G$ . Given  $i \leq k$ , the set of vertices at distance  $i$  from vertex  $u$  is denoted by  $G_i(u)$ .

As in the case of (undirected) graphs and digraphs, the degree/diameter problem for mixed graphs calls for finding the largest possible number of vertices  $N(r, z, k)$  in a mixed graph with maximum undirected degree  $r$ , maximum directed outdegree  $z$ , and diameter  $k$ . A bound for  $N(r, z, k)$  is called a Moore(-like) bound. It is obtained by counting the number of vertices of a *Moore tree*  $MT(u)$  rooted at a given vertex  $u$ , with depth equal to the diameter  $k$ , and assuming that for any vertex  $v$  there exists a unique shortest path of length at most  $k$  (with the usual meaning when we see  $G$  as a digraph) from  $u$  to  $v$ . The number of vertices in  $MT(u)$ , which is denoted by  $M(r, z, k)$ , was given by Buset, Amiri, Erskine, Miller, and Pérez-Rosés [2], and it is the following:

$$M(r, z, k) = A \frac{u_1^{k+1} - 1}{u_1 - 1} + B \frac{u_2^{k+1} - 1}{u_2 - 1}, \quad (1)$$

where

$$\begin{aligned} v &= (z + r)^2 + 2(z - r) + 1, \\ u_1 &= \frac{z + r - 1 - \sqrt{v}}{2}, & u_2 &= \frac{z + r - 1 + \sqrt{v}}{2}, \\ A &= \frac{\sqrt{v} - (z + r + 1)}{2\sqrt{v}}, & B &= \frac{\sqrt{v} + (z + r + 1)}{2\sqrt{v}}. \end{aligned}$$

This bound applies when  $G$  is totally regular with degrees  $(r, z)$ . Moreover, if we bound the total degree  $d = r + z$ , the largest number is always obtained when  $r = 0$  and  $z = d$ . That is, when the mixed graph has no (undirected) edges. In Table 1 we show the values of (1) when  $r = d - z$ , with  $0 \leq z \leq d$ , for different values of  $d$  and diameter  $k$ . In particular, when  $z = 0$ , the bound corresponds to the Moore bound for graphs (numbers in bold).

$d \setminus k$	1	2	3	4	5
1	<b>2</b>	$z + \mathbf{2}$	$2z + \mathbf{2}$	$z^2 + 2z + \mathbf{2}$	$2z^2 + 2z + \mathbf{2}$
2	<b>3</b>	$z + \mathbf{5}$	$4z + \mathbf{7}$	$z^2 + 9z + \mathbf{9}$	$5z^2 + 16z + \mathbf{11}$
3	<b>4</b>	$z + \mathbf{10}$	$6z + \mathbf{22}$	$z^2 + 22z + \mathbf{46}$	$8z^2 + 66z + \mathbf{94}$
4	<b>5</b>	$z + \mathbf{17}$	$8z + \mathbf{53}$	$z^2 + 41z + \mathbf{161}$	$11z^2 + 176z + \mathbf{485}$
5	<b>6</b>	$z + \mathbf{26}$	$10z + \mathbf{106}$	$z^2 + 66z + \mathbf{426}$	$14z^2 + 370z + \mathbf{1706}$

Table 1: Moore bounds according to (1).

## 2. A new upper bound

An alternative approach for computing the bound given by (1) is the following (see also [4]). Let  $G$  be a  $(r, z)$ -regular mixed graph with  $d = r + z$ . Given a vertex  $v$  and for  $i = 0, 1, \dots, k$ , let  $N_i = R_i + Z_i$  be the maximum possible number of vertices at distance  $i$  from  $v$ . Here,  $R_i$  is the number of vertices that, in the corresponding tree rooted at  $v$ , are adjacent by an edge to their parents; and  $Z_i$  is the number of vertices that are adjacent by an arc from their parents. Then,

$$N_i = R_i + Z_i = R_{i-1}((r-1) + z) + Z_{i-1}(r + z). \quad (2)$$

That is,

$$R_i = R_{i-1}(r-1) + Z_{i-1}r, \quad (3)$$

$$Z_i = R_{i-1}z + Z_{i-1}z, \quad (4)$$

or, in matrix form,

$$\begin{pmatrix} R_i \\ Z_i \end{pmatrix} = \begin{pmatrix} r-1 & r \\ z & z \end{pmatrix} \begin{pmatrix} R_{i-1} \\ Z_{i-1} \end{pmatrix} = \dots = \mathbf{M}^i \begin{pmatrix} R_0 \\ Z_0 \end{pmatrix} = \mathbf{M}^i \begin{pmatrix} 0 \\ 1 \end{pmatrix},$$

where  $\mathbf{M} = \begin{pmatrix} r-1 & r \\ z & z \end{pmatrix}$  and, by convenience,  $R_0 = 0$  and  $Z_0 = 1$ . Therefore,

$$N_i = R_i + Z_i = \begin{pmatrix} 1 & 1 \end{pmatrix} \mathbf{M}^i \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

Consequently, after summing a geometric matrix progression, the order of  $MT(u)$  turns out to be

$$M(r, z, k) = \sum_{i=0}^k N_i = \frac{1}{r+2z-2} \begin{pmatrix} 1 & 1 \end{pmatrix} (\mathbf{M}^{k+1} - \mathbf{I}) \begin{pmatrix} r \\ z \end{pmatrix}, \quad (5)$$

with  $r+2z \neq 2$ , that is, except for the cases  $(r, z) = (0, 1)$  and  $(r, z) = (2, 0)$ , which correspond to a directed and undirected cycle, respectively.

Alternatively, note that  $N_i$  satisfies an easy linear recurrence formula (see again Buset, El Amiri, Erskine, Miller, and Pérez-Rosés [2]). Indeed, from (2) and (4) we have that  $Z_i = z(N_{i-1} - Z_{i-1}) + zZ_{i-1} = zN_{i-1}$  and, hence,

$$\begin{aligned} N_i &= (r+z)N_{i-1} - R_{i-1} = (r+z)N_{i-1} - (N_{i-1} - Z_{i-1}) \\ &= (r+z-1)N_{i-1} + zN_{i-2}, \quad i = 2, 3, \dots \end{aligned} \quad (6)$$

with initial values  $N_0 = 1$  and  $N_1 = r+z$ .

In this context, Nguyen, Miller, and Gimbert [8] showed that the bound in (1) is not attained for diameter  $k \geq 3$  and, hence, that *mixed Moore graphs* do not exist in general. More precisely, they proved that there exists a pair of vertices  $u, v$  such that there are two different paths of length  $\leq k$  from  $u$  to  $v$ . When there exist exactly two such paths, the usual terminology is to say that  $v$  is the *repeat* of  $u$ , and this is denoted by writing  $\text{rep}(u) = v$  (see, for instance, Miller and Širáň [6]). Extending this concept, we denote by  $\text{Rep}(u)$  the set (or multiset) of vertices  $v$  such that there are  $\nu \geq 2$  paths of length  $\leq k$  from  $u$  to  $v$ , in such a way that each  $v$  appears  $\nu - 1$  times in  $\text{Rep}(u)$ . (In other words, we could say that vertex  $v$  is “repeated” or “revisited”  $\nu - 1$  times when reached from  $u$ .) Then, as a consequence, the number  $N$  of vertices of  $G$  must satisfy the bound

$$N \leq |MT(u)| - |\text{Rep}(u)| = M(r, z, k) - |\text{Rep}(u)|.$$

We use this simple idea in the proof of our main result.

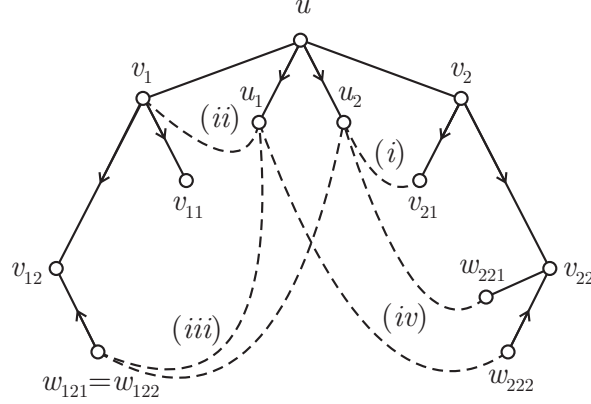


Figure 1: Repeated vertices in a  $(2,2)$ -regular mixed graph: (i)  $v_{21} \in \text{Rep}(u)$ ; (ii)  $v_{11} \in \text{Rep}(u)$ ; (iii)  $w_{121} \in \text{Rep}(u)$ ; (iv)  $w_{221} \in \text{Rep}(u)$ .

**Theorem 2.1.** *The order  $N$  of a  $(r, z)$ -regular mixed graph  $G$  with diameter  $k \geq 3$  satisfies the bound*

$$N \leq M(r, z, k) - r, \quad (7)$$

where  $M(r, z, k)$  is given by (1).

*Proof.* It is clear that we can assume that there are no parallel arcs or edges. Let  $u$  be a vertex with edges to the vertices  $v_1, \dots, v_r$  and arcs to the vertices  $u_1, \dots, u_z$ . For each  $i = 1, \dots, r$ , let  $v_{i1}, \dots, v_{iz}$  be the vertices adjacent (through arcs) from  $v_i$ . (The situation in the case  $r = z = 2$  is depicted in Figure 1, where the dashed lines represent paths.) Now, for some fixed  $i = 1, \dots, r$  and  $j = 1, \dots, z$ , let us consider the following possible cases for the distance from a vertex in  $\{u_1, \dots, u_z\}$  to vertex  $v_{ij}$ :

- (i) If, for some  $h = 1, \dots, z$ , we have  $\text{dist}(u_h, v_{ij}) < k$ , then there exist two paths of length at most  $k$  from  $u$  to  $v_{ij}$  and, hence,  $v_{ij} \in \text{Rep}(u)$  (note that this includes the case  $u_h = v_{ij}$ ).
- (ii) If, for some  $h = 1, \dots, z$ , we have  $\text{dist}(u_h, v_{ij}) = k$  and the shortest path from  $u_h$  to  $v_{ij}$  goes through  $v_i$ , then there are two paths of length  $\leq k$  from  $u$  to  $v_i$  (one of length 1 and the other of length  $k$ ). Hence,  $v_i \in \text{Rep}(u)$ . In fact, notice that, in this case,  $\text{dist}(u_h, v_{i\ell}) = k$  for every  $\ell = 1, \dots, z$ .

If, for every  $h = 1, \dots, z$ , we have  $\text{dist}(u_h, v_{ij}) = k$ , let  $w_{ij\ell}$  denote, for  $\ell = 1, \dots, z$ , the predecessor vertices to  $v_{ij}$  in the paths (of length  $k$ ) from every  $u_h$  to  $v_{ij}$  (see the dashed lines in Figure 1). Now we have again two cases:

- (iii) If, for some  $\ell, \ell' = 1, \dots, z$ , we have  $w_{ij\ell} = w_{ij\ell'}$ , then there are two paths of length  $k$  from  $u$  to  $w_{ij\ell}$ . Thus,  $w_{ij\ell} \in \text{Rep}(u)$ .
- (iv) Otherwise, since  $z^-(v_{ij}) = z$ , there must be at least one  $\ell$  such that  $w_{ij\ell}v_{ij}$  is an edge. But, in this case, there are two paths from  $u$  to  $w_{ij\ell}$  of length at most  $k(\geq 3)$  and, so,  $w_{ij\ell} \in \text{Rep}(u)$ .

As a consequence, we see that, for each  $i = 1, \dots, r$  there is a vertex, which is either  $v_i$ ,  $v_{ij}$ , or  $w_{ij\ell}$ , belonging to  $\text{Rep}(u)$ . Moreover, different values of  $i$  lead to different repeated vertices, so that the paths from  $u$  to them must be also different. In any case, the multiset  $\text{Rep}(u)$  has at least  $r$  elements, and the result follows.  $\square$

The new upper bound  $M(r, z, k) - r$  for diameter  $k \geq 3$  can be even improved for certain cases, as the next proposition states.

**Proposition 2.2.** *Let  $G$  be a  $(r, z)$ -regular mixed graph of diameter  $k \geq 3$  with order  $N$ . If  $r$  and  $z$  are odd, and  $k \equiv 2 \pmod{3}$ , then*

$$N \leq M(r, z, k) - r - 1. \quad (8)$$

*Proof.* The proof is based on a parity argument. Namely, since  $r$  is odd,  $N$  must be even. Thus, let us check the parity of  $M(r, z, k) - r = \sum_{i=0}^k N_i - r$ . Let  $\pi_i \in \{0, 1\}$  denote the parity of  $N_i$  in the obvious way. If  $z$  is odd, we have that  $\pi_0 = 1$ ,  $\pi_1 = 0$  and, from (6) we get the recurrence  $\pi_i = \pi_{i-1} + \pi_{i-2}$  for  $i \geq 2$ . This gives the following sequence for the  $\pi_i$ 's:  $1, 0, 1, 1, 0, 1, 1, 0, 1, 1, \dots$ . Thus,  $\sum_{i=0}^k N_i$  is even for every  $k \equiv 2 \pmod{3}$ . Then, as  $r$  is odd, we get the result.  $\square$

### 3. The case of $(1, 1)$ -regular mixed graphs with diameter three

In this section we show that the upper bound (7) is attained for exactly three mixed graphs in the case  $r = z = 1$  and  $k = 3$ .

**Proposition 3.1.** *Let  $G$  be a  $(1, 1)$ -regular mixed graph with diameter  $k = 3$  and maximum order  $N = 10$  given by (7). Then,  $G$  is isomorphic to one of the three mixed graphs depicted in Figure 2.*

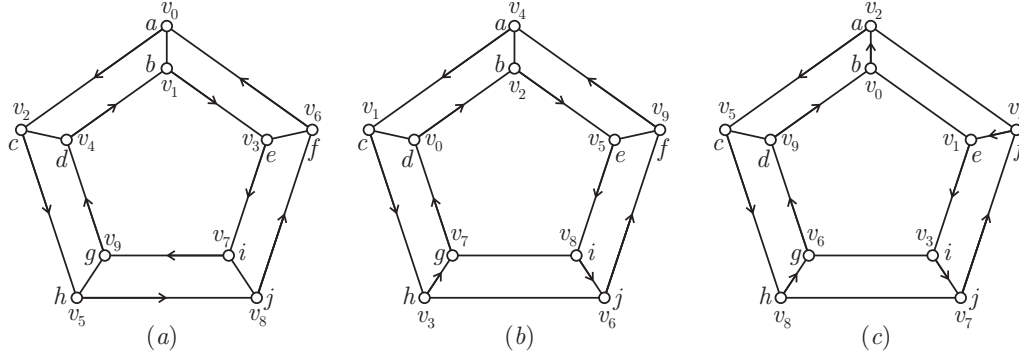


Figure 2: The unique three non-isomorphic  $(1,1)$ -regular mixed graphs with diameter  $k = 3$  and order  $N = 10$ .

*Proof.* We divide the proof according to the four cases (i)–(iv) given in Theorem 2.1. Let  $u$  be any vertex of  $G$ . The remaining vertices of  $G$  fall into one of the sets  $G_i(u)$ , according to their corresponding distance  $i \in \{1, 2, 3\}$  from  $u$ . Then,  $|G_1(u)| = 2$ , and it is easy to see that  $|G_2(u)| = 3$  and  $|G_3(u)| = 4$  since, otherwise,  $G$  would have order  $N < M(1, 1, 3) - 1 = 10$ . Now, observe that case (i) is impossible since  $\text{dist}(u_1, v_{11}) < 3$  would imply  $|G_3(u)| < 4$ . Also, case (iii) is not possible simply because  $z = 1$ . So, let us suppose that we are in case (ii), that is,  $\text{dist}(u_1, v_{11}) = 3$  and the shortest path from  $u_1$  to  $v_{11}$  goes through  $v_1$ . Hence,  $G$  contains one of the two induced mixed subgraphs depicted in Figure 3 (from now on, we follow the vertex labeling in this figure, where  $v_0 = u, v_2 = u_1$  and  $v_3 = v_{11}$ ). Next, we proceed in detail with case (iia) and we leave to the reader cases (iib) and (iv), where similar reasoning leads to the same mixed graphs.

Due to its regularity,  $G$  must contain the edge  $v_7 \sim v_8$ . Moreover, every vertex of  $G$  is at distance  $\leq 3$  from  $v_2$  except  $v_6$ . This means that there must exist an arc  $x \rightarrow v_6$ , where  $x \in \{v_8, v_9\}$ .

- Let  $x = v_8$ . Another arc  $y \rightarrow v_9$  is needed to have  $\text{dist}(v_1, v_9) \leq 3$ , where  $y \in \{v_6, v_7\}$ .
- If  $y = v_6 \rightarrow v_9$  we have just two possibilities to complete the regularity of the mixed graph:
  - The remaining arcs are  $v_7 \rightarrow v_0$  and  $v_9 \rightarrow v_4$ , which yield the mixed graph of Figure 4(iia1), which is isomorphic to the one in Figure 2(b).



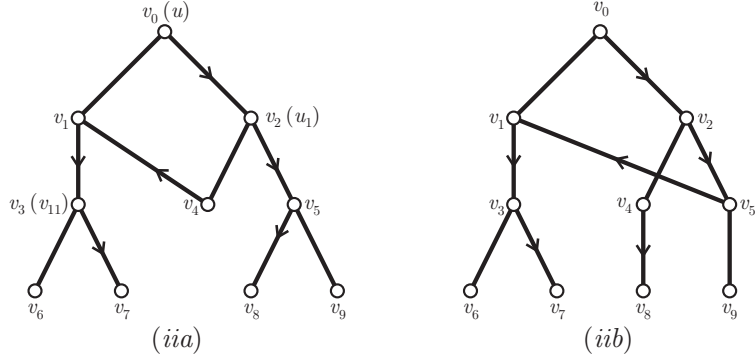


Figure 3: The two cases derived from (ii) according to Theorem 2.1 when  $r = 1, z = 1$  and  $k = 3$ .

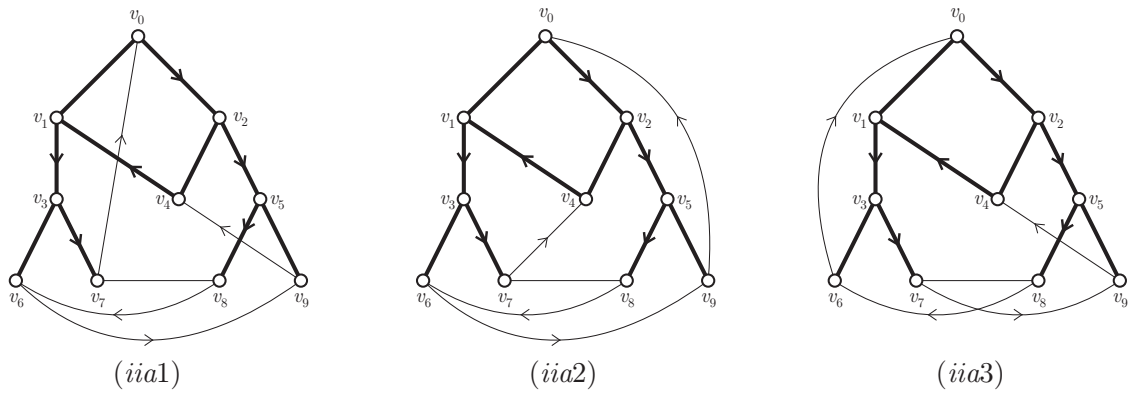


Figure 4: Three cases derived from (iia) giving non-isomorphic mixed graphs.

- The last arcs are  $v_7 \rightarrow v_4$  and  $v_9 \rightarrow v_0$ , in which case we obtain the mixed graph of Figure 4(iia2), which is isomorphic to the one in Figure 2(c).
- If  $y = v_7 \rightarrow v_9$ , we have again two possibilities:
  - The arcs  $v_6 \rightarrow v_0$  and  $v_9 \rightarrow v_4$  yield the mixed graph of Figure 4(iia3), which is isomorphic to the one in Figure 2(a).
  - The arcs  $v_6 \rightarrow v_4$  and  $v_9 \rightarrow v_0$  give rise to a mixed graph isomorphic to the one in Figure 2(b).

A scheme of the above cases is the following.

$$x = v_8 \rightarrow v_6 \Rightarrow \begin{cases} y = v_6 \rightarrow v_9 \Rightarrow \begin{cases} v_7 \rightarrow v_0 \ \& \ v_9 \rightarrow v_4 \rightsquigarrow (b) \\ \text{or} \\ v_7 \rightarrow v_4 \ \& \ v_9 \rightarrow v_0 \rightsquigarrow (c) \end{cases} \\ \text{or} \\ y = v_7 \rightarrow v_9 \Rightarrow \begin{cases} v_6 \rightarrow v_0 \ \& \ v_9 \rightarrow v_4 \rightsquigarrow (a) \\ \text{or} \\ v_6 \rightarrow v_4 \ \& \ v_9 \rightarrow v_0 \rightsquigarrow (b) \end{cases} \end{cases}$$

- Let  $x = v_9$ . We must add the arc  $v_7 \rightarrow v_9$  in order to have  $\text{dist}(v_1, v_9) \leq 3$ . Now, to complete the mixed graph we have two possibilities:
  - The arcs  $v_6 \rightarrow v_0$  and  $v_8 \rightarrow v_4$  yield a mixed graph isomorphic to the one in Figure 2(b).
  - The arcs  $v_6 \rightarrow v_4$  and  $v_8 \rightarrow v_0$  complete a mixed graph isomorphic to the one in Figure 2(c).

Schematically,

$$x = v_9 \rightarrow v_6 \Rightarrow v_7 \rightarrow v_9 \Rightarrow \begin{cases} v_6 \rightarrow v_0 \ \& \ v_8 \rightarrow v_4 \rightsquigarrow (b) \\ \text{or} \\ v_6 \rightarrow v_4 \ \& \ v_8 \rightarrow v_0 \rightsquigarrow (c) \end{cases}$$

This completes the proof. □

Note that the mixed graph in Figure 2(a) is the line digraph of the cycle  $C_5$  (seen as a digraph, so that each edge corresponds to a digon). It is also the Cayley graph of the dihedral group  $D_5 = \langle r, s \mid r^5 = s^2 = (rs)^2 = 1 \rangle$ , with generators  $r$  and  $s$ . The spectrum of this mixed graph is that of the  $C_5$  cycle plus a 0 with multiplicity 5. Namely,

$$\text{sp } G = \left\{ 2, \left(-\frac{1}{2} + \frac{\sqrt{5}}{2}\right)^2, 0^5, \left(-\frac{1}{2} - \frac{\sqrt{5}}{2}\right)^2 \right\}.$$

This is because  $G$  is the line digraph of  $C_5$ . As a consequence, the only difference between  $\text{sp } G$  and  $\text{sp } C_5$  are the additional 0's (see Balbuena, Ferrero, Marcote, and Pelayo [1].) In fact, the mixed graphs of Figures 2(b) and 2(c) are cospectral with  $G$ , and can be obtained by applying a recent

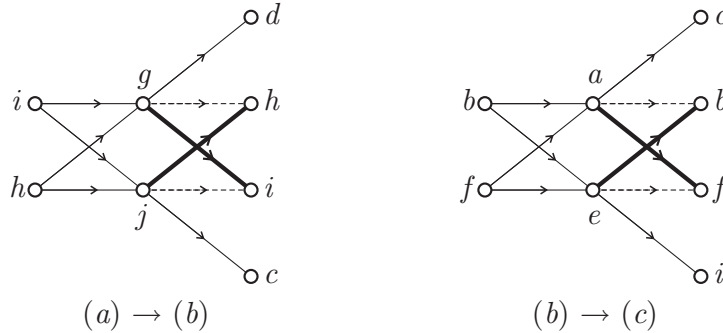


Figure 5: The method for obtaining the cospectral digraphs of Figure 2.

method to obtain cospectral digraphs with a locally line digraph. The right modifications to obtain the mixed graphs (b) and (c) from mixed graph (a) are depicted in Figure 5. For more details, see Dalfó and Fiol [3].

Two other interesting characteristics of these mixed graphs are the following:

- Each of the three mixed graphs is isomorphic to its converse (where the directions of the arcs are reversed).
- Each of these mixed graphs can be obtained as a proper orientation of the so-called Yutsis graph of the  $15j$  symbol of the second kind (see Yutsis, Levinson, and Vanagas [9]). This is also called the pentagonal prim graph. Notice that it has girth 4 and, curiously, its diameter is 3, in every of its considered orientations here.

The result of Proposition 3.1 could prompt us to look for a whole family of  $(1, 1)$ -regular mixed graphs attaining the upper bound  $M(1, 1, k) - 1$  for any diameter  $k \geq 3$ . Nevertheless, as a consequence of Proposition 2.2, this is not possible, since such a bound cannot be attained for some values of  $k$ .

**Corollary 3.2.** *Let  $G$  be a  $(1, 1)$ -regular mixed graph with  $N$  vertices and diameter  $k = 2 + 3s$  with  $s \geq 1$ . Then,*

$$N \leq \theta_1 \phi_1^{k+1} + \theta_2 \phi_2^{k+1} - 4, \quad (9)$$

where  $\theta_{1,2} = 1 \pm \frac{2}{\sqrt{5}}$  and  $\phi_{1,2} = \frac{1}{2}(1 \pm \sqrt{5})$ .

*Proof.* Apply Proposition 2.2 with  $r = z = 1$  and  $M(1, 1, k)$  computed from (1).  $\square$

Note that, in this last case, (6) yields the recurrence  $N_i = N_{i-1} + N_{i-2}$ , with  $N_0 = 1$  and  $N_1$ , so defining a Fibonacci sequence. In fact, with the usual numbering of such a sequence ( $F_1 = 1, F_2 = 1, F_3 = 2, \dots$ ), we have  $M(1, 1, k) = F_{k+4} - 2$  and so, for the case under consideration, (9) becomes

$$N \leq F_{k+4} - 4.$$

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