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.

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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 $u \to v$. 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 $\operatorname{dist}(u, v)$. Note that $\operatorname{dist}(u, v)$ may be different from $\operatorname{dist}(v, u)$ 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:

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

where

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

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).

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

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 $i = 0, 1, \ldots, k$, 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,

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

That is,

$$R_i = R_{i-1}(r-1) + Z_{i-1}r, \tag{3}$$
$$Z_i = R_{i-1}z + Z_{i-1}z, \tag{4}$$

or, in matrix form,

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

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

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

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

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

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,

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

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 $\mathrm{rep}(u) = v$ (see, for instance, Miller and Širáň [6]). Extending this concept, we denote by $\mathrm{Rep}(u)$ 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 $\mathrm{Rep}(u)$. (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

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

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

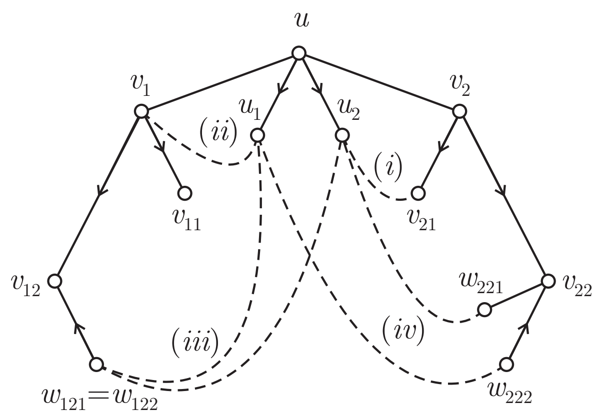

Figure 1: Repeated vertices in a $(2,2)$-regular mixed graph: (i) $v_{21} \in \mathrm{Rep}(u)$; (ii) $v_1 \in \mathrm{Rep}(u)$; (iii) $w_{121} \in \mathrm{Rep}(u)$; (iv) $w_{221} \in \mathrm{Rep}(u)$.

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

$$N \leq M(r,z,k) - r, \tag{7}$$

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 $v_1, \ldots, v_r$ and arcs to the vertices $u_1, \ldots, u_z$. For each $i = 1, \ldots, r$, let $v_{i1}, \ldots, v_{iz}$ 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 $i = 1, \ldots, r$ and $j = 1, \ldots, z$, let us consider the following possible cases for the distance from a vertex in $\{u_1, \ldots, u_z\}$ to vertex v_{ij}:

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

If, for every $h = 1, \dots, z$, we have $\mathrm{dist}(u_h, v_{ij}) = k$, let w_{ijl} 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, $w_{ij\ell} \in \mathrm{Rep}(u)$.

(*iv*) Otherwise, since $z^-(v_{ij}) = z$, there must be at least one ℓ 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, $w_{ij\ell} \in \mathrm{Rep}(u)$.

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 $\mathrm{Rep}(u)$. 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 $\mathrm{Rep}(u)$ has at least r elements, and the result follows. □

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 $k \equiv 2 \mod 3$, then*

$$N \leq M(r, z, k) - r - 1. \tag{8}$$

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 π_i's: $1, 0, 1, 1, 0, 1, 1, 0, 1, 1, \dots$ Thus, $\sum_{i=0}^{k} N_i$ is even for every $k \equiv 2 \mod 3$. Then, as r is odd, we get the result. □

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.*

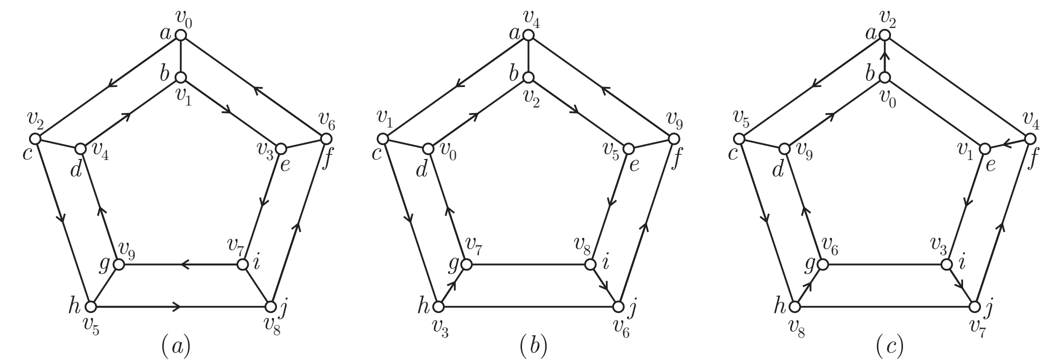

Figure 2: The unique three non-isomorphic $(1,1)$-regular mixed graphs with diameter $k = 3$ and order $N = 10$.

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 $\mathrm{dist}(u_1, v_{11}) < 3$ 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, $\mathrm{dist}(u_1, v_{11}) = 3$ 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 ≤ 3 from v_2 except v_6. This means that there must exist an arc $x \to v_6$, where $x \in \{v_8, v_9\}$.

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

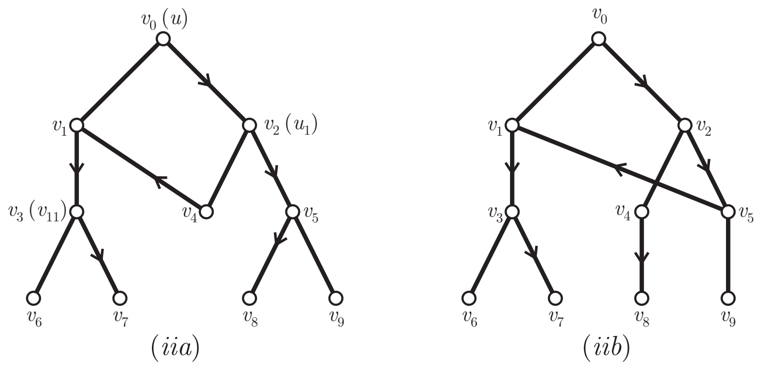

Figure 3: The two cases derived from (ii) according to Theorem 2.1 when $r = 1, z = 1$ and $k = 3$.

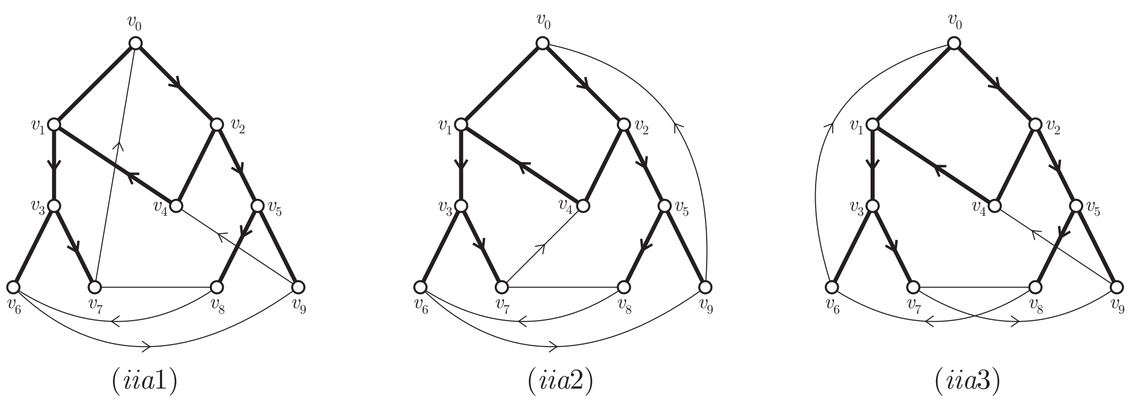

Figure 4: Three cases derived from (iia) giving non-isomorphic mixed graphs.

- The last arcs are $v_7 \to v_4$ and $v_9 \to v_0$, in which case we obtain the mixed graph of Figure 4$(iia2)$, which is isomorphic to the one in Figure 2(c).

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

A scheme of the above cases is the following.

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

- Let $x = v_9$. We must add the arc $v_7 \to v_9$ in order to have $\mathrm{dist}(v_1, v_9) \leq 3$. Now, to complete the mixed graph we have two possibilities:

  - The arcs $v_6 \to v_0$ and $v_8 \to v_4$ yield a mixed graph isomorphic to the one in Figure 2(b).
  - The arcs $v_6 \to v_4$ and $v_8 \to v_0$ complete a mixed graph isomorphic to the one in Figure 2(c).

  Schematically,

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

This completes the proof. $\square$

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 $D_5 = \langle r, s \,|\, r^5 = s^2 = (rs)^2 = 1 \rangle$, 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,

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

This is because G is the line digraph of C_5. As a consequence, the only difference between $\operatorname{sp} G$ and $\operatorname{sp} C_5$ 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

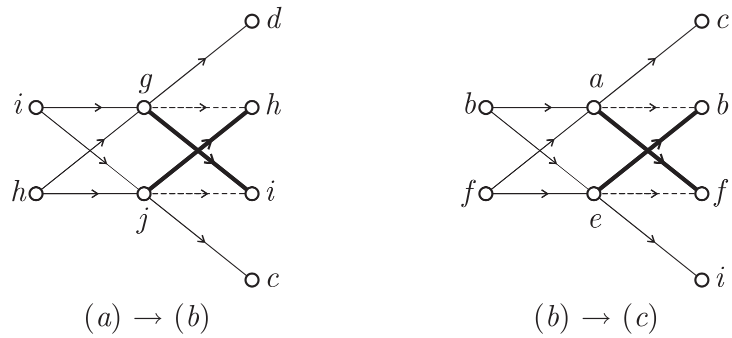

Figure 5: The method for obtaining the cospectral digraphs of Figure 2.

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,*

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

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 ($F_1 = 1$, $F_2 = 1$, $F_3 = 2,\ldots$), 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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