



## Extremal Graphs with Respect to Vertex Betweenness Centrality for Certain Graph Families

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**Abstract.** The betweenness centrality of a vertex in a graph is the sum of relative numbers of shortest paths that pass through that vertex. We study extremal values of vertex betweenness within various families of graphs. We prove that, in the family of 2-connected (resp. 3-connected) graphs on  $n$  vertices, the maximum betweenness value is reached for the maximum degree vertex of the fan graph  $F_{1,n-1}$  (resp. the wheel graph  $W_n$ ); the maximum betweenness values, their realizing vertices and extremal graphs are determined also for wider families of graphs of minimum degree at least 2 or 3, respectively, and, in addition, for graphs with prescribed maximum degree or prescribed diameter at least 3.

### 1. Introduction

The identification of vertices having a key role within large-scale graphs meets with an increasing interest connected with numerous applications in real-world networks. Measures of importance of objects within complex networks are formally expressed by so called *centrality indices*. According to the nature of relations between objects of the network and the criterion of importance, one can consider various centrality indices: degree, closeness, betweenness or eigenvector centrality.

As a centrality index, betweenness quantifies the appearance of a vertex as an intermediary on the shortest path between two other vertices. Due to the assumption that a flow (for example, transport or information flow) between vertices is propagated mainly along shortest paths of the network, the vertices that lie on many shortest paths can profit from the flow influence more than the vertices which are avoided by shortest paths. Brandes [5] gives a comprehensive survey and compares most recent variants of betweenness centrality. Some of them are the *proximal target betweenness* introduced by Borgatti, the *bounded-distance betweenness* defined by Borgatti and Everett [4] and the *edge betweenness*, as a natural extension of betweenness to edges, firstly discussed by Anthonisse [1] (see also [11]). Other variants of the general betweenness centrality are fundamentally different in their calculation and they are mostly based on the

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idea that a realistic betweenness measure should include non-shortest paths in addition to the shortest ones. The two most known measures of this type are the *flow-betweenness centrality* [3, 6, 13] and the *random walk betweenness centrality* [6, 17].

Besides practical applications, an attention is recently paid also to the graph-theoretical properties of betweenness centrality [9, 10, 18], as well as to its connection to the mean distance in graphs [7, 14, 15]. On the other hand, much less is known about values that the betweenness of vertices within a graph can reach, even in the case when all values are the same rational number (see [16]). In [11], it was shown that the maximal value of the betweenness centrality measure within a graph is  $\binom{n-1}{2}$  and it is attained if and only if the considered graph is isomorphic to the star, i.e.  $K_{1,n-1}$ . In this paper, we are interested in determining the maximum betweenness values within the various families of graphs, such as the families of graphs with prescribed maximum or minimum degree, 2-connected and 3-connected graphs, as well as graphs with diameter at least three.

## 2. Definitions and Notations

Before presenting the main results of our study, we give relevant graph-theoretical definitions and notations for considered graph families which underlie our work; further information can be found in [2, 8].

Throughout this paper, all graphs are assumed to be undirected, finite and connected, without loops or multiple edges. Given a graph  $G$ , we denote by  $n := |V(G)|$  the number of vertices and by  $m := |E(G)|$  the number of edges of  $G$ . A *path* between two vertices  $u, v \in V(G)$  (called  $(u, v)$ -path) is a sequence  $us_1s_2 \cdots s_kv$  of distinct vertices starting at  $u$  and ending at  $v$  such that each two consecutive vertices in this sequence form an edge in  $G$ . The *distance*  $d(u, v)$  between two vertices  $u$  and  $v$  in a graph  $G$  is the length of a shortest  $(u, v)$ -path in  $G$ . The *diameter*  $\text{diam}(G)$  of a graph  $G$  is the maximum distance between any pair of vertices  $u, v \in V(G)$ .

The join  $G_1 + G_2$  of graphs  $G_1$  and  $G_2$  with disjoint vertex sets  $V(G_1)$  and  $V(G_2)$  and edge sets  $E(G_1)$  and  $E(G_2)$  is the graph formed by graph union  $G_1 \cup G_2$  together with all the edges joining  $V(G_1)$  and  $V(G_2)$ . The disjoint union of  $k$  copies of a graph  $H$  is denoted by  $kH$ . The *fan*  $F_{r,s}$  is defined as the graph join  $\bar{K}_r + P_s$ , where  $\bar{K}_r$  is the empty graph on  $r$  vertices and  $P_s$  is the path on  $s$  vertices. The *wheel*  $W_n$  of order  $n$  is the graph join  $K_1 + C_{n-1}$ , where  $K_1$  is the singleton graph and  $C_{n-1}$  is the cycle on  $n - 1$  vertices. The *windmill*  $\text{Wd}(r, s)$  is the graph obtained by taking  $s$  copies of the complete graph  $K_r$  with a vertex in common. Thus, it has  $sr - s + 1$  vertices.

The *betweenness centrality*  $b_G(x)$  of a vertex  $x \in V(G)$  is the relative number of shortest paths between all pairs of vertices passing through  $x$ :

$$b_G(x) = \sum_{\substack{u,v \in V(G) \\ u \neq v \neq x}} \frac{\sigma_{u,v}^G(x)}{\sigma_{u,v}^G}, \tag{1}$$

where  $\sigma_{u,v}^G$  denotes the total number of shortest  $(u, v)$ -paths in  $G$  and  $\sigma_{u,v}^G(x)$  represents the number of shortest  $(u, v)$ -paths passing through  $x$ . The index  $G$  is omitted if  $G$  is known from the context. By  $\bar{b}(G)$ , we denote the average betweenness of a graph  $G$ , and by  $b_{\min}(G)$  (resp.  $b_{\max}(G)$ ) the smallest (resp. the largest) vertex betweenness within the graph  $G$ . If the considered graph  $G$  is a cycle on  $n$  vertices  $C_n$ , then, for every  $x \in V(C_n)$ , the following result holds:

$$b(x) = \begin{cases} \frac{(n-2)^2-1}{8} & \text{if } n \text{ is odd,} \\ \frac{(n-2)^2}{8} & \text{if } n \text{ is even.} \end{cases} \tag{2}$$

For a graph family  $\mathcal{H}$  and an integer  $n$ , let

$$B_{\max}(\mathcal{H}, n) := \max \{b_{\max}(G) : G \in \mathcal{H}, |V(G)| = n\}.$$

Then, within the family  $\mathcal{G}$  of all graphs, we have  $B_{\max}(\mathcal{G}, n) = \binom{n-1}{2}$ . In this paper, we consider the previously mentioned problem of maximization within several proper subfamilies of the family  $\mathcal{G}$  – the family  $\mathcal{G}^\Delta$  of all graphs with the maximum degree at most  $\Delta$ , the family  $\mathcal{G}_\delta$  of all graphs of minimum degree at least  $\delta$ , the families  $\mathcal{C}_2$  and  $\mathcal{C}_3$  of all 2- and 3-connected graphs and the family  $\mathcal{D}_D$  of graphs with diameter  $D$ . We present exact values and estimates for extremal values of maximum betweenness within graphs from these families, together with extremal graphs realizing these values.

### 3. Extremal Values and Extremal Graphs

In the subsequent proofs, we often use the calculation of the betweenness of a vertex  $x$  within a graph  $G$  based on the following: let  $\mathcal{V}$  be the set of all two-element subsets of  $V(G) \setminus \{x\}$ ,  $\mathcal{P}$  be the set of all pairs  $\{u, v\}$  from  $\mathcal{V}$  that form an edge in  $G$ ,  $\mathcal{Q}$  be the set of all pairs  $\{u, v\}$  from  $\mathcal{V} \setminus \mathcal{P}$  such that there is a 2-path  $uyv$  with  $y \neq x$ , and finally,  $\mathcal{R} = \mathcal{V} \setminus (\mathcal{P} \cup \mathcal{Q})$ . Thus, the previously defined subsets  $\mathcal{P}, \mathcal{Q}$  and  $\mathcal{R}$  are disjoint and moreover  $\mathcal{V} = \mathcal{P} \cup \mathcal{Q} \cup \mathcal{R}$ . Then

$$b_G(x) = \sum_{\{u,v\} \in \mathcal{P}} \frac{\sigma_{u,v}(x)}{\sigma_{u,v}} + \sum_{\{u,v\} \in \mathcal{Q}} \frac{\sigma_{u,v}(x)}{\sigma_{u,v}} + \sum_{\{u,v\} \in \mathcal{R}} \frac{\sigma_{u,v}(x)}{\sigma_{u,v}}. \tag{3}$$

Note that in (3) the first sum always contributes 0 to the betweenness of the vertex  $x$ . Each term in the second sum contributes at most  $1/2$  and each term of the third sum contributes at most 1.

Now, let  $G$  be a graph on  $n$  vertices,  $w$  be a vertex of  $G$  of maximum betweenness and let  $H = G - w$ . Denote by  $e_1(H)$  the number of adjacent pairs of vertices in  $H$  and by  $e_2(H)$  the number of pairs of vertices at distance 2 within the graph  $H$ . Since the contribution of the adjacent pairs of vertices is 0 and pairs of vertices at distance 2 can contribute at most  $1/2$ , using (3) we obtain

$$b(w) \leq 0 \cdot e_1(H) + \frac{1}{2} \cdot e_2(H) + 1 \cdot \left( \binom{n-1}{2} - e_1(H) - e_2(H) \right).$$

The above expression can be simplified to

$$b(w) \leq \frac{(n-1)(n-2)}{2} - e_1(H) - \frac{1}{2} \cdot e_2(H). \tag{4}$$

#### 3.1. The family $\mathcal{G}^\Delta$

For graphs with prescribed maximum degree, we have the following estimate:

**Proposition 3.1.** *If  $G$  is a graph of maximum degree  $\Delta$ , then*

$$b_{\max}(G) \leq \frac{\Delta-1}{2\Delta} (n-1)^2. \tag{5}$$

*Proof.* Let  $G$  be an  $n$ -vertex graph of maximum degree  $\Delta$  and  $x$  be its vertex of degree  $d$  such that  $b_G(x) = B_{\max}(\mathcal{G}^\Delta, n)$ . Let  $T$  be a spanning tree of  $G$  obtained by breadth-first search algorithm applied on  $G$  with the initial vertex (root)  $x$ . Note that  $\deg_T(x) = d$ . For each neighbour  $x_i$  of  $x$ , let  $T_i$  be the subtree of  $T$  rooted at  $x_i$ , and let  $t_i = |V(T_i)|$ ,  $i = 1, \dots, d$ . Then,  $\sum_{i=1}^d t_i = n - 1$ . It is not hard to see that the following properties hold:

- (a) No shortest path between two vertices  $u, v$  from the same subtree  $T_i$  contains  $x$ , i.e.  $\sigma_{u,v}^G(x) = \sigma_{u,v}^T(x) = 0$ .
- (b) For any two vertices  $u, v$  from distinct subtrees  $T_i, T_j$ , it holds  $\sigma_{u,v}^G(x) / \sigma_{u,v}^G \leq 1 = \sigma_{u,v}^T(x) / \sigma_{u,v}^T$ .

The observations (a) and (b) imply that no two vertices from distinct subtrees are adjacent in  $G$ , i.e. all  $xx_i$  are bridges. Hence,

$$b_G(x) = \sum_{i,j=1, i < j}^d t_i t_j \leq \binom{\Delta}{2} \left( \frac{n-1}{\Delta} \right)^2,$$

since the sum attains maximum when  $d = \Delta(G) = \Delta$  and all  $t_i$ 's are equal. This gives us the upper bound (5), which is attained when  $n - 1$  is divisible by  $\Delta$  and all subtrees  $T_i$  are of equal size.  $\square$

### 3.2. The families $C_2$ and $C_3$

In the following two propositions, we present the best upper bounds for the families of 2- and 3-connected graphs.

**Proposition 3.2.** *If  $G$  is a 2-connected graph on  $n$  vertices, then*

$$b_{\max}(G) \leq \frac{(n-3)^2}{2}.$$

Moreover, the bound is obtained only at the central vertex of the graph  $F_{1,n-1}$ .

*Proof.* Let  $G$  be a 2-connected graph on  $n$  vertices, let  $w$  be a vertex of  $G$  having the maximum betweenness centrality and let  $H = G - w$ . Since  $G$  is 2-connected,  $H$  is connected graph on  $n - 1$  vertices. For such a graph, it holds  $p(H) = e_1(H) + e_2(H)/2 \geq (3n - 7)/2$  with equality holding iff  $H$  is  $P_{n-1}$ . This is obviously true if  $\delta(H) \geq 3$ , and otherwise we have a vertex  $x$  of degree 1 or 2. So remove  $x$  and apply induction. Note that if  $x$  is of degree 2, then  $H - x$  may be disconnected (we leave the details to the reader as an easy exercise). Now, using (4) we obtain the following upper bound

$$b(w) \leq \frac{(n-1)(n-2)}{2} - p(H) \leq \frac{(n-1)(n-2)}{2} - \frac{3n-7}{2} = \frac{(n-3)^2}{2}.$$

By a routine check, it is easy to see that this bound is attained only if  $w$  is adjacent to every vertex of  $H$  and  $H$  is isomorphic to the path  $P_{n-1}$ . Therefore,  $G$  is isomorphic to  $F_{1,n-1}$ .  $\square$

**Proposition 3.3.** *If  $G$  is a 3-connected graph on  $n$  vertices, then*

$$b_{\max}(G) \leq \frac{(n-1)(n-5)}{2}.$$

Moreover the bound is obtained only at the central vertex of the wheel graph  $W_n$ .

*Proof.* Let  $G$  be a 3-connected graph on  $n$  vertices,  $w$  be a vertex of  $G$  of the maximum betweenness centrality and let  $H = G - w$ . Then, the connectivity of  $H$  is at least 2, so  $\delta(H) \geq 2$ , and it has at least  $n - 1$  edges. For such a graph, it holds  $p(H) = e_1(H) + e_2(H)/2 \geq (3n - 3)/2$  with equality holding iff  $H$  is  $C_{n-1}$ . This is obviously true if  $\delta(H) \geq 3$ , or it is a cycle. Otherwise we have a vertex  $x$  of degree 2 with neighbours  $y$  and  $z$ , where  $z$  is a 3-vertex. If  $y$  is of degree  $\geq 3$ , then consider the graph  $H'_1 = G - x$  and if  $y$  is of degree 2, then consider the graph  $H'_2 = H - x - y$ . Now, for  $i \in \{1, 2\}$  if the graph  $H'_i$  is 2-connected then apply induction, and otherwise, use the observation from the proof of the previous proposition that  $p(H_i) \geq 3(n - i) - 7$ . In both cases, the number of edges and the number of pairs of vertices on distance 2 that are in  $H$  and not in  $H_i$  assure to obtain the desired lower bound for  $p(H)$  (we leave the counting details to the reader as an easy exercise). Hence, based on the expression (4), the following holds

$$b(w) \leq \frac{(n-1)(n-2)}{2} - p(H) \leq \frac{(n-1)(n-2)}{2} - \frac{3n-3}{2} = \frac{(n-1)(n-5)}{2}.$$

By a routine check, it is easy to see that this bound is attained for the central vertex of an  $n$ -vertex wheel.  $\square$

### 3.3. The family $\mathcal{G}_\delta$

Now, we explore the family of graphs with prescribed minimum degree  $\delta$ .

**Proposition 3.4.** *If  $G$  is a graph on  $n$  vertices with minimum degree at least 2, then*

$$b_{\max}(G) \leq \frac{(n-1)(n-3) - 1 + (-1)^{n+1}}{2}.$$

The maximum for  $n$  odd is attained for the central vertex of the windmill graph on  $n$  vertices,  $Wd(3, (n-1)/2)$ , and the maximum for  $n$  even is attained for the maximum degree vertex of the graph obtained from the windmill graph  $Wd(3, (n-2)/2)$  on  $n - 1$  vertices by subdividing an edge joining two vertices of degree 2 by a new vertex of degree 2.

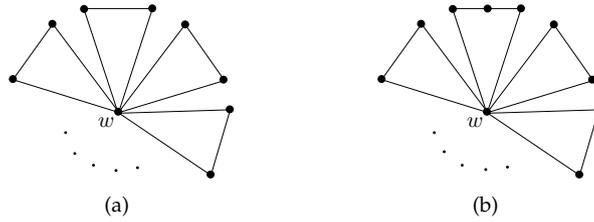


Figure 1: Extremal graphs within the family  $\mathcal{G}_2$ : (a) for  $n$  odd and (b) for  $n$  even.

*Proof.* Let  $G$  be a graph on  $n$  vertices with minimum degree at least 2,  $w$  be a vertex of  $G$  of maximum betweenness and let  $H = G - w$ . Then  $\delta(H) \geq 1$ . If  $n$  is odd, then  $H$  has at least  $(n - 1)/2$  edges, and if  $n$  is even, then either  $H$  has at least  $n/2$  edges and at least one pair of vertices of  $H$  at distance 2 or  $H$  has at least  $n/2 + 1$  edges. Hence, by the expression (4), for  $n$  odd we obtain the following upper bound:

$$b(w) \leq \frac{(n - 1)(n - 2)}{2} - \frac{n - 1}{2} = \frac{(n - 1)(n - 3)}{2},$$

and, for  $n$  even,

$$b(w) \leq \frac{(n - 1)(n - 2)}{2} - \frac{n}{2} - \frac{1}{2} = \frac{(n - 1)(n - 3) - 2}{2}.$$

The second part of the Theorem can be easily shown by the straightforward calculation of betweenness of maximum degree vertices within the previously mentioned windmill graphs. See Figures 1(a) and 1(b) for illustration.  $\square$

For the purposes of the following theorem, we define a new function  $\theta$  such that, for any integer  $n$ ,

$$\theta(n) = \begin{cases} 5/2 & \text{if } n \equiv 0 \pmod{3}, \\ 0 & \text{if } n \equiv 1 \pmod{3}, \\ 4/3 & \text{if } n \equiv 2 \pmod{3}. \end{cases} \tag{6}$$

Then the following result holds.

**Theorem 3.5.** *If  $G$  is a graph on  $n$  vertices with minimum degree at least 3, then*

$$b_{\max}(G) \leq \frac{(n - 1)(n - 4)}{2} - \theta(n). \tag{7}$$

*The maximum for  $n \equiv 1 \pmod{3}$  is attained for the central vertex of the windmill graph  $Wd(4, (n - 1)/3)$ , the maximum for  $n \equiv 2 \pmod{3}$  and  $n \equiv 0 \pmod{3}$  is attained for the maximum degree vertex of a graph which is obtained from the windmill graph by replacing one copy of the graph  $K_4$  by the graph of 4- and 5-sided pyramid, respectively.*

*Proof.* Let  $G$  be a graph on  $n$  vertices with minimum degree at least 3,  $w$  be a vertex of  $G$  of maximum betweenness and let  $H = G - w$ . Moreover, let  $e_2(H) = e_2^1(H) + e_2^2(H)$ , where  $e_2^1(H)$  is the number of those pairs of vertices at distance two for which there exists only one 2-path in  $H$  and  $e_2^2(H)$  the number of pairs at distance two that are joined with at least two 2-paths in  $H$ . Using an expression as (4), we have

$$b(w) \leq \frac{(n - 1)(n - 2)}{2} - (e_1(H) + \frac{1}{2} \cdot e_2^1(H) + \frac{2}{3} \cdot e_2^2(H)), \tag{8}$$

since the contribution of pairs at distance two that are joined with at least two 2-paths in  $H$  is at most  $1/3$ . The obtained upper bound is maximized, when the expression in the parentheses, denoted by  $p(H)$ ,

is minimized. Note that each adjacent pair of vertices in  $H$  contributes 1 to the value  $p(H)$ , each pair at distance two contributes  $1/2$  or  $2/3$ , depending on the number of 2-paths between them. Moreover, since  $\delta(H) \geq 2$ , it follows that  $e_1(H) \geq n - 1$ , and so  $p(H) \geq n - 1$ .

Now, we define a graph  $H^*$  in order to show that  $p(H^*)$  is minimal. Consider three different possibilities:

- (i). If  $n = 3k + 1$ , then let  $H^* = k C_3$  (see Figure 2(a)). Hence,  $H^*$  is a union of  $k$  cycles of length 3, in which case  $p(H^*)$  takes the value  $n - 1$ .
- (ii). If  $n = 3k + 2$ , then let  $H^* = (k - 1) C_3 \cup C_4$  (see Figure 2(b)). Thus,  $H^*$  contains one cycle of length 4 and  $k - 1$  cycles of length 3, in which case  $p(H^*)$  takes the value  $n - 1 + 4/3 = n + 1/3$ .
- (iii). If  $n = 3k$ , then let  $H^* = (k - 2) C_3 \cup C_5$  (see Figure 2(c)), in which case  $p(H^*)$  takes the value  $n - 1 + 5/2 = n + 3/2$ .

Note that  $p(H^*) \leq n + 3/2$ . In what follows, we prove that  $p(H)$  attains a minimum value if  $H$  is isomorphic to  $H^*$ . The main part of this will be to show that, if a graph  $H$  contains a vertex of degree greater than 2, then the value  $p(H)$  is greater than  $p(H^*)$ . First note that if the graph  $H$  contains a vertex of degree greater than 2, then  $H$  has at least  $n$  edges, each of which contributes 1 to  $p(H)$ . Therefore,  $p(H) \geq n$ .

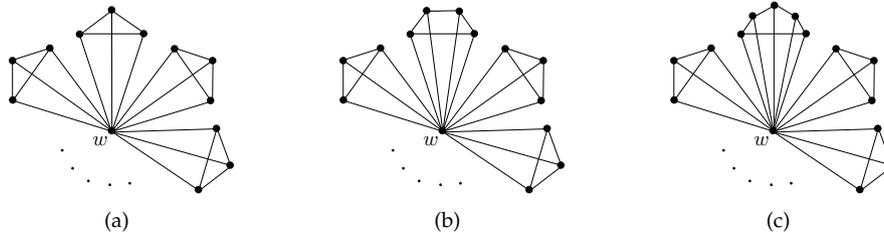


Figure 2: Extremal graphs within the family  $\mathcal{G}_3$ : (a)  $n \equiv 1 \pmod{3}$ , (b)  $n \equiv 2 \pmod{3}$  and (c)  $n \equiv 0 \pmod{3}$ .

**Claim 3.6.** *In  $H$ , there are no adjacent vertices both of degree at least 3.*

*Proof.* Suppose in contrary that there exists an edge  $uv \in E(H)$  such that both end-vertices  $u$  and  $v$  are of degree at least 3. Let  $H' = H - uv$ . Note that the pair  $u, v$  contributes 1 to the value  $p(H)$ , while the contribution of  $u, v$  to  $p(H')$  is at most  $2/3$ . Thus, the contribution of  $u, v$  to  $p(H')$  is strictly smaller than the contribution to  $p(H)$ . For any other pair of vertices  $x, y$  contribution remains unchanged or decreases. If  $x, y$  are adjacent in  $H$ , then they are adjacent in  $H'$  and the contribution of this pair stay unchanged after removing the edge  $uv$ . Suppose now that  $x, y$  are at distance 2 in  $H$ . If the distance grows after deleting  $uv$ , then the contribution of this pair drops to zero. If the distance remains unchanged in  $H'$ , then the contribution of  $x, y$  does not change or may drop from  $2/3$  to  $1/2$ . Thus,  $p(H') < p(H)$ .  $\square$

**Claim 3.7.** *In  $H$ , there are no vertices of degree at least 4.*

*Proof.* Suppose in contrary that there exists a vertex  $u \in V(H)$  such that  $\deg(u) \geq 4$ . By the previous claim, all neighbours of the vertex  $u$  are of degree 2. Note that each neighbour of  $u$  can be adjacent to at most 1 other neighbour of  $u$ . Let  $a, b, x$  and  $y$  be four neighbours of  $u$ . In case some pair of these four vertices is adjacent, we may assume that it is a pair  $a, b$ . Then the Cartesian product of two sets  $\{a, b\}$  and  $\{x, y\}$  constitutes four pairs of vertices which contribute at least  $1/2$  to  $p(H)$ . Thus,  $p(H) \geq 1 \cdot n + 4 \cdot 1/2 = n + 2 > n + 3/2 \geq p(H^*)$ .  $\square$

**Claim 3.8.** *In  $H$ , there are no vertices of degree 3.*

*Proof.* Suppose that there exists  $u \in V(H)$  of degree 3 and let  $a, b$ , and  $c$  be neighbours of  $u$ . Since each graph has an even number of vertices of odd degree, there exists another vertex  $v$  of degree 3 with neighbours, say  $x, y$  and  $z$ . By Claim 3.6,  $u$  and  $v$  are non-adjacent and all neighbours of  $u$  and  $v$  are of degree 2. Consider the following four possibilities:

- (a) Vertices  $u$  and  $v$  have no common neighbour. Since all neighbours of  $u$  are of degree 2, there are at least two pairs of neighbours of  $u$  (resp.  $v$ ) that are at distance 2, say  $a, c$  and  $b, c$  (resp.  $x, z$  and  $y, z$ ). Note that  $a$  and  $b$  (resp.  $x$  and  $y$ ) can be adjacent. Those four pairs contribute at least  $1/2$  to  $p(H)$ . Thus,  $p(H) \geq 1 \cdot n + 4 \cdot 1/2 = n + 2 > n + 3/2 \geq p(H^*)$ .
- (b) Vertices  $u$  and  $v$  have a common neighbour, say  $c = z$ . Pairs of vertices contained in the Cartesian product of two sets  $\{a, b, x, y\}$  and  $\{c\}$  are at distance 2 and each of them contribute  $1/2$  to  $p(H)$ . Hence,  $p(H) > n + 3/2 \geq p(H^*)$ .
- (c) Vertices  $u$  and  $v$  have two common neighbours, say  $b = y$  and  $c = z$ . Pairs of vertices contained in the Cartesian product of two sets  $\{a, x\}$  and  $\{b, c\}$  are at distance 2 and each of them contribute  $1/2$  to  $p(H)$ . Hence,  $p(H) > n + 3/2 \geq p(H^*)$ .
- (d) Vertices  $u$  and  $v$  have three common neighbours, i.e.  $a = x, b = y$  and  $c = z$ . Those five vertices induce  $K_{2,3}$ . Therefore, pairs of vertices  $\{a, b\}, \{a, c\}$  and  $\{b, c\}$  are at distance 2 and moreover, they are connected to each other by two 2-paths. Each of those pairs contribute  $2/3$  to the value  $p(H)$  and  $p(H) \geq 1 \cdot n + 3 \cdot 2/3 = n + 2 > n + 3/2 \geq p(H^*)$ .

□

Regarding the previous claims, the graph  $H$  is a 2-regular graph on  $n - 1$  vertices. Hence, it is a union of cycles. In what follows, we consider the following four possibilities:

- (a)  $H$  contains a cycle  $C_s$ , where  $s \geq 6$ . Then,  $p(C_s) = s + s/2$ . Now consider a graph  $C_3 \cup C_{s-3}$ . Since  $p(C_3 \cup C_{s-3}) = s + (s - 3)/2 < p(C_s)$ , it follows that  $H$  contains only cycles of length 3, 4 and 5.
- (b)  $H$  contains two cycles  $C_4$ . Since  $p(C_5 \cup C_3) = 8 + 5/2 < 8 + 8/3 = p(2C_4)$ , it follows that  $H$  contains at most one cycle of length 4.
- (c)  $H$  contains two cycles  $C_5$ . Since  $p(2C_3 \cup C_4) = 10 + 4/3 < 15 = p(2C_5)$ , it follows that  $H$  contains at most one cycle of length 5.
- (d)  $H$  contains  $C_4 \cup C_5$ . Since  $p(3C_3) = 9 < 9 + 4/3 + 5/2 = p(C_4 \cup C_5)$ , it follows that  $H$  is a union of cycles of length 3 and at most one cycle of length 4 or 5.

Therefore,  $p(H)$  attains minimum value if  $H$  is isomorphic to  $H^*$ . Using the upper bound defined in (8) and values  $p(H^*)$  calculated in (i), (ii) and (iii), the upper bound (7) is obtained. Moreover, the equality holds when  $H$  is isomorphic to  $H^*$  and  $w$  is adjacent to each vertex of  $H$ , which gives the graphs from the theorem. □

### 3.4. The family $\mathcal{D}_D$

Here, we consider the family  $\mathcal{D}_D$  of all graphs with diameter  $D$ . Since  $\mathcal{D}_1$  consists of complete graphs and  $\mathcal{D}_2$  contains all stars  $K_{1,n-1}$ , we have  $B_{\max}(\mathcal{D}_1, n) = 0$  and  $B_{\max}(\mathcal{D}_2, n) = \binom{n-1}{2}$ . We now consider the general case, i.e. the family  $\mathcal{D}_D$  for  $D \geq 3$  which is particularly interesting for the real-world networks that exhibit the small-world phenomenon, that is, the average distance between two object in the network is small (typically of the magnitude of logarithm of the number of objects) while the local edge density (quantified by clustering coefficient) is relatively high despite of the overall sparsity of the network.

Let  $\eta$  be a function such that, for any integer  $k$ ,  $\eta(2k) = 0$  and  $\eta(2k + 1) = -1/4$ .

**Theorem 3.9.** Let  $D$  be an integer such that  $D \geq 3$  and  $G$  be a graph with diameter  $D$ . Then,

$$b_{\max}(G) \leq \frac{(n - 1)(n - 2)}{2} - \frac{D(D - 2)}{4} + \eta(D).$$

Moreover, the maximum value is obtained only at the vertex with the largest degree, within the graph obtained by identifying a central vertex of the path  $P_{D+1}$  with the central vertex of the star graph  $K_{1,n-D-1}$ .

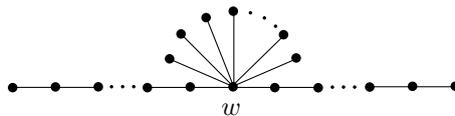


Figure 3: Extremal graph within the family  $\mathcal{D}_D$ , where  $D \geq 3$ .

*Proof.* Let  $G$  be a graph of order  $n$  and diameter  $D$  and let  $x$  be its vertex with the maximum betweenness value.

Suppose first that  $x$  lies on some diametral path  $P$  with end-vertices  $u$  and  $v$ , and let  $k = d(u, x)$ . Note that any pair of vertices, which lies on  $(u, x)$ -path, does not contribute to the sum in  $b(x)$ . This applies also to the  $(x, v)$ -path. As the contribution of any other vertex pair is at most 1, we obtain

$$b(x) \leq 0 \cdot \binom{k}{2} + 0 \cdot \binom{D-k}{2} + 1 \cdot \left( \binom{n-1}{2} - \binom{k}{2} - \binom{D-k}{2} \right).$$

It is easy to see that the expression in the parentheses is maximized for  $k = \lfloor D/2 \rfloor$ , giving  $b(x) \leq (n-1)(n-2)/2 - D(D-2)/4 + \eta(D)$ , where  $\eta(D)$  is equal to 0 for  $D$  even and  $-1/4$  otherwise. This also implies that the maximum is attained in the situation where  $x$  is a central vertex of  $P$  and the remaining  $n - D - 1$  vertices of  $G$  are of degree one and all are adjacent to  $x$ . Thus, the extremal graph within the family  $\mathcal{D}_D$  is obtained by identifying a central vertex of the path  $P_{D+1}$  with the central vertex of the star graph  $K_{1, n-D-1}$ .

Suppose now that the vertex  $x$  does not lie on any diametral path in  $G$ . In that case, for each pair of vertices which lies on a diametral path, there is no shortest path passing through the vertex  $x$ . Otherwise, if there is a shortest path between two vertices  $s, t$  passing through the vertex  $x$  and  $s$  and  $t$  belong to a diametral path, then obviously there exists a diametral path which contradicts our assumption. Therefore, there exist  $\binom{D}{2}$  pairs of vertices with the contribution 0 to the betweenness of the vertex  $x$ , i.e.

$$b(x) \leq 0 \cdot \binom{D}{2} + 1 \cdot \left( \binom{n-1}{2} - \binom{D}{2} \right) < \frac{(n-1)(n-2)}{2} - \frac{D(D-2)}{4} + \eta(D),$$

since  $D \geq 3$ . Hence, the maximal betweenness is attained in the case when  $x$  lies on the diametral path.  $\square$

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