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ON THE GRAPHS WITH MAXIMUM DISTANCE OR k-DIAMETER

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ABSTRACT. The distance of a set of vertices is the sum of the distances between pairs of vertices in the set. We define the k-diameter of a graph as the maximum distance of a set of k vertices; so the 2-diameter is the normal diameter and the n-diameter, where n is the order, is the distance of the graph. We complete the characterization of graphs with maximum distance given the order and size. We also determine the maximum size of a graph with given order and 3-diameter.

1. Introduction

An old problem is to characterize graphs of given order and size (number of edges) which attain the maximum value of a parameter. In 1962, Harary [4] determined the maximum size for a given order and diameter, and showed that the so-called path-complete graphs have maximum diameter given their order and size (but are in general not the only extremal graphs). More recently, Šoltés [6] showed that the path-complete graphs are also extremal graphs for the parameter distance (or transmission), given the order and size.

In this paper we refine Šoltés' result and show that almost always the path-complete graph is the only extremal graph. In contrast, we introduce the k-diameter of a graph, which generalizes both diameter and distance, and show that the path-complete graphs are seldom extremal for this parameter.

2. Distance measures and path-complete graphs

The *distance* between two vertices in a graph G is the number of edges in a shortest path between them. The *diameter* of G is the maximum distance

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between two vertices and is denoted $\operatorname{diam}(G)$. The *distance of the graph* (also called the transmission or total distance) is the sum over all pairs of vertices of their distances and is denoted $\sigma(G)$. The *status of a vertex* v is the sum of the distances from it to all other vertices and is denoted $\sigma(v)$. For general properties of these parameters, consult [1] or [7].

A natural generalization which appears not to have been studied is the following. The *distance of a set of vertices* is the sum of the distances between pairs of vertices in the set. Then we define the *k-diameter of the graph G* as the maximum distance of a set of k vertices and denote it by $d_k(G)$. So the normal diameter of G is its 2-diameter and the distance of G is its n-diameter where n is the order of G.

We are interested in graphs with maximum value of these parameters given their order and size.

By the graph operation of duplicating a vertex v, we mean introducing a new vertex v' and joining it to v and all neighbours of v. We say that H is an *expansion* of G if it is isomorphic to the graph obtained from G by repeatedly duplicating a vertex (not necessarily the same one each time).

We consider the expansions of paths: for positive integers $a_0, a_1, \dots, a_d$ we denote by $P[a_0, a_1, \dots, a_d]$ the graph formed from $d+1$ disjoint cliques A_i of orders a_i and joining all vertices in A_i and A_{i+1} for $0 \le i \le d-1$. The sets A_i are called the *levels* of $P[a_0, a_1, \dots, a_d]$.

Ore [5] characterized the *diameter-maximal* graphs: those graphs where the addition of any edge causes the diameter to decrease. He showed that, for diameter d, they are precisely the expansions of the path on $d+1$ vertices where the first and last vertices are not expanded; that is, $P[1, a_1, \dots, a_{d-1}, 1]$.

A *path-complete* graph is any expansion of the form $P[a_0, a_1, 1, \dots, 1]$. In other words, it is obtained from the disjoint union of a path and a complete graph by the addition of edges between one end-vertex of the path and a_1 vertices of the complete graph. It can easily be shown that there is a unique path-complete graph for a given order n and size $m \ge n-1$; we denote this by $PK_{n,m}$.

Harary observed that the solution to the diameter question was attained by the path-complete graph.

THEOREM 1. ([4]) *Let G be a connected graph with n vertices and m edges. Then* $\operatorname{diam}(G) \le \operatorname{diam}(PK_{n,m})$.

We note that for most n and m, $PK_{n,m}$ is not the only graph of order n and size m with maximum diameter: for example, for $m = n+1$ any one-vertex expansion of the path on n vertices has maximum diameter.

3. Graphs with maximum distance

Šoltés [6] showed that for every order n and size $m \in \{n-1, \dots, \binom{n}{2}\}$, the path-complete graph $PK_{n,m}$ has maximum distance. In fact, he proved an interesting extremal property of the path-complete graphs. For a graph G and integer $k \geq 2$, define $W_k(G)$ as the set of (unordered) pairs of *nonadjacent* vertices at distance at most k, and let $w_k(G) = |W_k(G)|$.

THEOREM 2. ([6]) *Let G be a connected graph of order n and diameter $d \geq 3$ and let $k \in \{2, \dots, d-1\}$. Then*

$$w_k(G) \geq \sum_{i=2}^{k} (n-i)\,.$$

Moreover, equality occurs for any path-complete graph.

We will need the following extension of Theorem 2.

LEMMA 3. *Let G be a connected graph of order n and diameter $d \geq 3$ and let $k \in \{2, \dots, d-1\}$. Then $w_k(G) = \sum_{i=2}^{k} (n-i)$ if and only if G is an expansion $P[a_0, a_1, \dots, a_d]$ of the following form:*

(a) *$k = d-1$ and all but two consecutive a_i are 1,*
or
(b) *$k = d-1$ and all but a_0 and a_d are 1,*
or
(c) *$k = d-2$ and all but a_0, a_1, a_{d-1} and a_d are 1, and at least one of a_1 or a_{d-1} is 1,*
or
(d) *$k \leq d-3$ and all but a_0, a_1, a_{d-1} and a_d are 1.*

Proof. We build on Šoltés' proof of the bound; so we start by recapping that proof. The bound is proved by induction on the order. The bound is true for the path, so we may assume G is not the path. Let P be a diametral path in G and let v be a non-cut-vertex which is not on P. Then $G - v$ is connected, has order $n-1$, and diameter $d' \geq d$.

So $G - v$ satisfies the bound of Theorem 2; that is,

$$w_k(G - v) \geq \sum_{i=2}^{k} (n-1-i)\,.$$

If a pair of vertices are nonadjacent in $G - v$, then they are nonadjacent in G; if they are at most distance k apart in $G - v$, then they are too in G. Thus

$W_k(G) \supseteq W_k(G-v)$. The bound will follow when we show that v is in at least $k-1$ pairs in $W_k(G)$.

Define a *mate* for v as a vertex nonadjacent to v but at distance at most k from v. Let x and y be the end-vertices of P and consider shortest paths P_x and P_y from v to x and y. There are two cases: If either path has length k or more, then there are $k-1$ mates for v on that path.

Otherwise all vertices on both paths apart from v and its successors are mates for v. Since the two paths combined constitute an x y walk, there are at least $d-2$ distinct vertices on P_x and P_y apart from v and its neighbours. Since we restricted $k \le d-1$, it follows that v has at least $k-1$ mates, and the bound is established.

Now, assume equality and that G is not a path (which is extremal). Then

(i) the graph $G-v$ is extremal,
(ii) the vertex v is in exactly $k-1$ pairs,
(iii) every pair in $W_k(G) - W_k(G-v)$ contains the vertex v.

By (i) and the induction hypothesis, $G-v$ is an expansion of the path. We claim that the neighbourhood of v is restricted to three consecutive levels of $G-v$: for otherwise there is a pair of vertices (distinct from v) whose distance apart is k in G, but is more than k in $G-v$, which contradicts (iii) above.

Further, the neighbourhood of v must be the union of one, two or three consecutive levels. For, otherwise then adding an edge joining v to another vertex of a level to which v is already adjacent reduces the number of mates. a contradiction of (ii).

In particular, the shortest paths P_x and P_y overlap in at most one vertex. So if one has length k or more, then the other one must have length 1. Hence, since G has diameter d, it then follows that v is adjacent to all vertices in the first two levels of $G-v$, or all in the first three levels and the remaining levels within distance k of v are singletons. This yields the group of expansions of paths given in (b) (d) above.

Otherwise (both P_x and P_y have length less than k), there are as above $d-2$ mates, and so by (ii) $d-2 = k-1$. That is, $k = d-1$. In particular, any level to which v is not adjacent must be singleton. Thus this yields the group of expansions of paths given in (a) above. □

Using Š o l t é s' ideas, from this we obtain the following theorem. (Observe that, for any graph G of order n and size m, $\sigma(G) \ge n(n-1) - m$ with equality if and only if $\operatorname{diam}(G) \le 2$.)

THEOREM 4. *Let G be a connected graph with n vertices and m edges. Then $\sigma(G)$ is maximum if and only if*

(a) *G is a path-complete graph $P[a_0, a_1, 1, \dots, 1]$,*

or

(b) *$m = \binom{n}{2} - (n-1)$ and G is $P[1, a_1, a_2, 1]$,*

or

(c) $m \geq \binom{n}{2} - (n-2)$.

P r o o f . Let D and d be the diameters of the graphs $PK_{n,m}$ and G respectively. If $d \leq 2$, then $\sigma(G) = n(n-1) - m \leq \sigma(PK_{n,m})$. If $\sigma(PK_{n,m}) = n(n-1) - m$, then $PK_{n,m}$ must have diameter at most 2, and so $m \geq \binom{n}{2} - (n-2)$. In this range of sizes, the graphs are automatically of diameter 2.

So assume $d \geq 3$. Then a little calculation (given in [6]) shows that

$$\sigma(G) = \binom{n}{2} + \sum_{k=1}^{d-1} \left(\binom{n}{2} - m - w_k(G) \right),$$

where $w_1(G) = 0$.

Now, consider the term $f_k(G) = \binom{n}{2} - m - w_k(G)$. This is always positive (since we restrict $k < d$). And by Theorem 2, $f_k(G) \leq f_k(PK_{n,m})$. Hence the summation for $\sigma(PK_{n,m})$ is term-by-term at least the summation for $\sigma(G)$, and has at least as many terms. It follows that $\sigma(G) = \sigma(PK_{n,m})$ if and only if $d = D$ and there is equality for $w_k(G)$ in the bound of Theorem 2 for each $k \in \{2, \dots, d-1\}$.

If $d=3$, then, by the above lemma, G is (up to symmetry) either $P[a_0, a_1, 1, 1]$, $P[1, a_1, a_2, 1]$ or $P[a_0, 1, 1, a_3]$. If $d \geq 4$, then by the above lemma, since we need equality for both $k = d-2$ and $k = d-1$, G is an expansion of the path with (up to symmetry) either all but a_0 and a_1 equal to 1 (the path-complete graph), or all but a_0 and a_d equal to 1.

But consider the graph $G[a_0, 1, \dots, 1, a_d]$ for $d \geq 3$: if $a_0, a_d \geq 2$, then this graph does not have maximum diameter. For, consider the graph G' formed as follows: let $v_0 v_1 \dots v_d$ be a diametral path of G and remove the edge $v_0 v_1$ and add the edge $v_{d-2} v_d$. The diameter of G' is $d+1$, and yet by Theorem 1 at most D; hence $d < D$.

So for $d \geq 3$, the only graphs with both maximum diameter and minimum $w_k(G)$ are those listed in the statement of the theorem. □

The path-complete graphs are also the extremal graphs for the problem of maximizing the status. E n t r i n g e r et al. [3] proved the bound; it is not hard to prove unique extremality.

THEOREM 5. *A vertex v has maximum status over all vertices in all connected graphs G with n vertices and m edges if and only if it is the vertex of minimum degree in the path-complete graph $PK_{n,m}$.*

Proof. By induction on n. Let G be a graph and let v be a vertex with maximum status. Let x be any neighbour of v.

If x is unique, then consider $G - v$. Clearly $\sigma_G(v) = n - 1 + \sigma_{G-v}(x)$ (where the subscript indicates the graph in which the status is measured). By the inductive hypothesis, the largest possible status for x in $G - v$ is uniquely the vertex of minimum degree in a path-complete graph on $n - 1$ vertices and $m - 1$ edges. Thus G is a path-complete graph.

Assume v has two or more neighbours. If there is a vertex y at distance 3 from v, then replace edge vx by edge xy; this increases the status of v, a contradiction. So every vertex is within distance 2 of v. If there are two vertices distinct from v that are nonadjacent, then replace xv by an edge joining them; again this increases the status of v, a contradiction. It follows that the graph $G - v$ is complete, and thus G is a path-complete graph. □

4. Graphs with maximum 3-diameter

We consider first the problem of maximum 3-diameter for a given order. This is obviously attained for a tree, but a few moments' thought shows:

THEOREM 6. *The maximum 3-diameter of a graph G on n vertices is $2(n-1)$, achieved by any tree with at most 3 end-vertices.*

Proof. Let T be any triple of vertices. Each edge of the tree G is in at most two of the shortest paths joining vertices of T; thus $d_3(G) \leq 2(n-1)$. Equality requires each edge to separate the triple; so equality is attained if and only if the tree has at most 3 end-vertices. □

The following result is similar to Ore's characterization of diameter-maximal graphs.

LEMMA 7. *Let G be a maximal graph with given order and 3-diameter. Then G is an expansion of one of the following:*

(a) *a path,*
(b) *a subdivision of the star with three end-vertices,*
(c) *the graph obtained by taking a triangle and three paths (possibly trivial) and identifying one end-vertex from each path with a different vertex of the triangle.*

Proof. Consider the triple $T = \{x, y, z\}$ of vertices with maximum distance in G. Define a *backbone* as the subgraph induced by the edges of three shortest paths, one for each pair of vertices in T. Let B be the backbone with the fewest edges.

It is clear that B is either the graph given in (a) or (b), or a subdivision of the graph given in (c). We show that in the latter case, the cycle in B is a triangle.

Suppose B contains a cycle but this cycle is not a triangle. Let the vertices on the cycle in B closest to x, y and z be x', y' and z' (necessarily distinct). These vertices divide the cycle into three edge-disjoint segments. Assume segment x' y' is the longest and z'–x' the shortest. By assumption segment x'–y' has length at least 2.

Let a be the vertex at distance two from y' on the x'–y' segment (possibly $a = x'$) and let b be the neighbour of y' on the y'–z' segment (possibly $b = z'$). See Figure 1. Now, if the edge ab is present, then this contradicts the minimality of B (delete the vertex between a and y' on the cycle). On the other hand, addition of the edge ab does not decrease any of the distances between vertices in the triple T, and so contradicts the maximality of G. Hence we have shown that the cycle in B is a triangle. So, B is one of the graphs listed in (a), (b) or (c) above.

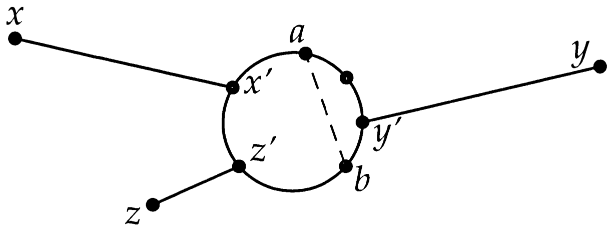

FIGURE 1. A non-minimum backbone.

Now, consider any other vertex u of G: it is adjacent to at most three vertices on any shortest path in G, and if it has three neighbours on the path then they are consecutive. Hence, $N(u) \cap B$ is a subset of the closed neighbourhood in B of some vertex v in B. By the maximality of G, the graph induced by $V(B) \cup \{u\}$ is obtained from B by duplicating the vertex v.

Repeated application of this argument shows that G is an expansion of B. $\square$

From this it follows:

THEOREM 8. *The maximum size of a graph with order* n *and* $d_3(G) = d$ *with* $d \in \{3, \dots, 2n-2\}$ *is*

$$m = \begin{cases} \binom{n-(d-5)/2}{2} + \frac{d-9}{2}, & d \geq 5,\ d \text{ odd}, \\ \binom{n-(d-6)/2}{2} + \frac{d-12}{2}, & d \geq 6,\ d \text{ even}, \\ \binom{n}{2} - 1, & d = 4, \\ \binom{n}{2}, & d = 3. \end{cases}$$

Proof. Obviously, G is maximal. By the above lemma, G is an expansion of a particular graph B. The maximum number of edges is obtained by always duplicating the vertex of maximum degree. So it remains to calculate the size in each case.

If the backbone B has a triangle, then the distance d of the triple T is odd, one vertex of the triangle is duplicated $n - (d+3)/2$ times, and the size is $m = \binom{n}{2}$ if $d = 3$, and

$$m = \binom{n - (d-5)/2}{2} + \frac{d-9}{2}$$

if $d \geq 5$. If the backbone B has no triangle, then the distance d of the triple T is even. If there is a vertex of degree 3 in B, then it is duplicated $n - (d+2)/2$ times, $d \geq 6$, and the size is

$$\binom{n - (d-6)/2}{2} + \frac{d-12}{2}.$$

If B is a path, and $d \geq 6$, then the size of G is smaller than that when B is not a path (except for $d = 2(n-1)$). But, for $d = 4$ this is the only possibility and when the middle vertex of the path of length 2 is duplicated $n-3$ times, the result has $m = \binom{n}{2} - 1$ edges. □

For d odd, it can be shown that the path-complete graph on this particular order and size (obtained by taking a path and expanding the penultimate vertex) is extremal. (The extremal triple is any triple containing the two initial end-vertices.)

However, for d even, the path-complete graph is not in general extremal. An example extremal graph for d even is constructed as follows. For $p \geq 2$ and $a \geq 1$, we define the broom (or comet) $B_{p,a}$ as the tree obtained by taking a path on p vertices and adding for one penultimate vertex (one adjacent to an end-vertex) $a-1$ new end-vertices adjacent to it. To obtain the extremal graph we take $B_{d/2,2}$ and expand the vertex of degree 3. (The triple of maximum distance is the three initial end-vertices.)

While we have not determined the maximum size for given k-diameter in general, it seems that, for k small relative to n, the above pattern may continue. In particular, consider a broom $B_{p,\lceil k/2\rceil}$ and expand the vertex of maximum degree. For suitable parity of distance, this is better than the path-complete graph.

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