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Diameter constraints in 2-distance graphs

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Abstract

For any finite, simple graph $G = (V, E)$, its 2-distance graph G_2 is a graph having the same vertex set V where two vertices are adjacent if and only if their distance is 2 in G. Connectivity and diameter properties of these graphs have been well studied. For example, it has been shown that if $\operatorname{diam}(G) = k \geq 3$ then $\lceil \left(\frac{1}{2}k\right) \rceil \leq \operatorname{diam}(G_2)$, and that this bound is sharp. In this paper, we prove that $\operatorname{diam}(G_2) = \infty$ (that is, G_2 is disconnected) or otherwise $\operatorname{diam}(G_2) \leq k + 2$. In addition, we show that this inequality is sharp for any even k, a result that we verify for some higher orders through judicious use of a SAT solver.

Keywords: graph operators; 2-distance; diameter bounds; connectivity; distance

1. Introduction

Given a finite, simple graph G, we let V and E denote the vertex set and the edge set of G, respectively. By $d_G(u, v)$ we denote *geodesic distance*, the length of a shortest path, between the vertices u and v in the graph G. The *diameter* of G, also denoted as $\operatorname{diam}(G)$, is the greatest geodesic distance between any two vertices in G. If G is disconnected, then $\operatorname{diam}(G) = \infty$. The *k-distance operator* D_k takes as input a simple graph G and outputs its *k-distance graph*, a graph having the same vertex set V but where any pair (u, v) has $d_{G_k}(u, v) = 1$ if and only if $d_G(u, v) = k$. The graph $D_k(G)$ is called the k-distance graph of G. A graph Y is *k-distance* if there exists a graph X such that $Y \cong D_k(X)$ (meaning that Y is isomorphic to $D_k(X)$). When ambiguity is impossible, we simply write G_k to refer to $D_k(G)$.

The general class of k-distance graphs was first introduced by Harary et al. [9] and are also known under the name of *exact distance powers* [3, 6]. Special cases for fixed k have been studied for their connectivity, diameter, and periodicity properties [10, 11, 12, 13, 5]. Known results in the literature are numerous. For example, the cubic self 2-distance graphs do not exist [1]. On the other hand, Azimi et al. [2] showed the complete set of graphs whose 2-distance graphs are simple paths or cycles. General characterizations were given by Ching and Garces [4] whereas Gaar and Krenn [7] characterized regular 2-distance graphs. Recognition under special constraints was shown to be polynomial-time by Bai et al. [3].

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Recently, Jafari and Musawi [11] conjectured that if $\operatorname{diam}(G) = k \geq 3$ then $\operatorname{diam}(G_2) \leq k + 2$, and proved it for $\operatorname{diam}(G) = 3$. Under the standard assumption that $\operatorname{diam}(G) = \infty$ when G is disconnected, we will prove that the statement is true when $\operatorname{diam}(G_2) \neq \infty$.

2. Preliminaries

Our graph theory notation basically follows that of Golumbic [8]. We write $G[S]$ to refer to the subgraph of G induced by the vertex set of S. For a graph H, we let $V(H)$ and $E(H)$ denote the vertex set and the edge set of H, respectively. For any $x \in V$, let $N_G(x) = \{y : \{x, y\} \in E\}$ be the (open) neighborhood of x and $N_G[x] = N(x) \cup \{x\}$ the closed neighborhood of x. We write $x \in N_G(S)$ to say that x is adjacent to some vertex in S while $x \notin S$. We write $x \in N_G[S]$ if $x \in N_G(S) \cup S$. We denote by $C_{N_G}(S)$ the *common neighborhood* of S in G. i.e. $C_{N_G}(S) = \bigcap_{v \in S} N_G(v)$.

A sequence of vertices $P = \langle u = x_0 x_1 \cdots x_{k-1} x_k = v \rangle$ is called a *walk* if $x_i \in N_G[x_{i+1}]$ for all $i \in \{0, 1, \ldots, k-1\}$. The *length* of a walk is the number of edges it contains. We say P is a *path* if the vertices $x_0, x_1, \ldots, x_k$ are all distinct. A walk with endpoints u and v may be called a u, v-walk. If $v \in N_G(v')$, then we denote by $P{-}v'$ the walk $\langle u = x_0 x_1 \cdots x_{k-1} x_k = v v' \rangle$. Similarly, if $P = \langle x_0 x_1 \cdots x_k \rangle$ and $P' = \langle y_0 y_1 \cdots y_q \rangle$ are walks and $x_k \in N_G(y_0)$, then we let $P{-}P' = \langle x_0 \cdots x_k y_0 \cdots y_q \rangle$. We write $P[x_i, x_j]$ where $(0 \leq i \leq j \leq k)$ for the subwalk $\langle x_i \cdots x_j \rangle$ of P. It is well known that we can extract a u, v-path from the subset of every u, v-walk. A *triangle* is a set of three vertices such that each vertex is adjacent to the other two.

3. Diameter Bounds

In this section, we show that the diameter of G imposes strong constraints on the diameter of G_2 (see Theorem 7). We need an easy way to refer to paths between G and its 2-distance graph in our proofs. For a basic example of the following definition, see Fig. 1.

Definition 1. *Let $P = \langle v_1 v_2 \cdots v_{k-1} v_k \rangle$ be a walk in G and let $p = k - (k \mod 2)$. If for each odd $i \in [1, k-2]$ we have that $P[v_i, v_{i+2}]$ is induced, then there exists a walk $\langle v_1 v_3 \cdots v_{p-2} v_p \rangle$ in G_2 that we denote by $D_2(P)$.*

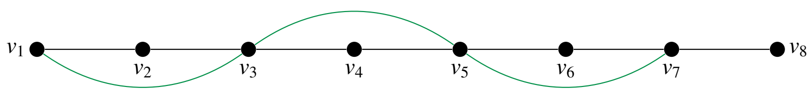

Fig. 1. Let $P = \langle v_1 v_2 \cdots v_8 \rangle$ in G, shown with black edges. The green edges are the edges of $D_2(P)$ by Definition 1.

We will prove our main theorem by showing that a graph G_2 having an exceedingly high diameter causes G to contain the complement of a path. This high edge-density subgraph will lead to a contradiction to $\operatorname{diam}(G)$. This result builds on a sequence of lemmas which we will now begin.

Lemma 2. *Let G be a graph with $\operatorname{diam}(G) = k \geq 3$, let $P_2 = \langle a_1 a_2 \cdots a_{k+3} a_{k+4} \rangle$ be a shortest path in G_2, and let $\ell = \lceil \left(\frac{k+4}{2} \right) \rceil$. Then, $a_1, a_{k+4} \in N_G(a_{\ell+1})$.*

Proof. To prove the statement, we will show that $\langle a_1, a_{\ell+1} \rangle$ and $\langle a_{k+1}, a_{\ell+1} \rangle$ exist and that all other cases result in a contradiction. For P_2 to exist in G_2, the graph G must contain a walk taking the form of $P = \langle a_1 b_1 a_2 b_2 a_3 \cdots a_{k+3} b_{k+3}$ $a_{k+4} \rangle$. We will first show that the shortest paths between vertices of $V(P_2)$ in G satisfy special constraints.

No shortest path in G has length exceeding $\operatorname{diam}(G)$. In particular, the subwalks $P[a_1, a_{\ell+1}]$ and $P[a_{\ell+1}, a_{k+4}]$ are not shortest paths because their lengths exceeds $\operatorname{diam}(G) = k$. Thus, there exist shortest paths $R = \langle a_1 = r_1 r_2 \cdots r_p = a_{\ell+1} \rangle$ and $R' = \langle a_{\ell+1} = r'_1 r'_2 \cdots r'_{p'} = a_{k+4} \rangle$ in G. In the remainder of the proof, we will frequently recall the fact that the length of $D_2(R)$ is at most $\lfloor \left(\frac{k}{2} \right) \rfloor$, which arises from the understanding that $D_2(R)$ is at most half the length of R by Definition 1.

We claim that the lengths of R and R' are odd. Suppose instead that $L = R$ (*resp.* $L = R'$) has an even length. Note that $\mu = (\ell + 1) - 1$ is the difference between the indices of $a_{\ell+1}$ and a_1. Moreover, $\omega = k + 4 - (\ell + 1)$ is the difference between the indices of a_{k+4} and $a_{\ell+1}$. We have that $D_2(L)$ is shorter than both $P_2[a_1, a_{\ell+1}]$ and $P_2[a_{\ell+1}, a_{k+4}]$ because $\lfloor\binom{k}{2}\rfloor$ (the greatest possible length of $D_2(L)$) is strictly less than both μ and ω, respectively, a fact easily verified for any value of $k \geq 3$. This is a contradiction to the assumption that P_2 is a shortest path. Fig. 2 shows an example for $k = 4$ and $L = R'$. We have proven our claim.

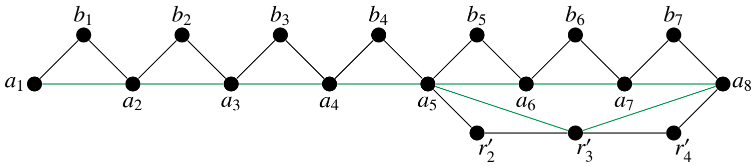

Fig. 2. Let $k = 4$. So, P_2 has length 7 and $\ell + 1 = 5$. Let the black edges denote $E(G)$ and let the green edges denote $E(G_2)$. A shortest a_5, a_8-path of length 4 in G causes $d_{G_2}(a_5, a_8) = 2$, a contradiction.

There is an important distinction between odd and even k. When k is odd, then R has length at most k. When k is even, then R has length at most $k - 1$ because we have shown that R may not have even length. Let $k' = k$ when k is odd, but $k' = k - 1$ when k is even. Later in the proof, we will need to use k' in order to reach a contradiction. We will arrive at a contradiction from assuming that the length of R or R' is greater than 1, and so the only possibility left is that both lengths are 1, i.e., they are edges. Note that r_{p-1} is the last endpoint of $D_2(R)$ because R has odd length. Consider two cases based on the incidence of r_{p-1} to R'.

Case 1: r_{p-1} is in the closed neighborhood of every vertex in R' in G. If $a_{k+4} = r_{p-1}$ then $D_2(R)$ is an a_1, a_{k+4}-path of length at most $\lfloor\binom{k}{2}\rfloor$, a contradiction to the assumption that $d_{G_2}(a_1, a_{k+4}) = k + 3$. Thus, $a_{k+4} \neq r_{p-1}$. Next, if $X = \langle a_{k+4} r_{p-1} a_{\ell+1} \rangle$ is an induced path in G then $D_2(X) = \langle a_{k+4} a_{\ell+1} \rangle$ gives $d_{G_2}(a_{k+4}, a_{\ell+1}) = 1$, a contradiction. So, X is not induced, meaning that X is a triangle in G, implying $a_{k+4} \in N_G(a_{\ell+1})$. Now $\langle a_{\ell+1} a_{k+4} \rangle$ is a shortest path in G, and therefore R' has length 1 (i.e. $R' = \langle a_{\ell+1} a_{k+4} \rangle$). Since the lengths of R and R' are odd, and we are considering the case where they are not both equal to 1, the length of R is 3 or greater.

Let $B = C_{N_G}(a_\ell, a_{\ell+1})$. For any $b \in B$, suppose that $b \notin N_G[r_{p-1}] \cup N_G[a_{k+4}]$. Observe that $D_2(R{-}b{-}R')$ has length at most $\lfloor\binom{k}{2}\rfloor + 2$, a contradiction to the assumption that $d_{G_2}(a_1, a_{k+4}) = k + 3$. Fig. 3 demonstrates this contradiction where $k = 4$ and $b = b_\ell$. Thus, $b \in N_G[r_{p-1}] \cup N_G[a_{k+4}]$ for any $b \in B$.

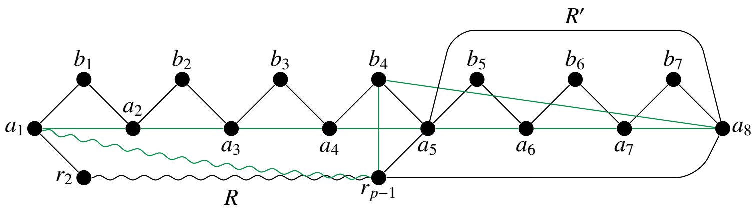

Fig. 3. In this example, we follow the assumptions set at the beginning of Case 1 of Lemma 2 where $k = 4$. Thus, $\text{diam}(G_2) = 7$, $\ell + 1 = 5$, and $k + 4 = 8$. Let the black edges denote $E(G)$ and let the green edges denote $E(G_2)$. Let $b_4 \notin N_G[r_{p-1}] \cup N_G[a_8]$. The green walk $D_2(R{-}b{-}R')$ has a length less than $d_{G_2}(a_1, a_8)$, a contradiction within the proof.

We claim that $r_{p-1} \in N_G[B]$. Suppose not. For a fixed $b \in B$ we have $r_{p-1} \notin N_G[b]$. Hence, $a_{k+4} \in N_G[b]$. If $a_{k+4} = b$, then $r_{p-1} \in N_G[b]$ (recall that $r_{p-1} \in N_G(a_{k+4})$), a contradiction. Therefore, $a_{k+4} \neq b$. Now G has a walk $Y = \langle a_{k+4} b a_\ell \rangle$ with all vertices distinct. If Y is induced then $D_2(Y)$ gives $d_{G_2}(a_{k+4}, a_\ell) = 1$, a contradiction. Therefore, Y is not induced, meaning that $a_{k+4} \in N_G(a_\ell)$ and so $R'{-}a_\ell$ is a path in G. The existence of $R'{-}a_\ell$ in G implies that $a_{k+4} \in C_{N_G}(a_\ell, a_{\ell+4})$ (i.e. $a_{k+4} \in B$). This immediately shows that $r_{p-1} \in N_G[B]$ because r_{p-1} neighbors $a_{k+4} \in R'$, a contradiction. We have proven our claim. We consider two specific subcases of the result of this claim.

Case 1.1: $r_{p-1} \in N_G(B)$. In particular, let $b' \in B$ and $r_{p-1} \in N_G(b')$. Recall that $r_p = a_{\ell+1}$. If $r_{p-1} = a_\ell$, then trivially $a_\ell \notin N_{G_2}(a_{\ell+1})$, a contradiction to the definition of P_2. Thus, $r_{p-1} \neq a_\ell$.

Next, we will prove that $r_{p-1} \in N_G(a_\ell)$. Suppose otherwise. Recalling the definition of k', note that $D_2(R)$ has length at most $\lfloor\binom{k'}{2}\rfloor$. There exists an a_1, a_ℓ-walk $Q = D_2(R{-}b'{-}a_\ell)$ of length at most $\lfloor\binom{k'}{2}\rfloor + 1$ in G_2. It is easy to verify that $\lfloor\binom{k'}{2}\rfloor + 1 < (\ell - 1) = (\lceil\binom{k+4}{2}\rceil - 1)$ for any $k \geq 3$. Consequently, the length of Q contradicts the assumption that $d_{G_2}(a_1, a_\ell) = \ell - 1$. Therefore, $r_{p-1} \in N_G(a_\ell)$. Now $r_{p-1} \in C_{N_G}(a_\ell, a_{k+4})$ (i.e. $r_{p-1} \in B$), a contradiction.

Case 1.2: $r_{p-1} \in B$. Note that $r_{p-1} \in N_G(a_\ell)$ by the definition of B. We also have that $a_\ell \in N_G(a_{k+4})$, otherwise $D_2(\langle a_\ell r_{p-1} a_{k+4}\rangle)$ gives $d_{G_2}(a_\ell, a_{k+4}) = 1$, a contradiction. Recall that R has length 3 or greater. Thus, r_{p-2} and r_{p-3} exist. If $r_{p-3} \in N_G(a_{k+4})$, then $\langle r_{p-3} a_{k+4} a_{\ell+1}\rangle$ has length at most 2 in G, a contradiction to the fact that R is a shortest path with $d_G(r_{p-3}, r_p) = 3$. Hence, $r_{p-3} \notin N_G(a_{k+4})$.

If $r_{p-2} \notin N_G(a_{k+4}) \cup N_G(a_\ell)$, then there exists $Q = \langle a_{k+4} r_{p-1} r_{p-2} r_{p-1} a_\ell\rangle$ in G; in fact, Q exists even if $r_{p-2} \in \{a_\ell, a_{k+4}\}$. Now $D_2(Q) = \langle a_{k+4} r_{p-2} a_\ell\rangle$ is an a_{k+4}, a_ℓ-walk of length at most 2 in G_2, a contradiction. We have shown that $r_{p-2} \in N_G(a_{k+4}) \cup N_G(a_\ell)$. In particular, we will show that $r_{p-2} \in N_G(a_\ell)$. Suppose not, and thus $r_{p-2} \in N_G(a_{k+4})$. Now $D_2(R[r_1, r_{p-2}]{-}a_{k+4})$ is an a_1, a_{k+4}-path of length at most $\lfloor\binom{k}{2}\rfloor$ in G_2, a contradiction. Therefore, $r_{p-2} \in N_G(a_\ell)$.

There exists $Q' = R[r_1, r_{p-2}]{-}a_\ell$ in G. If $r_{p-3} \notin N_G(a_\ell)$, then $D_2(Q')$ is an a_1, a_ℓ-path of length at most $\lfloor\binom{k'}{2}\rfloor$. Then, noting that $\lfloor\binom{k'}{2}\rfloor < (\ell - 1) = (\lceil\binom{k+4}{2}\rceil - 1)$ for any $k \geq 3$, observe that $D_2(Q')$ is shorter than $d_{G_2}(a_1, a_\ell) = \ell - 1$, a contradiction. Thus, $r_{p-3} \in N_G(a_\ell)$.

There exists $T = R[r_1, r_{p-3}]{-}a_\ell{-}a_{k+4}$ in G. Recalling that $r_{p-3} \notin N_G(a_{k+4})$, observe that $D_2(T)$ is an a_1, a_{k+4}-path of length at most $\lfloor\binom{k}{2}\rfloor$ in G_2, a contradiction.

Case 2: r_{p-1} is *not* in the closed neighborhood of every vertex in R' in G. Let r'_f be the first vertex in R' that is not in $N_G[r_{p-1}]$. Since r_{p-1} is adjacent to $a_{\ell+1} = r'_1$ by the definitions of R and R', clearly $f > 1$. There exists $T = R[r_1, r_{p-1}]{-}R'[r'_{f-1}, r'_{p'}]$ in G. Notice T is an a_1, a_{k+4}-walk with length no greater than $2k$.

It is straightforward to check that if f is even, then T has even length. Subsequently, from $D_2(T)$ we can extract an a_1, a_{k+4}-path having length at most k. This contradicts the assumption that $d_{G_2}(a_1, a_{k+4}) = k + 3$. So, f is odd.

Case 2.1: $f > 3$. Hence, $f \geq 5$ (since f cannot be even) and R' has length 5 or greater. There exists a walk $R'[r'_{p'}, r'_{f-1}]{-}\langle r_{p-1} r_p\rangle$ in G whose length is strictly less than the length of R', a contradiction to the assumption that R' is a shortest path in G.

Case 2.2: $f = 3$. So, $r'_3 = r'_f$ and $r'_2 = r'_{f-1}$. Notice that $\langle r_{p-1} r'_2 r'_3\rangle$ is induced in G. There exists $Q = R[r_1, r_{p-1}]{-}\langle r'_2 r'_3 r'_2 r'_1\rangle$ in G. It follows that $D_2(Q)$ is an $a_1, a_{\ell+1}$-walk with length at most $\tau = \lfloor\binom{k'}{2}\rfloor + 2$ in G_2. It is easy to verify that $\tau < \ell$ for any value of $k \geq 3$, a contradiction to $d_{G_2}(a_1, a_{\ell+1}) = \ell$. □

The following simple result will be useful in later proofs.

Proposition 3. *Given a graph G with $\mathrm{diam}(G) = k \geq 3$, let $P_2 = \langle a_1 a_2 \cdots a_{k+3} a_{k+4}\rangle$ be a shortest path in G_2, and let $i \in [3, k+2]$ such that $a_1, a_{k+4} \in N_G(a_i)$. The set $\{a_1, a_i, a_{k+4}\}$ induces a triangle in G.*

Proof. There exists a path $R = \langle a_1 a_i a_{k+4}\rangle$ in G. If $a_1 \notin N_G(a_{k+4})$, then $D_2(R) = \langle a_1 a_{k+4}\rangle$ exists in G_2, a contradiction to the assumption that P_2 is a shortest path. □

Next, we will show that any central vertex in P_2 that is adjacent to both the first and last vertices in P_2 infers the existence of two additional edges in G.

Lemma 4. *Under the hypothesis of Proposition 3 where $i > 3$, we have that $a_1, a_{k+4} \in N_G(a_{i-1})$.*

Proof. Let $b \in C_{N_G}(a_{i-1}, a_i)$ and $R = \langle a_1 a_i b a_i a_{k+4}\rangle$. By Proposition 3 we have that $a_1 \in N_G(a_{k+4})$. Suppose for the sake of contradiction that $b \notin N_G(a_1) \cup N_G(a_{k+4})$. Then, there exists a walk $D_2(R) = \langle a_1 b a_{k+4}\rangle$ (this walk exists even if $b \in \{a_1, a_{k+4}\}$). But, now we have that $d_{G_2}(a_1, a_{k+4}) \leq 2$, a contradiction. Thus, $b \in N_G(a_1) \cup N_G(a_{k+4})$.

Next, if $b \in N_G(a_1)$, then let $(u, v) = (a_1, a_{k+4})$; alternatively, if $b \in N_G(a_{k+4})$ then let $(u, v) = (a_{k+4}, a_1)$. Surely $u \in N_G(a_{i-1})$ when $b = u$ (trivially) or when $b \neq u$ (otherwise $D_2(\langle u b a_{i-1}\rangle) = \langle u a_{i-1}\rangle$ exists in G_2, a contradiction). Furthermore, we have $v \in N_G(a_{i-1})$ when $b = v$ (trivially) or when $b \neq v$ (otherwise $D_2(\langle v u a_{i-1}\rangle) = \langle v a_{i-1}\rangle$ exists in G_2, a contradiction). We have shown that $u, v \in N_G(a_{i-1})$, so we are done. □

Next, we will show that a graph satisfying the conclusions of Lemmas 2 and 4 contains a subgraph that induces the complement of a path. The existence of this structure will be vital for proving Theorem 7.

Theorem 5. *Let G have $\mathrm{diam}(G) = k \geq 3$ and let $P_2 = \langle a_1 a_2 \cdots a_{k+3} a_{k+4}\rangle$ be a shortest path in G_2. Then, $V(P_2)$ induces the complement of a path in G.*

Proof. For easier reference, let $A = V(P_2)$. Let $\ell = \lceil\left(\frac{k+4}{2}\right)\rceil$ and let $P_2^R = \langle a_{k+4}a_{k+3}\cdots a_1\rangle$ be a path in G_2 (that is, P_2^R is the reverse of P_2). By Lemma 2 we have that $a_1, a_{k+4} \in N_G(a_{\ell+1})$. By Proposition 3 where $i := \ell$ we have that $a_1 \in N_G(a_{k+4})$.

We will show by induction that, for each $3 \leq j \leq \ell$, we have $a_1, a_{k+4} \in N_G(a_j)$. The statement is true if $j = \ell$ because Lemma 4 is applicable by setting $P_2 := P_2$ and $i := \ell + 1$, giving $a_1, a_{k+4} \in N_G(a_\ell)$. Now suppose that $3 \leq j < \ell$. By the inductive hypothesis, $a_1, a_{k+4} \in N_G(a_{j+1})$. Then, Lemma 4 holds where $P_2 := P_2$, and $i := j + 1$, promising that $a_1, a_{k+4} \in N_G(a_j)$.

Next, we will also show by induction that, for each $\ell \leq j \leq k + 2$, we have $a_1, a_{k+4} \in N_G(a_j)$. The statement is true if $j = \ell$ because Lemma 4 is applicable by setting $P_2 := P_2^R$ and $i := \ell - 1$, giving $a_1, a_{k+4} \in N_G(a_\ell)$. Now suppose that $\ell < j \leq k + 2$. By the inductive hypothesis, $a_1, a_{k+4} \in N_G(a_{j-1})$. Then, Lemma 4 holds where $P_2 := P_2^R$ and $i := j - 1$, promising that $a_1, a_{k+4} \in N_G(a_j)$. We have proven our claim.

Observe now that both a_1 and a_{k+4} are in the closed neighborhood of every vertex in $A \setminus \{a_2, a_{k+3}\}$. We claim that for each $i, j \in [3, k + 2]$ such that $\text{abs}(i - j) > 1$ we have $a_i \in N_G(a_j)$. Suppose on the contrary that for some $i', j' \in [3, k + 2]$ where $\text{abs}(i' - j') > 1$ we have $a_{i'} \notin N_G(a_{j'})$. The existence of $D_2(\langle a_{i'}a_1a_{j'}\rangle) = \langle a_{i'}a_{j'}\rangle$ gives $d_{G_2}(a_{i'}, a_{j'}) = 1$, a contradiction. We have proven the claim. At this stage of the proof, $A \setminus \{a_2, a_{k+3}\}$ has been shown to induce the complement of a path in G.

We claim that $a_2 \in N_G(a_{k+4})$ and $a_{k+3} \in N_G(a_1)$. Note the symmetry of the fact that a_2 and a_{k+3} are the second and second to last vertices in P_2, respectively. W.l.o.g. suppose for the sake of contradiction that $a_2 \notin N_G(a_{k+4})$. Note that if $d_G(a_2, a_{k+4}) = 2$, then $d_{G_2}(a_2, a_{k+4}) = 1$, a contradiction. There exists a vertex $b_1 \in C_{N_G}(a_1, a_2)$ because we have assumed that $d_{G_2}(a_1, a_2) = 1$. Let $W = \langle a_{k+4}a_1b_1a_1a_\ell\rangle$ in G. If $b_1 \notin N_G(a_\ell) \cup N_G(a_{k+4})$, then $D_2(W) = \langle a_{k+4}b_1a_\ell\rangle$ is shorter than the assumed value of $d_{G_2}(a_\ell, a_{k+4})$, a contradiction (this is easily verified for any k, and is true even if $b_1 \in \{a_\ell, a_{k+4}\}$). But, $b_1 \in N_G(a_{k+4})$ gives $d_G(a_2, a_{k+4}) = 2$, a contradiction. Hence, it is necessary that $b_1 \in N_G(a_\ell)$. However, the existence of $\langle a_2b_1a_\ell\rangle$ in G implies that $d_{G_2}(a_2, a_\ell) = 1$, a contradiction. Thus, $a_2 \in N_G(a_\ell)$. Because $a_2 \notin N_G(a_{k+4})$, we have that the existence of $\langle a_2a_\ell a_{k+4}\rangle$ in G gives $d_{G_2}(a_2, a_{k+4}) = 1$, a contradiction. We have proven our claim.

Note the symmetry of the fact that a_2 and a_{k+3} are adjacent to a_{k+4} and a_1, respectively. We will prove that $a_2 \in N_G(u)$ for all $u \in A \setminus \{a_1, a_2, a_3, a_{k+3}, a_{k+4}\}$. This will similarly show that $a_{k+3} \in N_G(v)$ for all $v \in A \setminus \{a_{k+4}, a_{k+3}, a_{k+2}, a_2, a_1\}$. W.l.o.g. suppose for the sake of contradiction that $a_2 \notin N_G(u')$ for some $u' \in A \setminus \{a_1, a_2, a_3, a_{k+3}, a_{k+4}\}$. It follows that $\langle a_2a_{k+4}u'\rangle$ is an induced path in G that gives $d_{G_2}(a_2, u') = 1$, a contradiction. We have proven our claim.

In order to complete the proof, it remains to show that $a_2 \in N_G(a_{k+3})$. If not, then the induced path $\langle a_2a_4a_{k+3}\rangle$ in G gives $d_{G_2}(a_2, a_{k+3}) = 1$, a contradiction. □

The next lemma is crucial because it shows that the existence of $V(P_2)$, the complement of a path in G, applies special constraints on its neighboring vertices. More specifically, any such vertex has at least two edges between itself and $V(P_2)$, and these edges are incident to vertices that are far apart in P_2.

Lemma 6. *Given a graph G with* $\text{diam}(G) = k \geq 3$*, let $P_2 = \langle a_1a_2\cdots a_{k+3}a_{k+4}\rangle$ be a shortest path in G_2 and let $A \subseteq G$ be the subgraph induced by $V(P_2)$. Let $u \in N_G(A)$. Then, $N_G(u) \cap A \supseteq \{a_i, a_j\}$ such that $i, j \in [1, k + 4]$ and* $\text{abs}(i - j) > 2$.

Proof. We will prove the statement directly. By Theorem 5, A is the complement of a path. Let $u \in N_G(a_h)$ for any h. If $h = 1$, then let $S = \{a_h, a_{h+1}\}$; otherwise if $h = k + 4$, then let $S = \{a_{h-1}, a_h\}$; otherwise, let $S = \{a_{h-1}, a_h, a_{h+1}\}$. Next, let $a_s, a_t \in A \setminus S$ such that $i \notin \{s, t\}$ and $\text{abs}(s - t) > 2$ (it is easy to verify that such a pair a_s, a_t exists). There exists a walk $W = \langle a_sa_hua_ha_t\rangle$ in G. If $u \notin N_G(a_s) \cup N_G(a_t)$, then $D_2(W) = \langle a_sua_t\rangle$ exists in G_2, giving $d_{G_2}(a_s, a_t) = 2$, a contradiction to the assumption that $\text{abs}(s - t) > 2$. See Fig. 4 for an example of this contradiction. Therefore, $u \in N_G(a_s) \cup N_G(a_t)$. If $u \in N_G(a_s)$ and $\text{abs}(h - s) > 3$, then we are done by setting $(i, j) := (h, s)$. If $u \in N_G(a_t)$ and $\text{abs}(h - t) > 3$, then we are done by setting $(i, j) := (h, t)$. W.l.o.g. it remains for us to find appropriate (i, j) when $u \in N_G(a_t)$ and $\text{abs}(h - t) = 2$. We consider two cases based on the value of h.

Case 1: $1 < h < k+2$. Note that $d_{G_2}(a_{h-1}, a_{t+1}) = 4$. There exists a path $T = \langle a_{h-1}a_tua_ha_{t+1}\rangle$ in G. If $u \notin N_G(a_{h-1}) \cup N_G(a_{t+1})$, then $D_2(T) = \langle a_{h-1}ua_{t+1}\rangle$ gives $d_{G_2}(a_{h-1}, a_{t+1}) = 2$, a contradiction. Thus, $u \in N_G(a_{h-1}) \cup N_G(a_{t+1})$. If $u \in N_G(a_{h-1})$, then we are done by setting $(i, j) := (h - 1, t)$. But if $u \in N_G(a_{t+1})$, then we are done by setting $(i, j) := (h, t + 1)$.

Case 2: $h = 1$ or $h = k + 2$. More specifically, this means that either $(h, t) = (1, 3)$ or $(h, t) = (k + 2, k + 4)$. Due to the symmetry, finding indices that give us appropriate (i, j) in one of the two cases is enough to complete the proof. Hence, w.l.o.g. we may assume that $(h, t) = (1, 3)$. We will show that $u \in N_G(a_4) \cup N_G(a_7)$. Suppose not. There exists a path $R = \langle a_4 a_1 u a_3 a_7 \rangle$ in G. Then, $D_2(R) = \langle a_4 u a_7 \rangle$ gives $d_{G_2}(a_4, a_7) = 2$, a contradiction. Thus, $u \in N_G(a_4) \cup N_G(a_7)$. In particular, if $u \in N_G(a_4)$, then we are done by setting $(i, j) := (1, 4)$. But if $u \in N_G(a_7)$, then we are done by setting $(i, j) := (1, 7)$. □

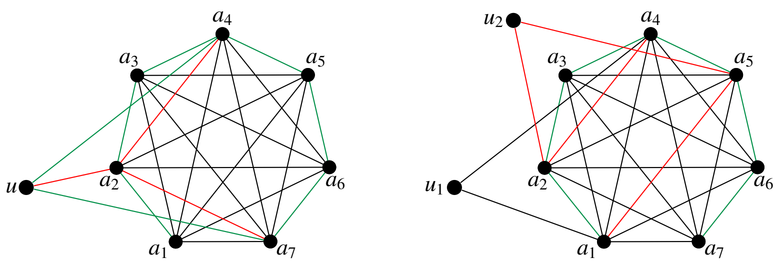

Fig. 4. The black and red edges belong to $E(G)$ and the green edges belong to $E(G_2)$. On the left, the graph shows a contradiction that occurs within the proof of Lemma 6 where $(k, h, s, t) = (3, 2, 4, 7)$. The red edges, in particular, denote W. On the right, we portray the proof of Theorem 7 where $k = 3$, $(b, d) = (1, 4)$, and $(p, q) = (2, 5)$. The red edges denote W within Case 1. Note that the path $D_2(W) = \langle a_1 u_2 a_4 \rangle$ exists but is not drawn.

We are prepared to prove our main result:

Theorem 7. *Given a graph $G = (V, E)$ with $\operatorname{diam}(G) = k \geq 3$, we have that either G_2 is disconnected or $\operatorname{diam}(G_2) \leq k + 2$.*

Proof. Suppose that G_2 is connected (and so G is also connected) and $\operatorname{diam}(G_2) > k+2$. Thus, G_2 contains a diametral path of length $k + 3$ or greater. This path necessarily contains a shortest path $P_2 = \langle a_1 a_2 \cdots a_{k+3} a_{k+4} \rangle$. By Theorem 5, we have that $V(P_2)$ induces the complement of a path in G. Let $A \subseteq G$ be the subgraph induced by $V(P_2)$ for simplicity. It is trivial to see that $\operatorname{diam}(A) = 2$. Since $\operatorname{diam}(G) = k$, there exists $S = N_G(A)$ where $S \neq \emptyset$.

We claim that $G \setminus (A \cup S) = \emptyset$. Suppose not. Let $u \in S$ and $v \in N_G(u) \setminus (A \cup S)$. By Lemma 6, $u \in S$ satisfies $N_G(u) \cap A = \{a_i, a_j\}$ such that $i, j \in [1, k + 4]$ and $\operatorname{abs}(i - j) > 2$. Clearly, for any $a \in A$ we have $d_G(u, a) \leq 2$. Consequently, there exists $T = \langle a_i u v u a_j \rangle$ in G. If $v \notin N_G(a_i) \cup N_G(a_j)$, then $D_2(T) = \langle a_i v a_j \rangle$ in G_2 gives $d_{G_2}(a_i, a_j) = 2$, a contradiction to the fact that $\operatorname{abs}(i - j) > 2$. Thus, $v \in N_G(a_i) \cup N_G(a_j)$, a contradiction to the fact that $v \notin S$. We have proven the claim.

It is easy to see that $|S| > 1$, otherwise $\operatorname{diam}(G[A \cup S]) = 2$, a contradiction. Next, we will prove that for all pairs $v_1, v_2 \in S$ we have $d_G(v_1, v_2) \leq 2$. On the contrary, suppose that some $u_1, u_2 \in S$ has $d_G(u_1, u_2) > 2$. Note that $C_{N_G}(u_1, u_2) = \emptyset$.

By Lemma 6 where $u := u_1$ there exists a set $N_G(u_1) \cap A \supseteq \{a_b, a_d\}$ satisfying $b, d \in [1, k + 4]$ and $\operatorname{abs}(b - d) > 2$. W.l.o.g. let $b < d$.

By Lemma 6 where $u := u_2$ there exists a set $N_G(u_2) \cap A \supseteq \{a_p, a_q\}$ satisfying $p, q \in [1, k + 4]$ and $\operatorname{abs}(p - q) > 2$. W.l.o.g. let $p < q$. Moreover, w.l.o.g. we may assume that $b < p$. Note that b, d, p, q are distinct because $C_{N_G}(u_1, u_2) = \emptyset$. Notice it is possible that $b+1 = p$, but it is not possible that $b+1 \in \{d, q\}$. Since $b+1 < q$, we have that $a_b \in N_G(a_q)$. We consider two cases:

Case 1: $p + 1 < d$. Thus, $a_p \in N_G(a_d)$. There exists a path $W = \langle a_b a_q u_2 a_p a_d \rangle$ in G. See the right graph in Fig. 4 for an example of this case. However, the existence of $D_2(W) = \langle a_b u_2 a_d \rangle$ gives $d_{G_2}(a_b, a_d) = 2$, a contradiction to the assumption that $\operatorname{abs}(b - d) > 2$. We have proven our claim that for all pairs $v_1, v_2 \in S$ we have $d_G(v_1, v_2) \leq 2$. Since we have also shown that $G \setminus (A \cup S) = \emptyset$, it immediately follows that $\operatorname{diam}(G) \leq 2$, a contradiction to the hypothesis that $\operatorname{diam}(G) = k$.

Case 2: $p + 1 \geq d$. In other words, we have that $a_p, a_q \in P_2[a_{d-1}, a_{k+4}]$. First, suppose that $p = b + 1$. Hence, $(b+1)+1 \geq d$. If $b+2 \in \{d, d+1\}$, then we contradict the fact that $\operatorname{abs}(b-d) > 2$. So, it is necessary that $b+2 > d+1$, but this clearly contradicts the assumption that $b < d$. We see that $p = b + 1$ leads to contradiction. It is necessary that

$p \neq b + 1$. Recalling also that $p > b$, we in fact have that $p > b + 1$ and thereby $a_b \in N_G(a_p)$. To simplify, we have shown that a_b and a_p are sufficiently far from one another in P_2 that they are adjacent in G.

Our assumption that $p + 1 \geq d$, combined with the fact that $\text{abs}(p - q) > 2$ and $p < q$, implies that $q \neq d + 1$. Thus, $a_q \in N_G(a_d)$. Stated plainly, a_q and a_d are far enough away in P_2 that they are adjacent in G. It has become evident that there exists a path $W = \langle a_b a_p u_2 a_q a_d \rangle$ in G. The existence of $D_2(W) = \langle a_b u_2 a_d \rangle$ gives $d_{G_2}(a_b, a_d) = 2$, a contradiction to the assumption that $\text{abs}(b - d) > 2$. We have proven our claim that for all pairs $v_1, v_2 \in S$ we have $d_G(v_1, v_2) \leq 2$. Since we have also shown that $G \setminus (A \cup S) = \emptyset$, it immediately follows that $\text{diam}(G) \leq 2$, a contradiction to the hypothesis that $\text{diam}(G) = k$. □

Combining our main theorem with the lower bound achieved in [11], we arrive at the following statement:

Theorem 8. *Let G have* $\text{diam}(G) = k \geq 3$. *Then, either* $\text{diam}(G_2) = \infty$ *or* $\lceil \left(\frac{1}{2}\right) k \rceil \leq \text{diam}(G_2) \leq k + 2$.

Proposition 9. *The upper bound of the inequality expressed by Theorem 8 is sharp when* $k = 3$ *or* $k > 3$ *is even.*

Proof. An example for $k = 3$ is provided in [11]. There exists a family of graphs showing that sharpness holds for any even $k > 3$. See Fig. 5, which shows a graph G having $\text{diam}(G) = 4$ and $\text{diam}(G_2) = 6$. By increasing the size of the largest cycle in G by 4 such that the triangle shares exactly one edge with the largest cycle, $\text{diam}(G)$ and $\text{diam}(G_2)$ increase by 2. It is easy to verify that this procedure can be repeated in order to generate any number of graphs satisfying the conclusion of the proposition. □

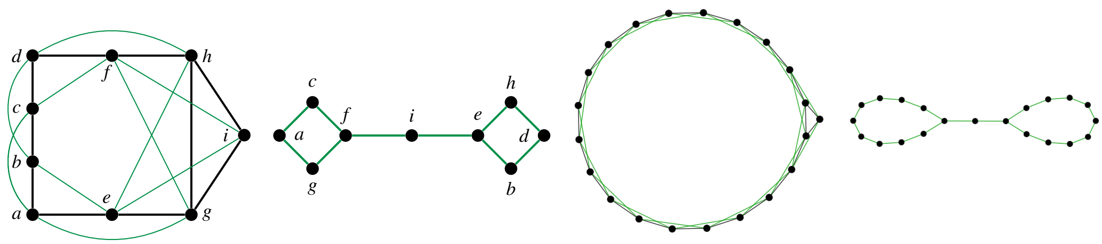

Fig. 5. These graphs exemplify Proposition 9 where $k = 4$ and $k = 10$. The left two graphs (drawn in order as G and then as G_2) have $\text{diam}(G) = 4$ and $\text{diam}(G_2) = 6$, where black edges denote $E(G)$ and green edges denote $E(G_2)$. The right two graphs have $\text{diam}(G) = 10$ and $\text{diam}(G_2) = 12$.

4. Computing Higher Order 2-distance Graphs

The use of brute-force to compute all 2-distance graphs is reliable up to 11 vertices, with results provided in Fig. 6. But, the run-time requirements increase exponentially beyond that. As it is apparent from the figure, graphs having $\text{diam}(G) = 2$ and $\text{diam}(G_2) = |V| - 1$ exist. For example, this property holds if G is the complement of a path that has $|V| \geq 4$.

Rather than using exhaustive search, 2-distance graphs with high $|V|$ can be computed with careful use of a SAT solver. In our implementation, we express $G = (V, E)$ and G_2 as adjacency matrices where True and False denote whether an edge exists. Henceforth, let $a_{i,j}$ be the (i, j)-th element in the adjacency matrix of G and let $b_{i,j}$ be the (i, j)-th element in the adjacency matrix of G_2. By definition,

$$b_{i,k} = \bigvee_j (a_{i,j} \wedge a_{j,k} \wedge \neg a_{i,k})$$

We fix $P_2 = \langle 0, 1, 2, 3, \ldots, k+1, k+2 \rangle$. Then, the first set of equations for the SAT solver fix the edges for P_2. That is, for all $b_{i,j} \in P_2$ we have $b_{i,j} = \text{True}$. For any $a, b \in P_2$, let $\mathscr{P}_{a,b,\ell}$ be the set of all a, b-paths of length ℓ in $(G_2 \setminus P_2) \cup \{a, b\}$. The set of equations that forbid shortcuts that would invalidate the diametral path P_2 can logically be expressed as

$$\bigwedge_{P \in \mathscr{P}_{a,b,\ell}} \neg\Big(\bigwedge_{(v,u) \in P} b_{v,u} \Big)$$

for all $\ell \leq |P_2|$. To eliminate the large number of isomorphic subgraphs in $\mathscr{P}_{a,b,\ell}$ in $H = G_2 \setminus P_2$, more edges can be fixed. Specifically, each nonisomorphic subgraph in H can be assigned its own satisfiability equation. Finally, an equation to eliminate the low-diameter $k = 2$ graphs is used, and is given by

$$\neg \bigwedge_{i,k} (a_{i,j} \wedge a_{j,k})$$

and means that if any path $\langle a_{i,j} a_{j,k} \rangle$ does not exist (i.e. $\mathrm{diam}(G) \neq 2$), then this expression will evaluate to True, and False otherwise.

After conversion of our logical equations to conjunctive normal form, we were able to perform an experiment restricted to $\mathrm{diam}(G_2) \geq 7$, $|V| = 13$, and $\mathrm{diam}(G) > 2$ (see Fig. 6). As opposed to the weeks required to exhaustively enumerate graphs on 13 vertices, we found results within one day.

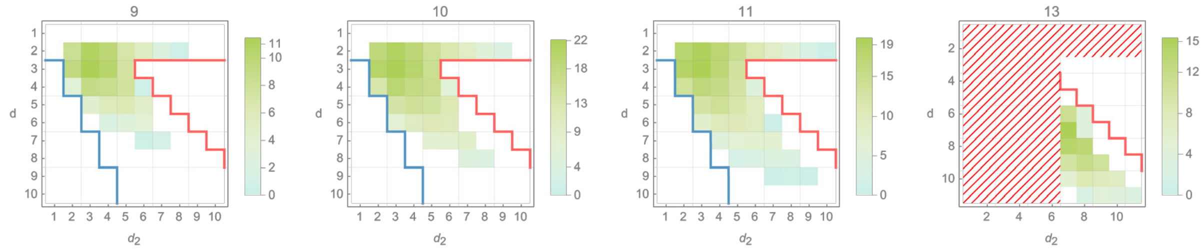

Fig. 6. Log scale plots showing the proportion of the diameters of G and G_2 where G belongs to the set of all graphs which are non-isomorphic, connected, and have fixed $|V|$. The top label corresponds to $|V|$. Axes labeled d and d_2 denote $\mathrm{diam}(G)$ and $\mathrm{diam}(G_2)$, respectively. The blue and red boundaries express the lower and upper bounds of the inequality from Theorem 8. The right-most plot demonstrates a large reduction in search space provided by our SAT equations for $|V| = 13$, allowing us to find 2-distance graphs that meet the sharp upper bound at $(d, d_2) = (6, 8)$ given by Theorem 8. The red region shows parameter ranges excluded by the equations.

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