

Diameter critical graphs

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Abstract

A graph is called diameter- k -critical if its diameter is k , and the removal of any edge strictly increases the diameter. In this paper, we prove several results related to a conjecture often attributed to Murty and Simon, regarding the maximum number of edges that any diameter- k -critical graph can have. In particular, we disprove a longstanding conjecture of Caccetta and Häggkvist (that in every diameter-2-critical graph, the average edge-degree is at most the number of vertices), which promised to completely solve the extremal problem for diameter-2-critical graphs.

On the other hand, we prove that the same claim holds for all higher diameters, and is asymptotically tight, resolving the average edge-degree question in all cases except diameter-2. We also apply our techniques to prove several bounds for the original extremal question, including the correct asymptotic bound for diameter- k -critical graphs, and an upper bound of $(\frac{1}{6} + o(1))n^2$ for the number of edges in a diameter-3-critical graph.

1 Introduction

An (x, y) -*path* is a path with endpoints x and y , and its *length* is its number of edges. We denote by $d_G(x, y)$ the smallest length of an (x, y) -path in a graph G , where we often drop the subscript if the graph G is clear from context. The *diameter* of G is the maximum of $d_G(x, y)$ over all pairs $\{x, y\}$. A graph G is said to be *diameter-critical* if for every edge $e \in G$, the deletion of e produces a graph $G - e$ with higher diameter.

The area of diameter-criticality is one of the oldest subjects of study in extremal graph theory, starting from papers of Erdős-Rényi [11], Erdős-Rényi-Sós [12], Murty-Vijayan [21], Murty [18–20], and Ore [22] from the 1960’s. Many problems in this domain were investigated, such as that of minimizing the number of edges subject to diameter and maximum-degree conditions (see, e.g., Erdős-Rényi [11], Bollobás [1, 2], Bollobás-Eldridge [3], Bollobás-Erdős [4]), controlling post-deletion diameter (Chung [8]), and vertex-criticality (Caccetta [5], Erdős-Howorka [9], Huang-Yeo [16], Chen-Füredi [7]), to name just a few.

The natural extremal problem of maximizing the number of edges (or equivalently, the average degree) in a diameter-critical graph also received substantial attention. Our work is inspired by the following long-standing conjecture of Ore [22], Plesník [23], Murty and Simon (see in [6]). A *diameter- k -critical* graph is a diameter-critical graph of diameter k .

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Conjecture 1.1. *For each n , the unique diameter-2-critical graph which maximizes the number of edges is the complete bipartite graph $K_{\lfloor n/2 \rfloor, \lceil n/2 \rceil}$.*

Successively stronger estimates were proved in the 1980's by Plesník [23], Caccetta-Häggkvist [6], and Fan [13], culminating in a breakthrough by Füredi [14], who used a clever application of the Ruzsa-Szemerédi (6,3) theorem to prove the exact (non-asymptotic) result for large n . As current quantitative bounds on the (6,3) theorem are of tower-type, the constraint on n is quite intense, and there is interest in finding an approach which is free of Regularity-type ingredients. For example, the recent survey by Haynes, Henning, van der Merwe, and Yeo [15] discusses recent work following a different approach based upon total domination, but we do not pursue that direction in this paper.

One hope for a Regularity-free method was proposed at around the origin of the early investigation. In their original 1979 paper, Caccetta and Häggkvist posed a very elegant stronger conjecture for a related problem, which would establish the extremal number of edges in diameter-2-critical graphs for all n . For an edge e , let its *edge-degree* $d(e)$ be the sum of the degrees of its endpoints, and let $\overline{d(e)}$ be the average edge-degree over all edges, so that in terms of the total number of edges m ,

$$\overline{d(e)} = \frac{1}{m} \sum_{uv \in E(G)} (d_u + d_v) = \frac{1}{m} \sum_{v \in V(G)} d_v^2.$$

Just as the Ore-Plesník-Murty-Simon problem sought to maximize the average vertex-degree over diameter-critical graphs, one can also ask to maximize the average edge-degree.

Conjecture 1.2. *(Caccetta-Häggkvist [6]; also see [14]) For any diameter-2-critical graph, the average edge-degree is at most the number of vertices.*

In terms of the numbers of vertices and edges (n and m), the conclusion of this conjecture is equivalent to:

$$\sum_v d_v^2 \leq nm.$$

Given the Caccetta-Häggkvist conjecture, Conjecture 1.1 then follows as an immediate consequence of convexity: $\sum d_v^2$ is at least n times the square of the average degree, and so Conjecture 1.2 implies that $nm \geq n(2m/n)^2$, giving $m \leq n^2/4$. In [6], Caccetta and Häggkvist proved the constant-factor approximation $\sum d_v^2 \leq \frac{6}{5}nm$, but there was no improvement for over three decades. Our first result indicates why: the Caccetta-Häggkvist conjecture is false. We demonstrate this by constructing a rich family of diameter-2-critical graphs, which may be of independent interest, as one challenge in the study of diameter-critical graphs is to find broad families of examples. (See our Constructions 2.1 and 2.2).

Theorem 1.3. *There is an infinite family of diameter-2-critical graphs for which*

$$\overline{d(e)} \geq \left(\frac{10}{9} - o(1) \right) n,$$

where $o(1)$ tends to 0 as n tends to infinity.

Since our construction opens a constant factor gap, this shows that the Caccetta-Häggkvist conjecture cannot be used to resolve the original problem. We were intrigued to study the best value of the constant multiplier on the Caccetta-Häggkvist conjecture, as it is a natural question in its own right, and proved that the $\frac{6}{5}$ factor from [6] was not sharp either.

Theorem 1.4. *There are absolute constants c and N such that for every diameter-2-critical graph with at least N vertices, the average edge-degree is at most $(\frac{6}{5} - c)$ times the number of vertices.*

On the other hand, it turns out that for all $k \geq 3$, the diameter- k -critical analogue of the Caccetta-Häggkvist conjecture holds precisely, and is tight.

Theorem 1.5. *For every diameter-critical graph with diameter at least 3, the average edge-degree is at most the number of vertices. This is asymptotically tight: for each fixed $k \geq 3$, there is an infinite family of graphs for which the average edge-degree is at least $(1 - o(1))$ times the number of vertices.*

As an immediate consequence, the earlier convexity argument proves that diameter-critical graphs with diameter at least 3 have at most $n^2/4$ edges, for all n . Regarding the maximum number of edges in diameter- k -critical graphs for $k \geq 3$, however, it was conjectured by Krishnamoorthy and Nandakumar [17] (who disproved an earlier conjecture of Caccetta and Häggkvist on this question) that a particular instance of the following construction is optimal (see Lemma 3.2 for a proof of diameter-criticality).

Construction 1.6. *Let a, b , and c be positive integers. Create a partition $V_0 \cup V_1 \cup \dots \cup V_k$ such that $|V_0| = a$, $|V_1| = |V_2| = \dots = |V_{k-1}| = b$ and $|V_k| = c$. Introduce edges by placing complete bipartite graphs between V_0 and V_1 , and between V_{k-1} and V_k , and placing b vertex-disjoint paths of length $k - 2$ from V_1 to V_{k-1} , each with exactly one vertex in V_i for every $1 \leq i \leq k - 1$.*

Krishnamoorthy and Nandakumar [17] observed that choosing $a = 1$, $b \approx \frac{n}{2(k-1)}$, and $c = n - a - b(k - 1)$ optimized the number of edges in this construction, yielding a total of $\frac{n^2}{4(k-1)} + o(n^2)$ edges. Our next result establishes a bound which deviates by an constant factor.

Theorem 1.7. *Every diameter- k -critical graph on n vertices has at most $\frac{3n^2}{k}$ edges.*

Finally, we investigated the case $k = 3$ in greater depth, as it is the first (asymptotically) unresolved diameter. The above construction produces a diameter-3-critical graph with $(\frac{1}{8} + o(1))n^2$ edges. We point out that there is a significantly different graph with the same asymptotic edge count: a clique $A := K_{n/2}$ together with a perfect matching (with $n/2$ edges) between A and its complement A^c . On the other hand, as observed above, our Theorem 1.5 immediately gives $n^2/4$ as an upper bound. We improve this to an intermediate value, and note that our proof applies in diameters greater than 3 as well (see remark at end of Section 6).

Theorem 1.8. *Every diameter-3-critical graph on n vertices has at most $\frac{n^2}{6} + o(n^2)$ edges.*

The rest of this paper is organized as follows. The next section contains constructions of families of diameter-2-critical graphs, which contain counterexamples to the Caccetta-Häggkvist conjecture. Section 3 resolves the Caccetta-Häggkvist conjecture for all diameters $k \geq 3$. In Section 4, we improve the upper bound on the diameter-2 Caccetta-Häggkvist result. Section 5 establishes an upper bound on the edge count for all diameters, which deviates by a constant factor (12) from all best known constructions. Finally, Section 6 proves a substantially stronger upper bound for the diameter-3 case.

Throughout our proofs, we will encounter and manipulate many paths. We will use ab to denote an edge, and abc , $abcd$, etc. to denote paths. If u and v are vertices of a path P , we will write uPv to denote the subpath of P with u and v as endpoints.

2 Diameter-2-critical constructions

In this section, we prove Theorem 1.3, by constructing a very rich family of diameter-2-critical graphs. Indeed, a major challenge in studying diameter-2-critical graphs is the lack of understanding of the menagerie of examples of such graphs. We proceed with a series of two constructions which give rise to a broad variety of examples.

Construction 2.1. *Let G be an arbitrary n -vertex graph for which both G and its complement have diameter at most 2. Create a new graph G' by taking two disjoint copies A and B of the set $V(G)$, placing an induced copy of G in A , placing an induced copy of the complement of G in B , and placing a perfect matching between A and B such that each edge in this matching joins a vertex in A to its copy in B . Then G' is diameter-2-critical.*

Proof. Select vertices $x \in A$ and $y \in B$ so that xy is not an edge of the perfect matching. Let $x' \in B$ and $y' \in A$ be the respective partners of x and y according to the perfect matching. Then, exactly one of $x'y$ and xy' is in G' , while xy is not, and thus distance between x and y is exactly 2. At the same time, vertices in the same part are at distance at most 2, since both G and its complement have diameter at most 2. Therefore, G' has diameter equal to 2.

Also, it is clear that upon deleting any matching edge xx' (where $x \in A$ and $x' \in B$), the distance between x and x' rises to at least 3. Deleting any edge xy in A increases the distance between x and y' above 2, where $y' \in B$ is the partner of $y \in A$, and so we conclude that G' is indeed diameter-2-critical. \square

At this point, although we can generate a wide variety of diameter-2-critical graphs, they do not yet bring $\sum d_v^2$ above nm . However, if one uses a very sparse graph G (with $o(n^2)$ edges) as the generator, one finds that $\sum d_v^2$ is asymptotically nm , while being very different from the balanced complete bipartite graph that also achieves that bound. As the balanced complete bipartite graph was quite a stable optimum, this second point creates the possibility for us to destabilize it. We exploit this by augmenting the construction with a third part.

Construction 2.2. *Let r be an arbitrary natural number, and let G be an n -vertex graph for which both G and its complement have diameter at most 2. Create G' from G as in Construction 2.1, and add a third disjoint set C of r vertices, with a complete bipartite graph between B and C . Then, the resulting $(2n + r)$ -vertex graph G'' is diameter-2-critical.*

Proof. We build upon our existing knowledge about G' . It is clear that each vertex of C is at distance at most 2 from every other vertex, and so G'' has diameter 2 as well. Also, the deletion of any edge yz with $y \in B$ and $z \in C$ would put z at distance greater than 2 from $y' \in A$ (the matching partner of $y \in B$). Therefore, G'' is diameter-2-critical, as claimed. \square

We build our counterexample to the Caccetta-Häggkvist conjecture by selecting suitable n and r , and using a sparse diameter-2 random graph G whose complement also has diameter 2. We saw that a property holds *asymptotically almost surely*, or a.a.s., if its probability tends to 1 as $n \rightarrow \infty$. The random graph $G_{n,p}$ is constructed by starting with n vertices, and taking each of the $\binom{n}{2}$ potential edges independently with probability p .

Lemma 2.3. *Let $2\sqrt{\frac{\log n}{n}} \leq p \leq 1 - 2\sqrt{\frac{\log n}{n}}$. Then, a.a.s., $G_{n,p}$ and its complement both have diameter at most 2, and all vertex degrees are at most $2np$.*

Proof. For any fixed pair of vertices, the probability that they have no common neighbors is exactly $(1 - p^2)^{n-2}$. A union bound over all pairs of vertices produces a total failure probability of at most $n^2 e^{-p^2(n-2)}$, which is clearly $o(1)$ because $p \geq 2\sqrt{\frac{\log n}{n}}$. Similarly, since $(1 - p) \geq 2\sqrt{\frac{\log n}{n}}$, we see that a.a.s., both $G_{n,p}$ and its complement have diameter at most 2. For the degrees, since a given vertex's degree is distributed as $\text{Bin}[n-1, p]$, the Chernoff inequality implies that the probability it exceeds $2np$ is at most $e^{-\Theta(np)}$, and another union bound over all vertices implies the result. \square

We are now ready to prove our first result, showing that there exist graphs which have $\sum d_v^2$ significantly greater than the product of their numbers of vertices and edges.

Proof of Theorem 1.3. Use $p = 2\sqrt{\frac{\log n}{n}}$ to create a random n -vertex graph G which satisfies the properties in Lemma 2.3. Use that in Construction 2.2 with $r = xn$ for some x . We will optimize the choice of x at the end. The total number of edges is then exactly $\binom{n}{2} + n + n(xn)$, because G and its complement together contribute exactly $\binom{n}{2}$ edges, the A - B matching contributes n edges, and $n(xn)$ edges come from the complete bipartite graph between B and C .

On the other hand, each vertex in B has degree at least $(1 - 2p)n + xn$, and each vertex in C has degree equal to n . Therefore, the sum of the squares of the vertex degrees is at least

$$(1 - o(1))n(1 + x)^2 n^2 + (xn)n^2 = (1 - o(1))n^3(1 + 3x + x^2).$$

The ratio between this and the product of the numbers of vertices and edges is at least

$$(1 - o(1)) \frac{n^3(1 + 3x + x^2)}{(2n + xn) \left(\frac{n^2 + n}{2} + xn^2 \right)} = (1 - o(1)) \frac{1 + 3x + x^2}{(2 + x) \left(\frac{1}{2} + x \right)}.$$

Substituting $x = 1$ gives a ratio of $\frac{10}{9} - o(1)$, proving Theorem 1.3, and it is easy to verify that this choice of x maximizes the final function on the right hand side. \square

3 Caccetta-Häggkvist for higher diameter

In this section, we prove Theorem 1.5, which resolves the analogue of the Caccetta-Häggkvist conjecture in diameters $k \geq 3$. The key concept which enables a number of our proofs is the following definition.

Definition 3.1. *In a graph G , an unordered vertex pair $\{x, y\}$ and an edge e are said to be k -associated if their distance $d_G(x, y)$ is at most k , but when e is deleted, their distance $d_{G-e}(x, y)$ becomes greater than k . A pair $\{x, y\}$ is called k -critical if there exists some edge e which is k -associated with $\{x, y\}$.*

Note that whenever an edge e is k -associated with a pair $\{x, y\}$, it immediately follows that e is part of every shortest path between x and y . When $k \geq 3$, there may be multiple shortest paths (all of the same length). It is convenient for us to have a single path to refer to for each $\{x, y\}$, and so for each k -critical pair $\{x, y\}$, we arbitrarily select one such shortest path and denote it P_{xy} . Let these P_{xy} be called *k -critical paths*. (We will have exactly one k -critical path per k -critical pair.) For each edge e , let $\mathcal{P}(e)$ be the set of all k -critical paths P_{xy} such that $\{x, y\}$ is k -associated with e . Observe that by the above, e is always on every $P_{xy} \in \mathcal{P}(e)$, and in diameter- k -critical graphs, $\mathcal{P}(e)$ is always nonempty.

In both this section and the next section, it will be useful to keep track of the 3-vertex subgraph statistics. For $0 \leq i \leq 3$, let \mathcal{T}_i be the set of unordered triples $\{x, y, z\}$ in $V(G)$ such that their induced subgraph $G[\{x, y, z\}]$ has exactly i edges. By counting the number of pairs (v, f) that vertex v is not incident to edge f , we see that

$$m(n-2) = 3|\mathcal{T}_3| + 2|\mathcal{T}_2| + |\mathcal{T}_1|, \quad (1)$$

which, together with the fact that

$$\sum_v \binom{d_v}{2} = 3|\mathcal{T}_3| + |\mathcal{T}_2|, \quad (2)$$

implies that

$$\sum_v d_v^2 - mn = 3|\mathcal{T}_3| - |\mathcal{T}_1|. \quad (3)$$

We are now ready to prove the diameter- k -critical analogue of the Caccetta-Häggkvist conjecture for $k \geq 3$.

Proof of Theorem 1.5, upper bound. Let G be a diameter k -critical graph with $k \geq 3$. Let $T = \{x, y, z\} \in \mathcal{T}_3$ be an arbitrary triangle in G . Writing xy to denote the edge with endpoints x and y , etc., select arbitrary $P_1 \in \mathcal{P}(xy)$, $P_2 \in \mathcal{P}(yz)$ and $P_3 \in \mathcal{P}(xz)$. We claim that P_1 , P_2 , and P_3 all have length k . Indeed, if, say, P_1 was a path of length at most $k-1$ from u to v via xy , then by using xz and zy instead of xy , we obtain an alternate path of length at most k , contradicting the k -association of xy and $\{u, v\}$.

The path P_1 contains an edge adjacent to xy . Without loss of generality, suppose that this edge is tx . It is clear that $t \neq z$. Label the endpoints of P_2 by u and v such that P_2 traverses u, y, z, v in that order. We claim that $t \notin P_2$. Indeed, if, say, $t \in uP_2y$, then since $t \neq y$, the

path uP_2txzP_2v has length at most k while avoiding the edge yz , contradicting the fact that $\{u, v\}$ is k -associated with yz . Thus $|V(P_2) \cup \{t\} \setminus T| \geq k$.

For each vertex $s \in V(P_2) \cup \{t\} \setminus T$, we choose an edge $f_s \in E(T)$ such that s and f_s form a triple $F_s \in \mathcal{T}_1$ as follows. For t , we have $ty \notin E(G)$ and $tz \notin E(G)$, as otherwise we could reroute P_1 between y and t either directly or via yzt , avoiding yx entirely, contradicting $P_1 \in \mathcal{P}(xy)$. So, the choice $f_t = yz$ produces $F_t = \{t, y, z\} \in \mathcal{T}_1$. For any $s \in V(P_2) \setminus T$ which is between u and y , clearly $sz \notin E(G)$. It also holds that $sx \notin E(G)$, as otherwise one could reroute P_2 via x to avoid yz , while maintaining length at most k . So $F_s := \{s, x, z\} \in \mathcal{T}_1$ by choosing $f_s = xz$. A similar argument handles the $s \in V(P_2) \setminus T$ which are between z and v .

The above argument actually showed that for the triple F_t , $f_t = yz$ and the edge xy was on all shortest paths between t and y . For every other triple F_s , either $f_s = xz$ and yz is on all shortest paths between s and z , or $f_s = xy$ and zy is on all shortest paths between s and y . In all of those cases, we have the property that

For any triple F_s , there exists an edge $f' \in E(T) - \{f_s\}$ such that f' is contained in all shortest (s, s') -paths, where $s' := V(f') \cap V(f_s)$.

Let $\mathcal{F}(T)$ be the collection of triples which arise in this way from T , i.e., $\mathcal{F}(T) = \{F_s : s \in V(P_2) \cup \{t\} \setminus T\}$. We claim that $\mathcal{F}(T) \cap \mathcal{F}(T') = \emptyset$ for distinct $T, T' \in \mathcal{T}_3$. To see this, assume for contradiction that it is not the case. Then there exists $\{s, x, y\} \in \mathcal{F}(T) \cap \mathcal{F}(T')$ for distinct triangles T, T' such that $xy \in E(G)$. As $xy \in E(T) \cap E(T')$ by definition, let $T := \{x, y, z\}$ and $T' := \{x, y, z'\}$ for distinct vertices z, z' . In light of the above observation, we may assume that xz is contained in all shortest (s, x) -paths, and yz' is contained in all shortest (s, y) -paths. Let P be a shortest (s, x) -path and P' be a shortest (s, y) -path, and assume without loss of generality that $|P| \leq |P'|$. Then $sPzy$ is an (s, y) -path of length $|P| \leq |P'|$ which does not contain yz' , a contradiction. This proves the claim.

Since $\mathcal{F}(T)$'s are disjoint subsets of \mathcal{T}_1 with at least k triples each, it follows that $|\mathcal{T}_1| \geq \sum_{T \in \mathcal{T}_3} |\mathcal{F}(T)| \geq k|\mathcal{T}_3| \geq 3|\mathcal{T}_3|$, completing the proof of the upper bound by (3). \square

For the other part of our Caccetta-Häggkvist-type result for diameter 3 and higher, we must construct graphs which asymptotically approach our bound. We do this by selecting specific parameters for Construction 1.6, and we include the following proof for completeness.

Lemma 3.2. *Construction 1.6 always produces a diameter- k -critical graph.*

Proof. We first verify that every pair of vertices $\{x, y\}$ has distance at most k . To see this, arbitrarily select vertices $u \in V_0$ and $v \in V_k$, allowing $\{u, v\}$ to possibly overlap with $\{x, y\}$. Observe that there is a path of length k from u to v which passes through x on the way, and a path of length k from v to u which passes through y on the way. Therefore, there is a closed walk (possibly repeating vertices or edges) from x back to itself via y , of length exactly $2k$, which implies that x and y are at distance at most k .

To verify criticality, we have two types of edges. Consider an edge xy in a matching, say with $x \in V_i$ and $y \in V_{i+1}$ where $1 \leq i \leq k-2$. If xy is deleted, then y can only reach V_0 by going all the way to V_k and then coming back, and so the distance between y and any vertex of V_0 rises above k . Now consider the other kind of edge xy , where $x \in V_0$ and $y \in V_1$, say. Let P be the unique path of length $k-2$ from V_1 to V_{k-1} with endpoint y , and let $y' \in V_{k-1}$ be the other endpoint of P . If edge xy is deleted, then one may verify that the distance between x and y' changes from $k-1$ to $k+1$, which completes our proof. \square

We now use Construction 1.6 to prove our lower bound on Caccetta-Häggkvist for diameter- k -critical graphs.

Proof of Theorem 1.5, lower bound. Let $k \geq 3$ be fixed. We build n -vertex graphs by using Construction 1.6 with $a = 1$, $b = 1$, and $c = n - k$. (We actually can select any sub-linear function $b = o(n)$, e.g., $b = \sqrt{n}$, to create a wider variety of asymptotically extremal constructions.) Then,

$$\sum_v d_v^2 = (1 + o(1))bn^2,$$

and the number of edges is $(1 + o(1))bn$, and so the ratio between $\sum d_v^2$ and the product of the numbers of vertices and edges indeed tends to 1 as $n \rightarrow \infty$. \square

4 Caccetta-Häggkvist upper bound for diameter 2

In this section, we prove Theorem 1.4, which improves the upper bound on the constant for the Caccetta-Häggkvist problem in the diameter-2 setting. Let c and N represent sufficiently small and sufficiently large absolute constants, respectively, throughout this section. We will make a series of claims which hold for large N and positive constants c_i , where $c_0 := c$ and c_i is a function of variables c_0, c_1, \dots, c_{i-1} tending to 0 as $c \rightarrow 0$. The eventual values of N and c_i can be explicitly calculated, although some of them will not be expressed in the proof to keep the main ideas clean.

Let G be an arbitrary diameter-2-critical graph with n vertices and m edges, where $n \geq N$. We will show that

$$\sum_{v \in V(G)} d_v^2 \leq \left(\frac{6}{5} - c\right) nm. \quad (4)$$

We use the notion of 2-critical paths from the beginning of Section 3, and following that section, we also define $\mathcal{P}(e)$ as the set of all 2-critical paths P_{xy} such that $\{x, y\}$ is 2-associated with the edge e . Since our diameter is always 2 in this section, we will write *associated* and *critical path* to refer to the concepts of 2-associated and 2-critical path.

Definition 4.1. Let $T \in \mathcal{T}_3$ be a triangle. We say that a vertex $v \notin T$ is a foot of T if there are some $x, y \in T$ such that the path vxy belongs to $\mathcal{P}(xy)$.

Lemma 4.2. Every triangle $T \in \mathcal{T}_3$ has at least 2 feet, and if v is a foot of T , then it is adjacent to exactly one vertex of T .

Proof. Consider any triangle $T := \{x, y, z\} \in \mathcal{T}_3$. For any edge (say xy) in T , every path $P \in \mathcal{P}(xy)$ must have length 2 (suppose it is $P = vxy$). Since the removal of xy is supposed to increase the distance between v and y above 2, we must have $vy, vz \notin E(G)$, as claimed. Now consider $\mathcal{P}(yz)$. This must contain a path of length 2, and the outside vertex cannot be v because v is adjacent to neither of $\{y, z\}$, so it produces another foot of T . \square

Definition 4.3. Given a triangle $T \in \mathcal{T}_3$, let $\mathcal{F}(T)$ be the collection of all triples $\{v, y, z\}$ in \mathcal{T}_1 where v is a foot of T , both y and z are in T , and v is not adjacent to either of $\{y, z\}$.

Lemma 4.4. For distinct triangles $T, T' \in \mathcal{T}_3$, $\mathcal{F}(T)$ and $\mathcal{F}(T')$ are disjoint.

Proof. Assume for contradiction that $\{v, y, z\} \in \mathcal{F}(T) \cap \mathcal{F}(T')$ such that $yz \in E(G)$. Then $T = \{x, y, z\}$ and $T' = \{x', y, z\}$ for distinct vertices x, x' . Without loss of generality, assume that vxy is a critical path in $\mathcal{P}(xy)$. However, $vx'y$ is also an (v, y) -path of length 2, which does not contain the edge xy , a contradiction. \square

Lemma 4.5. *Let \mathcal{T}_3^* be the set of triangles with at least three feet. To prove (4) and hence Theorem 1.4, it suffices to establish any one of the following two conditions:*

$$\text{(C1). } |\mathcal{T}_2| \geq \frac{5c}{2} \cdot nm \qquad \text{(C2). } |\mathcal{T}_3^*| \geq \frac{5c}{6} \cdot nm.$$

Proof. By Lemma 4.4 and Lemma 4.2, we have

$$|\mathcal{T}_1| \geq \sum_{T \in \mathcal{T}_3} |\mathcal{F}(T)| \geq 2|\mathcal{T}_3| + |\mathcal{T}_3^*|. \quad (5)$$

By (1) and (5), we see that

$$\begin{aligned} m(n-2) &= 3|\mathcal{T}_3| + 2|\mathcal{T}_2| + |\mathcal{T}_1| \\ mn &\geq 3|\mathcal{T}_3| + 2|\mathcal{T}_2| + (2|\mathcal{T}_3| + |\mathcal{T}_3^*|) + 2m \\ mn &\geq 5|\mathcal{T}_3| + |\mathcal{T}_3^*| + 2|\mathcal{T}_2| + 2m. \end{aligned} \quad (6)$$

Also, by doubling (2), we find

$$\begin{aligned} \sum_v d_v^2 - \sum_v d_v &= 6|\mathcal{T}_3| + 2|\mathcal{T}_2| \\ \sum_v d_v^2 &= 6|\mathcal{T}_3| + 2|\mathcal{T}_2| + 2m \\ \sum_v d_v^2 &\leq mn + |\mathcal{T}_3| - |\mathcal{T}_3^*|, \end{aligned} \quad (7)$$

where we used (6) for the last deduction.

Now suppose (C1) holds. Then by (6), we have $mn \geq 5|\mathcal{T}_3| + 5cnm$ and thus (7) implies that $\sum_v d_v^2 - nm \leq |\mathcal{T}_3| \leq (1/5 - c)nm$, giving (4). On the other hand, if (C2) holds, by (7) we have $\sum_v d_v^2 - nm \leq |\mathcal{T}_3| - \frac{5c}{6} \cdot nm$. To compare $|\mathcal{T}_3|$ with nm , we use (6) to obtain $nm \geq 5|\mathcal{T}_3| + \frac{5c}{6} \cdot nm$, and thus $\sum_v d_v^2 - nm \leq (1/5 - c)nm$, which again implies (4). \square

Our objective is now to show that at least one of (C1) and (C2) always holds, unless (4) holds directly. To this end, we first show that almost all edges have endpoints with similar neighborhoods. For the remainder of this section, we write $A\Delta B$ to denote the symmetric difference of sets A and B .

Lemma 4.6. *Define $c_1 := c^{1/4}$, and let \mathcal{E}_1 be the set of all edges uv such that $|N_u\Delta N_v| \leq c_1n$. If (C1) does not hold, then $|\mathcal{E}_1| \geq (1 - c_1)m$.*

Proof. Suppose on the contrary that there are at least c_1m edges uv satisfying $|N_u\Delta N_v| > c_1n$, but (C1) does not hold. Note that for any vertex $w \in N_u\Delta N_v$, the set $\{w, u, v\} \in \mathcal{T}_2$. Then $|\mathcal{T}_2| \geq \frac{(c_1m)(c_1n)}{2} > \frac{5c}{2} \cdot mn$, and so (C1) holds, contradiction. \square

Lemma 4.7. *Let \mathcal{E}_2 be the set of edges $uv \in \mathcal{E}_1$ such that u and v have at least $(1/2 + c_1)n$ common neighbors. If (C1) does not hold and neither does (4), then $|\mathcal{E}_2| \geq c_1m$.*

Proof. Suppose for contradiction that $|\mathcal{E}_2| < c_1m$. By Lemma 4.6, it holds that $|\mathcal{E}_1| \geq (1 - c_1)m$, and so, for sufficiently small constant c , we have

$$\begin{aligned} \sum_v d_v^2 &= \sum_{uv \in E(G)} (d_u + d_v) = \sum_{uv \in E(G)} (|N_u \Delta N_v| + 2|N_u \cap N_v|) \\ &\leq \sum_{uv \in \mathcal{E}_1} (c_1n + 2|N_u \cap N_v|) + \sum_{uv \notin \mathcal{E}_1} 2n \\ &\leq 3c_1mn + 2 \sum_{uv \in \mathcal{E}_2} |N_u \cap N_v| + 2 \sum_{uv \in \mathcal{E}_1 \setminus \mathcal{E}_2} |N_u \cap N_v| \\ &\leq 3c_1mn + 2c_1mn + 2m(1/2 + c_1)n = (1 + 7c_1)mn < \left(\frac{6}{5} - c\right)mn, \end{aligned}$$

that is, (4) holds, contradicting the assumption. \square

Lemma 4.8. *Define $c_2 := \sqrt{c}/4$. If (C1) does not hold, then $m \geq \frac{c_1}{2}n^2$ and $|\mathcal{E}_2| \geq c_2n^2$.*

Proof. Let H be the subgraph of G spanned by the edges of \mathcal{E}_2 , and let $h = |V(H)|/n$. Note that for $v \in V(H)$, $d_G(v) \geq (1/2 + c_1)n$. If $h \geq \frac{1}{4}$, then $m \geq \frac{1}{2} \sum d_G(v) \geq \frac{n^2}{16}$ and thus by Lemma 4.7, $|\mathcal{E}_2| \geq c_1m \geq \frac{c_1}{16}n^2 > c_2n^2$ as desired.

It remains to consider $h < \frac{1}{4}$. Every $v \in V(H)$ has at least $(1/2 + c_1 - h)n$ neighbors out of $V(H)$, implying that $m \geq |V(H)| \cdot (1/2 + c_1 - h)n = h(1/2 + c_1 - h)n^2$. Using Lemma 4.7, we find $\frac{(hn)^2}{2} \geq |\mathcal{E}_2| \geq c_1m \geq c_1h(1/2 + c_1 - h)n^2$, which shows that $(h - c_1)(1 + 2c_1) \geq 0$. Thus $\frac{1}{4} > h \geq c_1$, implying that $m \geq \frac{c_1}{4}n^2$ and $|\mathcal{E}_2| \geq c_1^2n^2/4 = c_2n^2$. \square

Lemma 4.9. *Define $c_3 := 40\sqrt{c}$. If (C1) does not hold, then there exists an edge $uv \in \mathcal{E}_2$ such that $N_u \cap N_v$ induces at least $(1 - c_3) \binom{|N_u \cap N_v|}{2}$ edges.*

Proof. By Lemma 4.8, there exists a matching M with edges from \mathcal{E}_2 of size at least $\frac{c_2}{2}n$. Suppose for contradiction that for every edge $uv \in M$, $N_u \cap N_v$ has at least $c_3 \binom{|N_u \cap N_v|}{2}$ non-adjacent pairs. Note that any non-adjacent pair $\{x, y\}$ in $N_u \cap N_v$ contributes two triples $\{u, x, y\}$ and $\{v, x, y\}$ to \mathcal{T}_2 . Therefore, we see that

$$|\mathcal{T}_2| \geq 2c_3 \binom{(1/2 + c_1)n}{2} |M| \geq \frac{c_2c_3}{8}n^3 \geq \frac{c_2c_3}{4}mn \geq \frac{5c}{2}mn,$$

that is, (C1) holds. \square

Lemma 4.10. *Define $c_4 := \sqrt{40}c^{1/4}$, suppose (C1) does not hold, and let uv be the edge from Lemma 4.9. Then $G[N_u \cap N_v]$ has an induced subgraph D with at least $(1/2 - c_4)n$ vertices and minimum degree at least $(1 - c_4)|D|$.*

Proof. Start with $D = G[N_u \cap N_v]$. As long as D has a vertex of degree less than $(1 - \sqrt{c_3})|D|$, delete it. At every stage of this procedure, $\sqrt{c_3}|D| \cdot (|N_u \cap N_v| - |D|)$ is at most the number of non-adjacent pairs in $N_u \cap N_v$. Our assumption on uv from Lemma 4.9 then implies that

$$\sqrt{c_3}|D| \cdot (|N_u \cap N_v| - |D|) \leq \frac{c_3}{2}|N_u \cap N_v|^2$$

must hold throughout the process. It is clear that this holds when $D = N_u \cap N_v$, and since the function $f(x) = x(M - x)$ is a downward-opening parabola, the process must stop well before D reaches $\frac{1}{2}|N_u \cap N_v|$. So, throughout the process,

$$\begin{aligned} \sqrt{c_3} \frac{|N_u \cap N_v|}{2} \cdot (|N_u \cap N_v| - |D|) &\leq \frac{c_3}{2} |N_u \cap N_v|^2 \\ |N_u \cap N_v| - |D| &\leq \sqrt{c_3} |N_u \cap N_v|, \end{aligned}$$

and we conclude that at the end, $|D| \geq (1 - \sqrt{c_3}) |N_u \cap N_v| \geq (1/2 - c_4) \cdot n$. \square

Definition 4.11. Let D be the subgraph produced by Lemma 4.10. For each edge $e \in E(D)$, since the endpoints of e form a triangle with u , there exists a path of length 2 in $\mathcal{P}(e)$, say $x'xy$ where $xy = e$, $x' \notin D$, and $x'y \notin E(G)$. We call any such x' an arm of edge e . Define the digraph \vec{D} on $V(D)$ as follows: for any edge $xy \in E(D)$, we place a directed edge from y to x to \vec{D} whenever xy has an arm x' such that $xx' \in E(G)$.

Note that each edge in D can produce either one or both directed edges in \vec{D} , i.e., between each pair of vertices, there can be zero, one, or two directed edges.

Lemma 4.12. Define $c_5 := 5\sqrt{c_4}$, and suppose (C1) does not hold. Let S be the set of vertices in \vec{D} with in-degree at least $4c_4|D|$. Then, for large $n \geq N$, $|S| > (1/2 - c_5)n$.

Proof. Let S^c be the complement of S in $V(D)$ and let $s = |S^c|/n$. Let $d^-(v)$ denote the in-degree of v in \vec{D} . By Lemma 4.10, the number of non-adjacent pairs in \vec{D} is less than $\frac{c_4}{2}|D|^2$, thus

$$\binom{sn}{2} - \frac{c_4}{2}|D|^2 \leq e(\vec{D}[S^c]) \leq \sum_{v \in S^c} d^-(v) \leq 4c_4|D| \cdot sn.$$

Thus, for large $n \geq N$, we have $\frac{s^2}{2} \leq \frac{c_4}{2} + 4c_4s + \frac{s}{2n} < 5c_4$, implying that $s < 4\sqrt{c_4}$. By Lemma 4.10 again, we see $|S| = |D| - |S^c| \geq (1/2 - c_4 - 4\sqrt{c_4})n > (1/2 - c_5)n$. \square

Definition 4.13. For each $x \in S$ and $x' \notin V(D)$ satisfying $xx' \in E(G)$, define $A_{x'}(x)$ to be the set of all vertices $y \in V(D)$ such that $x'xy \in \mathcal{P}(xy)$. We say $x \in S$ is rich if there exists some $x' \notin V(D)$ such that $|A_{x'}(x)| \geq 2c_4|D|$.

Observe that since any edge $\vec{y}\vec{x} \in \vec{D}$ has an arm $x' \notin V(D)$ such that $x'xy \in \mathcal{P}(xy)$, the union $\bigcup_{x'} A_{x'}(x)$ is just the in-neighborhood $N^-(x)$ of x in \vec{D} , which is of at least $4c_4|D|$ by Lemma 4.12.

Lemma 4.14. Suppose (C1) does not hold, and let X be the set of rich vertices in S . Then $|X| \geq (1 - \sqrt{c})|S|$ or (C2) holds.

Proof. Suppose for contradiction that there are at least $\sqrt{c}|S|$ vertices $x \in S$ such that $|A_{x'}(x)| < 2c_4|D|$ for every $x' \notin V(D)$ adjacent to x . Fix such a vertex x . Consider any $y \in N^-(x)$, say $y \in A_{x_1}(x)$ for $x_1 \notin V(D)$. By Lemma 4.10, y is non-adjacent at most $c_4|D|$ vertices in D . Since $|N^-(x)| \geq 4c_4|D|$ (by Lemma 4.12), we see that there are more than $c_4|D|$ vertices $y' \in N^-(x) \setminus A_{x'}(x)$ such that $yy' \in E(D)$.

We need the following property: for distinct $x_1, x_2 \notin V(D)$,

$$\text{If } y_1 \in A_{x_1}(x) \text{ and } y_2 \in A_{x_2}(x) \text{ such that } y_1y_2 \in E(D), \text{ then } \{y_1, y_2, x\} \in \mathcal{T}_3^*. \quad (8)$$

To see this, it is clear that $\{y_1, y_2, x\}$ is in \mathcal{T}_3 and x_1, x_2 are two feet of it; we can find a third foot of $\{y_1, y_2, x\}$ by considering the edge y_1y_2 .

By (8), every such $\{y, y', x\} \in \mathcal{T}_3^*$, and there are at least $\frac{1}{2}|N^-(x)| \cdot c_4|D|$ pairs $\{y, y'\}$. Thus, for every such vertex x , there are at least $\frac{1}{2}|N^-(x)| \cdot c_4|D| > (c_4|D|)^2$ triples in \mathcal{T}_3^* which contain x . So, by Lemmas 4.10 and 4.12, we have

$$|\mathcal{T}_3^*| \geq \frac{1}{3} \cdot \sqrt{c}|S| \cdot (c_4|D|)^2 > \frac{1}{3}\sqrt{c}(1/2 - c_5)c_4^2(1/2 - c_4)^2n^3 \geq \frac{\sqrt{c}}{13} \cdot c_4^2mn > \frac{5c}{6} \cdot mn,$$

that is, (C2) holds. \square

Lemma 4.15. *Suppose (C1) and (C2) do not hold. For each vertex $x \in X$, choose and fix an adjacent vertex $x' \notin V(D)$ for which $|A_{x'}(x)| \geq 2c_4|D|$. Then, every such x' is not adjacent to any vertex in its corresponding $X \setminus \{x\}$.*

Proof. Suppose for contradiction that x' is adjacent to some $y \in X \setminus \{x\}$. By Lemma 4.10, y is non-adjacent to at most $c_4|D|$ vertices in D . Thus there exists some vertex $z \in A_{x'}(x)$ such that $yz \in E(D)$. Then zyx' is a (z, x') -path not containing edge zx . On the other hand, $z \in A_{x'}(x)$ implies that $zxx' \in \mathcal{P}(zx)$, a contradiction. \square

We are now ready to combine all of the above steps to complete the proof of our improved upper bound for the diameter-2-critical Caccetta-Häggkvist conjecture.

Proof of Theorem 1.4. Let Y be the set of all x' as defined in Lemma 4.15. Note that by construction, Y is disjoint from X , and by that lemma, the bipartite subgraph $G[X, Y]$ induces a perfect matching, so

$$|Y| = |X| > (1 - \sqrt{c})(1/2 - c_5)n > (1/2 - 20c^{1/8})n.$$

Let $Z = V(G) \setminus (X \cup Y)$, and define t such that $|X| = |Y| = (1/2 - t)n$ and $|Z| = 2tn$ for some $0 \leq t \leq 20c^{1/8}$. Then for every $x \in X$, by Lemma 4.10, we have that

$$(1/2 - 10c^{1/4})n < (1 - c_4)(1/2 - c_4)n \leq d_G(x) \leq (1/2 + t)n.$$

So the total number of edges satisfies

$$\begin{aligned} m &\geq \frac{1}{2} \sum_{x \in X} d_G(x) + e(Y) \\ &\geq \frac{1}{2} \left(\frac{1}{2} - 10c^{1/4} \right) \left(\frac{1}{2} - t \right) n^2 + e(Y) \\ &\geq \left(\frac{1}{8} - 10c^{1/8} \right) n^2 + e(Y). \end{aligned}$$

Also, since every vertex in X or Y has degree at most $(1/2 + t)n$,

$$\begin{aligned}
\sum_v d_v^2 &\leq |X| \left(\frac{1}{2} + t\right)^2 n^2 + |Z|n^2 + \left(\frac{1}{2} + t\right) n \sum_{y \in Y} d_y \\
&= \left(\left(\frac{1}{2} - t\right) \left(\frac{1}{2} + t\right)^2 + 2t \right) n^3 + \left(\frac{1}{2} + t\right) n \cdot (2e(Y) + e(X, Y) + e(Y, Z)) \\
&\leq \left(\left(\frac{1}{2} - t\right) \left(\frac{1}{2} + t\right)^2 + 2t \right) n^3 + (1 + 2t)n \cdot e(Y) + \left(\frac{1}{2} + t\right) n \cdot \left(\frac{1}{2} - t\right) n \cdot (1 + 2tn) \\
&\leq \left(\frac{1}{8} + 4t + \frac{1}{4n}\right) n^3 + (1 + 2t)n \cdot e(Y),
\end{aligned}$$

where $t \leq 20c^{1/8}$. Therefore, it is clear that by choosing c sufficiently small and N sufficiently large, given $n \geq N$, we will have

$$\sum_v d_v^2 \leq \left(\frac{6}{5} - c\right) mn,$$

completing the proof. \square

5 Asymptotics for maximizing edges

Construction 1.6 established a family of diameter- k -critical graphs with $\frac{n^2}{4(k-1)} + o(n^2)$ edges. In this section, we show that estimate is tight up to a constant factor by proving Theorem 1.7, which upper-bounds the number of edges by $\frac{3n^2}{k}$.

Let $k \geq 2$ be fixed throughout this section. Recall from Definition 3.1 that an unordered pair $\{x, y\}$ and edge e are k -associated if the distance between x and y is at most k , but rises above k if e is deleted. In such a situation, if P is an (x, y) -path of length at most k , we also say that P and e are k -associated.

Lemma 5.1. *Let G be a diameter- k -critical graph. For any edge e , there exists a path P of length $\lceil \frac{k}{3} \rceil$ such that e is $\lceil \frac{k}{3} \rceil$ -associated with P .*

Proof. For any edge e , since G is diameter- k -critical, there exists a pair $\{u, v\}$ such that $d_G(u, v) \leq k$ and $d_{G-e}(u, v) > k$. Let L be a shortest (u, v) -path. If L has length at least $\lceil \frac{k}{3} \rceil$, then we can choose vertices $x, y \in V(L)$ such that $e \in xLy$ and xLy has length $\lceil \frac{k}{3} \rceil$. We claim that e and xLy are $\lceil \frac{k}{3} \rceil$ -associated. Indeed, if not, then there must exist an (x, y) -path M in $G - e$ of length at most $\lceil \frac{k}{3} \rceil$, and one can use M and L together to construct a path of length at most k from u to v avoiding e , contradiction.

It thus suffices to consider the case when L has length at most $\lceil \frac{k}{3} \rceil - 1$. Write $e = ab$ and consider the depth-first-search tree T with root a . We see that the depth of T is at least $\lceil \frac{k}{2} \rceil$, as otherwise $d_G(s, t) \leq d_G(a, s) + d_G(a, t) \leq 2(\lceil \frac{k}{2} \rceil - 1) < k$ for all pairs $\{s, t\}$, contradicting the fact that G has diameter k . Thus there exists a path P' from the root a to some vertex, say z , such that P' has length $\lceil \frac{k}{3} \rceil$. We define $P := P'$ if $e \in P'$ and $P := P' \cup \{e\} - z$ otherwise. Note that P is a path of length $\lceil \frac{k}{3} \rceil$, satisfying $e \in P$.

We will show that e is $\lceil \frac{k}{3} \rceil$ -associated with P . Let x, y be the endpoints of P . Suppose on the contrary that $\{x, y\}$ and e are not $\lceil \frac{k}{3} \rceil$ -associated; then there exists an (x, y) -path Q in $G - e$ such that $|Q| \leq \lceil \frac{k}{3} \rceil$. Then, by combining P and Q , we find that there is a walk of length at most $2\lceil \frac{k}{3} \rceil - 1$ from one endpoint of e , to x , to y , and then to the other endpoint of e , completely avoiding e . Therefore, if we follow L from u to the nearest endpoint of e , and then take this e -avoiding walk to the other endpoint of e , and finish along L to v , we find an e -avoiding walk from u to v of length at most $3\lceil \frac{k}{3} \rceil - 2 \leq k$. This contradicts $d_{G-e}(u, v) > k$, and completes the proof. \square

We are now ready to show that every diameter- k -critical graph has at most $\frac{3n^2}{k}$ edges.

Proof of Theorem 1.7. Consider an arbitrary diameter- k -critical graph G . Let us say that a pair $\{x, y\}$ and an edge e are *matched* in G if e is incident to at least one of x, y and all shortest (x, y) -paths contain e . We will estimate the number N of pairs $(\{x, y\}, e)$ such that $\{x, y\}$ and $e \in E(G)$ are matched in G .

By the definition, it is clear that any pair $\{x, y\}$ can only match at most two edges, implying that $N \leq 2\binom{n}{2} \leq n^2$. On the other hand, by Lemma 5.1, any edge ab is $\lceil \frac{k}{3} \rceil$ -associated with a path P of length $\lceil \frac{k}{3} \rceil$. Without loss of generality, suppose that P is an (x, y) -path such that x, a, b, y appear on P in order, where possibly $x = a$ or $b = y$. Then for any vertex $z \in xPa$, the edge ab is matched with $\{z, b\}$, and for any vertex $z \in bPy$, the edge ab is matched with $\{a, z\}$. This shows that every edge is matched with at least $|V(P)| - 1 = \lceil \frac{k}{3} \rceil$ many pairs, implying $\frac{k}{3}e(G) \leq N \leq n^2$ and therefore $e(G) \leq \frac{3n^2}{k}$. \square

6 Diameter 3

Throughout this section, let G be a diameter-3-critical graph on n vertices. We will prove that G has at most $\frac{n^2}{6} + o(n^2)$ edges. Since we will work exclusively with diameter-3 graphs, let us simply say that a pair $\{x, y\}$ of vertices and an edge e are *associated* if $d_G(x, y) \leq 3$ and $d_{G-e}(x, y) \geq 4$. Similarly, say that a pair $\{x, y\}$ is *critical* if there exists some edge e associated with $\{x, y\}$. For any critical pair $\{x, y\}$, we arbitrarily select one of the (x, y) -paths of the smallest length to be P_{xy} , its corresponding *critical path*. We refer to a critical pair $\{x, y\}$ and its corresponding critical path P_{xy} interchangeably, i.e., we also say e is associated with P_{xy} if e is associated with $\{x, y\}$. Note that P_{xy} must be of length at most 3 and contain all edges associated with $\{x, y\}$.

For every edge e , let $\mathcal{P}_1(e)$ be the set containing all critical paths P_{xy} associated with e . Since G is diameter 3-critical, $\mathcal{P}_1(e) \neq \emptyset$ for every edge e . A pair $\{x, y\}$ is *2-critical* if there exists a unique (x, y) -path of length at most 2, and such a path is also called *2-critical*. For every edge e , let $\mathcal{P}_2(e)$ be the set of all 2-critical paths containing e . The *multiplicity* of an edge e is defined as $m(e) := |\mathcal{P}_1(e)| + |\mathcal{P}_2(e)|$.

6.1 Critical paths with all edges associated

Let \mathcal{P} be the set of all critical paths P_{xy} that are associated with at least 2 edges. Since every (x, y) -path of length at most 3 must then contain those 2 edges, and P_{xy} has length at most 3, every edge in P_{xy} must actually be associated with P_{xy} , and thus P_{xy} is the unique (x, y) -path

of length at most 3. For a positive integer t , let \mathcal{P}_t be the set of all critical paths in \mathcal{P} with length 3, where the middle edge has multiplicity at least t and the two non-middle edges each have multiplicity less than t .

Inspired by the proof of Füredi [14] for the diameter-2 case, we use the “(6, 3)” theorem of Ruzsa and Szemerédi [24] to show that $|\mathcal{P}_t|$ is a lower order term compared to n^2 . Recall that a *3-uniform hypergraph* H is a pair $(V(H), E(H))$, where the *edge-set* $E(H)$ is a collection of 3-element subsets of $V(H)$, each of which is called a *3-edge*. H is *linear* if any two distinct 3-edges share at most one vertex. In a linear 3-uniform hypergraph, three 3-edges form a *triangle* if they form a structure isomorphic to $\{\{1, 2, 3\}, \{3, 4, 5\}, \{5, 6, 1\}\}$. Let $\text{RSz}(n)$ be the maximum number of 3-edges in a triangle-free, linear 3-uniform hypergraph on n vertices.

Theorem 6.1. (*Ruzsa and Szemerédi [24]*) $\text{RSz}(n) = o(n^2)$.

The proof of the following lemma parallels Füredi’s, differing mainly at the definition of the auxiliary hypergraph. We write out the proof for completeness.

Lemma 6.2. *For each positive integer t , $|\mathcal{P}_t| \leq 54t \cdot \text{RSz}(n)$.*

Proof. Consider a path $P_{xy} := xaby$ in \mathcal{P}_t . By definition, multiplicities $m(xa) < t$, $m(ab) \geq t$, $m(by) < t$, and edges xa, ab, by are all associated with P_{xy} , implying that xab and aby are 2-critical paths. Define the 3-uniform hypergraph H_1 such that $V(H_1) := V(G)$, and form the edge-set $E(H_1)$ by arbitrarily choosing exactly one of $\{x, a, y\}$ and $\{x, b, y\}$ for each path $xaby$ in \mathcal{P}_t , so that $|E(H_1)| = |\mathcal{P}_t|$. For a 3-edge $\{x, a, y\} \in E(H_1)$ obtained from the path $P_{xy} = xaby \in \mathcal{P}_t$, we call vertices a and x the *center* and *handle* of this 3-edge, respectively.

We claim that the number of 3-edges of H_1 intersecting $\{x, a, y\}$ in 2 elements is at most $2t - 2$. To see this, first observe that the critical pair $\{x, y\}$ does not appear in any other 3-edges of H_1 . Since $m(xa) < t$, edge xa (and hence the pair $\{x, a\}$) is contained in fewer than t critical paths in \mathcal{P} , implying that the number of 3-edges of H_1 containing $\{x, a\}$ is fewer than t . Also note that aby is 2-critical, so if $\{a, y\}$ is contained in some 3-edge of H_1 then aby (and in particular $\{b, y\}$) must be contained in the corresponding path in \mathcal{P}_t , but $\{b, y\}$ is contained in fewer than t paths in \mathcal{P}_t as $m(by) < t$. Therefore, the number of 3-edges of H_1 containing $\{a, y\}$ is at most $t - 1$, completing the proof of the claim.

We use a greedy algorithm to construct a linear 3-uniform hypergraph H_2 from H_1 as follows. Initially set $V(H_2) := V(G)$, $E(H_2) := \emptyset$ and $A := E(H_1)$. In each coming iteration, if A is empty, then stop; otherwise, choose a 3-edge $\{x, a, y\} \in A$, move it to $E(H_2)$ and then delete all 3-edges in A which intersect $\{x, a, y\}$ in 2 elements. When it ends, we obtain a linear 3-uniform hypergraph H_2 such that

$$|E(H_2)| \geq \frac{|E(H_1)|}{2t} = \frac{|\mathcal{P}_t|}{2t}. \quad (9)$$

A r -uniform hypergraph H is called *r -partite* if there is a partition $V(H) = V_1 \cup V_2 \cup \dots \cup V_r$ such that for each $e \in E(H)$ it holds for all $1 \leq i \leq r$ that $|e \cap V_i| = 1$. By randomly and independently placing each vertex into one of 3 parts, a simple expectation argument shows that there exists a 3-partite linear 3-uniform hypergraph H_3 with parts V_1, V_2, V_3 such that $V(H_3) = V(H_2)$, $E(H_3) \subset E(H_2)$ and

$$|E(H_3)| \geq \frac{3!}{3^3} |E(H_2)|. \quad (10)$$

Without loss of generality, we may assume that at least $1/6$ of the 3-edges of H_3 have center in V_2 and handle in V_1 . So there exists a spanning subhypegraph H_4 of H_3 satisfying

$$|E(H_4)| \geq \frac{1}{6}|E(H_3)| \quad (11)$$

and the property that if $\{v_1, v_2, v_3\}$ is a 3-edge of H_4 with $v_i \in V_i$, then it must be obtained from the critical path $v_1v_2vv_3 \in \mathcal{P}_t$, for some vertex v . By (9)–(11), we see

$$|\mathcal{P}_t| \leq 54t \cdot |E(H_4)|.$$

To complete the proof, it suffices to show that H_4 has no triangles. Suppose, on the contrary, that three 3-edges T_1, T_2, T_3 of H_4 form a triangle. Since H_4 is linear, we must have $|T_1 \cup T_2 \cup T_3| = 6$. It also holds for each $1 \leq i \leq 3$ that $|V_i \cap (T_1 \cup T_2 \cup T_3)| = 2$, as otherwise there is a common vertex in all of 3-edges. Let $V_i \cap (T_1 \cup T_2 \cup T_3) = \{a_i, b_i\}$. Without loss of generality, we may assume $T_1 \cap T_2 \cap V_1 = \{a_1\}$ such that $T_1 = \{a_1, a_2, a_3\}$ and $T_2 = \{a_1, b_2, b_3\}$. By symmetry, the only case to consider is $T_3 = \{b_1, a_2, b_3\}$. Then the construction of H_4 ensures that $a_1a_2 \in E(G)$ and there are critical paths $P_{a_1b_3} := a_1b_2ub_3$ and $P_{b_1b_3} := b_1a_2vb_3$ in \mathcal{P}_t for some u and v . Clearly $a_1a_2vb_3$ is an (a_1, b_3) -path of length 3 distinct from $P_{a_1b_3}$. But $P_{a_1b_3}$ should be the unique (a_1, b_3) -path of length at most 3 because $P_{a_1b_3} \in \mathcal{P}$. This contradiction finishes the proof. \square

6.2 Covering by critical paths

The key innovation in our proof for the diameter-3 case is a delicate accounting of critical paths and edges. We will construct a family \mathcal{F} of critical paths such that

$$\text{every edge in } G \text{ is associated with at least one path in } \mathcal{F}. \quad (12)$$

This family will be obtained by an iterative greedy algorithm. In the i -th iteration, we will enlarge \mathcal{F} by adding one or two critical paths that are selected according to several prescribed rules (see the algorithm below). We define the set $P(i)$ to keep track of the critical paths added in the i -th iteration, and for bookkeeping purposes, we also define sets $P^2(i)$ of some 2-critical paths relevant for the i -th iteration.

During this process, we also maintain an *unsettled set* U which contains edges of G not “essentially” contained in those paths in \mathcal{F} . Let us give the formal definition for U . We have $|\mathcal{P}_1(e)| \geq 1$ for every $e \in E(G)$, as G is diameter-3-critical, and thus it is possible that e is associated with several critical paths of \mathcal{F} added in different iterations. We say edge e is *settled* in iteration i , if i is the first iteration which adds one critical path associated with the edge e . Note that given an edge settled in i , that edge could be contained in some critical path added by previous iterations. Throughout the process, U is defined to be the up-to-date set consisting of all edges which are not settled yet. We define types for edges in U as follows. An edge $e \in U$ is of:

Type 1: if there exists a critical path $P \in \mathcal{P}_1(e)$ which contains at least two associated edges (including e) in U .

Type 2: if it is not of type 1 and there exists a critical path $Q \in \mathcal{P}_1(e)$ such that $|Q| = 3$ and e is the middle edge of Q .

Type 3: if its type is not in $\{1, 2\}$ and there exists some edge $f \in U$ such that e and f induce a 2-critical path.

Type 4: if its type is not in $\{1, 2, 3\}$ and there exists a critical path $R \in \mathcal{P}_1(e)$ such that $|R| = 3$ and e is not the middle edge of R .

Type 5: if its type is not in $\{1, 2, 3, 4\}$ and there exists a critical path in $\mathcal{P}_1(e)$ of length two.

Type 6: if its type is not in $\{1, 2, 3, 4, 5\}$. Note that if e is of type 6, then we must have $\mathcal{P}_1(e) = \{e\}$.

We now describe the greedy algorithm. Initially, set $\mathcal{F} := \emptyset$ and $U := E(G)$; we iterate until $U = \emptyset$. In the i -th iteration, let t_i be the smallest type that the edges in U have. (Note that when $t_i \geq 2$, $\mathcal{P}_1(e) \cap \mathcal{P}_1(f) = \emptyset$ for any $e, f \in U$.) We split into cases based upon the value of t_i :

- (C1). If $t_i = 1$, choose a critical path P_{xy} which contains at least two associated edges in U . Add P_{xy} to \mathcal{F} , update U by deleting all associated edges of P_{xy} , and then let $P(i) := \{P_{xy}\}$ and $P^2(i) := \{P_{xy} - x, P_{xy} - y\}$.
- (C2). If $t_i = 2$, choose an edge $e \in U$ and a critical path $P_{xy} \in \mathcal{P}_1(e)$ of length three such that e is the middle edge of P_{xy} . Add P_{xy} to \mathcal{F} , delete e from U , and let $P(i) := \{P_{xy}\}$ and $P^2(i) := \{P_{xy} - x, P_{xy} - y\}$.
- (C3). If $t_i = 3$:
 - (C3-1). If there exist $e, f \in U$ such that the path $P := e \cup f$ is in $\mathcal{P}_1(e)$, then choose a critical path $P' \in \mathcal{P}_1(f)$, add P, P' to \mathcal{F} , delete e, f from U , and let $P(i) := \{P, P'\}$ and $P^2(i) := \emptyset$. If there are multiple choices for e, f , choose one that maximizes $|P| + |P'|$.
 - (C3-2). Otherwise, choose edges $e, f \in U$ and critical paths $P \in \mathcal{P}_1(e), P' \in \mathcal{P}_1(f)$ such that $e \cup f$ is a 2-critical path. Add P, P' to \mathcal{F} , delete e, f from U , and let $P(i) := \{P, P'\}$ and $P^2(i) := \{e \cup f\}$.
- (C4). If $t_i = 4$, choose an edge $e \in U$ and a path $P_{xy} \in \mathcal{P}_1(e)$ of length three such that e is incident to x but not y . Add P_{xy} to \mathcal{F} , delete e from U , and let $P(i) := \{P_{xy}\}$ and $P^2(i) := \{P_{xy} - y\}$.
- (C5). If $t_i = 5$, choose an edge $e \in U$ and a path $P \in \mathcal{P}_1(e)$ of length two. Add P to \mathcal{F} , delete e from U , and let $P(i) := \{P\}$ and $P^2(i) := \{e\}$.
- (C6). If $t_i = 6$, then all edges in U are critical paths of length one. Choose any $e \in U$, add e to \mathcal{F} , delete e from U , and let $P(i) := \{e\}$ and $P^2(i) := \emptyset$.

When the algorithm stops, the obtained family \mathcal{F} clearly satisfies the property (12). In each iteration, at least one edge is deleted from U and thus settled, and one or two critical paths are added to \mathcal{F} . We also observe that for every edge e , as the algorithm is proceeding, the type of e is nondecreasing (until e is deleted from U). This is because the type of an edge could change from 1 or 3 to some larger k , but any type other than 1 or 3 will stay as it is. This also shows that the sequence $\{t_i\}$ is nondecreasing.

Lemma 6.3. *For every iteration i ,*

- (a) *Each path in $P(i)$ is critical, and each path in $P^2(i)$ is 2-critical. Each such path contains at least one edge settled in the i -th iteration.*
- (b) *For each path in $P^2(i)$, one of the following holds:*
 - *all edges of P are settled in iteration i ; or*
 - *P is of length two such that one edge of P is settled in iteration i and the other is settled in some previous iteration.*

Proof. We split into cases based upon which of (C1)–(C6) happened at the i -th iteration. First, we observe that (a) and (b) hold trivially if (C3) or (C6) occur. If (C1) or (C2) occurs, we see that the critical path P_{xy} must be in the set \mathcal{P} (see its definition in last subsection). Thus (a) and (b) both follow by the fact that all edges of P_{xy} are associated with P_{xy} . If (C4) occurs, by definition we see that $e \cup e' := P_{xy} - y$ is 2-critical. And we also have $e' \notin U$, as otherwise the type of e would be at most 3. Hence e' was settled before iteration i and the conclusions hold in this case. Lastly, if (C5) occurs, it is easy to verify that e indeed is 2-critical, finishing the proof. \square

Lemma 6.4. *All sets $P(i)$ and $P^2(i)$ are pairwise disjoint, and for all but at most $\frac{n}{2}$ iterations i , we have $|P(i) \cup P^2(i)| \geq 2$.*

Proof. We first prove the second part. It is clear from the algorithm that $|P(i) \cup P^2(i)| = 1$ if and only if $t_i = 6$. Let us consider the first iteration i when all edges in U are of type 6 (hence all critical paths of length one). We claim that this must be a matching. Indeed, suppose on the contrary that $e, f \in U$ share a common vertex. It is easy to verify that $e \cup f$ actually is 2-critical, implying that the type of e is at most 3, a contradiction. Thus, for all but the last $|U| \leq \frac{n}{2}$ iterations i , it holds that $|P(i) \cup P^2(i)| \geq 2$.

It remains to prove the first part, for which it is enough to show that $P(i) \cup P^2(i)$ is disjoint from $P(j) \cup P^2(j)$ when $i < j$. Since the sequence $\{t_i\}$ is nondecreasing, it holds that $t_i \leq t_j$. Consider any $P \in P(i) \cup P^2(i)$ and $Q \in P(j) \cup P^2(j)$, and suppose for contradiction that $P = Q$. First, consider the case when $P \in P^2(i)$. By Lemma 6.3, every edge of P is settled in iteration i or earlier, whereas there is at least one edge of Q settled in iteration j , so $Q \neq P$, contradiction.

We may therefore assume that $P \in P(i)$. If $Q \in P(j)$, then $P = Q$ actually contained at least two associated edges which were in U at time i , and hence we must have been in (C1) at time i . However, then we would have deleted all of P 's associated edges at that time, making it impossible to find Q in $P(j)$ later, contradiction.

Thus, we may assume that $Q \in P^2(j)$. By Lemma 6.3(a), at least one edge of P was settled at iteration i , and so Lemma 6.3(b) implies that $P = Q$ is of length 2, say $e \cup e'$, such that $P \in \mathcal{P}_1(e)$ and e and e' are settled in iterations i and j respectively. From the algorithm, we see that (C5) and (C6) do not produce paths of length 2 in $P^2(j)$, and so $t_j \leq 4$. On the other hand, we have that $t_i \notin \{1, 2, 4\}$. As $t_i \leq t_j$, it must be the case that $t_i = 3$ and $t_j = 4$, that is, (C3) occurs at time i and (C4) occurs at time j .

Since we must be in (C3) at time i , let f be the other settled edge in that iteration, and let $P' \in \mathcal{P}_1(f)$ be the other critical path in $P(i)$. Similarly, since we must be in (C4) at time

j , and e' is settled there, let $Q' \in \mathcal{P}_1(e')$ be the corresponding critical path from $P(j)$, so that $Q \subsetneq Q'$. From above, we had $e \cup e' = P \in \mathcal{P}_1(e)$, so e, e' form a candidate for (C3-1) in iteration i with $|P| = 2$ and $|Q'| = 3$. This shows that (C3-1) must occur at time i , when the two settled edges are e, f . Looking back on the algorithm, in (C3-1), the two paths in $P(i)$ are $e \cup f$, together with a critical path which is associated with either e or f . Since $e \cup e' = P \in P(i)$, it must be one of these. We see that $P \neq e \cup f$, because that would force $e' = f$, and f is settled at time i while e' is settled at time j . Therefore, P must be the other critical path in $P(i)$ rather than $e \cup f$. Since P has length 2, we conclude that the two paths in $P(i)$ both have length 2. Yet, as mentioned, e and e' gave rise to an alternate candidate for iteration i in which the two paths $P \in \mathcal{P}_1(e)$ and $Q' \in \mathcal{P}_1(e')$ had lengths 2 and 3, and since the algorithm sought to maximize the sum of path lengths in $P(i)$ at (C3-1), we have a contradiction. \square

6.3 Putting everything together

The previous section's accounting enables us to complete our proof with methods similar to Füredi's [14] diameter-2 argument. For a graph H , let $\text{Disj}(H)$ denote the set of pairs $\{u, v\}$ in $V(H)$ such that u and v have disjoint neighborhoods, and let $\text{disj}(H) := |\text{Disj}(H)|$. We say that a 2-critical path P is t -light if $|P| = 2$ and both its edges have multiplicity less than t . Recall from the beginning of Section 6 that we define the multiplicity $m(e)$ of an edge e to be the sum $|\mathcal{P}_1(e)| + |\mathcal{P}_2(e)|$, where $\mathcal{P}_1(e)$ is the set of critical paths associated with e and $\mathcal{P}_2(e)$ is the set of 2-critical paths containing e . We record two results from Füredi [14], which hold for arbitrary graphs H (not necessarily diameter-2-critical).

Lemma 6.5. *(Derived from Lemmas 2.1 and 3.3 of Füredi [14].) For any n -vertex graph H , $e(H) + \text{disj}(H) \leq n^2/2$, and the number of t -light 2-critical paths is less than $27t \cdot \text{RSz}(n)$ for any positive integer t .*

In the rest of the section, let G be a diameter-3-critical graph, and define $t := \sqrt{n^2/\text{RSz}(n)}$. By the Ruzsa-Szemerédi (6,3) Theorem (See Theorem 6.1), t tends to infinity as $n \rightarrow \infty$. Let G_0 be the n -vertex graph obtained from G by deleting

- (i) all edges of G whose multiplicity is at least t , and
- (ii) all edges which appear in a t -light 2-critical path of G .

By Lemma 6.5, at most $54t \cdot \text{RSz}(n)$ edges are deleted in (ii). To control the number deleted in (i), observe that $\sum m(e) < 3n^2$, because each critical path is associated with at most 3 edges and each 2-critical path contains at most 2 edges, and thus it follows from $\sum |\mathcal{P}_1(e)| \leq 3\binom{n}{2}$ and $\sum |\mathcal{P}_2(e)| \leq 2\binom{n}{2}$. So, we delete fewer than $3n^2/t$ edges in (i), producing

$$e(G) \leq e(G_0) + \frac{3n^2}{t} + 54t \cdot \text{RSz}(n), \quad (13)$$

and it is clear that, after deleting the edges in (i) and (ii) from G ,

$$\text{all 2-critical paths in } G \text{ of length two are destroyed in } G_0. \quad (14)$$

Lemma 6.6. *Every critical or 2-critical pair of G is contained in $\text{Disj}(G_0)$.*

Proof. Consider any 2-critical pair $\{x, y\}$ in G . If the 2-critical (x, y) -path P has length 1, then by definition $\{x, y\} \in \text{Disj}(G)$ and thus $\{x, y\} \in \text{Disj}(G_0)$. If it has length 2, then by (14), at least one edge of P is deleted in G_0 , implying that $\{x, y\} \in \text{Disj}(G_0)$.

Now consider any critical pair $\{x, y\}$. Note that the critical path P_{xy} is a shortest (x, y) -path. If $|P_{xy}| \leq 2$, then $\{x, y\}$ is also 2-critical. Thus, we may assume that $|P_{xy}| = 3$. This shows that $N_G(x) \cap N_G(y) = \emptyset$ and thus $\{x, y\} \in \text{Disj}(G_0)$. \square

Run our algorithm from the previous section on G , and let s be the number of iterations it runs for before it stops. By Lemma 6.3, every path in $P(i) \cup P^2(i)$ is either critical or 2-critical, which also uniquely determines a critical or 2-critical pair of G . Thus, by Lemmas 6.4 and 6.6, we obtain

$$\text{disj}(G_0) \geq \sum_i |P(i) \cup P^2(i)| \geq 2s - n/2. \quad (15)$$

Let $S(i)$ be the set of edges settled in iteration i , which were also still in G_0 . By property (12), every edge is settled in some iteration, which shows that $E(G_0)$ is a disjoint union of the sets $S(i)$.

Lemma 6.7. *For all but at most $54t \cdot \text{RSz}(n)$ iterations, we have $|S(i)| \leq 1$, and hence $e(G_0) = \sum |S(i)| \leq s + 54t \cdot \text{RSz}(n)$.*

Proof. Consider an arbitrary iteration i . If (C2), (C4), (C5) or (C6) occur, exactly one edge is settled, giving $|S(i)| \leq 1$ trivially. If (C3) occurs, then there are two edges e and f settled such that $e \cup f$ is a 2-critical path. By (14), at most one of e and f remains in G_0 , and thus it also holds that $|S(i)| \leq 1$. It remains to consider (C1). Then there are at least two edges settled in this iteration, all of which are associated with a single critical path, say P_{xy} . And such $P_{xy} \in \mathcal{P}$ (recall the definitions of \mathcal{P} and \mathcal{P}_t at the beginning of Section 6.1). If $|P_{xy}| = 2$, then such P_{xy} is also 2-critical, and thus $|S(i)| \leq 1$ by the same argument as in (C3). Only $|P_{xy}| = 3$ remains. Let $P_{xy} = xaby$. Note that xab and aby both are 2-critical. By the definition of G_0 , one can verify that at most one edge of P_{xy} can be in G_0 , unless it is the situation that $m(ab) \geq t$, $m(xa) < t$ and $m(by) < t$, that is, $P_{xy} \in \mathcal{P}_t$. Thus, $|S(i)| \leq 1$ if $P_{xy} \notin \mathcal{P}_t$ and $|S(i)| \leq 2$ otherwise. By Lemma 6.2, we see that $|\mathcal{P}_t| \leq 54t \cdot \text{RSz}(n)$. This completes the proof. \square

We are now ready to prove our final main result, that G has at most $n^2/6 + o(n^2)$ edges.

Proof of Theorem 1.8. Let G be an arbitrary diameter-3-critical graph. By (15) and Lemma 6.7, we find

$$\text{disj}(G_0) \geq 2e(G_0) - 108t \cdot \text{RSz}(n) - \frac{n}{2}.$$

Apply Lemma 6.5 to G_0 , we find

$$\frac{n^2}{2} \geq e(G_0) + \text{disj}(G_0) \geq 3e(G_0) - 108t \cdot \text{RSz}(n) - \frac{n}{2},$$

which, together with (13), implies that

$$e(G) \leq \frac{n^2}{6} + \frac{3n^2}{t} + 90t \cdot \text{RSz}(n) + \frac{n}{6} = \frac{n^2}{6} + \left(\frac{93n^2}{t} + \frac{n}{6} \right) = \frac{n^2}{6} + o(n^2),$$

where the equalities follow by the fact that $t = \sqrt{n^2/\text{RSz}(n)} \rightarrow \infty$ as $n \rightarrow \infty$. \square

Remark. The proofs in Section 6 actually work for any diameter-critical graph with diameter at least 3. The only information from diameter-3-critical graphs we need in the proof is that for each edge e , the set of 3-critical paths of e is nonempty. This clearly holds for all diameter-critical graphs with diameter at least 3. Therefore, for all such graphs G , we have $e(G) \leq n^2/6 + o(n^2)$ as well.

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