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Fakultät für Mathematik und Wirtschaftswissenschaften
Institut für Optimierung und Operations Research

Exponential Domination, Exponential Independence, and the Clustering Coefficient

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Simon Thomas Jäger

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Prof. Dr. Alexander Lindner

1. Gutachter
Prof. Dr. Dieter Rautenbach

2. Gutachter
Prof. Dr. Henning Bruhn-Fujimoto

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Preface

This cumulative dissertation contains four research papers.

The paper *Relating domination, exponential domination, and porous exponential domination* [18] is about exponential domination in graphs, which is a variant of domination in graphs. It contains results about various parameters in the context of exponential domination, and the proofs include some linear programming arguments. This paper is joint work with Michael A. Henning and Dieter Rautenbach and has been published in the journal *Discrete Optimization*.

The paper *Hereditary equality of domination and exponential domination* [19] is related to exponential domination, too. It contains a characterization of a hereditary class of graphs in terms of forbidden induced subgraphs. The results have been developed in collaboration with Michael A. Henning and Dieter Rautenbach and will be published in the journal *Discussiones Mathematicae Graph Theory*.

The definition of exponential domination inspired us to introduce a similar concept in the context of independence in graphs. In the paper *Exponential independence* [20], we define such a concept, as well as show several results for the corresponding parameter. This article has been created together with Dieter Rautenbach, and it has been published in the journal *Discrete Mathematics*.

In the last paper of this dissertation, we consider the so-called clustering coefficient. This parameter arises in the study of social networks. Motivated by a question posed by Watts [26] in 1999, we determine the maximum clustering coefficients among special graph classes in the article *Large values of the clustering coefficient* [14]. This paper is joint work with Michael Gentner, Irene Heinrich, and Dieter Rautenbach, and it has been published in *Discrete Mathematics*.

This dissertation consists of two parts. The first contains an overview of the attached research papers and the co-authors. Furthermore, we give a classification of our work in the field of research, recall some notation, as well as summarize our results. The second part contains the four research papers.

Contents

Part I

Introduction

1 Overview of Research Papers and Co-authors

Research Papers

- M.A. Henning, S. Jäger, D. Rautenbach, Relating domination, exponential domination, and porous exponential domination, Discrete Optimization 23 (2017) 81-92.
- M.A. Henning, S. Jäger, D. Rautenbach, Hereditary equality of domination and exponential domination, Discussiones Mathematicae Graph Theory (2016), doi:10.7151/dmgt.2006.
- S. Jäger, D. Rautenbach, Exponential independence, Discrete Mathematics 340 (2017) 2650-2658.
- M. Gentner, et al., Large values of the clustering coefficient, Discrete Mathematics 341 (2018) 119-125.

Co-authorship

- Michael Gentner: PhD student at the Institute of Optimization and Operations Research, Ulm University, Ulm, Germany.
- Irene Heinrich: PhD student at the Department of Mathematics, University of Kaiserslautern, Kaiserslautern, Germany.
- Prof. Dr. Michael A. Henning: Professor at the Department of Pure and Applied Mathematics, University of Johannesburg, Auckland Park, 2006, South Africa.
- Prof. Dr. Dieter Rautenbach: Professor at the Institute of Optimization and Operations Research, Ulm University, Ulm, Germany.

2 Summary

2.1 Field of Research

Domination in graphs is a very important and well-studied area in graph theory. In their famous book, *Fundamentals of Domination in Graphs* [16], Haynes, Hedetniemi, and Slater distinguish different variations of domination in graphs. A well-known example is *k-domination*, introduced by Fink and Jacobson [11] in 1985: for a positive integer k, a set D of vertices of a graph is k-dominating if every vertex not in D has at least k neighbors in D. A version of domination involving distances of vertices is *distance-k-domination*, defined by Henning [17] in 1998: for a positive integer k, a set D of vertices of a graph is distance-k-dominating if every vertex not in D has distance at most k from a vertex in D. Another version of domination at a distance is *broadcast domination*, which was introduced by Erwin [10] in 2004. There, a function f assigns to each vertex v of a graph a nonnegative integer $f(v)$, and v dominates all vertices at distance between 1 and $f(v)$. Slater [23] had studied a similar variant, where a vertex v is dominated by a set S of vertices if the distance between v and a vertex in S is at most $f(v)$. A variant of domination that combines k-domination and domination at a distance is *disjunctive domination* defined by Goddard et al. [15] in 2014: for a positive integer b, a set D of vertices is b-disjunctive dominating if every vertex not in D is adjacent to a vertex in D or has at least b vertices in D at distance 2 from it. Apparently, disjunctive domination only considers distances of at most two. Its definition was motivated by a more general variant of domination, *exponential domination*, which had been introduced by Dankelmann et al. [7] in 2009. In this variant of domination, the influence of the vertices in an exponential dominating set decreases exponentially with distance but, in contrast to other variations, is not bounded by distance. A related parameter is the so-called *(total) influence number* [9]. It also deals with exponential decay with respect to distance but has not been studied in the context of domination.

In the concept of exponential domination, each vertex in a set D of vertices sends some kind of signal that diminishes exponentially by the factor $\frac{1}{2}$ with distance. A vertex not in D is dominated if a sufficiently large amount of this signal arrives at it. This can be attained by a single dominating neighbor or by multiple dominating vertices at some distance. Dankelmann et al. [7] distinguish two versions: *exponential domination*, where vertices in the exponential dominating set block the signals of each other, and *porous exponential domination*, where no such blocking occurs.

Dankelmann et al. [7] are mainly interested in the first version. They prove lower and upper bounds for the corresponding parameter, the *exponential domination number*. In 2017, Bessy et al. [3] strengthen their results and provide further bounds. In a second paper, Bessy et al. [4] consider exponential domination in subcubic graphs. They describe an efficient algorithm to determine the exponential domination number in subcubic trees and prove that the exponential domination number is APX-hard for subcubic graphs. Besides that, exponential domination has been studied only for some specific graphs [2]. The porous version and the corresponding parameter, the *porous exponential domination number*, have not been studied extensively, yet. Thus, there are only few results for some special graphs [1, 5], and even the complexity of the porous exponential domination number on subcubic trees is unknown.

Another fundamental field in graph theory is independence in graphs. Many variants of domination in graphs have been analyzed in the context of independence in graphs. Similar to k-domination, for example, a set S of vertices is *k-independent* for some positive integer k if the maximum degree of the subgraph induced by S is at most $k-1$ [11]. A variant of independence in graphs related to distance-k-domination is the so-called *k-packing*: for a positive integer k, a set P of vertices of a graph G is a k-packing if every two distinct vertices in P have distance at least k in G [21]. The introduction of exponential domination by Dankelmann et al. [7] as a non-local variant of domination inspired us to the definition of *exponential independence* in the third paper of this dissertation.

As an application of exponential domination, Dankelmann et al. [7] mention the analysis of social networks. The exponential decay of signals can be seen as a model for the spreading of information, whose influence diminishes every time it is passed on. An important parameter for the analysis of graphs representing social networks is the so-called *clustering coefficient*. It quantifies the transitivity of a network, i. e. it measures the probability that neighbors of vertices are adjacent themselves. The clustering coefficient of a graph was proposed by Watts and Strogatz [24] in 1998. They considered so-called small-world networks, that is graphs that are locally highly clustered but globally keep properties of random graphs. The clustering coefficient has been studied a lot in the field of social network analysis [6, 22, 25, 26]. In 1999, Watts [26] posed a simple question: among all connected graphs of given order and size, which one maximizes the clustering coefficient? Fukami and Takahashi [12, 13] studied graphs that locally maximize the clustering coefficient, i. e. graphs whose clustering coefficient cannot be increased by switching edges. But Watts' original problem is still unsolved.

2.2 Notation

We mainly use the notation from the book *Graph Theory* [8]. In this section, we recall some basic terminology.

We consider finite, simple, and undirected graphs. Let G be a graph. The vertex set and the edge set of G are denoted by $V(G)$ and $E(G)$, respectively. The *order* $n(G)$ of G is the cardinality of $V(G)$, and the *size* $m(G)$ of G is the cardinality of $E(G)$. The neighborhood of a vertex v in G is denoted by $N_G(v)$, and the *degree* $d_G(v)$ of v is the cardinality of $N_G(v)$. If the degrees of all vertices in G are at most 3, then G is *subcubic*. A vertex of degree at most 1 in G is an *endvertex* of G. The *distance* $\mathrm{dist}_G(u, v)$ between two vertices u and v in G is the minimum number of edges of a path in G between u and v. If no such path exists, then let $\mathrm{dist}_G(u, v) = \infty$. The *diameter* $\mathrm{diam}(G)$ of G is the maximum distance between vertices of G. The minimum length of a cycle in G is the *girth* of G. A graph H is a *subgraph* of G if $V(H) \subseteq V(G)$ and $E(H) \subseteq E(G)$. If H is a subgraph of G and H contains all edges $xy \in E(G)$ with $x, y \in V(H)$, then H is called *induced*. If $U \subseteq V(G)$ is a set of vertices, then $G[U]$ denotes the induced subgraph of G with vertex set U. Let $\mathcal{F}$ be a set of graphs. If G does not contain any graph from $\mathcal{F}$ as an induced subgraph, then G is called $\mathcal{F}$*-free*. A set D of vertices of G is a *dominating set* of G if every vertex of G not in D has a neighbor in D [16]. The *domination number* $\gamma(G)$ of G is the minimum order of a dominating set of G. A set S of vertices of G is *independent* if no two vertices in S are adjacent. The *independence number* $\alpha(G)$ of G is the maximum order of an independent set of G.

2.3 Exponential Domination

Before summarizing the results of the first two articles in this dissertation, we state the precise definitions of exponential domination, its porous version, and the corresponding parameters from [7].

In order to model the above-mentioned blocking effects, Dankelmann et al. [7] define a new type of distance. Let D be a set of vertices of a graph G. For two vertices u and v of G, let $\mathrm{dist}_{(G,D)}(u,v)$ be the minimum number of edges of a path P in G between u and v such that D contains exactly one endvertex of P but no internal vertex of P. If no such path exists, then let $\mathrm{dist}_{(G,D)}(u,v) = \infty$.

The set D is an *exponential dominating set* of G if

$$\sum_{v \in D} \left(\tfrac{1}{2}\right)^{\mathrm{dist}_{(G,D)}(u,v)-1} \geq 1 \text{ for every vertex } u \text{ of } G,$$

where $\left(\frac{1}{2}\right)^{\infty} = 0$, and the *exponential domination number* $\gamma_e(G)$ of G is the minimum order of an exponential dominating set.

Similarly, D is a *porous exponential dominating set* of G if

$$\sum_{v \in D} \left(\tfrac{1}{2}\right)^{\mathrm{dist}_{G}(u,v)-1} \geq 1 \text{ for every vertex } u \text{ of } G,$$

and the *porous exponential domination number* $\gamma_e^*(G)$ of G is the minimum order of a porous exponential dominating set of G.

Relating Domination, Exponential Domination, and Porous Exponential Domination

The domination number, exponential domination number, and porous exponential domination number of a graph G satisfy

$$\gamma_e^*(G) \leq \gamma_e(G) \leq \gamma(G).$$

In the paper *Relating domination, exponential domination, and porous exponential domination* [18], we show results about the gaps in these inequalities and characterize the graphs providing equality in some of these inequalities. We formulate the integer linear program that corresponds to the problem of determining the porous exponential domination number. For a graph G, the *fractional porous exponential* *domination number* $\gamma^*_{e,f}(G)$ is defined as the optimum value of the relaxation of this program. The results in our paper mostly concern subcubic graphs. The reason for this is that Bessy et al. [4] provide a useful lemma, which implies that the influence arriving at a vertex in a subcubic graph is bounded from above. In general graphs, this is not true. Using the dual of the above-mentioned relaxed program, we show that for a subcubic tree the fractional porous exponential domination number only depends on the order of the tree. In detail, we prove that for a subcubic tree T with n vertices $\gamma^*_{e,f}(T) = \frac{n+2}{6}$. This implies a result shown by Bessy et al. [4] in 2016. Using another result of Bessy et al. [4], we conclude that $\gamma_e(T) \leq 2\gamma^*_{e,f}(T)$ for every subcubic tree T and show that this bound is tight. It follows that $\gamma_e(T) \leq 2\gamma^*_e(T)$ for every subcubic tree T. We believe that it is possible to replace the factor 2 by $\frac{3}{2}$, which would be tight. We formulate a conjecture about the subcubic trees T with $\gamma^*_e(T) = \gamma^*_{e,f}(T)$ and collect some properties of these trees. After characterizing the subcubic trees T with $\gamma_e(T) = \gamma^*_{e,f}(T)$, we prove lower bounds on the fractional porous exponential domination number for more general graphs — again by using linear programming techniques. Finally, we give a characterization of the subcubic trees T with $\gamma(T) = \gamma_e(T)$.

Hereditary Equality of Domination and Exponential Domination

For general graphs G, it is unknown how to decide efficiently whether $\gamma(G) = \gamma_e(G)$. In the paper *Hereditary equality of domination and exponential domination* [19], we give a characterization of a large subclass of the graphs with $\gamma(H) = \gamma_e(H)$ for every induced subgraph H of G. We describe this class in terms of forbidden induced subgraphs. Our results imply characterizations for trees and graphs of girth at least 5. In our proofs, we identify sets $\mathcal{F}$ of graphs, such that a graph G is $\mathcal{F}$-free if and only if $\gamma(H) = \gamma_e(H)$ for every induced subgraph H of G. In order to prove our results, we show that every component of an $\mathcal{F}$-free graph has domination number at most 2. In 1965, Wolk [27] gave a characterization of the largest hereditary class of graphs for which every component can be dominated by one vertex. Our results contribute to a similar problem: the characterization of the largest hereditary class of graphs for which every component can be dominated by at most two vertices. At the end of our paper, we pose three conjectures. First, that it is possible to characterize the graphs G with $\gamma(H) = \gamma_e(H)$ for every induced subgraph H of G by a finite set of forbidden induced subgraphs. Second, that each of these forbidden induced subgraphs has exponential domination number 2 and domination number 3. Finally, we conjecture that a graph G satisfies $\gamma(H) = \gamma_e(H)$ for every induced subgraph H of G if and only if $\gamma(H) = \gamma_e^*(H)$ for every induced subgraph H of G.

2.4 Exponential Independence

In the paper *Exponential independence* [20], we define a set S of vertices of a graph G to be *exponentially independent* if

$$\sum_{v \in S\setminus\{u\}} \left(\tfrac{1}{2}\right)^{\mathrm{dist}_{(G,S\setminus\{u\})}(u,v)-1} < 1 \text{ for every vertex } u \text{ in } S,$$

where $\left(\frac{1}{2}\right)^{\infty} = 0$, and $\mathrm{dist}_{(G,S\setminus\{u\})}(u,v)$ refers to the modified version of distance defined in section 2.3. The maximum order of an exponential independent set is the *exponential independence number* $\alpha_e(G)$ of G. After describing some basic observations about exponential independence, we prove a lower bound on $\alpha_e(G)$ depending on the diameter of a graph G and characterize the trees for which this lower bound holds with equality. We determine the exponential independence number for some special graphs, present an upper bound on $\alpha_e(G)$ depending on the order of a graph G, and give a full characterization of the extremal graphs. For subcubic trees T, we prove a lower bound on $\alpha_e(T)$ depending on the order of T. Furthermore, we characterize the class of graphs with $\alpha_e(H) = \alpha(H)$ for every induced subgraph H of a graph G in terms of forbidden induced subgraphs and give a full description of the trees T with $\alpha_e(T) = \alpha(T)$. Our results motivate to examine further problems related to exponential independence, such as an explicit characterization of the graphs G with $\alpha_e(G) = \alpha(G)$ or hardness results concerning the exponential independence number.

2.5 The Clustering Coefficient

When introducing the clustering coefficient, Watts and Strogatz [24] distinguish between a local and a global clustering coefficient. The former, the clustering coefficient of a vertex u, is defined as the number of edges in the neighborhood of u divided by the maximum possible number of edges in this neighborhood. In detail, the *clustering coefficient* $C_u(G)$ of a vertex u in a graph G is

$$C_u(G) = \begin{cases} \frac{m(G[N_G(u)])}{\binom{d_G(u)}{2}} & \text{, if } d_G(u) \geq 2, \\ 0 & \text{, otherwise.} \end{cases}$$

The global clustering coefficient is defined as the average of the local clustering coefficients of a graph. More precisely, the *clustering coefficient* $C(G)$ of a graph G is

$$C(G) = \frac{1}{n(G)} \sum_{u \in V(G)} C_u(G).$$

The paper *Large values of the clustering coefficient* [14] was inspired by a question posed by Watts [26], who asks for the connected graphs maximizing the clustering coefficient for given order and size. We prove upper bounds on the clustering coefficient for all connected regular graphs and for all connected subcubic graphs of a given order. To answer Watts' question in these cases, we give characterizations of all graphs for which these upper bounds hold with equality. Finally, we determine the value by which the clustering coefficient of a graph G increases at most when adding a single edge to G and observe that it might change from 0 to nearly 1.

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Part II

Research Papers

3 Relating Domination, Exponential Domination, and Porous Exponential Domination

M.A. Henning, S. Jäger, D. Rautenbach, Relating domination, exponential domination, and porous exponential domination, Discrete Optimization 23 (2017) 81-92, http://dx.doi.org/10.1016/j.disopt.2016.12.002, Reprinted with permission by Elsevier.

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Relating domination, exponential domination, and porous exponential domination

Michael A. Henning[a], Simon Jäger[b], Dieter Rautenbach[b,*]

[a] *Department of Pure and Applied Mathematics, University of Johannesburg, Auckland Park, 2006, South Africa*

[b] *Institute of Optimization and Operations Research, Ulm University, Ulm, Germany*

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The domination number $\gamma(G)$ of a graph G, its exponential domination number $\gamma_e(G)$, and its porous exponential domination number $\gamma_e^*(G)$ satisfy $\gamma_e^*(G) \leq \gamma_e(G) \leq \gamma(G)$. We contribute results about the gaps in these inequalities as well as the graphs for which some of the inequalities hold with equality. Relaxing the natural integer linear program whose optimum value is $\gamma_e^*(G)$, we are led to the definition of the fractional porous exponential domination number $\gamma_{e,f}^*(G)$ of a graph G. For a subcubic tree T of order n, we show $\gamma_{e,f}^*(T) = \frac{n+2}{6}$ and $\gamma_e(T) \leq 2\gamma_{e,f}^*(T)$. We characterize the two classes of subcubic trees T with $\gamma_e(T) = \gamma_{e,f}^*(T)$ and $\gamma(T) = \gamma_e(T)$, respectively. Using linear programming arguments, we establish several lower bounds on the fractional porous exponential domination number in more general settings.

1. Introduction

The references for the present paper are [1–13]. In [5] Dankelmann et al. introduce *exponential domination* as a variant of domination in graphs where the influence of the vertices in an *exponential dominating set* extends to any arbitrary distance but decays exponentially with that distance. They consider two parameters for a given graph G, its *exponential domination number* $\gamma_e(G)$, corresponding to a setting in which the different vertices in the exponential dominating set block each others influence, and its *porous exponential domination number* $\gamma_e^*(G)$, where such a blocking does not occur.

Unlike most other domination parameters [8], which are based on local conditions, exponential domination is a genuinely global concept. Compared to exponential domination, even notions such as distance

* Corresponding author.
E-mail addresses: mahenning@uj.ac.za (M.A. Henning), simon.jaeger@uni-ulm.de (S. Jäger), dieter.rautenbach@uni-ulm.de (D. Rautenbach).

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domination [10] appear as essentially local, because they can be reduced to ordinary domination by considering suitable powers of the underlying graph. The global nature of exponential domination makes it much harder, which might be the reason why there are only relatively few results about it [1–4]. While Bessy et al. [4] show that the exponential domination number is APX-hard for subcubic graphs and describe an efficient algorithm for subcubic trees, the complexity of the exponential domination number on general trees is unknown, and a hardness result does not seem unlikely. For the porous version, even less is known. There is not a single complexity result, and it is even unknown whether the porous exponential domination number of a given subcubic tree can be determined efficiently. Partly motivated by such difficulties, Goddard et al. define [7] *disjunctive domination* (see also [11–13]), which keeps the exponential decay of the influence but only considers distances one and two. Further related parameters known as *influence* and *total influence* [6] also have unknown complexity even for trees [9].

The two parameters of exponential domination and the classical domination number $\gamma(G)$ [8] of a graph G satisfy

$$\gamma_e^*(G) \leq \gamma_e(G) \leq \gamma(G).$$

In the present paper we contribute results about the gaps in these inequalities as well as the graphs for which some of the inequalities hold with equality. In order to obtain lower bounds we consider fractional relaxations and apply linear programming techniques.

Before stating our results and several open problems, we recall some notation and give formal definitions. We consider finite, simple, and undirected graphs. The vertex set and the edges set of a graph G are denoted by $V(G)$ and $E(G)$, respectively. The order $n(G)$ of G is the number of vertices of G. If all vertex degrees in G are at most 3, then G is subcubic. A vertex of degree at most 1 in G is an endvertex of G. A vertex in a rooted tree T is a leaf of T if it has no child in T. The distance $\mathrm{dist}_G(u,v)$ between two vertices u and v in G is the minimum number of edges of a path in G between u and v. If no such path exists, then let $\mathrm{dist}_G(u,v) = \infty$. The diameter $\mathrm{diam}(G)$ of G is the maximum distance between vertices of G. A set D of vertices of a graph G is a dominating set of G [8] if every vertex of G not in D has a neighbor in D, and the domination number $\gamma(G)$ of G is the minimum order of a dominating set of G. Similarly, for some set X of vertices of G, let $\gamma(G,X)$ be the minimum order of a set D of vertices such that every vertex in $X \setminus D$ has a neighbor in D. Note that $\gamma(G) = \gamma(G, V(G))$. For positive integers n and m, let $[n]$ be the set of the positive integers at most n, let P_n, C_n, and K_n be the path, cycle, and complete graph of order n, respectively, and, let $K_{n,m}$ be the complete bipartite graph with partite sets of orders n and m.

In order to capture the above-mentioned blocking effects that are a feature of exponential domination, we need a modified distance notion. Therefore, let D be a set of vertices of a graph G. For two vertices u and v of G, let $\mathrm{dist}_{(G,D)}(u,v)$ be the minimum number of edges of a path P in G between u and v such that D contains exactly one endvertex of P but no internal vertex of P. If no such path exists, then let $\mathrm{dist}_{(G,D)}(u,v) = \infty$. Note that, if u and v are distinct vertices in D, then $\mathrm{dist}_{(G,D)}(u,u) = 0$ and $\mathrm{dist}_{(G,D)}(u,v) = \infty$.

For a vertex u of G, let

$$w_{(G,D)}(u) = \sum_{v \in D} \left(\frac{1}{2}\right)^{\mathrm{dist}_{(G,D)}(u,v)-1}, \tag{1}$$

where $\left(\frac{1}{2}\right)^{\infty} = 0$. Note that $w_{(G,D)}(u) = 2$ for $u \in D$.

Dankelmann et al. [5] define the set D to be an *exponential dominating set* of G if

$$w_{(G,D)}(u) \geq 1 \quad \text{for every vertex } u \text{ of } G,$$

and the *exponential domination number* $\gamma_e(G)$ of G as the minimum order of an exponential dominating set. Similarly, they define D to be a *porous exponential dominating set* of G if

$$w^*_{(G,D)}(u) \geq 1 \quad \text{for every vertex } u \text{ of } G,$$

where

$$w^*_{(G,D)}(u) = \sum_{v \in D} \left(\frac{1}{2}\right)^{\mathrm{dist}_G(u,v)-1}, \tag{2}$$

and they define the *porous exponential domination number* $\gamma_e^*(G)$ of G as the minimum order of a porous exponential dominating set of G. Note that the definition of $w^*_{(G,D)}(u)$ involves the usual distance rather than $\mathrm{dist}_{(G,D)}(u,v)$, which reflects the absence of blocking effects. A dominating, exponential dominating, or porous exponential dominating set of minimum order is called *minimum*.

The parameter $\gamma_e^*(G)$ equals the optimum value of the following integer linear program

$$\begin{array}{llcll} \min & \displaystyle\sum_{u \in V(G)} x(u) & & & \\ s.t. & \displaystyle\sum_{u \in V(G)} \left(\frac{1}{2}\right)^{\mathrm{dist}_G(u,v)-1} \cdot x(u) & \geq & 1 & \forall v \in V(G) \\ & x(u) & \in & \{0,1\} & \forall u \in V(G). \end{array} \tag{3}$$

Relaxing (3), we obtain the following linear program

$$\begin{array}{llcll} \min & \displaystyle\sum_{u \in V(G)} x(u) & & & \\ s.t. & \displaystyle\sum_{u \in V(G)} \left(\frac{1}{2}\right)^{\mathrm{dist}_G(u,v)-1} \cdot x(u) & \geq & 1 & \forall v \in V(G) \\ & x(u) & \geq & 0 & \forall u \in V(G). \end{array} \tag{4}$$

Let the *fractional porous exponential domination number* $\gamma^*_{e,f}(G)$ of G be the optimum value of (4).

Clearly,

$$\gamma^*_{e,f}(G) \leq \gamma_e^*(G) \leq \gamma_e(G) \leq \gamma(G) \tag{5}$$

for every graph G.

Most of our results concern subcubic graphs. While exponential domination number is APX-hard already for subcubic graphs [4], there is the following fundamental lemma from [4], which will be an important technical tool throughout our paper.

Lemma 1 (*Bessy et al. [4]*). *Let G be a graph of maximum degree at most 3, and let D be a set of vertices of G.*

If u is a vertex of degree at most 2 in G, then $w_{(G,D)}(u) \leq 2$ with equality if and only if u is contained in a subgraph T of G that is a tree, such that rooting T in u yields a full binary tree and $D \cap V(T)$ is exactly the set of leaves of T.

The next section contains all our results as well as many closely related conjectures and open problems.

2. Results

In order to organize our results for the reader, we split this section into subsections.

2.1. Exact values and upper bounds for subcubic trees

Our first slightly surprising result is that the fractional porous exponential domination number of a subcubic tree only depends on its order.

Theorem 2. *If T is a subcubic tree of order n, then $\gamma^*_{e,f}(T) = \frac{n+2}{6}$.*

Proof. Let T be a subcubic tree of order n. If T has only one vertex u, then $x(u) = \frac{1}{2} = \frac{1+2}{6}$ is an optimum solution of (4). Hence, we may assume that $n \geq 2$. Let V_i be the set of vertices of degree i in T, and let $n_i = |V_i|$ for $i \in [3]$. Let T' arise from T by adding, for every vertex u in V_2, a new vertex p_u as well as the new edge up_u. By construction, T' is a tree of order $n + n_2$ that only has vertices of degree 1 and 3, and $D' = V_1 \cup \{p_u : u \in V_2\}$ is the set of all endvertices of T'.

Let v be an endvertex of T', and let u be the neighbor of v. Since $T' - v$ rooted in u is a full binary tree whose set of leaves is exactly $D' \setminus \{v\}$, Lemma 1 implies that $w_{(T'-v,D'\setminus\{v\})}(u) = 2$. Since $v \in D'$, this implies $w^*_{(T',D')}(v) = 2 + 1 = 3$. Similarly, if v is a vertex of degree 3 in T' whose neighbors are u_1, u_2, and u_3, then Lemma 1 implies that $w_{(T'-v,D')}(u_i) = 2$ for $i \in [3]$, which implies $w^*_{(T',D')}(v) = 1 + 1 + 1 = 3$. Altogether, we obtain that $w^*_{(T',D')}(v) = 3$ holds for every vertex v of T'.

Let $(x(u))_{u\in V(T)}$ be such that

$$x(u) = \begin{cases} \dfrac{1}{3}, & \text{if } u \text{ is an endvertex of } T, \\ \dfrac{1}{6}, & \text{if } u \text{ has degree 2 in } T, \text{ and} \\ 0, & \text{if } u \text{ has degree 3 in } T. \end{cases}$$

If u and v are vertices of T, then $\text{dist}_T(u, v) = \text{dist}_{T'}(u, v)$. Furthermore, if $u \in V_2$, then $\text{dist}_T(u, v) = \text{dist}_{T'}(p_u, v) - 1$.

This implies that

$$\begin{aligned} \sum_{u\in V(T)} \left(\frac{1}{2}\right)^{\text{dist}_T(u,v)-1} \cdot x(u) &= \frac{1}{3} \sum_{u\in V_1} \left(\frac{1}{2}\right)^{\text{dist}_T(u,v)-1} + \frac{1}{6} \sum_{u\in V_2} \left(\frac{1}{2}\right)^{\text{dist}_T(u,v)-1} \\ &= \frac{1}{3} \sum_{u\in V_1} \left(\frac{1}{2}\right)^{\text{dist}_{T'}(u,v)-1} + \frac{1}{3} \sum_{u\in V_2} \left(\frac{1}{2}\right)^{\text{dist}_{T'}(p_u,v)-1} \\ &= \frac{1}{3} \sum_{u\in D'} \left(\frac{1}{2}\right)^{\text{dist}_{T'}(u,v)-1} \\ &= \frac{1}{3} w^*_{(T',D')}(v) \\ &= 1 \end{aligned} \tag{6}$$

for every vertex v of T.

The dual linear program of (4) is

$$\begin{array}{llcll} \max & \displaystyle\sum_{v\in V(T)} y(v) & & & \\ s.t. & \displaystyle\sum_{v\in V(T)} \left(\frac{1}{2}\right)^{\text{dist}_T(u,v)-1} \cdot y(v) & \leq & 1 & \forall u \in V(T) \\ & y(v) & \geq & 0 & \forall v \in V(T). \end{array} \tag{7}$$

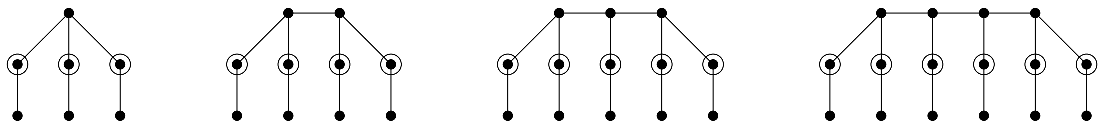

Fig. 1. Lemma 1 easily implies that every exponential dominating set D of the trees T shown above intersects the closed neighborhood of each endvertex. In fact, if u is an endvertex, v is the neighbor of u, w is the neighbor of v distinct from u, and D contains neither u nor v, then w has degree 2 in the subcubic graph $T-\{u,v\}$, and Lemma 1 applied to $T-\{u,v\}$ implies $w_{(T,D)}(u) = w_{(T,D)}(v)/2 = w_{(T,D)}(w)/4 \leq 1/2$. Therefore, the encircled vertices form a minimum exponential dominating set, and hence $\gamma_e(T) = \frac{n(T)+2}{3} = 2\gamma^*_{e,f}(T)$ for each shown tree T. Furthermore, it is easy to verify that $\gamma^*_e(T) = \gamma_e(T)$ for the two smallest trees T of orders 7 and 10.

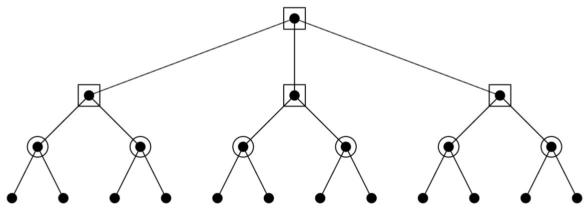

Fig. 2. A tree T with $\gamma_e(T) = 6$ and $\gamma^*_e(T) = \gamma^*_{e,f}(T) = 4$. The encircled vertices indicate a minimum exponential dominating set while the boxed vertices indicate a minimum porous exponential dominating set.

Therefore, setting $y(u) = x(u)$ for every vertex u of T, we obtain, by (6), that

- $(x(u))_{u\in V(T)}$ is a feasible solution of (4),
- $(y(u))_{u\in V(T)}$ is a feasible solution of (7), and that
- $\sum_{u\in V(T)} x(u) = \sum_{u\in V(T)} y(u)$,

that is, $(x(u))_{u\in V(T)}$ and $(y(u))_{u\in V(T)}$ are both optimum solutions of the respective linear programs.

Since $n_1 = n_3 + 2$, we obtain $n + 2 = n_1 + n_2 + n_3 + 2 = 2n_1 + n_2$ and, hence,

$$\gamma^*_{e,f}(T) = \sum_{u\in V(T)} x(u) = \frac{1}{3}n_1 + \frac{1}{6}n_2 = \frac{n+2}{6},$$

which completes the proof. $\square$

Bessy et al. [4] show $\frac{n+2}{6} \leq \gamma_e(T) \leq \frac{n+2}{3}$ for every subcubic tree T of order n. Note that the first of these two inequalities is an immediate consequence of Theorem 2, and that, combined with Theorem 2, the second of these inequalities implies the following.

Corollary 3. *If T is a subcubic tree of order n, then $\gamma_e(T) \leq 2\gamma^*_{e,f}(T)$.*

Fig. 1 illustrates an infinite family of trees showing that Corollary 3 is tight. Another immediate consequence of Corollary 3, namely $\gamma^*_e(T) \leq 2\gamma^*_{e,f}(T)$ for every subcubic tree T, is tight for the two smallest trees in this family, which implies that the integrality gap between the integer linear program (3) and its linear programming relaxation (4) is 2 for such trees. It seems possible that the integrality gap between (3) and (4) is bounded for all graphs of bounded maximum degree. Yet another consequence of Corollary 3 is that $\gamma_e(T) \leq 2\gamma^*_e(T)$ for every subcubic tree T. We believe that this estimate can be improved as follows.

Conjecture 4. *If T is a subcubic tree, then $\gamma_e(T) \leq \frac{3}{2}\gamma^*_e(T)$.*

The tree in Fig. 2 shows that the bound in Conjecture 4 would be tight.

2.2. Equality with the fractional relaxation in subcubic trees

The special tree in Fig. 2 also plays a role in our next conjecture.

Conjecture 5. *If T is a subcubic tree, then $\gamma_e^*(T) = \gamma_{e,f}^*(T)$ if and only if T is either $K_{1,3}$ or the tree in Fig. 2.*

We establish many quite restrictive properties of the trees considered in Conjecture 5.

Theorem 6. *Let T be a subcubic tree with $\gamma_e^*(T) = \gamma_{e,f}^*(T) > 1$. Let V_i be the set of vertices of degree i in T for $i \in [3]$. Let D be a minimum porous exponential dominating set of T.*

(i) $w^*_{(T,D)}(u) = 1$ *for every vertex* $u \in V_1 \cup V_2$.
(ii) $D \subseteq V_3$ *and* $N_T(V_1 \cup V_2) \subseteq V_3 \setminus D$.
(iii) T *does not contain a vertex u in V_1 and a vertex w in V_2 at distance* 2.
(iv) T *does not contain two vertices u_1 and u_2 in V_1 and a vertex v in V_2 such that* $\mathrm{dist}_T(u_1, u_2) = 2$ *and* $\mathrm{dist}_T(u_1, v) \in \{3, 4\}$.

Proof. Note that $\gamma_e^*(T) > 1$ implies that T is not a star.

(i) Let $(x(u))_{u\in V(T)}$ be such that

$$x(u) = \begin{cases} 1, & \text{if } u \in D, \text{ and} \\ 0, & \text{otherwise} \end{cases}$$

and let $(y(u))_{u\in V(T)}$ be as in the proof of Theorem 2. Since $\gamma_e^*(T) = \gamma_{e,f}^*(T)$, we obtain that $(x(u))_{u\in V(T)}$ is an optimum solution of (4), and $(y(u))_{u\in V(T)}$ is an optimum solution of (7). By the dual complementary slackness conditions, we obtain that $y(v) > 0$ for some $v \in V(T)$ implies

$$w^*_{(T,D)}(v) = \sum_{u\in V(G)} \left(\frac{1}{2}\right)^{\mathrm{dist}_T(u,v)-1} \cdot x(u) = 1.$$

Since $y(v) > 0$ if and only if $v \in V_1 \cup V_2$, the proof of (i) is complete.

(ii) Since $v \in D$ implies $w^*_{(T,D)}(v) \geq 2$, (i) implies $D \subseteq V_3$. If u in V_1 has a neighbor v in V_2, then $w^*_{(T,D)}(v) = 1$ implies the contradiction $w^*_{(T,D)}(u) = 2$. Hence, $N_T(V_1) \subseteq V_3$.

Suppose that T contains a path $uvwx$ with $d_T(v) = d_T(w) = 2$. Let T_v be the component of $T - w$ that contain v. Let $\alpha = w^*_{(T,D\cap V(T_v))}(v)$, and $\beta = w^*_{(T,D\setminus V(T_v))}(v)$. Clearly, $w^*_{(T,D\cap V(T_v))}(w) = \frac{1}{2}\alpha$, and $w^*_{(T,D\setminus V(T_v))}(w) = 2\beta$. Since $w^*_{(T,D)}(v) = \alpha + \beta = 1$ and $w^*_{(T,D)}(w) = \frac{1}{2}\alpha + 2\beta = 1$, we obtain $\beta = \frac{1}{3}$. By the definition (2) of w^*, we obtain that β is the finite sum of powers of 2, that is, $\beta = 2^{p_1} + \cdots + 2^{p_k}$ for suitable integers $p_1, \ldots, p_k$. Let $p = \max\{|p_1|, \ldots, |p_k|\}$. Since $\frac{1}{3} = 2^{p_1} + \cdots + 2^{p_k}$, we obtain $2^p = 3 \cdot (2^{p_1} + \cdots + 2^{p_k}) \cdot 2^p$. Note that $(2^{p_1} + \cdots + 2^{p_k}) \cdot 2^p$ is an integer. While the right hand side of this equation is divisible by 3, the left hand side is not, which is a contradiction. Hence, $N_T(V_2) \subseteq V_3$.

If $u \in V_1 \cup V_2$ has a neighbor in D, then $|D| = \gamma_e^*(T) > 1$ implies the contradiction $w^*_{(T,D)}(u) > 1$. Hence, $N_T(V_1 \cup V_2) \subseteq V_3 \setminus D$.

(iii) Let v be the common neighbor of u and w. By (ii), we have $v \in V_3 \setminus D$. Let T_v be the component of $T - w$ that contains v. Let $\alpha = w^*_{(T,D\cap V(T_v))}(v)$ and $\beta = w^*_{(T,D\setminus V(T_v))}(w)$. By (i), we obtain $w^*_{(T,D)}(u) = \frac{1}{2}\alpha + \frac{1}{4}\beta = 1$ and $w^*_{(T,D)}(w) = \frac{1}{2}\alpha + \beta = 1$, which implies $\alpha = 2$ and $\beta = 0$. Since $\beta = 0$, we obtain $D \setminus V(T_v) = \emptyset$. Now, if u' is an endvertex of T in the component of $T - v$ that contains w, then $w^*_{(T,D)}(u') \leq \frac{1}{4}\alpha < 1$, which is a contradiction.

(iv) First, we assume that $\mathrm{dist}_T(u_1, v) = 3$. Let u_1xyv be a path in T. By (ii), the vertices x and y belong to $V_3 \setminus D$. Let T_y be the component of $T - v$ that contains y. Let $\alpha = w^*_{(T,D\cap V(T_y))}(y)$ and $\beta = w^*_{(T,D\setminus V(T_y))}(v)$. By (i), we obtain $w^*_{(T,D)}(u_1) = w^*_{(T,D)}(u_2) = \frac{1}{4}\alpha + \frac{1}{8}\beta = 1$ and $w^*_{(T,D)}(v) = \frac{1}{2}\alpha + \beta = 1$, which implies $\frac{1}{4}\alpha + \frac{7}{8}\beta = \left(\frac{1}{2}\alpha + \beta\right) - \left(\frac{1}{4}\alpha + \frac{1}{8}\beta\right) = 0$. Since, by definition, α and β are non-negative, we obtain the contradiction $\alpha = \beta = 0$.

Next, we assume that $\mathrm{dist}_T(u_1, v) = 4$. Let u_1xyzv be a path in T. Let T_y be the component of $T - \{xy, yz\}$ that contains y, and let T_z be the component of $T - \{yz, zv\}$ that contains z. Let $\alpha = w^*_{(T,D\cap V(T_y))}(y), \beta = w^*_{(T,D\cap V(T_z))}(z)$, and $\gamma = w^*_{(T,D\setminus(V(T_y)\cup V(T_z)))}(v)$. By (i), we obtain $w^*_{(T,D)}(u_1) = w^*_{(T,D)}(u_2) = \frac{1}{4}\alpha + \frac{1}{8}\beta + \frac{1}{16}\gamma = 1$ and $w^*_{(T,D)}(v) = \frac{1}{4}\alpha + \frac{1}{2}\beta + \gamma = 1$, which implies $\frac{3}{8}\beta + \frac{15}{16}\gamma = 0$, and, hence, $\beta = \gamma = 0$, and $\alpha = 4$. Now, if u is an endvertex of T that lies in the component of $T - z$ that contains v, then $w^*_{(T,D)}(u) \le \frac{1}{8}\alpha < 1$, which is a contradiction. □

Our next result would be an immediate consequence of Conjecture 5.

Theorem 7. *If T is a subcubic tree, then $\gamma_e(T) = \gamma^*_{e,f}(T)$ if and only if T is $K_{1,3}$.*

Proof. If $T = K_{1,3}$, then $\gamma_e(T) = 1 = \frac{4+2}{6} = \gamma^*_{e,f}(T)$, which implies the sufficiency. In order to prove the necessity, let T be a subcubic tree with $\gamma_e(T) = \gamma^*_{e,f}(T)$. By (5), we have $\gamma_e(T) = \gamma^*_e(T) = \gamma^*_{e,f}(T)$. If $\gamma_e(T) = 1$, then $T \in \{P_1, P_2, P_3, K_{1,3}\}$. By Theorem 2, the only tree T in this set with $\gamma^*_{e,f}(T) = 1$ is $K_{1,3}$. Hence, we may assume that $\gamma_e(T) > 1$, which implies $\gamma^*_e(T) = \gamma^*_{e,f}(T) > 1$. Let D be a minimum exponential dominating set of T. Note that D is also a minimum porous exponential dominating set. Let u be an endvertex of T, and let v be the neighbor of u in T. Theorem 6(i) and (ii) imply $w^*_{(T,D)}(u) = 1$, $d_T(v) = 3$, and $u, v \notin D$. Now, $1 \le w_{(T,D)}(u) \le w^*_{(T,D)}(u) = 1$, which implies $w_{(T,D)}(u) = w^*_{(T,D)}(u) = 1$. Since $u, v \notin D$, we obtain $w_{(T,D)}(v) = w^*_{(T,D)}(v) = 2$. By Lemma 1 applied to the graph $T - u$ and the vertex v, which is of degree 2 in $T - u$, we obtain that the tree $T - u$ contains a full binary tree T' rooted in v such that $V(T') \cap D$ is exactly the set of leaves of T'. Since $v \notin D$, the tree T' has at least two leaves. Let u' be a leaf of T', and let v' be the parent of u' in T'. By Theorem 6(ii), we have $D \subseteq V_3$, implying that no leaf of T' is an endvertex of T. In particular, u' is not an endvertex of T. Let u'' be an endvertex of T in the component of $T - v'$ that contains u'. Since T' has more than one leaf, we obtain $w_{(T,D)}(u'') < w^*_{(T,D)}(u'')$. Nevertheless, by Theorem 6(i), we obtain $w^*_{(T,D)}(u'') = 1$, which implies the contradiction $1 \le w_{(T,D)}(u'') < w^*_{(T,D)}(u'') = 1$. □

It follows immediately from Theorem 7 that $K_{1,3}$ is the only subcubic tree T with $\gamma(T) = \gamma^*_{e,f}(T)$.

2.3. Lower bounds on the fractional relaxation

Our next result gives lower bounds on the fractional exponential domination number in more general settings. Again its proof relies on linear programming arguments.

Theorem 8. *Let G be a graph of order n, maximum degree Δ, and diameter d.*

(i) $\gamma^*_{e,f}(G) \ge \frac{d+3}{6}$.
(ii) *If $\Delta = 3$, then* $\gamma^*_{e,f}(G) \ge \frac{n}{2+3d}$.
(iii) *If $\Delta \ge 4$, then* $\gamma^*_{e,f}(G) \ge \left(\frac{\left(\frac{\Delta-1}{2}\right)-1}{\Delta\left(\frac{\Delta-1}{2}\right)^d-3}\right) n$.

Proof. (i) Let $P : x_0 \dots x_d$ be a shortest path of length d in G. Let $(y(u))_{u\in V(G)}$ be such that

$$y(u) = \begin{cases} \frac{1}{3}, & \text{if } u \text{ is an endvertex of } P,\\ \frac{1}{6}, & \text{if } u \text{ is an internal vertex of } P, \text{ and}\\ 0, & \text{if } u \text{ is in } V(G) \setminus V(P). \end{cases}$$

Let $u \in V(G)$.

If $u = x_i$ for some $i \in [d-1]$, then

$$\begin{aligned} &\sum_{v\in V(G)} \left(\frac{1}{2}\right)^{\mathrm{dist}_G(u,v)-1} \cdot y(v)\\ &= \sum_{v\in V(P)} \left(\frac{1}{2}\right)^{\mathrm{dist}_P(u,v)-1} \cdot y(v)\\ &= \underbrace{\left(\frac{1}{2}\right)^{i-1} \cdot \frac{1}{3} + \sum_{j=1}^{i-1} \left(\frac{1}{2}\right)^{i-j-1} \cdot \frac{1}{6}}_{=\frac{1}{3}} + \underbrace{\left(\frac{1}{2}\right)^{-1} \cdot \frac{1}{6}}_{=\frac{1}{3}} + \underbrace{\sum_{j=1}^{d-i-1} \left(\frac{1}{2}\right)^{j-1} \cdot \frac{1}{6} + \left(\frac{1}{2}\right)^{d-i-1} \cdot \frac{1}{3}}_{=\frac{1}{3}}\\ &= 1. \end{aligned}$$

Similarly, if $i \in \{0, d\}$, then we obtain $\sum_{v\in V(G)} \left(\frac{1}{2}\right)^{\mathrm{dist}_G(u,v)-1} \cdot y(v) = 1$.

Now, let $u \in V(G) \setminus V(P)$. By Lemma 4 in [5], there is a vertex $u' \in V(P)$ with $\mathrm{dist}_G(u, v) \geq \mathrm{dist}_G(u', v)$ for every vertex v of P. This implies

$$\begin{aligned} \sum_{v\in V(G)} \left(\frac{1}{2}\right)^{\mathrm{dist}_G(u,v)-1} \cdot y(v) &= \sum_{v\in V(P)} \left(\frac{1}{2}\right)^{\mathrm{dist}_G(u,v)-1} \cdot y(v)\\ &\leq \sum_{v\in V(P)} \left(\frac{1}{2}\right)^{\mathrm{dist}_G(u',v)-1} \cdot y(v)\\ &\leq 1. \end{aligned}$$

Altogether, we obtain that $(y(u))_{u\in V(G)}$ is a feasible solution for the dual of the linear program (4) (cf. (7) with "T" replaced by "G"), and, by weak duality, $\gamma^*_{e,f}(G) \geq \sum_{v\in V(G)} y(v) = \frac{d+3}{6}$.

(ii) and (iii) Let $(y(u))_{u\in V(G)}$ be such that $y(u) = y$ for every vertex u of G and some $y > 0$. Let $u \in V(G)$. Since there are at most $\Delta(\Delta-1)^{i-1}$ vertices at distance i from u for $i \in [d]$, we obtain

$$\begin{aligned} \sum_{v\in V(G)} \left(\frac{1}{2}\right)^{\mathrm{dist}_G(u,v)-1} \cdot y(v) &\leq 2y + \sum_{i=1}^{d} \Delta(\Delta-1)^{i-1} \left(\frac{1}{2}\right)^{i-1} y\\ &= \begin{cases} (2+3d)y, & \text{if } \Delta = 3, \text{ and}\\ \dfrac{\Delta\left(\frac{\Delta-1}{2}\right)^d - 3}{\left(\frac{\Delta-1}{2}\right) - 1} y, & \text{if } \Delta \geq 4. \end{cases} \end{aligned}$$

If $\Delta = 3$, then choosing $y = \frac{1}{2+3d}$ yields a feasible solution of the dual of (4), which implies $\gamma^*_{e,f}(G) \geq \frac{n}{2+3d}$. Similarly, if $\Delta \geq 4$, then choosing $y = \frac{\left(\frac{\Delta-1}{2}\right)-1}{\Delta\left(\frac{\Delta-1}{2}\right)^d-3}$ yields $\gamma^*_{e,f}(G) \geq \left(\frac{\left(\frac{\Delta-1}{2}\right)-1}{\Delta\left(\frac{\Delta-1}{2}\right)^d-3}\right) n$. $\square$

Since $\max\left\{\frac{d+3}{6}, \frac{n}{2+3d}\right\} \geq \frac{1}{6}\left(\sqrt{2n + \frac{49}{36}} + \frac{7}{6}\right)$, the following corollary is immediate.

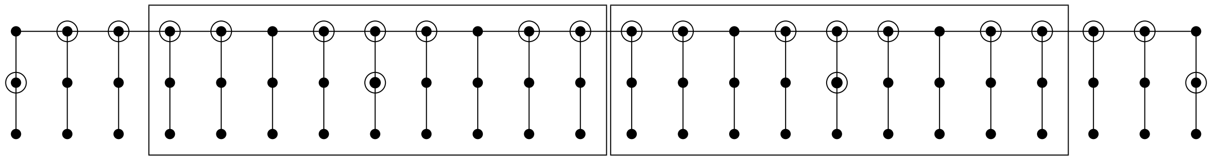

Fig. 3. A family of trees T for which $\gamma_e(T) = \gamma(T)$ and $\frac{\gamma_e^*(T)}{\gamma_e(T)} \leq \frac{8}{9} + o(n(T))$. The encircled vertices indicate some porous exponential dominating set.

Corollary 9. *If G is a subcubic graph of order n, then $\gamma^*_{e,f}(G) \geq \frac{1}{6}\left(\sqrt{2n + \frac{49}{36}} + \frac{7}{6}\right)$.*

Bessy et al. [4] proved that $\gamma_e(G) \geq \frac{n(G)}{6\log_2(n(G)+2)+4}$ for a connected cubic graph G, which is best possible up to the exponent of the log-term in the denominator. It is conceivable that similar lower bounds hold for $\gamma_e^*(G)$ or even $\gamma^*_{e,f}(G)$, which would greatly improve Corollary 9.

2.4. Subcubic trees T with $\gamma(T) = \gamma_e(T)$

Our next goal is a characterization of the subcubic trees T with $\gamma(T) = \gamma_e(T)$. As we have observed in the introduction, no efficient algorithms are known to determine the exponential domination number of general trees or the porous exponential number of subcubic trees. Therefore, it seems difficult to extend our characterization to all trees, or to characterize the subcubic trees T with $\gamma(T) = \gamma_e^*(T)$. The family of trees obtained by repeating the pattern indicated in Fig. 3 shows that the subcubic trees T with $\gamma(T) = \gamma_e^*(T)$ form a proper subset of those with $\gamma(T) = \gamma_e(T)$.

Let G be a graph. For a vertex x of G, let $\tau_G(x)$ be the minimum real value τ such that there is a set D of vertices of G with

- $|D| < \gamma_e(G)$,
- $x \notin D$,
- $w_{(G,D)}(u) + \left(\frac{1}{2}\right)^{\mathrm{dist}_{G-D}(x,u)} \cdot \tau \geq 1$ for every vertex u in $V(G) \setminus D$.

Now, we define three operations on trees. Let T and T' be two trees.

- *Operation 1*

  T arises from T' by *applying Operation 1* if T has an endvertex y with neighbor x such that $T' = T - y$, and x belongs to some minimum dominating set of T'.
- *Operation 2*

  T arises from T' by *applying Operation 2* if T contains a path xyz such that $\tau_{T'}(x) > 1$ or $\gamma(T', V(T') \setminus \{x\}) < \gamma(T')$, where y has degree 2 in T, z is an endvertex of T, and $T' = T - \{y, z\}$.
- *Operation 3*

  T arises from T' by *applying Operation 3* if T contains a path $wxyz$ such that x and y have degree 2 in T, z is an endvertex of T, $T' = T - \{x, y, z\}$, and $\tau_{T'}(w) > \frac{1}{2}$.

Let $\mathcal{T}$ be the family of subcubic trees that are obtained from P_1 by applying finite sequences of the above three operations.

Lemma 10. *If T' is a subtree of a subcubic tree T, then $\gamma_e(T') \leq \gamma_e(T)$.*

Proof. By an inductive argument, it suffices to consider the case that $T' = T - y$, where y is an endvertex of T. Let x be the neighbor of y. Let D be a minimum exponential dominating set of T. If $y \notin D$, then D is also an exponential dominating set of T'. If $y \in D$, then $x \notin D$, because D is minimum. Let $D' = (D \setminus \{y\}) \cup \{x\}$. Suppose that there is some vertex u with $w_{(T,D')}(u) < 1$. Clearly, $u \neq x$. Let e be the edge of the path P between u and x that is incident with x. Let T_x be the component of $T - e$ that contains x, and let $D_x = D \cap V(T_x)$. Since $w_{(T,D')}(u) < w_{(T,D)}(u)$, the path P does not intersect D. This implies

$$\begin{aligned} w_{(T,D')}(u) &= w_{(T,D)}(u) - w_{(T,D_x)}(u) + w_{(T,\{x\})}(u) \\ &= w_{(T,D)}(u) - \left(\frac{1}{2}\right)^{\mathrm{dist}_T(u,x)} \cdot w_{(T_x,D_x)}(x) + \left(\frac{1}{2}\right)^{\mathrm{dist}_T(u,x)-1}. \end{aligned}$$

Since $w_{(T,D')}(u) < w_{(T,D)}(u)$, this implies $w_{(T_x,D_x)}(x) > 2$, which contradicts Lemma 1. Hence, D' is an exponential dominating set of T'. Altogether, we obtain $\gamma_e(T') \leq \gamma_e(T)$. □

Lemma 11. *If $T \in \mathcal{T}$, then $\gamma_e(T) = \gamma(T)$.*

Proof. Note that $\gamma(P_1) = \gamma_e(P_1)$. By an inductive argument, it suffices to show that $\gamma(T) = \gamma_e(T)$ for every tree T that arises from some tree T' with $\gamma(T') = \gamma_e(T')$ by applying one of the above three operations.

First, let T arise from T' by applying Operation 1. Since x belongs to some minimum dominating set of T', we have $\gamma(T') = \gamma(T)$. By Lemma 10, we obtain

$$\gamma(T) = \gamma(T') = \gamma_e(T') \leq \gamma_e(T) \leq \gamma(T),$$

which implies $\gamma_e(T) = \gamma(T)$.

Next, let T arise from T' by applying Operation 2.

First, we assume that $\tau_{T'}(x) > 1$. By Lemma 10, we have $\gamma_e(T') \leq \gamma_e(T)$. Suppose that $\gamma_e(T') = \gamma_e(T)$. Let D be a minimum exponential dominating set of T. By Lemma 1, the set D must contain either y or z. Clearly, we may assume $y \in D$ and $z \notin D$. Let $D' = D \setminus \{y\}$. Since $|D'| < \gamma_e(T')$, the set D' is not an exponential dominating set of T', which implies that $x \notin D'$. Since

$$\begin{aligned} w_{(T,D)}(u) &= w_{(T,D')}(u) + \left(\frac{1}{2}\right)^{\mathrm{dist}_{T-D'}(u,y)-1} \\ &= w_{(T,D')}(u) + \left(\frac{1}{2}\right)^{\mathrm{dist}_{T'-D'}(u,x)} \cdot 1 \\ &\geq 1, \end{aligned}$$

for every vertex $u \in V(T') \setminus D'$, we obtain the contradiction that $\tau_{T'}(x) \leq 1$. Hence, $\gamma_e(T') + 1 \leq \gamma_e(T)$. Note that $\gamma(T) \leq \gamma(T') + 1$. Now,

$$\gamma(T) \leq \gamma(T') + 1 = \gamma_e(T') + 1 \leq \gamma_e(T) \leq \gamma(T),$$

which implies $\gamma_e(T) = \gamma(T)$.

Next, we assume that $\gamma(T', V(T') \setminus \{x\}) < \gamma(T')$. Let D' be a set of vertices of T' with $|D'| = \gamma(T', V(T') \setminus \{x\})$ such that every vertex in $(V(T') \setminus \{x\}) \setminus D'$ has a neighbor in D'. Since $D' \cup \{y\}$ is a dominating set of T, we obtain $\gamma(T) \leq \gamma(T', V(T') \setminus \{x\}) + 1 \leq \gamma(T')$. By Lemma 10, we obtain

$$\gamma_e(T) \leq \gamma(T) \leq \gamma(T') = \gamma_e(T') \leq \gamma_e(T),$$

which implies $\gamma_e(T) = \gamma(T)$.

Next, let T arise from T' by applying Operation 3. Clearly, $\gamma(T) = \gamma(T') + 1$. Suppose that $\gamma_e(T) \leq \gamma_e(T')$. Let D be a minimum exponential dominating set of T. By Lemma 1, the set D must contain either y or z.

Clearly, we may assume $y \in D$ and $z \notin D$. Arguing similarly as in the proof of Lemma 10, we may assume that $x \notin D$. Let $D' = D \setminus \{y\}$. Since $|D'| < \gamma_e(T')$, the set D' is not an exponential dominating set of T', which implies that $w \notin D'$. Since

$$\begin{aligned} w_{(T,D)}(u) &= w_{(T,D')}(u) + \left(\frac{1}{2}\right)^{\operatorname{dist}_{T-D'}(u,y)-1} \\ &= w_{(T,D')}(u) + \left(\frac{1}{2}\right)^{\operatorname{dist}_{T'-D'}(u,w)} \cdot \frac{1}{2} \\ &\geq 1, \end{aligned}$$

for every vertex $u \in V(T') \setminus D'$, we obtain the contradiction that $\tau_{T'}(w) \leq \frac{1}{2}$. Hence, $\gamma_e(T') + 1 \leq \gamma_e(T)$. Now,

$$\gamma(T) = \gamma(T') + 1 = \gamma_e(T') + 1 \leq \gamma_e(T) \leq \gamma(T),$$

which implies $\gamma_e(T) = \gamma(T)$. $\square$

Theorem 12. *If T is a subcubic tree, then $\gamma(T) = \gamma_e(T)$ if and only if $T \in \mathcal{T}$.*

Proof. Lemma 11 implies the sufficiency. In order to prove the necessity, suppose that T is a subcubic tree of minimum order such that $\gamma(T) = \gamma_e(T)$ and $T \notin \mathcal{T}$. Considering three applications of Operation 1 to P_1 implies $P_2, P_3, K_{1,3} \in \mathcal{T}$, that is, $\mathcal{T}$ contains all subcubic trees of diameter at most 2. Hence, the tree T has diameter at least 3. Let v be an endvertex of a longest path in T. The vertex v has a unique neighbor u in T.

Claim 1. *The vertex u has degree 2.*

Proof of Claim 1. Suppose that u has degree 3 in T. This implies that u has a neighbor w that is an endvertex of T distinct from v. Let $T' = T - w$. Clearly, u belongs to some minimum dominating set of T', which implies $\gamma(T) = \gamma(T')$. Since u has degree 2 in T', and is adjacent to the endvertex v, arguing as above (cf. Fig. 1), we obtain that T' has a minimum exponential dominating set D' that contains u. Since D' is also an exponential dominating set of T, we obtain $\gamma_e(T) \leq \gamma_e(T')$. By Lemma 10, we have $\gamma_e(T) = \gamma_e(T')$. Now, $\gamma(T') = \gamma(T) = \gamma_e(T) = \gamma_e(T')$. By the choice of T, we obtain $T' \in \mathcal{T}$. Since T arises from T' by applying Operation 1, we obtain $T \in \mathcal{T}$, which is a contradiction. $\square$

Let x be the neighbor of u distinct from v. Let $T'' = T - \{u, v\}$.

Claim 2. *$\tau_{T''}(x) > 1$ or $\gamma(T'', V(T'') \setminus \{x\}) < \gamma(T'')$.*

Proof of Claim 2. Suppose that $\tau_{T''}(x) \leq 1$ and $\gamma(T'', V(T'') \setminus \{x\}) \geq \gamma(T'')$. Arguing as above, we obtain that the first condition implies $\gamma_e(T) = \gamma_e(T'')$, and that the second condition implies $\gamma(T) = \gamma(T'') + 1$. Now, we obtain the contradiction $\gamma_e(T) = \gamma_e(T'') \leq \gamma(T'') < \gamma(T)$. $\square$

If $\gamma_e(T'') = \gamma(T'')$, then, by the choice of T, we have $T'' \in \mathcal{T}$, and, by Claim 2, the tree T arises from T'' by applying Operation 2, which implies the contradiction $T \in \mathcal{T}$. Hence, we may assume that $\gamma_e(T'') < \gamma(T'')$.

Clearly, $\gamma_e(T) \leq \gamma_e(T'') + 1$, and we obtain

$$\gamma(T) = \gamma_e(T) \leq \gamma_e(T'') + 1 \leq \gamma(T'') \leq \gamma(T),$$

which implies $\gamma(T'') = \gamma(T) = \gamma_e(T) = \gamma_e(T'') + 1$.

If x has degree 3, then, by the choice of v, either x has a neighbor that is an endvertex or there is a path $v'u'x$, where v' is an endvertex that is distinct from v. In both cases, T has a minimum dominating set that contains u and either x or u', which implies the contradiction $\gamma(T'') < \gamma(T)$. Hence, the vertex x has degree 2.

Let y be the neighbor of x that is distinct from u.

Let $T''' = T - \{x, u, v\}$. Clearly, $\gamma_e(T) \le \gamma_e(T''') + 1$.

Suppose that $\tau_{T'''}(y) \le \frac{1}{2}$. By adding u to the set D of vertices of T''' whose existence is guaranteed by $\tau_{T'''}(y) \le \frac{1}{2}$, we obtain $\gamma_e(T) \le \gamma_e(T''')$. Since T''' is a subtree of T'', Lemma 10 implies the contradiction

$$\gamma_e(T''') + 1 \le \gamma_e(T'') + 1 = \gamma_e(T) \le \gamma_e(T''').$$

Hence, $\tau_{T'''}(y) > \frac{1}{2}$, which implies $\gamma_e(T) = \gamma_e(T''') + 1$.

Since $\gamma(T) = \gamma(T''') + 1$, we obtain

$$\gamma_e(T''') = \gamma_e(T) - 1 = \gamma(T) - 1 = \gamma(T''').$$

By the choice of T, this implies that $T''' \in \mathcal{T}$, and that the tree T arises from T''' by applying Operation 3, which implies the contradiction $T \in \mathcal{T}$. □

A drawback of the above characterization is the use of the values $\tau_G(u)$ and conditions such as "$\gamma(T', V(T') \setminus \{x\}) < \gamma(T')$" in the definition of Operation 2. It is conceivable that these technical complications can be eliminated, and that a completely explicit (constructive) characterization is possible.

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4 Hereditary Equality of Domination and Exponential Domination

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HEREDITARY EQUALITY OF DOMINATION AND EXPONENTIAL DOMINATION

Michael A. Henning

Department of Pure and Applied Mathematics
University of Johannesburg
Auckland Park, 2006, South Africa

e-mail: mahenning@uj.ac.za

Simon Jäger

and

Dieter Rautenbach

Institute of Optimization and Operations Research
Ulm University, Ulm, Germany

e-mail: simon.jaeger@uni-ulm.de
dieter.rautenbach@uni-ulm.de

Abstract

We characterize a large subclass of the class of those graphs G for which the exponential domination number of H equals the domination number of H for every induced subgraph H of G.

Keywords: domination, exponential domination, hereditary class.

2010 Mathematics Subject Classification: 05C69.

1. Introduction

Domination in graphs is an important area within graph theory, and an astounding variety of different domination parameters are known [6]. Essentially all of these parameters involve merely local conditions, which makes them amenable to similar approaches and arguments. In [5] Dankelmann *et al.* introduce a truly non-local variant of domination, the so-called exponential domination, where the influence of vertices extends to any arbitrary distance within the graph but decays exponentially with that distance. There is relatively few research concerning exponential domination [1–4], and even apparently basic results require new and careful arguments.

As follows easily from the precise definitions given below, the exponential domination number of any graph is at most its domination number. Bessy *et al.* [4] show that computing the exponential domination number is APX-hard for subcubic graphs and describe an efficient algorithm for subcubic trees, but the complexity for general trees is unknown. It is not even known how to decide efficiently for a given tree T whether its exponential domination number $\gamma_e(T)$ equals its domination number $\gamma(T)$. In [8] we study relations between the different parameters of exponential domination and domination. Next to several bounds, we obtain a constructive characterization of the subcubic trees T with $\gamma_e(T) = \gamma(T)$. In view of the efficient algorithms to determine both parameters for such trees, the existence of a constructive characterization is not surprising, but, as said a few lines above, already for general trees all techniques from [3, 4, 8] completely fail.

Note that, since adding a universal vertex to any graph results in a graph G with $\gamma_e(G) = \gamma(G)$, the class of all graphs G that satisfy $\gamma_e(G) = \gamma(G)$ is not hereditary, and does not have a simple structure. The difficulty to decide whether $\gamma_e(G) = \gamma(G)$ for a given graph G motivates the study of the hereditary class $\mathcal{G}$ of graphs that satisfy this equality, that is, $\mathcal{G}$ is the set of those graphs G such that $\gamma_e(H) = \gamma(H)$ for every induced subgraph H of G. As for the well-known class of perfect graphs, the class $\mathcal{G}$ can be characterized by minimal forbidden induced subgraphs.

In the present paper we obtain such a characterization for a large subclass of $\mathcal{G}$, and pose several related conjectures.

Before we proceed to our results, we collect some notation. We consider finite, simple, and undirected graphs, and use standard terminology. The vertex set and the edge set of a graph G are denoted by $V(G)$ and $E(G)$, respectively. The order $n(G)$ of G is the number of vertices of G. For a vertex u of G, the neighborhood of u in G and the degree of u in G are denoted by $N_G(u)$ and $d_G(u)$, respectively. The distance $\text{dist}_G(X, Y)$ between two sets X and Y of vertices in G is the minimum length of a path in G between a vertex in X and a vertex in Y. If no such path exists, then let $\text{dist}_G(X, Y) = \infty$.

Let D be a set of vertices of a graph G. The set D is a dominating set of G [6] if every vertex of G not in D has a neighbor in D. The domination number $\gamma(G)$ of G is the minimum size of a dominating set of G. For two vertices u and v of G, let $\text{dist}_{(G,D)}(u, v)$ be the minimum length of a path P in G between u and v such that D contains exactly one endvertex of P but no internal vertex of P. If no such path exists, then let $\text{dist}_{(G,D)}(u, v) = \infty$. Note that, if u and v are distinct vertices in D, then $\text{dist}_{(G,D)}(u, u) = 0$ and $\text{dist}_{(G,D)}(u, v) = \infty$. For a vertex u of G, let

$$w_{(G,D)}(u) = \sum_{v \in D} \left(\frac{1}{2}\right)^{\mathrm{dist}_{(G,D)}(u,v)-1},$$

where $\left(\frac{1}{2}\right)^{\infty} = 0$. Dankelmann *et al.* [5] define the set D to be an *exponential dominating set* of G if $w_{(G,D)}(u) \geq 1$ for every vertex u of G, and the *exponential domination number* $\gamma_e(G)$ of G as the minimum size of an exponential dominating set of G. Note that $w_{(G,D)}(u) = 2$ for $u \in D$, and that $w_{(G,D)}(u) \geq 1$ for every vertex u that has a neighbor in D, which implies $\gamma_e(G) \leq \gamma(G)$.

The following Figure 1 contains forbidden induced subgraphs that relate to the considered subclasses of $\mathcal{G}$. Recall that P_k and C_k denote the path and cycle of order k, respectively.

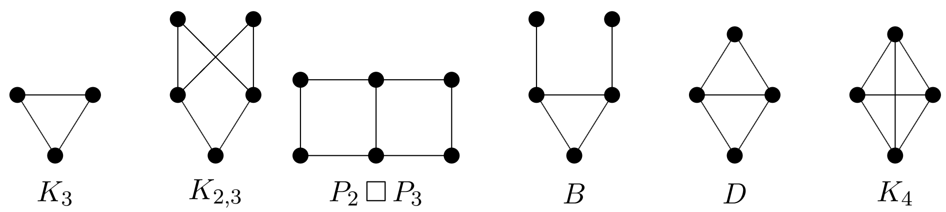

Figure 1. The graphs K_3, $K_{2,3}$, $P_2 \,\square\, P_3$, B (bull), D (diamond), and K_4.

Our main result is the following.

Theorem 1. *If G is a $\{B, D, K_4, K_{2,3}, P_2 \,\square\, P_3\}$-free graph, then $\gamma(H) = \gamma_e(H)$ for every induced subgraph H of G if and only if G is $\{P_7, C_7, F_1, \ldots, F_5\}$-free* (*cf. Figure* 2).

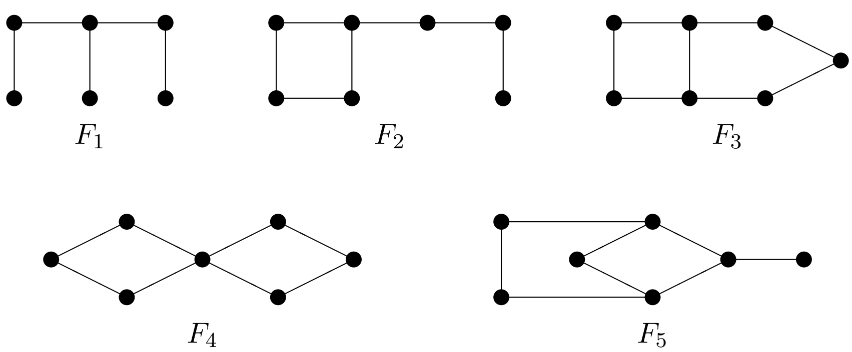

Figure 2. The graphs $F_1, \ldots, F_5$.

Since all graphs in $\{B, D, K_4, K_{2,3}, P_2 \square P_3\} \cup \{F_2, \ldots, F_5\}$ have girth at most 4, where the girth of a graph is the minimum length of a cycle in it, Theorem 1 has the following immediate corollary.

Corollary 2. *If G is a graph of girth at least 5, then $\gamma(H) = \gamma_e(H)$ for every induced subgraph H of G if and only if G is $\{P_7, C_7, F_1\}$-free.*

For the trees in $\mathcal{G}$, we achieve a complete characterization.

Corollary 3. *If T is a tree, then $\gamma(F) = \gamma_e(F)$ for every induced subgraph F of T if and only if T is $\{P_7, F_1\}$-free.*

All proofs and our conjectures are postponed to the next section.

2. Proofs and Conjectures

We split the proof of Theorem 1 into the triangle-free case and the non-triangle-free case. The triangle-free case is considered in the following lemma.

Lemma 4. *If G is a $\{K_3, K_{2,3}, P_2 \square P_3\}$-free graph, then $\gamma(H) = \gamma_e(H)$ for every induced subgraph H of G if and only if G is $\{P_7, C_7, F_1, \ldots, F_5\}$-free.*

Proof. Since $\gamma(H) > \gamma_e(H)$ for every graph H in $\{P_7, C_7, F_1, \ldots, F_5\}$, necessity follows. In order to prove sufficiency, suppose that G is a $\{K_3, K_{2,3}, P_2 \square P_3\} \cup \{P_7, C_7, F_1, \ldots, F_5\}$-free graph with $\gamma(G) > \gamma_e(G)$ of minimum order. By the choice of G, we have $\gamma(H) = \gamma_e(H)$ for every proper induced subgraph H of G. Clearly, G is connected. Since $\gamma_e(G) = 1$ if and only if $\gamma(G) = 1$, we obtain $\gamma_e(G) \geq 2$ and $\gamma(G) \geq 3$. Since G is $\{P_7, C_7\}$-free, either G is a tree or the girth g of G is at most 6.

Suppose that G is a tree. If G has at most one vertex of degree at least 3, then, since G is $\{P_7, F_1\}$-free, it arises from a path $P : u_1 \cdots u_\ell$ with $\ell \leq 6$ by attaching further endvertices to u_2. Since $\ell \leq 6$, the set $\{u_2, u_{\ell-1}\}$ is a dominating set of G, which contradicts $\gamma(G) \geq 3$. Hence, G has at least two vertices of degree at least 3. Let $P : u_1 \cdots u_\ell$ be a shortest path in G between two such vertices. Since G is F_1-free, it arises from P by attaching at least two further endvertices to u_1 and at least two further endvertices to u_ℓ. Since G is P_7-free, we obtain $\ell \leq 4$. This implies that the set $\{u_1, u_\ell\}$ is a dominating set of G, which contradicts $\gamma(G) \geq 3$. Hence, we may assume that G is not a tree. Let $C : x_1 x_2 x_3 \cdots x_g x_1$ be a shortest cycle of G, where we consider the indices modulo g. Let $R = V(G) \setminus V(C)$.

Suppose $g = 6$. Since $\gamma(C_6) = \gamma_e(C_6) = 2$, some vertex y in R has a neighbor x_i on C. Since $g = 6$, the vertex y has no further neighbor on C, implying that $G[\{y, x_{i-2}, x_{i-1}, x_i, x_{i+1}, x_{i+2}\}] = F_1$, contradicting the fact that G is F_1-free. Hence, $g < 6$.

Suppose $g = 5$. This implies that no vertex in R has more than one neighbor on C. If some vertex z has distance 2 from $V(C)$ in G and x_iyz is a path in G, then $G[\{z, y, x_{i-1}, x_i, x_{i+1}, x_{i+2}\}] = F_1$, which is a contradiction. Hence, every vertex in R has a unique neighbor on C. Suppose that there is some $i \in [5]$ such that x_i has a neighbor y_i in R and x_{i+1} has a neighbor y_{i+1} in R. Since $g = 5$, we note that $y_i \neq y_{i+1}$ and that the vertex y_i is not adjacent to y_{i+1}, implying that $G[\{x_{i-2}, x_{i-1}, x_i, x_{i+1}, y_i, y_{i+1}\}] = F_1$, which is a contradiction. This implies the existence of some index $i \in [5]$ such that $\{x_i, x_{i+2}\}$ is a dominating set of G, which contradicts $\gamma(G) \geq 3$. Hence, $g \leq 4$. Since G is K_3-free, this implies that $g = 4$.

Since G is $\{K_3, K_{2,3}\}$-free, no vertex in R has more than one neighbor on C, and since G is F_2-free, no vertex in R has distance more than 2 from $V(C)$.

Suppose that some vertex z has distance 2 from $V(C)$. Let x_1yz be a path in G. Suppose that x_2 has a neighbor u in R. Recall that u is not adjacent to any other vertex on C. Since G is $P_2 \,\square\, P_3$-free, the vertex u is not adjacent to y. If u is not adjacent to z, then $G[\{u, x_1, x_2, x_4, y, z\}] = F_1$, which is a contradiction. If u is adjacent to z, then $G[V(C) \cup \{u, y, z\}] = F_3$, which is a contradiction. Hence, by symmetry, we obtain $d_G(x_2) = d_G(x_4) = 2$.

Suppose that x_1 has a neighbor u in $R \setminus \{y\}$. Since G is $\{K_3, K_{2,3}\}$-free, the vertex u is not adjacent to any vertex in $\{x_2, x_3, x_4, y\}$. If u is not adjacent to z, then $G[\{x_1, x_2, x_3, u, y, z\}] = F_1$, which is a contradiction. If u is adjacent to z, then $G[V(C) \cup \{u, y, z\}] = F_4$, which is a contradiction. Hence, we obtain $d_G(x_1) = 3$.

Since $\{x_3, y\}$ is not a dominating set of G, and no vertex in R has distance more than 2 from $V(C)$, the degrees of x_1, x_2, and x_4 imply the existence of a path x_3uv, where v has distance 2 to $V(C)$, and v is not adjacent to y. Since $G[\{v, u, x_3, x_2, x_1, y, z\}]$ is neither P_7 nor C_7, the vertex u is adjacent to y or z. If u is adjacent to z, then, because G is K_3-free, $G[\{u, v, y, z, x_3, x_2\}] = F_1$, which is a contradiction. Hence, the vertex u is adjacent to y. If v is adjacent to z, then $G[\{u, v, y, z, x_1, x_2, x_3\}] = F_3$, which is a contradiction. Hence, the vertex v is not adjacent to z, and $G[\{u, v, y, z, x_3, x_2\}] = F_1$, which is a contradiction. Hence, every vertex in R has a unique neighbor on C.

Since $\gamma(G) > 2$, we may assume that x_i has a neighbor y_i in R for $i \in [3]$. Since G is $P_2 \,\square\, P_3$-free, the vertex y_2 is not adjacent to y_1 or y_3. Since G is F_5-free, the vertex y_1 is not adjacent to y_3. Now, $G[\{x_1, x_2, x_3, y_1, y_2, y_3\}] = F_1$, which is a contradiction, and completes the proof. ■

With Lemma 4 at hand, we now proceed to the proof of Theorem 1.

***Proof of Theorem* 1.** Necessity follows as above. In order to prove sufficiency, suppose that G is a $\{B, D, K_4, K_{2,3}, P_2 \,\square\, P_3\} \cup \{P_7, C_7, F_1, \ldots, F_5\}$-free graph with $\gamma(G) > \gamma_e(G)$ of minimum order. By the choice of G, we have $\gamma(H) = \gamma_e(H)$

for every proper induced subgraph H of G. Clearly, G is connected. Since $\gamma_e(G) = 1$ if and only if $\gamma(G) = 1$, we obtain $\gamma_e(G) \geq 2$ and $\gamma(G) \geq 3$.

By Lemma 4, G is not K_3-free, that is, the girth of G is 3.

We proceed with a series of claims. Let F be the graph that is obtained from the triangle $x_1x_2x_3$ and the path $y_1y_2y_3$ by adding the edge x_1y_1.

Claim 1. *F is not an induced subgraph of G.*

Proof. Suppose that F is an induced subgraph of G. Since $\{x_1, y_2\}$ is not a dominating set of G, there is a vertex u at distance 2 from the set $\{x_1, y_2\}$ in G.

We proceed with three subclaims.

Claim 1.1. *The vertex u is not adjacent to x_2 or x_3.*

Proof. Suppose that u is adjacent to x_2. Since G is D-free, the vertex u is not adjacent to x_3, and, since G is B-free, u is adjacent to y_1. If u is not adjacent to y_3, then $G[\{u, x_1, x_3, y_1, y_2, y_3\}] = F_1$, which is a contradiction. If u is adjacent to y_3, then $G[\{u, x_1, x_2, y_1, y_2, y_3\}] = P_2 \square P_3$, which is a contradiction. Hence, by symmetry, we obtain that u is not adjacent to x_2 or x_3. □

Claim 1.2. *The vertex u is not adjacent to y_1.*

Proof. Suppose that u is adjacent to y_1. Since G is F_1-free, the vertex u is adjacent to y_3. Since $\{x_1, y_3\}$ is not a dominating set of G, there is a vertex v at distance 2 from the set $\{x_1, y_3\}$. Suppose that v is adjacent to x_2. Since G is D-free, the vertex v is not adjacent to x_3, and, since G is B-free, v is adjacent to y_1. If v is adjacent to u, then $G[\{u, v, x_2, y_1, y_3\}] = B$, which is a contradiction. Hence, v is not adjacent to u, and, by symmetry, v is also not adjacent to y_2. Therefore, $G[\{u, v, x_1, x_2, y_1, y_2, y_3\}] = F_4$, which is a contradiction. Thus, by symmetry, v is not adjacent to x_2 or x_3. Next, suppose that v is adjacent to y_1. Since G is F_1-free, the vertex v is adjacent to both u and y_2, which yields the contradiction $G[\{u, v, y_1, y_2\}] = D$. Thus, v is not adjacent to y_1. Suppose that v is adjacent to u. If v is adjacent to y_2, then $G[\{u, v, y_1, y_2, y_3\}] = K_{2,3}$, which is a contradiction. If v is not adjacent to y_2, then $G[\{u, v, x_1, x_2, y_1, y_2\}] = F_1$, which is a contradiction. Thus, by symmetry, v is not adjacent to u or y_2, implying that v is at distance 2 from the set $\{u, x_1, x_2, x_3, y_1, y_2, y_3\}$.

Since the vertex v is at distance 2 from the set $\{x_1, y_3\}$ in G, there is a neighbor v' of v, that is adjacent to x_1 or to y_3 or to both x_1 and y_3. First, suppose that v' is not adjacent to x_1, implying that v' is adjacent to y_3. Suppose that v' is adjacent to y_1. If v' is adjacent to u, then $G[\{u, v', y_1, y_3\}] = D$, which is a contradiction. Thus, by symmetry, v' is adjacent to neither u nor y_2, implying that $G[\{u, v', y_1, y_2, y_3\}] = K_{2,3}$, which is a contradiction. Thus, v' is not adjacent to y_1. Since G is B-free, v' is not adjacent to u or y_2, which yields the contradiction $G[\{v, v', x_1, x_2, y_1, y_2, y_3\}] = P_7$. Therefore, v' is adjacent to x_1.

Since G is $\{B, K_4\}$-free, the vertex v' is not adjacent to x_2 or x_3. Since G is B-free, the vertex v' is not adjacent to y_1. Suppose that v' is not adjacent to y_3. If v' is not adjacent to u, then $G[\{u, v, v', x_1, x_2, y_1\}] = F_1$, which is a contradiction. Thus, by symmetry, v' is adjacent to both u and y_2, which yields the contradiction $G[\{u, v', y_1, y_2, y_3\}] = K_{2,3}$. Thus, v' is adjacent to y_3. Since G is F_1-free, the vertex v' is adjacent to both u and y_2, implying that $G[\{u, v, v', y_1, y_3\}] = B$, which is a contradiction. Therefore, u is not adjacent to y_1. □

Claim 1.3. *The vertex u is not adjacent to y_3.*

Proof. Suppose that u is adjacent to y_3. Since $\{x_1, y_3\}$ is not a dominating set of G, there is a vertex v at distance 2 from the set $\{x_1, y_3\}$ in G.

Suppose that v is adjacent to x_2. Since G is D-free, the vertex v is not adjacent to x_3. Since G is B-free, v is adjacent to y_1. If v is not adjacent to y_2, then $G[\{v, x_1, x_3, y_1, y_2, y_3\}] = F_1$, which is a contradiction. If v is adjacent to y_2, then we get the contradiction $G[\{x_2, v, y_1, y_2, y_3\}] = B$. Therefore, by symmetry, v is not adjacent to x_2 or x_3.

Next, suppose that v is adjacent to y_1. If v is not adjacent to y_2, then $G[\{v, x_1, x_2, y_1, y_2, y_3\}] = F_1$, which is a contradiction. If v is adjacent to y_2, then $G[\{v, x_1, y_1, y_2, y_3\}] = B$, which is a contradiction. Thus, v is not adjacent to y_1.

Next, suppose that v is adjacent to y_2. If v is not adjacent to u, then $G[\{u, v, x_1, y_1, y_2, y_3\}] = F_1$, which is a contradiction. If v is adjacent to u, then $G[\{u, v, x_1, x_2, y_1, y_2, y_3\}] = F_2$, which is a contradiction. Therefore, v is not adjacent to y_2, implying that v is at distance 2 from the set $\{x_1, x_2, x_3, y_1, y_2, y_3\}$.

If v is adjacent to u, then $G[\{u, v, x_1, x_2, y_1, y_2, y_3\}] = P_7$, which is a contradiction. Hence, v is not adjacent to u. Since the vertex v is at distance 2 from the set $\{x_1, y_3\}$ in G, there is a neighbor v' of v that is adjacent to x_1 or to y_3 or to both x_1 and y_3. Note that $v' \neq u$.

First, suppose that v' is not adjacent to x_1, implying that v' is adjacent to y_3. If v' is not adjacent to y_2, then analogous arguments as in Claim 1.1 and Claim 1.2 (with the vertex u replaced by the vertex v') show that y_3 is the only vertex in the set $\{x_1, x_2, x_3, y_1, y_2, y_3\}$ that is adjacent to v'. This in turn implies that $G[\{v, v', x_1, x_2, y_1, y_2, y_3\}] = P_7$, which is a contradiction. Hence, v' is adjacent to y_2. If v' is adjacent to y_1, then $G[\{v', y_1, y_2, y_3\}] = D$, which is a contradiction. Thus, v' is not adjacent to y_1, implying that $G[\{v, v', y_1, y_2, y_3\}] = B$, which is a contradiction. Therefore, v' is adjacent to x_1.

Since G is $\{D, K_4\}$-free, the vertex v' is not adjacent to x_2 or x_3. If v' is adjacent to y_1, then $G[\{v, v', x_1, x_2, y_1\}] = B$, which is a contradiction. Thus, v' is not adjacent to y_1. If v' is not adjacent to y_2, then $G[\{v, v', x_1, x_2, y_1, y_2\}] = F_1$, which is a contradiction. Thus, v' is adjacent to y_2. If v' is not adjacent to y_3, then $G[\{v, v', x_1, x_2, y_2, y_3\}] = F_1$, which is a contradiction. Thus, v' is adjacent to y_3, implying that $G[\{v, v', y_1, y_2, y_3\}] = B$, which is a contradiction. Therefore, u is not adjacent to y_3. □

We return to the proof of Claim 1. By Claims 1.1, 1.2 and 1.3, the vertex u is at distance 2 from the set $\{x_1, x_2, x_3, y_1, y_2, y_3\}$. Since the vertex u is at distance 2 from the set $\{x_1, y_2\}$ in G, there is a neighbor u' of u that is adjacent to x_1 or to y_2 or to both x_1 and y_2. First, suppose that u' is adjacent to x_1. Analogously as above, since G is $\{B, D, K_4\}$-free, the vertex u' is not adjacent to x_2, x_3 and y_1. If u' is not adjacent to y_2, then $G[\{u, u', x_1, x_2, y_1, y_2\}] = F_1$, which is a contradiction. Thus, u' is adjacent to y_2. If u' is adjacent to y_3, then $G[\{u, u', y_1, y_2, y_3\}] = B$, while, if u' is not adjacent to y_3, then $G[\{u, u', x_1, x_2, y_2, y_3\}] = F_1$. Since both cases produce a contradiction, we deduce that u' is not adjacent to x_1, implying that u' is adjacent to y_2. Since G is B-free, u' is not adjacent to y_1. If u' is not adjacent to y_3, then $G[\{u, u', x_1, y_1, y_2, y_3\}] = F_1$, which is a contradiction. If u' is adjacent to y_3, then $G[\{u, u', y_1, y_2, y_3\}] = B$, which is a contradiction. This completes the proof of Claim 1. $\square$

Claim 2. *If C is an arbitrary triangle in G, then every vertex is within distance 2 from $V(C)$.*

Proof. Let $C : x_1x_2x_3$ be a triangle in G. Suppose that there is a vertex y_3 at distance 3 from $V(C)$ in G. Let $x_1y_1y_2y_3$ be a shortest path in G from y_3 to $V(C)$. Since G is $\{D, K_4\}$-free, the vertex y_1 is adjacent to neither x_2 nor x_3, implying that F is an induced subgraph of G, which contradicts Claim 1. $\square$

Claim 3. *Every triangle contains at least one vertex of degree exactly 2 in G.*

Proof. Let $C : x_1x_2x_3$ be a triangle in G. Suppose that every vertex on C has degree at least 3 in G. Let $y_1, y_2, y_3 \in V(G) \setminus V(C)$ be neighbors of x_1, x_2, x_3, respectively. Since G is $\{D, K_4\}$-free, x_i is the only neighbor of y_i in $V(C)$ for $i \in [3]$. Since G is B-free, the vertices y_1, y_2 and y_3 induce a triangle C' in G. Suppose that there is a vertex $y \in V(G) \setminus (V(C) \cup V(C'))$ that is adjacent to a vertex on C, say x_1. Since G is $\{D, K_4\}$-free, x_1 is the only neighbor of y on C, and y is non-adjacent to some vertex y_j on C' with $j \in \{2, 3\}$, which implies the contradiction that $G[\{x_1, x_2, x_3, y, y_j\}] = B$. Hence, each vertex on C has degree exactly 3 in G. By symmetry, each vertex on C' has degree exactly 3 in G. Thus, $G = P_2 \,\Box\, C_3$, implying that $\gamma(G) = \gamma_e(G) = 2$, which is a contradiction. This completes the proof of Claim 3. $\square$

Claim 4. *Every triangle contains two vertices of degree exactly 2 in G.*

Proof. Let $C : x_1x_2x_3$ be a triangle in G and let $R = V(G) \setminus V(C)$. By Claim 3, the triangle C contains at least one vertex of degree exactly 2 in G. Renaming vertices if necessary, we may assume that x_1 has degree 2 in G. Suppose that both x_2 and x_3 have degree at least 3 in G. Since G is D-free, the vertices x_2 and x_3 have no common neighbor in R. Further, since G is B-free, every neighbor of

x_2 in R is adjacent to every neighbor of x_3 in R. Hence, since G is $\{D, K_{2,3}\}$-free, the degrees of x_2 and x_3 are exactly 3 in G. Let y_2 and y_3 in R be neighbors of x_2 and x_3, respectively. Recall that $\gamma(G) \geq 3$. Let w_2 be a vertex not dominated by $\{x_2, y_3\}$, and let w_3 be a vertex not dominated by $\{x_3, y_2\}$. By Claim 2, the vertex w_2 is within distance 2 from $V(C)$, implying that w_2 is adjacent to y_2. Analogously, the vertex w_3 is adjacent to y_3. Note that $w_2 \neq w_3$. If w_2 is adjacent to w_3, then $G[\{w_2, w_3, x_2, x_3, y_2, y_3\}] = P_2 \square P_3$. If w_2 is not adjacent to w_3, then $G[\{w_2, w_3, x_1, x_2, y_2, y_3\}] = F_1$. Both cases produce a contradiction, which completes the proof of Claim 4. □

Let $C : x_1x_2x_3$ be a triangle in G. By Claim 4, we may assume, renaming vertices if necessary, that x_2 and x_3 have degree 2 in G. Since $\gamma(G) \geq 3$, the vertex x_1 does not dominate $V(G)$. Let $D_2 = V(G) \setminus N_G[x_1]$. Claim 2 implies that every vertex in D_2 is at distance exactly 2 from x_1 in G. Let D_1 be the set of neighbors in $V(G) \setminus D_2$ of the vertices in D_2. Note that $D_1 \subset N_G(x_1)$. By Claim 4, the set D_1 is independent.

Claim 5. *Every vertex in D_2 has exactly one neighbor in D_1.*

Proof. Since D_1 is an independent set, and, since G is $K_{2,3}$-free, every vertex in D_2 has at most two neighbors in D_1. Suppose that a vertex w_1 in D_2 has two neighbors y_1, y_2 in D_1. Since $\{x_1, y_1\}$ is not a dominating set of G, there is a vertex $w_2 \in D_2$ that is not adjacent to y_1.

Claim 5.1. *The vertex w_2 is not adjacent to y_2.*

Proof. Suppose that w_2 is adjacent to y_2. Since $\{x_1, y_2\}$ is not a dominating set, there is a vertex w_3 in D_2 that is not adjacent to y_2. Suppose that w_3 is adjacent to y_1. If w_3 is not adjacent to w_2, then $G[\{x_1, x_2, y_1, y_2, w_2, w_3\}] = F_1$, which is a contradiction. Hence, w_3 is adjacent to w_2. If w_3 is adjacent to w_1, then, since G is D-free, w_1 is not adjacent to w_2, implying that $G[\{x_1, y_1, w_1, w_2, w_3\}] = B$, which is a contradiction. Thus, w_3 is not adjacent to w_1. If w_1 is not adjacent to w_2, then $G[\{x_1, x_2, y_1, w_1, w_2, w_3\}] = F_1$, while, if w_1 is adjacent to w_2, then $G[\{x_1, y_2, w_1, w_2, w_3\}] = B$. Since both cases produce a contradiction, we deduce that w_3 is not adjacent to y_1. Since G is $\{D, P_2 \square P_3\}$-free, the vertex w_3 is therefore adjacent to at most one of w_1 and w_2.

Let y_3 be a neighbor of w_3 in D_1. As observed earlier, every vertex in D_2 has at most two neighbors in D_1. In particular, w_1 is not adjacent to y_3. If w_3 is not adjacent to w_1, then $G[\{x_1, x_2, y_1, y_3, w_1, w_3\}] = F_1$, which is a contradiction. Thus, w_3 is adjacent to w_1, implying that w_3 is not adjacent to w_2. If w_2 is not adjacent to y_3, then $G[\{x_1, x_2, y_2, y_3, w_2, w_3\}] = F_1$, which is a contradiction. Hence, w_2 is adjacent to y_3. If w_1 and w_2 are not adjacent, then $G[\{x_1, y_1, y_2, y_3, w_1, w_2\}] = P_2 \square P_3$, which is a contradiction. Hence, w_1 and w_2

are adjacent, implying that $G[\{x_1, y_2, w_1, w_2, w_3\}] = B$, which is a contradiction. Therefore, w_2 is not adjacent to y_2. □

Recall that w_2 is not adjacent to y_1. By Claim 5.1, the vertex w_2 is not adjacent to y_2. Let y_4 be a neighbor of w_2 in D_1. Since every vertex in D_2 has at most two neighbors in D_1, the vertex w_1 is not adjacent to y_4. If w_1 is not adjacent to w_2, then $G[\{x_1, x_2, y_1, y_4, w_1, w_2\}] = F_1$, which is a contradiction. Hence, w_1 is adjacent to w_2. As $\{x_1, w_1\}$ is not a dominating set of G, there is a vertex w_4 in D_2 that is not adjacent to w_1. Since G is F_1-free, the vertex w_4 is adjacent to y_1 or to y_2 or to both y_1 and y_2. If w_4 is adjacent to y_1 and y_2, then $G[\{x_1, y_1, y_2, w_1, w_4\}] = K_{2,3}$, which is a contradiction. Hence, by symmetry, we may assume that w_4 is adjacent to y_1, but not to y_2. If w_4 is adjacent to w_2, then we get the contradiction $G[\{x_1, y_1, y_2, w_1, w_2, w_4\}] = P_2 \,\Box\, P_3$. If w_4 is not adjacent to w_2, then $G[\{x_1, x_2, y_1, y_4, w_2, w_4\}] = F_1$, which is a contradiction, and completes the proof of Claim 5. □

Let $D_1 = \{y_1, \ldots, y_k\}$, and, for $i \in [k]$, let w_i be a neighbor of y_i in D_2. If $k = 1$, then $\{x_1, y_1\}$ is a dominating set of G, which is a contradiction. Hence, $k \geq 2$. By Claim 5, the vertex y_i is the only neighbor of w_i in D_1 for $i \in [k]$. Since G is F_1-free, the vertices $w_1, \ldots, w_k$ induce a clique in G. Thus, by Claim 4, we obtain $k \leq 2$. This implies $k = 2$. Since G is F_1-free, each neighbor of y_i in D_2 is adjacent to every neighbor of y_{3-i} in D_2 for $i \in [2]$. If y_1 and y_2 both have only one neighbor in D_2, then $\{x_1, w_1\}$ is a dominating set of G, which is a contradiction. Hence, by symmetry, we may assume that the vertex y_1 has two neighbors w_1 and w_1' in D_2. Both w_1 and w_1' are adjacent to w_2. Since G is D-free, w_1 and w_1' are not adjacent. Since $\{x_1, w_2\}$ is not a dominating set of G, the vertex y_2 has a neighbor w_2' in D_2 that is different from w_2 and not adjacent to w_2. Thus, $G[\{w_1, w_1', w_2, w_2', y_1\}] = K_{2,3}$, which is a contradiction, and completes the proof of Theorem 1. ■

We close with a number of conjectures.

Conjecture 5. *There is a finite set $\mathcal{F}$ of graphs such that some graph G satisfies $\gamma(H) = \gamma_e(H)$ for every induced subgraph H of G if and only if G is $\mathcal{F}$-free.*

Conjecture 6. *The set $\mathcal{F}$ in Conjecture* 5 *can be chosen such that $\gamma(F) = 3$ and $\gamma_e(F) = 2$ for every graph F in $\mathcal{F}$.*

Our proof of Theorem 1 actually implies that every component of a graph that is $\{B, D, K_4, K_{2,3}, P_2 \,\Box\, P_3\} \cup \{P_7, C_7, F_1, \ldots, F_5\}$-free has domination number at most 2. Wolk [9] showed that the largest hereditary class of graphs for which every component has domination number 1 is the class of $\{P_4, C_4\}$-free graphs. A complete characterization of the largest hereditary class of graphs for which every component has domination number at most 2 in terms of minimal forbidden induced subgraphs seems to be a challenging and interesting problem, to which our results indirectly contribute.

Similar to the definition of an exponential dominating set, Dankelmann *et al.* [5] define a set D of vertices of a graph G to be a *porous exponential dominating set* of G if $w^*_{(G,D)}(u) \geq 1$ for every vertex u of G, where $w^*_{(G,D)}(u) = \sum_{v \in D} \left(\frac{1}{2}\right)^{\mathrm{dist}_G(u,v)-1}$. They define the *porous exponential domination number* $\gamma^*_e(G)$ of G as the minimum size of a porous exponential dominating set of G. Clearly, $\gamma^*_e(G) \leq \gamma_e(G) \leq \gamma(G)$ for every graph G.

Conjecture 7. *A graph G satisfies $\gamma(H) = \gamma_e(H)$ for every induced subgraph H of G if and only if $\gamma(H) = \gamma^*_e(H)$ for every induced subgraph H of G.*

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5 Exponential Independence

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Exponential independence

Simon Jäger, Dieter Rautenbach

Institute of Optimization and Operations Research, Ulm University, Ulm, Germany

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ABSTRACT

For a set S of vertices of a graph G, a vertex u in $V(G)\setminus S$, and a vertex v in S, let $\text{dist}_{(G,S)}(u,v)$ be the distance of u and v in the graph $G-(S\setminus\{v\})$. Dankelmann et al. (2009) define S to be an exponential dominating set of G if $w_{(G,S)}(u)\geq 1$ for every vertex u in $V(G)\setminus S$, where $w_{(G,S)}(u)=\sum_{v\in S}\left(\frac{1}{2}\right)^{\text{dist}_{(G,S)}(u,v)-1}$. Inspired by this notion, we define S to be an exponential independent set of G if $w_{(G,S\setminus\{u\})}(u) < 1$ for every vertex u in S, and the exponential independence number $\alpha_e(G)$ of G as the maximum order of an exponential independent set of G.

Similarly as for exponential domination, the non-local nature of exponential independence leads to many interesting effects and challenges. Our results comprise exact values for special graphs as well as tight bounds and the corresponding extremal graphs. Furthermore, we characterize all graphs G for which $\alpha_e(H)$ equals the independence number $\alpha(H)$ for every induced subgraph H of G, and we give an explicit characterization of all trees T with $\alpha_e(T)=\alpha(T)$.

1. Introduction

Independence in graphs is one of the most fundamental and well-studied concepts in graph theory. In the present paper we propose and study a version of independence where the influence of vertices decays exponentially with respect to distance. This new notion is inspired by the *exponential domination number*, which was introduced by Dankelmann et al. [5] and recently studied in [1–4]. Somewhat related parameters are the well-known *(distance) packing numbers* [8–10] and the *influence numbers* [6,7].

We consider finite, simple, and undirected graphs, and use standard terminology. The vertex set and the edge set of a graph G are denoted by $V(G)$ and $E(G)$, respectively. The order $n(G)$ of G is the number of vertices of G. The distance $\text{dist}_G(u,v)$ between two vertices u and v in a graph G is the minimum number of edges of a path in G between u and v. If no such path exists, then let $\text{dist}_G(u,v)=\infty$. The diameter $\text{diam}(G)$ of G is the maximum distance between vertices of G. A set of pairwise non-adjacent vertices of G is an independent set of G, and the maximum order of an independent set of G is the independence number $\alpha(G)$ of G.

Let S be a set of vertices of G. For two vertices u and v of G, let $\text{dist}_{(G,S)}(u,v)$ be the minimum number of edges of a path P in G between u and v such that S contains exactly one endvertex of P but no internal vertex of P. If no such path exists, then let $\text{dist}_{(G,S)}(u,v)=\infty$. Note that, if u and v are distinct vertices in S, then $\text{dist}_{(G,S)}(u,u)=0$ and $\text{dist}_{(G,S)}(u,v)=\infty$. For a vertex u of G, let

$$w_{(G,S)}(u)=\sum_{v\in S}\left(\frac{1}{2}\right)^{\text{dist}_{(G,S)}(u,v)-1}, \tag{1}$$

where $\left(\frac{1}{2}\right)^{\infty}=0$. Note that $w_{(G,S)}(u)=2$ for $u\in S$.

E-mail addresses: simon.jaeger@uni-ulm.de (S. Jäger), dieter.rautenbach@uni-ulm.de (D. Rautenbach).

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Dankelmann et al. [5] define a set S of vertices to be *exponential dominating* if

$$w_{(G,S)}(u) \geq 1 \text{ for every vertex } u \text{ in } V(G) \setminus S,$$

and the *exponential domination number* $\gamma_e(G)$ of G as the minimum order of an exponential dominating set. Analogously, we define S to be *exponential independent* if

$$w_{(G,S\setminus\{u\})}(u) < 1 \text{ for every vertex } u \text{ in } S,$$

that is, the accumulated exponentially decaying influence $w_{(G,S\setminus\{u\})}(u)$ of the remaining vertices in $S \setminus \{u\}$ that arrives at any vertex u in S is strictly less than 1. Let the *exponential independence number* $\alpha_e(G)$ of G be the maximum order of an exponential independent set. An (exponential) independent set of maximum order is *maximum*.

Our results comprise exact values for special graphs as well as tight bounds and the corresponding extremal graphs. Furthermore, we characterize all graphs G for which $\alpha_e(H)$ equals the independence number $\alpha(H)$ for every induced subgraph H of G, and we give an explicit characterization of all trees T with $\alpha_e(T) = \alpha(T)$. We conclude with several open problems.

2. Results

We start with some elementary observations concerning exponential independence. Clearly, every exponential independent set is independent, which immediately implies (i) of the following theorem. The quantity $w_{(G,S\setminus\{u\})}(u)$ does not behave monotonously with respect to the removal of vertices from S. Indeed, if G is a star $K_{1,n-1}$ with center v, and $S = V(G)$ for instance, then $w_{(G,S\setminus\{u\})}(u) = 1$ for every endvertex u of G but $w_{(G,S\setminus\{u,v\})}(u) = \frac{n-2}{2}$, which can be smaller or bigger than 1. In view of this observation part (iii) of the following theorem is slightly surprising.

Theorem 1. *Let G be a graph.*

(i) $\alpha_e(G) \leq \alpha(G)$.
(ii) *If H is a subgraph of G and $S \subseteq V(H)$ is an exponential independent set of G, then S is an exponential independent set of H.*
(iii) *A subset of an exponential independent set of G is an exponential independent set of G.*

Proof. (i) follows from the above observation. Since $\text{dist}_{(G,S\setminus\{u\})}(u, v) \leq \text{dist}_{(H,S\setminus\{u\})}(u, v)$ for every two vertices u and v in S, (ii) follows immediately from (1). We proceed to the proof of (iii). Let S be an exponential independent set of G. Let u and v be distinct vertices in S. In order to complete the proof, it suffices to show

$$w_{(G,S\setminus\{u,v\})}(u) \leq w_{(G,S\setminus\{u\})}(u). \tag{2}$$

For

$$\begin{aligned}
S_\infty &= \{w \in S \setminus \{u, v\} : \text{dist}_{(G,S\setminus\{u,v\})}(u, w) = \infty\}, \\
S_= &= \{w \in S \setminus \{u, v\} : \text{dist}_{(G,S\setminus\{u,v\})}(u, w) = \text{dist}_{(G,S\setminus\{u\})}(u, w) < \infty\}, \text{ and} \\
S_> &= \{w \in S \setminus \{u, v\} : \text{dist}_{(G,S\setminus\{u,v\})}(u, w) < \text{dist}_{(G,S\setminus\{u\})}(u, w)\},
\end{aligned}$$

we have $S = \{u, v\} \cup S_= \cup S_> \cup S_\infty$. If $S_> = \emptyset$, then (2) follows immediately from (1). Hence, we may assume that $S_> \neq \emptyset$. Let T be a subtree of G rooted in u such that

- $S_= \cup S_>$ is the set of all leaves of T,
- $\text{dist}_T(u, w) = \text{dist}_{(G,S\setminus\{u,v\})}(u, w)$ for every $w \in S_= \cup S_>$, and
- v is not an ancestor within T of any vertex in $S_=$.

Such a tree can easily be extracted from the union of paths P_w for $w \in S_= \cup S_>$, where P_w is a path of length $\text{dist}_{(G,S\setminus\{u,v\})}(u, w)$ between w and u that intersects $S \setminus \{u, v\}$ only in w, and that avoids v if $w \in S_=$. Since $S_> \neq \emptyset$, the vertex v belongs to T, and the set of leaves of T that are descendants of v is exactly $S_>$. The conditions imposed on T easily imply $\text{dist}_T(u, v) = \text{dist}_{(G,S\setminus\{u\})}(u, v)$. Let $T_>$ be the subtree of T rooted in v that contains v and all its descendants within T. Since S is exponential independent, we obtain $w_{(T_>,S_>)}(v) \leq w_{(G,S\setminus\{v\})}(v) < 1$, which implies

$$\begin{aligned}
w_{(G,S\setminus\{u,v\})}(u) &= w_{(T,S_=)}(u) + w_{(T,S_>)}(u) \\
&= w_{(T,S_=)}(u) + \left(\frac{1}{2}\right)^{\text{dist}_T(u,v)} w_{(T_>,S_>)}(v) \\
&< w_{(T,S_=)}(u) + \left(\frac{1}{2}\right)^{\text{dist}_{(G,S\setminus\{u\})}(u,v)} \\
&= \sum_{w\in S_=} \left(\frac{1}{2}\right)^{\text{dist}_{(G,S\setminus\{u\})}(u,w)-1} + \left(\frac{1}{2}\right)^{\text{dist}_{(G,S\setminus\{u\})}(u,v)}
\end{aligned}$$

$$< \sum_{w\in S_{=}\cup\{v\}} \left(\frac{1}{2}\right)^{\mathrm{dist}_{(G,S\setminus\{u\})}(u,w)-1}$$
$$\leq w_{(G,S\setminus\{u\})}(u),$$

which completes the proof. □

Our next result is a lower bound on the exponential independence number, for which we are able to characterize all extremal trees.

Theorem 2. *If G is a connected graph of order n and diameter* diam, *then*

$$\alpha_e(G) \geq \frac{2\mathrm{diam}+2}{5}. \tag{3}$$

Furthermore, if G is a tree, then (3) holds with equality if and only if G is a path and n is a multiple of 5.

Proof. Let $P : v_0v_1 \dots v_{\mathrm{diam}}$ be a shortest path of length diam in G. Let

$$S = \left\{v_{5i} : i \in \left\{0, \dots, \left\lfloor \frac{\mathrm{diam}}{5} \right\rfloor\right\}\right\} \cup \left\{v_{5i+2} : i \in \left\{0, \dots, \left\lfloor \frac{\mathrm{diam}-2}{5} \right\rfloor\right\}\right\}.$$

Let $v_i \in S$. Since P is a shortest path, we have $\mathrm{dist}_{(G,S\setminus\{v_i\})}(v_i, v_j) \geq |j-i|$ for every v_j in $S \setminus \{v_i\}$. By construction, the set S contains no neighbor of v_i, and S contains at most one of the two vertices v_{i-k} and v_{i+k} for every integer k at least 2. This implies $w_{(G,S\setminus\{v_i\})}(v_i) < \sum_{k=2}^{\infty}\left(\frac{1}{2}\right)^{k-1} = 1$. Hence, S is an exponential independent set of G, and

$$\alpha_e(G) \geq |S| = 1 + \left\lfloor \frac{\mathrm{diam}}{5} \right\rfloor + 1 + \left\lfloor \frac{\mathrm{diam}-2}{5} \right\rfloor \geq \frac{2\mathrm{diam}+2}{5}.$$

Now, let G be a path and let n be a multiple of 5, that is, $G = P_n$, where $P_n : v_0v_1 \dots v_{n-1}$. It is easy to verify that $\alpha_e(P_5) = 2 = \frac{2\mathrm{diam}+2}{5}$. Furthermore, if $n > 5$ and S is a maximum exponential independent set of G, then $S \cap \{v_0, v_1, v_2, v_3, v_4\}$ is an exponential independent set of P_5 and $S \setminus \{v_0, v_1, v_2, v_3, v_4\}$ is an exponential independent set of P_{n-5}. By an inductive argument, we obtain,

$$\frac{2n}{5} \leq \alpha_e(G) = \alpha_e(P_n) \leq \alpha_e(P_5) + \alpha_e(P_{n-5}) = 2 + \frac{2(n-5)}{5} = \frac{2n}{5},$$

which implies that paths whose order is a multiple of 5 satisfy (3) with equality.

Finally, let G be a tree with $\alpha_e(G) = \frac{2\mathrm{diam}+2}{5}$, and let P be as above. Since $\frac{2\mathrm{diam}+2}{5}$ is an integer, the order $\mathrm{diam}+1$ of P is a multiple of 5. Suppose that G is distinct from P. This implies that there is some vertex v_k of P that has a neighbor u that does not belong to P. Let $k = 5r + s$ for some $s \in \{0, 1, 2, 3, 4\}$. By symmetry, we may assume that $s \in \{0, 1, 2\}$. Let

$$\begin{aligned} S_0 &= \{v_i : i \in \{0, \dots, 5r-1\} \text{ with } i \bmod 5 \in \{0, 2\}\} \\ &\quad \cup \{v_i : i \in \{5r+5, \dots, \mathrm{diam}+1\} \text{ with } i \bmod 5 \in \{2, 4\}\}. \end{aligned}$$

If $s = 0$, then let $S = \{v_{5r+1}, v_{5r+4}, u\} \cup S_0$, and if $s \in \{1, 2\}$, then let $S = \{v_{5r}, v_{5r+4}, u\} \cup S_0$. The set S is an exponential independent set of G of order more than $\frac{2\mathrm{diam}+2}{5}$, which is a contradiction. Hence, G is a path and n is a multiple of 5, which completes the proof. □

For later reference, we include a fundamental lemma from [4]. Recall that a full binary tree is a rooted tree in which each vertex has either no or exactly two children.

Lemma 3 (*Bessy et al. [4]*)**.** *Let G be a graph of maximum degree at most 3, and let S be a set of vertices of G.*

If u is a vertex of degree at most 2 in G, then $w_{(G,S)}(u) \leq 2$ with equality if and only if u is contained in a subgraph T of G that is a tree, such that rooting T in u yields a full binary tree and $S \cap V(T)$ is exactly the set of leaves of T.

Our next result concerns the exponential independence numbers of some special graphs.

Theorem 4.

(i) *If P_n is the path of order n, then $\alpha_e(P_n) = \left\lceil \frac{2n}{5} \right\rceil$.*
(ii) *If C_n is the cycle of order n at least 5, then $\alpha_e(C_n) = \left\lfloor \frac{2n}{5} \right\rfloor$.*
(iii) *If T is a full binary tree of order n, then $\alpha_e(T) = \frac{n+1}{2}$. Furthermore, the set of leaves of T is the unique maximum exponential independent set of T.*

Proof. (i) By Theorem 2, $\alpha_e(P_n)$ is at least $\left\lceil \frac{2n}{5} \right\rceil$. For $n \leq 5$, it is easy to verify that $\alpha_e(P_n)$ is also at most $\left\lceil \frac{2n}{5} \right\rceil$. Now, let $n > 5$. Let P_n be the path $v_0v_1 \dots v_{n-1}$. Let S be a maximum exponential independent set of P_n. Since $S \cap \{v_0, v_1, v_2, v_3, v_4\}$ is an exponential independent set of P_5 and $S \setminus \{v_0, v_1, v_2, v_3, v_4\}$ is an exponential independent set of P_{n-5}, we obtain, by an inductive argument,

$$\alpha_e(P_n) \le \alpha_e(P_5) + \alpha_e(P_{n-5}) = 2 + \left\lceil \frac{2(n-5)}{5} \right\rceil = \left\lceil \frac{2n}{5} \right\rceil.$$

(ii) Let C_n be the cycle $v_1v_2\dots v_nv_1$. For $5 \le n \le 10$, it is easy to verify that $\alpha_e(C_n) = \left\lfloor \frac{2n}{5} \right\rfloor$, and that some maximum exponential independent set of C_n contains v_1 and v_3.

In order to show $\alpha_e(C_n) \ge \left\lfloor \frac{2n}{5} \right\rfloor$ for n at least 5, we prove, by induction on n, that C_n has an exponential independent set S_n of order $\left\lfloor \frac{2n}{5} \right\rfloor$ that contains v_1 and v_3. For $n \le 10$, this was already observed above. For $n > 10$, the set S_n defined as $S_{n-5} \cup \{v_{n-2}, v_{n-4}\}$ is an exponential independent set of order $\left\lfloor \frac{2n}{5} \right\rfloor$ that contains v_1 and v_3, which completes the proof of the lower bound.

In order to show $\alpha_e(C_n) \le \left\lfloor \frac{2n}{5} \right\rfloor$ for n at least 5, suppose, for a contradiction, that n is the smallest order at least 5 with $\alpha_e(C_n) > \left\lfloor \frac{2n}{5} \right\rfloor$. As observed above $n > 10$, which implies $\alpha_e(C_n) > 4$. It is easy to see that C_n has a maximum exponential independent set S_n that contains v_1 and v_3. Let $k \in [n]$ be minimum such that S_n contains two vertices in $\{v_{n-k+1}, \dots, v_n\}$. Clearly, $v_{n-k+1} \in S_n$, $v_{n-k} \notin S_n$, and $k \ge 5$. If $k = 5$, then $S_n \cap \{v_{n-4}, \dots, v_n\} = \{v_{n-4}, v_{n-2}\}$. This implies that $S_n \setminus \{v_{n-4}, v_{n-2}\}$ is an exponential independent set of C_{n-5}, which implies the contradiction $\alpha_e(C_{n-5}) > \left\lfloor \frac{2(n-5)}{5} \right\rfloor$. Similarly, if $k \ge 6$, then $S_n \setminus \{v_{n-k+1}, \dots, v_n\}$ is an exponential independent set of C_{n-k}, which implies the contradiction $\alpha_e(C_{n-k}) > \left\lfloor \frac{2(n-5)}{5} \right\rfloor$. This completes the proof of (ii).

(iii) Clearly, we may assume $n > 3$. Let L be the set of leaves of T. Note that $n = 2|L| - 1$. Let $v \in L$ and let u be the parent of u in T. If $w_{(T,L\setminus\{v\})}(v) \ge 1$, then $w_{(T,L\setminus\{v\})}(u) \ge 2$, and Lemma 3 implies that rooting $T - v$ in u yields a full binary tree. This implies the contradiction that T only has vertices of degree 1 and 3, while the root of T has degree 2. Hence, L is an exponential independent set of T, which implies $\alpha_e(T) \ge |L| = \frac{n+1}{2}$.

Suppose that T is a full binary tree of minimum order n such that either $\alpha_e(T) > \frac{n+1}{2}$ or $\alpha_e(T) = \frac{n+1}{2}$ but T has a maximum exponential independent set distinct from L. In both cases, T has a maximum exponential independent set S with $S \setminus L \ne \emptyset$. Let v be a vertex in $S \setminus L$ at maximum distance from the root of T. Let w and w' be the two children of v in T. Let T_w be the full binary subtree of T that contains w as well as all descendants of w in T, and is rooted in w. Let $S_w = S \cap V(T_w)$. By the choice of v, the set S_w contains only leaves of T_w. If S_w contains all leaves of T_w, then Lemma 3 implies $w_{(T,S\setminus\{v\})}(v) \ge w_{(T,S_w)}(v) = \frac{1}{2}w_{(T_w,S_w)}(w) = \frac{1}{2} \cdot 2 = 1$, which is a contradiction. Hence, the set $L \setminus S$ contains at least one leaf of T that is either w or a descendant of w, and, by symmetry, the set $L \setminus S$ also contains at least one leaf of T that is either w' or a descendant of w'. Hence, if ℓ_v leaves of T are descendants of v, then S contains at most $\ell_v - 2$ descendants of v. Let T' arise from T by removing all descendants of v. Since T' is a full binary tree of smaller order than T, the choice of T implies that $\alpha_e(T') = \frac{n(T')+1}{2}$. Note that $S \cap V(T')$ is an exponential independent set of T', and that v has exactly $2\ell_v - 2$ descendants. Therefore,

$$\begin{aligned}
|S| &\le |S \setminus V(T')| + |S \cap V(T')| \\
&\le (\ell_v - 2) + |S \cap V(T')| \\
&\le (\ell_v - 2) + \frac{n(T')+1}{2} \\
&= (\ell_v - 2) + \frac{n - (2\ell_v - 2) + 1}{2} \\
&< \frac{n+1}{2},
\end{aligned}$$

which is a contradiction. □

Our next result is an upper bound on the exponential independence number, for which we achieve a full characterization of the extremal graphs.

Theorem 5. *If G is a connected graph of order n, then*

$$\alpha_e(G) \le \frac{n+1}{2}$$

with equality if and only if G is a full binary tree.

Proof. We show the upper bound by induction on n. By Theorem 1(ii), we may assume that G is a tree T. If $n = 1$, then $\alpha_e(T) = 1 = \frac{n+1}{2}$. Now, let $n \ge 2$, and let S be a maximum exponential independent set of T. We root T in some vertex r. Let v be a vertex in S at maximum distance from r. If $v = r$, then $|S| = 1$, and the statement holds. Hence, we may assume that v and r are distinct. Let u be the parent of v.

First, we assume that v is the only descendant of u that belongs to S. Let T' arise from T by removing u together with all descendants of u, and let $S' = S \setminus \{v\}$. Clearly, S' is an exponential independent set of the tree T', and we obtain, by induction,

$$\alpha_e(T) = |S| = |S'| + 1 \le \alpha_e(T') + 1 \le \frac{n(T')+1}{2} + 1 \le \frac{n(T)+1}{2}.$$

Next, we assume that S contains some descendant of u distinct from v. Let S_u be the set of descendants of u that belong to S. By the choice of v, all vertices in S_u are children of u. Since S is exponential independent, we obtain $|S_u| = 2$, and $u \notin S$. Let T'' arise from T by removing all descendants of u, and let $S'' = (S \setminus S_u) \cup \{u\}$. If $w_{(T'',S''\setminus\{u\})}(u) \geq 1$, then $w_{(T,S\setminus\{v\})}(v) \geq \frac{1}{2}w_{(T'',S''\setminus\{u\})}(u) + \frac{1}{2} \geq 1$, which is a contradiction. If $w_{(T'',S''\setminus\{w\})}(w) \geq 1$ for some $w \in S'' \setminus \{u\}$, then $\text{dist}_{(T'',S''\setminus\{w\})}(w,u) = \text{dist}_{(T,S\setminus\{w\})}(w,x) - 1$ for every $x \in S_u$ and $|S_u| = 2$ imply

$$\begin{aligned} w_{(T,S\setminus\{w\})}(w) &= w_{(T'',S''\setminus\{w\})}(w) - \left(\frac{1}{2}\right)^{\text{dist}_{(T'',S''\setminus\{w\})}(w,u)-1} + \sum_{x\in S_u}\left(\frac{1}{2}\right)^{\text{dist}_{(T,S\setminus\{w\})}(w,x)-1} \\ &= w_{(T'',S''\setminus\{w\})}(w) \\ &\geq 1, \end{aligned}$$

which is a contradiction. Hence, S'' is an exponential independent set of T'', and we obtain, by induction,

$$\alpha_e(T) = |S| = |S''| + 1 \leq \alpha_e(T'') + 1 \leq \frac{n(T'')+1}{2} + 1 \leq \frac{n(T)+1}{2},$$

which completes the proof of the upper bound.

Next, we show that we have equality if and only if G is a full binary tree. By Theorem 4(iii), we only need to show that every connected graph G with $\alpha_e(G) = \frac{n+1}{2}$ is a full binary tree. Therefore, suppose that G is a connected graph of minimum order n with $\alpha_e(G) = \frac{n+1}{2}$ that is not a full binary tree.

Let T be a spanning tree of G. We will show first that T is a full binary tree. By Theorem 1(ii), we have $\frac{n+1}{2} = \alpha_e(G) \leq \alpha_e(T) \leq \frac{n+1}{2}$, which implies $\alpha_e(T) = \frac{n+1}{2}$. Let S be a maximum exponential independent set of G, and, hence, also of T. If the diameter of T is at most 2, then it is easy to see that either $\alpha_e(G) \neq \frac{n+1}{2}$ or G is a full binary tree, that is, the diameter of T is at least 3. Let w be the endvertex of a longest path P in T. Let v be the neighbor of w, and let u be the neighbor of v on P that is distinct from w. Let $T' = T - (N_T[v] \setminus \{u\})$, and let $S' = S \cap V(T')$. Note that all vertices in $N_T(v) \setminus \{u\}$ are endvertices of T.

First, we assume that v has degree 2 in T. Note that S' is an exponential independent set of T', the set S contains at most one of the two vertices v and w, and $n(T') = n-2$. This implies $\frac{n+1}{2} = \alpha_e(T) = |S| \leq |S'|+1 \leq \alpha_e(T')+1 \leq \frac{n(T')+1}{2}+1 = \frac{n+1}{2}$, which implies that $\alpha_e(T') = |S'| = \frac{n(T')+1}{2}$, and that S contains either w or v. By the choice of G, this implies that T' is a full binary tree. By Theorem 4(iii), the set S' is exactly the set of leaves of T'. If u is the root of T', then T is a full binary tree with root v, which is a contradiction. Hence, u is not the root of T'. Let u' be a leaf of T' that is either u or a descendant of u in T'. Let u' have distance d from the root r of T'. Let $u_0 \dots u_d$ with $u_0 = r$ and $u_d = u'$ be a path in T'. For $i \in [d]$, let u_i' be the child of u_{i-1} in T' that is distinct from u_i, let T_i' be the full binary subtree of T' that contains u_i' as well as all descendants of u_i' in T', and is rooted in u_i', and let $S_i' = S' \cap V(T_i')$. Since S_i' is exactly the set of leaves of T_i', Lemma 3 implies $w_{(T_i',S_i')}(u_i') = 2$ for $i \in [d]$. Since the distance in T' between u' and u_i' is $d-i+2$, this implies $w_{(T,S'\setminus\{u'\})}(u') = \sum_{i=1}^{d}\left(\frac{1}{2}\right)^{d-i+2} w_{(T_i',S_i')}(u_i') = \sum_{i=1}^{d}\left(\frac{1}{2}\right)^{i}$. Since the distance between w and u' is at most $d+1$, we obtain the contradiction $w_{(T,S\setminus\{u'\})}(u') \geq w_{(T,\{w\})}(u') + w_{(T,S'\setminus\{u'\})}(u') \geq \left(\frac{1}{2}\right)^{(d+1)-1} + \sum_{i=1}^{d}\left(\frac{1}{2}\right)^{i} = 1$. Hence, v has degree at least 3 in T.

If S contains at most one vertex from $N_T[v] \setminus \{u\}$, then $n(T') \leq n-3$ implies the contradiction $\frac{n+1}{2} = \alpha_e(T) = |S| \leq |S'| + 1 \leq \alpha_e(T') + 1 \leq \frac{n(T')+1}{2} + 1 = \frac{n}{2}$. Since S is an exponential independent set of T, it cannot contain either v and a neighbor of v or three neighbors of v. Hence, it follows that S contains exactly two vertices from $N_T(v) \setminus \{u\}$ but not v. Let $T'' = T - (N_T(v) \setminus \{u\})$, and let $S'' = S' \cup \{v\}$. Arguing as before, it follows that S'' is an exponential independent set of T''. Since $n(T'') \leq n-2$, we obtain $\frac{n+1}{2} = \alpha_e(T) = |S| = |S''| + 1 \leq \alpha_e(T'') + 1 \leq \frac{n(T'')+1}{2} + 1 \leq \frac{n+1}{2}$, which implies $\alpha_e(T'') = \frac{n(T'')+1}{2}$ and $n(T'') = n-2$. By the choice of G, it follows that T'' is a full binary tree, and that S'' is a maximum exponential independent set of T''. Since $v \in S''$, Theorem 4 implies that v is a leaf of T''. Now, also in this case, the tree T is a full binary tree.

Since T was an arbitrary spanning tree of G, it follows that every spanning tree of G is a full binary tree. This easily implies that $G = T$, that is, G is a full binary tree, which completes the proof. □

Theorem 2 implies that $\alpha_e(G)$ is at least $\Omega(\log_2(n(G)))$ for every connected cubic graph G. We conjecture that $\alpha_e(G)$ actually grows much faster than $\log_2(n(G))$. At least for subcubic trees, we obtain the following linear lower bound.

Theorem 6. *If T is a tree of order n and maximum degree at most 3, then $\alpha_e(T) \geq \frac{2n+8}{13}$.*

Proof. Clearly, we may assume that $n > 3$. Let T have n_i vertices of degree i for $i \in [3]$. Note that $n_1 \geq n_3 + 2$.

If $n_2 > 0$, then let S_1 be the set of all leaves of T, and, if $n_2 = 0$, then let S_1 be the set of all leaves of T except for exactly one. Arguing as in the proof of Theorem 4(iii), it follows that S_1 is an exponential independent set in T, which implies $\alpha_e(T) \geq n_1 - 1 \geq n_3 + 1$.

Let V_3 be the set of vertices of degree 3, and let $T' = T - N_T[V_3]$. Note that T' is a union of paths, and that $n(T') \geq n - 4n_3$. By Theorem 4(i), the forest T' has an exponential independent set S_2 of order at least $\frac{2n(T')}{5} \geq \frac{2n-8n_3}{5}$. We will show that S_2 is also exponential independent within T. Therefore, let u be a vertex of degree 1 in T' that has a neighbor v in $V(T) \setminus V(T')$. By construction, u and v have degree 2 in T, and v has a neighbor w of degree 3 in T. Let T_w be the component of $T - v$

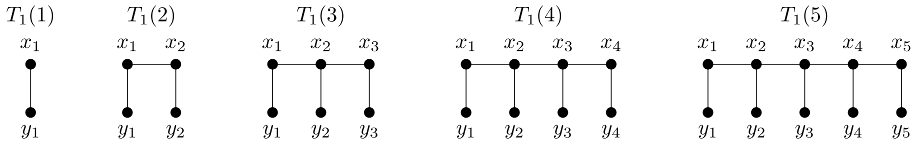

Fig. 1. The trees $T_1(k)$ for $k \in [5]$.

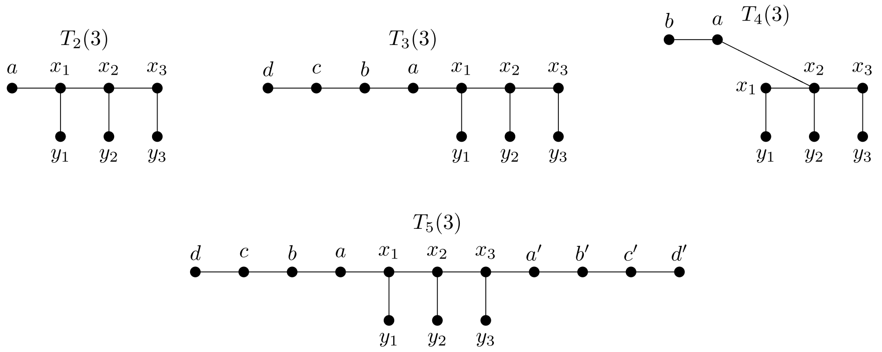

Fig. 2. The trees $T_k(3)$ for $k \in \{2, 3, 4, 5\}$.

that contains w, and let $S_w = S_2 \cap V(T_w)$. If $w_{(T,S_w)}(u) \geq \frac{1}{2}$, then $w_{(T_w,S_w)}(w) \geq 2$. By Lemma 3, this implies that S_w, and hence S_2, intersects $N_T[V_3]$, which is a contradiction. Hence, $w_{(T,S_w)}(u) < \frac{1}{2}$. Similarly, if u is a vertex of degree 0 in T', then $w_{(T,S_2\setminus\{u\})}(u) < \frac{1}{2}$ if u has degree 1 in T, and $w_{(T,S_2\setminus\{u\})}(u) < \frac{1}{2} + \frac{1}{2}$ if u has degree 2 in T. If $P = v_0 \dots v_\ell$ is a component of T' with $|V(P) \cap S_2| \geq 2$, and $v_i \in S_2$ is such that $S_2 \cap \{v_0, \dots, v_{i-1}\} = \emptyset$, then $w_{(T',S_2\setminus\{v_i\})}(v_i) \leq \frac{1}{2}$. Combining these observations, it follows easily that S_2 is an exponential independent set in T, which implies $\alpha_e(T) \geq \frac{2n-8n_3}{5}$.

Altogether, we obtain $\alpha_e(T) \geq \max\left\{n_3 + 1, \frac{2n-8n_3}{5}\right\} \geq \frac{2n+8}{13}$, which completes the proof. □

After the above bounds, exact values, and extremal graphs, we consider graphs G with $\alpha_e(G) = \alpha(G)$. We achieve full characterizations of all graphs for which every induced subgraph has this property, and also of all trees that have this property.

Recall that the *bull* is the unique graph B of order 5 with degree sequence 1, 1, 2, 3, 3.

Theorem 7. *If G is a graph, then $\alpha_e(H) = \alpha(H)$ for every induced subgraph H of G if and only if G is $\{K_{1,3}, P_5, B\}$-free.*

Proof. If $H \in \{K_{1,3}, P_5, B\}$, then $\alpha_e(H) = 2 < 3 = \alpha(H)$, which implies the necessity. In order to show the sufficiency, let G be a $\{K_{1,3}, P_5, B\}$-free graph. It suffices to show that $\alpha_e(G) = \alpha(G)$. Let S be a maximum independent set of G. If $|S| \leq 2$, then S is also exponential independent, which implies $\alpha_e(G) = \alpha(G)$. Hence, we may assume that $|S| \geq 3$. Possibly iteratively replacing elements of S by one of their neighbors, we may assume that S contains two vertices u and v at distance 2. Suppose that $S \setminus \{u, v\}$ contains a vertex w at distance 2 from u. If u, v, and w have a common neighbor, then the independence of S implies that G contains $K_{1,3}$ as an induced subgraph, which is a contradiction. Therefore, if $uv'v$ and $uw'w$ are shortest paths in G, then $v' \neq w'$ and $vw', wv' \notin E(G)$, which implies the contradiction that $\{u, v, w, v', w'\}$ induces P_5 or B. Hence, we may assume, by symmetry, that no vertex in S has two vertices in S at distance 2 from it. Let $w \in S \setminus \{u, v\}$. Since G is P_5-free, the distance of u and w is 3. Let $uv'v$ and $uw'w''w$ be shortest paths in G. Note that v is not adjacent to w''. If $v' = w'$, then $\{u, v, v', w''\}$ induces $K_{1,3}$, which is a contradiction. Hence, $v' \neq w'$. By symmetry, we may assume that v is not adjacent to w' and that v' is not adjacent to w''. Now, $\{u, v, v', w', w''\}$ induces P_5 or B, which is a contradiction and completes the proof. □

We proceed to the trees T with $\alpha_e(T) = \alpha(T)$.

For a positive integer k, let $T_1(k)$ be the tree illustrated in Fig. 1, that is, $T_1(k)$ has vertex set $\{x_1, \dots, x_k\} \cup \{y_1, \dots, y_k\}$, contains the path $x_1 \dots x_k$, and x_i is the only neighbor of y_i for $i \in [k]$.

Let $T_2(k)$ arise from $T_1(k)$ by adding a vertex a and the edge x_1a. Let $T_3(k)$ arise from $T_1(k)$ by adding the vertices a, b, c, and d, and the edges x_1a, ab, bc, and cd. For $k \geq 3$, let $T_4(k)$ arise from $T_1(k)$ by adding the vertices a and b, and the edges x_2a and ab. Finally, let $T_5(k)$ arise from $T_1(k)$ by adding the vertices a, b, c, d, a', b', c', and d', and the edges x_1a, ab, bc, cd, x_ka', $a'b'$, $b'c'$, $c'd'$. See Fig. 2 for an illustration.

Let

$$\mathcal{T} = \{P_1, P_8\} \cup \bigcup_{k\in\mathbb{N}} \left\{T_1(k), T_2(k), T_3(k), T_5(k)\right\} \cup \bigcup_{k\geq 3} \left\{T_4(k)\right\}.$$

Note that $\mathcal{T}$ contains the paths $P_1, P_2 = T_1(1), P_3 = T_2(1), P_4 = T_1(2), P_6 = T_3(1)$, and P_8.

Lemma 8. *Every tree $T \in \mathcal{T}$ satisfies $\alpha_e(T) = \alpha(T)$. Furthermore, if S is a maximum exponential independent set of T, then*

(i) $S \in \big\{\{y_1, \dots, y_k\}, \{x_1\} \cup \{y_2, \dots, y_k\}, \{x_k\} \cup \{y_1, \dots, y_{k-1}\}\big\}$ *if* $T = T_1(k)$,
(ii) $S = \{a, y_1, \dots, y_k\}$ *if* $T = T_2(k)$,
(iii) $S = \{b, d, y_1, \dots, y_k\}$ *if* $T = T_3(k)$ *with* $k \geq 2$,
(iv) $S = \{b, y_1, \dots, y_k\}$ *if* $T = T_4(k)$ *with* $k \geq 3$,
(v) $S = \{b, d, b', d', y_1, \dots, y_k\}$ *if* $T = T_5(k)$,
(vi) $S \in \big\{\{y_1, a, d\}, \{y_1, b, d\}\big\}$ *if* $T = P_6 = y_1x_1abcd$, *and*
(vii) $S = \{b, d, b', d'\}$ *if* $T = P_8 = dcbaa'b'c'd'$.

Proof. Let $T \in \mathcal{T}$. It is easy to see that $\alpha_e(P_n) = \alpha(P_n)$ for $n \in \{1, 2, 3, 4, 6, 8\}$. Furthermore, one easily checks that P_6 has only two distinct exponential independent sets of order 3, and that P_8 has a unique exponential independent set of order 4, which implies (vi) and (vii). Now, we may assume that $T \notin \{P_1, P_6, P_8\}$.

First, we assume that $T = T_1(k)$ for some positive integer k. Clearly, the set $\{y_1, \dots, y_k\}$ is a maximum independent set, which implies $\alpha(T) = k$. Since this set is also exponential independent, we obtain $\alpha_e(T) = \alpha(T) = k$. Now, let S be a maximum exponential independent set of T. For $k \in [2]$, it follows easily that S is as stated in (i). Now, let $k \geq 3$. Since S contains at most one of the two vertices x_i and y_i for each $i \in [k]$, the set S necessarily intersects each of the sets $\{x_i, y_i\}$ for $i \in [k]$ in exactly one vertex. If $x_i \in S$ for some $i \in \{2, \dots, k-1\}$, this implies that $y_{i-1}, y_{i+1} \in S$, which yields the contradiction that $w_{(T,S\setminus\{x_i\})}(x_i) \geq \frac{1}{2} + \frac{1}{2} = 1$. Hence, $\{y_i : 2 \leq i \leq k-1\} \subseteq S$. If $x_1, x_k \in S$, then $w_{(T,S\setminus\{x_1\})}(x_1) = \sum_{i=2}^{k-1} \left(\frac{1}{2}\right)^{i-1} + \frac{1}{2^{k-2}} = 1$, which is a contradiction. Hence, the set S is stated as in (i).

Next, we assume that $T = T_2(k)$ for some positive integer k. Again, the set of leaves is a maximum independent set of T, which is also exponential independent, and, hence, $\alpha_e(T) = \alpha(T) = k+1$. Now, let S be a maximum exponential independent set of T. If $a \notin S$, then S is an exponential independent set of $T - a = T_1(k)$, which contradicts $\alpha_e(T_1(k)) = k$. Hence, $a \in S$, which implies $x_1 \notin S$. For $k \in [2]$, it follows easily that S is as stated in (ii). Now, let $k \geq 3$. Since $S \setminus \{a\}$ is a maximum exponential independent set of $T - a = T_1(k)$, we obtain, by (i), that $\{y_1, \dots, y_{k-1}\} \subseteq S$. If $x_k \in S$, then $w_{(T,S\setminus\{a\})}(a) \geq 1$ follows similarly as above, which is a contradiction. Hence, the set S is as stated in (ii).

Next, we assume that $T = T_3(k)$ for some positive integer k. Since $T \neq P_6$, we have $k \geq 2$. As before, it follows easily that the set specified in (iii) is a maximum exponential independent set of T, and, hence, $\alpha_e(T) = \alpha(T) = k + 2$. Now, let S be a maximum exponential independent set of T. Necessarily, $|S \setminus \{a, b, c, d\}| = k$ and $|S \cap \{a, b, c, d\}| = 2$, which implies that S contains either a or b. If S contains a, then $S \setminus \{b, c, d\}$ is a maximum exponential independent set of $T_2(k)$, which, by (ii), implies $S \setminus \{b, c, d\} = \{a, y_1, \dots, y_k\}$. Now, we obtain the contradiction, $w_{(T,S\setminus\{a\})}(a) = w_{(T,S\setminus\{a,b,c,d\})}(a) + w_{(T,S\cap\{b,c,d\})}(a) \geq \frac{1}{2} + \frac{1}{4} + \frac{1}{4} = 1$. Hence, $b \in S$, which implies $S \cap \{a, b, c, d\} = \{b, d\}$, and $x_1 \notin S$. Since $S \setminus \{a, b, c, d\}$ is a maximum exponential independent set of $T - \{a, b, c, d\} = T_1(k)$, we obtain, by (i), that $\{y_1, \dots, y_{k-1}\} \subseteq S$. If $x_k \in S$, then $w_{(T,S\setminus\{a\})}(a) = 1$, which is a contradiction. Hence, the set S is as stated in (iii).

Next, we assume that $T = T_4(k)$ for some integer k at least 3. Since the set specified in (iv) is a maximum independent set and an exponential independent set, it is a maximum exponential independent set, and $\alpha_e(T) = \alpha(T)$. Now, let S be a maximum exponential independent set of T. Since S is a maximum independent set, it contains exactly one of the two vertices a and b. Since $T - \{a, b\} = T_1(k)$, part (i) implies that the set S' defined as $S \setminus \{a, b\}$ is a maximum exponential independent set of $T - \{a, b\}$. If $S' = \{x_1\} \cup \{y_2, \dots, y_k\}$, then $w_{(T,S\setminus\{x_1\})}(x_1) \geq w_{(T,\{y_2,y_3,b\})}(x_1) = 1$, which is a contradiction. If $S' = \{x_k\} \cup \{y_1, \dots, y_{k-1}\}$, then $w_{(T,S\setminus\{x_k\})}(x_k) \geq w_{(T,\{y_1,\dots,y_{k-1},b\})}(x_k) = 1$, which is a contradiction. Hence, by (i), $S' = \{y_1, \dots, y_k\}$. Furthermore, by symmetry between b and y_1, we obtain $S = \{b, y_1, \dots, y_k\}$, that is, the set S is as stated in (iv).

Finally, if $T = T_5(k)$ for some positive integer k, very similar arguments as above imply that $\alpha_e(T) = \alpha(T)$, and that every maximum exponential independent set is as specified in (v). $\square$

Theorem 9. *If T is a tree, then $\alpha_e(T) = \alpha(T)$ if and only if $T \in \mathcal{T}$.*

Proof. In view of Lemma 8, it remains to show that every tree T with $\alpha_e(T) = \alpha(T)$ belongs to $\mathcal{T}$. Therefore, suppose that T is a tree of minimum order such that $\alpha_e(T) = \alpha(T)$ but $T \notin \mathcal{T}$. Let S be a maximum exponential independent set of T. Since $P_1, P_2, P_3 \in \mathcal{T}$, and $\alpha_e(K_{1,n-1}) = 2 < n - 1 = \alpha(K_{1,n-1})$ for $n \geq 3$, we may assume that T has diameter at least 3. Therefore, if w is an endvertex of a longest path in T, then the unique neighbor v of w has exactly one neighbor u that is not an endvertex of T. Let T' be the component of $T - v$ that contains u. Note that T' is not P_1. We consider different cases.

Case 1 $d_T(v) \geq 4$.

Clearly, $\alpha(T) \geq \alpha(T') + (d_T(v) - 1) \geq \alpha(T') + 3$. Since S contains at most 2 vertices from $N_T[v] \setminus \{u\}$, and $S \cap V(T')$ is an exponential independent set of T', we obtain $\alpha_e(T) \leq \alpha_e(T') + 2$, which yields the contradiction $\alpha(T) \geq \alpha(T') + 3 \geq \alpha_e(T') + 3 > \alpha_e(T)$, which completes the proof in this case.

Case 2 $d_T(v) = 3$.

Let $N_T(v) = \{u, w, w'\}$. As before, we obtain that $\alpha(T) \geq \alpha(T') + 2$ and $\alpha_e(T) \leq \alpha_e(T') + 2$, which implies $\alpha(T) \geq \alpha(T') + 2 \geq \alpha_e(T') + 2 \geq \alpha_e(T) = \alpha(T)$. Since equality holds throughout this inequality chain, we have $\alpha(T') = \alpha_e(T')$ and

$\alpha_e(T) = \alpha_e(T') + 2$. By the choice of T, the condition $\alpha(T') = \alpha_e(T')$ implies that $T' \in \mathcal{T}$. Furthermore, $\alpha_e(T) = \alpha_e(T') + 2$ implies that $S \cap \{v, w, w'\} = \{w, w'\}$, and that $S' = S \setminus \{w, w'\}$ is a maximum exponential independent set of T'. Since $w_{(T,\{w,w'\})}(u) = 1$, we obtain $u \notin S'$.

First, we assume that $T' = P_8 = dcbaa'b'c'd'$. By Lemma 8, we have $S' = \{b, d, b', d'\}$. By symmetry, we may assume that $u \in \{a, c\}$. In both cases $w_{(T,\{d,w,w'\})}(b) \geq 1$, which is a contradiction.

Next, we assume that $T' = T_1(k)$. Since $u \notin S'$, we obtain that either $u = x_i$ for some $i \in [k]$ or $u = y_j$ for some $j \in \{1, k\}$. If $u = y_j$ for some $j \in \{1, k\}$, then $x_j \in S'$, and $w_{(T,(S'\setminus\{x_j\})\cup\{w,w'\})}(x_j) \geq 1$, which is a contradiction. Hence, $u = x_i$ for some $i \in [k]$. If $i \in \{1, k\}$, then $T = T_2(k+1) \in \mathcal{T}$, which is a contradiction. Hence, $2 \leq i \leq k-1$. Using Lemma 8, we obtain the contradiction $w_{(T,S\setminus\{y_i\})}(y_i) \geq 4 \cdot \frac{1}{4} = 1$.

Next, we assume that $T' = T_2(k)$. By Lemma 8, we have $S' = \{a, y_1, \ldots, y_k\}$. Since $u \notin S'$, we have $u = x_i$ for some $i \in [k]$, which implies the contradiction $w_{(T,S\setminus\{y_i\})}(y_i) \geq w_{(T,\{w,w'\})}(y_i) + w_{(T,\{a,y_1,\ldots,y_{i-1}\})}(y_i) = 2 \cdot \frac{1}{4} + \left(\frac{1}{4} + \cdots + \frac{1}{2^i} + \frac{1}{2^i}\right) = 1$.

Next, we assume that $T' = T_3(k)$. By Lemma 8, we have $S' = \{b, d, y_1, \ldots, y_k\}$ for $k \geq 2$. For $k = 1$, that is, $T' = P_6$, Lemma 8(vi) implies that, after suitably renaming the vertices of T', we have $S' = \{b, d, y_1, \ldots, y_k\}$. Since $u \notin S'$, we have $u \in \{a, c\}$ or $u = x_i$ for some $i \in [k]$. In the former case, $w_{(T,\{d,w,w'\})}(b) \geq 1$, and in the latter case, $w_{(T,S\setminus\{b\})}(b) \geq w_{(T,\{d,w,w'\})}(b) + w_{(T,\{y_1,\ldots,y_i\})}(b) = \frac{1}{2} + 2 \cdot \frac{1}{2^{i+2}} + \left(\frac{1}{4} + \cdots + \frac{1}{2^{i+1}}\right) = 1$.

Next, we assume that $T' = T_4(k)$ for some $k \geq 3$. By Lemma 8, we have $S' = \{b, y_1, \ldots, y_k\}$. Since $u \notin S'$, we have $u \in \{a, x_1\}$ or $u = x_i$ for some $i \in \{2, \ldots, k\}$. If $u = a$, then $w_{(T,S\setminus\{b\})}(b) \geq w_{(T,\{w,w',y_1,y_2,y_3\})}(b) = 3 \cdot \frac{1}{4} + 2 \cdot \frac{1}{8} = 1$. Similarly, if $u = x_1$, then $w_{(T,S\setminus\{y_1\})}(y_1) \geq 1$. Finally, if $u = x_i$ for some $i \geq 2$, then $w_{(T,S\setminus\{y_i\})}(y_i) \geq w_{(T,\{w,w',b\})}(y_i) + w_{(T,\{y_1,\ldots,y_{i-1}\})}(y_i) = 2 \cdot \frac{1}{4} + \frac{1}{2^i} + \left(\frac{1}{4} + \cdots + \frac{1}{2^i}\right) = 1$.

Finally, we assume that $T' = T_5(k)$. By Lemma 8, we have $S' = \{b, d, b', d', y_1, \ldots, y_k\}$. Since $u \notin S'$, we have $u \in \{a, c, a', c'\}$ or $u = x_i$ for some $i \in \{1, \ldots, k\}$. If $u \in \{a, c\}$, then $w_{(T,S\setminus\{b\})}(b) \geq w_{(T,\{d,w,w'\})}(b) = 1$, if $u \in \{a', c'\}$, then $w_{(T,S\setminus\{b'\})}(b') \geq 1$, and if $u = x_i$, then $w_{(T,S\setminus\{b\})}(b) \geq w_{(T,\{d,w,w'\})}(b) + w_{(T,\{y_1,\ldots,y_i\})}(b) = \frac{1}{2} + 2 \cdot \frac{1}{2^{i+2}} + \left(\frac{1}{4} + \cdots + \frac{1}{2^{i+1}}\right) = 1$, which completes the proof in this case.

Case 3 $d_T(v) = 2$.

Let $N_T(v) = \{u, w\}$. As before, we obtain that $\alpha(T) \geq \alpha(T') + 1$ and $\alpha_e(T) \leq \alpha_e(T') + 1$, which implies $\alpha(T) \geq \alpha(T') + 1 \geq \alpha_e(T') + 1 \geq \alpha_e(T) = \alpha(T)$. Again, equality holds throughout this inequality chain, and we obtain that $\alpha(T') = \alpha_e(T')$, $\alpha_e(T) = \alpha_e(T') + 1$, $T' \in \mathcal{T}$, and $S' = S \setminus \{v, w\}$ is a maximum exponential independent set of T'. Clearly, we may assume that $S \cap \{v, w\} = \{w\}$.

First, we assume that $T' = P_8 = dcbaa'b'c'd'$. By Lemma 8, we have $S' = \{b, d, b', d'\}$. Regardless of which vertex in $\{d, c, b, a, a', b', c', d'\}$ is u, either $w_{(T,S\setminus\{b\})}(b) \geq 1$ or $w_{(T,S\setminus\{b'\})}(b') \geq 1$.

Next, we assume that $T' = T_1(k)$. If $u \in \{x_1, x_k\}$, then $T = T_1(k+1) \in \mathcal{T}$. If $u \in \{y_1, y_k\}$, then either $k = 1$ and $T = P_4 \in \mathcal{T}$, or $k \geq 2$ and $T = T_3(k-1) \in \mathcal{T}$. If $u \in \{x_2, x_{k-1}\}$, then $T = T_4(k) \in \mathcal{T}$. If $u = y_i$ for some $i \in \{2, \ldots, k-1\}$, then, by Lemma 8, $y_i \in S'$ and $w_{(T,S\setminus\{y_i\})}(y_i) \geq w_{(T,\{w,y_{i-1},y_{i+1}\})}(y_i) = 1$. Finally, if $u = x_i$ for some $i \in \{3, \ldots, k-2\}$, then, by Lemma 8, $y_i \in S'$ and $w_{(T,S\setminus\{y_i\})}(y_i) \geq w_{(T,\{w,y_{i-1},y_{i+1},y_{i-2},y_{i+2}\})}(y_i) = 1$.

Next, we assume that $T' = T_2(k)$. If $u \in \{a, y_1, \ldots, y_k\}$, then, by Lemma 8, $w_{(T,S\setminus\{u\})}(u) = \frac{1}{2} + w_{(T,S'\setminus\{u\})}(u) \geq \frac{1}{2} + \frac{1}{2} = 1$. If $u = x_k$, then $T = T_2(k+1) \in \mathcal{T}$. Finally, if $u = x_i$ for some $i \in [k-1]$, then, by Lemma 8, $y_i \in S'$ and $w_{(T,S\setminus\{y_i\})}(y_i) \geq w_{(T,\{w,y_{i+1}\})}(y_i) + w_{(T,\{a,y_1,\ldots,y_{i-1}\})}(y_i) = 2 \cdot \frac{1}{4} + \left(\frac{1}{4} + \cdots + \frac{1}{2^i} + \frac{1}{2^i}\right) = 1$.

Next, we assume that $T' = T_3(k)$. If $u \in \{a, b, c, d\}$, then, by Lemma 8, $w_{(T,S\setminus\{b\})}(b) \geq w_{(T,\{w\})}(b) + w_{(T,\{d,y_1\})}(b) \geq 1$. If $u = x_k$, then $T = T_3(k+1) \in \mathcal{T}$. If $u = y_k$, then either $k = 1$ and $T = P_8 \in \mathcal{T}$, or $k \geq 2$ and $T = T_5(k-1) \in \mathcal{T}$. If $u = y_i$ for some $i \in [k-1]$, then $y_i \in S'$ and $w_{(T,S\setminus\{y_i\})}(y_i) \geq \frac{1}{2} + 2 \cdot \frac{1}{4} = 1$. Finally, if $u = x_i$ for some $i \in [k-1]$, then $w_{(T,S\setminus\{b\})}(b) \geq w_{(T,\{d,w\})}(b) + w_{(T,\{y_1,\ldots,y_{i+1}\})}(b) = \frac{1}{2} + \frac{1}{2^{i+2}} + \left(\frac{1}{4} + \cdots + \frac{1}{2^{i+2}}\right) = 1$.

Next, we assume that $T' = T_4(k)$ for some $k \geq 3$. If $u \in \{b, y_1, \ldots, y_k\}$, then, by Lemma 8, $u \in S'$ and $w_{(T,S\setminus\{u\})}(u) = \frac{1}{2} + w_{(T,S'\setminus\{u\})}(u) \geq \frac{1}{2} + \frac{1}{2} = 1$. If $u = x_1$ and $k = 3$, then $T = T_4(4) \in \mathcal{T}$. If $u = x_1$ and $k \geq 4$, then $w_{(T,S\setminus\{y_2\})}(y_2) \geq w_{(T,\{b,w,y_1,y_3,y_4\})}(y_2) = 3 \cdot \frac{1}{4} + 2 \cdot \frac{1}{8} = 1$. If $u = a$, we obtain similar contradictions. If $u = x_k$, then $T = T_4(k+1) \in \mathcal{T}$. Finally, if $u = x_i$ for some $i \in \{2, \ldots, k-1\}$, then $y_i \in S'$ and $w_{(T,S\setminus\{y_i\})}(y_i) \geq w_{(T,\{y_{i+1},w\})}(y_i) + w_{(T,\{b,y_1,\ldots,y_{i-1},w\})}(y_i) = 2 \cdot \frac{1}{4} + \left(\frac{1}{4} + \cdots + \frac{1}{2^i} + \frac{1}{2^i}\right) = 1$.

Finally, we assume that $T' = T_5(k)$. If $u \in \{b, d, b', d', y_1, \ldots, y_k\}$, then, by Lemma 8, $u \in S'$ and $w_{(T,S\setminus\{u\})}(u) = \frac{1}{2} + w_{(T,S'\setminus\{u\})}(u) \geq \frac{1}{2} + \frac{1}{2} = 1$. If $u \in \{a, c\}$, then $w_{(T,S\setminus\{b\})}(b) \geq w_{(T,\{d,w,y_1\})}(b) = 1$. If $u \in \{a', c'\}$, we obtain a similar contradiction. Finally, if $u = x_i$ for some $i \in [k]$, then $w_{(T,S\setminus\{b\})}(b) \geq w_{(T,\{w,d\})}(b) + w_{(T,\{y_j : 1 \leq j \leq \min\{i+1,k\}\}\cup\{b'\})}(b) = \frac{1}{2} + \frac{1}{2^{i+2}} + \left(\frac{1}{4} + \cdots + \frac{1}{2^{i+2}}\right) = 1$, which completes the proof. □

3. Conclusion

Our results motivate several open problems. It seems interesting to characterize all extremal graphs for Theorem 2. In view of Theorem 5, one can study upper bounds for graphs of larger minimum degree. As stated before Theorem 6, we conjecture that $\alpha_e(G)$ grows faster than $\log_2(n(G))$ for cubic graphs. Can the graphs G with $\alpha_e(G) = \alpha(G)$ be recognized efficiently? Are there hardness results concerning $\alpha_e(G)$, and efficient algorithms for restricted graph classes such as trees?

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6 Large Values of the Clustering Coefficient

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Note

Large values of the clustering coefficient

Michael Gentner [a], Irene Heinrich [b], Simon Jäger [a], Dieter Rautenbach [a,*]

[a] Institute of Optimization and Operations Research, Ulm University, Ulm, Germany
[b] Department of Mathematics, University of Kaiserslautern, Kaiserslautern, Germany

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ABSTRACT

A prominent parameter in the context of network analysis, originally proposed by Watts and Strogatz (1998), is the clustering coefficient of a graph G. It is defined as the arithmetic mean of the clustering coefficients of its vertices, where the clustering coefficient of a vertex u of G is the relative density $m(G[N_G(u)])/\binom{d_G(u)}{2}$ of its neighborhood if $d_G(u)$ is at least 2, and 0 otherwise. It is unknown which graphs maximize the clustering coefficient among all connected graphs of given order and size.

We determine the maximum clustering coefficients among all connected regular graphs of a given order, as well as among all connected subcubic graphs of a given order. In both cases, we characterize all extremal graphs. Furthermore, we determine the maximum increase of the clustering coefficient caused by adding a single edge.

1. Introduction

Watts and Strogatz [8] proposed the clustering coefficient of a graph in order to quantify the corresponding property of networks. For a vertex u of a simple, finite, and undirected graph G, let the *clustering coefficient* of u in G be

$$C_u(G) = \begin{cases} \frac{m(G[N_G(u)])}{\binom{d_G(u)}{2}}, & \text{if } d_G(u) \geq 2, \text{ and} \\ 0, & \text{otherwise,} \end{cases}$$

where $N_G(u)$ denotes the neighborhood $\{v \in V(G) : uv \in E(G)\}$ of u in the graph G whose vertex set is $V(G)$ and whose edge set is $E(G)$, $d_G(u)$ denotes the degree $|N_G(u)|$ of u in G, $G[N_G(u)]$ denotes the subgraph of G induced by $N_G(u)$, and $m(G[N_G(u)])$ denotes the size of this subgraph, that is, $m(G[N_G(u)])$ equals exactly the number of triangles of G that contain the vertex u.

Furthermore, let the *clustering coefficient* of G be the average

$$C(G) = \frac{1}{n(G)} \sum_{u \in V(G)} C_u(G)$$

of the clustering coefficients of its $n(G) = |V(G)|$ vertices.

For an integer ℓ, let $[\ell]$ denote the set of all positive integers at most ℓ.

While the clustering coefficient received a lot of attention within social network analysis [1,5–7], some fundamental mathematical problems related to it are still open. It is unknown [4,7], for instance, which graphs maximize the clustering coefficient among all connected graphs of a given order and size.

* Corresponding author.
E-mail addresses: michael.gentner@uni-ulm.de (M. Gentner), heinrich@mathematik.uni-kl.de (I. Heinrich), simon.jaeger@uni-ulm.de (S. Jäger), dieter.rautenbach@uni-ulm.de (D. Rautenbach).

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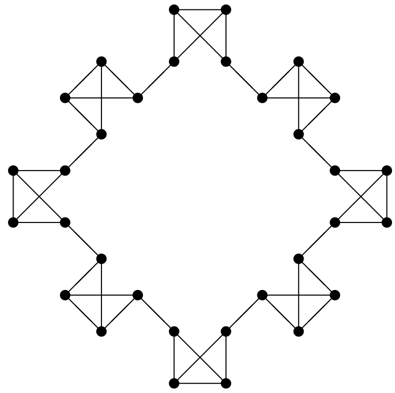


Fig. 1. The unique graph $G(3, 8)$ with the largest clustering coefficient among all connected 3-regular graphs of order 24.

Watts [6,7] suggested the so-called *connected caveman* graphs as a possible extremal construction. For integers k and ℓ at least 2, these arise from ℓ disjoint copies $G_1, \ldots, G_\ell$ of $K_{k+1} - e$, the complete graph of order $k + 1$ minus one edge, arranged cyclically by adding, for every i in $[\ell]$, an edge between one of the two vertices of degree $k - 1$ in G_i and one of the $k - 1$ vertices of degree k in G_{i+1}, where the indices are identified modulo ℓ. Actually, it is rather obvious that these graphs do not have the largest clustering coefficient among all connected graphs of given order and size, because removing the edge between G_1 and G_2, and adding a new edge between the two vertices of degree $k - 1$ in G_1, increases the clustering coefficient.

Fukami and Takahashi [2,3] considered *clustering coefficient locally maximizing graphs* whose clustering coefficient cannot be increased by some local operations such as an edge swap.

In the present paper we determine the maximum clustering coefficients among all connected regular graphs of a given order, as well as among all connected subcubic graphs of a given order. In both cases, we characterize all extremal graphs. Furthermore, we determine the maximum increase of the clustering coefficient caused by adding a single edge.

2. Results

We introduce a slightly modified version of the connected caveman graphs. For integers k and ℓ with $k \geq 3$ and $\ell \geq 2$, let $G(k, \ell)$ be the k-regular connected graph that arises from ℓ disjoint copies $G_1, \ldots, G_\ell$ of $K_{k+1} - e$ arranged cyclically by adding, for every i in $[\ell]$, an edge between a vertex in G_i and a vertex in G_{i+1}, where the indices are identified modulo ℓ. Note that $G(k, \ell)$ is uniquely determined up to isomorphism by the requirement of k-regularity. See Fig. 1 for an illustration.

Theorem 1. *Let k and n be integers with $n \geq k + 2$ and $k \geq 3$. If G is a connected k-regular graph of order n, then*

$$C(G) \leq 1 - \frac{6}{k(k+1)}$$

with equality if and only if $n/(k + 1)$ is an integer and G equals $G(k, n/(k + 1))$.

Proof. Let G be a connected k-regular graph of order n. For a non-negative integer i, let V_i be the set of vertices u of G with $m(G[N_G(u)]) = \binom{k}{2} - i$. Since G is connected and has order at least $k + 2$, no vertex has a complete neighborhood, that is, V_0 is empty. For a set U of vertices of G, let $\sigma(U) = \sum_{u \in U} C_u(G)$. In order to obtain a useful decomposition of G, we consider some special graphs. For $k \leq 4$, one such graph suffices, while for $k \geq 5$, two more are needed.

Let $G_1, \ldots, G_r$ be a maximal collection of disjoint subgraphs of G that are all copies of $K_{k+1} - e$. Let $A = V(G_1) \cup \cdots \cup V(G_r)$ and $R = V(G) \setminus A$. Note that every vertex in A has at most one neighbor in R. Suppose that R contains a vertex u from V_1. Since every vertex in $N_G(u)$ has at least two neighbors in the closed neighborhood $N_G[u]$ of u, the subgraph G_{r+1} of G induced by $N_G[u]$ does not intersect A and is a copy of $K_{k+1} - e$. Now, $G_1, \ldots, G_r, G_{r+1}$ contradicts the maximality of the above collection, which implies that R does not intersect V_1.

Since each G_i contains $k - 1$ vertices from V_1 and two vertices whose neighborhood induces $K_1 \cup K_{k-1}$, and $|A| = r(k + 1)$, we have

$$\sigma(A) = \sum_{i \in [r]} \sum_{u \in V(G_i)} C_u(G) = r \left((k-1) \frac{\binom{k}{2} - 1}{\binom{k}{2}} + 2 \frac{\binom{k-1}{2}}{\binom{k}{2}} \right) = |A| \left(1 - \frac{6}{k(k+1)} \right).$$

Since R does not intersect V_1, we have

$$\sigma(R) = \sum_{u\in R} C_u(G) \le |R| \frac{\binom{k}{2} - 2}{\binom{k}{2}} = |R| \left(1 - \frac{4}{(k-1)k}\right).$$

First, let $k \le 4$. Since $1 - \frac{4}{(k-1)k} < 1 - \frac{6}{k(k+1)}$ in this case, we obtain

$$\begin{aligned} C(G) &= \frac{1}{n(G)}(\sigma(A) + \sigma(R)) \\ &\le \frac{1}{n(G)}(|A| + |R|)\left(1 - \frac{6}{k(k+1)}\right) \\ &= 1 - \frac{6}{k(k+1)}, \end{aligned}$$

with equality if and only if $A = V(G)$ and $R = \emptyset$, which implies that $k + 1$ divides n, and G equals $G(k, n/(k + 1))$.

Now, let $k \ge 5$. In this case, we need to refine the partition of $V(G)$ into A and R further. Let $G_1, \ldots, G_r$, A, and R be exactly as above, and recall that R does not intersect V_1. Let $H_1, \ldots, H_s$ be a maximal collection of disjoint subgraphs of $G[R]$ that are all copies of the two possible graphs that arise from K_{k+1} by removing two edges. Let $B = V(H_1) \cup \cdots \cup V(H_s)$, and $S = V(G)\setminus(A\cup B)$. Note that every vertex in $A\cup B$ has at most two neighbors in S. Suppose that S contains a vertex u from V_2. Since $k \ge 5$, every vertex in $N_G(u)$ has at least three neighbors in the closed neighborhood $N_G[u]$ of u. Hence, the subgraph H_{s+1} of G induced by $N_G[u]$ does not intersect $A \cup B$ and is a copy of one of the two possible graphs that arise from K_{k+1} by removing two edges. Now, $H_1, \ldots, H_s, H_{s+1}$ contradicts the maximality of the above collection, which implies that S does not intersect $V_1 \cup V_2$.

If H_i for some i in $[s]$ is a copy of K_{k+1} minus two non-incident edges, then H_i contains $k - 3$ vertices from V_2 and four vertices whose neighborhood induces a graph that arises from $K_1 \cup (K_{k-1} - e)$ by adding at most two edges, which implies

$$\sigma(V(H_i)) \le (k-3)\frac{\binom{k}{2} - 2}{\binom{k}{2}} + 4\frac{\binom{k-1}{2} - 1 + 2}{\binom{k}{2}} = \frac{k^3 - 13k + 28}{(k-1)k}.$$

If H_i for some i in $[s]$ is a copy of K_{k+1} minus two incident edges, then H_i contains $k - 2$ vertices from V_2, two vertices whose neighborhood induces a graph that arises from $K_1 \cup K_{k-1}$ by adding at most one edge, and one vertex whose neighborhood induces a graph that arises from $K_1 \cup K_1 \cup K_{k-2}$ by adding at most one edge, which implies

$$\sigma(V(H_i)) \le (k-2)\frac{\binom{k}{2} - 2}{\binom{k}{2}} + 2\frac{\binom{k-1}{2} + 1}{\binom{k}{2}} + \frac{\binom{k-2}{2} + 1}{\binom{k}{2}} = \frac{k^3 - 13k + 24}{(k-1)k}.$$

Using $|B| = s(k + 1)$, we obtain

$$\sigma(B) = \sum_{i\in[s]} \sigma(V(H_i)) \le |B| \frac{k^3 - 13k + 28}{(k-1)k(k+1)} = |B| \left(1 - \frac{12k - 28}{(k-1)k(k+1)}\right).$$

Since S does not intersect $V_1 \cup V_2$, we have

$$\sigma(S) \le |S| \frac{\binom{k}{2} - 3}{\binom{k}{2}} = |S| \left(1 - \frac{6}{(k-1)k}\right).$$

Since

$$\max\left\{1 - \frac{12k - 28}{(k-1)k(k+1)}, 1 - \frac{6}{(k-1)k}\right\} < 1 - \frac{6}{k(k+1)}$$

for $k \ge 5$, we obtain

$$\begin{aligned} C(G) &= \frac{1}{n(G)}(\sigma(A) + \sigma(B) + \sigma(S)) \\ &\le \frac{1}{n(G)}(|A| + |B| + |S|)\left(1 - \frac{6}{k(k+1)}\right) \\ &= 1 - \frac{6}{k(k+1)}, \end{aligned}$$

with equality if and only if $A = V(G)$ and $B = S = \emptyset$, which implies that $k + 1$ divides n, and G equals $G(k, n/(k + 1))$. This completes the proof. □

Recall that the *diamond* is the unique graph with degree sequence 2, 2, 3, 3.

Theorem 2. *If G is a connected subcubic graph of order n at least 6, then*

$$C(G) \leq \begin{cases} \frac{7}{12} + \frac{12}{12n}, & \text{if } n \equiv 0 \bmod 4, \\ \frac{7}{12} + \frac{13}{12n}, & \text{if } n \equiv 1 \bmod 4, \\ \frac{7}{12} + \frac{14}{12n}, & \text{if } n \equiv 2 \bmod 4, \text{ and} \\ \frac{7}{12} + \frac{11}{12n}, & \text{if } n \equiv 3 \bmod 4. \end{cases} \tag{1}$$

Proof. Let $\mathcal{G}$ be the set of all connected subcubic graphs of order n at least 6. We assume that G is chosen within $\mathcal{G}$ in such a way that

(i) its clustering coefficient $C(G)$ is as large as possible,
(ii) subject to condition (i), the size $m(G)$ of G is as small as possible, and,
(iii) subject to conditions (i) and (ii), the number of triangles in G that contain at most one vertex of degree 2 in G is as small as possible.

We establish a series of structural properties of G.

Claim 1. *Every subgraph D of G that is a diamond is induced and forms an endblock.*

Proof of Claim 1. Let D be a subgraph of G that is a diamond. Since G is subcubic, connected, and of order more than 4, the subgraph D is induced, that is, the two vertices of degree 2 in D are non-adjacent in G. If all vertices in D have degree 3 in G, then contracting D to a single vertex u, adding a new triangle xyz, and adding the new edge ux yields a graph G' in $\mathcal{G}$ with $C(G') \geq C(G) + \frac{1}{3n}$, contradicting the choice of G. Note that the two neighbors of u in G' that are distinct from x may be adjacent, in which case $C(G') > C(G) + \frac{1}{3n}$. In view of the order, this implies that D contains exactly one vertex of degree 2, and, hence, forms an endblock of G. □

Claim 2. *Every edge of G that lies in some cycle also lies in some triangle.*

Proof of Claim 2. If the edge uv of G lies in some cycle but in no triangle, then removing uv yields a graph G' in $\mathcal{G}$ with $C(G') \geq C(G)$ and $m(G') < m(G)$, contradicting the choice of G. Note that, if some triangle of G contains u or v, then $C(G') > C(G)$. □

Claim 3. *Every block of G is K_2, K_3, or a diamond.*

Proof of Claim 3. Suppose, for a contradiction, that B is a block of G that is neither K_2, nor K_3, nor a diamond. Note that every edge of B lies in some cycle, and, hence, by Claim 2, also lies in some triangle. Let uvw be a triangle in B. Since B is not K_3, we may assume that u has a neighbor x in $V(B) \setminus \{v, w\}$. Since the edge ux of B lies in some triangle, we may assume that x and v are adjacent. Since B is not a diamond, we may assume, by symmetry, that x has a neighbor y in $V(B) \setminus \{u, v, w\}$. Since the edge xy of B lies in some triangle, we obtain that y is adjacent to u or v, contradicting the assumption that G is subcubic. □

Let $\mathcal{D}$ be the set of blocks of G that are diamonds. For $i \in \{2, 3\}$, let $\mathcal{I}_i$ be the set of blocks of G that are triangles that contain exactly i vertices of degree 3 in G. Let $\mathcal{I} = \mathcal{I}_2 \cup \mathcal{I}_3$. Finally, let $\mathcal{S}$ be the set of vertices of G that do not lie in some triangle and have degree at most 2 in G.

The triangles in $\mathcal{I}$ are called *inner triangles*. By condition (iii), G has as few inner triangles as possible given the other conditions.

If $u \in \mathcal{S}$ has degree 2, then *resolving u* means to remove u from G, and to connect its two neighbors by a new edge. If $u \in \mathcal{S}$ has degree 1, then *resolving u* simply means to remove u from G. Note that resolving some vertex from $\mathcal{S}$ yields a connected subcubic graph G' of order $n - 1$ with $C(G') \geq C(G)$.

Claim 4. *Either $\mathcal{D}$ or $\mathcal{I}$ is empty.*

Proof of Claim 4. Suppose, for a contradiction, that G contains a diamond D and an inner triangle T. By Claim 1, D contains a vertex u of degree 2 in G. Let v be a neighbor of u. If $T \in \mathcal{I}_2$, then contracting T to a single vertex w, removing u, adding a new triangle xyz, and adding the new edge xw yields a graph G' in $\mathcal{G}$ with $C(G') = C(G) + \frac{1}{3n}$, contradicting the choice of G. If $T \in \mathcal{I}_3$, then contracting T to a single vertex, removing u, adding a new triangle xyz, and adding the new edge xv yields a graph G' in $\mathcal{G}$ with $C(G') = C(G) + \frac{1}{3n}$, contradicting the choice of G. □

Claim 5. $|\mathcal{D}| \le 2$.

Proof of Claim 5. Suppose, for a contradiction, that G has three blocks B_1, B_2, and B_3 that are diamonds. By Claim 1, these are all endblocks, and removing the three vertices, say v_1, v_2, and v_3, of degree 2 in G from B_1, B_2, and B_3, adding a new triangle xyz, and adding a new edge between x and one of the two neighbors of v_1 in B_1 yields a graph G' in $\mathcal{G}$ with $C(G') = C(G) + \frac{2}{3n}$, contradicting the choice of G. □

Claim 6. *$\mathcal{S}$ is empty.*

Proof of Claim 6. Suppose, for a contradiction, that $\mathcal{S}$ contains some vertex u.

If $\mathcal{I}_2$ contains a triangle T, then resolving u, contracting T to a single vertex v, adding a new triangle xyz, and adding the new edge xv yields a graph G' in $\mathcal{G}$ with $C(G') \ge C(G) + \frac{2}{3n}$, contradicting the choice of G. If $\mathcal{I}_3$ contains a triangle T, then resolving u, contracting T to a single vertex v, adding a new triangle xyz, and then replacing one of the edges incident with v, say vw, with the two new edges xv and yw yields a graph G' in $\mathcal{G}$ with $C(G') \ge C(G) + \frac{2}{3n}$, contradicting the choice of G. Hence, we may assume that G has no inner triangles.

If G has a block B that is a triangle, then B is an endblock, and resolving u, adding a new vertex v, and adding two new edges between v and the two vertices of degree 2 in B yields a graph G' in $\mathcal{G}$ with $C(G') \ge C(G) + \frac{1}{3n}$, contradicting the choice of G. Hence, we may assume that G has no blocks that are triangles.

If G has two blocks B_1 and B_2 that are diamonds, then B_1 and B_2 are endblocks by Claim 1, and resolving u, removing the two vertices, say v_1 and v_2, of degree 2 in G from B_1 and B_2, respectively, adding a new triangle xyz, and adding a new edge between x and one of the two neighbors of v_1 in B_1 yields a graph G' in $\mathcal{G}$ with $C(G') \ge C(G) + \frac{1}{n}$, contradicting the choice of G. Hence, since G is not a tree, we may assume that G has exactly one endblock B that is a diamond, and all other blocks of G are K_2 s. In this case $C(G) = \frac{8}{3n}$. Since $\mathcal{G}$ contains a graph G' with two endblocks that are triangles, we obtain $C(G') \ge \frac{14}{3n} > C(G)$, contradicting the choice of G. □

Recall that the *paw* is the unique graph with degree sequence $1, 2, 2, 3$.

Claim 7. $|\mathcal{I}| \le 1$.

Proof of Claim 7. Suppose, for a contradiction, that G has two inner triangles T_1 and T_2.

If $T_1, T_2 \in \mathcal{I}_3$, then contracting both triangles to single vertices u_1 and u_2, adding a new paw P, and then replacing one of the edges incident with u_1, say u_1v, with the two new edges xu_1 and xv, where x is the vertex of degree 1 in P, yields a graph G' in $\mathcal{G}$ with $C(G') = C(G) + \frac{1}{3n}$, contradicting the choice of G.

If $T_1 \in \mathcal{I}_2$ and $T_2 \in \mathcal{I}_3$, then contracting both triangles to single vertices u_1 and u_2, adding a new diamond D, and adding the new edge xu_1, where x is a vertex of degree 2 in D, yields a graph G' in $\mathcal{G}$ with $C(G') = C(G)$, $m(G') = m(G)$, and less inner triangles than G, contradicting the choice of G.

If $T_1, T_2 \in \mathcal{I}_2$, then replacing T_1 with an edge between the two vertices, say a and b, outside of T_1 that have neighbors in T_1, adding a new triangles xyz, and adding the new edge xu_2, where u_2 is the vertex in T_2 of degree 2 in G, yields a graph G' in $\mathcal{G}$ with $C(G') = C(G)$, $m(G') = m(G)$, and less inner triangles than G, contradicting the choice of G. Note that, in this last construction, the vertices a and b are non-adjacent in G by Claim 3, and two triangles that contributed to $\mathcal{I}_2$ are replaced by one that contributes to $\mathcal{I}_3$. □

For $t(G) = (|\mathcal{D}|, |\mathcal{I}_2|, |\mathcal{I}_3|)$, the above claims imply $t(G) \in \{(0, 0, 0), (1, 0, 0), (2, 0, 0), (0, 0, 1), (0, 1, 0)\}$. For each of these cases, we can determine $C(G)$ exactly. Let k be the number of vertices of G that do not lie in a triangle.

If $t(G) = (i, 0, 0)$ for some $i \in \{0, 1, 2\}$, then G arises from a tree of order $2k + 2$ with k vertices of degree 3 and $k + 2$ endvertices, by replacing $k+2-i$ endvertices with triangles and i endvertices with diamonds, and we obtain $n = 4k+6+i$, and

$$C(G) = \frac{1}{n}\left(\frac{7}{3}(k+2-i) + \frac{8}{3}i\right) = \frac{7}{12} + \frac{14-3i}{12n}.$$

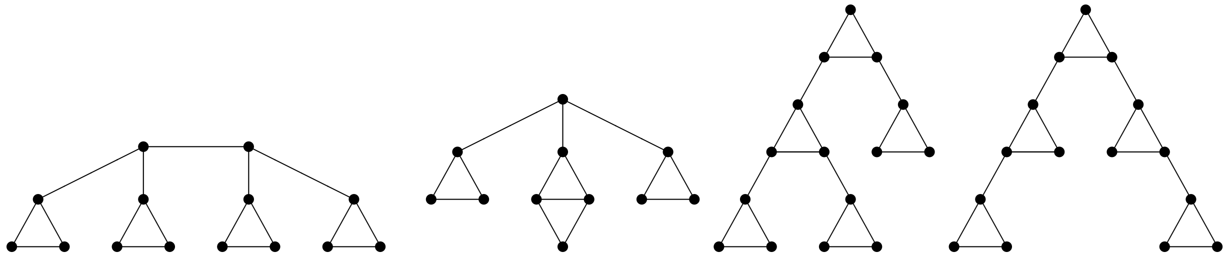
If $t(G) = (0, 0, 1)$, then G arises from a tree of order $2k+4$ with $k+1$ vertices of degree 3 and $k+3$ endvertices, by replacing all endvertices as well as one internal vertex with triangles, and we obtain $n = 4k + 12$, and

$$C(G) = \frac{1}{n}\left(\frac{7}{3}(k+3) + 1\right) = \frac{7}{12} + \frac{1}{n}.$$

If $t(G) = (0, 1, 0)$, then G arises from a tree of order $2k + 3$ with k vertices of degree 3, one vertex of degree 2, and $k + 2$ endvertices, by replacing all endvertices as well as the vertex of degree 2 with triangles, and we obtain $n = 4k + 9$, and

$$C(G) = \frac{1}{n}\left(\frac{7}{3}(k+2) + \frac{5}{3}\right) = \frac{7}{12} + \frac{13}{12n}.$$

Considering the different parities of n modulo 4, the desired result follows. □



$(0,0,0)$ $(1,0,0)$ $(0,1,1)$ $(0,3,0)$

Fig. 2. Some graphs in $\mathcal{B}_0$ of type $(0, 0, 0)$, $(1, 0, 0)$, $(0, 1, 1)$, and $(0, 3, 0)$.

Our next goal is the characterization of all extremal graphs for (1). Therefore, let $\mathcal{B}_0$ be the set of all connected subcubic graphs G of order at least 6 such that

- every block of G is K_2, K_3, or a diamond,
- every block of G that is a diamond is an endblock of G, and
- every vertex of degree at most 2 lies in a triangle.

Note that the last condition implies that the set denoted by $\mathcal{S}$ above is empty.

Let the *type* $t(G)$ of a graph G in $\mathcal{B}_0$ be the 3-tuple (d, i_2, i_3), where d is the number of blocks of G that are diamonds, and, for j in $\{2, 3\}$, i_j is the number of blocks of G that are triangles that contain exactly j vertices of degree 3 in G.

Let

$$\mathcal{B} = \Big\{G \in \mathcal{B}_0 : t(G) \in \{(0, 0, 0), (1, 0, 0), (0, 1, 0), (0, 0, 1), (0, 1, 1), (0, 2, 0), (0, 3, 0)\}\Big\}.$$

See Fig. 2 for some illustrations.

Theorem 3. *If G is a connected subcubic graph of order at least 6, then G satisfies (1) with equality if and only if $G \in \mathcal{B}$.*

Proof. First, let $G \in \mathcal{B}$. For $t(G) \in \{(0, 0, 0), (1, 0, 0), (0, 1, 0), (0, 0, 1)\}$, we verified at the end of the proof of Theorem 2 that (1) holds with equality. For $t(G) \in \{(0, 1, 1), (0, 2, 0), (0, 3, 0)\}$, very similar simple calculations imply the same.

Now, let G satisfy (1) with equality. Similarly as above, let $\mathcal{G}$ be the set of all connected subcubic graphs of order $n(G)$. We consider the claims from the proof of Theorem 2. Clearly, Claim 1 still holds. Suppose, for a contradiction, that Claim 2 fails, that is, G has some edge uv that lies in some cycle but in no triangle. Iteratively removing from G first the edge uv, and then further edges that lie in cycles but not in triangles as long as possible yields a graph G' in $\mathcal{G}$ with $C(G') \geq C(G)$ such that every edge of G' that lies in some cycle also lies in some triangle. Now, the argument from the proof of Claim 3 applies, and, hence, $G' \in \mathcal{B}_0 \subseteq \mathcal{G}$. By (1) for G', we obtain $C(G') = C(G)$, which, as observed in the proof of Claim 2, implies that u and v are vertices of G' that do not lie in some triangle and have degree at most 2 in G'. Arguing as in the proof of Claim 6, we obtain the existence of a graph G'' in $\mathcal{G}$ with $C(G'') > C(G') = C(G)$, which contradicts (1) for G''. Hence, Claim 2 holds. Considering their respective proofs, it follows that also Claims 3, 4, 5, and 6 hold. Let the type $t(G)$ of G be (d, i_2, i_3). By Claim 5, $d \leq 2$. If $d = 2$, then, by Claim 4, $i_2 = i_3 = 0$, and the calculation at the end of the proof of Theorem 2 implies the contradiction that (1) does not hold with equality. Hence, $d \in \{0, 1\}$, and, if $d = 1$, then, by Claim 4, $i_2 = i_3 = 0$. If $i_3 \geq 2$, then arguing as in the proof of Claim 7 yields the existence of a graph G' in $\mathcal{G}$ with $C(G') > C(G)$, which is a contradiction. Hence, $i_3 \leq 1$. If $i_2 \geq 4$, then arguing as in the proof of Claim 7 yields the existence of a graph G' in $\mathcal{G}$ with $C(G') = C(G)$ that is of type $(d', i_2', i_3') = (d, i_2 - 4, i_3 + 2)$. Now, as observed above, $i_3' \geq 2$ implies the existence of a graph G'' in $\mathcal{G}$ with $C(G'') > C(G') = C(G)$, which is a contradiction. Hence, $i_2 \leq 3$. Finally, if $i_2 \geq 2$ and $i_3 = 1$, then arguing as in the proof of Claim 7 yields the existence of a graph G' in $\mathcal{G}$ with $C(G') = C(G)$ that is of type $(d', i_2', i_3') = (d, i_2 - 2, i_3 + 1)$. Again, as observed above, $i_3' \geq 2$ implies a contradiction. Hence, $i_3 = 1$ implies $i_2 \leq 1$. Altogether, it follows that $G \in \mathcal{B}$, which completes the proof. $\square$

Our final result shows that adding a single edge can increase the clustering coefficient of a graph from 0 to almost 1, which means that it is a rather sensitive parameter.

Theorem 4. *If G is a graph of order n at least 3, and u and v are non-adjacent vertices in G, then*

$$C(G + uv) \leq C(G) + \left(1 - \frac{2}{n} + \frac{4}{n(n-1)}\right)$$

with equality if and only if G is $K_{2,n-2}$, and u and v are of degree $n - 2$ in G.

Proof. Since the statement is trivial if $d_G(u) = 0$ or $d_G(v) = 0$, we may assume that neither u nor v is isolated in G. Let $G' = G + uv$.

If w is a common neighbor of u and v in G, then the degree of w in G' equals the degree of w in G but $G'[N_{G'}(w)]$ contains exactly one edge more than $G[N_G(w)]$, which implies

$$C_w(G') - C_w(G) = \frac{1}{\binom{d_G(w)}{2}} \le 1$$

with equality if and only if $d_G(w) = 2$.

If $d_G(u) \ge 2$, then

$$\begin{aligned}
C_u(G') - C_u(G) &= \frac{m(G'[N_{G'}(u)])}{\binom{d_{G'}(u)}{2}} - \frac{m(G[N_G(u)])}{\binom{d_G(u)}{2}} \\
&= \frac{m(G[N_G(u)]) + |N_G(u) \cap N_G(v)|}{\binom{d_G(u)+1}{2}} - \frac{m(G[N_G(u)])}{\binom{d_G(u)}{2}} \\
&= \frac{2(d_G(u)-1)|N_G(u) \cap N_G(v)| - 4m(G[N_G(u)])}{(d_G(u)+1)d_G(u)(d_G(u)-1)} \\
&\le \frac{2(d_G(u)-1)d_G(u) - 4m(G[N_G(u)])}{(d_G(u)+1)d_G(u)(d_G(u)-1)} \\
&\le \frac{2}{d_G(u)+1}
\end{aligned}$$

with equality if and only if $N_G(u) \subseteq N_G(v)$ and $N_G(u)$ is independent.

If $d_G(u) = 1$, then

$$C_u(G') - C_u(G) \le 1 = \frac{2}{d_G(u)+1}$$

with equality if and only if $N_G(u) \subseteq N_G(v)$ and $N_G(u)$ is independent.

We obtain that

$$\begin{aligned}
n(C(G') - C(G)) &= (C_u(G') - C_u(G)) + (C_v(G') - C_v(G)) + \sum_{w \in N_G(u) \cap N_G(v)} (C_w(G') - C_w(G)) \\
&\le \frac{2}{d_G(u)+1} + \frac{2}{d_G(v)+1} + |N_G(u) \cap N_G(v)|
\end{aligned}$$

with equality if and only if $N_G(u) = N_G(v)$ is independent and every vertex in $N_G(u)$ has degree 2 in G, that is, G is $K_{2,n-2}$, and u and v are of degree $n-2$ in G. Since $d := \min\{d_G(u), d_G(v)\} \le n-2$ and the function $f : \mathbb{N} \to \mathbb{R} : d \mapsto \frac{4}{d+1} + d$ is strictly increasing, we conclude

$$\begin{aligned}
n(C(G') - C(G)) &\le \frac{2}{d_G(u)+1} + \frac{2}{d_G(v)+1} + |N_G(u) \cap N_G(v)| \\
&\le \frac{4}{d+1} + d \\
&\le \frac{4}{n-1} + n - 2,
\end{aligned}$$

which completes the proof. □

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