Note

On diameter and inverse degree of a graph

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**Abstract**

The inverse degree \( r(G) \) of a finite graph \( G = (V, E) \) is defined as \( r(G) = \sum_{v \in V} \frac{1}{\deg v} \), where \( \deg v \) is the degree of vertex \( v \). We establish inequalities concerning the sum of the diameter and the inverse degree of a graph which for the most part are tight. We also find upper bounds on the diameter of a graph in terms of its inverse degree for several important classes of graphs. For these classes, our results improve bounds by Erdős et al. (1988) [5], and by Dankelmann et al. (2008) [4].

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**1. Introduction**

Let \( G = (V, E) \) be a finite, connected, undirected graph. The distance \( d_G(u, v) \) between two vertices \( u, v \) of \( G \) is the length of a shortest \( u-v \) path in \( G \), and the diameter is \( \text{diam}(G) = \max\{d_G(u, v) : u, v \in V\} \). The neighborhood \( N(v) \) of a vertex \( v \) is the set \( \{x \in V : d_G(v, x) = 1\} \). The degree \( \deg v \) of \( v \) is the cardinality of \( N(v) \). The inverse degree \( r(G) \) of \( G \) is defined as \( r(G) = \sum_{v \in V} \frac{1}{\deg v} \). For notions not defined here refer the reader to [1]. The inverse degree (also known as the sum of reciprocals of degrees) first attracted attention through numerous conjectures generated by the computer programme Graffiti [7]. Since then its relationship with other graph invariants, such as diameter, edge-connectivity, matching number, Wiener index has been studied by several authors (see, for example [2,9,5,4,6]).

Amongst the conjectures made by Graffiti are predictions on bounds on the sum of the inverse degree and other graph invariants. For instance, conjectures on the bounds of \( r(G) + \mu(g), r(G) + R(G) \), where \( \mu(G) \) is the average distance and \( R(G) \) is the Randic Index of \( G \), were generated. In [3] the conjecture listed as Conjecture 25 in [7] which states that \( \text{rad}(G) \leq r(G) + \mu(G) \), where \( \text{rad}(G) \) is the radius of \( G \), was disproved. Although some conjectures by Graffiti were disproved (see also [5,7,9]), they led to relations between parameters that seemed to have no obvious inter-dependence. In [9] best bounds on the sum of the inverse degree and the matching number \( r(T) + \alpha'(T) \) of a tree \( T \) are given. On the other hand, until now no bounds on more significant combinations of graph invariants have been reported. The aim of the present note, among other things, is to make a contribution in this direction.

Turning to bounds on the diameter in terms of order and inverse degree, our starting point is the following bound by Erdős, Pach and Spencer [5].

**Theorem 1.** Let \( G \) be a connected graph of order \( n \), diameter \( \text{diam}(G) \), average distance \( \mu(G) \) and inverse degree \( r(G) \). Then

\[
\text{diam}(G) \leq (6r(G) + o(1)) \frac{\log n}{\log \log n}.
\]

Moreover, there exist graphs for which

\[
\left( \frac{2}{9} \lceil \frac{r(G)}{3} \rceil + o(1) \right) \frac{\log n}{\log \log n} \leq \mu(G) \leq \text{diam}(G).
\]

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The bound (1) was later improved by a factor of about 2 by Dankelmann, Swart and van den Berg [4] who showed that
\[ \text{diam}(G) \leq (3r(G) + 2 + o(1)) \frac{\log n}{\log \log n}. \] (2)

The construction given in the second part of Theorem 1 confirms that, for an arbitrary graph \( G \), there is no constant \( \alpha \) for which \( \text{diam}(G) \leq \alpha \cdot r(G) \). It is therefore natural to ask whether there exist classes of graphs for which \( \text{diam}(G) \leq \alpha \cdot r(G) \) for some constant \( \alpha \) and hence providing improvements on (2) for such classes of graphs. In this article, we will focus our attention to bounds on the diameter in terms of the inverse degree for some important classes of graphs such as planar graphs, regular graphs, chemical graphs, and trees. Chemical graphs, for instance, represent the structure of organic molecules and thus have a maximum degree of 4, carbon atoms being 4-valent and double bonds being counted as single edges. Formally, a chemical graph is a graph with a maximum degree of 4. Molecular structure-descriptor such as the Randić Index (defined as \( R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{\deg u \cdot \deg v}} \), whose flavor is similar to that of the inverse degree, were studied intensively for these classes of graphs (see, for example the book by Li and Gutman [8], and references cited therein).

2. Main results

**Theorem 2.** Let \( T \) be a tree of order \( n > 2 \) and diameter \( \text{diam}(T) \). Then
\[ \frac{n}{2} + \frac{\sqrt{2} \cdot \sqrt{n}}{2} \leq \text{diam}(T) + r(T) \leq \frac{3}{2}n. \]

The upper bound is tight. The lower bound is close to best possible in the sense that there exist graphs \( T_n \) satisfying the hypothesis of the theorem such that \( \text{diam}(T_n) + r(T_n) = \frac{n}{2} + 2\sqrt{n} - 1 + O(1) \).

**Theorem 3.** Let \( T \) be a tree with diameter \( d \) and \( s \) leaves. Let \( q \) and \( \varepsilon \), \( 0 \leq \varepsilon < d - 1 \), be unique integers for which \( s - 2 = q(d - 1) + \varepsilon \). Then
\[ r(T) \geq s + \frac{d - 1}{q + 2} - \frac{\varepsilon}{(q + 2)(q + 3)}. \]

Moreover the bound is sharp for all values of \( d \) and \( s \).

**Corollary 1.** Let \( T \) be a tree with diameter \( d \) and \( s \) leaves. Let \( q \) and \( \varepsilon \), \( 0 \leq \varepsilon < d - 1 \), be the unique integers satisfying \( s - 2 = q(d - 1) + \varepsilon \). Then
\[ d \leq q + 2 \frac{r(T)}{(q + 1)^2} - \frac{q^2 + 5q + 5}{(q + 1)^2(q + 3)} \varepsilon + \frac{q^2 - 3}{(q + 1)^2}. \]

Moreover the bound is sharp for all values of \( d \) and \( s \).

**Theorem 4.** Let \( G \) be a \( k \)-regular connected graph, \( k \geq 3 \). Then
\[ \text{diam}(G) \leq 3 \left( 1 - \frac{1}{k + 1} \right) r(G) + 1 - \frac{6}{k + 1}, \]
and this inequality is tight.

The bounds presented below seem not best possible; we will conjecture sharp bounds at the end of this note.

**Theorem 5.** Let \( G \) be a connected chemical graph. Then
\[ \text{diam}(G) \leq 3r(G) + 3. \]

**Theorem 6.** Let \( G \) be a connected planar graph of order \( n > 2 \). Then
\[ \text{diam}(G) \leq 6r(G) - 3 - \frac{4}{n - 2}. \]

3. Known results

The following result was proved for example in [2].

**Lemma 1.** Let \( a_1, a_2, \ldots, a_p \) be positive reals with \( \sum_{i=1}^{p} a_i \leq A \). Then
\[ \sum_{i=1}^{p} \frac{1}{a_i} \geq \frac{p^2}{A}. \quad \square \]
We will make use of Euler's formula:

\[ m = n + f - 2, \]

for a planar graph of order \( n \), size \( m \) and with \( f \) faces.

### 4. An elementary bound on \( \text{diam}(T) + r(T) \)

Let \( T \) be a tree of order \( n \). Then \( \sum_{v \in V(T)} \deg v = 2(n - 1) \). It follows by Lemma 1 that \( r(T) = \sum_{v \in V(T)} \frac{1}{\deg v} \geq \frac{n^2}{2(n-1)} \).

\[ \text{diam}(T) = \text{max} \{d(v_1, v_2) | v_1, v_2 \in V(T)\} \]

Thus since \( \text{diam}(T) \geq 1 \), on one hand we have \( \text{diam}(T) + r(T) \geq \frac{n}{2} + \frac{3}{2} + \frac{1}{2(n-1)} \). On the other hand, by bounding each of \( \text{diam}(T) \) and \( r(T) \) separately and adding, we have \( \text{diam}(T) + r(T) \leq \frac{n}{2} + \frac{3}{2} + \frac{1}{2(n-1)} \leq \text{diam}(T) + r(T) \leq 2n - 1 \).

We will improve these bounds and show that

\[ \frac{n}{2} + \frac{\sqrt{2n}}{2} \leq \text{diam}(T) + r(T) \leq \frac{3}{2}n. \]

### 5. Proof of Theorem 2

The following lemma, which gives a sharp lower bound on the number of leaves of a tree in terms of order and diameter, will be required in the proof of Theorem 2.

**Lemma 2.** Let \( T \) be a tree of order \( n > 2 \) and diameter \( \text{diam}(T) \). Then the bound

\[ s(T) \geq \frac{2n}{\text{diam}(T)} - 1 \]

on the number of leaves of \( T \) holds.

**Proof.** We prove the result by induction on the order \( n \) of \( T \). The result can easily be verified for \( n = 3 \). Assume that the result holds for any tree with less than \( n \) vertices. If \( T \) is a path, then \( s(T) = 2 \geq \frac{2n}{(n-1)} - 1 \), as required. Thus, we assume that \( T \) is not a path. Let \( v_0 v_1 \ldots v_{\text{diam}(T)} \) be a diametral path of \( T \). Since \( T \) is not a path, let \( k \in \{1, 2, \ldots, \text{diam}(T) - 1\} \) be the smallest integer such that \( \deg_{T} v_k \geq 3 \). Assume wlog that \( v_k \) is closer to \( v_0 \) than to \( v_{\text{diam}(T)} \), i.e., \( k \leq \text{diam}(T) - k \) so that \( 2k \leq \text{diam}(T) \). Let \( T' = T - \{v_0, v_1, v_2, \ldots, v_{k-1}\} \). Clearly \( \text{diam}(T') \leq \text{diam}(T) \), and since \( \deg_{T} v_k \geq 3 \) we have \( s(T') = s(T') + 1 \). This, in conjunction with the induction hypothesis yields

\[ s(T) = s(T') + 1 \geq \frac{2n}{\text{diam}(T)} - 1 + 1 \geq \frac{2n}{\text{diam}(T)} - \frac{2k}{\text{diam}(T)} \geq \frac{2n}{\text{diam}(T)} - \frac{\text{diam}(T)}{\text{diam}(T)}, \]

as claimed. \( \square \)

Recall the statement of the lower bound in Theorem 2.

**Lower bound of Theorem 2.** Let \( T \) be a tree of order \( n > 2 \) and diameter \( \text{diam}(T) \). Then \( \frac{n}{2} + \frac{\sqrt{2n}}{2} \leq \text{diam}(T) + r(T) \).

**Proof.** Denote the diameter of \( T \) by \( d \) and let \( P = v_0 v_1 \ldots v_d \) be a diametral path of \( T \). Let \( P' = \{v_1, v_2, \ldots, v_{d-1}\} \). Let \( S \) be the set of all leaves of \( T \) and \( s \) be the cardinality of \( S \). Denote the set \( V(T) - S - P' \) by \( R \). Hence \( V(T) = S \cup P' \cup R \) and so

\[ r(T) = \sum_{x \in S} \frac{1}{\deg x} + \sum_{x \in P'} \frac{1}{\deg x} + \sum_{x \in R} \frac{1}{\deg x}. \]

Note that

\[ \sum_{x \in S} \deg x + \sum_{x \in P'} \deg x + \sum_{x \in R} \deg x = 2|E(T)| = 2n - 2. \]

(3)

Since for all \( x \in P' \) we have \( \deg x \geq 2 \), it follows that \( \sum_{x \in P'} \deg x \leq 2n - s - 2d \). Consequently by Lemma 1 we have

\[ \sum_{x \in R} \frac{1}{\deg x} \geq \frac{|R|^2}{2n - s - 2d} = \frac{(n - d - s + 1)^2}{2n - s - 2d}. \]

(4)
Making use of (3), and noting that for all \( x \in R, \deg x \geq 2 \) we obtain \( \sum_{x \in P} \deg x \leq 2d + s - 4 \). This, in conjunction with Lemma 1 yields

\[
\sum_{x \in P} \frac{1}{\deg x} \geq \frac{|P'|^2}{2d + s - 4} = \frac{(d - 1)^2}{2d + s - 4}.
\]  

(5)

Using (4) and (5) we deduce that

\[
diam(T) + r(T) = d + \sum_{x \in S} \frac{1}{\deg x} + \sum_{x \in R} \frac{1}{\deg x} + \sum_{x \in P} \frac{1}{\deg x} \\
\geq d + s + \frac{(n - d - s + 1)^2}{2n - s - 2d} + \frac{(d - 1)^2}{2d + s - 4}.
\]

Let \( f(d, s) \) \( = d + s + \frac{(n - d - s + 1)^2}{2n - s - 2d} + \frac{(d - 1)^2}{2d + s - 4} \). Subject to the condition \( s \geq \frac{2n}{d} - 1 \) given in Lemma 2, a simple differentiation shows that

\[
f(d, s) \geq \frac{n}{2} + \sqrt{2} \sqrt{n} - 1,
\]

establishing the lower bound.

To see that the lower bound is close to best possible, let \( n \) be a positive integer such that \( n - 1 \) is an even perfect square. Let \( T_n \) be the tree obtained by taking a disjoint vertex \( v \) and \( 2\sqrt{n} - 1 \) disjoint copies of the path \( P_{\frac{\sqrt{n} - 1}{2}} \) (of order \( \frac{\sqrt{n} - 1}{2} \)) and joining \( v \) by an edge to one end vertex of each copy of \( P_{\frac{\sqrt{n} - 1}{2}} \). A simple calculation shows that \( r(T_n) + diam(T_n) = \frac{n}{2} + \sqrt{2} \sqrt{n} - 1 + O(1) \). □

**Upper bound of Theorem 2.** Let \( T \) be a tree of order \( n > 2 \) and diameter \( diam(T) \). Then \( diam(T) + r(T) \leq \frac{3}{2} n \) and the bound is tight.

**Proof.** Assume the notation above. Then

\[
r(T) = \sum_{x \in S} \frac{1}{\deg x} + \sum_{x \in V(T) - S} \frac{1}{\deg x} \leq s + \sum_{x \in V(T) - S} \frac{1}{2} \leq s + \frac{n - s}{2}.
\]

This, in conjunction with \( d \leq n - s + 1 \), yields \( diam(T) + r(T) \leq \frac{3}{2} n + 1 - \frac{s}{2} \). From \( s \geq 2 \), we obtain the desired upper bound which is attained by a path. □

**Corollary 2.** Let \( G \) be a connected graph of order \( n \) and diameter \( diam(G) \). Then

\[
2 + \frac{1}{n - 1} \leq diam(G) + r(G) \leq \frac{3}{2} n
\]

and the bound is sharp.

**Proof.** Clearly, \( 1 \leq diam(G) \) and \( \frac{n}{n - 1} \leq r(G) \) from which we deduce the lower bound. Let \( T \) be a spanning tree of \( G \). Then \( \deg_G x \geq \deg_T x \) for all \( x \in V \). It follows that

\[
r(G) = \sum_{x \in V} \frac{1}{\deg_G x} \leq \sum_{x \in V} \frac{1}{\deg_T x} = r(T).
\]

Note also that \( diam(G) \leq diam(T) \). This, in conjunction with Theorem 2, yields

\[
diam(G) + r(G) \leq diam(T) + r(T) \leq \frac{3}{2} n,
\]

as desired. Both inequalities are tight; the lower bound is achieved by the complete graph whereas the upper bound is achieved by a path. □

6. Proofs of Theorems 3–6

6.1. The Family \( T_{d,s} \)

We first define, for \( d \geq 2, s \geq 2 \), a family of trees \( T_{d,s} \) with diameter \( d \) and \( s \) leaves. For this purpose, let \( q \) and \( \varepsilon, \ 0 \leq \varepsilon < d - 1 \), be the unique integers satisfying \( s - 2 = q(d - 1) + \varepsilon \). Let \( H \) be the graph obtained by taking a path \( P_{d+1} \) of length \( d \) and attaching \( q \) leaves to every non-leaf vertex of \( P_{d+1} \). Let \( W \subset V(H) \) be a subset of cardinality \( \varepsilon \) with vertices \( v \)
satisfying \( \deg_{H} v = q + 2 \). Let \( T_{W} \) be the tree obtained by taking \( H \) and attaching a unique leaf vertex to every vertex in \( W \). \( T_{d,s} \) is the family \( \{ T_{W} : W \subset V(H) \} \). (See, for example Fig. 1.) A simple calculation shows that

\[
\begin{aligned}
r(T) & = s + \left( \frac{d-1}{q+2} - \frac{r}{(q+2)(q+3)} \right) \\
& \geq s + \frac{d-1}{q+2} - \frac{r}{(q+2)(q+3)}.
\end{aligned}
\]

Moreover the bound is sharp for all values of \( d \) and \( s \).

\section*{Proof of Claim 1.}

\begin{equation}
\begin{aligned}
\deg_{H} x = \deg_{H} x & \quad \text{for all } x \notin \{ v_{i}, u \}.
\end{aligned}
\end{equation}

Thus since \( \deg_{H} u \geq 2 \),

\[
\begin{aligned}
r(H) - r(H') &= \frac{1}{\deg_{H} v_{i}} + \frac{1}{\deg_{H} u} - \frac{1}{\deg_{H'} v_{i}} \\
& = \frac{1}{\deg_{H} v_{i}} + \frac{1}{\deg_{H} u} - \frac{1}{\deg_{H} v_{i} + \deg_{H} u - 2} \\
& > 0;
\end{aligned}
\]

contradicting the minimality of \( H \).

\section*{Proof of Claim 2.}

\begin{equation}
| \deg_{H} v_{i} - \deg_{H} v_{j} | \leq 1 \quad \text{for all } i, j \in \{ 1, \ldots, d - 1 \}.
\end{equation}

Thus \( \deg_{H} v_{i} \geq 3 \). Let \( u \) be a neighbour of \( v_{j} \) that is not on \( P \). By Claim 1 \( u \) is a leaf vertex. Now let \( H' = H - u_{v_{j}} + u_{v_{i}} \). Then clearly \( H' \) has diameter \( d \) and \( s \) leaves. Moreover, \( \deg_{H} x = \deg_{H} x \) for all \( x \notin \{ v_{i}, v_{j} \} \).Thus since \( \deg_{H} v_{i} \geq 2 \), we have

\[
\begin{aligned}
r(H) - r(H') &= \frac{1}{\deg_{H} v_{i}} + \frac{1}{\deg_{H} v_{j}} - \left( \frac{1}{\deg_{H} v_{i}} + \frac{1}{\deg_{H} v_{j}} \right) \\
& = \frac{1}{\deg_{H} v_{i}} + \frac{1}{\deg_{H} v_{j}} - \left( \frac{1}{\deg_{H} v_{i} + 1} + \frac{1}{\deg_{H} v_{j} - 1} \right) \\
& > 0;
\end{aligned}
\]

contradicting the minimality of \( H \).

\section*{We conclude from Claim 1 and Claim 2 that \( H \in T_{d,s} \). It follows that

\[
\begin{aligned}
r(T) & \geq r(H) \\
& = s + \frac{d-1}{q+2} - \frac{r}{(q+2)(q+3)},
\end{aligned}
\]

as desired.}

The bound of the theorem is tight for all values of \( d \) and \( s \) since it is attained by each tree \( T \in T_{d,s} \).

\section*{Corollary 3.}

Let \( T \) be a tree with diameter \( d \) and \( s \) leaves. Let \( q \) and \( \epsilon \), \( 0 \leq \epsilon < d - 1 \), be unique integers satisfying \( s - 2 = q(d - 1) + \epsilon \). Then

\[
d \leq \frac{q + 2}{(q + 1)^{2}} r(T) - \frac{q^{2} + 5q + 5}{(q + 1)^{2}(q + 3)} \epsilon + \frac{q^{2} - 3}{(q + 1)^{2}}.
\]

Moreover the bound is sharp for all values of \( d \) and \( s \).
By the previous theorem, $r(T) \geq s + \frac{d-1}{q+2} - \frac{s}{(q+2)(q+3)}$. Noting that $s = q(d-1) + \varepsilon + 2$, the corollary is established upon re-arranging the terms. The inequality is tight since every tree $T \in T_{d,\varepsilon}$ attains the bound. □

Recall the statement of Theorem 4.

**Theorem 4.** Let $G$ be a $k$-regular connected graph, $k \geq 3$. Then $\text{diam}(G) \leq 3 \left(1 - \frac{1}{k+1}\right) r(G) + 1 - \frac{6}{k+1}$, and this inequality is tight.

**Proof.** Let $P = v_0v_1 \ldots v_d$ be a diametral path and let $d + 1 = 3q + r$, where $q \in \mathbb{Z}$ and $0 \leq r \leq 5$. For $i = 0, 1, 2, \ldots, d$, let $N_i := \{x : d(x, v_0) = i\}$.

**Claim 3.** Let $c \in \{1, 2, \ldots, d-4\}$ be a fixed integer and $M_c := \bigcup_{i=c+1}^{c+4} N_i$. Then

$$\sum_{v \in M_c} \frac{1}{\deg v} \geq 2.$$

**Proof of Claim 3.** Denote by $S_c$ the set $\{v_c, v_{c+1}\}$ of vertices on $P$. Let $n_j, j = 2, 3, 4$, be the number of vertices of $S_c$ of degree $j$; hence $n_2 + n_3 + n_4 = 2$ and $\sum_{v \in S_c} \frac{1}{\deg v} = \frac{n_2}{2} + \frac{n_3}{3} + \frac{n_4}{4}$. Since $N(v_c) \cap N(v_{c+3}) = \emptyset$, we have $|N(S_c) \setminus V(P)| \geq n_3 + 2n_4$. Letting $F_c = \{v_{c-1}, v_{c+1}, v_{c+2}, v_{c+4}\}$, and recalling that the maximum degree is 4, it follows that

$$\sum_{v \in M_c} \frac{1}{\deg v} \geq \sum_{v \in N(S_c) \setminus V(P)} \frac{1}{\deg v} + \sum_{v \in S_c} \frac{1}{\deg v} + \sum_{v \in F_c} \frac{1}{\deg v}$$

$$\geq \frac{n_3 + 2n_4}{4} + \left(\frac{n_2}{2} + \frac{n_3}{3} + \frac{n_4}{4}\right) + \frac{4}{4}$$

$$= 1 + \frac{1}{12}(6n_2 + 7n_3 + 9n_4)$$

$$= 2 + \frac{1}{12}(n_3 + 3n_4) \geq 2,$$

as claimed. □

By Claim 3, we now have

$$r(G) \geq \sum_{v \in \bigcup_{i=0}^{d-1} M_{d+i+1}} \frac{1}{\deg v} + r \geq 2q + \frac{r}{4} \geq \frac{d}{3} - 1,$$

from which the bound follows.

To see that the coefficient 3 of $r(G)$ in the bound is close to best possible, consider the graph $G_4$ in Fig. 2. □
Recall the statement of Theorem 6.

**Theorem 6.** Let $G$ be a connected planar graph of order $n > 2$. Then

$$\text{diam}(G) \leq 6r(G) - 3 - \frac{4}{n - 2}.$$ 

**Proof.** Let $n$, $m$ be the order and size of $G$, respectively. By Euler’s formula, one deduces that $m \leq 3n - 6$. Thus $\sum_{v \in V} \deg v = 2m \leq 6n - 12$. Applying Lemma 1 and the fact that $\text{diam}(G) \leq n - 1$, we get $r(G) \geq \frac{n^2}{6n-12} \geq \frac{\text{diam}(G)}{6} + \frac{1}{2} + \frac{2}{3n-6}$, and the bound follows upon re-arranging the inequality. \( \square \)

**Remark.** The bounds given in Theorems 5 and 6 seem not best possible. We conjecture that, for chemical and planar graphs, essentially the bound for 4-regular and 3-regular graphs apply respectively.

**Conjecture 1.** Let $G$ be a connected chemical graph with diameter $\text{diam}(G)$ and inverse degree $r(G)$. Then

$$\text{diam}(G) \leq \frac{12}{5} r(G) + O(1),$$

and this inequality is tight.

**Conjecture 2.** Let $G$ be a connected planar graph with diameter $\text{diam}(G)$ and inverse degree $r(G)$. Then

$$\text{diam}(G) \leq \frac{9}{4} r(G) + O(1),$$

and this inequality is tight.

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