On the Relation Between Degree Distance and Eccentric Connectivity Index

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Abstract

The relation between the degree distance DD(G) and the eccentric connectivity index $\xi^c(G)$ of a graph G is studied. Sharp lower and upper bounds on DD(G)involving $\xi^c(G)$ are determined. A Nordhaus-Gaddum type result on DD(G) in terms of $\xi^c(G)$ and the first Zagreb index is proposed for connected graphs G with connected complements. A sharp upper bound on DD(T) involving $\xi^c(T)$ is given for trees of given order. It is proved that the difference $DD(T) - \xi^c(T)$ on trees with the same order is minimized on caterpillars. Effect on the degree distance versus the eccentric connectivity index of a tree under edge contractions is also investigated.

1 Introduction

The usage of different graphical invariants for establishing correlations of chemical structures with physical properties, chemical reactivity, or biological activity, has a long history. Many of these invariants, often addressed to as *topological indices*, are based on distances in molecular graphs, cf. the survey [22]. Another approach is to use vertex degrees, the reader can start investigating such topoplogical indices with the paper [10] and references therein. It is then only one step to combine these two groups and consider degree-distance based topological indices. An important index of the latter form is the *degree distance index* of a graph G defined as

$$DD(G) = \sum_{u \neq v} (\deg(u) + \deg(v))d(u, v), \qquad (1)$$

where deg(x) denotes the degree of a vertex x, and d(x, y) is the shortest-path distance between vertices x and y. The degree distance index was independently proposed by Dobrynin and Kochetova [6] and Gutman [8] and well investigated afterwards. For instance, its extremal properties were studied in [6,17–19], while for its recent studies see [1,2,4,7].

The second index of our interest here is the *eccentric connectivity index* introduced by Sharma, Goswami and Madan [16] and defined for a graph G with

$$\xi^{c}(G) = \sum_{v \in V(G)} \deg(v)\varepsilon(v), \qquad (2)$$

where $\varepsilon(v)$ denotes the *eccentricity* of v, that is, the distance between v and a farthest vertex from v. See [12,13,24] for basic properties of the eccentric connectivity index including extremal graphs and various bounds in terms of other graph invariants. We especially point out to the papers [3,5] in which the eccentric connectivity index is compared with the Wiener index and with the Zagreb indices, respectively. Further, for current investigations of the eccentric connectivity index see [11,14,15,20,21,23]. Now, setting D(v) to denote the sum of distances between v and the other vertices of a graph G, that is, D(v) denotes the *total distance* of the vertex v, the definition (1) can be equivalently rewritten as follows:

$$DD(G) = \sum_{v \in V(G)} \deg(v)D(v).$$
(3)

Looking at (2) and (3), it appears natural to compare the degree distance index with the eccentric connectivity index. In the next section we bound the degree distance index of G

in terms of the eccentric connectivity and the first Zagreb index of G. We also prove an additive Nordhaus-Gaddum type result on DD(G) for (connected) graphs with connected complements. Then, in Section 3, we prove a sharp upper bound on the degree distance index of trees as a function of the eccentric connectivity index. Moreover, we show that the minimum difference between the degree distance and the eccentric connectivity index in the class of trees of the same order is achieved on caterpillars. In the final section we investigate how the degree distance and the eccentric connectivity index of a tree change under the edge contraction.

In the rest of the introduction we list some further definitions and give some notation. Graphs considered in this paper are connected. The order and the size of a graph Gwill be denoted with n(G) and m(G), respectively. The minimum and the maximum vertex eccentricity of G are the radius $\operatorname{rad}(G)$ of G and the diameter diam(G) of G. The maximum and the minimum degree of vertices of G are denoted by $\Delta(G)$ and $\delta(G)$, respectively. The complement of G will be denoted with \overline{G} . Finally, when speaking of a graph invariant on a graph G and when necessary to avoid confusion with other graph(s), we will write G in the subscript of the invariant. For instance, instead of deg(u) and d(u, v) we will write deg_G(u) and $d_G(u, v)$, respectively.

2 Bounds for general graphs

We first bound the degree distance index of G in terms of the eccentric connectivity and the first Zagreb index of G. For this recall that the *first Zagreb index* $M_1(G)$ of a graph G is the sum of the squares of the degrees of G, cf. [9].

Theorem 2.1 If G is a connected graph, then

$$\xi^{c}(G) + M_{1}(G) - 2m(G) \le DD(G) \le M_{1}(G) + (n(G) - 1 - \delta(G))\xi^{c}(G)$$

The left equality holds if and only of $G = K_{n(G)}$, the right equality holds if and only if G is regular with diam $(G) \leq 2$.

Proof. Set n = n(G). If v is a vertex of G, then, simply because the distance from v to any of its non-neighbors is at least 2, we infer that

$$\varepsilon(v) - 1 \le D(v) - \deg(v) \le (n - \deg(v) - 1)\varepsilon(v).$$
(4)

Multiplying the above inequalities with deg(v) we get

$$\deg(v)\varepsilon(v) - \deg(v) \le \deg(v)D(v) - \deg(v)^2 \le \deg(v)(n - \deg(v) - 1)\varepsilon(v),$$

from which the inequalities follow by summing over all vertices of G.

The left equality in (4) holds if and only if $\deg(v) = n - 1$. As this must hold for every vertex of G, we get that G is a complete graph when the left equality holds. The right equality in (4) holds if and only if $\varepsilon(v) \leq 2$. Hence the equality part of the theorem. \Box

The degree distance index of G can also be bounded from below only in terms of the eccentric connectivity index.

Theorem 2.2 If G is a graph with $n(G) \ge 4$, then $DD(G) \ge 2\xi^{c}(G) + 2m(G)(n(G) - 4)$. Moreover, equality holds if and only if $G = P_4$ or G is a graph obtained by removing a perfect matching of $K_{n(G)}$.

Proof. Let v be a vertex of G. Considering the vertices on a selected longest path starting from v, we see that

$$D(v) \geq (1 + \dots + \varepsilon(v)) + (n(G) - \varepsilon(v) - 1))$$

= $\binom{\varepsilon(v) + 1}{2} + (n(G) - \varepsilon(v) - 1)$
= $\frac{1}{2}(\varepsilon(v)(\varepsilon(v) - 1) + 6) + n(G) - 4.$

Suppose first that $n(G) \ge 5$. Then it is straightforward to verify that $D(v) \ge \frac{1}{2}(\varepsilon(v)(\varepsilon(v) - 1) + 6) + n(G) - 4 \ge 2\varepsilon(v) + n(G) - 4$ holds. Summing over all vertices we get the inequality of the theorem.

If $\varepsilon(v) \neq 2$, we have $D(v) > 2\varepsilon(v) + n(G) - 4$. Moreover in the case $\varepsilon(v) = 2$ and $\deg(v) \leq n(G) - 3$ we get $D(v) \geq n(G) + 1 > 2\varepsilon(v) + n(G) - 4$. Thus $D(v) = 2\varepsilon(v) + n(G) - 4$ holds if and only if $\varepsilon(v) = 2$ and $\deg(v) = n(G) - 2$.

Checking the six connected graphs of order 4 we see that the inequality holds for all of them, where the equality holds only for C_4 and P_4 .

To conclude the section we give an additive Nordhaus-Gaddum type result on DD(G)for (connected) graphs with connected complements.

Theorem 2.3 If G is a connected graph with a connected complement, then

 $DD(G) + DD(\bar{G}) \le M_1(G) + M_1(\bar{G}) + (n(G) - 1 - \delta(G))\xi^c(G) + \Delta(G)\xi^c(\bar{G}).$

Moreover, equality holds if both G and \overline{G} are regular graphs of diameter 2.

Proof. Let v be a vertex of G and set n = n(G). Then

$$D_G(v) \le \deg(v) + (n - \deg(v) - 1)\varepsilon_G(v), \qquad (5)$$

$$D_{\bar{G}}(v) \le (n - \deg(v) - 1) + \deg(v)\varepsilon_{\bar{G}}(v).$$
(6)

Multiplying these two inequalities with $\deg(v)$ and $n - \deg(v) - 1$, respectively, we have

$$\begin{aligned} \deg(v)D_G(v) &+ (n - \deg(v) - 1)D_{\bar{G}}(v) \leq \deg(v)^2 + \deg(v)(n - \deg(v) - 1)\varepsilon_G(v) \\ &+ (n - \deg(v) - 1)^2 + \deg(v)(n - \deg(v) - 1)\varepsilon_{\bar{G}}(v) \\ &= \deg(v)^2 + (n - \deg(v) - 1)^2 + (n - 1)\deg(v)\varepsilon_G(v) \\ &- \deg(v)^2\varepsilon_G(v) + \deg(v)(n - 1 - \deg(v))\varepsilon_{\bar{G}}(v) \\ &\leq \deg(v)^2 + (n - \deg(v) - 1)^2 + (n - 1 - \delta(G))\deg(v)\varepsilon_G(v) \\ &+ \Delta(G)(n - 1 - \deg(v))\varepsilon_{\bar{G}}(v) \,. \end{aligned}$$

Summing over all vertices of G, the inequality follows.

If diam(G) = 2, then equality holds in (5), and if diam(\overline{G}) = 2, the same is true in (6). Moreover, the inequality in the computation above becomes equality if $\delta(G) = \Delta(G)$. Hence equality in Theorem 2.3 holds if both G and \overline{G} are regular graphs of diameter 2.

3 Trees

In this section we first give a sharp upper bound on the degree distance index of trees as a function of the eccentric connectivity index. Then, in our second main result, we prove that the minimum difference between the degree distance and the eccentric connectivity index in the class of trees of the same order is achieved on caterpillars. For the first main result two lemmas are needed.

Lemma 3.1 If x is a vertex of tree T, then

$$\sum_{y \in V(T)} \deg(y) d(x, y) = 2D(x) - n(T) + 1.$$

Proof. For a vertex $u \in V(T)$, let $N_k(u)$ be the set of vertices at distance k from x. Since no pair of vertices from $N_k(x)$ have a common neighbor in $N_{k+1}(x)$, we have $|N_{k+1}(u)| = \sum_{v \in N_k(u)} (\deg(v) - 1), k \ge 1$. Thus

$$D(x) = \sum_{k=1}^{\varepsilon(x)} k |N_k(x)| = \deg(x) + \sum_{k=1}^{\varepsilon(x)-1} \left[(k+1) \sum_{y \in N_k(x)} (\deg(y) - 1) \right]$$

= $\deg(x) + \sum_{y \in V(T-x)} (d(x,y) + 1)(\deg(y) - 1)$
= $\deg(x) + \sum_{y \in V(T-x)} \deg(y)d(x,y) - D(x)$
+ $2(n(T) - 1) - \deg(x) - (n(T) - 1),$

and the result follows.

Lemma 3.2 If x is a pendant vertex of T and T' = T - x, then

$$DD(T) - DD(T') = 4D_T(x) - 2n(T) + 2$$

Proof. Let y be the neighbor (support) of x. Then we have:

$$DD(T) - DD(T') = \sum_{z \in V(T)} \deg_T(z) d_T(z, x) + \sum_{z \in V(T-x)} d(z, y) + D_T(x)$$
$$= \sum_{z \in V(T)} \deg_T(z) d_T(z, x) + D_T(y) - 1 + D_T(x).$$

Using Lemma 3.1 and the fact that $D_T(x) = D_T(y) + n(T) - 2$, we get

$$DD(T) - DD(T') = 2D_T(x) - (n(T) - 1) + D_T(x) - (n(T) - 2) - 1 + D_T(x)$$

= $4D_T(x) - 2(n(T) - 1)$,

which was to be proved.

For our first main result, besides the above lemmas, we also need the following known result.

Theorem 3.3 [13, Theorem 5] If T is a tree with $\operatorname{diam}(T) = d$ and n(T) = n, then

$$\xi^{c}(T) \geq \begin{cases} n(d+1) + \frac{1}{2}d^{2} - 2d - 1; & d \text{ even}, \\ n(d+2) + \frac{1}{2}d^{2} - 3d - \frac{3}{2}; & d \text{ odd}. \end{cases}$$

Now all is ready for the first main result of this section.

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Theorem 3.4 If T is a tree of order $n \ge 3$, then

$$DD(T) \le \frac{4}{3}n\xi^{c}(T) - (n-1)(n+4).$$

Moreover, equality holds if and only if T is a star.

Proof. We prove the result by induction on the order of T. One can easily verify that the result is true if n = 3 and that the equality holds if T is a star.

Assume that n > 3 and that the result holds for all trees of order less than n. As we have already dealt with stars, we may also suppose that $\operatorname{diam}(T) = d \ge 3$. Let xbe a vertex of eccentricity d. Clearly, x is a leaf and let T' = T - x. By the induction hypothesis,

$$DD(T') \le \frac{4}{3}(n-1)\xi^c(T') - (n-2)(n+3).$$
(7)

If y is the neighbor of x in T, then we have

$$\xi^c(T) - \xi^c(T') \ge \varepsilon(x) + \varepsilon(y) = 2d - 1$$
.

Moreover

$$D_T(x) \le (1+2+\dots+d-1) + (n-d)d = nd - \binom{d+1}{2}.$$

Combining this inequality with Lemma 3.2 and setting X = DD(T) - DD(T') we get the following estimates:

$$\begin{aligned} X &\leq 4nd - 4\binom{d+1}{2} - 2(n-1) \\ &\leq \frac{4}{3}(n-1)\xi^c(T') - (n-2)(n+3) + 4nd - 4\binom{d+1}{2} - 2(n-1) \\ &\leq \frac{4}{3}(n-1)(\xi^c(T) - 2d+1) - (n-2)(n+3) + 4nd - 4\binom{d+1}{2} - 2(n-1) \\ &= \frac{4}{3}n\xi^c(T) - (n-1)(n+4) - \frac{4}{3}\xi^c(T) + \frac{4}{3}n(d+1) - 2d^2 + \frac{2}{3}d + \frac{8}{3}, \end{aligned}$$

where, to obtain the second inequality above, we have used the fact that by (7) we have $\frac{4}{3}(n-1)\xi^{c}(T') - (n-2)(n+3) \ge 0.$

Now it is sufficient to show that

$$\frac{4}{3}\xi^c(T) \ge \frac{4}{3}n(d+1) - 2d^2 + \frac{2}{3}d + \frac{8}{3}.$$

Applying Theorem 3.3 and setting $Y = \frac{4}{3}\xi^c(T) - \frac{4}{3}n(d+1) + 2d^2 - \frac{2}{3}d - \frac{8}{3}$ we get

$$Y \geq -\frac{4}{3}n(d+1) + 2d^2 - \frac{2}{3}d - \frac{8}{3} + \frac{4}{3} \begin{cases} n(d+1) + \frac{1}{2}d^2 - 2d - 1; & d \text{ even} \\ n(d+2) + \frac{1}{2}d^2 - 3d - \frac{3}{2}; & d \text{ odd} \end{cases}$$
$$= \begin{cases} \frac{8}{3}d^2 - \frac{10}{3}d - 4; & d \text{ even} \\ \frac{8}{3}d^2 + \frac{4}{3}n - \frac{14}{3}(d+1); & d \text{ odd} \end{cases}$$
$$> 0.$$

We conclude that if T is not a star, then the claimed inequality is strict.

Recall that a *catterpilar* is a tree T that contains a path P such that each vertex from $V(T) \setminus V(P)$ is adjacent to a vertex of P. Then the second main result of this section reads as follows.

Theorem 3.5 If n is a positive integer, then $\min\{DD(T) - \xi^c(T) : T \text{ tree with } n(T) = n\}$ is attained on caterpillars.

Proof. Assume that T is not a caterpillar. Let P be a diametrical path of T. Let u be a non-pendant vertex of T which is farthest from P, and let $z \in V(P)$ be the vertex on P which is closest to u. Let $d_T(u, z) = d$. Since T is not a caterpillar, $d \ge 1$. Let v be the neighbor of u on the u, z-path, and let T_z be the maximal subtree of T that contains z and no other vertex of P. Consider the following transformation. Let $S = N(u) - \{v\}$ and let $|S| = s \ge 1$. Construct a tree T' from T by removing the edges between u and the vertices of S and then connecting vertex v to each vertex of S. See Fig. 1 for an example of this construction where the subtree T_z is induced by the black vertices.

It is clear that distances between the vertices from V(G) - S are the same in T and T'. Also, the distance between a vertex from S and the vertices not in S except u decrease by 1, while for each vertex $w \in S$ we have $d_{T'}(u, w) = 2$ and $d_T(u, w) = 1$. From these observations we deduce that

$$DD(T) - DD(T') = \sum_{x \in \{u,v\}} \left[\deg_T(x) D_T(x) - \deg_{T'}(x) D_{T'}(x) \right] + \sum_{j \in S} \left[\deg_T(j) D_T(j) - \deg_{T'}(j) D_{T'}(j) \right] + \sum_{\substack{j \in V(T) - S \\ j \notin \{u,v\}}} \left[\deg_T(j) \left(D_T(j) - D_{T'}(j) \right) \right]$$



Figure 1. Constructing T' from T

$$= \left((s+1)D_T(u) - (D_T(u)+s) \right) + \left(\deg_T(v)D_T(v) - (\deg_T(v)+s)(D_T(v)-s) \right) + \sum_{j \in S} (n-s-2) + \sum_{\substack{j \in V(T)-S \\ j \notin \{u,v\}}} \deg_T(j)s = s(D_T(u)-1) + s(\deg_T(v) - D_T(v)+s) + s(n-s-2) + s \left[2(n-1) - (\deg_T(v)+2s+1) \right] = s \left[D_T(u) - D_T(v) + 3n(-2s) - 6 \right] = s \left[n-2s-2+3n(-2s)-6 \right] = s(4n-4s-8).$$

The described transformation decreases the eccentricity of each vertex in S by 1, while the other vertices (not equal to u or to v) have the same eccentricity and degree in both T and T'. Thus we get

$$\begin{aligned} \xi^{c}(T) - \xi^{c}(T') &= \sum_{x \in \{u,v\}} \left[\deg_{T}(x)\varepsilon_{T}(x) - \deg_{T'}(x)\varepsilon_{T'}(x) \right] \\ &+ \sum_{j \in S} (\varepsilon_{T}(j) - \varepsilon_{T'}(j)) \\ &= \left[(s+1)\varepsilon_{T}(u) - \varepsilon_{T}(u) + \deg_{T}(v)\varepsilon_{T}(v) - (s + \deg_{T}(v))\varepsilon_{T}(v) \right] + s \\ &= s(\varepsilon_{T}(u) - \varepsilon_{T}(v)) + s = 2s \,. \end{aligned}$$

Since T is not a caterpillar we have $n - s \ge 6$ and hence

$$DD(T) - DD(T') = s(4n - 4s - 8) > 2s = \xi^{c}(T) - \xi^{c}(T')$$

that is, $DD(T') - \xi^c(T') < DD(T) - \xi^c(T)$. Repeating the construction until a caterpillar is obtained proves the result.

Let B(n,d) denotes the tree obtained from a path $P : v_1v_2 \cdots v_{d+1}$ with attaching n-d-1 pendant vertices to vertex $v_{\lfloor \frac{n}{2} \rfloor}$.

Conjecture. Among trees of of given order n and diameter d, graph B(n, d) gets the minimum value of $DD - \xi^c$.

4 Contracting edges in trees

Let e = uv be an edge of graph G. Then we denote by G.e the graph obtained from G by contracting e. In this section we investigate how the degree distance and the eccentric connectivity index of a tree change under the edge contraction.

For our first main result of the section we need the following straightforward lemma, where, for an edge e = uv, we use the notation n_u for the number of vertices closer to uthan to v. The notation n_v has the analogous meaning.

Lemma 4.1 If e = uv is an edge of a tree T, then $D_T(u) - D_T(v) = n_v - n_u$.

Theorem 4.2 If e = uv is an edge of a tree T of order n, then

$$DD(T) - DD(T.e) = 4n_v(n_u - 1) + 4D_T(u) - 2(n - 1).$$

Proof. Let T_u and T_v be the components (trees) of T - uv containing u and v, respectively. Setting W = DD(T) - DD(T.e), we can compute as follows:

$$\begin{split} W &= \sum_{x \in V(T_u - u)} \deg_T(x) (D_T(x) - D_{T.e}(x)) + \sum_{y \in V(T_v - v)} \deg_T(y) (D_T(y) - D_{T.e}(y)) \\ &+ \deg_T(u) D_T(u) + \deg_T(v) D_T(v) - (\deg_T(u) + \deg_T(v) - 2) (D_T(u) - n_v) \\ &= \sum_{x \in V(T_u - u)} \deg_T(x) (n_v + d_T(x, u)) + \sum_{y \in V(T_v - v)} \deg_T(y) (n_u - 1 + d_T(y, u)) \\ &+ \deg_T(u) D_T(u) + \deg_T(v) D_T(v) - (\deg_T(u) + \deg_T(v) - 2) (D_T(u) - n_v) \\ &= n_v \sum_{x \in V(T_u - u)} \deg_T(x) + (n_u - 1) \sum_{y \in V(T_v - v)} \deg_T(y) \\ &+ \sum_{x \in V(T)} \deg_T(x) d_T(x, u) - \deg_T(v) + \deg_T(u) D_T(u) + \deg_T(v) D_T(v) \\ &- (\deg_T(u) + \deg_T(v) - 2) (D_T(u) - n_v) \\ &= n_v (2n_u - \deg_T(u) - 1) + (n_u - 1) (2n_v - \deg_T(v) - 1) \\ &+ (2D_T(u) - (n(T) - 1) - \deg_T(v)) \\ &+ \deg_T(v) (D_T(v) - D_T(u) + n_v) + \deg_T(u) n_v + 2 (D_T(u) - n_v) \\ &= 4n_u n_v - (n_u + n_v) + 4D_T(u) - 4n_v \\ &- n(T) + 2 + \deg_T(v) (D_T(v) - D_T(u) + n_v - n_u) \,. \end{split}$$

The result now follows by an application of Lemma 4.1.

For the second main result of the section recall that the *center* C(G) of a graph G is the set of vertices of G with minimum eccentricity. It is well-known that if T is a tree, then $|C(T)| \in \{1, 2\}$. Moreover, if |C(T)| = 2, then the two central vertices are adjacent.

Theorem 4.3 If e = uv is an edge of a tree T, where $\varepsilon(u) \ge \varepsilon(v)$, then

$$2n_u + 2\varepsilon(v) - 1 \le \xi^c(T) - \xi^c(T.e) \le 2(n(T) + \varepsilon(u) - 2).$$

Moreover, the right-hand side equality holds if and only if $C(T) = \{u, v\}$.

Proof. Suppose first that $\varepsilon(u) = \varepsilon(v)$. Then necessarily both u and v are central vertices, that is, $C(T) = \{u, v\}$. Contracting the edge uv, the eccentricity of each vertex is decreased by 1 and hence

$$\begin{aligned} \xi^c(T) - \xi^c(T.e) &= \left(\sum_{x \in V(T) - \{u,v\}} \deg_T(x)\right) + \deg_T(u)\varepsilon(u) + \deg_T(v)\varepsilon(v) \\ &- (\deg_T(u)\deg_T(v) - 2)(\varepsilon(u) - 1) \\ &= 2(n(T) - 1) + 2(\varepsilon(u) - 1) \,. \end{aligned}$$

Suppose now that $\varepsilon(u) > \varepsilon(v)$. Then contracting the edge uv, the eccentricity of each vertex in T_u is decreased by 1 and for vertices in T_v it is decreased by at most 1. Moreover $\varepsilon(u) = \varepsilon(v) + 1$. Thus

$$\begin{aligned} \xi^{c}(T) - \xi^{c}(T.e) &\geq \sum_{x \in V(T_{u}-u)} \deg_{T}(x) + \deg_{T}(u)\varepsilon(u) \\ &+ \deg_{T}(v)\varepsilon(v) - (\deg_{T}(u)\deg_{T}(v) - 2)(\varepsilon(v)) \\ &= 2n_{u} - 1 - \deg_{T}(u) + \deg_{T}(u)(\varepsilon(u) - \varepsilon(v)) + 2\varepsilon(v) \\ &= 2n_{u} + 2\varepsilon(v) - 1. \end{aligned}$$

As for the right-hand side inequality for the case when $\varepsilon(u) > \varepsilon(v)$, we proceed as follows:

$$\begin{split} \xi^c(T) - \xi^c(T.e) &\leq \sum_{x \in V(T) - \{u,v\}} \deg_T(x) + \deg_T(u)\varepsilon(u) + \deg_T(v)\varepsilon(v) \\ &- (\deg_T(u) \deg_T(v) - 2)(\varepsilon(v)) \\ &= 2(n(T) - 1) - \deg_T(v) + 2\varepsilon(v) \\ &= 2(n(T) + \varepsilon(u) - 2) - \deg_T(v) \,, \end{split}$$

which completes the argument.

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