Maximum Modulus of Independence Roots of Graphs and Trees

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Abstract

The *independence polynomial* of a graph is the generating polynomial for the number of independent sets of each size and its roots are called *independence roots*. We bound the maximum modulus, $\mathrm{maxmod}(n)$, of an independence root over all graphs on n vertices and the maximum modulus, $\mathrm{maxmod}_T(n)$, of an independence root over all trees on n vertices in terms of n. In particular, we show that

$$\frac{\log_3(\mathrm{maxmod}(n))}{n} = \frac{1}{3} + o(1)$$

and

$$\frac{\log_2(\mathrm{maxmod}_T(n))}{n} = \frac{1}{2} + o(1).$$

1 Introduction

The *independence number* of a graph G, denoted $\alpha(G)$, is the maximum size of an independent of G. The *independence polynomial* of G, denoted $i(G,x)$, is the generating polynomial for the number of independence sets of each size:

$$i(G,x) = \sum_{k=0}^{\alpha(G)} i_k x^k,$$

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where i_k denotes the number of independent sets of size k in G. (When dealing with the independence polynomials of multiple graphs, we will distinguish the coefficients with a superscript to avoid confusion, so that i_k^G is the number of independent sets of size k in G.) The roots of $i(G,x)$ are called the *independence roots* of G.

The independence polynomial was first introduced by Gutman and Harary in 1983 [15] and has been a fascinating object of study ever since (see Levit and Mandrescu's survey [18]). One topic that has generated much research is on the independence roots [1, 2, 4, 5, 7, 9, 10, 19, 23].

The roots of other graph polynomials have also been of interest and the nature and location in $\mathbb{C}$ of these roots can vary considerably depending on the polynomial (see [20]). Determining bounds on the moduli of these roots is an important question. In 1992, the first author and Colbourn [3] conjectured that the roots of reliability polynomials lie in the unit disk. The Brown-Colbourn conjecture stood for 12 years until it was shown to be false (although just barely) in [25]. It was later shown that if G is a connected graph on n vertices and q is a reliability root, then $|q| \leq n-1$, yet the largest known reliability root has modulus approximately 1.113486 [6]. It is still believed that the reliability roots are bounded by some constant although the problem remains open. A polynomial that is more closely related to the independence polynomial is the edge cover polynomial and it was recently shown that its roots are bounded, in fact contained in the disk $|z| < \frac{(2+\sqrt{3})^2}{1+\sqrt{3}}$ [11]. In contrast, the collection of all roots of independence polynomials [5], domination polynomials [8], and chromatic polynomials [28] are each dense in $\mathbb{C}$.

Although these polynomials have roots with arbitrarily large moduli, an interesting question to ask is: for fixed n, how large can the modulus of a root of one of these polynomials be for a graph in n vertices? Sokal [27] showed that all simple graphs on n vertices have their chromatic roots contained in the disk $|z| \leq 7.963907(n-1)$, so that the maximum moduli of chromatic roots grows at most linearly in n. The growth rate of domination roots is unknown. There has been work done on bounding the independence roots; for example, it was shown in [7] that for fixed α, the largest modulus of an independence root of a graph with independence number α on n vertices is $\left(\frac{n}{\alpha-1}\right)^{\alpha-1} + O(n^{\alpha-2})$. Although this bound is tight, the $O(n^{\alpha-2})$ term hides enough information to make it unclear if the maximum moduli of independence roots is a polynomial in n or exponential in n. In this paper, we consider the problem of fixing n as the number of vertices and determining the maximum modulus of an independence root over all

graphs on n vertices. We will show that the growth rate is indeed exponential. To that end, let $\mathrm{maxmod}(n)$ denote the maximum modulus of an independence root over all graphs on n vertices and $\mathrm{maxmod}_T(n)$ denote the maximum modulus of an independence root over all trees on n vertices. We show that, in contrast to Sokal's linear bound for chromatic roots, $\mathrm{maxmod}(n)$ and $\mathrm{maxmod}_T(n)$ are both exponential in n: in Section 2, we prove that

$$3^{\frac{n-r+3}{3}} \leq \mathrm{maxmod}(n) \leq 3^{\frac{n}{3}} + n - 1,$$

where $1 \leq r \leq 3$, while in Section 3, we prove that

$$2^{\frac{n-1}{2}} \leq \mathrm{maxmod}_T(n) \leq 2^{\frac{n-1}{2}} + \frac{n-1}{2}$$

if n is odd and

$$2^{\frac{n-6}{2}} \leq \mathrm{maxmod}_T(n) \leq 2^{\frac{n-2}{2}} + \frac{n}{2}$$

if n is even.

We shall need some notation. The number of maximum independent sets in G is denoted by $\xi(G)$. The number of maximal independent sets in G is denoted $\mu(G)$. Note that $\xi(G) = i^G_{\alpha(G)}$, the leading coefficient of the independence polynomial of G. For $S \subseteq V(G)$, let $G - S$ be the graph obtained from G by deleting all vertices of S as well as their incident edges. If $S = \{v\}$, we will use the shorthand, $G - v$ to denote $G - \{v\}$.

2 Bounds on the maximum modulus of independence roots

To bound the roots of independence polynomials, we will make extensive use of the classical Eneström-Kakeya Theorem which uses the ratios of consecutive coefficients of a given polynomial to describe an annulus in $\mathbb{C}$ that contains all its roots.

Theorem 2.1 (Eneström-Kakeya [12, 17]) *If $f(x) = a_0 + a_1 x + \cdots + a_n x^n$ has positive real coefficients, then all complex roots of f lie in the annulus $r \leq |z| \leq R$ where*

$$r = \min\left\{ \frac{a_i}{a_{i+1}} : 0 \leq i \leq n-1 \right\} \ \textit{and} \ R = \max\left\{ \frac{a_i}{a_{i+1}} : 0 \leq i \leq n-1 \right\}.$$

We will also need to make use of two basic results on computing the independence polynomial.

Proposition 2.2 ([15]) *If G and H are graphs and $v \in V(G)$, then:*

i) $i(G,x) = i(G - v,x) + x \cdot i(G - N[v],x).$

ii) $i(G \cup H,x) = i(G,x)i(H,x).$

Note that from Proposition 2.2, $\xi(G \cup H) = \xi(G) \cdot \xi(H)$. Our proofs are inductive and often require upper bounds $\xi(G)$ for all graphs on n vertices, a collection of which can be found in [16].

Theorem 2.3 ([22]) *If G is a graph of order $n \geq 2$, then*

$$\xi(G) \leq \mu(G) \leq g(n) = \begin{cases} 3^{\frac{n}{3}} & \text{if } n \equiv 0 \mod 3 \\ 4 \cdot 3^{\frac{n-4}{3}} & \text{if } n \equiv 1 \mod 3 \\ 2 \cdot 3^{\frac{n-2}{3}} & \text{if } n \equiv 2 \mod 3 \end{cases}.$$

Note that an easy corollary of this is that for a graph on n vertices, $\xi(G) \leq \mu(G) \leq 3^{\frac{n}{3}}$, since $\xi(K_1) = \mu(K_1) = 1 \leq 3^{\frac{1}{3}}$, $3^{\frac{n}{3}} \geq 4 \cdot 3^{\frac{n-4}{3}}$, and $3^{\frac{n}{3}} \geq 2 \cdot 3^{\frac{n-2}{3}}$ for all $n \geq 1$.

Proposition 2.4 *For all $n \geq 1$,*

$$\text{maxmod}(n) \geq \begin{cases} 3^{\frac{n-3}{3}} & \text{if } n \equiv 0 \mod 3 \\ 3^{\frac{n-1}{3}} & \text{if } n \equiv 1 \mod 3 \\ 3^{\frac{n-2}{3}} & \text{if } n \equiv 2 \mod 3 \end{cases}.$$

Proof The proof is in three cases depending on n mod 3. Each relies on independence polynomials of the graphs G_0, G_1, and G_2, respectively, in Figure 1 where G_1 is obtained by joining a central vertex to all but one vertex in each of k copies of K_3, G_0 is obtained by joining one vertex in K_2 to the central vertex in G_1, and G_2 is obtained by joining one vertex in another copy of K_2 to the central vertex in G_0. Note that the orders of G_0, G_1, and G_2 are congruent to 0, 1, and 2,
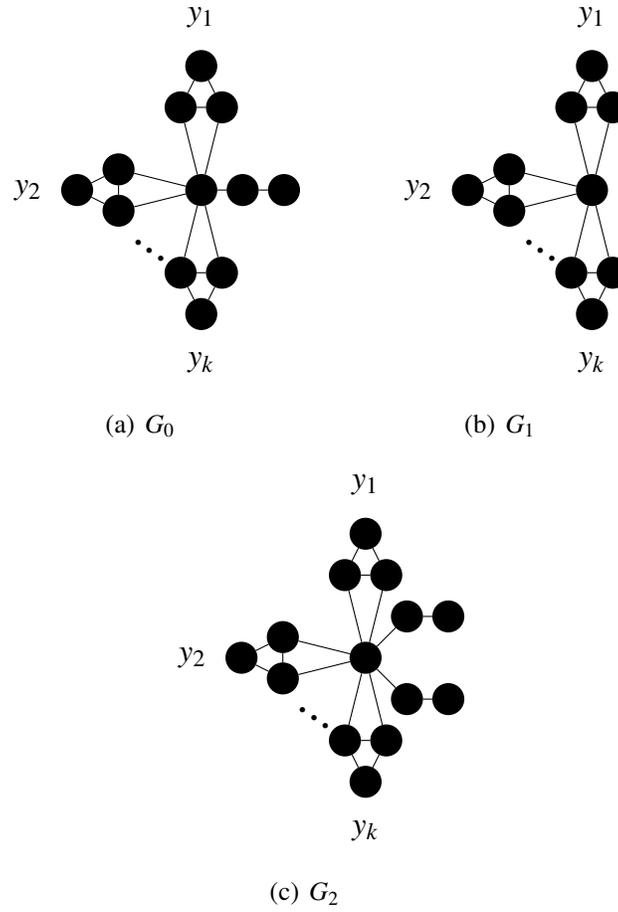
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(a) G_0 (b) G_1

(c) G_2

Figure 1: Graphs with independence roots of large moduli.

respectively, mod 3. We then use the Intermediate Value Theorem (IVT) to find that each has a real root of large modulus.

From Proposition 2.2, it easily follows that

$$i(G_0,x) = (1+3x)^k(1+2x)+x(1+x)^{k+1}$$
$$i(G_1,x) = (1+3x)^k+x(1+x)^k$$
$$i(G_2,x) = (1+3x)^k(1+2x)^2+x(1+x)^{k+2}.$$

It is now straightforward to determine that

$$\operatorname{sign}\left(\lim_{x \to -\infty} i(G_0, x) \right) = (-1)^k$$

$$\operatorname{sign}\left(\lim_{x \to -\infty} i(G_1, x) \right) = (-1)^{k+1}$$

$$\operatorname{sign}\left(\lim_{x \to -\infty} i(G_2, x) \right) = (-1)^{k+1}.$$

We now prove the lower bounds for $\operatorname{maxmod}(n)$ by exhibiting, in each one of the cases, a graph with a real independence root with modulus larger than the bound.

Case 0: $n \equiv 0 \mod 3$

If $n = 3$, then we can use the quadratic formula to find that P_3 has a real independence root with modulus approximately $2.618 > 1$. So we may assume that $n \geq 6$ and thus $k \geq 1$ for our analysis of G_0. For all $k \geq 1$, we have that

$$i(G_0, -3^k) = \left(1 - 3^{k+1}\right)^k \left(1 - 2 \cdot 3^{k+1}\right) - 3^k \left(1 - 3^k\right)^k$$
$$= (-1)^k \left[(1 - 3^k)\left((3^{k+1} - 1)^k - (3^{k+1} - 3)^k\right) - 3^k(3^k - 1)^k\right]$$

which has the same sign as $(-1)^{k+1}$ since $0 > (3^{k+1} - 1)^k - (3^{k+1} - 3)^k$. Thus, $i(G_0, x)$ alternates sign on $(-\infty, -3^k]$ and by the IVT and since $k = \frac{n-3}{3}$, $i(G_0, x)$ has a root in the interval $(-\infty, -3^{\frac{n-3}{3}})$.

Case 1: $n \equiv 1 \mod 3$

If $n = 1$, then K_1 is the only graph to consider and the result clearly holds. So we may assume that $n \geq 4$ and therefore $k \geq 1$ for our analysis of G_1. Since $i(G_1, -3^k) = (-1)^k((3^{k+1} - 1)^k - (3^{k+1} - 3)^k)$, it follows that $i(G_1, -3^k)$ has the same sign as $(-1)^k$. Thus $i(G_1, x)$ alternates sign on $(-\infty, -3^k]$ and by IVT it must have a root in the interval $(-\infty, -3^{\frac{n-1}{3}})$.

Case 2: $n \equiv 2 \mod 3$

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If $n = 2$, then the graph $\overline{K_2}$ has and -1 as an independence root and $|-1| = 1 = 3^0$. If $n = 5$, then P_5 has a real independence root of modulus approximately 5.0489173 which is greater than 3. So we may assume $n \geq 8$ and therefore $k \geq 1$ for the our analysis of the graph G_2. We now have,

$$\begin{aligned}
i(G_2, -3^k) &= (-1)^k \left[(1 - 2 \cdot 3^k)^2 (3^{k+1} - 1)^k - 3^k (1 - 3^k)^2 (3^k - 1)^k \right] \\
&= (-1)^k \left[(1 - 4 \cdot 3^k + 4 \cdot 3^{2k})(3^{k+1} - 1)^k - (1 - 3^k)^2 (3^{k+1} - 3)^k \right] \\
&= (-1)^k \left[(1 - 4 \cdot 3^k + 3^{2k} + 3^{2k+1})(3^{k+1} - 1)^k - (1 - 3^k)^2 (3^{k+1} - 3)^k \right] \\
&= (-1)^k \left[(1 - 3^k)^2 \left((3^{k+1} - 1)^k - (3^{k+1} - 3)^k \right) + \right. \\
&\qquad \left. (3^{2k+1} - 2 \cdot 3^k)(3^{k+1} - 1)^k \right]
\end{aligned}$$

which has sign $(-1)^k$ since $(3^{k+1} - 1)^k - (3^{k+1} - 3)^k > 0$, $(1 - 3^k)^2 > 0$, and $(3^{2k+1} - 2 \cdot 3^k)(3^{k+1} - 1)^k > 0$.

Therefore, IVT gives that $i(G_2, x)$ must have a root in the interval $(-\infty, -3^{\frac{n-2}{3}})$. This completes the proof. ∎

Therefore, $\mathrm{maxmod}(n)$ is at least exponential in n. We require the next two lemmas to put an upper bound on $\mathrm{maxmod}(n)$.

Lemma 2.5 *For all graphs G with at least one edge, there exists a non-isolated vertex v such that $\alpha(G) = \alpha(G - v) \geq \alpha(G - N[v]) + 1$.*

Proof Let G be a graph with at least one edge. It is clear that for any vertex v of G, $\alpha(G) \geq \alpha(G - N[v]) + 1$, since any maximum independent set in $G - N[v]$ will still be independent in G with the addition of v. Suppose that for all vertices $v \in V(G)$, that $\alpha(G) > \alpha(G - v)$. Then every vertex belongs to every maximum independent set. However, G has at least one edge, so the vertices incident with this edge cannot belong to the same independent set, which contradicts both of these vertices being in every maximum independent set. Therefore, there exists some $v \in V(G)$ incident with some edge such that

$$\alpha(G) = \alpha(G - v) \geq \alpha(G - N[v]) + 1.$$

∎

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Lemma 2.6 *If G is a graph on n vertices such that $\xi(G) = 1$, then $i_{\alpha(G)-1} \leq 3^{\frac{n}{3}} + n - 1$.*

Proof Let G be a graph on n vertices such that $\xi(G) = 1$. Every independent set of size $\alpha(G) - 1$ is either maximal or is a subset of the one independent set of size $\alpha(G)$. Therefore, $i_{\alpha(G)-1} \leq \mu(G) - 1 + \alpha(G) \leq 3^{\frac{n}{3}} + n - 1$ (subtracting 1 from $\mu(G)$ to account for the one maximum independent set) by the note following Theorem 2.3. ∎

Theorem 2.7 *For all $n \geq 1$, $\mathrm{maxmod}(n) \leq 3^{\frac{n}{3}} + n - 1$.*

Proof We actually prove the stronger result that for a graph on n vertices, the ratios of coefficients, given by R in the statement of Theorem 2.1 (the Eneström-Kakeya Theorem), of its independence polynomial are bounded above by $3^{\frac{n}{3}} + n - 1$. It then follows directly from the Eneström-Kakeya Theorem that the roots are bounded by this value. We proceed by induction on n.

The results hold for graphs on $n \leq 5$ vertices by straightforward checking the ratios of consecutive coefficients of the independence polynomials of all 52 graphs in Maple. Now suppose the result holds for all $3 \leq k < n$, and let G be a graph on n vertices. If G has no edges, then we are done, since G has only -1 as an independence root in this case. Therefore, suppose G has at least one edge. Let v be a nonisolated vertex in G such that $\alpha(G) = \alpha(G - v) \geq \alpha(G - N[v]) + 1$, noting that v exists by Lemma 2.5. Now, by Proposition 2.2,

$$
\begin{aligned}
i(G,x) &= i(G-v,x) + x \cdot i(G-N[v],x) \\
&= \sum_{k=0}^{\alpha(G-v)} i_k^{G-v} x^k + x \sum_{k=0}^{\alpha(G-N[v])} i_k^{G-N[v]} x^k \\
&= 1 + \sum_{k=1}^{\alpha(G-v)} i_k^{G-v} x^k + \sum_{k=1}^{\alpha(G-N[v])+1} i_{k-1}^{G-N[v]} x^k. \quad (1)
\end{aligned}
$$

We now have two cases.

Case 1: $\alpha(G) = \alpha(G-v) = \alpha(G-N[v]) + 1$.

In this case, (1) gives

$$i(G,x) = 1 + \sum_{k=1}^{\alpha(G-v)} \left(i_k^{G-v} + i_{k-1}^{G-N[v]} \right) x^k.$$

This gives the following ratios between coefficients,

$$\frac{1}{n} \text{ and } \frac{i_k^{G-v} + i_{k-1}^{G-N[v]}}{i_{k+1}^{G-v} + i_k^{G-N[v]}} \text{ for } k = 1, 2, \ldots, \alpha(G-N[v]).$$

For all $n \geq 1$, $\frac{1}{n} < 3^{\frac{n}{3}} + n - 1$, and by the inductive hypothesis,

$$\frac{i_k^{G-v} + i_{k-1}^{G-N[v]}}{i_{k+1}^{G-v} + i_k^{G-N[v]}} < \frac{\left(3^{\frac{n-1}{3}} + n - 2 \right) i_{k+1}^{G-v} + \left(3^{\frac{n-|N[v]|}{3}} + n - 1 - |N[v]| \right) i_k^{G-N[v]}}{i_{k+1}^{G-v} + i_k^{G-N[v]}}$$

$$\leq \frac{\left(3^{\frac{n-1}{3}} + n - 2 \right) \left(i_{k+1}^{G-v} + i_k^{G-N[v]} \right)}{i_{k+1}^{G-v} + i_k^{G-N[v]}}$$

$$= 3^{\frac{n-1}{3}} + n - 2$$

$$< 3^{\frac{n}{3}} + n - 1.$$

Case 2: $\alpha(G) = \alpha(G-v) > \alpha(G-N[v]) + 1.$

In this case, the independence polynomial is obtained from (1) as, In this case, (1) gives

$$i(G,x) = 1 + \sum_{k=1}^{\alpha(G-N[v])+1} \left(i_k^{G-v} + i_{k-1}^{G-N[v]} \right) x^k + \sum_{\alpha(G-N[v])+2}^{\alpha(G-v)} i_k^{G-v} x^k.$$

This gives four different forms for $\frac{i_k^G}{i_{k+1}^G}$. The first two, namely $\frac{1}{n}$ and $\frac{i_k^{G-v} + i_{k-1}^{G-N[v]}}{i_{k+1}^{G-v} + i_k^{G-N[v]}}$, are less than or equal to $3^{\frac{n}{3}} + n - 1$ for each $k = 1, 2, \ldots, \alpha(G-N[v])$ by the same argument as Case 1. This leaves,

$$\frac{i_{\alpha(G-N[v])+1}^{G-v} + i_{\alpha(G-N[v])}^{G-N[v]}}{i_{\alpha(G-N[v])+2}^{G-v}}, \text{ and } \frac{i_k^{G-v}}{i_{k+1}^{G-v}} \text{ for } k \geq \alpha(G-N[v]) + 2$$

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By the inductive hypothesis, $\frac{i_k^{G-v}}{i_{k+1}^{G-v}} \leq 3^{\frac{n-1}{3}} + n - 2 < 3^{\frac{n}{3}} + n - 1$, so we are left only

with $\frac{i_{\alpha(G-N[v])+1}^{G-v} + i_{\alpha(G-N[v])}^{G-N[v]}}{i_{\alpha(G-N[v])+2}^{G-v}}$.

In this case, we first show that $|N[v]| \geq 3$. As v is not isolated, $|N[v]| \geq 2$. If $|N[v]| = 2$, then v is a leaf, and since v was chosen such that $\alpha(G) = \alpha(G - v) \geq \alpha(G - N[v]) + 1$, v is not in every maximum independent set in G. But every maximum independent set in G must contain either v or its neighbour, so $\alpha(G - v) = \alpha(G - N[v]) + 1$ as covered in Case 1. Therefore, we may assume $|N[v]| \geq 3$. We also note that

$$\frac{i_{\alpha(G-N[v])+1}^{G-v} + i_{\alpha(G-N[v])}^{G-N[v]}}{i_{\alpha(G-N[v])+2}^{G-v}} = \frac{i_{\alpha(G-N[v])+1}^{G-v}}{i_{\alpha(G-N[v])+2}^{G-v}} + \frac{\xi(G-N[v])}{i_{\alpha(G-N[v])+2}^{G-v}}.$$

There are three subcases to consider.

Case 2a: $\alpha(G - N[v]) + 2 < \alpha(G - v) = \alpha(G)$.

If $\alpha(G - N[v]) + 2 < \alpha(G - v)$, then $G - v$ has an independent set of size $\alpha(G - N[v]) + 3$. Therefore, $i_{\alpha(G-N[v])+2}^{G-v} \geq \alpha(G - N[v]) + 3 \geq 3$, since any independent set of size k, contains at least $\binom{k}{k-1} = k$ independent sets of size $k - 1$. Now by the inductive hypothesis and the note following Theorem 2.3,

$$\frac{i_{\alpha(G-N[v])+1}^{G-v}}{i_{\alpha(G-N[v])+2}^{G-v}} + \frac{\xi(G-N[v])}{i_{\alpha(G-N[v])+2}^{G-v}} \leq 3^{\frac{n-1}{3}} + n - 2 + \frac{\xi(G-N[v])}{3}$$

$$\leq 3^{\frac{n-1}{3}} + n - 2 + 3^{\frac{n-|N[v]|-3}{3}}$$

$$\leq 3^{\frac{n-1}{3}} + n - 2 + 3^{\frac{n-6}{3}}$$

$$= 3^{\frac{n}{3}}\left(3^{\frac{-1}{3}} + \frac{1}{9}\right) + n - 2$$

$$\leq 3^{\frac{n}{3}} + n - 1.$$

Case 2b: $\alpha(G - N[v]) + 2 = \alpha(G - v) = \alpha(G)$ and $|N[v]| \geq 4$.

In this case, by the inductive hypothesis and the note following Theorem 2.3,

$$\frac{i^{G-v}_{\alpha(G-N[v])+1}}{i^{G-v}_{\alpha(G-N[v])+2}} + \frac{\xi(G-N[v])}{i^{G-v}_{\alpha(G-N[v])+2}} \le 3^{\frac{n-1}{3}} + n - 2 + \xi(G-N[v])$$

$$\le 3^{\frac{n-1}{3}} + n - 2 + 3^{\frac{n-|N[v]|}{3}}$$

$$\le 3^{\frac{n-1}{3}} + n - 2 + 3^{\frac{n-4}{3}}$$

$$= 3^{\frac{n}{3}}\left(3^{\frac{-1}{3}} + 3^{\frac{-4}{3}}\right) + n - 2$$

$$< 3^{\frac{n}{3}} + n - 1.$$

Case 2c: $\alpha(G-N[v]) + 2 = \alpha(G-v)$ and $|N[v]| = 3$.

We break this final case into two subcases bases on the size of $i^{G-v}_{\alpha(G-N[v])+2}$. First, if $i^{G-v}_{\alpha(G-N[v])+2} \ge 2$, then by the inductive hypothesis and the note following Theorem 2.3,

$$\frac{i^{G-v}_{\alpha(G-N[v])+1}}{i^{G-v}_{\alpha(G-N[v])+2}} + \frac{\xi(G-N[v])}{i^{G-v}_{\alpha(G-N[v])+2}} \le 3^{\frac{n-1}{3}} + n - 2 + \frac{\xi(G-N[v])}{2}$$

$$\le 3^{\frac{n-1}{3}} + n - 2 + \frac{3^{\frac{n-3}{3}}}{2}$$

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

$$\le 3^{\frac{n}{3}} + n - 1.$$

Note if some maximum independent set in G contained v, then this set with v removed would be an independent set of size $\alpha(G) - 1 = \alpha(G-N[v]) + 1$ in $G - N[v]$, which is a contradiction. Therefore, the maximum independent sets in G and $G - v$ are exactly the same sets and, in particular, $\xi(G) = \xi(G-v)$. Now, if

$$1 = i^{G-v}_{\alpha(G-N[v])+2} = \xi(G-v) = \xi(G),$$

then Lemma 2.6 applied to G gives a bound on $i^G_{\alpha(G)-1}$ in the last line of the following,

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$$\frac{i^{G-v}_{\alpha(G-N[v])+1} + i^{G-N[v]}_{\alpha(G-N[v])}}{i^{G-v}_{\alpha(G-N[v])+2}} = \frac{i^{G}_{\alpha(G)-1}}{i^{G}_{\alpha(G)}}$$

$$= i^{G}_{\alpha(G)-1}$$

$$\leq 3^{\frac{n}{3}} + n - 1.$$

Now, if z is an independence root of G, then, by the Eneström-Kakeya Theorem, $|z| \leq 3^{\frac{n}{3}} + n - 1$. ∎

Proposition 2.4 and Theorem 2.7 give the following corollary.

Corollary 2.8

$$\frac{\log_3(\mathrm{maxmod}(n))}{n} = \frac{1}{3} + o(1).$$

∎

3 Bounds for trees of order n

Now that we have determined bounds on $\mathrm{maxmod}(n)$, a natural extension of this is to determine the *largest* modulus an independence root can obtain among all graphs of order n in a specific family of graphs. In particular, the bound we obtained for $\mathrm{maxmod}(n)$ seems to be much too large when we restrict our attention to trees. In this section, we consider $\mathrm{maxmod}_T(n)$, the maximum modulus of an independence root over all trees on n vertices.

Let T_k be the tree obtained by gluing k copies of P_3 together at a leaf (see Figure 2). This tree is known [26] to have the largest number of maximal independent sets among trees on $2k+1$ vertices and we will show that it also has the largest ratio of consecutive coefficients among all such trees, and therefore provides an upper bound on $\mathrm{maxmod}_T(n)$.

Theorem 3.1 ([29]) *If G is a tree of order $n \geq 2$, then*

$$\xi(G) \leq t'(n) = \begin{cases} 2^{\frac{n-3}{2}} & \text{if } n \text{ is odd} \\ \\ 2^{\frac{n-2}{2}} + 1 & \text{if } n \text{ is even} \end{cases}.$$
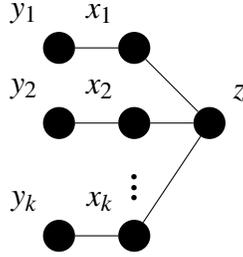
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Figure 2: The tree T_k on $2k+1$ vertices that has independence root in $[-2^k - k, -2^k)$.

We need to extend our notation to $\mathrm{maxmod}_F(n)$, the maximum modulus of an independence root of a forest of order n; clearly $\mathrm{maxmod}_T(n) \leq \mathrm{maxmod}_F(n)$. The following lemma will be required in proving an upper bound on the ratio of consecutive coefficients of the independence polynomials of forests.

Lemma 3.2 *If F is a forest on n vertices, $n \geq 2$, and $v \in V(F)$, then*

$$\frac{\xi(F)}{\xi(F-v)} \leq \begin{cases} 2^{\frac{n-3}{2}} + 1 & \text{if } n \text{ is odd} \\ \\ 2^{\frac{n-2}{2}} + 1 & \text{if } n \text{ is even} \end{cases}.$$

Proof   Let $F = H_1 \cup H_2 \cup \cdots \cup H_k$, where $k \geq 1$, and each H_i is a connected component of F. Suppose, without loss of generality, that $v \in H_k$. Then

$$F - v = H_1 \cup H_2 \cup \cdots H_{k-1} \cup F',$$

where F' is the forest obtained from deleting v from H_k (note that if v was an isolated vertex in F, then F' may have no vertices and $\xi(H_k) = 1$). Now we have,

$$\frac{\xi(F)}{\xi(F-v)} = \frac{\xi(H_1) \cdot \xi(H_2) \cdots \xi(H_k)}{\xi(H_1) \cdot \xi(H_2) \cdots \xi(H_{k-1}) \cdot \xi(F')}$$

$$= \frac{\xi(H_k)}{\xi(F')}$$

$$\leq \xi(H_k)$$

$$\leq \max\{t'(i) : 1 \leq i \leq n\} \qquad \text{(from Theorem 3.1)}$$

$$= \begin{cases} \max\left\{2^{\frac{n-(2i+1)}{2}} + 1 : i = 1, 2, \ldots, n\right\} & \text{if } n \text{ is odd} \\ \\ \max\left\{2^{\frac{n-2i}{2}} + 1 : i = 1, 2, \ldots, n\right\} & \text{if } n \text{ is even} \end{cases}$$

$$= \begin{cases} 2^{\frac{n-3}{2}} + 1 & \text{if } n \text{ is odd} \\ \\ 2^{\frac{n-2}{2}} + 1 & \text{if } n \text{ is even} \end{cases}.$$

∎

Theorem 3.3 *For $n \geq 1$,*

$$\mathrm{maxmod}_F(n) \leq \begin{cases} 2^{\frac{n-1}{2}} + \frac{n-1}{2} & \text{if } n \text{ is odd} \\ \\ 2^{\frac{n-2}{2}} + \frac{n}{2} & \text{if } n \text{ is even} \end{cases}.$$

Proof   As in the proof of Theorem 2.7, we actually prove a stronger result, bounding the ratios of consecutive coefficients. The Eneström-Kakeya Theorem then applies to obtain the bound the roots. We proceed by induction on n.

For $n = 1, 2, 3, 4$ the results hold by checking all forests of order at most 4. Suppose the result holds for all $4 \leq k \leq n-1$ and let F be a forest on n vertices. Note that if $F = \overline{K_n}$, then the largest ratio of consecutive coefficients of $i(F, x)$ can easily be verified to be n which is less than the result in either case, so suppose F has at least one edge and therefore at least one leaf. Let v be a leaf of F and let u be adjacent to v. Note that $\alpha(F - \{u, v\}) \leq \alpha(F - v) \leq \alpha(F - \{u, v\}) + 1$ and for our argument, we assume that $\alpha(F - v) = \alpha(F - \{u, v\})$ as our arguments will hold (and be even shorter) when $\alpha(F - v) = \alpha(F - \{u, v\}) + 1$. To simplify

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notation, let $\alpha = \alpha(F - v) = \alpha(F - \{u,v\})$. By Proposition 2.2, we have

$$i(F,x) = i(F - v,x) + x \cdot i(F - \{u,v\},x)$$

$$= \sum_{k=0}^{\alpha} i_k^{F-v} x^k + x \sum_{k=0}^{\alpha} i_k^{F-\{u,v\}} x^k$$

$$= 1 + \sum_{k=1}^{\alpha} \left(i_k^{F-v} + i_{k-1}^{F-\{u,v\}} \right) x^k + i_{\alpha}^{F-\{u,v\}} x^{\alpha+1}. \tag{2}$$

We need to show that $\dfrac{i_k^F}{i_{k+1}^F}$ is bounded above by the desired value and from (2),
we see that $\dfrac{i_k^F}{i_{k+1}^F}$ can take on the following forms,

$$\frac{1}{n}, \; \frac{i_k^{F-v} + i_{k-1}^{F-\{u,v\}}}{i_{k+1}^{F-v} + i_k^{F-\{u,v\}}} \text{ for } k = 1,2,\ldots\alpha(F - \{u,v\}) - 1, \text{ and } \frac{i_{\alpha}^{F-v} + i_{\alpha-1}^{F-\{u,v\}}}{i_{\alpha}^{F-\{u,v\}}}.$$

The first ratio, $\frac{1}{n}$, clearly satisfies the desired bound regardless of the parity of
n. We now only need to verify the remaining two forms of $\dfrac{i_k^F}{i_{k+1}^F}$. We will do this in
two cases depending on the parity of n.

Case 1: n is odd.

We apply the inductive hypothesis to get,

$$\frac{i_k^{F-v} + i_{k-1}^{F-\{u,v\}}}{i_{k+1}^{F-v} + i_k^{F-\{u,v\}}} \leq \frac{\left(2^{\frac{n-3}{2}} + \frac{n-1}{2}\right) i_{k+1}^{F-v} + \left(2^{\frac{n-3}{2}} + \frac{n-3}{2}\right) i_k^{F-\{u,v\}}}{i_{k+1}^{F-v} + i_k^{F-\{u,v\}}}$$

$$\leq \frac{\left(2^{\frac{n-3}{2}} + \frac{n-1}{2}\right) \left(i_{k+1}^{F-v} + i_k^{F-\{u,v\}}\right)}{i_{k+1}^{F-v} + i_k^{F-\{u,v\}}}$$

$$= 2^{\frac{n-3}{2}} + \frac{n-1}{2}$$

$$< 2^{\frac{n-1}{2}} + \frac{n-1}{2}.$$

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For the last ratio, we have,

$$\frac{i_\alpha^{F-v} + i_{\alpha-1}^{F-\{u,v\}}}{i_\alpha^{F-\{u,v\}}} = \frac{i_\alpha^{F-v}}{i_\alpha^{F-\{u,v\}}} + \frac{i_{\alpha-1}^{F-\{u,v\}}}{i_\alpha^{F-\{u,v\}}}$$

$$\leq \frac{\xi(F-v)}{\xi(F-\{u,v\})} + 2^{\frac{n-3}{2}} + \frac{n-3}{2} \quad \text{(by the inductive hypothesis)}$$

$$\leq 2^{\frac{n-3}{2}} + 1 + 2^{\frac{n-3}{2}} + \frac{n-3}{2} \quad \text{(by the Lemma 3.2)}$$

$$= 2^{\frac{n-1}{2}} + \frac{n-1}{2}.$$

Therefore, the result holds when n is odd by the Eneström-Kakeya Theorem.

Case 2: Suppose that n is even.

Then we apply the inductive hypothesis to get,

$$\frac{i_k^{F-v} + i_{k-1}^{F-\{u,v\}}}{i_{k+1}^{F-v} + i_k^{F-\{u,v\}}} \leq \frac{\left(2^{\frac{n-2}{2}} + \frac{n-2}{2}\right) i_{k+1}^{F-v} + \left(2^{\frac{n-4}{2}} + \frac{n-2}{2}\right) i_k^{F-\{u,v\}}}{i_{k+1}^{F-v} + i_k^{F-\{u,v\}}}$$

$$\leq \frac{\left(2^{\frac{n-2}{2}} + \frac{n-2}{2}\right)\left(i_{k+1}^{F-v} + i_k^{F-\{u,v\}}\right)}{i_{k+1}^{F-v} + i_k^{F-\{u,v\}}}$$

$$= 2^{\frac{n-2}{2}} + \frac{n-2}{2}$$

$$< 2^{\frac{n-2}{2}} + \frac{n}{2}.$$

For the last ratio, we have,

$$\frac{i_\alpha^{F-v} + i_{\alpha-1}^{F-\{u,v\}}}{i_\alpha^{F-\{u,v\}}} = \frac{i_\alpha^{F-v}}{i_\alpha^{F-\{u,v\}}} + \frac{i_{\alpha-1}^{F-\{u,v\}}}{i_\alpha^{F-\{u,v\}}}$$

$$\leq \frac{\xi(F-v)}{\xi(F-\{u,v\})} + 2^{\frac{n-4}{2}} + \frac{n-2}{2} \quad \text{(by the inductive hypothesis)}$$

$$\leq 2^{\frac{n-4}{2}} + 1 + 2^{\frac{n-4}{2}} + \frac{n-2}{2} \quad \text{(by the Lemma 3.2)}$$

$$= 2^{\frac{n-2}{2}} + \frac{n}{2}.$$

Therefore, the result holds when n is even by the Eneström-Kakeya Theorem. ∎

Corollary 3.4 *For $n \geq 1$,*

$$\text{maxmod}_T(n) \leq \begin{cases} 2^{\frac{n-1}{2}} + \frac{n-1}{2} & \text{if } n \text{ is odd} \\[2ex] 2^{\frac{n-2}{2}} + \frac{n}{2} & \text{if } n \text{ is even} \end{cases}.$$

■

We remark that, at least in terms of the bounds on the ratio of consecutive coefficients, this is best possible as there are forests that achieve these bounds. Let n be odd, and consider the graph $T_{\frac{n-1}{2}}$ as previously defined and pictured in Figure 2. The independence polynomial of this tree has $2^{\frac{n-1}{2}} + \frac{n-1}{2}$ as its last ratio of consecutive coefficients. If n is even then look at the forest $T_{\frac{n-2}{2}} \cup K_1$, whose independence polynomial has $2^{\frac{n-2}{2}} + \frac{n}{2}$ as its last ratio of consecutive coefficients.

We have shown that the bounds on the ratio of consecutive coefficients are tight, but are these bounds tight on the roots? It is not always the case that the upper bound on the moduli of the roots of a polynomial is tight, even for trees and forests. Take for example, the tree $K_{1,30}$ which has 30 as an upper bound on the roots from Eneström-Kakeya but its actual root of largest modulus is approximately 2.023777128. It gets even worse when we consider taking the disjoint union of k copies of $K_{1,30}$. This forest will have the same root of maximum modulus but the bound on the root from Eneström-Kakeya is $30k$, which is unbounded. Fortunately, it turns out that the bound we found in Theorem 3.3 is asymptotically tight when n is odd.

For the case where n is even in the next proof we require the definition of the tree T'_k as shown in Figure 3. Let T'_k be the graph obtained by adding two leaves to each vertex in K_2 and then gluing a leaf of the resulting graph to the central vertex of T_k.

Proposition 3.5 *For all $n \geq 1$,*

$$\text{maxmod}_T(n) \geq \begin{cases} 2^{\frac{n-1}{2}} & \text{if } n \text{ is odd} \\[2ex] 2^{\frac{n-6}{2}} & \text{if } n \text{ is even} \end{cases}.$$
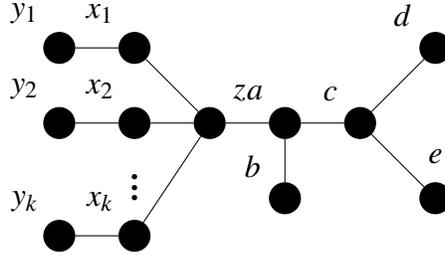
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Figure 3: The tree T'_k on $2(k+3)$ vertices that has an independence root in $[-2^{k+1} - k - 4, -2^k)$.

Proof   The proof is similar to the proof of Proposition 2.4, finding trees that have real independence roots of large modulus.

Case 1: n is odd.

If $n = 1$, then the result clearly holds so we may assume $n \geq 1$. Let $n = 2k+1$ (note $k \geq 1$), so that $k = \frac{n-1}{2}$, and set $T = T_k$ as in Figure 2. A simple calculation via Proposition 2.2 shows that $i(T, x) = (1 + 2x)^k + x(1 + x)^k$. We will use the Intermediate Value Theorem to show that $i(T, x)$ has a real root to the left of -2^k. Now,

$$i(T, -2^k) = (1 - 2^{k+1})^k - 2^k(1 - 2^k)^k$$
$$= (-1)^k \left((2^{k+1} - 1)^k - (2^{k+1} - 2)^k \right),$$

so $i(T, -2^k)$ has the same sign as $(-1)^k$. On the other hand, $i(T, x)$ has sign $(-1)^{k+1}$ as x tends to ∞We now compute the limit as x tends to $-\infty$. Thus, $i(T_k, x)$ alternates sign on $(-\infty, -2^k]$, so by IVT it must have a real root in the interval $(-\infty, -2^k)$. We remark that from Theorem 3.3, that $i(T, x)$ actually has a real root in the interval $[-2^k - k, -2^k)$.

Case 2: n is even.

For $n = 2$ and 4, the result is clear. For $n \geq 6$, we will show that T'_k, the graph in Figure 3, has a real root to the left of -2^k. Let $n = 2(k+3)$ for $k \geq 0$. If $k = 0$, then $i(T'_k, x) = (1 + x)^2(1 + 4x + x^2)$ which has roots -1, $-2 + \sqrt{3}$, and $-2 - \sqrt{3}$, with $-2 - \sqrt{3}$ being to the left of $-2^{\frac{6-6}{2}} = -1$). If $k = 1$, then $i(T'_k, x) = x^5 + 9x^4 +$

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$22x^3 + 21x^2 + 8x + 1$, which has its largest root at approximately -5.7833861, which is to the left of $-2^{\frac{8-6}{2}} = -4$. Since the result holds for $k = 0, 1$, we may now assume that $k \geq 2$.

Using Proposition 2.2, we find that

$$i(T'_k, x) = (1 + 2x)^k (1 + 5x + 6x^2 + 2x^3) + x(1 + x)^k (1 + 4x + 4x^2 + x^3).$$

Let $g(x) = 1 + 5x + 6x^2 + 2x^3$ and $h(x) = 1 + 4x + 4x^2 + x^3$. We can easily verify that $g(x) < 0$ for all $x \leq -2$ and $h(x) < 0$ for all $x \leq -3$. Moreover, $h(x) = g(x) - x(x+1)^2$. We consider the function

$$f(x) = (-2x - 1)^k (1 + 5x + 6x^2 + 2x^3) + x(-x - 1)^k (1 + 4x + 4x^2 + x^3),$$

so that $i(T'_k, x) = (-1)^k f(x)$. Now,

$$
\begin{aligned}
f(-2^k) &= (2^{k+1} - 1)^k g(-2^k) - 2^k (2^k - 1)^k h(-2^k) \\
&= (2^{k+1} - 1)^k g(-2^k) - 2^k (2^k - 1)^k (g(-2^k) + 2^k (1 - 2^k)^2) \\
&= g(-2^k)((2^{k+1} - 1)^k - (2^{k+1} - 2)^k) - 2^{2k}(2^k - 1)^{k+2}
\end{aligned}
$$

and since $g(-2^k)$ and $-2^{2k}(2^k - 1)^{k+2}$ are both negative for $k \geq 2$, it follows that $f(-2^k) < 0$. Therefore, $i(T'_k, x)$ has sign $(-1)^k (-1) = (-1)^{k+1}$. On the other hand, $i(T'_k, x)$ has sign $(-1)^{k+4} = (-1)^k$ as x tends to ∞. Thus, by the IVT, $i(T'_k, x)$ has a real root to the left of -2^k. From, Theorem 3.3 and the Eneström-Kakeya Theorem, $i(T, x)$ has no roots in $(-\infty, -2^{k+1/2} - k - 3)$, so $i(T'_k, x)$ has a root in the interval $[-2^{k+1/2} - k - 3, -2^k)$.

∎

Tables 1 and 2 show values of $\mathrm{maxmod}_T(n)$ for small values of n in comparison to our bounds.

Although the bounds on $\mathrm{maxmod}_T(n)$ are not as tight for even n as for odd n, Corollary 3.4 and Proposition 3.5 give the following corollary for all n.

Corollary 3.6
$$\frac{\log_2(\mathrm{maxmod}_T(n))}{n} = \frac{1}{2} + o(1).$$

∎

n	$2^{\frac{n-1}{2}}$	$\mathrm{maxmod}_T(n)$	$2^{\frac{n-1}{2}}+\frac{n-1}{2}$	n	$2^{\frac{n-6}{2}}$	$\mathrm{maxmod}_T(n)$	$2^{\frac{n-2}{2}}+\frac{n}{2}$
3	2	2.61803398900000	3	2	0.25	0.5	2
5	4	5.04891733952231	6	4	0.5	1.77423195656734	4
7	8	9.49699733952714	11	6	1	3.732050808	7
9	16	17.9705962347393	20	8	2	5.78338611675281	12
11	32	34.4632033453548	37	10	4	10.0833151322046	21
13	64	66.9662907779610	70	12	64	18.5001015662614	38
15	128	131.473379027662	135	14	8	34.9710040067543	71
17	256	259.980782682655	264	16	16	67.4665144832128	136

Table 1: Comparing $\mathrm{maxmod}_T(n)$ to our bounds for odd n

Table 2: Comparing $\mathrm{maxmod}_T(n)$ to our bounds for even n

4   Conclusion and Open Problems

We were able to prove upper and lower bounds on $\mathrm{maxmod}(n)$ and $\mathrm{maxmod}_T(n)$ for all n but questions remain about tightening our bounds for all graphs and about the growth rate of the moduli of independence roots for other families of graphs.

One highly structured and highly interesting family of graphs is the family of well-covered graphs [13, 14, 24], that is, graphs with all maximal independent sets of the same size. For each well-covered graph with independence number α, it is known that all of its independence roots lie in the disk $|z| \leq \alpha$ and there are well-covered graphs with independence roots arbitrarily close to the boundary [4]. This difference between the independence roots of graphs and well-covered graphs begs the question of what happens for well-covered trees? Finbow et al. [14] showed that every well-covered tree is obtained by attaching a leaf to every vertex of another tree. This construction of attaching a leaf to every vertex in a graph G is know as the graph star operation, the resulting graph denoted G^*. Levit and Mandrescu [19] proved a formula for $i(G^*, x)$ in terms of $i(G, x)$ for all graphs G. Using Maple and nauty [21], we were able exploit this formula to verify that all well-covered trees on $n \leq 40$ vertices have their independence roots contained in the unit disk!

This makes it extremely tempting to conjecture that the independence roots of all well-covered trees are contained in the unit disk. However, the relationship between the independence roots of a tree and the independence roots of its well-covered extension are bound by the properties of Möbius transformations (this relationship was used by the authors in [1, 2]). Drawing on the theory of these

transfomrations, it can be shown that any tree T with independence roots to the right of the line $\text{Re}(z) = \frac{1}{2}$, will yield a well-covered tree T^* with independence roots outside of the unit disk. It was shown in [1], that there are trees with independence roots arbitrarily far in the right half of $\mathbb{C}$, therefore, there are well-covered trees with independence roots outside of the unit disk. The tantalizing question remains:

Question 4.1 *What is the maximum modulus of an independence root of a well-covered tree on n vertices?*

Our bounds on $\log_3(\text{maxmod}(n))$ and $\log_2(\text{maxmod}_T(n))$ are very good asymptotically and a fairly good estimate for all n. Nevertheless, from computations with Maple and nauty [21], we have the following conjectures.

Conjecture 4.2 *If G is a graph on n vertices, then for $n \geq 3$,*

$$
\text{maxmod}(n) \leq \begin{cases} 2 \cdot 3^{\frac{n-3}{3}} + \frac{n}{3} & \text{if } n \equiv 0 \mod 3 \\[2mm] 3^{\frac{n-1}{3}} + \frac{n-1}{3} & \text{if } n \equiv 1 \mod 3 \\[2mm] 4 \cdot 3^{\frac{n-5}{3}} + \frac{n+1}{3} & \text{if } n \equiv 2 \mod 3 \end{cases}
$$

Conjecture 4.3 *The graphs G_0, G_1, and G_2 are the only graphs to achieve $\text{maxmod}(n)$.*

Conjecture 4.4 *If T is a tree on n vertices with $n \geq 6$ even , then,*

$$
\text{maxmod}_T(n) \leq 2^{\frac{n-4}{2}} + \frac{n+2}{2}
$$

Conjecture 4.5 *The trees $T_{\frac{n-1}{2}}$ and $T'_{\frac{n-6}{2}}$ (see Figures 2 and 3) are the only trees to achieve $\text{maxmod}_T(n)$ for n odd and even respectively.*

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