On the Characteristic Set, Centroid, and Centre for a Tree

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Abstract

Given a tree T, we consider a pair of vertices (u, v) where u is a centroid of T, v is a characteristic vertex of T, and such that the distance between them, denoted $d(u, v)$, is smallest over all such pairs. We define $\delta_{\text{centroid}}(T) = d(u, v)$ and $\delta_{\text{centroid}}(n) = \max_T \delta_{\text{centroid}}(T)$, where the maximum is taken over all trees T on n vertices. Analogous definitions are also given for $\delta_{\text{centre}}(T)$ and $\delta_{\text{centre}}(n)$

We show that for each $n \geq 12$, there is a broom T on n vertices such that $\delta_{\text{centroid}}(T) = \delta_{\text{centroid}}(n)$ and a broom T' on n vertices such that $\delta_{\text{centre}}(T') = \delta_{\text{centre}}(n)$. We also prove that the sequences $\frac{\delta_{\text{centroid}}(n)}{n}$ and $\frac{\delta_{\text{centre}}(n)}{n}$ are convergent, and find their limits. We rely on the characterisation of characteristic vertices in terms of Perron branches in order to establish our results.

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This paper is dedicated to the memory of Marvin Marcus.

1 Introduction and preliminaries

Suppose that T is a tree on n vertices, and denote its Laplacian matrix by L. It is straightforward to see that L is positive semidefinite, with 0 as a simple eigenvalue. The smallest positive eigenvalue of L is known as the *algebraic connectivity* of the tree, and here we denote it by $a(T)$. Suppose that x is an eigenvector of L

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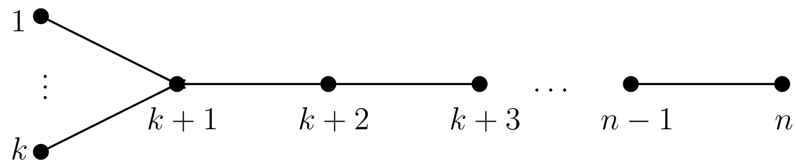

Figure 1: The broom $T_{k,n}$

corresponding to the eigenvalue $a(T)$. A remarkable result of Fiedler [3] shows that precisely one of two cases holds.
i) There is a unique vertex j of T such that $x_j = 0$, and j is adjacent to k for some vertex k with $x_k \neq 0$. When this is the case, T is called a *type 1 tree*, and j is its *characteristic vertex*.
ii) There is a unique pair of adjacent vertices j, k of T such that $x_j x_k < 0$. When this is the case, T is called a *type 2 tree*, and the vertices j and k are its *characteristic vertices*.
In either of cases i) and ii), the set consisting of the characteristic vertices of T is known as the *characteristic set*. If it happens that $a(T)$ is a multiple eigenvalue of L, then on the face of it, it would seem that both the type of tree and the characteristic set could depend on the particular choice of the eigenvector x. However, as is shown in [5], in fact every $a(T)$–eigenvector yields the same type of tree, and the same characteristic set.

Suppose that T is a tree, and that v is a vertex of T. A *branch* at v is one of the connected components of the forest $T \setminus v$. Recall that a vertex v of a tree T on n vertices is a *centroid* if it has the property that each branch at v contains at most $\lfloor \frac{n}{2} \rfloor$ vertices. It is well–known that for any tree on $n \geq 2$ vertices, either there is a unique centroid, or there are exactly two centroids, and they are adjacent. Similarly, a vertex v of a tree on $n \geq 2$ vertices is a *centre* if $\max_u d(v, u) = \min_w \max_u d(w, u)$ (here $d(a, b)$ is the distance between vertices a and b). Again, it is well–known that for any tree on $n \geq 2$ vertices, either there is a unique centre, or there are exactly two centres, and they are adjacent. Evidently v is a centre of T if and only if it is a centre of one (indeed, every) longest path in T.

In [6], Merris considers the location of the characteristic set of a tree in relation to both the centroid and the centre. In particular, he gives two intriguing examples, both of which are instances of the family of trees known as brooms, which we now describe. Given $n \geq 2$ and k with $1 \leq k \leq n - 1$, the broom $T_{k,n}$ is formed from the path on $n - k$ vertices by appending k pendent vertices to one end point of that path. Figure 1 illustrates, and note that henceforth we will take the vertices of $T_{k,n}$ to be labelled as in that figure. With this notation in place, Merris' examples show that for $T_{5,11}$, the characteristic set and the centroid are disjoint, and for $T_{7,13}$, the characteristic set and the centre are disjoint. Motivated by Merris' intriguing examples, we investigate the following two quantities for trees in this paper:
i) the maximum possible distance between the characteristic set and the centroid (taken over all trees on n vertices);

ii) the maximum possible distance between the characteristic set and the centre (taken over all trees on n vertices).
For each quantity we show that the maximum is attained for a broom. We also describe the asymptotics for both quantities as $n \to \infty$.

We now recall a useful definition developed in [5]. Fix a vertex j of a tree T; for each branch B at j, the principal submatrix (say L_B) of L corresponding to the vertices of B is an irreducible M–matrix, consequently L_B^{-1} is a positive matrix. (We refer the reader to [1] for definitions and basic facts on M–matrices.) We say that the Perron value of L_B^{-1} is the *Perron value of the branch* B. We note in passing that the Perron value of the branch B is the reciprocal of the smallest eigenvalue of L_B. A branch B at j is said to be a *Perron branch at* j if its Perron value is maximum among the Perron values of all branches at j. The following result summarises some helpful facts about Perron branches. The proofs can be found in [5].

Lemma 1.1. *Let T be a tree on vertices $1, \ldots, n$.*
a) Suppose that at some vertex j of T there are two or more Perron branches. Then T is a type 1 tree and j is its characteristic vertex.
b) Suppose that there is a unique Perron branch at every vertex of T. Then there is a unique pair of adjacent vertices j and k such that the unique Perron branch at j is the branch containing k, and the unique Perron branch at k is the branch containing j. Further, T is a type 2 tree, with j and k as its characteristic vertices.
c) Suppose that T is a tree and l is not a characteristic vertex of T. Then there is a unique Perron branch at l, and it is the one containing the characteristic vertex or vertices of T.

Let T be a tree. For any vertex u of T, let $d_c(u)$ be the distance between u and the nearest characteristic vertex of T. Let $\delta_{\text{centroid}}(T) = \max\{d_c(u) | u \text{ is a centroid of} T\}$, and let $\delta_{\text{centre}}(T) = \max\{d_c(u) | u \text{ is a centre of} T\}$. Finally, we let

$$\delta_{\text{centroid}}(n) = \max\{\delta_{\text{centroid}}(T) | T \text{ is a tree on } n \text{ vertices}\}$$

and

$$\delta_{\text{centre}}(n) = \max\{\delta_{\text{centre}}(T) | T \text{ is a tree on } n \text{ vertices}\}.$$

The following two examples show that $\delta_{\text{centroid}}(n) \geq 1$ for $n \geq 11$ and that $\delta_{\text{centre}}(n) \geq 1$ for $n \geq 14$. In both examples, we make use of the fact (shown in [5]) that for the bottleneck matrix of a branch that consists of a path on k vertices, the corresponding Perron value is given by $\frac{1}{2(1-\cos(\frac{\pi}{2k+1})}$.

Example 1.1. Consider the tree $T_{\lceil \frac{n-1}{2} \rceil, n}$, and observe that vertex $\lceil \frac{n-1}{2} \rceil + 1$ is the unique centroid. Consider vertex $\lceil \frac{n-1}{2} \rceil + 2$ and note that there are two branches at vertex $\lceil \frac{n-1}{2} \rceil + 2$: a path on $\lfloor \frac{n-3}{2} \rfloor$ vertices having Perron value $r_1 = \frac{1}{2\left(1-\cos\left(\frac{\pi}{2\lfloor \frac{n-3}{2} \rfloor + 1}\right)\right)}$, and a star with $\lceil \frac{n-1}{2} \rceil$ pendent vertices. It is easily seen that this latter branch has Perron value r_2 bounded above by $\lceil \frac{n+3}{2} \rceil$.

Since $\cos(\theta) > 1 - \frac{\theta^2}{2}$ for any $\theta > 0$, we find that

$$r_1 > \left(\frac{2\lfloor \frac{n-3}{2} \rfloor + 1}{\pi} \right)^2 .$$

It is readily determined that for any $n \geq 11$, we have

$$r_1 > \left(\frac{2\lfloor \frac{n-3}{2} \rfloor + 1}{\pi} \right)^2 > \left\lceil \frac{n+3}{2} \right\rceil \geq r_2.$$

Consequently when $n \geq 11$, the unique Perron branch at u is the path on $\lfloor \frac{n-3}{2} \rfloor$ vertices. We conclude that the centroid, vertex $\lceil \frac{n-1}{2} \rceil + 1$, is not a characteristic vertex in that case.

Example 1.2. Consider the tree $T_{n-6,n}$, which has a unique centre $n-3$, i.e., the middle vertex on the paths of length 6 (there are $n-6$ such paths). We claim that $n-3$ is not a characteristic vertex of T when $n \geq 14$.

To see the claim, consider the vertex $n-4$. Observe that at $n-4$ there are two branches: a path of length 3 and a star on $n-5$ vertices. The former branch has a bottleneck matrix with Perron value $\frac{1}{2\left(1-\cos\left(\frac{\pi}{9}\right)\right)} \approx 8.2909\ldots$. The latter branch has the bottleneck matrix given by

$$\left[\begin{array}{c|c} I + J_{n-6} & \mathbf{1} \\ \hline \mathbf{1}^T & 1 \end{array} \right],$$

where J_k denotes the $k \times k$ all ones matrix and $\mathbf{1}$ is an all ones vector. Evidently the Perron value of this branch is bounded below by $n-5$. It now follows that if $n \geq 14$, then the unique Perron branch at $n-4$ is the one containing the vertex of maximum degree. Consequently $n-3$ cannot be a characteristic vertex.

The following useful result will assist us in developing our results. In that result and elsewhere, we use $u \sim v$ to indicate that vertices u and v are adjacent.

Lemma 1.2. *Let T be a tree and suppose that u is a vertex of T that is not a characteristic vertex. Let v be the characteristic vertex of T that is closest to u, say with $d_c(u) = d$, and denote the path from u to v by $u \equiv u_0 \sim u_1 \sim \ldots \sim u_{d-1} \sim u_d \equiv v$. Let $B_j, j = 1, \ldots, l$ be a collection of branches at u that do not contain any characteristic vertices, and denote the direct sum of the corresponding bottleneck matrices by M. Form $\hat{T}$ from T by replacing the branches $B_1, \ldots, B_l$ by another collection of branches $\hat{B}_1, \ldots, \hat{B}_p$, and denote the direct sum of the corresponding bottleneck matrices by $\hat{M}$. If $\hat{M}$ is entrywise dominated by a principal submatrix of M, then $d_c(u) \leq \hat{d}_c(u)$, where $\hat{d}_c(u)$ denotes the distance in $\hat{T}$ from u to the closest vertex in the characteristic set.*

Proof. Consider the branches of T at u_{d-1}, and observe that by Lemma 1.1, the unique Perron branch at u_{d-1} is the one containing u_d (equivalently, v). From the construction of $\hat{T}$, we find that the branch (in $\hat{T}$) at u_{d-1} containing u_0 cannot be a Perron branch at u_{d-1}. It now follows that in $\hat{T}$, the unique Perron branch at u_{d-1} is the branch containing u_d. Since all characteristic vertices of $\hat{T}$ lie in the branch at u_{d-1} containing u_d, we deduce that $\hat{d}_c(u) \geq d = d_c(u)$. □

The following result is a consequence of Theorem 1 in [4]. Here we employ the following notation: for square nonnegative matrices A and B (not necessarily of the same order) we write $A << B$ if there is a permutation matrix Q such that QAQ^T is entrywise dominated by a principal submatrix of B, with strict inequality in at least one position if A and B have the same order.

Proposition 1.1. *Let T be a tree, v a vertex of T, and B a branch at v that does not contain all of the characteristic vertices of T. Form a new tree $\hat{T}$ by replacing the branch B at v by another branch $\hat{B}$ at v. Let M be the bottleneck matrix for B in T and let $\hat{M}$ be the bottleneck matrix for $\hat{B}$ in $\hat{T}$. Suppose that $M << \hat{M}$. Then the characteristic vertices of $\hat{T}$ are either on the path joining the characteristic vertices of T to v, or they are in the new branch $\hat{B}$.*

Suppose that T is a tree and that B is a branch at vertex v, say with w as the vertex in B adjacent to v. The *depth* of B is equal to $\max_{u \in B} d(w, u)$. Suppose that B is a branch on m vertices with depth k that is not a broom, and consider a branch $\tilde{B}$, also on m vertices with depth k that is a broom. It is straightforward to show (say by induction on $m - k$) that $M << \tilde{M}$, where M and $\tilde{M}$ are the bottleneck matrices for B and $\tilde{B}$, respectively.

2 Maximum distance between the centroid and the characteristic set

The following result identifies a family of trees that attain the maximum distance between the centroid and the characteristic set.

Theorem 2.1. *Suppose that $n \geq 12$. Then $\delta_{\text{centroid}}(n) = \delta_{\text{centroid}}(T_{\lfloor \frac{n}{2} \rfloor, n})$.*

Proof. Let T be a tree on n vertices such that $\delta_{\text{centroid}}(n) = \delta_{\text{centroid}}(T)$. Let u and v be the centroid and characteristic vertex, respectively, of T such that $d(u, v) = \delta_{\text{centroid}}(T)$. From Example 1.1, $u \neq v$ so that $d(u, v) \geq 1$. Observe that each branch of T at u contains at most $\frac{n}{2}$ vertices, and that the unique Perron branch at u is the one containing v. Form T_1 from T by replacing all of the non-Perron branches at u by collections of pendent vertices (comprising the same total number of vertices), each of which is adjacent to u. By Lemma 1.2, $d_c(u) \geq \delta_{\text{centroid}}(n)$, and u is still a centroid of T_1, so we see that in fact $d_c(u) = \delta_{\text{centroid}}(n)$. Suppose for concreteness that there are k pendent vertices adjacent to u in T_1. In T_1, label the branches at v

as $B_1, \dots, B_l$, where we take B_1 to be the branch containing u. Letting $\rho(\bullet)$ denote the Perron value of a branch, we see that $\rho(B_1) \le \max_{j=2,\dots,l} \rho(B_j)$.

Next form T_2 from T_1 by replacing the Perron branch at u by a path on $n-k-1$ vertices, and let v' be the vertex on that path whose distance to u is $d(u,v)$. Denote the branch at v' containing u by B_1' and denote the other branch at v' by B_2'. Observe that $\rho(B_1') \le \rho(B_1) \le \max_{j=2,\dots,l} \rho(B_j) \le \rho(B_2')$. If $\rho(B_1') = \rho(B_2')$, then T_2 is a type 1 tree with v' as its unique characteristic vertex; if $\rho(B_1') < \rho(B_2')$, then necessarily v' is a characteristic vertex, otherwise every characteristic vertex of T_2 is in B_2', which in turn yields $d(u,v) < \delta_{\text{centroid}}(T_2)$, a contradiction. In either case we see that v' is a characteristic vertex, and that $\delta_{\text{centroid}}(n) = \delta_{\text{centroid}}(T_2) = \delta_{\text{centroid}}(T_{k,n})$.

Since u is a centroid of $T_{k,n}$, we find that $n-k-1 \le \frac{n}{2}$, so that $k \ge \frac{n-2}{2}$. If $k = \frac{n-2}{2}$, we find that the non-pendent neighbour of u is also a centroid of $T_{k,n}$, contrary to our original assumption that $d(u,v) = \delta_{\text{centroid}}(T)$. Hence $k \ge \frac{n-1}{2}$. Suppose that it were the case that $k \ge \frac{n+1}{2}$. Then we could remove one of the pendent vertices adjacent to u and appended it at the end of the Perron component at u. The resulting tree $T_{k-1,n}$ still would have u as a centroid, and applying Lemma 1.2 (for deleting a pendent vertex adjacent to u), followed by Proposition 1.1 (for appending a pendent vertex at the end of the Perron component at u) as above it follows that $d_c(u) = \delta_{\text{centroid}}(n)$, i.e. $\delta_{\text{centroid}}(T_{k-1,n}) = \delta_{\text{centroid}}(n)$. Repeating that process if necessary, it follows that for a tree $T_{l,n}$ with $\frac{n}{2} \ge l \ge \frac{n-1}{2}$, we have $\delta_{\text{centroid}}(T_{l,n}) = \delta_{\text{centroid}}(n)$. Considering the cases that n is odd and even respectively, we find that $\delta_{\text{centroid}}(T_{\lfloor \frac{n}{2} \rfloor,n}) = \delta_{\text{centroid}}(n)$, as desired. $\square$

Next, we want to consider the asymptotics of $\delta_{\text{centroid}}(n)$. The following technical result will assist with our later analysis. Below we use I_k to denote the $k \times k$ identity matrix.

Lemma 2.1. *Consider the irreducible nonsingular M-matrix M of order $k+l$ given by:*

$$M = \left[\begin{array}{c|cccccc} I_k & -\mathbf{1} & 0 & & \dots & & 0 \\ \hline -\mathbf{1}^T & k+1 & -1 & & & & \\ 0^T & -1 & 2 & -1 & & & \\ 0^T & & -1 & 2 & -1 & & \\ \vdots & & & \ddots & \ddots & \ddots & \\ 0^T & & & & -1 & 2 & -1 \\ 0^T & & & & & -1 & 2 \end{array}\right].$$

Let λ be the smallest eigenvalue of M. Then $\lambda = 2(1-\cos(\theta_*))$, where θ_* is the unique solution in the interval $(0, \frac{\pi}{2l+3}]$ of the equation

$$f_l(\theta) \equiv \tan\left(\frac{\pi}{2} - (l+1)\theta\right) + \tan\left(\frac{\theta}{2}\right) - \frac{2k(1-\cos(\theta))}{\sin(\theta)(2(k-1)(1-\cos(\theta))+1)} = 0. \quad (1)$$

Proof. We will proceed by producing an all–positive eigenvector of M associated with $2(1-\cos(\theta_*))$, then appeal to the fact that for an irreducible symmetric M–matrix, the only eigenvalue for which there is a positive eigenvector is the smallest eigenvalue.

We begin by showing that (1) has a solution in the interval $(0, \frac{\pi}{2l+3}]$. To that end, consider $f_l(\theta)$ in (1) as a function of θ. First, we claim that $f_l(\frac{\pi}{2l+3}) < 0$. To see the claim, we first note that it is straightforward to verify that the inequality $f_l(\frac{\pi}{2l+3}) < 0$ is equivalent to

$$\tan(\tau) - \frac{k(1-\cos(2\tau))}{\sin(2\tau)(2(k-1)(1-\cos(2\tau))+1)} < 0, \tag{2}$$

where $\tau = \frac{\pi}{2(2l+3)}$. Using the double angle formulas for $\cos(2\tau)$ and $\sin(2\tau)$, (2) simplifies to $4(k-1)\sin^2(\tau)+1 < k$, i.e. $|\sin(\tau)| < \frac{1}{2}$. Since $0 < \tau \le \frac{\pi}{10}$ we have $\sin(\tau) < \frac{1}{2}$, and (2) now follows, completing the proof of the claim. Evidently f is continuous for $\theta \in (0, \frac{\pi}{2l+3}]$. Since $f_l(\frac{\pi}{2l+3}) < 0$ while $f_l(\theta) \to \infty$ as $\theta \to 0^+$, it now follows from the intermediate value theorem that (1) has a solution in the interval $(0, \frac{\pi}{2l+3}]$.

Let θ_* be a solution to (1) in $(0, \frac{\pi}{2l+3}]$. Let $\lambda = 2(1-\cos(\theta_*))$, and for each $j = 1, \dots, l$, let $v_j = \sin((l+1-j)\theta_*)$. Set $v_0 = \frac{v_1}{1-\lambda}$, and consider the vector

$$v = \begin{bmatrix} v_0 \mathbf{1} \\ \hline v_1 \\ v_2 \\ \vdots \\ v_l \end{bmatrix}.$$

Evidently v is a positive vector, and an uninteresting exercise reveals that $Mv = \lambda v$. Since v is positive and M is an M–matrix, we find that λ is in fact the smallest eigenvalue of M. Finally, we note that if there were another solution $\hat{\theta} \ne \theta_*$ to (2) (in the interval $(0, \frac{\pi}{2l+3}]$), then, analogous to the construction of v, we would be able to construct a positive eigenvector $\hat{v}$ of M corresponding to an eigenvalue $\hat{\lambda} \ne \lambda$, a contradiction. We thus deduce that θ_* is the unique solution to (2) in the $(0, \frac{\pi}{2l+3}]$. □

The final result of this section gives the asymptotics for $\delta_{\text{centroid}}(n)$.

Theorem 2.2. *Let z be the unique root of the equation $\tan(z) + z = 0$ that lies in the interval $(\frac{\pi}{2}, \pi]$. We have $\lim_{n\to\infty} \frac{\delta_{\text{centroid}}(n)}{n} = \frac{1}{2} - \frac{\pi}{4z}$.*

Proof. From Theorem 2.1, the maximum distance between the centroid and the characteristic set for a tree on n vertices occurs for $T_{k,n}$ with $k = \lfloor \frac{n}{2} \rfloor$. Henceforth we take $k = \lfloor \frac{n}{2} \rfloor$, and as usual we label the vertices of $T_{k,n}$ as in Figure 1. Suppose that $k + l$ is the characteristic vertex of $T_{k,n}$ that is closest to a centroid. Observe that $l \le n-k-l$, otherwise the unique Perron branch at vertex $k+l$ contains vertex $k+l-1$, not vertex $k+l+1$, a contradiction. In particular we have $l \le \frac{n-k}{2} \le \frac{n+1}{4}$.

Let θ_{l-1} be the unique root of f_{l-1} in the interval $(0, \frac{\pi}{2l+1}]$ and let θ_l be the unique root of f_l in the interval $(0, \frac{\pi}{2l+3}]$. Observe that if $T_{k,n}$ is a type 1 tree with $k+l$ as the characteristic vertex, then necessarily $\theta_{l-1} = \frac{\pi}{2(n-k-l)+1}$. On the other hand, if $T_{k,n}$ is a type 2 tree with $(k+l) \sim (k+l+1)$ as the end vertices of the characteristic edge, then $\theta_{l-1} > \frac{\pi}{2(n-k-l)+1}$ and $\theta_l < \frac{\pi}{2(n-k-l)-1}$. Observe that in either case, we have $\theta_{l-1} \ge \frac{\pi}{2(n-k-l)+1}$ and $\theta_l < \frac{\pi}{2(n-k-l)-1}$. Since f_{l-1} and f_l have unique roots in the intervals $(0, \frac{\pi}{2l+1}]$ and $(0, \frac{\pi}{2l+3}]$ respectively, it follows that $\theta_{l-1} \ge \frac{\pi}{2(n-k-l)+1}$ if and only if

$$f_{l-1}\left(\frac{\pi}{2(n-k-l)+1}\right) \ge 0. \tag{3}$$

Similarly, $\theta_l < \frac{\pi}{2(n-k-l)-1}$ if and only if

$$f_l\left(\frac{\pi}{2(n-k-l)-1}\right) < 0. \tag{4}$$

We thus deduce that if $k+l$ is the characteristic vertex of $T_{k,n}$ that is closest to a centroid, then

$$\begin{aligned}
&\tan\left(\frac{\pi}{2} - \frac{\pi l}{2(n-k-l)+1}\right) + \tan\left(\frac{\pi}{2(2(n-k-l)+1)}\right) \\
&- \frac{2k\left(1-\cos\left(\frac{\pi}{2(n-k-l)+1}\right)\right)}{\sin\left(\frac{\pi}{2(n-k-l)+1}\right)\left(2(k-1)\left(1-\cos\left(\frac{\pi}{2(n-k-l)+1}\right)\right)+1\right)} \ge 0 \\
&> \tan\left(\frac{\pi}{2} - \frac{\pi(l+1)}{2(n-k-l)-1}\right) + \tan\left(\frac{\pi}{2(2(n-k-l)-1)}\right) \\
&- \frac{2k\left(1-\cos\left(\frac{\pi}{2(n-k-l)-1}\right)\right)}{\sin\left(\frac{\pi}{2(n-k-l)-1}\right)\left(2(k-1)\left(1-\cos\left(\frac{\pi}{2(n-k-l)-1}\right)\right)+1\right)}.
\end{aligned} \tag{5}$$

For each n, define $r_n = \frac{l}{n}$, and note that since $l \le \frac{n+1}{4}$, we have $r_n \le \frac{1}{4} + \frac{1}{4n}$.

Observe that (5) can then be rewritten as

$$\begin{aligned}
&\tan\left(\frac{\pi}{2} - \frac{\pi r_n}{2(1-\frac{k}{n}-r_n)+\frac{1}{n}}\right) + \tan\left(\frac{\pi}{2n(2(1-\frac{k}{n}-r_n)+\frac{1}{n})}\right) \\
&-\frac{2k\left(1-\cos\left(\frac{\pi}{n(2(1-\frac{k}{n}-r_n)+\frac{1}{n})}\right)\right)}{\sin\left(\frac{\pi}{n(2(1-\frac{k}{n}-r_n)+\frac{1}{n})}\right)\left(2(k-1)\left(1-\cos\left(\frac{\pi}{n(2(1-\frac{k}{n}-r_n)+\frac{1}{n})}\right)\right)+1\right)} \geq 0 \\
&> \tan\left(\frac{\pi}{2} - \frac{\pi r_n + \frac{1}{n}}{2(1-\frac{k}{n}-r_n)-\frac{1}{n}}\right) + \tan\left(\frac{\pi}{2n(2(1-\frac{k}{n}-r_n)-\frac{1}{n})}\right) \\
&-\frac{2k\left(1-\cos\left(\frac{\pi}{n(2(1-\frac{k}{n}-r_n)-\frac{1}{n})}\right)\right)}{\sin\left(\frac{\pi}{n(2(1-\frac{k}{n}-r_n)-\frac{1}{n})}\right)\left(2(k-1)\left(1-\cos\left(\frac{\pi}{n(2(1-\frac{k}{n}-r_n)-\frac{1}{n})}\right)\right)+1\right)}. \qquad (6)
\end{aligned}$$

Observe that r_n is a bounded sequence, and so has at least one convergent subsequence. Let n_j be an increasing subsequence of natural numbers such that r_{n_j} converges, say to r, as $j \to \infty$. Necessarily $0 \leq r \leq \frac{1}{4}$. In fact it must be the case that $r > 0$, otherwise there is a further subsequence $r_{n_{j_p}}$ such that as $p \to \infty$, either

$$\tan\left(\frac{\pi}{2} - \frac{\pi r_{n_{j_p}} + \frac{1}{n_{j_p}}}{2(1-\frac{k}{n_{j_p}}-r_{n_{j_p}})-\frac{1}{n_{j_p}}}\right) \to \infty$$

or

$$\tan\left(\frac{\pi}{2} - \frac{\pi r_{n_{j_p}}}{2(1-\frac{k}{n_{j_p}}-r_{n_{j_p}})+\frac{1}{n_{j_p}}}\right) \to -\infty,$$

both of which violate (6). Hence we have $r > 0$. Consider (6) where we take $n = n_j, k = \lfloor \frac{n_j}{2} \rfloor$ and $r_n = r_{n_j}$. Taking a limit as $j \to \infty$, we find from (6) that

$$-\tan\left(\frac{\pi}{2} + \frac{\pi r}{2(\frac{1}{2}-r)}\right) - \frac{\pi}{4(\frac{1}{2}-r)} \geq 0 \geq -\tan\left(\frac{\pi}{2} + \frac{\pi r}{2(\frac{1}{2}-r)}\right) - \frac{\pi}{4(\frac{1}{2}-r)}. \quad (7)$$

Consequently, $\tan\left(\frac{\pi}{2} + \frac{\pi r}{2(\frac{1}{2}-r)}\right) + \frac{\pi}{4(\frac{1}{2}-r)} = 0$. Since $0 < r \leq \frac{1}{4}$, we have $\frac{\pi}{2} < \frac{\pi}{4(\frac{1}{2}-r)} \leq \pi$. In particular, letting z be the unique root of the equation $\tan(z) + z = 0$ that lies in the interval $(\frac{\pi}{2}, \pi]$ we have $r = \frac{1}{2} - \frac{\pi}{4z}$. Inspecting the argument above, we see that any convergent subsequence of r_n converges to $\frac{1}{2} - \frac{\pi}{4z}$, from which we deduce that in fact the entire sequence r_n is convergent, with limit given by $\frac{1}{2} - \frac{\pi}{4z}$. □

Remark 2.1. From computations we find that $z \approx 2.0287578381104339\ldots$ so that $\frac{1}{2} - \frac{\pi}{4z} \approx 0.112867465675962\ldots$.

3 Maximum distance between the centre and the characteristic set

In this section we consider the distance between the centre and the characteristic set for a tree. Some of the approaches of section 2 will carry over to the present section, though there are some subtle differences between the two problems.

Theorem 3.1. *Suppose that $n \geq 12$. Then for some $2 \leq k \leq n-2, \delta_{\text{centre}}(n) = \delta_{\text{centre}}(T_{k,n})$.*

Proof. Let T be a tree on n vertices such that $\delta_{\text{centre}}(n) = \delta_{\text{centre}}(T)$. Let u and v be the centre and characteristic vertex, respectively, of T such that $d(u,v) = \delta_{\text{centre}}(T)$. By Example 1.2, $u \neq v$ so that $d(u,v) \geq 1$. Denote by P an induced path in T of maximum length, recall that u is a centre of P, and denote the (end point) pendent vertices of P by w_1 and w_2.

We claim that without loss of generality we may assume that u and v are on a path P of maximum length. To see the claim, we suppose that v is not on P, and let v_0 denote the vertex on P that is closest to v. Without loss of generality we assume that $d(u,w_1) \leq d(v_0,w_1)$. Observe that at v, there is at least one Perron branch $\tilde{B}$ that does not contain v_0, otherwise v is not the closest characteristic vertex to u. Select a vertex v_1 on P such that $d(v_1,w_2) = d(v_0,w_2) - d(v_0,v)$, and note that $d(v_1,w_2) \geq 1$, since we are assuming that v is not on a path of maximum length that includes u.

Form $\hat{T}$ from T by deleting the branch at v_1 that contains w_2, and appending that same branch at v. Note also that u is a centre in $\hat{T}$ that is closest to v, and that u and v are on a path of maximum length in $\hat{T}$. Further, in $\hat{T}$, neither the branch at v containing v_0, nor the branch at v containing w_2 is a Perron branch; also the branch $\tilde{B}$ at v is still a Perron branch at v in $\hat{T}$. From this we deduce that v must be a characteristic vertex of $\hat{T}$, otherwise all characteristic vertices of T are in $\tilde{B}$, so that $\delta_{\text{centre}}(\hat{T}) > \delta_{\text{centre}}(T) = \delta_{\text{centre}}(n)$, a contradiction. This establishes the claim.

Henceforth we suppose that in T, the vertices u and v are on a path P of maximum length. Let B_u be the branch at v containing u, and note that as above it is not a Perron branch at v. Construct T_1 from T as follows: delete all vertices in B_u that are not on P, and append those vertices as pendent vertices adjacent to v. By Lemma 1.2 and the fact that pendent vertices cannot be Perron branches in a tree on more than 3 vertices, we deduce that v is a characteristic vertex of T_1 that is closest to u. In T_1 denote the branches at v not containing u by $B_1, \ldots, B_k$. Next we construct T_2 from T_1 by successively replacing, for each $j = 1, \ldots, k$, each B_j by the corresponding broom on $|B_j|$ vertices whose depth coincides with that of B_j. By Proposition 1.1 (repeatedly applied) and the fact that $d(u,v) = \delta_{\text{centre}}(n)$, we deduce that $\delta_{\text{centre}}(T_2) = \delta_{\text{centre}}(n)$, with u and v as the centre and characteristic vertex that are closest together. Note that if $k = 1$, then T_2 is a broom, and we are done.

Suppose now that $k \geq 2$. Let $\overline{B}_1$ be a branch at v not containing u and having maximum depth, and let $\overline{B}_l$ be a Perron branch at v. Consider a branch $\overline{B}_j$ at v that is not a unique Perron branch, and such that $j \geq 2$. Note that if we modify T_2 by deleting $\overline{B}_j$ and appending $|\overline{B}_j|$ pendent vertices adjacent to the next–to–pendent vertex in $\overline{B}_l$, then the resulting tree still has u as a centre, and v as the closest characteristic vertex to that centre (otherwise we exceed $\delta_{\text{centre}}(n)$). Perform this operation repeatedly for each such $\overline{B}_j$, and denote the resulting tree by T_3. Evidently $\delta_{\text{centre}}(T_3) = \delta_{\text{centre}}(n)$, with u and v as the centre and characteristic vertex that are closest together. In particular if $l = 1$, (i.e. $\overline{B}_1$ was a Perron branch in T_2) then T_3 is a broom, and we are done.

The last case to consider is that in T_3 there are just three branches at v: the branch containing u, a non–Perron branch $\overline{B_1}$, and a Perron branch $\tilde{B}$ whose depth is less than that of $\overline{B_1}$. Construct T_4 as follows. Delete $\overline{B_1}$, and successively append its vertices into $\tilde{B}$ so that the depth of the resulting branch coincides with the depth of $\overline{B_1}$. Arguing as above we find that in T_4, u and v as the centre and characteristic vertex that are closest together. Note that in T_4, v has degree 2. We now construct T_5 from T_4 by replacing the branch B' at v that does not contain u by the broom on $|B'|$ vertices having the same depth as B'. Evidently T_5 is a broom, and as above it follows that $\delta_{\text{centre}}(T_5) = \delta_{\text{centre}}(n)$. $\square$

The following sequence of technical results will assist us in determining the asymptotic behaviour of $\frac{\delta_{\text{centre}}(n)}{n}$.

Lemma 3.1. *Fix $c \in (0,1)$ and consider the function $\phi(r) = \tan\left(\frac{(1-c)\pi}{2(1-r)}\right) + \frac{c\pi}{2(1-r)}$ for $r \in \left(c, \frac{c+1}{2}\right)$.*
a) For each $c \in (0,1) \exists! r \in \left(c, \frac{c+1}{2}\right)$ such that $\phi(r) = 0$.
b) Considering r as a function of c in a), r is differentiable with respect to c for $c \in (0,1)$.
c) As $c \to 0^+, r \to \frac{1}{2}$.
d) As $c \to 1^-, r \to 1$.

Proof. a) Observe that as $r \to c^+$, $\frac{(1-c)\pi}{2(1-r)} \to \frac{\pi}{2}^+$, so that $\phi(r) \to -\infty$. As $r \to \left(\frac{c+1}{2}\right)^+$, $\frac{(1-c)\pi}{2(1-r)} \to \pi$, so $\phi(r) \to \frac{c\pi}{1-c} > 0$. Hence by the Intermediate Value Theorem, there is at least one $r \in \left(c, \frac{c+1}{2}\right)$ such that $\phi(r) = 0$. Since $\frac{d\phi}{dr} = \frac{(1-c)\pi}{2(1-r)^2} \sec^2\left(\frac{(1-c)\pi}{2(1-r)}\right) + \frac{c\pi}{2(1-r)^2} > 0$, we deduce that the solution to $\phi(r) = 0$ in the interval $\left(c, \frac{c+1}{2}\right)$ is unique.
b) Since $\frac{d\phi}{dr} = \frac{(1-c)\pi}{2(1-r)^2} \sec^2\left(\frac{(1-c)\pi}{2(1-r)}\right) + \frac{c\pi}{2(1-r)^2} > 0$, we find from implicit differentiation that r is differentiable as a function of c and that

$$\frac{dr}{dc} = -\frac{\frac{d\phi}{dc}}{\frac{d\phi}{dr}} = -\left(\frac{-\frac{\pi}{2(1-r)}\left(1 - \sec^2\left(\frac{(1-c)\pi}{2(1-r)}\right)\right)}{\frac{(1-c)\pi}{2(1-r)^2}\sec^2\left(\frac{(1-c)\pi}{2(1-r)}\right) + \frac{c\pi}{2(1-r)^2}}\right).$$

c) Let c_j be a sequence of positive numbers that converges to 0, and for each $j \in \mathbb{N}$, let $r_j \in \left(c_j, \frac{c_j+1}{2}\right)$ be the corresponding solution to $\phi(r) = 0$. Then for each $j \in \mathbb{N}, \tan\left(\frac{(1-c_j)\pi}{2(1-r_j)}\right) = -\frac{c_j\pi}{2(1-r_j)} \equiv z_j$. Note that $z_j \to 0^-$. Further, since $\frac{\pi}{2} < \frac{(1-c_j)\pi}{2(1-r_j)} < \pi$, we find that $\frac{(1-c_j)\pi}{2(1-r_j)} = \pi + \arctan(z_j)$. Consequently,

$$r_j = 1 - \frac{(1-c_j)\pi}{2(\pi + \arctan(z_j))},$$

and since $c_j, z_j \to 0$, we find that $r_j \to \frac{1}{2}$. It now follows that as $c \to 0^+, r \to \frac{1}{2}$.
d) Since $c < r < \frac{c+1}{2}$, we have $0 < \frac{c+1}{2} - r < \frac{1-c}{2}$. Thus, as $c \to 1^-, r \to 1$. □

Lemma 3.2. *For each $c \in (0,1)$ let $g(c) = \frac{c+1}{2} - r$, where $r \in \left(c, \frac{c+1}{2}\right)$ is the solution to $\phi(r) = 0$ guaranteed by Lemma 3.1. Extend g to $[0,1]$ by setting $g(0) = 0$ and $g(1) = 0$. Then g is continuous on $[0,1]$ and differentiable on $(0,1)$. Suppose that $c_0 \in (0,1)$ is such that $\left.\frac{dg}{dc}\right|_{c_0} = 0$. Then*

$$g(c_0) = \frac{\pi c_0}{4}\left(\pi c_0 - \sqrt{\pi^2 c_0^2 - 4(1-c_0)}\right) - \frac{1-c_0}{2}.$$

In particular, it must be the case that $c_0 \geq \frac{2\sqrt{\pi^2+1}}{\pi^2} - 1$.

Proof. From Lemma 3.1 b) it follows that g is differentiable on $(0,1)$. By Lemma 3.1 c) and d) , we find that as $c \to 0^+, g(c) \to 0$, and as $c \to 1^-, g(c) \to 0$. Consequently g is continuous on $[0,1]$.

Next, suppose that $c_0 \in (0,1)$ and that $\left.\frac{dg}{dc}\right|_{c_0} = 0$. For ease of notation in the remainder of the argument, we introduce a dummy function w via $w(c) = \frac{\pi}{2(1-r)}$ (here and elsewhere we express the explicit dependence of r on c). Evidently $\left.\frac{dg}{dc}\right|_{c_0} = 0$ if and only if $\left.\frac{dr}{dc}\right|_{c_0} = \frac{1}{2}$. Since $\frac{dr}{dc} = \frac{dr}{dw}\frac{dw}{dc}$, and $\frac{dr}{dw} = \frac{\pi}{2w^2}$, we find that $\left.\frac{dr}{dc}\right|_{c_0} = \frac{1}{2}$ if and only if $dw\frac{dw}{dc} = \frac{w^2}{\pi}$. Using implicit differentiation on the equation $\phi(w) = 0$, we find that

$$\frac{dw}{dc} = -\frac{w\sec^2((1-c)w) + w}{(1-c)\sec^2((1-c)w) + c}.$$

From the facts that $\sec^2((1-c)w) = \tan^2((1-c)w) + 1$, and $\tan((1-c)w) = -cw$ (since $\phi(w) = 0$), it now follows that $\frac{dw}{dc}$ can be rewritten as

$$\frac{dw}{dc} = \frac{c^2w^3}{1 + c^2(1-c)w^2}.$$

We thus deduce that if $\left.\frac{dg}{dc}\right|_{c_0} = 0$, then

$$\frac{w(c_0)^2}{\pi} = \frac{c_0^2 w(c_0)^3}{1 + c_0^2(1-c_0)w(c_0)^2},$$

which in turn yields

$$c_0^2(1-c_0)w(c_0)^2 - \pi c_0^2 w(c_0) + 1 = 0. \tag{8}$$

Considering the left side of (8) as a quadratic in w we observe that its vertex is $\frac{\pi}{2(1-c_0)}$, so that necessarily $w(c_0)$ is the larger of the two roots of (8). We thus deduce that

$$w(c_0) = \frac{\pi c_0 + \sqrt{\pi^2 c_0^2 - 4(1-c_0)}}{2c_0(1-c_0)};$$

the expression

$$g(c_0) = \frac{\pi c_0}{4}\left(\pi c_0 - \sqrt{\pi^2 c_0^2 - 4(1-c_0)}\right) - \frac{1-c_0}{2}$$

now follows by substitution and simplification. □

Lemma 3.3. *Let $w(c)$ be defined as in Lemma 3.2. There is a unique $c_0 \in \left(\frac{2\sqrt{\pi^2+1}}{\pi^2} - 1, 1\right)$ such that*

$$w(c_0) = \frac{\pi c_0 + \sqrt{\pi^2 c_0^2 - 4(1-c_0)}}{2c_0(1-c_0)}. \tag{9}$$

Proof. For each $c \in \left(\frac{2\sqrt{\pi^2+1}}{\pi^2} - 1, 1\right)$, we define the function $\omega(c)$ via

$$\omega(c) = \frac{\pi c + \sqrt{\pi^2 c^2 - 4(1-c)}}{2c(1-c)}.$$

We claim that the equation $\phi(\omega(c)) = 0$ has a unique solution on $\left(\frac{2\sqrt{\pi^2+1}}{\pi^2} - 1, 1\right)$. First note that as $c \to (\frac{2\sqrt{\pi^2+1}}{\pi^2} - 1)^+, (1-c)\omega(c) \to \frac{\pi}{2}^+$, so that $\phi(\omega(c)) \to -\infty$. Also, as $c \to 1^-, (1-c)\omega(c) \to \pi^-$, so that $\phi(\omega(c)) \to \infty$. Hence there is at least one $c \in \left(\frac{2\sqrt{\pi^2+1}}{\pi^2} - 1, 1\right)$ such that $\phi(\omega(c)) = 0$.

Next, we show the uniqueness of c_0 in (9) by showing that $\phi(\omega(c))$ is increasing in c. We have

$$\frac{d\phi(\omega(c))}{dc} = \sec^2((1-c)\omega(c))\left(-w + (1-c)\frac{d\omega}{dc}\right) + \left(w + c\frac{d\omega}{dc}\right).$$

Since $c^2(1-c)\omega^2 - \pi c^2\omega + 1 = 0$, we find from implicit differentiation that

$$\frac{d\omega}{dc} = \frac{2\pi\omega - (2-3c)\omega^2}{2c(1-c)\omega - \pi c}.$$

It now follows readily that

$$w + c\frac{d\omega}{dc} = \frac{c\omega(\pi + c\omega)}{2c(1-c)\omega - \pi c} > 0$$

and that

$$-w + (1-c)\frac{d\omega}{dc} = \frac{\omega(2-c)(\pi-(1-c)\omega)}{2c(1-c)\omega - \pi c} > 0.$$

Consequently, $\frac{d\phi(\omega(c))}{dc} > 0$, so that there is a unique $c_0 \in \left(\frac{2\sqrt{\pi^2+1}}{\pi^2} - 1, 1\right)$ satisfying (9). $\square$

Remark 3.1. Based on numerical calculations, it turns out that for c_0 satisfying (9), we have $c_0 \approx 0.48165092839814441\ldots$, and $g(c_0) \approx 0.137326240400131\ldots$.

Remark 3.2. Consider a sequence of trees T_{k_j,n_j} such that $\frac{k_j}{n_j} \to 1$ as $j \to \infty$. Since no pendent vertex of a tree on more than two vertices can be either a centre or a characteristic vertex, it follows that $\delta_{\text{centre}}(T_{k_j,n_j}) \le n_j - k_j - 2$ for each $j \in \mathbb{N}$. We deduce then that $\frac{\delta_{\text{centre}}(T_{k_j,n_j})}{n_j} \to 0$ as $j \to \infty$.

Theorem 3.2. *Consider the sequence* $\frac{\delta_{\text{centre}}(n)}{n}$*, and let* $\frac{\delta_{\text{centre}}(n_j)}{n_j}$ *be a convergent subsequence of it. Then*

$$\lim_{j\to\infty} \frac{\delta_{\text{centre}}(n_j)}{n_j} \le \frac{\pi c_0}{4}\left(\pi c_0 - \sqrt{\pi^2 c_0^2 - 4(1-c_0)}\right) - \frac{1-c_0}{2}, \tag{10}$$

where c_0 is the unique solution to (9).

Proof. By Theorem 3.1, for all sufficiently large $n \in \mathbb{N}$ we have $\delta_{\text{centre}}(n) = \delta(T_{k,n})$ for some k. Consequently, for the convergent subsequence in the statement, we have $\frac{\delta_{\text{centre}}(n_j)}{n_j} = \frac{\delta(T_{k_j,n_j})}{n_j}$ for some corresponding subsequence k_j. For each $j \in \mathbb{N}$, denote the characteristic vertex of T_{k_j,n_j} that is closest to a centre by $k_j + l_j$. Observe that both $\frac{k_j}{n_j}$ and $\frac{k_j+l_j}{n_j}$ are bounded, and so by considering a further subsequence of T_{k_j,n_j} if necessary, we may assume that both $\frac{k_j}{n_j}$ and $\frac{k_j+l_j}{n_j}$ are convergent, say with $\lim_{j\to\infty} \frac{k_j}{n_j} = c$ and $\lim_{j\to\infty} \frac{k_j+l_j}{n_j} = r$. Observe that we then have $\lim_{j\to\infty} \frac{\delta_{\text{centre}}(n_j)}{n_j} = \lim_{j\to\infty} \frac{\delta(T_{k_j,n_j})}{n_j} = \frac{c+1}{2} - r$.

By Remark 3.2, we see that if $c = 1$, then $\lim_{j\to\infty} \frac{\delta_{\text{centre}}(n_j)}{n_j} = \lim_{j\to\infty} \frac{\delta(T_{k_j,n_j})}{n_j} = 0$. Henceforth we assume that $c \in [0,1)$. By applying the technique of the proof of Theorem 2.2, we find that $\tan\left(\frac{(1-c)\pi}{2(1-r)}\right) + c\frac{\pi}{2(1-r)} = 0$. Thus, $\lim_{j\to\infty} \frac{\delta_{\text{centre}}(n_j)}{n_j} = g(c)$ for some $c \in [0,1]$, where $g(c)$ is defined in Lemma 3.2. From Lemmas 3.2 and 3.3, it follows that g attains its maximum on $[0,1]$ at the unique solution c_0 to (9). Consequently, $\lim_{j\to\infty} \frac{\delta_{\text{centre}}(n_j)}{n_j} = g(c) \le g(c_0)$, and the conclusion follows. $\square$

Theorem 3.3. *Let c_0 be the unique solution to (9). For the sequence of trees $T_{\lfloor c_0 n\rfloor,n}$, we have*

$$\lim_{n\to\infty} \frac{\delta_{\text{centre}}(T_{\lfloor c_0 n\rfloor,n})}{n} = \frac{\pi c_0}{4}\left(\pi c_0 - \sqrt{\pi^2 c_0^2 - 4(1-c_0)}\right) - \frac{1-c_0}{2}.$$

Proof. Set $k = \lfloor c_0 n \rfloor$. The centre of $T_{\lfloor c_0 n \rfloor, n}$ is readily seen to consist of vertex $\frac{n-k+2}{2}$ if $n-k$ is even, and to consist of vertices $\frac{n-k+1}{2}, \frac{n-k+3}{2}$ if $n-k$ is odd. Observe that as $n \to \infty$, $\frac{n-k+2}{2n}$, $\frac{n-k+1}{2n}$, and $\frac{n-k+3}{2n}$ all approach c_0. Having determined the asymptotic behaviour of the centre of $T_{\lfloor c_0 n \rfloor, n}$, it remains only to do the same for its characteristic vertices.

From the techniques used in section 2, we find that if $f_{l-1}\left(\frac{\pi}{2(n-k-l)+1}\right) > 0$, then the Perron component at vertex $k+l$ is the path component at that vertex, and if $f_{l-1}\left(\frac{\pi}{2(n-k-l)+1}\right) < 0$, then the Perron component at vertex $k+l$ is the broom component at that vertex. Our goal is to localise the characteristic vertices of $T_{\lfloor c_0 n \rfloor, n}$ by showing that there are indices l_1, l_2 such that $f_{l_1-1}\left(\frac{\pi}{2(n-k-l_1)+1}\right) > 0$, $f_{l_2-1}\left(\frac{\pi}{2(n-k-l_2)+1}\right) < 0$ such that as $n \to \infty$, $\frac{k+l_1}{2n}, \frac{k+l_2}{2n} \to r$, where $r = 1 - \frac{\pi}{2w(c_0)}$. This will show that the characteristic vertices of $T_{\lfloor c_0 n \rfloor, n}$ lie on the path between vertices $k+l_1$ and $k+l_2$, and that if j_n is a sequence of characteristic vertices of $T_{\lfloor c_0 n \rfloor, n}$, then $\frac{j_n}{n} \to r$ as $n \to \infty$.

To that end, we will write $k = nc_0 - \epsilon_c$, where the explicit dependence of k and ϵ_c on n will be suppressed. Observe that $\epsilon_c \in [0,1]$ for all n. Fix an $M > 0$, and consider an $l \in \mathbb{N}$ such that $rn - k - M \le l \le rn - k + M$; note that since $c_0 < r$, such an l exists for all sufficiently large n. Observe that $k + l$ can be written as $k + l = rn + \epsilon_r$ (here we suppress the explicit dependence of ϵ_r on n), where $|\epsilon_r| \le M$ for all n. In particular, we have $\frac{\epsilon_r}{n} \to 0$ as $n \to \infty$. With this notation and hypothesis in place, we want to estimate $f_{l-1}\left(\frac{\pi}{2(n-k-l)+1}\right)$ to terms in $\frac{1}{n}$, and neglect all terms of order $\frac{1}{n^2}$ and smaller.

First, note that $\tan\left(\frac{\pi}{2(2(n-k-l)+1)}\right) = \frac{\pi}{2(2(n-k-l)+1)} + O\left(\frac{1}{n^2}\right) = \frac{\pi}{4(1-r)n} + O\left(\frac{1}{n^2}\right)$.

Next, observe that $\frac{2k\left(1-\cos\left(\frac{\pi}{2(n-k-l)+1}\right)\right)}{\sin\left(\frac{\pi}{2(n-k-l)+1}\right)} = \left(\frac{k\pi}{2(n-k-l)+1}\right) + O\left(\frac{1}{n^2}\right)$. Also,

$$2(k-1)\cos\left(\frac{\pi}{2(n-k-l)+1}\right) + 1 = 1 + k\left(\frac{\pi}{2(n-k-l)+1}\right)^2 + O\left(\frac{1}{n^2}\right).$$

Consequently, we find that

$$\begin{aligned}
&\frac{2k\left(1-\cos\left(\frac{\pi}{2(n-k-l)+1}\right)\right)}{\sin\left(\frac{\pi}{2(n-k-l)+1}\right)\left((k-1)\cos\left(\frac{\pi}{2(n-k-l)+1}\right)+1\right)} = \\
&\frac{k\pi}{2(n-k-l)+1}\left(1 - k\left(\frac{\pi}{2(n-k-l)+1}\right)^2\right) + O\left(\frac{1}{n^2}\right) \\
&= \frac{k\pi}{2(n-k-l)+1} - k^2\left(\frac{\pi}{2(n-k-l)+1}\right)^3 + O\left(\frac{1}{n^2}\right).
\end{aligned}$$

Observe that

$$\frac{k\pi}{2(n-k-l)+1} = \frac{\pi\left(c_0 - \frac{\epsilon_c}{n}\right)}{2(1-r-\frac{\epsilon_r}{n})+\frac{1}{n}} =$$
$$\frac{\pi\left(c_0 - \frac{\epsilon_c}{n}\right)}{2(1-r)}\left(1+\frac{\epsilon_r}{n(1-r)}-\frac{1}{2n(1-r)}\right)+O\left(\frac{1}{n^2}\right) =$$
$$\frac{\pi c_0}{2(1-r)} - \frac{\pi c_0}{2(1-r)}\frac{\epsilon_c}{n} + \frac{\pi c_0}{2(1-r)}\left(\frac{\epsilon_r}{n(1-r)}-\frac{1}{2n(1-r)}\right)+O\left(\frac{1}{n^2}\right).$$

Further, it is straightforward to determine that

$$k^2\left(\frac{\pi}{2(n-k-l)+1}\right)^3 = \frac{\pi^3 c_0^2}{8(1-r)^2 n}+O\left(\frac{1}{n^2}\right).$$

Consequently, we find that

$$\frac{2k\left(1-\cos\left(\frac{\pi}{2(n-k-l)+1}\right)\right)}{\sin\left(\frac{\pi}{2(n-k-l)+1}\right)\left((k-1)\cos\left(\frac{\pi}{2(n-k-l)+1}\right)+1\right)} =$$
$$\frac{\pi c_0}{2(1-r)} - \frac{\pi c_0}{2(1-r)}\frac{\epsilon_c}{n} + \frac{\pi c_0}{2(1-r)}\left(\frac{\epsilon_r}{n(1-r)}-\frac{1}{2n(1-r)}\right) - \frac{\pi^3 c_0^2}{8(1-r)^2 n}+O\left(\frac{1}{n^2}\right).$$

Finally, we need to estimate $\tan\left(\frac{\pi}{2}-\frac{l\pi}{2(n-k-l)+1}\right)$, or equivalently, $-\tan\left(\frac{\pi}{2}+\frac{l\pi}{2(n-k-l)+1}\right) = -\tan\left(\frac{\pi((2(n-k)+1)}{2(2(n-k-l)+1)}\right)$. Note that

$$\frac{\pi((2(n-k)+1)}{2(2(n-k-l)+1)} = \frac{\pi\left(1-\frac{k}{n}+\frac{1}{2n}\right)}{2\left(1-\frac{k+l}{n}\right)+\frac{1}{n}} =$$
$$\frac{\pi\left(1-c_0+\frac{\epsilon_c}{n}+\frac{1}{2n}\right)}{2(1-r)\left(1-\frac{\epsilon_r}{n(1-r)}+\frac{1}{2n(1-r)}\right)} =$$
$$\frac{\pi\left(1-c_0+\frac{\epsilon_c}{n}+\frac{1}{2n}\right)\left(1+\frac{\epsilon_r}{n(1-r)}-\frac{1}{2n(1-r)}\right)}{2(1-r)}+O\left(\frac{1}{n^2}\right) =$$
$$\frac{\pi(1-c_0)}{2(1-r)}+\frac{\pi}{2(1-r)}\left(\frac{\epsilon_c}{n}+\frac{1}{2n}\right)+\frac{\pi(1-c_0)}{2(1-r)}\left(\frac{\epsilon_r}{n(1-r)}-\frac{1}{2n(1-r)}\right)+O\left(\frac{1}{n^2}\right).$$

Consequently, from Taylor's theorem we have

$$\begin{aligned}\tan\left(\frac{\pi((2(n-k)+1)}{2(2(n-k-l)+1)}\right) &= \tan\left(\frac{\pi(1-c_0)}{2(1-r)}\right)+\sec^2\left(\frac{\pi(1-c_0)}{2(1-r)}\right)\left[\frac{\pi}{2(1-r)}\left(\frac{\epsilon_c}{n}\right.\right. \\ &+ \left.\left.\frac{1}{2n}\right)+\frac{\pi(1-c_0)}{2(1-r)}\left(\frac{\epsilon_r}{n(1-r)}-\frac{1}{2n(1-r)}\right)\right]+O\left(\frac{1}{n^2}\right).\end{aligned}$$

Assembling the estimates above, we have

$$\begin{aligned}
f_{l-1}\left(\frac{\pi}{2(n-k-l)+1}\right) &= \tan\left(\frac{\pi}{2} - l\frac{\pi}{2(n-k-l)+1}\right) + \tan\left(\frac{\frac{\pi}{2(n-k-l)+1}}{2}\right) \\
&- \frac{2k(1-\cos(\frac{\pi}{2(n-k-l)+1}))}{\sin(\frac{\pi}{2(n-k-l)+1})(2(k-1)(1-\cos(\frac{\pi}{2(n-k-l)+1}))+1)} \\
&= -\left(\tan\left(\frac{\pi(1-c_0)}{2(1-r)}\right) + \sec^2\left(\frac{\pi(1-c_0)}{2(1-r)}\right)\left[\frac{\pi}{2(1-r)}\left(\frac{\epsilon_c}{n}\right.\right.\right. \\
&+ \left.\frac{1}{2n}\right) + \left.\left.\left.\frac{\pi(1-c_0)}{2(1-r)}\left(\frac{\epsilon_r}{n(1-r)} - \frac{1}{2n(1-r)}\right)\right]\right) + \frac{\pi}{4(1-r)n} \\
&- \left[\frac{\pi c_0}{2(1-r)} - \frac{\pi c_0}{2(1-r)}\frac{\epsilon_c}{n} + \frac{\pi c_0}{2(1-r)}\left(\frac{\epsilon_r}{n(1-r)} - \frac{1}{2n(1-r)}\right)\right. \\
&- \left.\frac{\pi^3 c_0^2}{8(1-r)^2 n}\right] + O\left(\frac{1}{n^2}\right).
\end{aligned}$$

Since

$$-\tan\left(\frac{\pi(1-c_0)}{2(1-r)}\right) - \frac{\pi c_0}{2(1-r)} = 0,$$

we find that

$$\begin{aligned}
f_{l-1}\left(\frac{\pi}{2(n-k-l)+1}\right) &= -\sec^2\left(\frac{\pi(1-c_0)}{2(1-r)}\right)\left[\frac{\pi}{2(1-r)}\left(\frac{\epsilon_c}{n} + \frac{1}{2n}\right)\right. \\
&+ \left.\frac{\pi(1-c_0)}{2(1-r)}\left(\frac{\epsilon_r}{n(1-r)} - \frac{1}{2n(1-r)}\right)\right] \\
&+ \frac{\pi}{4(1-r)n} - \left[-\frac{\pi c_0}{2(1-r)}\frac{\epsilon_c}{n} + \frac{\pi c_0}{2(1-r)}\left(\frac{\epsilon_r}{n(1-r)} - \frac{1}{2n(1-r)}\right)\right. \\
&- \left.\frac{\pi^3 c_0^2}{8(1-r)^3 n}\right] + O\left(\frac{1}{n^2}\right) \\
&= -\sec^2\left(\frac{\pi(1-c_0)}{2(1-r)}\right)\frac{\pi}{2(1-r)}\left(\frac{1}{2n} - \frac{(1-c_0)}{2n(1-r)}\right) \\
&+ \frac{\pi}{4(1-r)n} + \frac{\pi c_0}{2(1-r)}\frac{1}{2n(1-r)} + \frac{\pi^3 c_0^2}{8(1-r)^3 n} \\
&+ \frac{\epsilon_c}{n}\left(-\frac{\pi}{2(1-r)}\sec^2\left(\frac{\pi(1-c_0)}{2(1-r)}\right) + \frac{\pi c_0}{2(1-r)}\right) \\
&- \frac{\epsilon_r}{n}\left(\frac{\pi(1-c_0)}{2(1-r)^2}\sec^2\left(\frac{\pi(1-c_0)}{2(1-r)}\right) + \frac{\pi c_0}{2(1-r)^2}\right) + O\left(\frac{1}{n^2}\right).
\end{aligned}$$

Define α, β, γ as follows:

$$\begin{aligned}
\alpha &= -\sec^2\left(\frac{\pi(1-c_0)}{2(1-r)}\right)\frac{\pi}{2(1-r)}\left(\frac{1}{2}-\frac{(1-c_0)}{2(1-r)}\right) \\
&+ \frac{\pi}{4(1-r)}+\frac{\pi c_0}{2(1-r)}\frac{1}{2(1-r)}+\frac{\pi^3 c_0^2}{8(1-r)^3}; \\
\beta &= -\frac{\pi}{2(1-r)}\sec^2\left(\frac{\pi(1-c_0)}{2(1-r)}\right)+\frac{\pi c_0}{2(1-r)}; \\
\gamma &= \frac{\pi(1-c_0)}{2(1-r)^2}\sec^2\left(\frac{\pi(1-c_0)}{2(1-r)}\right)+\frac{\pi c_0}{2(1-r)^2}.
\end{aligned}$$

Observe that $\beta < 0$ and $\gamma > 0$. With this notation in place we see that

$$f_{l-1}\left(\frac{\pi}{2(n-k-l)+1}\right) = \frac{1}{n}\left(\alpha+\beta\epsilon_c-\gamma\epsilon_r\right)+O\left(\frac{1}{n^2}\right).$$

Suppose that we choose l_1 via the relation $n-k-l_1 = \lfloor (1-r)n\rfloor + \lfloor \frac{\alpha+\beta}{\gamma}\rfloor - 1$. Observe that the corresponding value of ϵ_r is given by $\lfloor (1-r)n\rfloor - (1-r)n + \lfloor \frac{\alpha+\beta}{\gamma}\rfloor - 1$. Then $\alpha+\beta\epsilon_c-\gamma\epsilon_r \geq \alpha+\beta-\gamma\epsilon_r \geq \alpha+\beta-\gamma(\lfloor\frac{\alpha+\beta}{\gamma}\rfloor - 1) > 0$. We thus deduce that for all sufficiently large n, $f_{l_1-1}\left(\frac{\pi}{2(n-k-l_1)+1}\right) > 0$.

Next, choose l_2 via the relation $n-k-l_2 = \lceil (1-r)n\rceil + \lceil \frac{\alpha}{\gamma}\rceil + 1$. The corresponding ϵ_r is given by $\lceil (1-r)n\rceil - (1-r)n + \lceil\frac{\alpha}{\gamma}\rceil + 1$. Then we have $\alpha+\beta\epsilon_c-\gamma\epsilon_r \leq \alpha-\gamma\epsilon_r \leq \alpha-\gamma(\lceil\frac{\alpha}{\gamma}\rceil+1) < 0$. Hence, for all sufficiently large n, $f_{l_2-1}\left(\frac{\pi}{2(n-k-l_2)+1}\right) < 0$.

We have thus shown that for all sufficiently large values of n, the characteristic vertices of $T_{\lfloor c_0 n\rfloor, n}$ lie on the path from $k+l_1$ to $k+l_2$. Since $\frac{k+l_1}{n}, \frac{k+l_2}{n} \to r$ as $n\to\infty$, the desired conclusion now follows.

□

We now establish the asymptotics for $\frac{\delta_{\text{centre}}(n)}{n}$.

Corollary 3.3.1. *Let c_0 be the unique solution to (9). We have*

$$\lim_{n\to\infty}\frac{\delta_{\text{centre}}(n)}{n} = \frac{\pi c_0}{4}\left(\pi c_0 - \sqrt{\pi^2 c_0^2 - 4(1-c_0)}\right) - \frac{1-c_0}{2}.$$

Proof. Take any sequence $n_j \in \mathbb{N}$ such that $\frac{\delta_{\text{centre}}(n_j)}{n_j}$ converges, say to limit m. Since $\delta_{\text{centre}}(n_j) \geq \delta_{\text{centre}}(T_{\lfloor c_0 n_j\rfloor, n_j})$ for each $j\in\mathbb{N}$, we deduce from Theorem 3.3 that

$$m = \lim_{j\to\infty}\frac{\delta_{\text{centre}}(n_j)}{n_j} \geq \lim_{j\to\infty}\frac{\delta_{\text{centre}}(T_{\lfloor c_0 n_j\rfloor, n_j})}{n_j} = \frac{\pi c_0}{4}\left(\pi c_0 - \sqrt{\pi^2 c_0^2 - 4(1-c_0)}\right) - \frac{1-c_0}{2}.$$

On the other hand, from Theorem 3.2, we also have

$$m = \lim_{j\to\infty}\frac{\delta_{\text{centre}}(n_j)}{n_j} \leq \frac{\pi c_0}{4}\left(\pi c_0 - \sqrt{\pi^2 c_0^2 - 4(1-c_0)}\right) - \frac{1-c_0}{2},$$

from which we conclude that

$$\lim_{j\to\infty}\frac{\delta_{\mathrm{centre}}(n_j)}{n_j}=\frac{\pi c_0}{4}\left(\pi c_0-\sqrt{\pi^2 c_0^2-4(1-c_0)}\right)-\frac{1-c_0}{2}.$$

Since every convergent subsequence of $\frac{\delta_{\mathrm{centre}}(n)}{n}$ has limit $\frac{\pi c_0}{4}\left(\pi c_0-\sqrt{\pi^2 c_0^2-4(1-c_0)}\right)-\frac{1-c_0}{2}$, the desired conclusion follows. □

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