Linear Algebra and its Applications 639 (2022) 135–158

Contents lists available at ScienceDirect

Linear Algebra and its Applications

www.elsevier.com/locate/laa

Perron values and classes of trees

Enide Andrade [a], Lorenzo Ciardo [b], Geir Dahl [c,*]

[a] Center for Research and Development in Mathematics and Applications, Department of Mathematics, University of Aveiro, Portugal
[b] Department of Computer Science, University of Oxford, UK
[c] Department of Mathematics, University of Oslo, Norway

ARTICLE INFO

Article history:
Received 23 June 2021
Accepted 7 January 2022
Available online 12 January 2022
Submitted by S. Kirkland

MSC:
05C50
15A18
05C05
05C40

Keywords:
Perron value
Laplacian matrix
Bottleneck matrix
Tree
Special trees

ABSTRACT

The bottleneck matrix M of a rooted tree T is a combinatorial object encoding the spatial distribution of the vertices with respect to the root. The spectral radius of M, known as the Perron value of the rooted tree, is closely related to the theory of the algebraic connectivity. In this paper, we investigate the Perron values of various classes of rooted trees by making use of combinatorial and linear-algebraic techniques. This results in multiple bounds on the Perron values of these classes, which can be straightforwardly applied to provide information on the algebraic connectivity.

1. Introduction

Let T be a rooted tree having root r and order n whose vertices are labelled $1, 2, \dots, n$, and consider the symmetric matrix M of order n whose (i, j)'th entry m_{ij} is the number

* Corresponding author.
E-mail addresses: enide@ua.pt (E. Andrade), lorenzo.ciardo@cs.ox.ac.uk (L. Ciardo), geird@math.uio.no (G. Dahl).

https://doi.org/10.1016/j.laa.2022.01.005

of vertices in T that simultaneously lie in the path $\mathcal{P}_i$ joining i to r and in the path $\mathcal{P}_j$ joining j to r. Equivalently, following [3], M may be defined as $M = N^T N$, where N is the *path matrix* of T, i.e., the $n \times n$ $(0, 1)$-matrix whose j'th column is the incidence vector of $\mathcal{P}_j$ for $j \leq n$ (that is, it contains ones in rows corresponding to vertices in $\mathcal{P}_j$ and zeros elsewhere). The root of a tree in the figures of the paper is denoted by a square. The vertices of T can be ordered so that N is upper triangular with ones on the diagonal. The matrix M is referred to as the *bottleneck matrix* of T. Its spectral radius, known as the *Perron value* of T and denoted by $\rho(T)$ (or $\rho(M)$), is closely linked to the theory of algebraic connectivity and characteristic set of trees. Let T' be an unrooted tree and pick a vertex v of T'. Removing v from T', along with all edges incident to v, results in a forest. A *branch* at v is a connected component of such a forest, considered as a rooted tree whose root is the vertex adjacent to v in T'; a *Perron branch* at v is a branch at v having maximum Perron value. The bottleneck matrices of the branches at v can be obtained as the diagonal blocks of the inverse of the principal submatrix of the Laplacian matrix L of T' resulting from removing the row and column corresponding to v. This connects their spectral radii to the spectrum of L and, in particular, to the algebraic connectivity $a(T')$ – i.e., the second smallest eigenvalue of L – as described in the next result.

Theorem 1.1 *([13]). Let T' be an unrooted tree with more than one vertex. Exactly one of two cases can occur.*

1. *There exists exactly one vertex z having $k \geq 2$ Perron branches $B_1, B_2, \ldots, B_k$ at z. T' is said to be a type I tree and z is its characteristic vertex. Moreover, in this case,*

$$a(T') = \frac{1}{\rho(B_i)} \quad (i = 1, 2, \ldots, k).$$

2. *There exists exactly one edge pq such that the unique Perron branch B_p at p contains q and the unique Perron branch B_q at q contains p. T' is said to be a type II tree and p, q are its characteristic vertices. Moreover, in this case,*

$$a(T') = \frac{1}{\rho\left(M_p - \gamma J\right)} = \frac{1}{\rho\left(M_q - (1-\gamma) J\right)},$$

where M_p (resp. M_q) is the bottleneck matrix of B_p (resp. B_q), J is the all-ones matrix, and γ is a real number such that $0 < \gamma < 1$.

Due to its suitability to express connectivity for graphs, the algebraic connectivity has been extensively studied since its introduction by Fiedler [8] (for example, see [7,9,10]). Theorem 1.1 asserts that the Perron values of the branches of a tree play a central role in determining its algebraic connectivity and characteristic set. More specifically, investigating the algebraic connectivity through the lenses of Perron values rather than directly studying the spectrum of the Laplacian matrix yields two advantages:

1. Unlike the Laplacian matrix, the bottleneck matrix is entrywise positive; this opens the possibility of using the Perron-Frobenius theory to study its spectral radius and the corresponding eigenspace.
2. The variational expression for the maximum (or minimum) eigenvalue of a Hermitian matrix coming from the Courant-Fischer-Weyl principle is simpler than the corresponding expression for the other eigenvalues. In particular, the Rayleigh quotient of M with any nonzero real vector yields a lower bound on $\rho(M)$.

Unfortunately, analytic expressions for the spectral radii of bottleneck matrices are only available for very specific classes of rooted trees. Let S_n be the rooted star on n vertices having the central vertex as the root, and let P_n be the rooted path on n vertices having one of the endpoints as the root. From [1,3,13], we have the following expressions for their Perron values:

$$\rho(S_n) = \frac{1}{2}\left(n + 1 + \sqrt{n^2 + 2n - 3}\right), \tag{1}$$

$$\rho(P_n) = \frac{1}{2}\left(1 - \cos\left(\frac{\pi}{2n+1}\right)\right)^{-1}. \tag{2}$$

A main purpose of this work is to provide bounds on the Perron values of various classes of rooted trees by using diverse combinatorial and spectral tools. Through Theorem 1.1, the bounds we obtain can be straightforwardly turned into bounds for the algebraic connectivity of classes of unrooted trees. Below are listed the different techniques applied in the paper.

- In Section 2, we prove a general result on the spectral radius of symmetric matrices having a specific 2×2 block structure, and we use it to obtain upper bounds for the Perron value of generic rooted trees (Corollary 2.3) as well as of split-paths (Corollary 2.4), broom trees (Corollary 2.5), and Fiedler roses (Corollary 2.6).
- In Section 3, the focus is on families of "composite" rooted trees, which may be obtained from simpler building blocks through certain natural operations that are consistent with the behaviour of the Perron value. This results in upper and lower bounds for starlike trees (Proposition 3.3) and regular caterpillars (Proposition 3.4).
- In Section 4, we make use of a bound for the spectral radius of nonnegative irreducible symmetric matrices from [4,16] and the interlacing of the eigenvalues for the quotient matrix of a symmetric partitioned matrix [11] to obtain an upper and a lower bound on the Perron value of broom trees, respectively.
- The theory of the *combinatorial Perron parameters* – developed in [3,2] to provide close and computationally efficient approximations of the Perron value – is the core of Section 5. These parameters are lower bounds on the Perron value coming from the variational characterization of the eigenvalues of Hermitian matrices. The distance vector of a rooted tree T is $d = (d_1, d_2, \ldots, d_n)$, where d_j is the number of vertices (note: not edges) in the path $\mathcal{P}_j$ joining j to the root. When M is the bottleneck

matrix of T, two combinatorial parameters were introduced in [3], namely $\rho_c(M)$ (or $\rho_c(T)$) and $\pi_d(M)$ (or $\pi_d(T)$) and a third one, $\pi_e(M)$ (or $\pi_e(T)$), was introduced in [2]:
(i) $\rho_c(M) = \frac{\|Nd\|^2}{\|d\|^2} = \frac{d^TMd}{d^Td}$;
(ii) $\pi_d(M) = \frac{\|Md\|}{\|d\|}$;
(iii) $\pi_e(M) = \frac{\|Me\|}{\|e\|}$, where e is the all-ones vector.
An alternative expression for $\rho_c(M)$ is $\rho_c(M) = (\sum_i \sigma_i^2)/(\sum_i d_i^2)$, where $\sigma_i = \sum_{j:j \preceq i} d_j$ and $j \preceq i$ means that j is below i in the sense that the path $\mathcal{P}_i$ is contained in the path $\mathcal{P}_j$. Each of the parameters (i)–(iii) gives a lower bound on the Perron value of T, and their combinatorial nature makes it possible to obtain closed formulae for certain classes of rooted trees. In Section 5, we use this strategy focusing on the parameters (i) and (iii) and, as a result, we obtain lower bounds on the Perron value of broom trees and regular caterpillars.

We point out here that the unifying aspect of this work lies in the results rather than the techniques adopted. In fact, to obtain tight bounds for each different class of rooted trees requires to efficiently exploit the specific combinatorial structure of the class; this results in a variety of different proof strategies. On the other hand, the scope of these techniques is wider than the examples investigated in the current work: Many other classes of rooted trees can be addressed with combinations and suitable modifications of the tools considered here. Hence, we believe this exposition can serve as a starting point for future investigations of the Perron value and the algebraic connectivity of other families of trees.

Notation: We treat vectors in $\mathbb{R}^n$ as column vectors and identify these with real n-tuples. The all-ones matrix of size $n \times n$ is denoted by J_n. We let $e_{(k)}$ denote the all-ones (column) vector of dimension k; we sometimes omit the subscript. The transpose of a matrix A is denoted by A^T. The Euclidean norm of a vector x is $\|x\| = (x^Tx)^{1/2}$. We will need the following well-known formulae for the sums of the k'th power of the first n natural numbers for $k = 1, 2, 3, 4$:

$$\begin{aligned} S_n^{(1)} &:= \sum_{i=1}^n i &&= \tfrac{n^2+n}{2} \\ S_n^{(2)} &:= \sum_{i=1}^n i^2 &&= \tfrac{n(n+1)(2n+1)}{6} = \tfrac{2n^3+3n^2+n}{6} \\ S_n^{(3)} &:= \sum_{i=1}^n i^3 &&= \tfrac{n^4+2n^3+n^2}{4} \\ S_n^{(4)} &:= \sum_{i=1}^n i^4 &&= \tfrac{6n^5+15n^4+10n^3-n}{30}. \end{aligned} \tag{3}$$

2. The spectral radius of certain block matrices

In this section we prove a quite general result that gives an upper bound for the spectral radius of symmetric matrices with a specific 2×2 block structure, and use this to find an upper bound on the Perron value of certain families of rooted trees.

Let

$$M = \begin{bmatrix} A & B \\ B^T & C \end{bmatrix} \tag{4}$$

where (i) A and C are symmetric matrices of order k and ℓ, respectively, so B is of size $k \times \ell$, and (ii) $B = wq^T$ where $w \in \mathbb{R}^k$ and $q \in \mathbb{R}^\ell$. This means that B has rank at most 1. M is symmetric, and therefore has real eigenvalues. We establish the following upper bound on the spectral radius of M, expressed in terms of the spectral radii of A and C.

Theorem 2.1. *Let M be as in (4). Then*

$$\rho(M) \leq \frac{1}{2}(\rho(A) + \rho(C)) + \frac{1}{2}\sqrt{(\rho(A) - \rho(C))^2 + 4\|w\|^2\|q\|^2}. \tag{5}$$

Moreover, if $\rho(A)\rho(C) > \|w\|^2\|q\|^2$, then the upper bound in (5) is strictly smaller than $\rho(A) + \rho(C)$.

Proof. Consider the 2×2 symmetric matrix

$$K = \begin{bmatrix} \rho(A) & \|q\|\|w\| \\ \|q\|\|w\| & \rho(C) \end{bmatrix}.$$

Let $\lambda_{\max}(X)$ and $\lambda_{\min}(X)$ denote the maximum and minimum eigenvalue of a symmetric matrix X, respectively. Suppose first that $\rho(M) = \lambda_{\max}(M)$. Then, letting x be a corresponding eigenvector of norm 1, we have $x^T Mx = \rho(M)$. Partition x according to M as $x = (y, z)$, let $x' = (\|y\|, \|z\|)$, and observe that $\|x'\|^2 = \|y\|^2 + \|z\|^2 = \|x\|^2 = 1$. We obtain

$$\begin{aligned}
\rho(M) = x^T Mx = \begin{bmatrix} y^T & z^T \end{bmatrix} \begin{bmatrix} A & wq^T \\ qw^T & C \end{bmatrix} \begin{bmatrix} y \\ z \end{bmatrix} &= y^T Ay + z^T Cz + 2y^T wq^T z \\
&\leq \lambda_{\max}(A)\|y\|^2 + \lambda_{\max}(C)\|z\|^2 + 2|y^T w||q^T z| \\
&\leq \rho(A)\|y\|^2 + \rho(C)\|z\|^2 + 2\|y\|\|w\|\|q\|\|z\| \\
&= [\,\|y\| \quad \|z\|\,] \begin{bmatrix} \rho(A) & \|q\|\|w\| \\ \|q\|\|w\| & \rho(C) \end{bmatrix} \begin{bmatrix} \|y\| \\ \|z\| \end{bmatrix} \\
&= x'^T Kx' \leq \lambda_{\max}(K)\|x'\|^2 = \lambda_{\max}(K).
\end{aligned}$$

A standard formula for the eigenvalues of a symmetric 2×2 matrix gives the desired inequality (5). Suppose now that $\rho(M) = -\lambda_{\min}(M)$. Observe that

$$\rho(-M) = \rho(M) = -\lambda_{\min}(M) = \lambda_{\max}(-M).$$

We can then apply the argument above to $-M$ to find

$$\begin{aligned}\rho(M) = \rho(-M) &\leq \frac{1}{2}(\rho(-A) + \rho(-C)) + \frac{1}{2}\sqrt{(\rho(-A) - \rho(-C))^2 + 4\|-w\|^2\|q\|^2} \\ &= \frac{1}{2}(\rho(A) + \rho(C)) + \frac{1}{2}\sqrt{(\rho(A) - \rho(C))^2 + 4\|w\|^2\|q\|^2},\end{aligned}$$

as wanted.

If $\rho(A)\rho(C) > \|w\|^2\|q\|^2$, then $\det(K) > 0$, and the entry in position $(1,1)$ in K is positive (as A is nonzero), so K is positive definite. Then the eigenvalues of K are positive, and their sum equals the trace $\rho(A) + \rho(C)$. Therefore $\lambda_{\max}(K) < \rho(A) + \rho(C)$, and the proof is complete. □

Remark 2.2. In Theorem 2.1 one may assume without loss of generality that $\rho(A) \geq \rho(C)$. This is seen by simultaneous row and column permutations which gives

$$M' = \begin{bmatrix} C & B^T \\ B & A \end{bmatrix}.$$

Notice that $\rho(M') = \rho(M)$. □

Let $T = (V, E)$ be a rooted tree, with root r, and let p be a vertex in T. We shall assume that $p \neq r$ and that p is not a pendent vertex, so $F_p = \{v : v \preceq p, v \neq p\}$ is nonempty. Let T_p denote the induced subtree with vertices $\{v : v \preceq p\}$ with root p and let T' be the subtree induced by $V - F_p$ with root r; these two trees have only vertex p in common. Order the vertices in T such that all the vertices in $V - F_p$ are before all the vertices in F_p, and for each of these vertex sets we order according to distance from the root. Then the bottleneck matrix M of T has the block form in (4), i.e.,

$$M = \begin{bmatrix} A & B \\ B^T & C \end{bmatrix}$$

where A is the bottleneck matrix of T', and C is the truncated bottleneck matrix of T_p (where the row and column corresponding to p are deleted) plus a constant block. So, A and C are symmetric. Concerning B, each row corresponds to a vertex $u \in T'$ and the entry b_{uv} in the column corresponding to a vertex $v \in T_p$, $v \neq p$, is

$$b_{uv} = |\mathcal{P}_u \cap \mathcal{P}_v| = |\mathcal{P}_u \cap \mathcal{P}_p|$$

which is the number of common vertices in $\mathcal{P}_u$ and $\mathcal{P}_p$, and independent of v. Thus, each row in B is constant, so $B = we^T$ where $w = (|\mathcal{P}_u \cap \mathcal{P}_p| : u \in T')$. Note that w can be viewed as a "projection" of the paths $\mathcal{P}_u$ onto the path $\mathcal{P}_p$ for $u \in T'$. The upper bound in Theorem 2.1 then holds for the Perron value of T, with $\|q\|^2 = \|e\|^2 = \ell = |V(T_p)| - 1$.

Example 1. We illustrate the construction above for the special case when $\ell = 1$. Then T_p is an edge, say pp', so $|V| = k + 1$ and $w = (|\mathcal{P}_u \cap \mathcal{P}_p| : u \in T')$. Let s be the distance of the root to p, so $d_p = s$ and $d_{p'} = s + 1$. The bottleneck matrix is

$$M = \begin{bmatrix} A & w \\ w^T & s+1 \end{bmatrix}$$

and (5) gives

$$\rho(M) \le \beta := \frac{1}{2}(\rho(A) + s + 1) + \frac{1}{2}\sqrt{(\rho(A) - s - 1)^2 + 4\|w\|^2}.$$

We note that $\beta \le \rho(A) + \|w\|$ (due to the basic inequality $\sqrt{a+b} \le \sqrt{a} + \sqrt{b}$).

For the rooted path P_n, the bound β is almost tight. For instance, when $n = 21$, the Perron value $\rho(P_n) = \rho(M) = 187.4262$ and $\beta = 187.6282$. Here β is computed based on $\rho(P_{n-1}) = (1/2)(1 - \cos(\pi/(2n-1)))^{-1}$, see [3,13]. □

In the remaining part of this section we use the previous approach based on Theorem 2.1 to find an upper bound on the Perron value of rooted trees. First, we develop a technique for general trees, and then we consider three different classes of trees.

2.1. Bounds for general trees

Let T be a rooted tree and M its bottleneck matrix. We now give a technique for finding an upper bound on $\rho(M)$. Note that the technique applies to *any* tree.

The starting point is the approach above based on Theorem 2.1. Also, we know that T may be constructed by the general tree-construction procedure: (i) Start with a single vertex (the root); this is the initial tree, and (ii) successively add a new vertex and attach to the existing tree by an edge to some existing vertex. The tree construction procedure means that we can repeatedly use Theorem 2.1 as explained in Example 1. Let the tree-construction procedure result in the trees

$$T^{(1)}, T^{(2)}, \ldots, T^{(n)} = T,$$

where $T^{(1)}$ consists in the root $r = v_1$ and, for $i = 2, 3, \ldots, n$, $T^{(i)}$ is obtained from $T^{(i-1)}$ by adding vertex v_i and an edge to a vertex v_h (in $T^{(i-1)}$) for some $h < i$. Note that there may be many tree constructions giving the same tree T, by different vertex orderings. Let $M^{(i)}$ be the bottleneck matrix of $T^{(i)}$, and let $w^{(i)} = (|\mathcal{P}_u \cap \mathcal{P}_{v_h}| : u \in T^{(i-1)})$, where we (for convenience) view paths as vertex sets in the final tree T. Finally, let $s^{(i)}$ be the distance of the root to v_h. So

$$M^{(i)} = \begin{bmatrix} M^{(i-1)} & w^{(i)} \\ (w^{(i)})^T & s^{(i)} + 1 \end{bmatrix}. \tag{6}$$

We define (recursively)

$$\rho^{(1)} = 1,$$
$$\rho^{(i)} = \frac{1}{2}(\rho^{(i-1)} + s^{(i)} + 1) + \frac{1}{2}\sqrt{(\rho^{(i-1)} - s^{(i)} - 1)^2 + 4\|w^{(i)}\|^2} \quad (2 \leq i \leq n).$$

Corollary 2.3. *The following upper bound on the Perron value $\rho(M^{(i)})$ holds*

$$\rho(M^{(i)}) \leq \rho^{(i)} \quad (i = 1, 2, \ldots, n). \tag{7}$$

In particular, $\rho(T) \leq \rho^{(n)}$.

Proof. We prove this by induction on i. For $i = 1, 2$, or 3, a direct verification shows that (7) holds. Let $i \geq 4$, and assume that $\rho(M^{(i-1)}) \leq \rho^{(i-1)}$.

We first prove the following inequality

$$\rho(M^{(i-1)}) \geq s^{(i)} + 1. \tag{8}$$

To do so, let $s = s^{(i)}$. Assume first that $s \geq 3$. Then

$$\rho(M^{(i-1)}) \geq \rho(P_s) \geq \rho_c(P_s) = (1/5)(2s^2 + 2s + 1) \geq s + 1.$$

Here the first inequality holds as the bottleneck matrix of the path P_s is componentwise smaller than $M^{(i-1)}$ so the same ordering holds for the spectral radii (see Theorem 8.1.18 in [12]). The second inequality and expression concerns the combinatorial Perron value ρ_c, see the Introduction and [3]. The final inequality is by simple algebra. Thus, (8) holds for $s \geq 3$, and it remains to verify (8) when $s \leq 2$. If $T^{(i-1)}$ contains a vertex with distance 3 to the root (where, as usual, by distance we mean the number of vertices in the shortest path), then $\rho(M^{(i-1)}) \geq \rho(P_3) \geq \rho_c(P_3) = (1/5)(2\cdot 3^2 + 2\cdot 3 + 1) = 5 > 3 \geq s+1$, as desired. Otherwise, the maximum distance to the root is at most 2, so $T^{(i-1)}$ is a star with at least 3 vertices. So, $\rho(M^{(i-1)}) \geq \rho(S_3) \geq \rho_c(S_3) = 3 + 6/9 > 3 \geq s + 1$, as desired. This completes the proof of (8).

We can now finish the induction proof, by using the induction assumption $\rho(M^{(i-1)}) \leq \rho^{(i-1)}$ and Theorem 2.1 on the block matrix (6). This gives

$$\begin{aligned}
\rho(M^{(i)}) &\leq \tfrac{1}{2}(\rho(M^{(i-1)}) + s^{(i)} + 1) + \tfrac{1}{2}\sqrt{(\rho(M^{(i-1)}) - (s^{(i)} + 1))^2 + 4\|w^{(i)}\|^2} \\
&\leq \tfrac{1}{2}(\rho^{(i-1)} + s^{(i)} + 1) + \tfrac{1}{2}\sqrt{(\rho(M^{(i-1)}) - s^{(i)} - 1)^2 + 4\|w^{(i)}\|^2} \\
&\leq \tfrac{1}{2}(\rho^{(i-1)} + s^{(i)} + 1) + \tfrac{1}{2}\sqrt{(\rho^{(i-1)} - s^{(i)} - 1)^2 + 4\|w^{(i)}\|^2} \\
&= \rho^{(i)},
\end{aligned}$$

and the proof is complete. □

We have done extensive computational tests with the bounding procedure of Corollary 2.3. Perhaps surprisingly, the upper bounds are very good. Thus, it seems that the

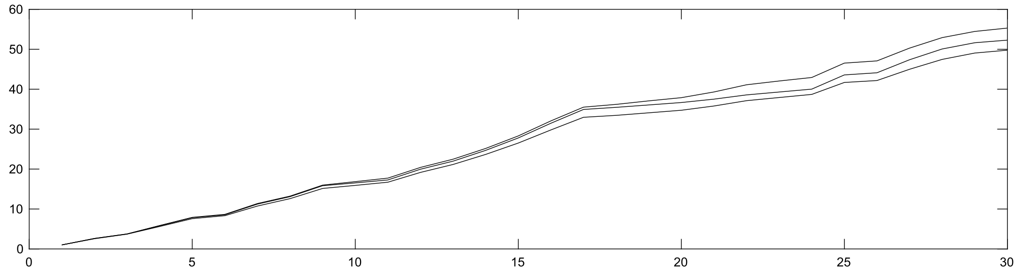

Fig. 1. Random tree; lower and upper bounds on $\rho(M^{(i)})$, $i = 1, 2, \ldots, 30$.

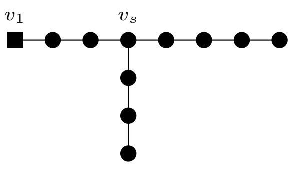

Fig. 2. Split-path $P(8, 3; 4)$.

error in each tree extension is small, and this shows the usefulness of Theorem 2.1. As an illustration, we show results for a test with $n = 30$ for a random tree T, constructed using the tree construction where the attaching vertex was chosen uniformly at random in each step. Fig. 1 shows three curves, corresponding to $\rho(M^{(i)})$ (middle curve), $\rho^{(i)}$ (upper curve), and the known lower bound $\pi_e(M^{(i)})$ (lower curve). Let the relative gap be defined as RG = (100 × (upper bound - exact value) / exact value) %. The relative gap for the final tree $T = T^{(30)}$, comparing $\rho(M^{(i)})$ to $\rho^{(i)}$, is 5.78%. A similar experiment for the path P_{30} gave relative gap 0.62%, and for the star S_{30} we got 0.029%. Many experiments have been done and for $n = 30$ the gaps vary typically between 1% and 11%. The gap seems to increase very slowly as a function of the tree order n. Random trees with the same number of vertices show very similar performance. Finally, we remark that for a given tree T, one might improve the bound by trying different tree constructions each leading to T.

2.2. Split-paths

Let s, ℓ, k be positive integers such that $s+\ell \leq k$. Consider the path $P_k = v_1, v_2, \ldots, v_k$ and add another path $P_{\ell+1}$ at vertex v_s of the first path, by identifying v_s with the root (first vertex) of $P_{\ell+1}$. Let $P(k, \ell; s)$ be the resulting rooted tree, which we call a *split-path* (see Fig. 2). It has $k + \ell$ vertices, and the root is v_1. Note that the distances (number of vertices) in $P(k, \ell; s)$ from the root to each of the two other pendent vertices are k and $s + \ell$. Then, its bottleneck matrix can be partitioned into the block form:

$$M = \begin{bmatrix} A^{(k)} & B \\ B^T & C \end{bmatrix}, \tag{9}$$

where $A^{(k)}$, B, C have dimensions $k \times k$, $k \times \ell$, and $\ell \times \ell$, respectively, and

$$A^{(k)} = \begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & 2 & 2 & \cdots & 2 \\ 1 & 2 & 3 & \cdots & 3 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 2 & 3 & \cdots & k \end{bmatrix}, \; B = \begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \\ 2 & 2 & 2 & \cdots & 2 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ s & s & s & \cdots & s \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ s & s & s & \cdots & s \end{bmatrix}, \tag{10}$$

and $C = s \times J_\ell + A^{(\ell)}$ (where $A^{(\ell)}$ is defined like $A^{(k)}$ but is of order ℓ). Notice that $A^{(k)}$ is the bottleneck matrix of the path P_k, so we have an exact expression for $\rho(A^{(k)})$.

Corollary 2.4. *For the split-path $P(k, \ell; s)$,*

$$\rho(M) \leq \tfrac{1}{2}(\rho(A^{(k)}) + s\ell + \rho(A^{(\ell)})) + \tfrac{1}{2}\sqrt{(\rho(A^{(k)}) - \alpha)^2 + 4\ell(S_s^{(2)} + (k-s)s^2)}$$

where $S_s^{(2)} = \sum_{i=1}^{s} i^2$ and $\alpha = \max\{s + \rho(A^{(\ell)}), s\ell + (1/6)(2\ell^2 + 3\ell + 1)\}$.

Proof. We have $w = (1, 2, \ldots, s, \ldots, s)$ so $\|w\|^2 = \sum_{i=1}^{s} i^2 + (k-s)s^2$. Moreover, let $x = (x_1, x_2, \ldots, x_\ell)$ be the Perron vector of $A^{(\ell)}$, with $\|x\| = 1$. Then

$$x^T J_\ell x = \sum_{i,j} x_i x_j = \sum_i x_i \sum_j x_j \geq \sum_i x_i \geq 1$$

because $0 < x_i < 1$ so $x_i > x_i^2$ for each i, and therefore $\sum_i x_i \geq \sum_i x_i^2 = 1$. Therefore,

$$x^T C x = x^T s J_\ell x + x^T A^{(\ell)} x \geq s + \rho(A^{(\ell)}).$$

Next, let $y = (1/\sqrt{\ell}) e_{(\ell)}$, so $\|y\| = 1$. Then,

$$y^T C y = s(1/\ell) e_{(\ell)}^T J_\ell e_{(\ell)} + (1/\ell) e_{(\ell)}^T A^{(\ell)} e_{(\ell)} = s\ell + (1/6)(2\ell^2 + 3\ell + 1).$$

So, using Rayleigh quotients we get

$$\rho(C) \geq \max\{x^T C x, y^T C y\} \geq \alpha.$$

Observe that, as $k \geq s + \ell$,

$$\rho(A^{(k)}) \geq \rho(s J_{(k-s)} + A^{(k-s)}) \geq \rho(s J_{(\ell)} + A^{(\ell)}) = \rho(C).$$

This implies that

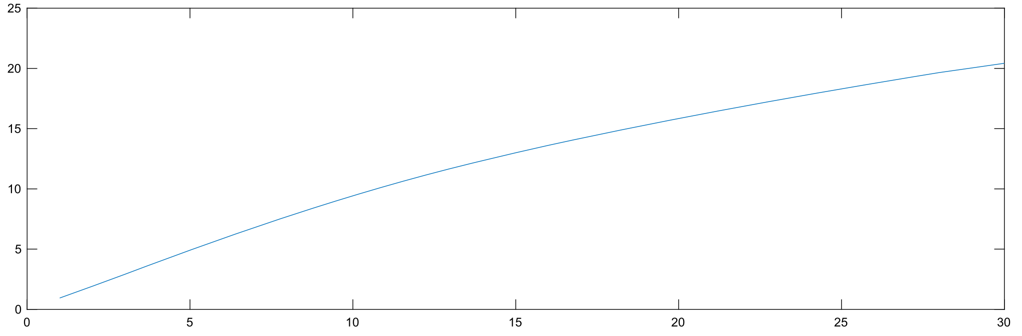

Fig. 3. Split-path $k = 50$, $\ell = 20$. On the y-axis, relative gap for $1 \leq s \leq 30$.

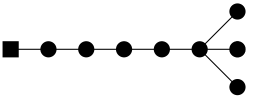

Fig. 4. Broom tree $B(6, 3)$.

$$(\rho(A^{(k)}) - \rho(C))^2 \leq (\rho(A^{(k)}) - \alpha)^2.$$

Then the inequality follows from Theorem 2.1. □

We have tested computationally the quality of the bound in Corollary 2.4. Fig. 3 shows test cases for split-paths where $k = 50$, $\ell = 20$. We varied s from 1 to $k - \ell = 30$; the x-axis shows s and the y-axis shows RG. Note that RG is increasing in s. The average RG was 12.3% and the maximum RG was 20.4%. A general experience is that the quality of the bound improves as k becomes significantly larger than $s + \ell$. This can also be explained from the formula, as in this case $\rho(A^{(k)})$ dominates in the expression.

2.3. Broom trees

Let $B(k, \ell)$ be the broom tree which is obtained from a path P_k of length k by adding ℓ vertices and attaching each of these to one of the end vertices of the path (see Fig. 4). Let the root of the tree be the other end vertex in the path (so it has degree 1). Then, the bottleneck matrix of $B(k, \ell)$ can be partitioned into the block form

$$M = \begin{bmatrix} A^{(k)} & B \\ B^T & C \end{bmatrix}, \tag{11}$$

where $A^{(k)}$, B, C have dimensions $k \times k$, $k \times \ell$, and $\ell \times \ell$, respectively, and

k	ℓ	average RG	maximum RG
25	$1 \leq \ell \leq 50$	0.095%	0.2%
100	$1 \leq \ell \leq 200$	0.094%	0.2%

Fig. 5. Computational results, RG for broom trees $B(k, \ell)$.

$$A^{(k)} = \begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & 2 & 2 & \cdots & 2 \\ 1 & 2 & 3 & \cdots & 3 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 2 & 3 & \cdots & k \end{bmatrix}, \; B = \begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \\ 2 & 2 & 2 & \cdots & 2 \\ 3 & 3 & 3 & \cdots & 3 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ k & k & k & \cdots & k \end{bmatrix}, \tag{12}$$

and $C = k \times J_\ell + I_\ell$. Here $A^{(k)}$ is the bottleneck matrix of the path P_k, so we have an exact expression for $\rho(A^{(k)})$. Moreover, $\rho(C) = k\ell + 1$. Recall that $S_k^{(2)} = \sum_{i=1}^{k} i^2$.

Corollary 2.5. *For the broom $B(k, \ell)$*

$$\rho(M) \leq \tfrac{1}{2}(\rho(A^{(k)}) + k\ell + 1) + \tfrac{1}{2}\sqrt{(\rho(A^{(k)}) - k\ell - 1)^2 + 4\ell S_k^{(2)}}\,.$$

Proof. This follows from Theorem 2.1. □

We tested computationally the quality of the bound in Corollary 2.5. Some results for $k = 25$ and $k = 100$, and varying ℓ are shown in Fig. 5. The relative gap RG was defined in Subsection 2.1. It was observed that the RG is monotonically increasing as a function of ℓ, so the maximum value was obtained for the largest ℓ in the interval. The maximum RG was about 0.2%. Several experiments indicate that the upper bound in Corollary 2.5 is very good.

2.4. Rose trees

Rose trees, also called Fiedler roses, were introduced by Evans [6] and were recently studied in connection to algebraic connectivity, [1]. See also some work in [15].

Let h, t, ℓ be natural numbers. A *rose tree* $R(h, t, \ell)$ is the graph obtained from the path $P_{h+t+1} = v_1, v_2, \ldots, v_{h+t+1}$ and the star S_ℓ by connecting the vertex v_{h+1} of the path by an edge to the center v_{h+t+2} of the star. Let $v_{h+t+3}, \ldots, v_n$ be the other vertices of the star where $n = h + t + \ell + 1$. The rose tree has n vertices and the root is vertex v_1. If $t = h$, then it is called a *perfect rose tree* [1] and it is just denoted by $R(h, \ell)$. An example of perfect rose tree can be seen in Fig. 6.

Now, order the vertices according to the subscripts, so $v_1, v_2, \ldots, v_n$. For a rose tree (or a perfect rose tree) the bottleneck matrix has the form as in (9) with $A^{(k)}$ and B as in (10), where $A^{(k)}$ has order $k = h + t + 1$, and $s = h + 1$. Additionally, $C = s \times J_\ell + M^{(\ell)}$, where $M^{(\ell)}$ is the bottleneck matrix of the star S_ℓ.

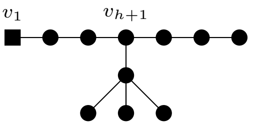

Fig. 6. Perfect rose tree $R(3, 4)$.

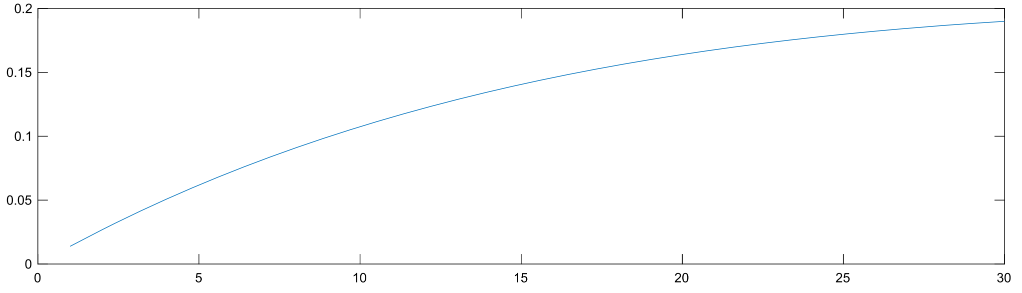

Fig. 7. Fiedler roses with $h = t = 50$. On the y-axis, relative gap (RG) of the bound in Corollary 2.6, for $1 \leq \ell \leq 30$.

Corollary 2.6. *For every rose tree $R(h, t, \ell)$ with $\ell \leq t$*

$$\rho(M) \leq \frac{1}{2}(\rho(A^{(k)}) + (h+1)\ell + \rho(M^{(\ell)})) + \frac{1}{2}\sqrt{(\rho(A^{(k)}) - \alpha)^2 + 4\ell(S^{(2)}_{h+1} + t(h+1)^2)}$$

where $k = h + t + 1$ and $\alpha = (h+1)\ell + (\ell^2 + \ell - 1)/\ell$.

Proof. This may be shown similarly to Corollary 2.4 with one difference being that the computed α is different. Moreover, the assumption $\ell \leq t$ implies that a principal submatrix of $A^{(k)}$ is componentwise larger than or equal to C, so $\rho(A^{(k)}) \geq \rho(C)$. □

We did computational experiments to study the quality of the bound in Corollary 2.6. For $h = t = 50$, so perfect rose trees, we let ℓ vary with $1 \leq \ell \leq 30$. The resulting average relative gap (RG) was 0.054%. The RG is monotonically increasing as a function of ℓ and the maximum value, for $\ell = 30$, was about 0.19%, see Fig. 7.

3. Bounds from tree constructions: starlike trees and regular caterpillars

Certain classes of rooted trees have the property that they can be obtained – either directly or recursively – by combining simpler trees through some natural constructions. In this section, we apply the results obtained in [5] on the Perron values of two such constructions – rooted sums and products – to the classes of starlike trees and regular caterpillars. This yields simple bounds on their Perron values that would be harder to obtain by directly looking at the combinatorial structure of their bottleneck matrices.

Given ℓ rooted trees $T_1, T_2, \ldots, T_\ell$ having roots $r_1, r_2, \ldots, r_\ell$, their *rooted sum* $\boxplus_{i=1}^{\ell} T_i$ is the rooted tree obtained by joining $r_1, r_2, \ldots, r_\ell$ to an additional vertex r, which we take as the root. Given two rooted trees T_1 and T_2, their *rooted product* $T_1 \boxtimes T_2$ is the rooted tree obtained from T_1 by identifying each of its vertices with the root of a copy of T_2. We let the root of $T_1 \boxtimes T_2$ be the root of the copy of T_2 identified with the root of T_1. In [5], certain upper and lower bounds for the Perron value of these constructions were obtained. For completeness, we state those results below.

Proposition 3.1 *([5]). Let $T_1, T_2, \ldots, T_\ell$ be rooted trees having orders $n_1, n_2, \ldots, n_\ell$, and let $n = \sum_{i=1}^{\ell} n_i + 1$. Then*

$$\max_{1\le i\le \ell} \rho(T_i) \le \rho\left(\boxplus_{i=1}^{\ell} T_i\right) \le \max_{1\le i\le \ell} \rho(T_i) + n.$$

We remark that the bounds in Proposition 3.1 come from the analysis of the *neckbottle matrix* – a matrix that has the same spectrum as the bottleneck matrix and is in some cases easier to study since, unlike the bottleneck matrix, it can have zero blocks.

The quantity $H(T)$ appearing in the next result is the *Perron entropy* of the rooted tree T. It was defined in [5] as $H(T) = (e^T w)^2/\|w\|^2$, where w is a Perron vector for the bottleneck matrix of T.

Proposition 3.2 *([5]). Let T_1 and T_2 be rooted trees having orders n_1 and n_2. Then*

$$\begin{aligned} &(i) && \rho(T_1 \boxtimes T_2) \ge n_2\rho(T_1); \\ &(ii) && \rho(T_1 \boxtimes T_2) \ge \rho(T_2) + (\rho(T_1) - 1)H(T_2); \\ &(iii) && \rho(T_1 \boxtimes T_2) < n_2\rho(T_1) + \rho(T_2). \end{aligned}$$

The proofs of Proposition 3.3 and Proposition 3.4 exploit the fact that starlike trees and regular caterpillars can be obtained through the constructions considered above: A starlike tree is a rooted sum of stars, while a regular caterpillar can be seen both as a (recursive) rooted sum and as a rooted product of suitable rooted trees.

Let $n_1, n_2, \ldots, n_k$ be positive integers. The *starlike tree* $S(n_1, n_2, \ldots, n_k)$ is the rooted tree that results from the stars $S_{n_1}, S_{n_2}, \ldots, S_{n_k}$ by connecting their centers to an extra vertex r which we take as the root, see [14]. An example of starlike tree can be seen in Fig. 8.

Proposition 3.3. *Let $n = \sum_{i=1}^{k} n_i + 1$ and suppose $n_M = \max_{i=1,\ldots,k} n_i$. Then*

$$\begin{aligned} \frac{1}{2}(n_M + 1 + \sqrt{n_M^2 + 2n_M - 3}) &\le \rho(S(n_1, n_2, \ldots, n_k)) \\ &\le n + \frac{1}{2}(n_M + 1 + \sqrt{n_M^2 + 2n_M - 3}). \end{aligned}$$

Proof. Observe that

$$S(n_1, n_2, \ldots, n_k) = \boxplus_{i=1}^{k} S_{n_i}.$$

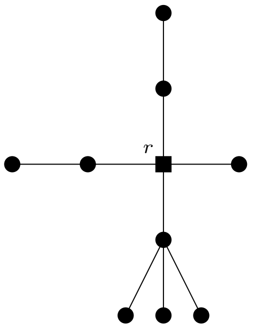

Fig. 8. Starlike tree $S(2, 1, 4, 2)$.

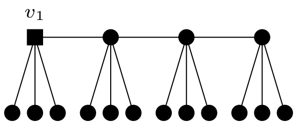

Fig. 9. Regular caterpillar $C_{4,3}$.

The result then follows from Proposition 3.1 and the known formula (1) for the Perron value of stars. □

A *caterpillar* $C(n_1, n_2, \ldots, n_k)$ is a rooted tree consisting of a path $P = v_1, v_2, \ldots, v_k$ for some k and, for each $i \leq k, n_i \geq 0$ additional vertices attached to v_i. P is called the *central path* and v_1 is the root of the tree. We consider here a special case of caterpillars where $n_1 = n_2 = \cdots = n_k = p > 0$, which we call *regular caterpillars* (see Fig. 9). Let us denote such a tree by $C_{k,p}$. Observe that the number of vertices in $C_{k,p}$ is $n = k + pk$.

Proposition 3.4. *Let $k \geq 1$, $p \geq 1$ be integers. Then*

$$\begin{aligned} &U1.\ \ \rho(C_{k,p}) \leq 1 + (p+1)\tfrac{k^2+k}{2} \\ &U2.\ \ \rho(C_{k,p}) < (p+1)\rho(P_k) + \rho(S_{p+1}) \\ &L1.\ \ \rho(C_{k,p}) \geq (p+1)\rho(P_k) \\ &L2.\ \ \rho(C_{k,p}) \geq \rho(S_{p+1}) + (\rho(P_k) - 1)H(S_{p+1}) \end{aligned}$$

where

$$H(S_{p+1}) = \frac{\left(p^2 + 4p + 3\right)\sqrt{p^2 + 4p} + p^3 + 6p^2 + 9p + 2}{(p+3)\sqrt{p^2 + 4p} + p^2 + 5p + 4}. \tag{13}$$

Proof. We first prove U1 by induction on k. If $k = 1$, $C_{k,p} = S_{p+1}$. Using either the exact expression for the Perron value of stars or the bound $\rho(S_n) \leq 1 + n$ pointed out in [5, Example 2], we see that

$$\rho(C_{k,p}) = \rho(S_{p+1}) \leq p + 2 = 1 + (p+1)\frac{k^2 + k}{2}.$$

Let now $k \geq 2$, and suppose the bound in U1 holds for regular caterpillars whose central path length is at most $k - 1$. Let $\mathcal{E}$ be the trivial rooted tree (of order 1). Observe that $C_{k,p} = \boxplus_{i=1}^{p+1} T_i$, where $T_i = \mathcal{E}$ for $i = 1, 2, \ldots, p$, and $T_{p+1} = C_{k-1,p}$. Using Proposition 3.1 and the inductive hypothesis, we find

$$\rho(C_{k,p}) = \rho\left(\boxplus_{i=1}^{p+1} T_i\right) \le (p+1)k + \max_{1\le i\le p+1} \rho(T_i) = (p+1)k + \rho(C_{k-1,p})$$
$$\le (p+1)k + 1 + (p+1)\frac{(k-1)^2 + (k-1)}{2} = 1 + (p+1)\frac{k^2+k}{2}.$$

We next explain the details in this computation. The first equality is true because $C_{k,p} = \boxplus_{i=1}^{p+1} T_i$. The first inequality is Proposition 3.1. The second equality is true because the bottleneck matrix of $\mathcal{E}$ (i.e., the matrix [1]) is a principal submatrix of the bottleneck matrix of $\rho(C_{k-1,p})$, and hence $\rho(\mathcal{E}) \le \rho(C_{k-1,p})$. Therefore, $\max_{1\le i\le p+1} \rho(T_i) = \rho(C_{k-1,p})$. The last inequality follows by applying the inductive hypothesis on $\rho(C_{k-1,p})$, and the last equality is a simplification.

To prove the other three bounds, we observe that $C_{k,p} = P_k \boxtimes S_{p+1}$, and we directly apply Proposition 3.2. The Perron entropy $H(S_{p+1})$ of the star S_{p+1} was computed in [5, Proposition 2.4] and yields the expression (13). The Perron values of the star and the path are given in (1) and (2), respectively. □

Observation 3.5. Both the two upper bounds (U1 and U2) and the two lower bounds (L1 and L2) in Proposition 3.4 are incomparable. For example, for the regular caterpillar $C_{2,1}$, the values of the bounds in U1, U2, L1, and L2 are 7, 7.854..., 5.236..., and 5.683..., respectively (while the true value is $\rho(C_{2,1}) = 5.783\ldots$). However, for $C_{6,2}$, we find the values 64, 55.353..., 51.621..., and 51.435... (while the true value is $\rho(C_{6,2}) = 52.292\ldots$). □

Observation 3.6. Using the expression for the combinatorial Perron value ρ_c of the path, we obtain

$$\rho(P_k) \ge \rho_c(P_k) = \frac{2k^2+2k+1}{5} > \frac{2}{5}(k^2+k). \tag{14}$$

Here the first inequality follows from the fact that ρ_c is a lower bound on ρ, as stated in the Introduction. The expression $\rho_c(P_k) = (2k^2+2k+1)/5$ was found in [3, Proposition 3.1].

Combining the bounds U1 and L1 of Proposition 3.4 and using (14), we find the following simple interval for the Perron value of $C_{k,p}$:

$$\rho(C_{k,p}) \in \left[0.4(p+1)(k^2+k), 0.5(p+1)(k^2+k)+1\right].$$

The upper bound in the expression above is U1 from Proposition 3.4. The lower bound follows from L1 by plugging in it the lower bound on $\rho(P_k)$ stated in (14). □

4. Further bounds for the Perron value of broom trees

In this section we present lower and upper bounds for the Perron value of the broom trees $B(k,\ell)$, which we already considered in Section 2.3.

Let T be a rooted tree of order n and let $M=[m_{ij}]$ be its bottleneck matrix. Let also $R=(r_1,r_2,\dots,r_n)$ be the row-sum vector of M, so that $R=Me$. From [4,16], we have that

$$\left((1/n)\sum_{i=1}^{n} r_i^2\right)^{1/2} \le \rho(M) \le \max_{1\le j\le n}\sum_{i=1}^{n} m_{ij}\sqrt{\frac{r_j}{r_i}}. \tag{15}$$

Observe that the lower bound in (15) is $\|Me\|/\|e\|=\pi_e(M)$. We now focus on the upper bound in (15). Notice that the maximum in its expression is necessarily attained in a pendent vertex. We can apply this bound to the rooted broom to obtain the following result.

Proposition 4.1. *Let $B(k,\ell)$ be a rooted broom, and let M be its bottleneck matrix. Then*

$$\rho(M) \le k\ell+1+\sum_{i=1}^{k}\sqrt{i\,\frac{k^2+k+2k\ell+2}{2k+2\ell-i+1}}.$$

Proof. Based on what we noticed above, we can let the vertex j attaining the maximum in (15) be one of the ℓ extra pendent vertices. Observe that if $\alpha>k$

$$r_\alpha=\sum_{i=1}^{k} i+(\ell-1)k+k+1=\frac{1}{2}(k^2+k+2k\ell+2)$$

and if $1\le\alpha\le k$

$$r_\alpha=\sum_{i=1}^{\alpha} i+(k+\ell-\alpha)\alpha=\frac{1}{2}(2k\alpha+2\ell\alpha-\alpha^2+\alpha).$$

Hence, we can write the upper bound in (15) as

$$\begin{aligned}\sum_{i=1}^{k+\ell} m_{ij}\sqrt{\frac{r_j}{r_i}} &= \sum_{i=1}^{k} m_{ij}\sqrt{\frac{r_j}{r_i}}+\sum_{\substack{k+1\le i\le k+\ell\\ i\ne j}} m_{ij}\sqrt{\frac{r_j}{r_i}}+m_{jj}\sqrt{\frac{r_j}{r_j}}\\ &= \sum_{i=1}^{k} i\sqrt{\frac{k^2+k+2k\ell+2}{2ki+2\ell i-i^2+i}}+\sum_{\substack{k+1\le i\le k+\ell\\ i\ne j}} k+k+1\end{aligned}$$

$$= k\ell + 1 + \sum_{i=1}^{k} \sqrt{i \frac{k^2 + k + 2k\ell + 2}{2k + 2\ell - i + 1}}$$

as desired. □

We tested computationally the upper bound in Proposition 4.1 on the same test cases as for the bound in Corollary 2.5. Both for $k = 25$ and $k = 100$ the average RG was ca 23%, so the bound in Proposition 4.1 is clearly inferior to the other.

The next result gives a lower bound for the Perron value of $B(k, \ell)$. This bound depends only on the eigenvalues of a 2×2 matrix. The tool used here is the interlacing of eigenvalues for the quotient matrix of a symmetric partitioned matrix [11, p. 594]. Let $n_1, n_2, \ldots, n_r$ be positive integers, and define $n = \sum_{i=1}^{r} n_i$. Consider the partitioning of a symmetric matrix M of order n into blocks

$$M = [M_{ij}]_{1 \le i,j \le r},$$

where M_{ij} is a matrix of size $n_i \times n_j$ and $M_{ij} = M_{ji}^T$ $(i, j \le r)$. The quotient matrix $Q = [q_{ij}]$ of M is the $r \times r$ matrix whose (i, j)'th entry is the average of the row sums of M_{ij}, that is:

$$q_{ij} = \frac{1}{n_i} e_{(n_i)}^T M_{ij} e_{(n_j)} \quad (i, j \le r).$$

As shown in [11, Corollary 2.3], all the eigenvalues of Q interlace the eigenvalues of M.

Lemma 4.2. [11] *Let M be a symmetric partitioned matrix of order n with eigenvalues $\beta_1 \ge \beta_2 \ge \cdots \ge \beta_n$ and let Q be its quotient matrix of order $r < n$ with eigenvalues $\nu_1, \nu_2, \ldots, \nu_r$. Then $\beta_i \ge \nu_i \ge \beta_{n-r+i}$ for $i = 1, 2, \ldots, r$.*

We now prove the mentioned lower bound on $\rho(M)$, when M is the bottleneck matrix of $B(k, \ell)$.

Proposition 4.3. *Let M be the bottleneck matrix of a rooted broom $B(k, \ell)$. Then*

$$\rho(M) \ge \gamma(k, \ell)$$

where

$$\gamma(k,\ell) = \frac{1}{2}\left\{\frac{2k^2+3k+1}{6} + \ell k + 1 + \left[\left(\frac{2k^2+3k+1}{6} - (\ell k+1)\right)^2 + \ell(k+1)(k^2+k)\right]^{1/2}\right\}.$$

Proof. The bottleneck matrix M of $B(k, \ell)$ can be partitioned into block form as shown in (11) and (12). Then, the entries of the quotient matrix are

$$\begin{aligned} q_{11} &= \tfrac{1}{k}\left[\sum_{i=1}^{k} i^2\right], \\ q_{12} &= \tfrac{1}{k}\left[\left(\tfrac{k^2+k}{2}\right)\ell\right], \\ q_{21} &= \tfrac{1}{\ell}\left[\ell\left(\tfrac{k^2+k}{2}\right)\right], \\ q_{22} &= \tfrac{1}{\ell}\left[\ell(\ell k+1)\right] \end{aligned}$$

so that the quotient matrix is

$$\begin{bmatrix} \frac{2k^2+3k+1}{6} & \frac{\ell(k+1)}{2} \\ \frac{k^2+k}{2} & \ell k+1 \end{bmatrix}.$$

Since, as is readily seen, for a nonnegative 2×2 matrix

$$\rho\left(\begin{bmatrix} a_{ii} & a_{ij} \\ a_{ji} & a_{jj} \end{bmatrix}\right) = \frac{1}{2}\left\{a_{ii} + a_{jj} + \left[(a_{ii} - a_{jj})^2 + 4a_{ij}a_{ji}\right]^{1/2}\right\},$$

it follows by interlacing that

$$\rho(M) \geq \frac{1}{2}\left\{\frac{2k^2+3k+1}{6} + \ell k + 1 + \left[\left(\frac{2k^2+3k+1}{6} - (\ell k+1)\right)^2 + \ell(k+1)(k^2+k)\right]^{1/2}\right\}. \quad \square$$

Remark 4.4. From Proposition 4.3, by dropping some nonnegative terms, we obtain a simple lower bound on $\gamma(k, \ell)$ (and, hence, on $\rho(M)$):

$$\begin{aligned} \gamma(k, \ell) &\geq \frac{1}{2}\left\{\frac{2k^2+3k+1}{6} + \ell k + 1 + \left[\left(\frac{2k^2+3k+1}{6} - (\ell k+1)\right)^2\right]^{1/2}\right\} \\ &= \frac{2k^2+3k+1}{6}, \end{aligned}$$

and this simple lower bound approximates $\gamma(k, \ell)$ well when ℓ is small compared to k. $\square$

5. Combinatorial Perron parameters for some classes of trees

In this section, we present exact values for some of the combinatorial Perron parameters introduced in [2] and [3]. In particular, we present the exact value for $\pi_e(T)$ when T is a broom tree, as well as the exact values for $\pi_e(T)$ and $\rho_c(T)$ when T is a regular caterpillar. These parameters were demonstrated to be good lower bounds for the Perron values of these rooted trees (see [2,3]). All the exact expressions obtained here were tested using MATLAB and Maple.

5.1. Broom trees

In [2], the combinatorial Perron value $\rho_c(B(k,\ell))$ of a broom tree $B(k,\ell)$ was determined. Here, we compute $\pi_e(B(k,\ell))$.

Proposition 5.1. *Consider the broom $B(k,\ell)$. Then*

$$\pi_e(B(k,\ell)) = \frac{1}{\sqrt{k+\ell}}\sqrt{\Psi_1+\Psi_2}$$

where

$$\Psi_1 = \frac{1}{30}k + \frac{1}{6}k^2 + \frac{1}{3}k^3 + \frac{2}{15}k^5 + \frac{1}{3}k^4 + \frac{7}{12}k^2\ell + \frac{1}{6}\ell^2 k + \frac{5}{12}\ell\, k^4 + \frac{5}{6}\ell\, k^3 + \frac{1}{3}\ell^2 k^3 + \frac{1}{2}\ell^2 k^2 + \frac{1}{6}k\ell,$$
$$\Psi_2 = \ell\left(\frac{k^2+k}{2} + \ell k + 1\right)^2.$$

Proof. First note that the bottleneck matrix M of $B(k,\ell)$ satisfies

$$Me = \begin{bmatrix} p \\ q \end{bmatrix},$$

where $p = (p_i) \in \mathbb{R}^k$ and $q = (q_i) \in \mathbb{R}^\ell$ are given by

$$p_i = \sum_{j=1}^{i} j + i(k-i) + i\ell \qquad i = 1, 2, \ldots, k,$$
$$q_i = \frac{k^2+k}{2} + \ell k + 1 \qquad i = 1, 2, \ldots, \ell.$$

Therefore,

$$\pi_e(B(k,\ell)) = \frac{1}{\sqrt{k+\ell}}\sqrt{\sum_{i=1}^{k}\left(\sum_{j=1}^{i} j + i(k-i) + i\ell\right)^2 + \ell\left(\frac{k^2+k}{2} + \ell k + 1\right)^2}.$$

Setting

$$\Psi_1 = \sum_{i=1}^{k}\left(\sum_{j=1}^{i} j + i(k-i) + i\ell\right)^2 \quad \text{and} \quad \Psi_2 = \ell\left(\frac{k^2+k}{2} + \ell k + 1\right)^2$$

and using the expressions in (3) yields the desired result. □

5.2. Regular caterpillars

In this section, we calculate $\rho_c(C_{k,p})$ and $\pi_e(C_{k,p})$, where $C_{k,p}$ is the regular caterpillar considered in Section 3. Recall that the order of $C_{k,p}$ is $n = k + pk$.

Proposition 5.2. *For the regular caterpillar $C_{k,p}$, we have*

$$\rho_c(C_{k,p}) = \frac{\phi_2}{\phi_1},$$

where

$$\begin{aligned}\phi_1 =& \frac{1}{6}(2k^3 + 9k^2 + 13k)p + \frac{1}{6}(2k^3 + 3k^2 + k),\\ \phi_2 =& \frac{1}{30}k + \frac{1}{6}k^2 + \frac{1}{3}k^4 + \frac{1}{3}k^3 + \frac{12}{5}pk + \frac{29}{12}k^2p + \frac{3}{4}k^4p^2 + \frac{13}{12}k^4p + \frac{3}{2}k^3p^2 + \frac{11}{6}k^3p\\ &+ \frac{5}{4}k^2p^2 + \frac{11}{30}p^2k + \frac{2}{15}k^5 + \frac{2}{15}k^5p^2 + \frac{4}{15}k^5p.\end{aligned}$$

Proof. We shall use the alternative expression for ρ_c found in [3]: $\rho_c(C_{k,p}) = (\sum_i \sigma_i^2)/(\sum_i d_i^2)$, where d_i is the number of vertices in the path $\mathcal{P}_i$ joining i to the root, $\sigma_i = \sum_{j:j\preceq i} d_j$, and $j \preceq i$ means that j is below i in the sense that the path $\mathcal{P}_i$ is contained in the path $\mathcal{P}_j$. The vector $d = (d_i)$ for $C_{k,p}$ has the following expression:

$$d = (1, 2, \dots, k, \underbrace{2, \dots, 2}_{p}, \underbrace{3, \dots, 3}_{p}, \dots, \underbrace{k+1, k+1, \dots, k+1}_{p}).$$

Therefore,

$$\begin{aligned}\phi_1 = \sum_{i=1}^{n} d_i^2 = S_k^{(2)} + \sum_{i=1}^{k} p(i+1)^2 = (1+p)S_k^{(2)} + 2pS_k^{(1)} + kp\\ = \frac{1}{6}(2k^3 + 9k^2 + 13k)p + \frac{1}{6}(2k^3 + 3k^2 + k).\end{aligned}$$

Now we calculate the numerator $\sum_{i=1}^{n} \sigma_i^2$. For $i \in \{1, \dots, k\}$,

$$\begin{aligned}\sigma_i^2 &= (\sum_{j:j\preceq i} d_j)^2 = (\sum_{j=i}^{k} j + \sum_{j=i}^{k} p(j+1))^2 = (\sum_{j=i}^{k} j + p\sum_{j=i}^{k} j + p\sum_{j=i}^{k} 1)^2\\ &= \left(\frac{(p+1)(k+i)(k-i+1)}{2} + p(k-i+1)\right)^2\\ &= \frac{(p+1)^2}{4}i^4 + \left(-\frac{(p+1)^2}{2} + p(p+1)\right)i^3\end{aligned}$$

$$+\left(\frac{(p+1)^2}{4}(-2k^2-2k+1)+p(p+1)(-k-2)+p^2\right)i^2$$
$$+\left(\frac{(p+1)^2}{4}(2k^2+2k)+p(p+1)(-k^2+1)+p^2(-2k-2)\right)i$$
$$+\left(\frac{(p+1)^2}{4}(k^4+2k^3+k^2)+p(p+1)(k^3+2k^2+k)+p^2(k^2+2k+1)\right).$$

We obtain

$$\begin{aligned}
\phi_2 &= \sum_{i=1}^{n}\sigma_i^2=\sum_{i=1}^{k}\sigma_i^2+\sum_{i=k+1}^{n}\sigma_i^2\\
&= \frac{(p+1)^2}{4}\left(\frac{6k^5+15k^4+10k^3-k}{30}\right)\\
&\quad+\left(-\frac{(p+1)^2}{2}+p(p+1)\right)\left(\frac{k^4+2k^3+k^2}{4}\right)\\
&\quad+\left(\frac{(p+1)^2}{4}(-2k^2-2k+1)+p(p+1)(-k-2)+p^2\right)\left(\frac{2k^3+3k^2+k}{6}\right)\\
&\quad+\left(\frac{(p+1)^2}{4}(2k^2+2k)+p(p+1)(-k^2+1)+p^2(-2k-2)\right)\left(\frac{k^2+k}{2}\right)\\
&\quad+\left(\frac{(p+1)^2}{4}(k^4+2k^3+k^2)+p(p+1)(k^3+2k^2+k)+p^2(k^2+2k+1)\right)k\\
&\quad+p(2^2+3^2+\ldots+(k+1)^2)\\
&= \frac{1}{30}k+\frac{1}{6}k^2+\frac{1}{3}k^4+\frac{1}{3}k^3+\frac{12}{5}pk+\frac{29}{12}k^2p+\frac{3}{4}k^4p^2+\frac{13}{12}k^4p+\frac{3}{2}k^3p^2+\frac{11}{6}k^3p\\
&\quad+\frac{5}{4}k^2p^2+\frac{11}{30}p^2k+\frac{2}{15}k^5+\frac{2}{15}k^5p^2+\frac{4}{15}k^5p,
\end{aligned}$$

as desired. □

Proposition 5.3. *For the regular caterpillar $C_{k,p}$, we have*

$$\pi_e(C_{k,p})=\sqrt{\frac{4\,(p+1)^3\,k^4+10\,(p+1)^3\,k^3+(10p^3+50p^2+50p+10)\,k^2+(5p^3+45p^2+45p+5)\,k+p^3+13p^2+43p+1}{30p+30}}.$$

Proof. Observe, as noted in the proof of Proposition 3.4, that $C_{k,p}=P_k\boxtimes S_{p+1}$. Letting M_1 and M_2 denote the bottleneck matrices of P_k and S_{p+1}, respectively, and using [5, Proposition 4.8], we find that the bottleneck matrix of $C_{k,p}$ is (permutationally similar to)

$$M=I_k\otimes M_2+(M_1-I_k)\otimes J_{p+1},$$

where $\otimes$ denotes the Kronecker product of matrices. Observe that M_1 corresponds to $A^{(k)}$ in (12), while $M_2 = J_{p+1} + I_{p+1} - e_1 e_1^T$ (with e_1 the first standard unit vector of size $p+1$). Hence,

$$\begin{aligned} M &= I_k \otimes (J_{p+1} + I_{p+1} - e_1 e_1^T) + (A^{(k)} - I_k) \otimes J_{p+1} \\ &= A^{(k)} \otimes J_{p+1} + I_k \otimes (I_{p+1} - e_1 e_1^T). \end{aligned}$$

Since $e_{(n)} = e_{(k)} \otimes e_{(p+1)}$, using the well-known multiplication rules for Kronecker products, we obtain

$$\begin{aligned} Me_{(n)} &= (A^{(k)} \otimes J_{p+1} + I_k \otimes (I_{p+1} - e_1 e_1^T))(e_{(k)} \otimes e_{(p+1)}) \\ &= (A^{(k)} e_{(k)}) \otimes (J_{p+1} e_{(p+1)}) + (I_k e_{(k)}) \otimes ((I_{p+1} - e_1 e_1^T) e_{(p+1)}) \\ &= (p+1)\vartheta \otimes e_{(p+1)} + e_{(k)} \otimes e_{(p+1)} - e_{(k)} \otimes e_1, \end{aligned}$$

where we have denoted $A^{(k)} e_{(k)}$ by ϑ for the sake of simplicity. As a consequence, we find

$$\begin{aligned} &\|Me_{(n)}\|^2 = (Me_{(n)})^T Me_{(n)} \\ =&[(p+1)\vartheta^T \otimes e_{(p+1)}^T + e_{(k)}^T \otimes e_{(p+1)}^T - e_{(k)}^T \otimes e_1^T] \\ &\times [(p+1)\vartheta \otimes e_{(p+1)} + e_{(k)} \otimes e_{(p+1)} - e_{(k)} \otimes e_1] \\ =&(p+1)^2(\vartheta^T\vartheta)(e_{(p+1)}^T e_{(p+1)}) + (p+1)(\vartheta^T e_{(k)})(e_{(p+1)}^T e_{(p+1)}) - (p+1)(\vartheta^T e_{(k)})(e_{(p+1)}^T e_1) \\ &+ (p+1)(e_{(k)}^T \vartheta)(e_{(p+1)}^T e_{(p+1)}) + (e_{(k)}^T e_{(k)})(e_{(p+1)}^T e_{(p+1)}) - (e_{(k)}^T e_{(k)})(e_{(p+1)}^T e_1) \\ &- (p+1)(e_{(k)}^T \vartheta)(e_1^T e_{(p+1)}) - (e_{(k)}^T e_{(k)})(e_1^T e_{(p+1)}) + (e_{(k)}^T e_{(k)})(e_1^T e_1) \\ =&(p+1)^3\vartheta^T\vartheta + (p+1)^2\vartheta^T e_{(k)} - (p+1)\vartheta^T e_{(k)} + (p+1)^2 e_{(k)}^T \vartheta + k(p+1) - k \\ &- (p+1)e_{(k)}^T\vartheta - k + k \\ =&(p+1)^3\vartheta^T\vartheta + (2p^2 + 2p)\vartheta^T e_{(k)} + kp. \end{aligned}$$

Observe that

$$\vartheta^T e_{(k)} = e_{(k)}^T A^{(k)} e_{(k)} = \sum_{i=1}^{k} i^2 = S_k^{(2)}.$$

Moreover, the i'th entry of ϑ is

$$\vartheta_i = \sum_{j=1}^{i} j + i(k-i) = i(k - i/2 + 1/2)$$

so that

$$\vartheta^T\vartheta = \sum_{i=1}^{k} \vartheta_i^2 = \sum_{i=1}^{k} \left[i^2(k-i/2+1/2)^2\right] = \sum_{i=1}^{k} \left[i^2\left(k^2+i^2/4+1/4-ik+k-i/2\right)\right]$$
$$= (1/4)S_k^{(4)} - (k+1/2)S_k^{(3)} + (k^2+k+1/4)S_k^{(2)}.$$

The result follows by using the formulae (3) and recalling that

$$\pi_e(C_{k,p}) = \frac{\|Me_{(n)}\|}{\|e_{(n)}\|} = \frac{\|Me_{(n)}\|}{\sqrt{k+pk}}. \quad \square$$

Declaration of competing interest

No competing interest.

Acknowledgements

We thank two referees for a number of very useful comments and suggestions.

Enide Andrade is supported by Portuguese funds through the CIDMA - Center for Research and Development in Mathematics and Applications, and the Portuguese Foundation for Science and Technology (FCT-Fundação para a Ciência e a Tecnologia), within project UIDB/04106/2020. Lorenzo Ciardo was supported by a University of Oslo PhD Fellowship and by funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (grant agreement No 714532).

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