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Locating the eigenvalues of trees

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ABSTRACT

We give an $O(n)$ method that computes, for any tree T and interval (α, β), how many eigenvalues of T lie within the interval. Our method is based on Sylvester's Law of Inertia. We use our algorithm to show that the nonzero eigenvalues of a caterpillar are simple. It follows that caterpillars having b back nodes, where $b > 2\sqrt{\Delta - 1}$, are not integral. We also show that among the regular caterpillars $C(b,k)$ formed by adjoining k legs to each of b back nodes, all positive roots are in the interval $\left(\sqrt{k} - 1, \sqrt{k} + 2\right)$, and $C(b,k)$ is not integral if $b > 2$.

1. Introduction

Given $G = (V, E)$, an undirected graph with vertices $V = (v_1, \ldots, v_n)$ and edge set E, the *adjacency matrix* $A = [a_{ij}]$ of G is the $n \times n$ 0–1 matrix for which $a_{ij} = 1$ if and only if v_i is adjacent to v_j (that is, there is an edge between v_i and v_j). A value λ is an *eigenvalue* of G if $\det(\lambda I_n - A) = 0$, and since A is real symmetric its eigenvalues are real. A graph G is called *integral* if all its eigenvalues are integers. In this paper, a graph is always a *tree*, i.e., a connected, acyclic graph. It is well-known that if λ is an eigenvalue of a tree T, then $-\lambda$ is also an eigenvalue ([2], Lemma 1).

Eigenvalues of trees have been studied in [8–12]. The main idea of our paper, which we describe in Section 2, is an algorithm for computing the number of eigenvalues in any interval (α, β) for a tree T. Of course, this can be done by other methods. For example, one could obtain the characteristic polynomial $\chi(\lambda)$ of T and then compute the Sturm sequence of χ. But to just obtain χ, requires $O(n \log^2 n)$ time [3]. Our method is simple and takes only $O(n)$ operations. It is based on diagonalizing the matrix $A + \alpha I$, and is inspired by the bottom-up algorithms in [5,6].

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As an application, we obtain some new results about *caterpillars*. For purposes of this paper, a caterpillar is a tree formed by taking a path P_b and adding *at least one leaf* to each node in the path. We call the nodes in P_b *back* nodes, and we call the appendant leaves *legs*. In Section 4, we show that the nonzero eigenvalues of a caterpillar are simple. It follows that a caterpillar having b back nodes where $b > 2\sqrt{\Delta - 1}$ is not integral. In Section 5, we consider so-called regular caterpillars $C(b, k)$, formed by adding exactly k legs to each node in P_b. We show that all positive eigenvalues are in the interval $\left(\sqrt{k} - 1, \sqrt{k} + 2\right)$, and that $C(b, k)$ is not integral if $b > 2$.

2. Diagonalizing $A + \alpha I$

Let T be a tree with adjacency matrix A, and let (α_1, α_2) be a real interval. Our goal is to compute the number of eigenvalues of T in (α_1, α_2). This seems difficult to do directly.

We consider the matrix $B_\alpha = A + \alpha I$ for some scalar α. Recall that two real symmetric matrices R and S are *congruent* if there exists a nonsingular matrix P with $R = P^T SP$. We compute a diagonal matrix D which is congruent to B_α, as follows.

The tree is rooted at an arbitrary vertex, and vertices are ordered $v_1, \ldots, v_n$ so that if v_i is a child of v_k then $k > i$. We store with each vertex v, its diagonal value $d(v)$. Initially, $d(v) = \alpha$, for all $v \in V$. The algorithm, shown in Figure 1, then processes the vertices bottom-up, operating directly on the tree.

If a parent v_k has all children with nonzero diagonal elements, each child may be used to annihilate its own two off-diagonal entries. For example, if node v_j, with parent v_k has diagonal value $d(v_j) \neq 0$, then the following row and column operations remove the one's at entries kj and jk.

$$R_k \leftarrow R_k - \frac{1}{d(v_j)} R_j$$
$$C_k \leftarrow C_k - \frac{1}{d(v_j)} C_j$$

```
Input:  tree T, scalar α
Output:  diagonal matrix D congruent to A(T) + αI

Algorithm Diagonalize(T, α)
   initialize d(v) := α, for all vertices v
   order vertices bottom up
   for  k = 1 to n
      if v_k is a leaf then continue
      else if d(c) ≠ 0 for all children c of v_k then
         d(v_k) := d(v_k) − Σ 1/d(c), summing over all children of v_k
      else
         select one child v_j of v_k for which d(v_j) = 0
         d(v_k) := −1/2
         d(v_j) := 2
         if v_k has a parent v_l, remove the edge v_k v_l.
   end loop
```

Fig. 1. Diagonalizing $A + \alpha I$.

The ordering of the vertices avoids fill-in. Assuming all children c of node v_k have nonzero diagonal values, then collectively

$$d(v) - \sum_{c \in C} \frac{1}{d(c)}. \tag{1}$$

The difficulty occurs when there exists a child v_j of v_k with $d(v_j) = 0$. Assume v_i and v_j are children of v_k, whose parent is v_l. One such child v_j having $d(v_j) = 0$ is selected. The vertex v_j may be used to annihilate the two off-diagonal entries of any other child v_i, as follows:

$$\begin{aligned} R_i &\leftarrow R_i - R_j \\ C_i &\leftarrow C_i - C_j \end{aligned}$$

The vertex v_j is then used to also annihilate the two entries representing the edge between v_k and its parent v_l:

$$\begin{aligned} R_l &\leftarrow R_l - R_j \\ C_l &\leftarrow C_l - C_j \end{aligned}$$

These last two operations effectively remove the edge from v_k to its parent v_l. Although this disconnects the graph, it is not a problem. At this point, the submatrix with rows and columns i, j, k, l has been transformed as

$$\begin{array}{c} i \\ j \\ k \\ l \end{array} \begin{bmatrix} c & & 1 & \\ & 0 & 1 & \\ 1 & 1 & \alpha & 1 \\ & & 1 & \alpha \end{bmatrix} \longrightarrow \begin{array}{c} i \\ j \\ k \\ l \end{array} \begin{bmatrix} c & & 0 & \\ & 0 & 1 & \\ 0 & 1 & \alpha & 0 \\ & & 0 & \alpha \end{bmatrix}$$

Next, the following operations

$$\begin{aligned} R_k &\leftarrow R_k - \frac{\alpha}{2} R_j \\ C_k &\leftarrow C_k - \frac{\alpha}{2} C_j \end{aligned}$$

produce:

$$\begin{array}{c} i \\ j \\ k \\ l \end{array} \begin{bmatrix} c & & 0 & \\ & 0 & 1 & \\ 0 & 1 & 0 & 0 \\ & & 0 & \alpha \end{bmatrix}$$

And then the operations

$$\begin{aligned} R_j &\leftarrow R_j + R_k \\ C_j &\leftarrow C_j + C_k \\ R_k &\leftarrow R_k - \frac{1}{2} R_j \\ C_k &\leftarrow C_k - \frac{1}{2} C_j \end{aligned}$$

yield the diagonalized form

$$\begin{array}{c} i \\ \\ j \\ \\ k \\ \\ l \end{array} \begin{bmatrix} c & & 0 & \\ & 2 & 0 & \\ 0 & 0 & -\frac{1}{2} & 0 \\ & & 0 & \alpha \end{bmatrix}$$

The particular values 2 and $-\frac{1}{2}$ are not too important, but their signs are important. The net effect is that $d(v_j) = -\frac{1}{2}$ and $d(v_k) = 2$. If v_k is not the root, then the edge incident to its parent is removed. All other children of v_k are unaffected, including those that might also have zero values. The above comments justify the Theorem 1.

Theorem 1. *For inputs T, α, where T is a tree with adjacency matrix A, algorithm* `Diagonalize` *computes a diagonal matrix D, which is congruent to $A + \alpha I$.*

The following theorem is sometimes called Sylvester's Law of Inertia.

Theorem 2 ([1, p. 336])**.** *Two $n \times n$ real symmetric matrices are congruent if and only if they have the same number of positive eigenvalues and the same number of negative eigenvalues.*

Theorem 3. *Let D be the diagonal matrix produced by* `Diagonalize` *$(T, -\alpha)$, for T a tree.*

(i) The number of positive entries in D is the number of eigenvalues of T greater than α.
(ii) The number of negative entries in D is the number of eigenvalues of T less than α.
(iii) If there are j zero entries in D, then α is an eigenvalue of T with multiplicity j.

Proof. Let A be the adjacency matrix of T, having eigenvalues

$$\lambda_1 \geqslant \lambda_2 \cdots \geqslant \lambda_n \tag{2}$$

and let

$$\beta_1 \geqslant \beta_2 \cdots \geqslant \beta_n \tag{3}$$

be the eigenvalues of $B_{-\alpha}$. Note that $\beta_i = \lambda_i - \alpha$. Thus $\lambda_i > \alpha$ if and only if $\beta_i > 0$. Now let

$$d_1, d_2, \ldots, d_n \tag{4}$$

be the diagonal elements of D. By Theorem 1, D and $B_{-\alpha}$ are congruent. By Theorem 2, the number of positive values in (4) is exactly the same number of positive terms in (3), which is the same number of terms in (2) that are greater than α. This establishes part **i**. Part **ii** is similar. To establish part **iii**, if 0 appears in (4) j times, then by Theorem 2, it appears in (3) j times as well. Thus α appears j times in (2). □

Corollary 1. *The number of eigenvalues in an interval (α_1, α_2) is the number of positive entries in the diagonalization of $B_{-\alpha_1}$, minus the number of negative entries in the diagonalization of $B_{-\alpha_2}$.*

This observation shows that we may determine the number of eigenvalues in a finite interval by making two calls to algorithm `Diagonalize`.

3. Example

As an example, consider the tree shown in the left of Fig. 2. Setting $\alpha = 0$ we diagonalize and obtain the forest in the right side of the figure, concluding that the original tree has two positive eigenvalues.

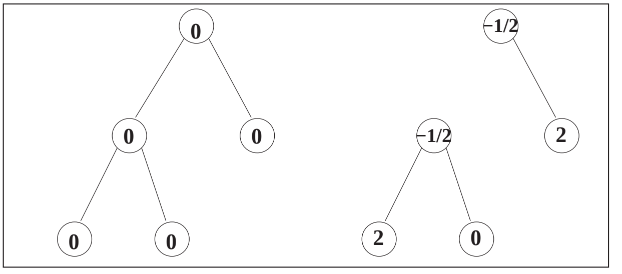

Fig. 2. Two positive eigenvalues.

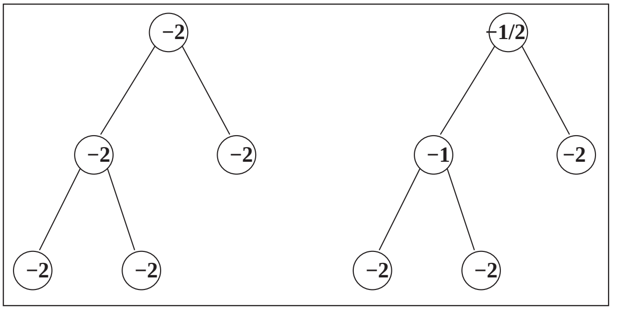

Fig. 3. All eigenvalues less than 2.

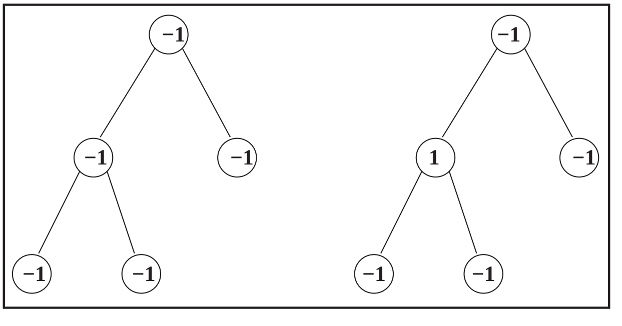

Fig. 4. One eigenvalue greater than 1.

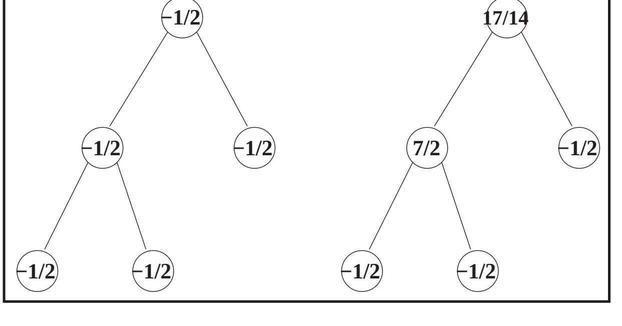

Fig. 5. Two eigenvalues greater than $\frac{1}{2}$.

The computation in Fig. 3 shows that no eigenvalue is greater than 2. From the computation shown in Fig. 4, we learn that one positive eigenvalue is greater than 1. In Fig. 5 we learn that two are greater than $\frac{1}{2}$. We can conclude that one positive eigenvalue is in $\left(\frac{1}{2}, 1\right)$ and one is in (1,2). It can be shown that this tree has eigenvalues $0, \pm\sqrt{2 \pm \sqrt{2}}$.

4. Caterpillars

Let C be a caterpillar whose back nodes are $v_1, \ldots, v_n$. Caterpillars having only one back node and k legs are *stars* with nonzero eigenvalues $\pm\sqrt{k}$, and hence are integral when k is a perfect square. Caterpillars having two back nodes with k_1 and k_2 legs are known [12] to be integral if and only if there exist integers a and b such that

$$\begin{aligned} k_1 + k_2 + 1 &= a^2 + b^2 \\ k_1 k_2 &= a^2 b^2 \end{aligned} \tag{5}$$

It is easy to show that when $k = k_1 = k_2$, the caterpillar will be integral if and only if $4k + 1$ is a perfect square. In studying the Diophantine system (5), Graham found all possible solutions, and characterized them as values of Chebyshev polynomials [4].

From here on, we will root caterpillars at their right-most back node and diagonalize from left to right.

Lemma 1. *If $\lambda \neq 0$ is an eigenvalue of a caterpillar C, then* `Diagonalize` *with input (C, λ) produces exactly one zero entry, at the root of C.*

Proof. At least one zero must appear on the diagonal. Since the caterpillar's legs were initially $\lambda \neq 0$, they will never change and will remain nonzero. If a zero appears on any back node the algorithm will replace it by 2 unless it appears at the root, in which case the algorithm will leave it unchanged. □

Lemma 2. *In tree a T having maximum degree Δ we have $\lambda_1 \leqslant 2\sqrt{\Delta - 1}$.*

Proof. See [7], Proposition 3.1 (iii). □

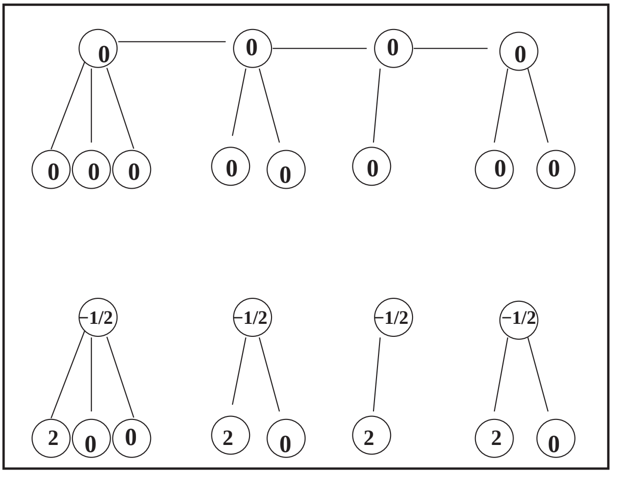

Fig. 6. Diagonalized caterpillar with $\alpha = 0$.

Theorem 4. *In any caterpillar, the nonzero eigenvalues are simple. Moreover, a caterpillar having b back nodes has b positive eigenvalues and b negative eigenvalues.*

Proof. Let λ be a nonzero eigenvalue of a caterpillar. By Lemma 1, only one zero will appear on the diagonal. By Theorem 3(iii), since the diagonal has a single zero, λ is simple. To prove the second statement, let $\alpha = 0$, and observe that the algorithm will produce exactly b positive values and b negative values. This is illustrated in Fig. 6. $\square$

Corollary 2. *In a caterpillar C having b back nodes, and having maximum degree* Δ*, there must exist non-integer eigenvalues if* $b > 2\sqrt{\Delta - 1}$.

Proof. By Theorem 4, C has b positive distinct eigenvalues. By Lemma 2, they are bounded by $2\sqrt{\Delta - 1}$. There are exactly $\lfloor 2\sqrt{\Delta - 1} \rfloor$ positive integers in this range, and $b > \lfloor 2\sqrt{\Delta - 1} \rfloor$. By the pigeon-hole principle at least one eigenvalue must be non-integer. $\square$

5. Regular caterpillars

Let $C(b, k)$ be the caterpillar with b back nodes $v_1, \ldots, v_b$, each of which have $k \geqslant 1$ legs. We call these *regular* caterpillars. As usual, we diagonalize from left to right. If the nodes are initialized with α, denote by α_i the (diagonal) value which occurs at back node v_i. Assuming that $\alpha_1, \alpha_2, \ldots, \alpha_{b-1}$ are all nonzero, we have, using (1),

$$\alpha_1 = \alpha - \frac{k}{\alpha} = \frac{\alpha^2 - k}{\alpha} \tag{6}$$

$$\alpha_2 = \alpha - \frac{k}{\alpha} - \frac{1}{\alpha_1} = \alpha_1 - \frac{1}{\alpha_1} \tag{7}$$

$$\vdots$$

$$\alpha_b = \alpha_1 - \frac{1}{\alpha_{b-1}} \tag{8}$$

Lemma 3. *All positive eigenvalues of* $C(b, k)$ *are greater than* $\sqrt{k} - 1$.

Proof. We may assume $k > 1$, for otherwise the statement is trivially true. From Theorem 3, it suffices to show that the values (6)–(8) are all positive when $\alpha = -\sqrt{k} + 1$. Note that

$$\alpha_1 = \frac{\alpha^2 - k}{\alpha} = \frac{1 - 2\sqrt{k}}{1 - k} = \frac{1 - \sqrt{k}}{1 - \sqrt{k}} + \frac{\sqrt{k}}{\sqrt{k} - 1} > 2.$$

By induction, suppose that $\alpha_j > 1$. Then $\alpha_{j+1} = \alpha_1 - \frac{1}{\alpha_j} > 2 - 1 = 1$, completing the proof. $\square$

Lemma 4. *All eigenvalues of* $C(b, k)$ *are less than* $\sqrt{k} + 2$.

Proof. Again by Theorem 3, it suffices to prove that the values (6)–(8) are all negative when $\alpha = -\sqrt{k} - 2$. Note $\alpha \neq 0$ since $k > 0$. Then

$$\alpha_1 = \frac{\alpha^2 - k}{\alpha} = \frac{\left(-\sqrt{k} - 2\right)^2 - k}{-\sqrt{k} - 2} = \frac{4 + 4\sqrt{k}}{-\sqrt{k} - 2} = \frac{2\left(2 + \sqrt{k}\right)}{-2 - \sqrt{k}} < -2.$$

By induction, if $\alpha_j < -1$ then $\alpha_{j+1} = \alpha_1 - \frac{1}{\alpha_j} < -2 + 1 < -1$, completing the proof. $\square$

From Lemma 3 and Lemma 4, we have:

Theorem 5. *All positive eigenvalues of $C(b,k)$ are located in the interval* $\left(\sqrt{k}-1, \sqrt{k}+2\right)$.

Corollary 3. *For $b \geqslant 3$ and $k \geqslant 1$, no caterpillar $C(b,k)$ is integral.*

Proof. Since there are only two integer values in the interval

$$\left(\sqrt{k}-1, \sqrt{k}+2\right),$$

and there are $b \geqslant 3$ distinct eigenvalues of $C(b,k)$ in this interval, at least one of them has to be non-integral. □

6. Conclusions

Our method for locating eigenvalues is efficient and simple enough that it can be performed by hand for small trees. By using the algorithm, together with a binary search, one can approximate a single eigenvalue. The diagonalization method does not depend on all diagonal elements initially being equal, so the method has potential for other kinds of matrices, for example the Laplacian. Theorem 5 can be used, along with interlacing, to approximate eigenvalues of non-regular caterpillars since any caterpillar can be sandwiched between two regular caterpillars.

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