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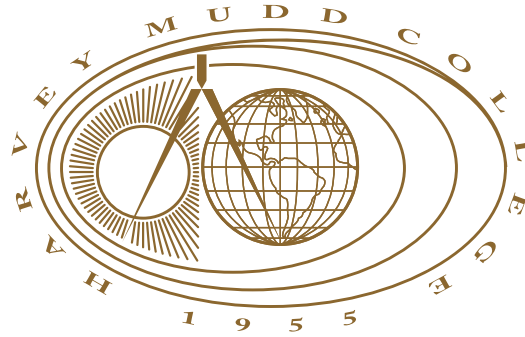
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# The Singular Values of the Exponentiated Adjacency Matrices of Broom-Tree Graphs

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May, 2006

**HARVEY MUDD**  
**C O L L E G E**

Department of Mathematics

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# Abstract

In this paper, we explore the singular values of adjacency matrices  $\{A_n\}$  for a particular family  $\{G_n\}$  of graphs, known as broom-trees. The singular values of a matrix  $M$  are defined to be the square roots of the eigenvalues of the symmetrized matrix  $M^T M$ . The matrices we are interested in are the symmetrized adjacency matrices  $A_n^T A_n$  and the symmetrized exponentiated adjacency matrices  $B_n^T B_n = (e^{A_n} - I)^T (e^{A_n} - I)$  of the graphs  $G_n$ . The application of these matrices in the HITS algorithm for Internet searches suggests that we study whether the largest two eigenvalues of  $A_n^T A_n$  (or those of  $B_n^T B_n$ ) can become close or in fact coincide.

We have shown that for one family of broom-trees, the ratio of the two largest eigenvalues of  $B_n^T B_n$  as the number  $n$  of nodes (more specifically, the length  $\ell$  of the graph) goes to infinity is bounded below one. This bound shows that for these graphs, the second largest eigenvalue remains bounded away from the largest eigenvalue. For a second family of broom-trees it is not known whether the same is true. However, we have shown that for that family a certain later eigenvalue remains bounded away from the largest eigenvalue. Our last result is a generalization of this latter result.



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# Acknowledgments

I would like to thank Professor Lesley Ward for her tireless efforts and for motivating my work on this thesis. Without her, none of this would have been possible. I am also sincerely grateful to Claire Connelly for her expertise in  $\text{\LaTeX}$ . A big thanks to Böttcher and Grudsky for writing their book on Toeplitz matrices as it was the most used reference in this thesis.



# Chapter 1

## Introduction

This thesis addresses the multiplicity of the largest, or leading, eigenvalue of particular  $n \times n$  matrices in the limit as  $n \rightarrow \infty$ . Chapter 1 contains the question that will be the main focus of this thesis and an application of this problem. In Chapter 2 are some examples of the objects we will consider. Chapter 3 is an interesting section on the numbering of the nodes in a graph. Chapter 4 contains some definitions fundamental to the proofs in this thesis. In Chapter 5 we show our final results for this problem as described in the abstract. Chapter 6 has two conjectures on the eigenvalues of  $B^TB$  and an open question relating to this thesis. The appendix contains the MATLAB m-file we used to calculate the eigenvalues and leading eigenvectors of  $B^TB$  and  $BB^T$ . The bibliography is annotated to explain the significance of each reference.

### 1.1 The Question

A graph  $G$  is made up of vertices, or nodes, and edges connecting them. The corresponding adjacency matrix is denoted  $A = A(G)$ . See Chapter 2 for examples.

**Definition 1.1.** A *directed graph*, or *digraph*, is a graph whose edges are directed. A *simple* directed graph is a directed graph having no repeated edges.

In this thesis, we will consider only simple directed graphs.

**Definition 1.2.** The *adjacency matrix* of a simple directed graph is a matrix  $A$  where the  $a_{ij}$ th entry is 1 if there is a directed edge from vertex  $i$  to vertex  $j$  and 0 otherwise. (See Chapter 2 for examples.)

## 2 Introduction

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We will also consider the matrix  $B$  defined by

$$B = e^A - I = A + A^2/2! + A^3/3! + \dots$$

We call  $B$  the *exponentiated adjacency matrix* of the graph  $G$ . In (Farahat et al., 2006), it is proven that the matrices  $BB^T$  and  $B^TB$  have simple, or nonrepeated, leading eigenvalues if the graph  $G$  is weakly connected. For some graphs, the leading eigenvalues of  $AA^T$  and  $A^TA$  are repeated. (For any matrix  $M$ ,  $M^TM$  and  $MM^T$  have the same eigenvalues. See Theorem 2.1.)

**Definition 1.3.** The *leading or dominant eigenvalue* of a matrix whose eigenvalues are real is the largest eigenvalue of the matrix. Similarly, a *leading eigenvector* is an eigenvector in the eigenspace corresponding to the leading eigenvalue. For an  $n \times n$  matrix whose eigenvalues are real, we denote the eigenvalues as

$$\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n.$$

We will use  $\vec{v}_i(M)$  to denote an eigenvector of  $M$  corresponding to  $\lambda_i(M)$ . The notation  $\alpha(h, \ell, b)$  will denote the ratio  $\lambda_2/\lambda_1$  of  $B^TB$  corresponding to the graph  $G_{h,\ell,b}$ .

**Definition 1.4.** A *simple* eigenvalue is one which is not repeated.

As the number of nodes  $n$  goes to infinity for a particular family of graphs, it can be observed that the second leading eigenvalue  $\lambda_2 = \lambda_2(B^TB)$  of  $B^TB$  becomes increasingly close to the leading eigenvalue  $\lambda_1 = \lambda_1(B^TB)$  of  $B^TB$ . As observed in (Farahat et al., 2006), the eigenvalues of  $B^TB$  are real and non-negative since  $B^TB$  is real and symmetric; the same is true for  $A^TA$ .

**Definition 1.5.** A matrix  $M$  is *symmetric* if  $M = M^T$ .

If the ratio of  $\lambda_2$  to  $\lambda_1$  is not bounded above by a number less than one, then “in the limit” the leading eigenvalue will be repeated. Since this applies to the eigenvalues of  $B^TB$ , the same is true for the singular values of  $B$ .

**Definition 1.6.** (Böttcher and Grudsky, 2000, page 78) The  *$i$ th singular value* of a matrix  $M$  is the square root of the  *$i$ th eigenvalue* of  $M^TM$ . That is,

$$\sigma_i(M) = \sqrt{\lambda_i(M^TM)}.$$

In this thesis we will mostly discuss the eigenvalues of matrices  $M^TM$ ; we emphasize that this is equivalent to discussing the singular values of  $M$ .

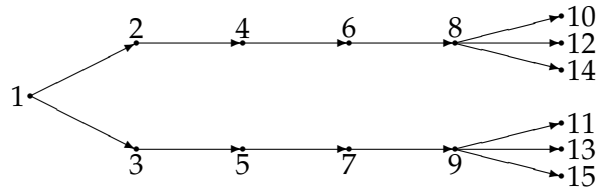


Figure 1.1: The graph  $G_{h,\ell,b} = G_{2,4,3}$ .

Several authors have found upper bounds for leading eigenvalues of the adjacency matrices of certain trees and other graphs. For instance, Hofmeister finds upper bounds for the leading and second leading eigenvalues of an adjacency matrix based on the number of vertices of a tree in (Hofmeister, 1997). A lower bound on the leading eigenvalue and an upper bound on the second leading eigenvalue would put an upper bound on the ratio of the two. There are also several articles on improved bounds, bounds on the eigenvalues of other types of graphs, Laplacian eigenvalues, etc. (See the bibliography.) Böttcher and Grudsky (Böttcher and Grudsky, 2000) discuss bounds on the singular values of Toeplitz matrices  $T$  (Definition 4.1), which are equivalent to bounds on the eigenvalues of  $T^T T$ . As far as the author of this thesis knows, no other bounds are known for the eigenvalues of the symmetrized adjacency matrix  $A^T A$  nor for the eigenvalues of  $B$  or  $B^T B$ .

We define the degree of a vertex in a directed graph.

**Definition 1.7.** In a directed graph, the *in-degree* of a vertex  $v$  is the number of edges pointing to  $v$ . The *out-degree* of a vertex  $v$  is the number of edges pointing away from  $v$ . The *degree* (or *total degree*) of a vertex  $v$  is the sum of the in-degree and out-degree of  $v$ .

We denote by  $G_{h,\ell,b}$  the family of directed trees that we consider in this thesis. Here  $h$ ,  $\ell$ , and  $b$  are positive integers. One node in  $G_{h,\ell,b}$  has out-degree  $h$  and in-degree zero. Each of the  $h$  nodes it points to begins a chain of  $\ell + 1$  nodes, each of which has in-degree one and each of which except the  $\ell^{\text{th}}$  has out-degree one. The  $\ell^{\text{th}}$  node in each of these chains has out-degree  $b$ .

The example  $G_{2,4,3}$  from this family of trees is shown in Figure 1.1. When viewing these graphs with the first node at the top and the  $h$  handles extending down, they look like brooms with multiple handles. This is where the name *broom-tree graphs* comes from. The parameters  $h$ ,  $\ell$ , and  $b$  that are taken directly from the structure of the graph correspond to the



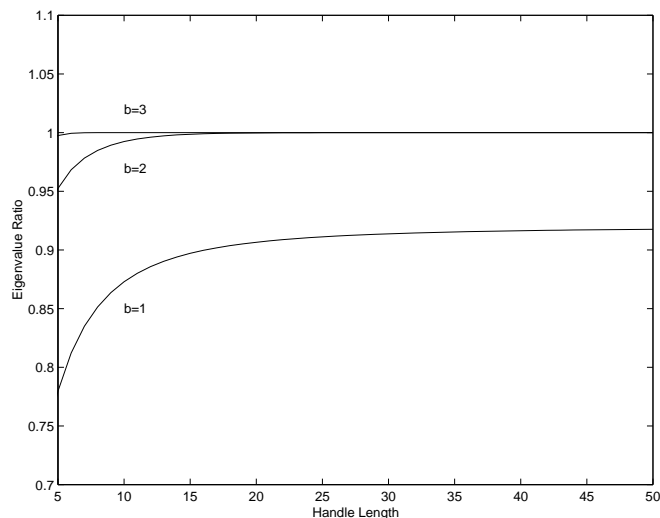


Figure 1.2: The ratio  $\lambda_2/\lambda_1$  of  $B^TB$  for different values of  $b$  (Farahat et al., 2006).

number of handles, the length, and the number of bristles at the end of each handle of the graph, respectively. We do not consider broom-trees in which different handles have different numbers of bristles.

For the family of trees  $G_{h,\ell,b}$ , as  $\ell \rightarrow \infty$ , the leading and second leading eigenvalues of  $B^TB$  seem to become increasingly close. Specifically, numerical experiments using Matlab (Farahat et al., 2006) suggest that  $\lambda_2/\lambda_1$  tends to one for  $b = 1, 2$ , and  $3$ . The results can be seen in Figure 1.2. The question addressed in this thesis is whether  $\lambda_2/\lambda_1$  does in fact have limit 1, as  $\ell \rightarrow \infty$ , for subfamilies of these graphs.

## 1.2 Application: The HITS Internet Search Algorithm

Internet search engines such as Google and Teoma use particular algorithms to rank web pages based on their relevance to a given search query. Teoma for instance, which has now merged with Ask.com, uses the Hypertext Induced Topic Search, or HITS, algorithm developed by Kleinberg in (Kleinberg, 1999). Briefly stated, this algorithm uses the symmetrized adjacency matrix  $A^TA$  of the graph of web pages to calculate the rankings of the pages in the graph. When the leading eigenvalue of  $A^TA$  is repeated,

the ranking of these web pages is not unique (Farahat et al., 2006). This implies that the same search query entered at different times, or on a different computer, could potentially produce web pages ranked in different orders. To prevent the repetition of the dominant eigenvalue, the matrix  $B^TB$  can be used in place of  $A^TA$ , where  $B$  is as defined above (Farahat et al., 2006).

Here is a more detailed explanation of the HITS algorithm. A search term, or query, is fed into the algorithm by the user. An algorithm that finds pages that mention the query is used to retrieve the set  $S$  consisting of these pages. This set  $S$  is then enlarged to a set  $T$  by adding in pages that link to or are linked to by pages in  $S$ . Kleinberg (Kleinberg, 1999) calls  $S$  the *root set* and  $T$  the *base set*. Typically,  $T$  has 3000–5000 pages. (This is different from Google’s PageRank algorithm in that PageRank first ranks all of the pages in its database, currently about 8 billion pages of the 11.5 billion indexable pages on the Internet (Gulli and Signorini, 2005), instead of looking at a subset of the pages (Brin and Page, 1998).) HITS now ranks the pages of  $T$  in the following way. The pages in  $T$  and the links between them are represented by a graph  $G$  where the pages in  $T$  are the nodes of  $G$  and the hyperlinks between the pages are the (directed) edges of  $G$ . The nodes are numbered.

To each page HITS assigns two nonnegative numbers less than or equal to one, known as the authority weight and the hub weight of the page. The authority and hub vectors are normalized column vectors that contain these values, where the  $i^{\text{th}}$  entry is the weight for the  $i^{\text{th}}$  page in  $G$ . The authority weight measures the worth of the information on the webpage about the given search term. A page that is a good authority would have an authority weight close to one (since the vectors are normalized); a poor authority would have an authority weight close to zero. The hub weight tells whether or not the web page points to good authorities. A hub weight close to one indicates a good hub.

The authority and hub vectors are initialized uniformly. The initial authority vector  $\vec{a}_0$  and the initial hub vector  $\vec{h}_0$  look like

$$\vec{a}_0 = \vec{h}_0 = \begin{bmatrix} 1/\sqrt{n} \\ 1/\sqrt{n} \\ \vdots \\ 1/\sqrt{n} \end{bmatrix},$$

where  $n$  is the number of nodes of  $G$ . The notation  $\vec{a}_0(i)$  (or similarly  $\vec{h}_0(i)$ ) denotes the  $i^{\text{th}}$  entry of the initial authority (hub) vector, which corresponds to the initial authority (hub) weight of node  $i$ . Then the HITS algorithm

updates the authority vector such that, for node  $i$ , the new authority weight  $\tilde{a}_1(i)$  is the sum of the current authority weights of all nodes  $j$  that node  $i$  points to:

$$\tilde{a}_1(i) = \sum_{j:j \rightarrow i} \vec{h}_0(j),$$

where  $j \rightarrow i$  means that there is a link from node  $j$  to node  $i$ . The hub vector is updated similarly; the new hub weight  $\tilde{h}_1(i)$  for node  $i$  is the sum of the current authority weights of all nodes  $j$  that node  $i$  points to:

$$\tilde{h}_1(i) = \sum_{j:i \rightarrow j} \tilde{a}_1(j).$$

Both vectors are then normalized so that

$$\vec{a}_1 = \frac{\tilde{a}_1}{\|\tilde{a}_1\|} \quad \text{and} \quad \vec{h}_1 = \frac{\tilde{h}_1}{\|\tilde{h}_1\|}.$$

This iteration is repeated until  $\vec{h}_n = \vec{h}_{n+1}$  and  $\vec{a}_n = \vec{a}_{n+1}$  up to some tolerance level. The sequence of computation is then  $h_0, a_1, h_1, a_2, h_2, a_3, \dots$

Let  $A$  denote the adjacency matrix of the graph  $G$ . In terms of  $A$ , the algorithm described above can be rewritten as follows. At the  $k^{\text{th}}$  iteration,

$$\vec{a}_k = \phi_k A^T \vec{h}_{k-1}, \tag{1.1}$$

$$\vec{h}_k = \psi_k A \vec{a}_k, \tag{1.2}$$

where  $\phi_k, \psi_k \in \mathbb{R}_+$  are normalization constants chosen to ensure

$$\sum_{i=1}^n \vec{a}_k(i)^2 = \sum_{i=1}^n \vec{h}_k(i)^2 = 1.$$

Focusing on the authority vector, we deduce from equation (1.1) and equation (1.2) that

$$\vec{a}_k = \phi_k \psi_{k-1} A^T A \vec{a}_{k-1}. \tag{1.3}$$

Since  $A^T A$  is a symmetric matrix ( $(A^T A)^T = A^T (A^T)^T = A^T A$ ), the following theorems apply. The proofs of these theorems can be found in (Poole, 2003).

**Theorem 1.1** (The Spectral Theorem). *Let  $M$  be an  $n \times n$  matrix with real entries. Then  $M$  is symmetric if and only if it is orthogonally diagonalizable. In particular, a real symmetric matrix  $M$  is diagonalizable.*

In particular, our  $n \times n$  matrices  $A^T A$ ,  $A A^T$ ,  $B^T B$ , and  $B B^T$  each have  $n$  real eigenvalues with full geometric multiplicity.

**Theorem 1.2.** *Let  $M$  be an  $n \times n$  diagonalizable matrix with dominant eigenvalue  $\lambda_1$ . Then for most nonzero vectors  $\vec{x}_0$ , the sequence of vectors  $\vec{x}_k$  defined by*

$$\vec{x}_1 = \frac{M\vec{x}_0}{\|M\vec{x}_0\|}, \vec{x}_2 = \frac{M\vec{x}_1}{\|M\vec{x}_1\|}, \vec{x}_3 = \frac{M\vec{x}_2}{\|M\vec{x}_2\|}, \dots, \vec{x}_k = \frac{M\vec{x}_{k-1}}{\|M\vec{x}_{k-1}\|}, \dots$$

*approaches a dominant eigenvector of  $M$ . The vectors  $\vec{x}_0$  for which this is not true have a zero component in the direction of the dominant eigenvector or eigenspace.*

This iterative method is called the *power method*, and this form of the power method uses Rayleigh quotients (Poole, 2003, page 312). In particular, the sequence  $\{\vec{a}_k\}$  determined by equation (1.3) converges to a dominant eigenvector  $\vec{v}_1$  of  $A^T A$ . Similarly, the sequence of hub vectors converges to a dominant eigenvector of  $A A^T$ .

The ranking of the webpages in  $T$  in order from the best to the worst authority on the given query is read off from the dominant eigenvector  $\vec{v}_1$  of  $A^T A$  found by the power method, as follows. Since the entries of  $\vec{v}_1$  are understood as the authority weights of the webpages in  $T$ , if the largest entry of  $\vec{v}_1$  is the  $i^{\text{th}}$  entry, then the  $i^{\text{th}}$  webpage is the best authority on the given query and would be ranked first. The second largest entry of  $\vec{v}_1$  corresponds to the webpage that is the second best authority, and so on.

If the dominant eigenvalue  $\lambda_1(A^T A)$  is repeated, there can be multiple linearly independent eigenvectors associated with this eigenvalue. The power method will then converge to an eigenvector in this eigenspace, but the one it converges to depends on the initial vector  $\vec{a}_0$ . Therefore, for Internet search rankings to be unique, it is imperative that the dominant eigenvalue of the matrix used in the iteration be simple. The rate of convergence of the HITS algorithm also depends on the ratio  $\lambda_2/\lambda_1$  of  $A^T A$ . The closer this ratio is to one, the more slowly the algorithm will converge, and vice versa. So, to have a fast algorithm that yields a unique ranking of webpages, it would be good for this ratio always to be less than one.

As noted above, it is shown in (Farahat et al., 2006) that if the HITS algorithm uses the matrix  $B = e^A - I$  instead of  $A$ , the leading eigenvalue of  $B^T B$  is simple (assuming  $G$  is weakly connected), so  $\lambda_2(B^T B)/\lambda_1(B^T B) < 1$ , and the modified "Exponentiated Input to HITS" algorithm yields a unique authority vector.



## Chapter 2

### Examples

In this chapter we present five examples of graphs  $G$  with their adjacency matrices  $A$  and exponentiated adjacency matrices  $B$ . We discuss the related eigenvalues and eigenvectors. We also present a little more theory. Table 2.1 contains the ratios  $\lambda_2/\lambda_1$  of  $B^T B$  for the graphs  $G_{h,\ell,1}$  where  $1 \leq h \leq 6$ ,  $1 \leq \ell \leq 12$ , and  $b = 1$ .

The trees  $G_{h,\ell,b}$  under consideration in this paper are what we call broom trees. The parameters of these trees are the number of handles, the length of each handle, and the number of bristles on the end of each handle. (The name originally came from looking at the trees with the first node at the top and the handles going down to the bristles, like a set of brooms tied together at the top.) Figure 2.1 shows an example of the tree  $G_{2,3,1}$  within this family of trees. This graph has an adjacency matrix that is  $9 \times 9$ , since there are  $n = 9$  nodes.

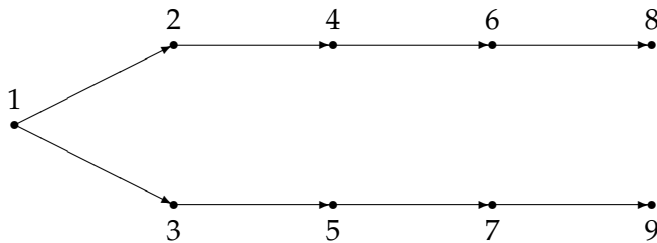


Figure 2.1: The graph  $G_{2,3,1}$ .

This graph is denoted  $G_{2,3,1}$  since it has two handles ( $h = 2$ ), length (including the bristle)  $\ell = 3$ , and one bristle at the end of each handle

( $b = 1$ ). The adjacency matrix for the graph  $G_{2,3,1}$  is

$$A = \begin{bmatrix} 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

The  $i$ th row of the adjacency matrix corresponds to the nodes that node  $i$  points to, while the  $j$ th column shows the nodes that point to node  $j$ . The exponentiated adjacency matrix is

$$B = \begin{bmatrix} 0 & 1 & 1 & 1/2 & 1/2 & 1/3! & 1/3! & 1/4! & 1/4! \\ 0 & 0 & 0 & 1 & 0 & 1/2 & 0 & 1/3! & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1/2 & 0 & 1/3! \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1/2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1/2 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

The eigenvalues of  $A^T A$ , in decreasing order, are 2, 1, 1, 1, 1, 1, 1, 0, and 0. Also, the eigenvalues of  $B^T B$ , rounded to four decimal places, are 3.1421, 2.0625, 1.6674, 0.9604, 0.8002, 0.5048, 0.4771, 0, and 0. The authority and hub vectors calculated using the exponentiated adjacency matrix are

$$\vec{a} = \vec{v}_1(B^T B) = \begin{bmatrix} 0 \\ 0.4634 \\ 0.4634 \\ 0.4197 \\ 0.4197 \\ 0.2886 \\ 0.2886 \\ 0.1604 \\ 0.1604 \end{bmatrix}, \quad \vec{h} = \vec{v}_1(B B^T) = \begin{bmatrix} 0.8215 \\ 0.3333 \\ 0.3333 \\ 0.2081 \\ 0.2081 \\ 0.0905 \\ 0.0905 \\ 0 \\ 0 \end{bmatrix}.$$

From these vectors, we can see that if the graph  $G_{2,3,1}$  were the base set  $T$  for a given query with the edges representing the hyperlinks, then nodes 2 and 3 would be the best authorities for that query and node 1 would be the best hub. The ratio of the second largest to largest eigenvalue, denoted in general by  $\alpha(h, \ell, b) = \lambda_2(B^T B) / \lambda_1(B^T B)$ , is  $\alpha(2, 3, 1) = 0.6564$ .

A confusion that can easily arise is between the eigenvalues of  $A$  and the eigenvalues of  $A^T A$ . Note that in all of the examples in this paper, the eigenvalues of  $A$  are identically zero (hence  $A$  is nilpotent) while those of  $A^T A$  are not all zero. Similarly, the singular values mentioned in this paper are those of the matrix  $A$ ; see Definition 1.6 for further clarification.

**Definition 2.1.** A *nilpotent* matrix is a square matrix  $M$  such that  $M^n$  is the zero matrix for some positive integer  $n$ . In fact, a matrix is nilpotent if and only if its eigenvalues are all zero.

It is also important to note that the eigenvalues of  $A^T A$  are the same as the eigenvalues of  $A A^T$ , and similarly those of  $B^T B$  are the same as those of  $B B^T$ . This is a special case of the following theorem.

**Theorem 2.1.** For any  $n \times n$  matrices  $A$  and  $B$ ,  $AB$  has the same eigenvalues as  $BA$ .

*Proof.* As suggested in Exercise 16 (Shifrin and Adams, 2002, §6.1), consider the  $2n \times 2n$  matrix

$$M = \begin{bmatrix} tI & A \\ B & tI \end{bmatrix}$$

where  $t \in \mathbb{R}$ . Left-multiply  $M$  by either

$$A' = \begin{bmatrix} tI & -A \\ 0 & I \end{bmatrix} \quad \text{or} \quad B' = \begin{bmatrix} I & 0 \\ -B & tI \end{bmatrix}$$

to get

$$A'M = \begin{bmatrix} t^2 I - AB & 0 \\ B & tI \end{bmatrix} \quad \text{and} \quad B'M = \begin{bmatrix} tI & A \\ 0 & t^2 I - BA \end{bmatrix}.$$

Then, taking determinants in each equation, we obtain

$$\begin{aligned} t^n \det(M) &= t^n \det(t^2 I - AB), \\ t^n \det(M) &= t^n \det(t^2 I - BA). \end{aligned}$$

So  $AB$  and  $BA$  have the same characteristic polynomial, and thus, the same eigenvalues.  $\square$

Note, however, that  $AB$  and  $BA$  may have different *eigenvectors* corresponding to the same eigenvalue.

Figure 2.2 shows a broom tree in which  $b = 2$ . Here, the adjacency matrix is  $13 \times 13$ .



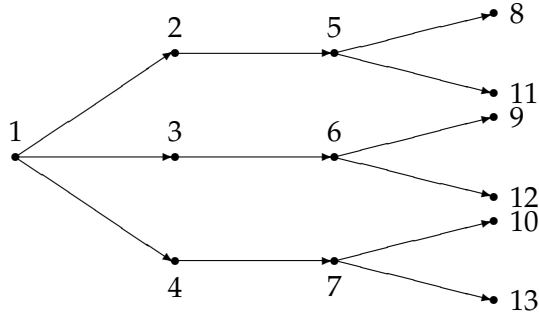


Figure 2.2: The graph  $G_{3,2,2}$ .

The number of handles of this tree is  $h = 3$ , the length is  $\ell = 2$ , and the number of bristles on each handle is  $b = 2$ . The adjacency matrix  $A$  of  $G_{3,2,2}$  is

$$A = \begin{bmatrix} 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

The exponentiated adjacency matrix  $B$  is

$$B = \begin{bmatrix} 0 & 1 & 1 & 1 & 1/2 & 1/2 & 1/2 & 1/3! & 1/3! & 1/3! & 1/3! & 1/3! & 1/3! & 1/3! \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1/2 & 0 & 0 & 1/2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1/2 & 0 & 0 & 1/2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

Here, the eigenvalues of  $A^T A$  are 3, 2, 2, 2, 1, 1, 1, and 0 with multiplicity six; the eigenvalues of  $B^T B$  are 4.7014, 2.7808, 2.7808, 2.1105, 0.7192, 0.7192,

0.6047, and 0 with multiplicity six. The authority and hub vectors are

$$\vec{a} = \vec{v}_1(B^TB) = \begin{bmatrix} 0 \\ 0.3915 \\ 0.3915 \\ 0.3915 \\ 0.3050 \\ 0.3050 \\ 0.3050 \\ 0.2086 \\ 0.2086 \\ 0.2086 \\ 0.2086 \\ 0.2086 \\ 0.2086 \end{bmatrix}, \quad \vec{h} = \vec{v}_1(BB^T) = \begin{bmatrix} 0.8489 \\ 0.2369 \\ 0.2369 \\ 0.2369 \\ 0.1924 \\ 0.1924 \\ 0.1924 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}.$$

Again, the best authorities are nodes 2, 3, and 4 and the best hub is node 1. The ratio of the second largest eigenvalue to the largest eigenvalue of  $B^TB$  is  $\alpha(3,2,2) = 0.5915$ .

$\ell$	$h$					
	1	2	3	4	5	6
1	0.37162	0.35961	0.25000	0.19098	0.15436	0.12948
2	0.46565	0.53828	0.38680	0.29919	0.24334	0.20488
3	0.56377	0.65641	0.48033	0.37338	0.30431	0.25648
4	0.64665	0.73118	0.53991	0.42036	0.34276	0.28895
5	0.71296	0.77936	0.57824	0.45040	0.36430	0.30965
6	0.76434	0.81223	0.60371	0.47030	0.38353	0.32333
7	0.80427	0.83501	0.62128	0.48399	0.39470	0.33275
8	0.83549	0.85146	0.63383	0.49377	0.40267	0.33947
9	0.86020	0.86368	0.64309	0.50099	0.40856	0.34443
10	0.87994	0.87292	0.65005	0.50641	0.41298	0.34816
11	0.89595	0.88013	0.65546	0.51062	0.41641	0.35106
12	0.90905	0.88580	0.65970	0.51393	0.41911	0.35333

Table 2.1: The ratios  $\alpha(h, \ell, 1) = \lambda_2(B^TB)/\lambda_1(B^TB)$  for the symmetrized exponentiated adjacency matrices  $B^TB$  for graphs  $G_{h,\ell,1}$ .

Table 2.1 shows the ratios  $\alpha(h, \ell, 1)$  of  $\lambda_2(B^TB)$  to  $\lambda_1(B^TB)$  for the graphs

$G_{h,\ell,1}$  for varying  $h$  and  $\ell$ . For instance, the entry 0.30431 for  $\ell = 3$  and  $h = 5$  means that for the graph  $G_{5,3,1}$  with five handles of length three including the one bristle, the ratio  $\alpha(5,3,1) = \lambda_2(B^TB)/\lambda_1(B^TB)$  of the largest two eigenvalues of  $B^TB$  is 0.30431. It is interesting to note that this ratio tends to decrease along a row (that is, as the number of handles increases) and increase along a column (as the length of the handles increases). However, from  $\ell = 2$  to  $\ell = 9$ , this ratio increases as  $h$  increases from one to two.

We present three more examples of graphs and the corresponding matrices and eigenvalues.

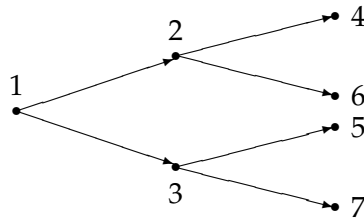


Figure 2.3: A binary tree.

Figure 2.3 shows a binary tree. This tree fits into our family of broom-tree graphs and is the one denoted by  $G_{2,1,2}$ . The associated matrices and

the eigenvalues of  $A^T A$  and  $B^T B$  are as follows.

$$\begin{aligned}
 A &= \begin{bmatrix} 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}, & B &= \begin{bmatrix} 0 & 1 & 1 & .5 & .5 & .5 & .5 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}, \\
 A^T A &= \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 \end{bmatrix}, & B^T B &= \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & .5 & .5 & .5 & .5 \\ 0 & 1 & 1 & .5 & .5 & .5 & .5 \\ 0 & .5 & .5 & 1.25 & .25 & 1.25 & .25 \\ 0 & .5 & .5 & .25 & 1.25 & .25 & 1.25 \\ 0 & .5 & .5 & 1.25 & .25 & 1.25 & .25 \\ 0 & .5 & .5 & .25 & 1.25 & .25 & 1.25 \end{bmatrix}, \\
 AA^T &= \begin{bmatrix} 2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}, & BB^T &= \begin{bmatrix} 3 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 2 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}, \\
 \lambda(A^T A) &= \{2, 2, 2, 0, 0, 0, 0\}, & \lambda(B^T B) &= \{4, 2, 1, 0, 0, 0, 0\}.
 \end{aligned}$$

The ratio of the largest two eigenvalues of  $A^T A$  is 1 while this ratio for  $B^T B$  is 0.5. This is an example where the HITS algorithm could return improper weights for the ranked web pages using  $A^T A$  but not using  $B^T B$ , since the largest eigenvalue is repeated in the first case and not in the second.

The example shown in Figure 2.4 is a slightly modified version of the previous one. We will call this tree the 3-2 tree for reasons that are clear from the figure.

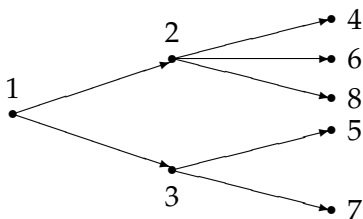


Figure 2.4: A 3-2 tree.

Again, the associated matrices and eigenvalues are below.

$$A = \begin{bmatrix} 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}, \quad B = \begin{bmatrix} 0 & 1 & 1 & .5 & .5 & .5 & .5 & .5 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix},$$

$$A^T A = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 \end{bmatrix},$$

$$B^T B = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & .5 & .5 & .5 & .5 & .5 \\ 0 & 1 & 1 & .5 & .5 & .5 & .5 & .5 \\ 0 & .5 & .5 & 1.25 & .25 & 1.25 & .25 & 1.25 \\ 0 & .5 & .5 & .25 & 1.25 & .25 & 1.25 & .25 \\ 0 & .5 & .5 & 1.25 & .25 & 1.25 & .25 & 1.25 \\ 0 & .5 & .5 & .25 & 1.25 & .25 & 1.25 & .25 \\ 0 & .5 & .5 & 1.25 & .25 & 1.25 & .25 & 1.25 \end{bmatrix},$$

$$A A^T = \begin{bmatrix} 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix},$$

$$B B^T = \begin{bmatrix} 3.25 & 1.5 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1.5 & 3 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix},$$

$$\lambda(A^T A) = \{3, 2, 2, 0, 0, 0, 0, 0\},$$

$$\lambda(B^T B) = \{4.8316, 2.3708, 1.0476, 0, 0, 0, 0, 0\}.$$

The ratio of the largest two eigenvalues is 0.6667 for  $A^T A$  and is 0.4907 for  $B^T B$ .

The last example is a diamond (Figure 2.5). The associated adjacency

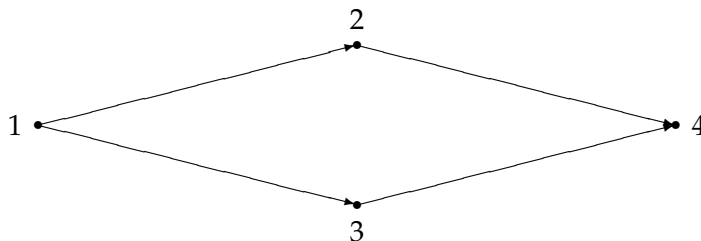


Figure 2.5: A diamond.

matrices and eigenvalues are

$$\begin{aligned}
 A &= \begin{bmatrix} 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{bmatrix}, & B &= \begin{bmatrix} 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \\
 A^T A &= \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 2 \end{bmatrix}, & B^T B &= \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 \\ 0 & 1 & 1 & 3 \end{bmatrix}, \\
 A A^T &= \begin{bmatrix} 2 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, & B B^T &= \begin{bmatrix} 3 & 1 & 1 & 0 \\ 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \\
 \lambda(A^T A) &= \{2, 2, 0, 0\}, & \lambda(B^T B) &= \{4, 1, 0, 0\}.
 \end{aligned}$$

It is interesting to note that the symmetries of the diamond graph are also apparent in the symmetries of the matrices. The shape of the graph remains the same whether it is reflected across the horizontal or vertical axis. This is also apparent algebraically:

$$\begin{aligned}
 B^T B &= W(B B^T)W, \\
 A^T A &= W(A A^T)W
 \end{aligned}$$

## 18 Examples

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where

$$W = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}.$$

## Chapter 3

# Renumbering of Nodes

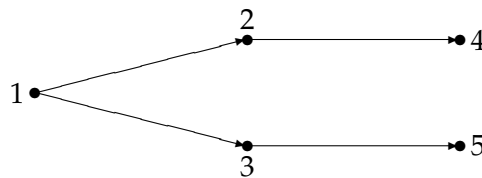


Figure 3.1: A numbering of the graph  $G_{2,1,1}$ .

The reader may wonder: what is the significance of the way the nodes are numbered? The numbering convention we have used throughout this paper is for convenience only. Renumbering the nodes of any graph should not change the eigenvalues of the adjacency matrix. For our graphs, it makes sense that renumbering the nodes should permute the rows of the dominant eigenvectors of  $B^TB$  and  $BB^T$  since the  $i$ th entry in the eigenvector corresponds to the authority or hub weight of node  $i$ . It turns out that the effect of renumbering the graph is to permute the columns and rows of the adjacency matrix using a permutation matrix, which encodes the changes made in the renumbering.

**Definition 3.1.** A *permutation matrix* is a matrix obtained by permuting the rows (or columns) of an  $n \times n$  identity matrix.

It follows from the definition that a permutation matrix is nonsingular and the determinant is always  $\pm 1$ . In addition, if the permutation of the rows of the identity matrix is identical to the permutation of the columns, the permutation matrix  $P$  satisfies  $P^TP = PP^T = I$ .



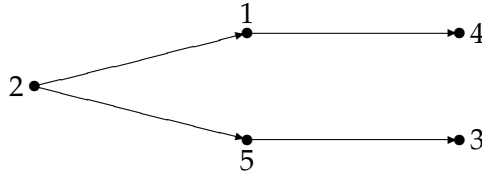


Figure 3.2: Example 1.

It is helpful to look at specific examples. Let  $A$  be the adjacency matrix of the graph in Figure 3.1, with the numbering shown there, so that

$$A = \begin{bmatrix} 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

In Example 1 (Figure 3.2), we have swapped the numbers of nodes 1 and 2 and the numbers of nodes 3 and 5. This will swap the corresponding rows and columns of the adjacency matrix. The process by which this happens is a pre- and post-multiplication of the adjacency matrix by the corresponding permutation matrix, that is, if  $A'$  is the permuted adjacency matrix, then  $A = PA'P$ . For this example,

$$A' = \begin{bmatrix} 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{bmatrix} \quad \text{and} \quad P = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{bmatrix}.$$

It is the case that, for the permutation matrices which encode the renumbering of a tree,  $A' = PAP$  since  $P = P^{-1}$ . If  $P^2 \neq I$ , then the matrix  $PAP$  is not an adjacency matrix for a tree. So  $P$  must be symmetric and involutory if it encodes a renumbering of a tree.

**Definition 3.2.** An *involutory* matrix is a square matrix  $M$  such that  $M^2 = I$ . An involutory matrix is its own inverse matrix.

It is easy to show that the characteristic polynomials of a matrix  $M$  and its permuted matrix  $M'$  are the same, which implies that the eigenvalues of

$M$  and  $M'$  are equal:

$$\begin{aligned}
 \det(M - \lambda I) &= \det(PM'P - \lambda PP) \\
 &= \det(P(M' - \lambda I)P) \\
 &= \det(P)^2 \det(M' - \lambda I) \\
 &= (\pm 1)^2 \det(M' - \lambda I) \\
 &= \det(M' - \lambda I).
 \end{aligned}$$

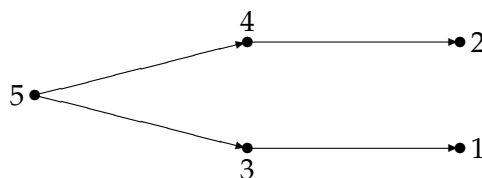


Figure 3.3: Example 2.

Figure 3.3 shows the nodes of the same tree numbered in reverse order. Again we can see that  $P^2 = I$ . This example has

$$A' = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 \end{bmatrix} \quad \text{and} \quad P = \begin{bmatrix} 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

Again, we have that  $A = PA'P$ .

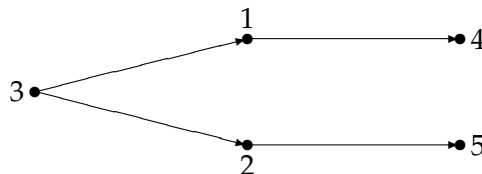


Figure 3.4: Example 3.

In our last example, shown in Figure 3.4, we consider a renumbering of the same tree where the swapping is of more than two nodes. Here, we

have cycled nodes 1, 2, and 3. In this case, we can write the permutation of  $A$  by  $A' = P_r A P_c$  where  $P_r$  is a permutation of rows corresponding to the desired row swaps in  $A$  and  $P_c$  is the column permutation matrix. Fortunately, there is still a way to find one  $P$  that is symmetric and involutory where  $A = PA'P$ . Here, the matrices are

$$A' = \begin{bmatrix} 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}, \quad P = \begin{bmatrix} 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix},$$

$$P_r = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}, \quad P_c = \begin{bmatrix} 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

With the properties of these permutation matrices, we can also show some interesting results about  $A^T A$ ,  $B = e^A - I$ , and  $B^T B$ .

**Theorem 3.1.** *Let  $P$  be a permutation matrix that is involutory, and let  $A$  be the adjacency matrix of a graph  $G_{h,\ell,b}$ . If  $A = PA'P$ , then  $A^T A = P(A')^T(A')P$  and  $(A')^T(A') = PA^T A P$ .*

*Proof.* Let  $A = PA'P$ . Then

$$\begin{aligned} A^T A &= (PA'P)^T (PA'P) \\ &= (P(A')^T P)(PA'P) \\ &= P(A')^T P P A' P \\ &= P(A')^T (A') P. \end{aligned}$$

Since  $P$  is involutory,  $(A')^T(A') = PA^T A P$ . □

**Theorem 3.2.** *Let  $P$  be a permutation matrix that is involutory and  $A$  be the adjacency matrix corresponding to a graph  $G_{h,\ell,b}$  and  $B = e^A - I$ . If  $A' = PAP$ , then  $PBP = B'$ ,  $B = PB'P$ , and  $B^T B = P(B')^T(B')P$ .*

*Proof.* Let  $A = PA'P$ . Then

$$\begin{aligned}
 PBB &= P(e^A - I)P \\
 &= P\left(A + \frac{1}{2!}A^2 + \frac{1}{3!}A^3 + \dots\right)P \\
 &= PAP + \frac{1}{2!}PAPPAP + \frac{1}{3!}PAPPAPPAP + \dots \\
 &= A' + \frac{1}{2!}(A')^2 + \frac{1}{3!}(A')^3 + \dots \\
 &= e^{A'} - I \\
 &= B'.
 \end{aligned}$$

$B = PB'P$  follows from  $P$  being involutory and  $B^TB = P(B')^T(B')P$  follows as in the proof of Theorem 3.1.  $\square$

To summarize, when the nodes of a broom-tree graph are renumbered, the new adjacency matrix  $A'$  is related to the old adjacency matrix  $A$  by a pre- and post-multiplication by the appropriate permutation matrix. The matrices  $A$  and  $A'$  have the same eigenvalues; the same is true for the two matrices  $A^TA$  and  $(A')^T(A')$ , and for the two matrices  $B = e^A - I$  and  $B' = e^{A'} - I$ , and for the two matrices  $B^TB$  and  $(B')^T(B')$ . The entries of the leading eigenvectors of  $B^TB$  and of  $(B')^T(B')$  are permuted in the same way as the numbers of the nodes, so that a given entry always corresponds to the same node.



## Chapter 4

# Toeplitz Matrices

In this chapter we introduce Toeplitz matrices, both finite and infinite, and present some of their properties. We use the following definitions and theorems to give upper bounds for the ratios described in the theorems of Chapter 5.

**Definition 4.1.** A *Toeplitz matrix* is a square matrix which has constant values along negative-sloping diagonals, i.e., a matrix of the form

$$T_n(a) = \begin{bmatrix} a_0 & a_{-1} & a_{-2} & \cdots & a_{-n+1} \\ a_1 & a_0 & a_{-1} & & \\ a_2 & a_1 & a_0 & \ddots & \vdots \\ \vdots & & \ddots & \ddots & a_{-1} \\ a_{n-1} & \cdots & a_1 & a_0 & \end{bmatrix} \quad (4.1)$$

for  $2n - 1$  real or complex numbers  $a_k, k = -n + 1, \dots, -1, 0, 1, \dots, n - 1$ , or for an infinite matrix

$$T(a) = \begin{bmatrix} a_0 & a_{-1} & a_{-2} & \cdots \\ a_1 & a_0 & a_{-1} & \cdots \\ a_2 & a_1 & a_0 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}. \quad (4.2)$$

Before defining the symbol of a Toeplitz matrix, we recall that  $L^\infty$  of a space  $X$  denotes the space of essentially bounded complex-valued functions on  $X$ , with the  $L^\infty$ -norm (see for example (Folland, 1999)). Also  $\ell^2$  is the space of square-summable sequences of complex numbers:

$$\ell^2 := \left\{ \{a_n\} \in \mathbb{C} \mid \sum_{n=1}^{\infty} a_n^2 < \infty \right\},$$

with the  $\ell^2$ -norm defined by

$$\|\{a_n\}\|_2 := \left( \sum_{n=1}^{\infty} a_n^2 \right)^{1/2}.$$

**Definition 4.2.** (Böttcher and Grudsky, 2000, page 3) If there is a function  $a$  in  $L^\infty$  of the unit circle satisfying

$$a_n = \frac{1}{2\pi} \int_0^{2\pi} a(e^{i\theta}) e^{-in\theta} d\theta, \quad n \in \mathbb{Z}, \quad (4.3)$$

for  $a_n$  in equations (4.1) and (4.2), then this function is unique. We therefore denote the matrix (4.2) and the operator it induces on  $\ell^2$  by  $T(a)$ . The function  $a$  in this context is referred to as the *symbol* of the Toeplitz matrix or operator  $T(a)$ . The symbol for any Toeplitz matrix with entries  $\{a_n\}$  is

$$a(e^{i\theta}) = \sum_{n=-\infty}^{\infty} a_n e^{ni\theta},$$

or

$$a(z) = \sum_{n=-\infty}^{\infty} a_n z^n,$$

where  $z := e^{i\theta}$ .

**Definition 4.3.** The *operator norm* of a linear operator  $T : V \rightarrow W$ , where  $V$  and  $W$  are normed vector spaces, is the largest factor by which  $T$  stretches an element of  $V$ :

$$\|T\| = \sup_{\|v\|=1} \|Tv\|.$$

When  $T$  is given by a matrix,  $Tv = Mv$ , and  $\|v\|$  is the  $\ell^2$ -norm, then  $\|T\|$  is the largest singular value of  $M$ . That is,

$$\sigma_1(M) = \sqrt{\lambda_1(M^T M)} = \|M\|.$$

For a Toeplitz matrix, the operator norm is equal to the maximum of the absolute value of the symbol for all unit vectors, as stated in (Böttcher and Grudsky, 2000, equation (1.12)).

**Definition 4.4.** Let  $M_n$  be an  $n \times n$  matrix. A *principal submatrix*  $M_{n-1}$  of  $M_n$  is obtained by omitting one row and the corresponding column of  $M_n$ .

**Definition 4.5.** (Böttcher and Grudsky, 2000, page 79) For  $j \in \{0, 1, \dots, n\}$ , let  $\mathcal{F}_j^{(n)}$  denote the collection of all  $n \times n$  matrices of rank at most  $j$ . The  $j$ th approximation number  $a_j(M_n)$  of an  $n \times n$  matrix  $M_n$  is defined by

$$a_j(M_n) = \text{dist}(M_n, \mathcal{F}_j^{(n)}) := \min\{\|M_n - F_n\| : F_n \in \mathcal{F}_j^{(n)}\}.$$

It is easy to see that  $\|M_n\| = a_0(M_n) \geq a_1(M_n) \geq \dots \geq a_n(M_n) = 0$ .

The next two equations are also used to prove Theorems 5.1 and 5.2. Equations (4.4) and (4.5) are equations (1.12) and (2.12) in (Böttcher and Grudsky, 2000), respectively. Let  $T_n(a)$  be the  $n \times n$  Toeplitz matrix with symbol  $a$ , let  $T(a)$  be the infinite Toeplitz matrix obtained by extending  $T_n$  indefinitely to the right and downward, and let  $\|\cdot\|_\infty$  be the  $L^\infty$ -norm. Then

$$\|T(a)\|_{\text{ess}} = \|a\|_\infty \quad (4.4)$$

and

$$\lim_{n \rightarrow \infty} \|T_n(a)\| = \|T(a)\|. \quad (4.5)$$

The following theorem is used in the proof of Theorem 5.1.

**Theorem 4.1.** (Böttcher and Grudsky, 2000, page 79) If  $M_n$  is an  $n \times n$  matrix, then

$$\sigma_j(M_n) = a_{j-1}(M_n)$$

for every  $j \in \{1, 2, \dots, n\}$ . (Note: The indexing we use in this thesis is slightly different from that used in (Böttcher and Grudsky, 2000).)

Here is an interesting theorem relating the eigenvalues of a matrix to the eigenvalues of a principal submatrix of that matrix.

**Theorem 4.2.** (Cauchy's Interlace Theorem, (Fisk, 2005)) If  $M$  is a Hermitian matrix and  $N$  is a principal submatrix of  $M$ , then the eigenvalues of  $N$  interlace the eigenvalues of  $M$ . That is, if  $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$  are the eigenvalues of  $M$  and  $\mu_2 \geq \mu_3 \geq \dots \geq \mu_n$  are the eigenvalues of  $N$ , then

$$\lambda_1 \geq \mu_2 \geq \lambda_2 \geq \dots \geq \mu_{n-1} \geq \lambda_{n-1} \geq \mu_n \geq \lambda_n.$$

We recall that a square matrix  $M$  is Hermitian if it is self-adjoint, that is, if  $M$  is equal to its conjugate transpose  $M^H$ .





## Chapter 5

# Results: Bounds on Ratios of Eigenvalues

In this chapter we begin by proving three useful lemmas about the structure of matrices of the form  $A^T A$  and  $A A^T$ . The heart of the chapter is the following three results. First, for the broom-tree graphs  $G_{h,\ell,1}$ , with  $h$  handles, one bristle at the end of each handle, and length  $\ell$  increasing to infinity, the ratio  $\lambda_2(B^T B)/\lambda_1(B^T B)$  of the second to the first eigenvalues of the symmetrized exponentiated adjacency matrix  $B^T B$  remains bounded above by a constant less than one. Second, for the broom-tree graphs  $G_{h,\ell,2}$ , with  $h$  handles, two bristles at the end of each handle, and length  $\ell$  increasing to infinity, the ratio  $\lambda_{h+2}(B^T B)/\lambda_1(B^T B)$  of the  $(h+2)^{\text{nd}}$  to the first eigenvalues of  $B^T B$  remains bounded below one. Third, for the broom tree  $G_{h,\ell,b}$ , with  $h$  handles,  $b$  bristles at the end of each handle, and length  $\ell$  increasing to infinity, the ratio  $\lambda_{h(b-1)+2}/\lambda_1$  of the  $(h(b-1)+2)^{\text{nd}}$  to the first eigenvalues of  $B^T B$  remains bounded below one. In Chapter 6 we discuss the open question of the behavior as  $\ell \rightarrow \infty$  of the ratio  $\lambda_2(B^T B)/\lambda_1(B^T B)$  when  $b \geq 2$ .

### 5.1 Useful Lemmas

The following lemmas are results that aid in the calculation of the entries in the types of matrices we are interested in studying.

**Lemma 5.1.** For every  $n \times m$  matrix  $M$ ,

$$(M^T M)_{ij} = \text{col}_i M \cdot \text{col}_j M,$$

$$(M M^T)_{ij} = \text{row}_i M \cdot \text{row}_j M.$$

*Proof.* Let  $\vec{v}_1, \dots, \vec{v}_m$  denote the columns of  $M$  so that

$$M = [\vec{v}_1 \ \vec{v}_2 \ \cdots \ \vec{v}_m],$$

$$M^T = \begin{bmatrix} \vec{v}_1^T \\ \vec{v}_2^T \\ \vdots \\ \vec{v}_m^T \end{bmatrix}.$$

Therefore, by simple matrix multiplication,  $(M^T M)_{ij} = \vec{v}_i^T \vec{v}_j = \vec{v}_i \cdot \vec{v}_j$  where  $\vec{v}_i$  is the  $i$ th column of  $M$ . The second part of the proof is identical except the row and column vectors are reversed.  $\square$

**Lemma 5.2.** Let  $G_{h,\ell,1}$  be the broom-tree graph with  $h$  handles of length  $\ell$  with only one bristle at the end of each handle. Let  $A$  be the adjacency matrix of  $G_{h,\ell,1}$ . Then  $AA^T$  is diagonal, and so the eigenvalues of  $AA^T$  are its diagonal entries.

*Proof.* By Lemma 5.1, the entries of  $AA^T$  are the dot products of the rows. Since there is no more than one 1 in each column of  $A$ ,  $(\text{row } i) \cdot (\text{row } j) = 0$  when  $i \neq j$ . Therefore, the only possible nonzero entries of  $AA^T$  are when  $i = j$ , yielding exactly the entries on the main diagonal of  $AA^T$ . So  $AA^T$  is diagonal. (The fact that the eigenvalues are on the diagonal is a result of basic linear algebra.)  $\square$

**Lemma 5.3.** Let  $G_{h,\ell,1}$  be the broom-tree graph with  $h$  handles of length  $\ell$  and only one bristle at the end of each handle,  $b = 1$ . Let  $A$  be the adjacency matrix of  $G_{h,\ell,1}$ . Then the entries of  $A^T A$  are 0's and 1's, and  $A^T A$  is block-diagonal of the specific form shown below.

*Proof.* Using Lemma 5.1, we can construct the following formula for the entries of  $A^T A$ :

$$(A^T A)_{ij} = \begin{cases} 1, & \text{if column } i \text{ of } A = \text{column } j \text{ of } A; \\ 0, & \text{otherwise.} \end{cases}$$

Therefore, since columns 2 through  $h + 1$  are the same (they have a one in the first row and zeros everywhere else), there will be an  $h \times h$  matrix

whose entries are all ones, in the position after the first row and column, and ones will run down the rest of the diagonal of  $A^T A$ . The remaining entries of  $A^T A$  are zero. That is,  $A^T A$  will look like

$$A^T A = \begin{bmatrix} 0 & 0 & \dots & & & 0 \\ 0 & 1 & \dots & 1 & & 0 \\ & \vdots & 1 & \vdots & & \\ \vdots & 1 & \dots & 1 & & \vdots \\ & & & & 1 & \\ & & & & & \ddots & 0 \\ 0 & 0 & \dots & & 0 & 1 \end{bmatrix}.$$

□

### 5.2 Graphs With One Bristle

In this section we establish an upper bound, strictly less than one, for the ratio  $\lambda_2(B^T B) / \lambda_1(B^T B)$ , when the number of handles in the broom tree is fixed at  $h \geq 2$ , the number of bristles on each handle is fixed at  $b = 1$ , and the length  $\ell$  of the handles tends to infinity.

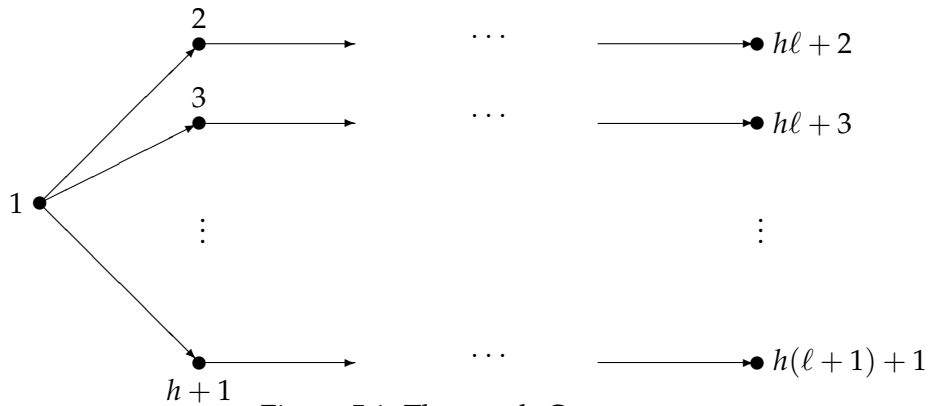


Figure 5.1: The graph  $G_{h, \ell, 1}$ .

Theorem 5.1 was proven for broom trees with two handles,  $h = 2$ , by Estelle Basor and Kent Morrison of California Polytechnic State University, San Luis Obispo. I have modified the proof to extend to any  $h \geq 2$ .

**Theorem 5.1.** Let  $G_{h,\ell,1}$  be the directed graph shown in Figure 5.1 where  $h$  is fixed and  $b = 1$ . Also let  $\lambda_j(M)$  denote the  $j^{\text{th}}$  largest eigenvalue of an  $n \times n$  matrix  $M$  and let  $B = e^A - I$  where  $A$  is the adjacency matrix corresponding to  $G_{h,\ell,1}$ . Then, for  $\ell$  sufficiently large,

$$\frac{\lambda_2(B^T B)}{\lambda_1(B^T B)} < 0.94430081$$

for all natural numbers  $h$  and  $\ell$ . In particular, for fixed  $h$  as  $\ell \rightarrow \infty$ , the ratio  $\lambda_2(B^T B) / \lambda_1(B^T B)$  remains bounded above by a constant less than one.

*Proof.* The  $n \times n$  adjacency matrix for  $G_{h,\ell,1}$  is

$$A = \begin{bmatrix} 0 & 1 & \cdots & 1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & & 0 & 1 & 0 & & 0 & 0 \\ 0 & 0 & & 0 & 0 & 1 & & 0 & 0 \\ \vdots & & & & & & \ddots & & \vdots \\ 0 & 0 & & 0 & 0 & 0 & & 1 & 0 \\ 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & 1 \\ 0 & 0 & & 0 & 0 & 0 & & 0 & 0 \\ \vdots & & & & & & & & \vdots \\ 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & 0 \end{bmatrix}$$

where  $n = h(\ell + 1) + 1$  is the number of nodes of  $G$ . There are  $h$  ones in the first row corresponding to the links from node 1 to the  $h$  handles in  $G_{h,\ell,1}$ . The matrix  $B_{h,\ell,1} = e^A - I$  is

$$B_{h,\ell,1} = \begin{bmatrix} 0 & 1 & \cdots & 1 & \frac{1}{2} & \cdots & \frac{1}{2} & \frac{1}{3!} & \cdots & \frac{1}{3!} & \cdots & \frac{1}{m!} & \cdots & \frac{1}{m!} \\ 0 & \cdots & \cdots & 0 & 1 & \cdots & 0 & \frac{1}{2} & \cdots & 0 & \cdots & \frac{1}{(m-1)!} & \cdots & 0 \\ \vdots & & & & & \ddots & \vdots & & & \ddots & \vdots & & \ddots & \vdots \\ & & & & & & 1 & 0 & \cdots & \frac{1}{2} & & & & \frac{1}{(m-1)!} \\ 0 & \cdots & & & & & & & & & & \cdots & & 0 \\ \vdots & & & & & & & & & & & & & \vdots \\ 0 & \cdots & & & & & & & & & & \cdots & & 0 \end{bmatrix}.$$

Again, in the first row, each non-zero entry is repeated  $h$  times, because the graph has  $h$  handles.

We begin by obtaining a lower bound for the largest singular value of  $B_{h,\ell,1}$ . Take a unit vector  $x \in \mathbb{R}^n$  such that  $\|B_{h,\ell,1}\| = \|B_{h,\ell,1}x\|$ . Now we let

$y = [x_1, x_2, \dots, x_n, 0, \dots, 0]^T \in \mathbb{R}^{n+h}$ . Then  $\|B_{h,\ell,1}x\| = \|B_{h,\ell+1,1}y\|$ . Therefore, since  $\|y\| = 1$ , we obtain

$$\begin{aligned} \|B_{h,\ell,1}\| &= \|B_{h,\ell,1}x\| \\ &= \|B_{h,\ell+1,1}y\| \\ &\leq \|B_{h,\ell+1,1}\| \|y\| \\ &= \|B_{h,\ell+1,1}\|. \end{aligned}$$

By a similar argument,  $\|B_{h,\ell,1}\| \leq \|B_{h+1,\ell,1}\|$ . Using MATLAB, we find that  $\|B_{2,3,1}\| \approx 1.77261 > 1.77$ . Since the operator norm of a matrix is its largest singular value,

$$\sigma_1(B_{2,3,1}) = \sqrt{\lambda_1(B_{2,3,1}^T B_{2,3,1})} > 1.77$$

for  $h \geq 2$  and  $\ell \geq 3$ .

Next we obtain an upper bound for the second largest singular value of  $B_{h,\ell,1}$ . Let the lower right principal submatrix of  $B_{h,\ell,1}$  be denoted  $T_n$ . Note that  $T_n$  is a Toeplitz matrix of size  $h(\ell+1) \times h(\ell+1)$ . The matrix representation of the Toeplitz operator  $T$  is the infinite matrix obtained by extending  $T_n$  indefinitely to the right and downward. Let  $z = e^{i\theta}$ . The symbol for  $T$  is the function

$$z^{-h} + \frac{1}{2}z^{-2h} + \dots + \frac{1}{m!}z^{-mh} + \dots = e^{1/z^h} - 1 \quad (m = 1, 2, 3, \dots)$$

since  $a(e^{i\theta}) = a(z) = e^{1/z^h} - 1$  is the function satisfying equation (4.3) for the entries of  $T_n$ . Then from Definition 4.5 and Theorem 4.1, we get the following relations for an  $n \times n$  matrix  $M_n$ :

$$\sigma_2(M_n) = a_1(M_n) = \text{dist}(M_n, \mathcal{F}_1^{(n)}) := \min\{\|M_n - F_n\| : F_n \in \mathcal{F}_1^{(n)}\}.$$

This says that the second singular value  $\sigma_2(B_{h,\ell,1})$  is the distance from  $B_{h,\ell,1}$  to the set of matrices of rank at most one. Now, we can write  $B_{h,\ell,1}$  as the sum of a rank one matrix and an augmented Toeplitz matrix. The rank one matrix is the  $n \times n$  matrix, where  $n$  is the number of nodes of  $G_{h,\ell,1}$ , that has the same first row as  $B_{h,\ell,1}$  and zeros for all other entries. The augmented Toeplitz matrix, denoted  $C_n$ , is the Toeplitz matrix  $T_n$  with an additional row of zeros at the top and column of zeros on the left. Therefore

$$B_{h,\ell,1} = \begin{bmatrix} \text{rank one} \\ \text{matrix} \end{bmatrix} + \left[ \begin{array}{c|ccc} 0 & 0 & \cdots & 0 \\ 0 & & & \\ \vdots & & & \\ 0 & & & T_n \end{array} \right],$$

and so

$$B_{h,\ell,1} - \begin{bmatrix} \text{rank one} \\ \text{matrix} \end{bmatrix} = C_n.$$

Thus  $\|C_n\| \geq \sigma_2(B_{h,\ell,1})$ . But  $\|C_n\| = \|T_n\|$  since the matrices  $C_n$  and  $T_n$  differ only by a row and column of zeros. Equations (4.4) and (4.5) in (Böttcher and Grudsky, 2000) imply that, for  $z \in \mathbb{C}$ ,

$$\lim_{n \rightarrow \infty} \|T_n\| = \|T\| = \max_{|z|=1} |e^{1/z^h} - 1|.$$

We now show that the maximum value is  $e - 1$ , and that it occurs at  $z = 1$ . Let  $f_h(z) = e^{z^{-h}} - 1$ . Then, since  $z = e^{i\theta}$  is complex,

$$f_h(e^{i\theta}) = e^{e^{-i\theta}} - 1.$$

Let

$$g_h(\theta) := |f_h(\theta)|^2 = e^{(e^{-i\theta} + e^{i\theta})} - e^{e^{i\theta}} - e^{e^{-i\theta}} + 1.$$

Then

$$g'_h(\theta) = ihe^{i\theta} e^{e^{-i\theta}} - ihe^{-i\theta} e^{e^{i\theta}}.$$

So  $g'_h(\theta) = 0$  if and only if

$$e^{e^{-i\theta}} e^{i2h\theta} = e^{e^{i\theta}}.$$

Equivalently,

$$\begin{aligned} e^{i2h\theta} &= e^{(e^{i\theta} - e^{-i\theta})} = e^{2i \sin(h\theta)}, \\ 2ih\theta &= 2i \sin(h\theta) + 2ik\pi, \quad k \in \mathbb{Z}, \\ h\theta &= \sin(h\theta) + k\pi, \end{aligned}$$

and so

$$\theta = \frac{k\pi}{h}, \quad k \in \mathbb{Z}.$$

Now

$$f_h(e^{ik\pi/h}) = \begin{cases} e - 1, & \text{if } k \text{ is even;} \\ e^{-1} - 1, & \text{if } k \text{ is odd.} \end{cases}$$

Therefore

$$\max_{|z|=1} |e^{1/z^h} - 1| = e - 1,$$

independent of the value of  $h$ .

We conclude that, for  $n$  sufficiently large,  $\|T_n\| \leq e - 1 < 1.72$ . Therefore, by Definition 4.3,  $\sigma_2(B_{h,\ell,1}) \leq \|C_n\| = \|T_n\| < 1.72$ .

These results imply that

$$\frac{\sigma_2(B_{h,\ell,1})}{\sigma_1(B_{h,\ell,1})} < \frac{1.72}{1.77} = 0.97175141\dots$$

and by Definition 1.6,

$$\frac{\lambda_2(B_{h,\ell,1}^T B_{h,\ell,1})}{\lambda_1(B_{h,\ell,1}^T B_{h,\ell,1})} < 0.94430081.$$

□

This theorem says that the lowest curve in Figure 1.2 (where  $b = 1$ ) does remain bounded by a constant less than one as  $\ell \rightarrow \infty$ .

### 5.3 Graphs With Two Bristles

Generalizing the ideas in the previous section, I have proved the following theorem for broom-tree graphs with  $b = 2$ . This theorem says that for a fixed  $h$  as  $\ell \rightarrow \infty$ , the ratio  $\lambda_{h+2}/\lambda_1$  of  $B^T B$  is bounded above by a constant less than one.

**Theorem 5.2.** *Let  $G_{h,\ell,2}$  be the directed graph shown in Figure 5.2 where  $h$  is fixed and  $b = 2$ . As usual let  $\lambda_i(M)$  denote the  $i^{\text{th}}$  largest eigenvalue of an  $n \times n$  matrix  $M$  and let  $B = e^A - I$  where  $A$  is the adjacency matrix of  $G_{h,\ell,2}$ . Then, for  $\ell$  sufficiently large,*

$$\frac{\lambda_{h+2}(B^T B)}{\lambda_1(B^T B)} < 0.85512776.$$

*Proof.* The adjacency matrix for  $G_{h,\ell,2}$  is



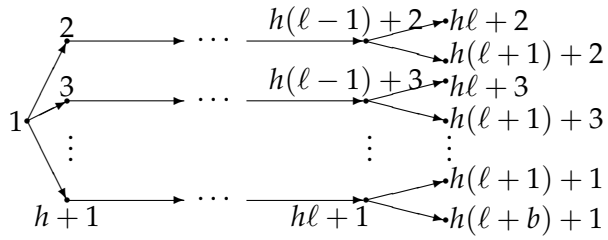


Figure 5.2: The graph  $G_{h,\ell,2}$ .

$$A = \begin{bmatrix} 0 & 1 & \dots & 1 & 0 & \dots & \dots & \dots & \dots & \dots & \dots & \dots & 0 \\ \vdots & & & 0 & 1 & 0 & & & & & & & \vdots \\ & & & & & 1 & & & & & & & \\ & & & & & & \ddots & & & & & & \\ & & & & & & & 1 & 0 & \dots & 0 & 1 & \\ & & & & & & & 1 & 0 & \dots & 0 & 1 & \\ & & & & & & & & \ddots & & & & \\ & & & & & & & & & 1 & 0 & \dots & 0 & 1 \\ 0 & \dots & \dots & \dots & \dots & \dots & \dots & 0 & \dots & \dots & \dots & \dots & 0 \\ \vdots & & & & & & & \vdots & & & & & \vdots \\ 0 & \dots & \dots & \dots & \dots & \dots & \dots & 0 & \dots & \dots & \dots & \dots & 0 \end{bmatrix}.$$

The exponentiated adjacency matrix  $B_{h,\ell,2} = e^A - I$ , where there are  $h$  of each non-zero value in the first row except for the last value where there are  $2h$  entries of this value, is

$$B = \begin{bmatrix} 0 & 1 & \dots & 1 & \frac{1}{2!} & \dots & \frac{1}{2!} & \frac{1}{3!} & \dots & \frac{1}{3!} & \dots & \dots & \dots & \dots & \frac{1}{(\ell+b-1)!} \\ \vdots & & & & 1 & & & \frac{1}{2!} & & \frac{1}{3!} & & & & & \\ & & & & & 1 & & \frac{1}{2!} & & \frac{1}{3!} & & & & & \\ & & & & & & \ddots & & & & & & & & \\ & & & & & & & \frac{1}{m!} & 0 & \dots & 0 & \frac{1}{m!} & & & \\ & & & & & & & & \ddots & & & & & & \\ & & & & & & & & & \frac{1}{m!} & 0 & \dots & 0 & \frac{1}{m!} & \\ & & & & & & & & & & \vdots & & & & \\ & & & & & & & 1 & 0 & \dots & 0 & 1 & & & \\ & & & & & & & & \ddots & & & & & & \\ & & & & & & & & & 1 & 0 & \dots & 0 & 1 & \\ & & & & & & & & & 0 & \dots & \dots & & 0 & \\ \vdots & & & & & & & & & \vdots & & & & \vdots & \\ 0 & \dots & \dots & \dots & \dots & \dots & \dots & 0 & \dots & \dots & \dots & \dots & \dots & 0 & \end{bmatrix}.$$

By the corresponding argument in the proof of Theorem 5.1, we have that  $\|B_{h,\ell,2}\| \leq \|B_{h,\ell+1,2}\|$  and  $\|B_{h,\ell,2}\| \leq \|B_{h+1,\ell,2}\|$  for all  $h \geq 1$  and  $\ell \geq 1$ . Using MATLAB, we find that  $\|B_{2,3,2}\| \approx 1.8705 > 1.86$ . Therefore, since

$$\sigma_1(B_{2,3,2}) = \sqrt{\lambda_1(B_{2,3,2}^T B_{2,3,2})} > 1.86,$$

we obtain

$$\lambda_1(B_{h,\ell,2}^T B_{h,\ell,2}) \geq \lambda_1(B_{2,3,2}^T B_{2,3,2}) > 3.46$$

for all  $h \geq 2$  and  $\ell \geq 3$ .

Now,  $B_{h,\ell,2}$  can be written as the sum of a Toeplitz matrix and a rank  $h + 1$  matrix. It is easiest to see by an example; we show this sum for the

graph  $G_{2,3,2}$ :

$$B_{2,3,2} = \begin{bmatrix} 0 & 0 & 1 & 0 & \frac{1}{2!} & 0 & \frac{1}{3!} & 0 & \frac{1}{4!} & 0 & \frac{1}{4!} \\ 0 & 0 & 0 & 1 & 0 & \frac{1}{2!} & 0 & \frac{1}{3!} & 0 & \frac{1}{4!} & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & \frac{1}{2!} & 0 & \frac{1}{3!} & 0 & \frac{1}{4!} \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & \frac{1}{2!} & 0 & \frac{1}{3!} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & \frac{1}{2!} & 0 & \frac{1}{3!} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & \frac{1}{2!} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & \frac{1}{2!} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \\
 + \begin{bmatrix} 0 & 1 & 0 & \frac{1}{2!} & 0 & \frac{1}{3!} & 0 & \frac{1}{4!} & 0 & \frac{1}{4!} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{1}{8} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{1}{8} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{1}{3} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{1}{3} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{1}{2} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

The differences between this example and the general case  $h \geq 2$  are the number of zeros before the first one in the first row and the number of zeros between each of the nonzero terms in each row. The terms in the last  $h$  columns of the rank  $h + 1$  matrix are terms in the sequence given by  $a_0 = 1$ ,  $a_n = \frac{1}{(n+1)!} - \frac{1}{n!}$  for  $n \geq 1$ . Then, if  $T_n$  ( $n$  being the number of nodes in  $G_{h,\ell,2}$ ) represents the Toeplitz part of  $B_{h,\ell,2}$ , we have

$$T_n = B_{h,\ell,2} - \begin{bmatrix} \text{rank } h + 1 \\ \text{matrix} \end{bmatrix}.$$

Notice that here  $T_n$  is  $n \times n$ , while the  $T_n$  in the proof of Theorem 5.1 was  $(n - 1) \times (n - 1)$ .

From Definition 4.5 and Theorem 4.1,

$$\begin{aligned} \sigma_{h+2}(M_n) &= a_{h+1}(M_n) \\ &= \text{dist}(M_n, \mathcal{F}_{h+1}^{(n)}) \\ &:= \min\{\|M_n - F_n\| : F_n \in \mathcal{F}_{h+1}^{(n)}\}. \end{aligned} \tag{5.1}$$

In particular, for  $M_n = B_{h,\ell,2}$ , we obtain the inequality

$$\begin{aligned}\sigma_{h+2}(B_{h,\ell,2}) &\leq \|B_{h,\ell,2} - \begin{bmatrix} \text{rank } h + 1 \\ \text{matrix} \end{bmatrix}\| \\ &= \|T_n\|,\end{aligned}$$

since the quantity  $\|B_{h,\ell,2} - \begin{bmatrix} \text{rank } h + 1 \\ \text{matrix} \end{bmatrix}\|$  falls into the set over which we are minimizing in equation 5.1.

The symbol (Definition 4.2) for  $T$ , the infinite matrix obtained by extending  $T_n$  indefinitely to the right and downward, is

$$z^{-h} + \frac{1}{2!}z^{-2h} + \cdots + \frac{1}{m!}z^{-mh} + \cdots = e^{1/z^h} - 1 \quad (m = 1, 2, 3, \dots).$$

Again, equations (4.4) and (4.5) from (Böttcher and Grudsky, 2000) imply that

$$\lim_{n \rightarrow \infty} \|T_n\| = \|T\| = \max_{|z|=1} |e^{1/z^h} - 1| = e - 1,$$

where the maximum value  $e - 1$  occurs at  $z = 1$  as shown in the proof of the previous theorem. So, for  $\ell$  sufficiently large,  $\|T_n\| \leq e - 1 < 1.72$  and  $\sigma_{h+2}(B_{h,\ell,2}) \leq \|T_n\| < 1.72$ . Therefore

$$\frac{\sigma_{h+2}(B_{h,\ell,2})}{\sigma_1(B_{h,\ell,2})} < \frac{1.72}{1.86} \approx 0.92473118,$$

and so

$$\frac{\lambda_{h+2}(B_{h,\ell,2}^T B_{h,\ell,2})}{\lambda_1(B_{h,\ell,2}^T B_{h,\ell,2})} < 0.85512776$$

for  $\ell$  sufficiently large. □

To summarize, Theorem 5.2 shows that for  $b = 2$  and fixed  $h \geq 2$ , the ratio of the  $(h + 2)^{\text{nd}}$  to the first eigenvalue of  $B^T B$  remains bounded above by a constant less than one as the length  $\ell$  of the graph  $G_{h,\ell,2}$  tends to infinity.

## 5.4 Graphs with Multiple Bristles

We conclude with our most general result, which subsumes Theorems 5.1 and 5.2 as special cases. This theorem says that for fixed  $h$  and  $b$  as  $\ell \rightarrow \infty$ , the ratio  $\lambda_{h(b-1)+2}/\lambda_1$  of  $B^T B$  is bounded above by a constant less than one.

**Theorem 5.3.** Let  $G_{h,\ell,b}$  be the general broom-tree graph with  $h$  handles,  $b$  bristles, and length  $\ell$ . Fix  $h \geq 2$  and  $b \geq 1$ . As usual let  $\lambda_j(M)$  denote the  $j^{\text{th}}$  largest eigenvalue of an  $n \times n$  matrix  $M$ , and let  $B = e^A - I$  where  $A$  is the adjacency matrix of  $G_{h,\ell,b}$ . Then there is a constant  $c_0 = c_0(h, b) < 1$  such that for  $\ell$  sufficiently large,

$$\frac{\lambda_{h(b-1)+2}(B^T B)}{\lambda_1(B^T B)} < c_0 < 1.$$

*Proof.* The proof is almost exactly the same as that of Theorem 5.2. We sketch the main points.

First,  $\|B_{h,\ell,b}\| \leq \|B_{h,\ell,b+1}\|$  for all  $b \geq 1$  by the same argument used earlier for the cases of increasing  $h$  and increasing  $\ell$ . Using MATLAB we find  $\|B_{2,3,1}\| \approx 1.77261 > 1.77$ . Hence,

$$\lambda_1(B_{h,\ell,b}^T B_{h,\ell,b}) > 1.77^2$$

for all  $h \geq 2$ ,  $\ell \geq 3$ , and  $b \geq 1$ .

Careful analysis of the form of  $B_{h,\ell,b}$  shows that  $B_{h,\ell,b}$  can be written as the sum of a Toeplitz matrix  $T_n$  and a matrix of rank  $h(b-1) + 1$ . So, as before,

$$\sigma_{h(b-1)+2}(B_{h,\ell,b}) \leq \|T_n\|.$$

The symbol of the corresponding infinite matrix  $T$  is the same as that in Theorem 5.2, and so again

$$\|T_n\| \leq e - 1 < 1.72.$$

Thus

$$\frac{\lambda_{h(b-1)+2}(B^T B)}{\lambda_1(B^T B)} < \frac{1.72^2}{1.77^2} \approx 0.94430081,$$

for  $\ell$  sufficiently large. □

## Chapter 6

# Open Questions and Future Work

Here we discuss some potential future work.

### 6.1 Two Conjectures About $\lambda_1$ and $\lambda_2$

From observations made when calculating the ratios  $\lambda_2/\lambda_1$ , I propose the following conjectures. We do not examine these conjectures for  $b > 1$ .

**Conjecture 6.1.** *Consider the graph  $G_{h,\ell,1}$  with  $b = 1$ . Fix  $h$ . Then there is a constant  $c$  such that*

$$\lambda_1(B^T B) \leq c$$

for all  $\ell$ .

This conjecture says that as  $\ell \rightarrow \infty$ , the leading eigenvalue of  $B^T B$  approaches or is equal to  $c$ .

**Conjecture 6.2.** *Let  $G_{h,\ell,1}$  denote the broom-tree graph with  $h$  handles of length  $\ell$  with one bristle at the end of each handle ( $b = 1$ ). As usual let  $\lambda_i(M)$  denote the  $i^{\text{th}}$  largest eigenvalue of an  $n \times n$  matrix  $M$  and let  $B = e^A - I$  where  $A$  is the adjacency matrix of  $G_{h,\ell,1}$ . Fix  $\ell$ . Then*

$$\lambda_2(B^T B) = \lambda_1(\tilde{B}^T \tilde{B}),$$

where  $\tilde{B}$  is the lower right principal submatrix of  $B$ , and  $\lambda_2(B^T B)$  is independent of  $h$ . Further, for  $h > 1$ , the multiplicity of  $\lambda_2(B^T B)$  is  $h - 1$ .

$\ell$	$h$							
	1		2		3		4	
	$\lambda_1$	$m$	$\lambda_2$	$m$	$\lambda_2$	$m$	$\lambda_2$	$m$
1	1.6404	1	1	1	1	2	1	3
2	2.0625	1	1.6404	1	1.6404	2	1.6404	3
3	2.3247	1	2.0625	1	2.0625	2	2.0625	3
4	2.4913	1	2.3247	1	2.3247	2	2.3247	3

Table 6.1: Leading or second leading eigenvalues and their multiplicities  $m$  of  $B^TB$  for the graph  $G_{h,\ell,1}$  with different values of  $h$  and  $\ell$ .

Table 6.1 shows leading eigenvalues of  $B^TB$  for graphs with  $h = 1$  and the second leading eigenvalues of  $B^TB$  for graphs with  $h = 2, 3, 4$ . The pattern is made clear from this table. The following describes a possible approach to proving this conjecture. The idea is that the second leading eigenvalue of  $B^TB$  can be obtained by removing the first node of  $G_{h,\ell,1}$  and finding the leading eigenvalue of  $B^TB$  for the new graph.

## 6.2 Back to the Original Question

Our original goal was to find upper bounds, strictly less than one, for the ratio  $\lambda_2/\lambda_1$  of the second eigenvalue to the first eigenvalue of the matrix  $B^TB = (e^A - I)^T(e^A - I)$  for broom-tree graphs, as the length  $\ell$  goes to infinity. We achieved this goal for broom-tree graphs with any number  $h \geq 2$  of handles, and with only one bristle ( $b = 1$ ) at the end of each handle (Theorem 5.1). For broom-tree graphs with more bristles ( $b \geq 2$ ), we obtained instead upper bounds on the ratio  $\lambda_{h(b-1)+2}/\lambda_1$  involving a specific later eigenvalue of  $B^TB$  (Theorems 5.2 and 5.3). Why does the method of proof used for Theorem 5.1 not extend to obtain a bound on  $\lambda_2/\lambda_1$  when  $b \geq 2$ ?

The technique for finding a lower bound for the leading eigenvalue of  $B^TB$  for the graph in Figure 5.2 is analogous to the technique used to find the lower bound in the proof of Theorem 5.1. I will show why the technique for finding an upper bound for the second leading eigenvalue used in that proof will not hold when  $b \geq 2$ .

From the theory contained in the proof of Theorem 5.1, we can estimate the operator norm of any  $B_{h,\ell,b}$  for large enough  $\ell$ . For example, using

MATLAB we find that  $\|B_{2,3,2}\| = 1.870499 > 1.87$ . It is, at this point, unclear whether these values are strictly increasing as the variables  $h$ ,  $\ell$ , and  $b$  are increasing.

The problem with the second part of the proof when  $b > 1$  is that, because of the structure of the graph  $G_{h,\ell,b}$ , there is no way to write  $B_{h,\ell,b}$  as the sum of a Toeplitz matrix and a rank one matrix. Numerical methods might help to find a useful upper bound on  $\lambda_2(B^TB)$  for different values of  $b$ . Other linear algebra theory such as the Lanczos method might also help to find such a bound.

My intuition is that for  $b \geq 2$ , the ratio  $\lambda_2/\lambda_1$  of  $B^TB$  probably does tend to one as  $\ell$  goes to infinity. For now, this remains an open question.





## Appendix A

# MATLAB Code to Determine Eigenvalues and Eigenvectors

I wrote this m-file for MATLAB (with the aid of Keith Soleberg) to make the calculations of the eigenvalues and dominant eigenvectors of  $B^T B$  and  $BB^T$  faster and easier. The file takes the parameters  $h$ ,  $\ell$ , and  $b$  of the broom tree as inputs and returns the eigenvalues of  $B^T B$ , which are the same as the eigenvalues of  $BB^T$  by Theorem 2.1, as well as the dominant eigenvectors associated with  $B^T B$  and  $BB^T$  which correspond to the authority and hub vectors discussed in the introduction.

```
1 function xx=lambda(H,L,B)
2
3 %find size of A
4 n=H*(L+B)+1;
5
6 %A=n by n zero matrix
7 A=zeros(n);
8
9 %define nonzero entries in first row of A
10 A(1,2:H+1)=ones(1,H);
11
12 %define nonzero entries in rows 2 through h(l-1)
13 for k=H+2:H*L+1
14     A(k-H,k)=1;
15 end
16
17 %define nonzero entries on first slope of bristle part
18 for m=2:H*L+1
```

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```
19     A(m, m+H)=1;
20 end
21
22 %define nonzero entries on remaining slopes of bristle part
23 for q=1:B-1
24     for p=2:H+1
25         A(H*(L-1)+p, H*(L+1)+p+(q-1)*H)=1;
26     end
27 end
28
29 %calculate B
30 V=expm(A)-eye(n);
31
32 %calculate eigenvalues and vectors of BB^T
33 [B,D]=eig(V*V. ');
34
35 %put eigenvalues in a row vector
36 E=zeros(1,n);
37 for j=1:n
38     E(1, j)=D(j, j);
39 end
40 display('Eigenvalues of BB^T are:')
41 E
42
43 %find placement of largest eigenvalue of BB^T
44 [F,G]=max(E);
45 display('Dominant Eigenvector of BB^T');
46 B(:,G)
47
48 %find eigenvalues and vectors of B^TB
49 [J,K]=eig(V.'*V);
50 M=zeros(1,n);
51 for j=1:n
52     M(1, j)=K(j, j);
53 end
54
55 %find placement of largest eigenvalue of B^TB
56 [P,Q]=max(M);
57 display('Dominant Eigenvector of B^TB');
58 J(:,Q)
```

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