



# A new type of lower bound for the largest eigenvalue of a symmetric matrix

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## Abstract

Let  $A_{m \times m}$  denote a symmetric matrix. We present an order expansion (4) based on Lagrange series that allows us to improve the classical bound  $\frac{1}{m} \sum_{i=1}^m \sum_{j=1}^m a_{ij} \leq \lambda_{\max}(A)$ .  
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## 1. Introduction

Let  $\lambda_{\min}(A) \leq \lambda_{m-1} \leq \dots \leq \lambda_2 \leq \lambda_{\max}(A)$  denote the ordered, real eigenvalues of a symmetric  $m \times m$  matrix  $A$ . The largest eigenvalue can be expressed [4, p. 549] as

$$\lambda_{\max}(A) = \max_{x \neq 0} \frac{x^T A x}{x^T x}, \quad (1)$$

where  $\frac{x^T A x}{x^T x}$  is called the Rayleigh quotient. The maximum in (1) is only attained if  $x$  is the eigenvector belonging to  $\lambda_{\max}(A)$ . Hence, for any other vector  $y$  that is not the corresponding eigenvector, it holds that

$$\frac{y^T A y}{y^T y} \leq \lambda_{\max}(A)$$

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from which the commonly used lower bound,

$$\frac{u^T Au}{m} = \frac{1}{m} \sum_{i=1}^m \sum_{j=1}^m a_{ij} \leq \lambda_{\max}(A) \tag{2}$$

follows for the choice  $y = u$ , where  $u = [1 \ 1 \ \dots \ 1]^T$  is the  $m \times 1$  all-one vector.

The main result of this article is

**Theorem 1.1.** *Consider a symmetric matrix  $A_{m \times m}$  and define  $T = \frac{1}{\sqrt{m}} \max_{1 \leq j \leq m} (a_{jj} + \sum_{i=1; i \neq j}^m |a_{ij}|)$ . For any real number  $t \geq T$  and  $\lambda_0 = t\sqrt{m}$ , the largest eigenvalue of  $A$  can be bounded from below by*

$$\frac{N_1}{m} + 2 \left( \frac{N_3}{2m} - \frac{N_1 N_2}{m^2} + \frac{N_1^3}{2m^3} \right) \lambda_0^{-2} + O(t^{-4}) \leq \lambda_{\max}(A), \tag{3}$$

where  $N_k = u^T A^k u = \sum_{i=1}^m \sum_{j=1}^m (A^k)_{ij}$  and  $N_0 = m$ .

Although the theorem is stated with order term  $O(t^{-4})$ , the method of [Appendix B](#) allows us to sharpen the classical bound to any desired order  $O(t^{-2j})$ , where  $j$  is a positive integer. If the  $\lambda_0^{-2}$  term and the order term are ignored, we find the classical bound (2).

In the theory on the spectra of graphs, numerous lower and upper bounds for the largest eigenvalue  $\lambda_{\max}(A)$  of the adjacency matrix  $A$  of a graph  $G$  exist (see e.g. [6, Appendix B]). In a graph,  $N_k$  is the total number of walks of length  $k$  [6, Appendix B] and the degree of node  $k$  is  $d_k(A) = \sum_{j=1}^m (A)_{kj}$ . Then, the first few  $N_k$  are  $N_1 = 2L_A$ , where  $L_A$  is the number of links in  $G$  and  $N_2 = D_A = \sum_{k=1}^m d_k^2(A)$ . For graphs, we show in Section 3 that (3) can be rephrased as

$$\frac{2L_A}{m} + 2 \left( \frac{N_3}{2m} - \frac{2L_A D_A}{m^2} + \frac{4L_A^3}{m^3} \right) \lambda_0^{-2} + O(N^{-2}) \leq \lambda_{\max}(A) \tag{4}$$

for any  $N \geq 2m$  and where  $\lambda_0 = \sqrt{(N - m)m}$ . Equality in the classical bound (2) is attained in regular graphs where each node has the same degree  $r$  and where  $\lambda_{\max}(A) = \frac{2L_A}{m} = r$ . Thus, for regular graphs, the coefficient of the  $\lambda_0^{-2}$  term in (4) is precisely zero.

In Section 2, Theorem 1.1 is proved. Section 3 discusses the applications to graphs, while Section 4 revisits Theorem 1.1 from the viewpoint of perturbation theory.

## 2. Proof of Theorem 1.1

The ingredients of the proof of Theorem 1.1 rely on the possibility to compute the largest eigenvalue  $\lambda_{\max}(A_t)$  and the smallest eigenvalue  $\lambda_{\min}(A_t)$  of the symmetric matrix

$$A_t = \begin{bmatrix} A_{m \times m} & t \cdot u_{m \times 1} \\ t \cdot (u^T)_{1 \times m} & 0 \end{bmatrix},$$

where  $t \in \mathbb{R}$  and on Lemma A.1 that yields

$$\lambda_{\max}(A_t) + \lambda_{\min}(A_t) \leq \lambda_{\max}(A). \tag{5}$$

The sequel is devoted to the computation of  $\lambda_{\max}(A_t)$  and  $\lambda_{\min}(A_t)$ . Lemma A.1 restricts the validity of the analysis to symmetric matrices.

The characteristic polynomial of  $A_t$  is

$$\det(A_t - \lambda I)_{(m+1) \times (m+1)} = \begin{bmatrix} (A - \lambda I)_{m \times m} & t \cdot u_{m \times 1} \\ t \cdot (u^T)_{1 \times m} & -\lambda \end{bmatrix}.$$

The general relation (15) gives

$$\det(A_t - \lambda I) = \det(A - \lambda I)_{m \times m} \det(-\lambda - t^2(u^T)_{1 \times m}((A - \lambda I)_{m \times m})^{-1}u_{m \times 1}).$$

For any matrix  $X$ , the sum of all its elements is  $s_X = u^T X u = \sum_{i=1}^n \sum_{j=1}^n x_{ij}$ . Let us denote by  $s_\lambda$  the sum of all elements of the resolvent  $(A - \lambda I)^{-1}$ , then

$$\det(A_t - \lambda I) = -(\lambda + t^2 s_\lambda) \det(A - \lambda I)_{m \times m}. \tag{6}$$

An explicit expression for  $s_\lambda$  is given in (24).

Consider the expansion of the resolvent of  $A$ ,

$$(A - \lambda I)^{-1} = \frac{1}{-\lambda} \left( I - \frac{A}{\lambda} \right)^{-1} = -\frac{1}{\lambda} \sum_{k=0}^{\infty} \frac{A^k}{\lambda^k} = -\frac{1}{\lambda} \left( I + \frac{A}{\lambda} + \frac{A^2}{\lambda^2} + \dots \right) \tag{7}$$

such that

$$s_\lambda = -\frac{1}{\lambda} \sum_{i=1}^m \sum_{j=1}^m \sum_{k=0}^{\infty} \frac{(A^k)_{ij}}{\lambda^k} = -\frac{1}{\lambda} \sum_{k=0}^{\infty} \frac{1}{\lambda^k} \sum_{i=1}^m \sum_{j=1}^m (A^k)_{ij} = -\frac{1}{\lambda} \sum_{k=0}^{\infty} \frac{N_k}{\lambda^k}.$$

Introduced into the equation  $\lambda + s_\lambda t^2 = 0$ , gives

$$\lambda + s_\lambda t^2 = \lambda - \frac{t^2}{\lambda} \left( m + \sum_{k=1}^{\infty} \frac{N_k}{\lambda^k} \right) = 0 \tag{8}$$

or,

$$\lambda = \pm t \sqrt{m \left( 1 + \sum_{k=1}^{\infty} \frac{N_k}{m \lambda^k} \right)}. \tag{9}$$

If  $t$  is large and  $m$  fixed, (9) reveals that the first order expression,  $\lambda_0 = \pm t \sqrt{m}$  is accurate up to  $O(1)$ . Gerschgorin’s Theorem [7, p. 71] shows that each eigenvalue of the (symmetric) matrix  $A$  lies in at least one of the  $1 \leq j \leq m$  intervals  $\left( a_{jj} - \sum_{i=1; i \neq j}^m |a_{ij}|, a_{jj} + \sum_{i=1; i \neq j}^m |a_{ij}| \right)$ .

Hence, if  $t > T = \frac{1}{\sqrt{m}} \max_{1 \leq j \leq m} \left( a_{jj} + \sum_{i=1; i \neq j}^m |a_{ij}| \right)$ , then relation (9) further shows that the largest eigenvalues of  $A_t$  in absolute value are the roots of  $\lambda + s_\lambda t^2 = 0$ . This observation leads to a lower bound for  $t \geq T$ .

### 2.1. Lagrange series for the zero of (8)

We solve the equation  $f(\lambda) = \lambda + s_\lambda t^2 \simeq \lambda - t^2 \left( \frac{m}{\lambda} + \frac{N_1}{\lambda^2} + \frac{N_2}{\lambda^3} \right) = 0$  by Lagrange expansion first<sup>1</sup> up to  $O(t^{-2})$  while the general method is outlined in Appendix B. The zero  $\zeta(\lambda_0)$  of  $f(\lambda)$  around  $\lambda_0 = t \sqrt{m}$  can be written as a Lagrange series [3, II, pp. 88]. Since  $f(\lambda)$  is known up to order  $O(t^{-2})$ , only three terms in the general Lagrange series are needed,

<sup>1</sup> The same result can be obtained by two iterations in Newton-Raphson’s method.

$$\zeta(\lambda_0) \approx \lambda_0 - \frac{f(\lambda_0)}{f'(\lambda_0)} - \frac{f''(\lambda_0)}{2f'(\lambda_0)} \left( \frac{f(\lambda_0)}{f'(\lambda_0)} \right)^2 \tag{10}$$

to guarantee that the zero is also accurate up to order  $O(t^{-2})$ . Indeed,

$$\begin{aligned} f(\lambda_0) &= -\frac{N_1}{m} - \frac{N_2}{mt\sqrt{m}} + O(t^{-2}), \\ f'(\lambda_0) &= 2 + \frac{2N_1}{mt\sqrt{m}} + O(t^{-2}), \\ f''(\lambda_0) &= -\frac{2}{t\sqrt{m}} + O(t^{-2}) \end{aligned}$$

and  $f'''(\lambda_0) = O(t^{-2})$ . After substitution in (10) and some reorganization, the extreme eigenvalues of  $A_t$  are, accurate up to order  $O(t^{-2})$  for large  $t$ ,

$$\lambda_{\max}(A_t) = t\sqrt{m} + \frac{N_1}{2m} + \left( \frac{N_2}{2m} - \frac{3N_1^2}{8m^2} \right) \frac{1}{t\sqrt{m}} + O(t^{-2}) \tag{11}$$

and

$$\lambda_{\min}(A_t) = -t\sqrt{m} + \frac{N_1}{2m} - \left( \frac{N_2}{2m} - \frac{3N_1^2}{8m^2} \right) \frac{1}{t\sqrt{m}} + O(t^{-2}), \tag{12}$$

where the last expression is obtained analogously from (10) for  $\lambda_0 = -t\sqrt{m}$ . The method presented in Appendix B allows us to compute  $\zeta(\lambda_0)$  to any desired order in  $t$ , although the amount of computations rapidly becomes impressive. Computed up to  $O(t^{-3})$ , we find

$$\zeta(\lambda_0) = \lambda_0 + \frac{N_1}{2m} + \left( \frac{N_2}{2m} - \frac{3N_1^2}{8m^2} \right) \frac{1}{\lambda_0} + \left( \frac{N_3}{2m} - \frac{N_1N_2}{m^2} + \frac{N_1^3}{2m^3} \right) \frac{1}{\lambda_0^2} + O(t^{-3}), \tag{13}$$

where  $\lambda_{\max}(A_t)$  and  $\lambda_{\min}(A_t)$  follow for  $\lambda_0 = t\sqrt{m}$  and  $\lambda_0 = -t\sqrt{m}$ , respectively.

Finally, our Theorem 1.1, in particular the bound (3), is proved by combining the bound (5) and equation (13).

### 3. Application to the spectra of graphs

Since  $A_t$  is not an adjacency matrix for  $t \neq 1$ , we consider the adjacency matrix of the  $G$ -connected  $m$  star topology with  $N$  nodes,

$$A_{mstarG} = \begin{bmatrix} A_{m \times m} & J_{m \times (N-m)} \\ J_{(N-m) \times m} & O_{(N-m) \times (N-m)} \end{bmatrix},$$

where  $J$  is the all-one matrix and  $A_{m \times m}$  is the adjacency matrix of an arbitrary graph  $G$  that connects  $m$  nodes. Each of those  $m$  nodes is connected to each of the  $N - m$  other nodes in the topology called  $mstarG$ . We note that the bi-partite structure of  $A_{mstarG}$  is crucial. Similarly as above, we find

$$\det(A_{mstarG} - \lambda I) = \det(A - \lambda I)_{m \times m} (-1)^{N-m} \lambda^{N-m-1} (\lambda + s_\lambda(N - m)),$$

where  $t^2 = N - m$ . Hence, by modifying the size of the matrix  $A_{mstarG}$ , the zeros of the same function  $f(\lambda) = \lambda + s_\lambda(N - m)$  are the maximum and minimum eigenvalue of  $A_{mstarG}$ . Moreover, since the largest eigenvalue of  $A$  (for any graph) is smaller than the maximum degree  $d_{\max}(A) \leq m - 1$ , a tighter bound for  $N$  compared to  $t$  is found,  $N \geq 2m$ . The general result is then given in (4).

**Example.** The spectrum of a  $m$ -fully meshed star topology where  $A = J - I$  can be computed exactly as

$$\begin{aligned}
 (\lambda_{\max})_{m\text{star}} &= \sqrt{m(N - m) + \left(\frac{m - 1}{2}\right)^2} + \frac{m - 1}{2}, \\
 (\lambda_{\min})_{m\text{star}} &= -\sqrt{m(N - m) + \left(\frac{m - 1}{2}\right)^2} + \frac{m - 1}{2}
 \end{aligned}$$

and with an eigenvalue at  $-1$  with multiplicity  $m - 1$  and at  $0$  with multiplicity  $N - m - 1$ . Comparing (13) with the exact result of a  $m$ -fully meshed star topology,

$$\begin{aligned}
 (\lambda_{\max})_{m\text{star}} &= \sqrt{m(N - m) + \left(\frac{m - 1}{2}\right)^2} + \frac{m - 1}{2} \\
 &= \sqrt{(N - m)m} + \frac{m - 1}{2} + \frac{1}{2} \left(\frac{m - 1}{2}\right)^2 \frac{1}{\sqrt{(N - m)m}} + O(N^{-3/2})
 \end{aligned}$$

shows, indeed, that (13) is correct, since  $N_1 = \frac{m(m-1)}{2}$ ,  $N_2 = m(m - 1)^2$  and  $N_3 = m(m - 1)^3$  for the complete graph  $K_m$ .

#### 4. Perturbation theory

Consider the symmetric matrix

$$B = \begin{bmatrix} O_{m \times m} & u_{m \times 1} \\ (u^T)_{1 \times m} & 0 \end{bmatrix}$$

that represents the adjacency matrix of the bi-partite graph  $K_{m,1}$  or the star topology, a central node that connects  $m$  other, not interconnected nodes. The eigenvalues of  $B$  are well-known:  $-\sqrt{m}$ ,  $\sqrt{m}$  and  $0$  with multiplicity  $m - 1$ . The corresponding eigenvectors to the eigenvalue  $\sqrt{m}$  and  $-\sqrt{m}$  are  $v = [u_{1 \times m} \quad \sqrt{m}]^T$  and  $w = [u_{1 \times m} \quad -\sqrt{m}]^T$ , respectively. Hence, apart from the zero eigenvalues, the eigenvalues of  $tB$  are precisely  $\lambda_0 = \pm t\sqrt{m}$ .

Further, we can write

$$A_t = tB + A_0 = t \left( B + \frac{1}{t}A_0 \right)$$

which implies that the eigenvalues of  $A_t$  are equal to those of  $B + \frac{1}{t}A_0$  multiplied by  $t$ . Since we know the eigenvalues of  $B$  exactly, and if  $t$  is sufficiently large, perturbation theory [2,7] can be applied. Since  $B + zA_0$  is analytic in  $z$ , real symmetric on the real axis, all eigenvalues of  $B + zA_0$  are analytic functions of  $z$  in the neighborhood of the real axis ( $\text{Im}z = 0$ ). Hence, there exists a real number  $R > 0$ , for which  $B + zA_0$  has two, simple eigenvalues  $\lambda_+(z)$  and  $\lambda_-(z)$  with Taylor expansion around  $\sqrt{m}$  and  $-\sqrt{m}$ ,

$$\begin{aligned}
 \lambda_+(z) &= \sqrt{m} + \sum_{k=1}^{\infty} \alpha_k z^k \quad |z| < R, \\
 \lambda_-(z) &= -\sqrt{m} + \sum_{k=1}^{\infty} \beta_k z^k \quad |z| < R,
 \end{aligned}$$

where all coefficients  $\alpha_k$  and  $\beta_k$  are real. Perturbation theory [7, p. 69] gives explicitly the first order coefficients as

$$\alpha_1 = \frac{v^T Av}{v^T v} = \frac{u^T Au}{2m} \quad \text{and} \quad \beta_1 = \frac{w^T Aw}{w^T w} = \frac{u^T Au}{2m}.$$

Thus,

$$\alpha_1 = \beta_1 = \frac{N_1}{2m}.$$

For sufficiently small  $z$ ,  $\lambda_+(z)$  and  $\lambda_-(z)$  are the maximum and minimum eigenvalue of  $B + zA_0$ . Hence, with (5), we obtain

$$\begin{aligned} \lambda_{\max}(A) &\geq t \left( \lambda_+ \left( \frac{1}{t} \right) + \lambda_- \left( \frac{1}{t} \right) \right) = \sum_{k=1}^{\infty} (\alpha_k + \beta_k) t^{1-k} \\ &= \frac{N_1}{m} + \frac{(\alpha_2 + \beta_2)}{t} + \frac{(\alpha_3 + \beta_3)}{t^2} + \sum_{k=4}^{\infty} (\alpha_k + \beta_k) t^{1-k}. \end{aligned}$$

The specific (bi-partite) structure of  $A_t$  enables us to write the characteristic polynomial (6) explicitly, from which we deduce, for sufficiently large  $t$ , that both  $t\lambda_+(t^{-1})$  and  $t\lambda_-(t^{-1})$  are zeros of the function  $f(\lambda) = \lambda + s_\lambda t^2$ . If  $y(t)$  is a zero of  $\lambda + s_\lambda t^2 = 0$ , which is even in  $t$ , then also  $y(-t)$  is a zero, which shows that  $t\lambda_+(t^{-1}) = -t\lambda_-(-t^{-1})$ . The zeros of  $f(\lambda)$  can be expanded in a Lagrange series around  $\lambda_0 = \pm t\sqrt{m}$ . By also expanding the coefficients of this Lagrange series into a power series expansion in  $\lambda_0$  as shown in Appendix B, all coefficients  $\alpha_k$  can be computed and we indeed find that  $\lambda_+(t^{-1}) = -\lambda_-(-t^{-1})$ . Hence,

$$\begin{aligned} t \left( \lambda_+ \left( \frac{1}{t} \right) + \lambda_- \left( \frac{1}{t} \right) \right) &= 2 \sum_{k=0}^{\infty} \alpha_{2k+1} t^{-2k} \\ &= \frac{N_1}{m} + \frac{2\alpha_3}{t^2} + 2 \sum_{k=2}^{\infty} \alpha_{2k+1} t^{-2k}. \end{aligned}$$

If  $\alpha_3 = \frac{N_3}{2m} - \frac{N_1 N_2}{m^2} + \frac{N_1^3}{2m^3} > 0$ , a tighter lower bound for  $\lambda_{\max}(A)$  than the classical  $\lambda_{\max}(A) \geq \frac{N_1}{m}$  is obtained.

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**Appendix A. Results from linear algebra**

From the Schur identity

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix} = \begin{bmatrix} I & O \\ CA^{-1} & I \end{bmatrix} \begin{bmatrix} A & B \\ O & D - CA^{-1}B \end{bmatrix} \tag{14}$$

we find that

$$\det \begin{bmatrix} A & B \\ C & D \end{bmatrix} = \det A \det(D - CA^{-1}B) \tag{15}$$

and  $D - CA^{-1}B$  is called the Schur complement of  $A$ .

**Lemma A.1.** *If*

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

*is a real symmetric matrix, where A and B are square, and consequently symmetric, matrices, then*

$$\lambda_{\max}(X) + \lambda_{\min}(X) \leq \lambda_{\max}(A) + \lambda_{\max}(B) \tag{16}$$

**Proof.** See e.g. [1, p. 56]. □

**Appendix B. Characteristic coefficients of a complex function**

If  $f(z)$  has a Taylor series around  $z_0$ ,

$$f(z) = \sum_{k=0}^{\infty} f_k(z_0)(z - z_0)^k \quad \text{with} \quad f_k(z_0) = \frac{1}{k!} \left. \frac{d^k f(z)}{dz^k} \right|_{z=z_0}$$

then the general relation where  $G(z)$  is analytic around  $f(z_0)$  is

$$G(f(z)) = G(f(z_0)) + \sum_{m=1}^{\infty} \left( \sum_{k=1}^m \frac{1}{k!} \left. \frac{d^k G(p)}{dp^k} \right|_{p=f(z_0)} s[k, m]_{f(z)}(z_0) \right) (z - z_0)^m, \tag{17}$$

where the characteristic coefficient [5] of a complex function  $f(z)$  is

$$s[k, m]_{f(z)}(z_0) = \sum_{\sum_{i=1}^k j_i = m; j_i > 0} \prod_{i=1}^k f_{j_i}(z_0)$$

which obeys the recursion relation

$$\begin{aligned} s[1, m]_{f(z)}(z_0) &= f_m(z_0), \\ s[k, m]_{f(z)}(z_0) &= \sum_{j=1}^{m-k+1} f_j(z_0) s[k-1, m-j]_{f(z)}(z_0) \quad (k > 1). \end{aligned} \tag{18}$$

The zero  $\zeta(z_0)$  of  $f(z)$  closest to  $z_0$  is given [5] in terms of the coefficients  $f_k(z_0)$  of the series expansion of  $f(z)$  around  $z_0$  as

$$\begin{aligned} \zeta(z_0) = f^{-1}(0) = z_0 - \frac{f_0(z_0)}{f_1(z_0)} \\ + \sum_{n=2}^{\infty} \left[ \sum_{k=1}^{n-1} \frac{(-1)^k \binom{n+k-1}{k-1}}{k(f_1(z_0))^k} s^*[k, n-1]_{f(z)}(z_0) \right] \left( -\frac{f_0(z_0)}{f_1(z_0)} \right)^n, \end{aligned} \tag{19}$$

where  $s^*[k, m] = s[k, m]_{f_m \rightarrow f_{m+1}}$  denotes that the index of all Taylor coefficients appearing in (18) is augmented by 1. Explicitly summing the first five terms ( $n \leq 5$ ),

$$\begin{aligned} \zeta(z_0) \approx & z_0 - \frac{f_0(z_0)}{f_1(z_0)} - \frac{f_2(z_0)}{f_1(z_0)} \left( \frac{f_0(z_0)}{f_1(z_0)} \right)^2 + \left[ -2 \left( \frac{f_2(z_0)}{f_1(z_0)} \right)^2 + \frac{f_3(z_0)}{f_1(z_0)} \right] \left( \frac{f_0(z_0)}{f_1(z_0)} \right)^3 \\ & + \left[ -5 \left( \frac{f_2(z_0)}{f_1(z_0)} \right)^3 + 5 \frac{f_3(z_0)}{f_1(z_0)} \frac{f_2(z_0)}{f_1(z_0)} - \frac{f_4(z_0)}{f_1(z_0)} \right] \left( \frac{f_0(z_0)}{f_1(z_0)} \right)^4 \\ & + \left[ -14 \left( \frac{f_2(z_0)}{f_1(z_0)} \right)^4 + 21 \frac{f_3(z_0)}{f_1(z_0)} \left( \frac{f_2(z_0)}{f_1(z_0)} \right)^2 - 3 \left( \frac{f_3(z_0)}{f_1(z_0)} \right)^2 \right. \\ & \left. - 6 \frac{f_4(z_0)}{f_1(z_0)} \frac{f_2(z_0)}{f_1(z_0)} + \frac{f_5(z_0)}{f_1(z_0)} \right] \left( \frac{f_0(z_0)}{f_1(z_0)} \right)^5. \end{aligned} \tag{20}$$

Appendix B.1. Lagrange expansion

The zero of  $f(\lambda) = \lambda + s_\lambda t^2 = 0$  will be computed using the Lagrange series which can be efficiently computed to any order with characteristic coefficients [5]. The Lagrange expansion (19) in terms of characteristic coefficients needs the Taylor coefficients of  $f(\lambda)$  around  $\lambda_0 = \pm t\sqrt{m}$ ,

$$f_n(\lambda_0) = \frac{1}{n!} \frac{d^n}{d\lambda^n} \left( \lambda - t^2 \sum_{k=0}^{\infty} \frac{N_k}{\lambda^{k+1}} \right) \Big|_{\lambda=\lambda_0}.$$

For  $n = 0$ ,

$$f_0(\lambda_0) = \lambda_0 - t^2 \sum_{k=0}^{\infty} \frac{N_k}{\lambda_0^{k+1}} = -t^2 \sum_{k=1}^{\infty} \frac{N_k}{\lambda_0^{k+1}}$$

because  $\lambda_0 - \frac{t^2 m}{\lambda_0} = 0$  and,

$$f_0(\lambda_0) = -\frac{1}{m} \sum_{k=0}^{\infty} \frac{N_{k+1}}{\lambda_0^k}. \tag{21}$$

Similarly, for  $n = 1$ ,

$$f_1(\lambda_0) = 1 + t^2 \sum_{k=0}^{\infty} \frac{(k+1)N_k}{\lambda_0^{k+2}} = 2 + \frac{1}{m} \sum_{k=1}^{\infty} \frac{(k+1)N_k}{\lambda_0^k} \tag{22}$$

and, for all  $n > 1$ ,

$$f_n(\lambda_0) = \frac{(-1)^{n+1} t^2}{\lambda_0^{n+1}} \sum_{k=0}^{\infty} \binom{n+k}{k} \frac{N_k}{\lambda_0^k}, \tag{23}$$

We now confine ourselves to computing the zero  $\zeta(\lambda_0)$  of  $f(\lambda)$  accurate up to order  $O(t^{-2q})$ , where  $q$  is fixed, but specified later. Since  $\lambda_0 = O(t)$ , for  $f_n(\lambda_0)$  to be accurate up to order  $O(t^{-2q})$ , we need to take in the computation  $k = 2(q - 1) - n$  terms in the  $k$ -sums. Also, it follows that  $2(q - 1) > n$  derivatives or Taylor coefficients in the Lagrange series are needed. The Lagrange expansion (19) indicates that we need order expansions for  $(f_1(\lambda_0))^{-k}$  and  $\left( \frac{f_0(z_0)}{f_1(z_0)} \right)^n$ . Both of these expansions can be given in terms of characteristic coefficients. Applying

$$g^{-k}(z) = g_0^{-k} + \sum_{m=1}^{\infty} \left( \sum_{n=1}^m (-1)^n \binom{n+k-1}{n} g_0^{-k-n} s[n, m] \right) z^m$$



to (22), we have, with  $z = \lambda_0^{-1}$  and  $g_0 = 2$  and  $g_n = \frac{(n+1)}{m} N_n$  for  $n > 0$ , that

$$(f_1(\lambda_0))^{-k} = 2^{-k} + \sum_{m=1}^{\infty} \left( \sum_{n=1}^m (-1)^n \binom{n+k-1}{n} \frac{s[n, m]_{g(z)}}{2^{k+n}} \right) \lambda_0^{-m}.$$

Similarly, applying

$$h^n(z) = h_0^n + \sum_{m=1}^{\infty} \left( \sum_{k=1}^m \binom{n}{k} h_0^{n-k} s[k, m] \right) z^m$$

to (21), we obtain, with  $z = \lambda_0^{-1}$  and with  $h_n = -\frac{N_{n+1}}{m}$  for  $n \geq 0$ , that

$$(f_0(\lambda_0))^n = \frac{(-1)^n N_1^n}{m^n} \left( 1 + \sum_{m=1}^{\infty} \left( \sum_{k=1}^m \binom{n}{k} \frac{(-m)^k s[k, m]_{h(z)}}{N_1^k} \right) \lambda_0^{-m} \right).$$

The quotient  $\left( \frac{f_0(z_0)}{f_1(z_0)} \right)^n$  follows by Cauchy’s product rule for series,

$$\begin{aligned} \left( \frac{f_0(z_0)}{f_1(z_0)} \right)^n &= \frac{(-1)^n N_1^n}{m^n 2^n} \left( 1 - \frac{n}{m} \left( \frac{-m N_2}{N_1} + N_1 \right) \lambda_0^{-1} \right. \\ &\quad + \frac{(-1)^n N_1^n}{m^n 2^n} \sum_{r=2}^{\infty} \left( \sum_{k=1}^r \binom{n}{k} \frac{(-m)^k s[k, r]_{h(z)}}{N_1^k} \right. \\ &\quad + \sum_{j=1}^r (-1)^j \binom{j+n-1}{j} \frac{s[j, r]_{g(z)}}{2^j} \\ &\quad + \sum_{q=1}^{r-1} \left( \sum_{j=1}^{r-q} (-1)^j \binom{j+n-1}{j} \frac{s[j, r-q]_{g(z)}}{2^j} \right) \\ &\quad \left. \times \left( \sum_{k=1}^q \binom{n}{k} \frac{(-m)^k s[k, q]_{h(z)}}{N_1^k} \right) \right) \lambda_0^{-r}. \end{aligned}$$

Explicitly up to order  $O(t^{-3})$ ,

$$\begin{aligned} \left( \frac{f_0(z_0)}{f_1(z_0)} \right)^n &= \frac{(-1)^n N_1^n}{m^n 2^n} \left( 1 + \frac{n}{m} \left( \frac{m N_2}{N_1} - N_1 \right) \right) \lambda_0^{-1} \\ &\quad + \frac{(-1)^n N_1^n}{m^n 2^n} \left( \frac{n N_3}{N_1} + \frac{n(n-1) N_2^2}{2 N_1^2} - \frac{(3n+2n^2) N_2}{2m} + \frac{n(n+1) N_1^2}{2m^2} \right) \lambda_0^{-2}. \end{aligned}$$

Let us compute the zero of  $f(\lambda) = \lambda + s_\lambda t^2 = 0$  up to  $O(t^{-3})$ . For  $q = 3/2$ , we need for each derivative  $n < 4$ , only  $k = 4 - n$  terms. The corresponding Lagrange series is

$$\begin{aligned} \zeta(\lambda_0) &= \lambda_0 - \frac{f_0(\lambda_0)}{f_1(\lambda_0)} - \frac{f_2(\lambda_0)}{f_1(\lambda_0)} \left( \frac{f_0(\lambda_0)}{f_1(\lambda_0)} \right)^2 \\ &\quad + \left[ -2 \left( \frac{f_2(\lambda_0)}{f_1(\lambda_0)} \right)^2 + \frac{f_3(\lambda_0)}{f_1(\lambda_0)} \right] \left( \frac{f_0(\lambda_0)}{f_1(\lambda_0)} \right)^3 + O(t^{-3}). \end{aligned}$$

We list the separate terms,

$$\begin{aligned} \frac{f_0(z_0)}{f_1(z_0)} &= \frac{-N_1}{2m} \left( 1 + \frac{1}{m} \left( \frac{mN_2}{N_1} - N_1 \right) \lambda_0^{-1} + \left( \frac{N_3}{N_1} - \frac{5N_2}{2m} + \frac{N_1^2}{m^2} \right) \lambda_0^{-2} \right), \\ \left( \frac{f_0(\lambda_0)}{f_1(\lambda_0)} \right)^2 &= \frac{N_1^2}{4m^2} \left( 1 + \frac{2}{m} \left( \frac{mN_2}{N_1} - N_1 \right) \lambda_0^{-1} + O(\lambda_0^{-2}) \right), \\ \left( \frac{f_0(z_0)}{f_1(z_0)} \right)^3 &= \frac{-N_1^3}{8m^3} (1 + O(\lambda_0^{-1})) \end{aligned}$$

and

$$\begin{aligned} \frac{f_2(\lambda_0)}{f_1(\lambda_0)} &= - \left( \frac{1}{2} - \frac{N_1}{2m} \lambda_0^{-1} + \left( \frac{N_1^2}{2m^2} - \frac{3N_2}{2m} \right) \lambda_0^{-2} \right) \left( \frac{1}{\lambda_0} + \frac{3N_1}{m\lambda_0^2} \right) \\ &= - \left( \frac{1}{2} \lambda_0^{-1} + \frac{N_1}{m} \lambda_0^{-2} \right), \\ \left( \frac{f_2(\lambda_0)}{f_1(\lambda_0)} \right)^2 &= \frac{1}{4} \lambda_0^{-2} \end{aligned}$$

and

$$\frac{f_3(\lambda_0)}{f_1(\lambda_0)} = \left( 2^{-1} - \frac{N_1}{2m} \lambda_0^{-1} + \left( \frac{N_1^2}{2m^2} - \frac{3N_2}{2m} \right) \lambda_0^{-2} \right) \lambda_0^{-2} = \frac{1}{2} \lambda_0^{-2}.$$

Combined yields the final result (13).

**Appendix C. A finite sum expression for  $s_\lambda$**

Since  $A$  is symmetric,  $A^k = X \text{diag}(\lambda_j^k) X^T$  where the columns of the orthogonal matrix  $X$  consists of eigenvectors  $x_j$  of  $A$ ,

$$(A - \lambda I)^{-1} = -\frac{1}{\lambda} X \left( \text{diag} \left( \sum_{k=0}^{\infty} \frac{\lambda_j^k}{\lambda^k} \right) \right) X^T = -X \text{diag} \left( \frac{1}{\lambda - \lambda_j} \right) X^T.$$

Then,

$$s_\lambda = u(A - \lambda I)^{-1} u^T = - \sum_{j=1}^m \frac{(\sum_{k=1}^m x_{j;k})^2}{\lambda - \lambda_j}. \tag{24}$$

Unless the all-one vector  $u$  is an eigenvector of  $A$ ,  $(\sum_{k=1}^m x_{j;k})^2 \neq 0$ . Hence, in that case

$$\det(A_t - \lambda I) = - \det(A - \lambda I)_{m \times m} \left( \lambda - t^2 \sum_{j=1}^m \frac{(\sum_{k=1}^m x_{j;k})^2}{\lambda - \lambda_j} \right)$$

and no eigenvalue of  $A$  is a zero of  $f(\lambda) = \lambda - t^2 \sum_{j=1}^m \frac{(\sum_{k=1}^m x_{j;k})^2}{\lambda - \lambda_j}$ .

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