

Some Laplacian eigenvalues can be computed by matrix perturbation

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Abstract

Matrix perturbation theory is applied to the matrix $W(\zeta) = \tilde{\Delta} + \zeta\tilde{A}$, where \tilde{A} is the $N \times N$ symmetric, weighted adjacency matrix of an undirected graph G on N nodes with corresponding weighted degree diagonal matrix $\tilde{\Delta}$ and ζ is the perturbation parameter. Assuming that node q has a unique weighted degree $\tilde{d}_q = \sum_{j=1}^N \tilde{a}_{qj}$, a power series in ζ of an eigenvalue $\lambda(W(\zeta))$, expanded around \tilde{d}_q , is deduced and its first four coefficients are computed explicitly.

In the unweighted case, A (without tilde) is the zero-one, symmetric adjacency matrix with corresponding diagonal matrix Δ with nodal degrees. Choosing the perturbation parameter $\zeta = -1$ yields $W(-1) = \Delta - A$, which is the Laplacian matrix of the undirected graph G . Unfortunately, the power series does not converge for $\zeta = -1$. However, after Euler summation, the resulting eigenvalue perturbation expansion is found to converge, when d_q is a high and unique degree, to a Laplacian eigenvalue.

1 Introduction

We consider the matrix $W(\zeta) = W + \zeta B$. Perturbation theory, outlined in Appendix A, assumes that the perturbation parameter ζ is sufficiently small so that we may regard $W(\zeta)$ as the perturbation of the original symmetric matrix W by a matrix B , which is not necessarily symmetric. We limit ourselves to a simple eigenvalue $\lambda(W)$ of the matrix W with multiplicity one.

Here, we apply the perturbation theory in Appendix A to a weighted Laplacian $\tilde{Q} = \tilde{\Delta} - \tilde{A}$, where \tilde{A} is a weighted adjacency matrix and the diagonal matrix is $\tilde{\Delta} = \text{diag}(\tilde{A}u)$, where u is the all-one vector. In the unweighted case, we omit the tilde and write the Laplacian $Q = \Delta - A$, where A is the $N \times N$ zero-one, symmetric adjacency matrix of a simple graph G without self-loops, i.e. $a_{jj} = 0$ for any node j in the graph G . The graph G has N nodes and L links. Thus, in our case, the matrix $W = \tilde{\Delta}$ and the perturbing matrix $B = \tilde{A}$. Hence, $W(\zeta) = \tilde{\Delta} + \zeta\tilde{A}$ and $W(-1) = \tilde{Q}$. The entire challenge is caused by the relatively large perturbation parameter ζ , which may lead to an excessive number of terms in the eigenvalue expansion (7) and, even worse, to a diverging series, in case the radius of convergence of (7) is smaller than 1.

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2 Coefficients and convergence of the perturbation power series

The diagonal matrix $\tilde{\Delta}$ has a rather obvious spectral structure. The eigenvalue $\lambda_j(W) = \tilde{d}_j$ is equal to the j -th diagonal element of $\tilde{\Delta}$, which corresponds to the nodal strength $\tilde{d}_j = \left(\tilde{A}u\right)_j$ of node j . The corresponding, normalized eigenvector e_j is the basic vector with all zeros, except an entry 1 for the j -th component, i.e. $(e_j)_k = \delta_{jk}$, where the Kronecker $\delta_{jk} = 1$ if $k = j$, else $\delta_{jk} = 0$. The eigenvalue $\lambda_j(W)$ can possess a multiplicity m_j , but the orthogonal eigenvector matrix remains the identity matrix I , which greatly avoids complications of Jordan forms in the general case.

In order to allow direct application of the perturbation theory in Appendix A, we assume that $\lambda_q = \tilde{d}_q$ is a simple eigenvalue, i.e. the weighted degree should be simple and only node q in the graph G has a degree equal to \tilde{d}_q .

The first perturbation coefficient c_1 in (14) translates to

$$\tilde{c}_1(q) = e_q^T \tilde{A}e_q = \tilde{a}_{qq} = 0$$

and, in general, $x_k^T Bx_q$ translates to $e_k^T \tilde{A}e_q = \tilde{a}_{kq} \geq 0$. The second perturbation coefficient in (19) becomes

$$\tilde{c}_2(q) = \sum_{k=1; k \neq q}^n \frac{(\tilde{a}_{kq})^2}{\tilde{d}_q - \tilde{d}_k}$$

and in the unweighted case

$$c_2(q) = \sum_{k=1; k \neq q}^n \frac{a_{kq}}{d_q - d_k} = \sum_{k \in \mathcal{N}_q} \frac{1}{d_q - d_k}$$

where \mathcal{N}_q is the set of all direct neighbors of node q . Thus, the perturbation coefficient $c_2(q)$ is the sum of the reciprocal degree difference with d_q over all direct neighbors of node q . Using $\sum_{k=1; k \neq q}^n a_{kq} = d_q$, the degree of node q , we can bound c_2 as

$$|c_2(q)| < \max_{\substack{1 \leq k \leq n \\ k \neq q}} \frac{d_q}{|d_q - d_k|} = d_q = (A^2)_{qq}$$

The third perturbation coefficient in (21) reduces, with $\tilde{a}_{qq} = 0$, to

$$\tilde{c}_3(q) = \sum_{r=1; r \neq q}^n \frac{\tilde{a}_{rq}}{\tilde{d}_q - \tilde{d}_r} \sum_{k=1; k \neq q}^n \frac{\tilde{a}_{kq}\tilde{a}_{kr}}{\tilde{d}_q - \tilde{d}_k}$$

and in the unweighted case

$$c_3(q) = \sum_{r=1; r \neq q}^n \sum_{k=1; k \neq q}^n \frac{a_{rq}}{(d_q - d_r)} \frac{a_{qk}}{(d_q - d_k)} a_{kr} = \sum_{r \in \mathcal{N}_q} \sum_{k \in \mathcal{N}_q \cap \mathcal{N}_r} \frac{1}{d_q - d_r} \frac{1}{d_q - d_k}$$

which is the sum of the product of reciprocal degree differences over all mutually connected neighbors of node q . We bound c_3 as

$$\begin{aligned} |c_3(q)| &= \left| \sum_{r=1; r \neq q}^n \sum_{k=1; k \neq q}^n \frac{a_{rq}}{d_q - d_r} \frac{a_{qk}a_{kr}}{d_q - d_k} \right| \leq \sum_{r=1; r \neq q}^n \sum_{k=1; k \neq q}^n \frac{a_{rq}}{|d_q - d_r|} \frac{a_{qk}a_{kr}}{|d_q - d_k|} \\ &< \max_{\substack{1 \leq k \leq n \\ k \neq q}} \frac{1}{|d_q - d_k|^2} \sum_{r=1}^n a_{rq} \sum_{k=1}^n a_{qk}a_{kr} \end{aligned}$$

With $\sum_{r=1}^n a_{rq} \sum_{k=1}^n a_{qk} a_{kr} = \sum_{r=1}^n a_{rq} (A^2)_{qr} = (A^3)_{qq}$, the number of closed walks of length 3 from node j back to itself [4], we find

$$|c_3(q)| < \max_{\substack{1 \leq k \leq n \\ k \neq q}} \frac{(A^3)_{qq}}{|d_q - d_k|^2} \leq (A^3)_{qq}$$

The fourth perturbation coefficient in (22) reduces, with $\tilde{a}_{qq} = 0$, to

$$\tilde{c}_4(q) = \sum_{r=1; r \neq q}^n \frac{\tilde{a}_{rq}}{\tilde{d}_q - \tilde{d}_r} \sum_{l=1; l \neq q}^n \frac{\tilde{a}_{rl}}{\tilde{d}_q - \tilde{d}_l} \sum_{k=1; k \neq q}^n \frac{\tilde{a}_{kq} \tilde{a}_{kl}}{\tilde{d}_q - \tilde{d}_k} - \sum_{r=1; r \neq q}^n \frac{(\tilde{a}_{rq})^2}{(\tilde{d}_q - \tilde{d}_r)^2} \sum_{k=1; k \neq q}^n \frac{(\tilde{a}_{kq})^2}{\tilde{d}_q - \tilde{d}_k}$$

and in the unweighted case

$$c_4(q) = \sum_{r=1; r \neq q}^n \frac{a_{rq}}{d_q - d_r} \sum_{l=1; l \neq q}^n \frac{a_{rl}}{d_q - d_l} \sum_{k=1; k \neq q}^n \frac{a_{kq} a_{kl}}{d_q - d_k} - \sum_{r=1; r \neq q}^n \frac{a_{rq}}{(d_q - d_r)^2} \sum_{k=1; k \neq q}^n \frac{a_{kq}}{d_q - d_k}$$

Conservatively bounding yields

$$\begin{aligned} |c_4(q)| &< \sum_{r=1; r \neq q}^n \sum_{l=1; l \neq q}^n \sum_{k=1; k \neq q}^n \frac{a_{rq}}{|d_q - d_r|} \frac{a_{rl}}{|d_q - d_l|} \frac{a_{kq} a_{kl}}{|d_q - d_k|} \\ &< \max_{\substack{1 \leq k \leq n \\ k \neq q}} \frac{1}{|d_q - d_k|^3} \sum_{r=1}^n \sum_{l=1}^n \sum_{k=1}^n a_{qr} a_{rl} a_{lk} a_{kq} = \max_{\substack{1 \leq k \leq n \\ k \neq q}} \frac{(A^4)_{qq}}{|d_q - d_k|^3} \leq (A^4)_{qq} \end{aligned}$$

If $d_q = d_{\max}$, then $c_2(q)$ and $c_3(q)$ are positive, but the sign of $c_4(q)$ may be negative. In summary, up to order ζ^4 , we find that the eigenvalue expansion $\xi_q(\zeta)$ in (8) of the matrix $\Delta + \zeta A$ around degree d_q is

$$\begin{aligned} \xi_q(\zeta) &= d_q + \zeta^2 c_2(q) + \zeta^3 c_3(q) + \zeta^4 c_4(q) + O(\zeta^5) \\ &= d_q + \zeta^2 \sum_{k=1; k \neq q}^n \frac{a_{kq}}{d_q - d_k} + \zeta^3 \sum_{r=1; r \neq q}^n \frac{a_{rq}}{d_q - d_r} \sum_{k=1; k \neq q}^n \frac{a_{qk} a_{kr}}{d_q - d_k} \\ &\quad + \zeta^4 \left(\sum_{r=1; r \neq q}^n \frac{a_{rq}}{d_q - d_r} \sum_{l=1; l \neq q}^n \frac{a_{rl}}{d_q - d_l} \sum_{k=1; k \neq q}^n \frac{a_{kq} a_{kl}}{d_q - d_k} - \sum_{r=1; r \neq q}^n \frac{a_{rq}}{(d_q - d_r)^2} \sum_{k=1; k \neq q}^n \frac{a_{kq}}{d_q - d_k} \right) + O(\zeta^5) \end{aligned} \tag{1}$$

Assuming that $|c_j(q)| \leq (A^j)_{qq}$ holds for any integer j , then the eigenvalue expansion in (8) of the matrix $\Delta + \zeta A$,

$$\xi_q(\zeta) = d_q + \zeta^2 c_2(q) + \zeta^3 c_3(q) + \zeta^4 c_4(q) + \cdots = d_q + \sum_{j=2}^{\infty} c_j(q) \zeta^j$$

is bounded as

$$|\xi_q(\zeta)| < d_q + \sum_{j=2}^{\infty} (A^j)_{qq} \zeta^j = d_q + \left(\sum_{j=2}^{\infty} A^j \zeta^j \right)_{qq}$$

Introducing the eigenvalue decomposition $A = X\Lambda X^T = \sum_{k=1}^N \lambda_k(A) x_k x_k^T$, where x_k is the normalized eigenvector of A belonging to eigenvalue $\lambda_k(A)$ and assuming the ordering $\lambda_1(A) \geq \lambda_2(A) \geq \dots \geq \lambda_N(A)$, then

$$\sum_{j=2}^{\infty} A^j \zeta^j = \sum_{k=1}^N x_k x_k^T \sum_{j=2}^{\infty} (\lambda_k(A) \zeta)^j$$

The geometric j -series converges, provided $|\lambda_k(A) \zeta| < 1$ for any k , i.e. $|\zeta| < \frac{1}{\lambda_1(A)}$, which is smaller than 1 in any connected graph G of size $N > 2$, because $\lambda_1(A) \geq d_{av} = \frac{2L}{N}$ (see e.g. [4]). The bounds $|c_j(q)| \leq (A^j)_{qq}$ are conservative, because, if $d_q \neq d_{\max}$, then there will be negative terms in each sum of the coefficients $c_j(q)$ for $j \geq 2$. Nevertheless, numerical computations indeed reveal that the expansion $\xi_q(-1) = d_q + \sum_{j=2}^{\infty} (-1)^j c_j(q)$, corresponding to an eigenvalue of the Laplacian $Q = \Delta - A$ around degree d_q (assumed to be unique or simple), diverges. For $N = 10$ and $N = 20$, we found numerically that the first 4 coefficients $c_k(q)$ decrease and just from $c_5(q)$ on increase. Limiting the series $\xi_{q;K}(-1) = d_q + \sum_{j=2}^K (-1)^j c_j(q)$ up to $K = 4$ terms seems “reasonably” accurate and limiting a divergent series (as in Stirling’s approximation [5]) to the point where the terms start increasing may be meaningful. Numerical evaluation seems that the accuracy of $\xi_{q;K}(-1)$ improves with increasing size N of the graph, but for not too high density $p = \frac{L}{\binom{N}{2}}$.

Instead of summing $\xi_q(-1) = d_q + \sum_{j=2}^{\infty} c_j(-1)^j$, Euler summation [2]

$$\xi_q(-1) = d_q + \sum_{m=2}^{\infty} \left(\sum_{k=2}^m \binom{m-1}{k-1} (-1)^k c_k \right) \frac{1}{2^m} \quad (2)$$

yields considerably better results: for sufficiently large K , the sum

$$\xi_{q;K}(-1) = d_q + \sum_{m=2}^K \left(\sum_{k=2}^m \binom{m-1}{k-1} (-1)^k c_k \right) \frac{1}{2^m} \rightarrow \mu_k$$

for some integer k and μ_k is close to d_q , where the eigenvalues of the Laplacian matrix Q are $\mu_1 \geq \mu_2 \geq \dots \geq \mu_N = 0$. In particular, we found numerically that the largest eigenvalue μ_1 is retrieved from $d_q = d_{\max}$, even with 4 coefficients, quite accurately! In addition, Euler summation (2) also seems to converge for other large degrees. On the other hand, expansion around $d_q = d_{\min}$ is considerably less accurate and Euler summation (2) does not seem to converge anymore. In other words, if the number of terms $K = 4$ in (2) is limited and the node q has a sufficiently large degree d_q (that is unique), then

$$\begin{aligned} \xi_{q;4}(-1) &\approx d_q + \frac{11}{16}c_2 - \frac{5}{16}c_3 + \frac{1}{16}c_4 \\ &= d_q + \frac{11}{16} \sum_{k=1; k \neq q}^n \frac{a_{kq}}{d_q - d_k} - \frac{5}{16} \sum_{r=1; r \neq q}^n \frac{a_{rq}}{d_q - d_r} \sum_{k=1; k \neq q}^n \frac{a_{qk}a_{kr}}{d_q - d_k} \\ &\quad + \frac{1}{16} \left(\sum_{r=1; r \neq q}^n \frac{a_{rq}}{d_q - d_r} \sum_{l=1; l \neq q}^n \frac{a_{rl}}{d_q - d_l} \sum_{k=1; k \neq q}^n \frac{a_{kq}a_{kl}}{d_q - d_k} - \sum_{r=1; r \neq q}^n \frac{a_{rq}}{(d_q - d_r)^2} \sum_{k=1; k \neq q}^n \frac{a_{kq}}{d_q - d_k} \right) \end{aligned} \quad (3)$$

is a reasonable estimate for a Laplacian eigenvalue μ_k . There exist many bounds on Laplacian eigenvalues. The Brouwer-Haemers bound [1] is $\mu_k \geq d_{(k)} - k + 2$, where $d_{(k)}$ is the k -th largest degree in the graph, i.e. $d_{(1)} \geq d_{(2)} \geq \dots \geq d_{(N)}$. An upper bound for the largest Laplacian eigenvalue [4] is

$\mu_1 \leq \min(N, \max_{l \in \mathcal{L}}(d_{l^+} + d_{l^-}))$, where d_{l^+} and d_{l^-} are the nodal degrees at the left- and right-hand node of a link l ; clearly $d_{l^+} + d_{l^-} \leq 2d_{\max}$. We hope that the approximation (3) may lead to sharper bounds.

The Euler summation of the matrix perturbation series in (2) bears resemblance to Lagrange series, where expansions around different points may converge to a same zero. Lagrange's series for the inverse $f^{-1}(z)$ of a function $f(z)$ is [3, II, pp. 88]

$$f^{-1}(z) = z_0 + \sum_{m=1}^{\infty} \frac{1}{m!} \left[\frac{d^{m-1}}{dw^{m-1}} \left(\frac{w - z_0}{f(w) - f(z_0)} \right)^m \right] \Big|_{w=z_0} (z - f(z_0))^m \quad (4)$$

A zero y of $f(z)$, obeying $f(y) = 0$ and $y = f^{-1}(0)$, has the Lagrange series

$$y = f^{-1}(0) = z_0 + \sum_{m=1}^{\infty} \frac{1}{m!} \left[\frac{d^{m-1}}{dw^{m-1}} \left(\frac{w - z_0}{f(w) - f(z_0)} \right)^m \right] \Big|_{w=z_0} (-f(z_0))^m$$

provided that z_0 is sufficiently close to y , else the Lagrange series may diverge or converge towards a different, more nearby zero of $f(z)$. Since the characteristic polynomial $c_Q(z) = \det(Q - zI) = \sum_{k=0}^N \gamma_k z^k = \prod_{k=1}^N (\mu_k - z)$ corresponds to the function $f(z)$, it is tempting to infer by comparing the Euler summation (2) and the Lagrange series (4) of $\mu_k = c_Q^{-1}(0)$ that $z_0 = d_q$, $c_Q(d_q) = -\frac{1}{2}$ and $\sum_{k=2}^m \binom{m-1}{k-1} (-1)^k c_k = \frac{1}{m!} \left[\frac{d^{m-1}}{dw^{m-1}} \left(\frac{w-d_q}{c_Q(w)+\frac{1}{2}} \right)^m \right] \Big|_{w=d_q}$. However, we are unable to prove this speculation.

3 Numerical examples

The recursion in (15) and (18) in Appendix A becomes, for $r \neq q$,

$$\begin{cases} \beta_{1r} = \frac{a_{rq}}{d_q - d_r} \\ \beta_{jr} = \frac{1}{d_r - d_q} \sum_{l=1; l \neq q}^N \left\{ \sum_{k=1}^{j-2} \beta_{kr} \beta_{j-k-1, l} a_{ql} - \beta_{j-1, l} a_{rl} \right\} \quad \text{for } j > 1 \end{cases}$$

and the coefficients (17) for $j > 1$ are

$$c_j(q) = \sum_{k=1; k \neq q}^N \beta_{j-1, k} a_{qk} \quad (5)$$

which can be computed up to any desired value of j .

Example 1 A tree on $N = 5$ nodes, with the adjacency matrix

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

has a degree vector $d = (3, 1, 1, 1, 2)$ and Laplacian eigenvalue vector $\mu = (4.17009, 2.31111, 1., 0.518806, 0)$. The infinite series (2) does not seem to converge, but the Euler sum (3) up to $K = 4$ terms equals $\xi_{5;4}(-1) = 2.125$ for $d_5 = 2$ and $\xi_{5;5}(-1) = 2.375$ for $K = 5$ terms and $\xi_{1;4}(-1) = 4.21875$ for

$d_1 = 3$. Also, all odd coefficients $c_{2m+1}(q) = 0$ in (5) for odd $m \geq 0$ are zero, possibly agreeing with the fact [4, p. 133] that the characteristic polynomial of the adjacency matrix of a tree is even, $c_{A_{\text{tree}}}(z) = \det(A_{\text{tree}} - zI) = c_{A_{\text{tree}}}(-z)$.

Example 2 An instance of an Erdős-Rényi graph $G_p(N)$ on $N = 20$ nodes and link density $p = 0.3$ has the adjacency matrix

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

degree vector

$$d = (4, 4, 8, 3, 7, 4, 12, 4, 7, 6, 7, 6, 10, 6, 6, 6, 6, 5, 4, 5)$$

ranked in decreasing order as (12, 10, 8, 7, 7, 7, 6, 6, 6, 6, 6, 6, 5, 5, 4, 4, 4, 4, 4, 3) to see uniqueness and Laplacian eigenvalue vector

$$\begin{aligned} \mu = & (13.3514, 11.6199, 9.80641, 9.32872, 7.6586, 7.46193, 7.11613, 6.92149, \\ & 6.3782, 6.07484, 5.80058, 5.29648, 4.59557, 4.05486, 3.58036, 3.50647 \\ & 2.83079, 2.39082, 2.22645, 0) \end{aligned}$$

The Euler summation $\xi_{q;K}(-1)$ in (2), in short $\xi_{q;K}$, seems to converge for node $q = 13$ and $d_q = 10$. Indeed, $\xi_{13;K}$ as function of the number K of terms converges to $\mu_2 = 11.6199$ as

$$\begin{aligned} \xi_{13;2} &= 10.48154762 & \xi_{13;7} &= 11.61206362 & \xi_{13;12} &= 11.61699285 & \xi_{13;17} &= 11.62009681 \\ \xi_{13;3} &= 11.00138889 & \xi_{13;8} &= 11.62002740 & \xi_{13;13} &= 11.61921713 & \xi_{13;18} &= 11.61968541 \\ \xi_{13;4} &= 11.33195709 & \xi_{13;9} &= 11.61508019 & \xi_{13;14} &= 11.62029217 & \xi_{13;19} &= 11.61958213 \\ \xi_{13;5} &= 11.49508126 & \xi_{13;10} &= 11.61181587 & \xi_{13;15} &= 11.62070805 & \xi_{13;20} &= 11.61970380 \\ \xi_{13;6} &= 11.57496760 & \xi_{13;11} &= 11.61364728 & \xi_{13;16} &= 11.62057580 & \xi_{13;30} &= 11.61991367 \end{aligned}$$

The Euler summation $\xi_{q;K}$ converges faster for node $q = 7$ with the maximum degree $d_q = 12$. Indeed, $\xi_{7;K}$ as function of K converges to $\mu_1 = 13.3514$ as

$$\begin{array}{llll} \xi_{7;2} = 12.55684524 & \xi_{7;7} = 13.32451888 & \xi_{7;12} = 13.35071509 & \xi_{7;17} = 13.35134956 \\ \xi_{7;3} = 12.92105159 & \xi_{7;8} = 13.33893469 & \xi_{7;13} = 13.35094032 & \xi_{7;18} = 13.35137642 \\ \xi_{7;4} = 13.10777862 & \xi_{7;9} = 13.34549561 & \xi_{7;14} = 13.35114508 & \xi_{7;19} = 13.35138894 \\ \xi_{7;5} = 13.22029144 & \xi_{7;10} = 13.34889571 & \xi_{7;15} = 13.35126516 & \xi_{7;20} = 13.35139125 \\ \xi_{7;6} = 13.28981543 & \xi_{7;11} = 13.35029701 & \xi_{7;16} = 13.35131598 & \xi_{7;30} = 13.35139267 \end{array}$$

where all presented digits of $\xi_{7;30}$ are correct. For node $q = 3$ with degree $d_3 = 8$, the Euler summation (2) seems to diverge. Indeed, $\xi_{3;K}$ initially tends to converge to $\mu_3 = 9.80641$, but diverges for larger K ,

$$\begin{array}{llll} \xi_{3;2} = 8.937500000 & \xi_{3;7} = 9.961090970 & \xi_{3;12} = 7.834417220 & \xi_{3;17} = 20.15673862 \\ \xi_{3;3} = 9.593750000 & \xi_{3;8} = 9.152494535 & \xi_{3;13} = 11.10756619 & \xi_{3;18} = 19.02124175 \\ \xi_{3;4} = 9.541536458 & \xi_{3;9} = 9.649234801 & \xi_{3;14} = 13.44103998 & \xi_{3;19} = -15.77306388 \\ \xi_{3;5} = 9.632552083 & \xi_{3;10} = 10.87231670 & \xi_{3;15} = 5.881312597 & \xi_{3;20} = -0.7480476187 \\ \xi_{3;6} = 10.14137146 & \xi_{3;11} = 9.574716849 & \xi_{3;16} = 3.636664041 & \xi_{3;30} = -1883.697136 \end{array}$$

All mentioned values of $\xi_{q;4}$, corresponding to the explicitly form in (3), indicate that (3) is a reasonably accurate estimate for a Laplacian eigenvalue.

4 Conclusion

Quite remarkably, we discovered that the Euler summation (2) seems to converge, for some suitably chosen node q with large and unique degree d_q , to a Laplacian eigenvalue μ_k . Convergence does not always happen. For smaller (and unique) degrees, the Euler summation (2) seems to diverge most of the time. Perhaps, a better tuning of the Euler summation¹ may be needed.

Apart from unique degree nodes, it would be desirable to know the graph properties for which the Euler summation (2) converges to Laplacian eigenvalues. More generally, under which matrix conditions does Euler summation (6) of the perturbation eigenvalue series in (8) in Appendix A converge, when the power series itself diverges.

Finally, the extension of spectral matrix theory to multiple eigenvalues is placed on the agenda of future research.

References

- [1] A. E. Brouwer and W. H. Haemers. A lower bound for the Laplacian eigenvalues of a graph: Proof of a conjecture by Guo. *Linear Algebra and its Applications*, 429:2131–2135, 2008.
- [2] G. H. Hardy. *Divergent Series*. Oxford University Press, London, 1948.

¹The more general Euler transform of $f(z) = f_0 + \sum_{m=1}^{\infty} f_m z^m$ disposes of a tuneable parameter t ,

$$f(z) = f_0 + \sum_{m=1}^{\infty} \left[\sum_{k=1}^m \binom{m-1}{k-1} f_k t^{m-k} \right] \left(\frac{z}{1+tz} \right)^m \quad (6)$$

that was chosen equal to $t = -1$ in (2).

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A Perturbation Theory

We confine ourselves to simple eigenvalues of a symmetric matrix, in which case the perturbation theory is relatively simple [6, pp. 60-70]. Perturbation theory for non-symmetric matrices and for eigenvalues with higher multiplicity is more involved and omitted.

A.1 Perturbation theory around a simple eigenvalue

Let us consider the matrix $A(\zeta) = A + \zeta B$. Perturbation theory assumes that the real number ζ is sufficiently small so that we may regard $A(\zeta)$ as the perturbation of the original $n \times n$ symmetric matrix A , not necessarily an adjacency matrix, by an $n \times n$ matrix B , which is not necessarily symmetric. We denote by $x(\zeta)$ the $n \times 1$ eigenvector of $A(\zeta)$ belonging to the eigenvalue $\lambda(\zeta)$. As shown in [6, pp. 60-70], both $x(\zeta)$ and $\lambda(\zeta)$ are analytic functions of ζ around zero and can be represented by a power series

$$x(\zeta) = x + \zeta z_1 + \zeta^2 z_2 + \dots = \sum_{j=0}^{\infty} z_j \zeta^j \quad (7)$$

$$\lambda(\zeta) = \lambda + \zeta c_1 + \zeta^2 c_2 + \dots = \sum_{j=0}^{\infty} c_j \zeta^j \quad (8)$$

where $x(0) = x = z_0$ is the eigenvector of A and $\lambda(0) = \lambda = c_0$ is its corresponding simple eigenvalue. We omit considerations about the convergence radius of the above power series. We choose $x = x_q$ as the normalized eigenvector of A corresponding to $\lambda = \lambda_q$.

The eigenvalue equation of $A(\zeta)$ is

$$(A + \zeta B) x(\zeta) = \lambda(\zeta) x(\zeta)$$

After introducing the power series (7) and (8), we obtain

$$(A + \zeta B) \left(x_q + \sum_{j=1}^{\infty} z_j \zeta^j \right) = \sum_{j=0}^{\infty} c_j \zeta^j \sum_{j=0}^{\infty} z_j \zeta^j$$

The left-hand side equals

$$\begin{aligned} (A + \zeta B) \left(x_q + \sum_{j=1}^{\infty} z_j \zeta^j \right) &= A x_q + \sum_{j=1}^{\infty} A z_j \zeta^j + \zeta B x_q + \sum_{j=1}^{\infty} B z_j \zeta^{j+1} \\ &= \lambda_q x_q + (A z_1 + B x_q) \zeta + \sum_{j=2}^{\infty} (A z_j + B z_{j-1}) \zeta^j \end{aligned}$$

while the Cauchy product of the right-hand side gives

$$\sum_{j=0}^{\infty} c_j \zeta^j \sum_{j=0}^{\infty} z_j \zeta^j = \sum_{j=0}^{\infty} \left(\sum_{k=0}^j c_{j-k} z_k \right) \zeta^j = \lambda_q x_q + (c_1 x_q + \lambda_q z_1) \zeta + \sum_{j=2}^{\infty} \left(\sum_{k=0}^j c_{j-k} z_k \right) \zeta^j$$

Equating corresponding powers in ζ yields, for $j = 1$,

$$Az_1 + Bx_q = \lambda_q z_1 + c_1 x_q \quad (9)$$

and, for $j > 1$,

$$Az_j + Bz_{j-1} = \sum_{k=0}^j c_{j-k} z_k = c_j x_q + \sum_{k=1}^{j-1} c_{j-k} z_k + \lambda_q z_j \quad (10)$$

Relations (9) and (10) are the results of complex function theory. The solution for the $n \times 1$ vectors $\{z_j\}_{j \geq 1}$ in (7) and the coefficients c_k in (8) now requires linear algebra.

A.2 Scaling of the eigenvector $x(\zeta)$

Since the vector z_j can be written as a linear combination of the eigenvectors x_k of A , we have

$$z_j = \sum_{k=1}^n \beta_{jk} x_k \quad (11)$$

where the coefficients $\beta_{jm} = x_m^T z_j = z_j^T x_m \neq \beta_{mj}$. The particular case $j = 0$, where $z_0 = x_q$, indicates that $\beta_{0k} = \delta_{kq}$. Thus, the eigenvector in (7) is rewritten as

$$x(\zeta) = \sum_{j=0}^{\infty} z_j \zeta^j = \sum_{k=1}^n \left(\sum_{j=0}^{\infty} \beta_{jk} \zeta^j \right) x_k = \left(\sum_{j=0}^{\infty} \beta_{jq} \zeta^j \right) x_q + \sum_{k=1; k \neq q}^n \left(\sum_{j=0}^{\infty} \beta_{jk} \zeta^j \right) x_k$$

and

$$x(\zeta) = \left(1 + \sum_{j=1}^{\infty} \beta_{jq} \zeta^j \right) x_q + \sum_{k=1; k \neq q}^n \left(\sum_{j=1}^{\infty} \beta_{jk} \zeta^j \right) x_k$$

We can always scale an eigenvector by a scalar $\alpha \neq 0$, which we choose here as $\alpha = 1 + \sum_{j=1}^{\infty} \beta_{jq} \zeta^j$, assuming that the power series converges to a value different than -1 . The latter condition can always be met for sufficiently small $|\zeta|$ and we arrive at

$$\alpha^{-1} x(\zeta) = x_q + \sum_{k=1; k \neq q}^n \left(\frac{\sum_{j=1}^{\infty} \beta_{jk} \zeta^j}{1 + \sum_{j=1}^{\infty} \beta_{jq} \zeta^j} \right) x_k$$

If we choose $\beta_{jq} = x_q^T z_j = z_0^T z_j = 0$ for $j \geq 1$ and recall that $\beta_{0q} = 1$, then $\alpha = 1$ and we simplify the computation by requiring that any ‘‘perturbation’’ vector z_j for $j \geq 1$ is orthogonal to the eigenvector x_q of the matrix A .

If we choose a different scaling by requiring a normalized eigenvector, such as $x^T(\zeta) x(\zeta) = 1$, then it implies that

$$1 = x^T(\zeta) x(\zeta) = \sum_{j=0}^{\infty} z_j^T \zeta^j \sum_{m=0}^{\infty} z_m \zeta^m = \sum_{j=0}^{\infty} \left(\sum_{m=0}^j z_m^T z_{j-m} \right) \zeta^j$$

and equating corresponding powers in ζ leads, for $j = 0$, to $z_0^T z_0 = 1$, which is satisfied for any normalized eigenvector $z_0 = x_q$ of A and, for $j > 0$, to $0 = \sum_{m=0}^j z_m^T z_{j-m}$. The latter condition means that $z_0^T z_1 = 0$ and furthermore that $z_0^T z_j = -\frac{1}{2} \sum_{m=1}^{j-1} z_m^T z_{j-m}$ for $j \geq 2$. In summary, the normalization of the eigenvector $x(\zeta)$ imposes conditions on the scalar products $z_0^T z_j$ for all $j \geq 1$. Choosing a different scaling leads to a different computational scheme and the art consists of choosing the most appropriate conditions on $z_0^T z_j$.

A.3 Evaluation of the power series coefficients c_k and vectors z_j

After expressing the relations (9) and (10) with (11) in terms of the normalized eigenvectors x_1, x_2, \dots, x_n of the matrix A and taking the eigenvalue equation $Ax_k = \lambda_k x_k$ into account, we obtain the set of linear equations

$$c_1 x_q = \sum_{k=1}^n \beta_{1k} (\lambda_k - \lambda_q) x_k + Bx_q \quad (12)$$

and, for $j > 1$,

$$c_j x_q = \sum_{k=1}^n \beta_{jk} (\lambda_k - \lambda_q) x_k + \sum_{k=1}^n \beta_{j-1,k} Bx_k - \sum_{l=1}^n \sum_{k=1}^{j-1} c_{j-k} \beta_{kl} x_l \quad (13)$$

in the unknown numbers $\{c_k\}_{k \geq 1}$ and $\{\beta_{jk}\}_{j \geq 1; k \geq 1}$. As eigenvector scaling, we choose $\beta_{jq} = x_q^T z_j = z_0^T z_j = 0$ for $j \geq 1$, which is computationally, the simplest choice.

Pre-multiplying (12) with the vector x_r^T , using $x_r^T x_q = \delta_{rq}$ yields

$$c_1 \delta_{rq} = \beta_{1r} (\lambda_r - \lambda_q) + x_r^T Bx_q$$

In particular, if $r = q$, then

$$c_1 = x_q^T Bx_q \quad (14)$$

else,

$$\beta_{1r} = \frac{x_r^T Bx_q}{\lambda_q - \lambda_r} \quad \text{for } r \neq q \quad (15)$$

The expression (15) emphasizes that the eigenvalue λ_q must be simple, which is a basic limitation of the presented perturbation method. Hence, it follows from (11) that

$$z_1 = \sum_{k=1}^N \beta_{1k} x_k = \sum_{k=1; k \neq q}^N \frac{x_k^T Bx_q}{\lambda_q - \lambda_k} x_k + \beta_{1q} x_q$$

With our eigenvector scaling choice $\beta_{1q} = 0$, we find the first order expansion in ζ ,

$$\begin{cases} x(\zeta) = x_q + \zeta \sum_{k=1; k \neq q}^N \frac{x_k^T Bx_q}{\lambda_q - \lambda_k} x_k + O(\zeta^2) \\ \lambda(\zeta) = \lambda_q + \zeta x_q^T Bx_q + O(\zeta^2) \end{cases}$$

Pre-multiplying (13) with the vector x_r^T analogously leads, for $j > 1$, to

$$c_j \delta_{rq} = \beta_{jr} (\lambda_r - \lambda_q) + \sum_{k=1}^n \beta_{j-1,k} x_r^T Bx_k - \sum_{k=1}^{j-1} c_{j-k} \beta_{kr}$$

In particular, if $r = q$, then

$$c_j = \sum_{k=1}^n \beta_{j-1,k} x_q^T B x_k - \sum_{k=1}^{j-1} c_{j-k} \beta_{kq}$$

else

$$\beta_{jr} = \frac{1}{\lambda_r - \lambda_q} \left\{ \sum_{k=1}^{j-1} c_{j-k} \beta_{kr} - \sum_{k=1}^n \beta_{j-1,k} x_r^T B x_k \right\} \quad \text{for } r \neq q \quad (16)$$

With our eigenvector scaling choice $\beta_{jq} = 0$ for $j > 0$, the first recursive equation in the coefficients c_k simplifies considerably to

$$c_j = \sum_{k=1; k \neq q}^n \beta_{j-1,k} x_q^T B x_k \quad \text{for } j > 1 \quad (17)$$

Substituting the explicit form of the coefficients c_j in (17) into (16) yields, for $j > 1$,

$$\beta_{jr} = \frac{1}{\lambda_r - \lambda_q} \sum_{l=1; l \neq q}^n \left\{ \sum_{k=1}^{j-1} \beta_{kr} \beta_{j-k-1,l} x_q^T B x_l - \beta_{j-1,l} x_r^T B x_l \right\} \quad \text{for } r \neq q$$

The scaling choice $\beta_{0,l} = \delta_{lq}$ and $\beta_{jq} = 0$ for $j \geq 1$ simplifies, for $r \neq q$, to a recursion in β_{jr}

$$\beta_{jr} = \frac{\beta_{j-1;r} x_q^T B x_q}{\lambda_r - \lambda_q} + \frac{1}{\lambda_r - \lambda_q} \sum_{l=1; l \neq q}^n \left\{ \sum_{k=1}^{j-2} \beta_{kr} \beta_{j-k-1,l} x_q^T B x_l - \beta_{j-1,l} x_r^T B x_l \right\} \quad (18)$$

which can be iterated up to any desired integer value of j .

For example, if $j = 2$, then (irrespective of the choice of scaling)

$$c_2 = \sum_{k=1}^n \beta_{1k} x_q^T B x_k - c_1 \beta_{1q} = \sum_{k=1; k \neq q}^n \beta_{1k} x_q^T B x_k$$

and

$$\beta_{2r} = \frac{1}{\lambda_r - \lambda_q} \left\{ \beta_{1r} x_q^T B x_q - \sum_{k=1}^n \beta_{1k} x_r^T B x_k \right\} \quad \text{for } r \neq q$$

Using (15) results in

$$c_2 = \sum_{k=1; k \neq q}^n \frac{(x_k^T B x_q)^2}{\lambda_q - \lambda_k} \quad (19)$$

and

$$\beta_{2r} = \frac{1}{\lambda_q - \lambda_r} \sum_{k=1; k \neq q}^n \frac{(x_k^T B x_q)(x_k^T B x_r)}{\lambda_q - \lambda_k} - \frac{(x_r^T B x_q)(x_q^T B x_q)}{(\lambda_q - \lambda_r)^2} \quad \text{for } r \neq q \quad (20)$$

Moreover, we can use β_{2r} immediately in $c_3 = \sum_{k=1; k \neq q}^n \beta_{2k} x_q^T B x_k$ in (17),

$$c_3 = \sum_{r=1; r \neq q}^n \frac{x_q^T B x_r}{\lambda_q - \lambda_r} \sum_{k=1; k \neq q}^n \frac{(x_k^T B x_q)(x_k^T B x_r)}{\lambda_q - \lambda_k} - \sum_{r=1; r \neq q}^n \frac{(x_r^T B x_q)^2 (x_q^T B x_q)}{(\lambda_q - \lambda_r)^2} \quad (21)$$

illustrating that, in general, the eigenvalue expansion (8) can always be computed, with the same efforts, one order higher in ζ than the eigenvector expansion (7). Indeed, the coefficient c_j in (17) only depends on $\beta_{j-1,k}$ and not on β_{jk} as z_j in (11).

If $j = 3$, then (18) becomes, for $r \neq q$,

$$\begin{aligned}
\beta_{3r} &= \frac{\beta_{2r} x_q^T B x_q}{\lambda_r - \lambda_q} + \frac{1}{\lambda_r - \lambda_q} \sum_{l=1}^n \{ \beta_{1r} \beta_{1l} x_q^T B x_l - \beta_{2l} x_r^T B x_l \} \\
&= -\frac{x_q^T B x_q}{(\lambda_q - \lambda_r)^2} \sum_{k=1; k \neq q}^n \frac{(x_k^T B x_q)(x_k^T B x_r)}{\lambda_q - \lambda_k} + \frac{(x_r^T B x_q)(x_q^T B x_q)^2}{(\lambda_q - \lambda_r)^3} \\
&\quad - \frac{x_r^T B x_q}{(\lambda_q - \lambda_r)^2} \sum_{k=1; k \neq q}^n \frac{(x_k^T B x_q)^2}{\lambda_q - \lambda_k} + \frac{1}{\lambda_q - \lambda_r} \sum_{l=1; l \neq q}^n \frac{x_r^T B x_l}{\lambda_q - \lambda_l} \sum_{k=1; k \neq q}^n \frac{(x_k^T B x_q)(x_k^T B x_l)}{\lambda_q - \lambda_k} \\
&\quad - \frac{x_q^T B x_q}{\lambda_q - \lambda_r} \sum_{k=1; k \neq q}^n \frac{(x_k^T B x_q)(x_k^T B x_r)}{(\lambda_q - \lambda_k)^2}
\end{aligned}$$

The coefficient $c_4 = \sum_{k=1; k \neq q}^n \beta_{3k} x_q^T B x_k$ in (17) is

$$\begin{aligned}
c_4 &= - \sum_{r=1; r \neq q}^n \frac{(x_q^T B x_r)(x_q^T B x_q)}{(\lambda_q - \lambda_r)^2} \sum_{k=1; k \neq q}^n \frac{(x_k^T B x_q)(x_k^T B x_r)}{\lambda_q - \lambda_k} + \sum_{r=1; r \neq q}^n \frac{(x_r^T B x_q)^2 (x_q^T B x_q)^2}{(\lambda_q - \lambda_r)^3} \\
&\quad - \sum_{r=1; r \neq q}^n \frac{(x_r^T B x_q)^2}{(\lambda_q - \lambda_r)^2} \sum_{k=1; k \neq q}^n \frac{(x_k^T B x_q)^2}{\lambda_q - \lambda_k} + \sum_{r=1; r \neq q}^n \frac{x_q^T B x_r}{\lambda_q - \lambda_r} \sum_{l=1; l \neq q}^n \frac{x_r^T B x_l}{\lambda_q - \lambda_l} \sum_{k=1; k \neq q}^n \frac{(x_k^T B x_q)(x_k^T B x_l)}{\lambda_q - \lambda_k} \\
&\quad - \sum_{r=1; r \neq q}^n \frac{(x_q^T B x_r)(x_q^T B x_q)}{\lambda_q - \lambda_r} \sum_{k=1; k \neq q}^n \frac{(x_k^T B x_q)(x_k^T B x_r)}{(\lambda_q - \lambda_k)^2}
\end{aligned}$$

The first and last sum are the same and we obtain

$$\begin{aligned}
c_4 &= (x_q^T B x_q)^2 \sum_{r=1; r \neq q}^n \frac{(x_r^T B x_q)^2}{(\lambda_q - \lambda_r)^3} - 2(x_q^T B x_q) \sum_{r=1; r \neq q}^n \frac{(x_q^T B x_r)}{(\lambda_q - \lambda_r)^2} \sum_{k=1; k \neq q}^n \frac{(x_k^T B x_q)(x_k^T B x_r)}{\lambda_q - \lambda_k} \\
&\quad - \sum_{r=1; r \neq q}^n \frac{(x_r^T B x_q)^2}{(\lambda_q - \lambda_r)^2} \sum_{k=1; k \neq q}^n \frac{(x_k^T B x_q)^2}{\lambda_q - \lambda_k} \\
&\quad + \sum_{r=1; r \neq q}^n \frac{x_q^T B x_r}{\lambda_q - \lambda_r} \sum_{l=1; l \neq q}^n \frac{x_r^T B x_l}{\lambda_q - \lambda_l} \sum_{k=1; k \neq q}^n \frac{(x_k^T B x_q)(x_k^T B x_l)}{\lambda_q - \lambda_k} \tag{22}
\end{aligned}$$

If $\lambda_q = \lambda_1$ is the largest eigenvalue of a symmetric matrix A , then we observe that the coefficient c_2 in (19) is positive. Consequently, if ζ is sufficiently small so that the remainder of the series in (8) obeys $\left| \sum_{j=3}^{\infty} c_j \zeta^j \right| < c_2 \zeta^2$, then the first order perturbation $\lambda(\zeta) \geq \lambda_1 + \zeta x_1^T B x_1$ is a lower bound.