EIGENVALUE BOUNDS OF THE KIRCHHOFF LAPLACIAN

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Abstract. We prove the inequality $\lambda_k \leq d_k + d_{k-1}$ for all the eigenvalues $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$ of the Kirchhoff Laplacian of a finite simple graph with vertex degrees $d_1 \leq d_2 \leq \cdots \leq d_n$ and assuming $d_0 = 0$. A consequence is that the pseudo determinant $\text{Det}(K)$ counting the number of rooted spanning trees has an upper bound $2^n \prod_{k=1}^n d_k$ and that $\det(1+K)$ counting the number of rooted spanning forests has an upper bound $2^n \prod_{k=1}^n (1+d_k)$.

1. The theorem

1.1. Let $G = (V, E)$ be a **finite simple graph** with n vertices. Denote by $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$ the ordered list of eigenvalues of the **Kirchhoff matrix** $K = B - A$, where B is the diagonal vertex degree matrix with ordered vertex degrees $d_1 \leq d_2 \leq \cdots \leq d_n$ and where A is the adjacency matrix of G.

1.2. We assume $d_0 = 0$ so that $d_1 + d_0 = d_1$ and prove

Theorem 1. $\lambda_k \leq d_k + d_{k-1}$, *for all* $1 \leq k \leq n$.

The case $d = n$ is the **spectral radius** estimate $\lambda_n \leq d_n + d_{n-1}$ of Anderson and Morley [1] which we will use in the proof. The case $k = 1$ is obvious because $\lambda_1 = 0$ and $k = 2$ is a special case of the Schur-Horn inequality [5] as $\lambda_2 = \lambda_1 + \lambda_2 \leq d_1 + d_2$. Already the case $\lambda_3 \leq d_3 + d_2$ appears to be new as it goes beyond the Schur-Horn inequality. Note that any estimate on the spectral radius λ_n provides upper bounds on λ_k and there are many improvements since the ground breaking Anderson-Morley paper [35, 16, 43, 10, 19, 37, 28, 29, 44]. They would give better upper bounds also for λ_k but look less elegant.

1.3. Already the corollary $\lambda_k \leq 2d_k$ is stronger than what the **Gershgorin circle theorem** [14, 42] gives in this case: the circle theorem provides in every interval $[0, 2d_k]$ at least one eigenvalue λ_l of K. It does not need to be the k'th one. In the Kirchhoff case, where the Gershgorin circles are nested, 0 is always in the spectrum. Theorem (1) gives more information. The spectral data $\lambda_1 = 0, \lambda_2 = 10, \lambda_3 = 10$ for example are Gershgorin compatible to $d_1 = 1, d_2 = 3, d_3 = 7$ because there is an eigenvalue in each closed ball $[0, 2], [0, 6]$ and $[0, 14]$. But these data contradict Theorem (1) as $\lambda_2 = 2d_2 + 4$. Theorem 1 keeps the eigenvalues more aligned with the degree sequence, similarly as the Schur-Horn theorem does.

1.4. An application is that the pseudo determinant $\text{Det}(K) = \prod_{k=2}^n \lambda_k$ which by the Kirchhoff-Cayley **matrix tree theorem** count the number of rooted spanning trees has an upper bound $2^n \prod_k d_k$ and that $\det(1+K)$ by the Chebotarev-Shamis matrix forest theorem count the number of rooted spanning forests has an upper bound $2^n \prod_k (1 + d_k)$. These determinant inequalities do not follow from the Gershgorin nor from the Schur-Horn inequalities. We like to rephrase the determinant bounds as bound on the spectral potential $U(z) = (1/n) \log \det(K - z) \leq$

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$2 + (1/n)\log\det(M - z)$, where $M = \mathrm{Diag}(d_1, \dots, d_n)$ is the diagonal matrix and $z \leq 0$ is real. We made use of Theorem (1) to show that $U(z)$ has a Barycentric limit. It bounds the potential U of the interacting system with the potential $(1/n)\log\det(M - z)$ of the non-interacting system where M can be thought of as the Kirchhoff matrix of a non-interacting system where we have d_k self-loops at vertices k, even-so the tree and forest interpretations do not make sense any more.

2. The proof

2.1. If we make he statement slightly stronger, also the induction assumption becomes more powerful. Let $\mathcal{K}$ the class of symmetric matrices which are obtained as principal submatrices of a Kirchhoff matrices of a finite simple graph obtained by deleting the rows and columns to a maximal diagonal entry. In other words, we close the class of Kirchhoff matrices under the operation of taking principal submatrices. The stronger statement is that for all $A \in \mathcal{K}$, the eigenvalues λ_k and diagonal entries d_k, when ordered in an ascending order, satisfy $\lambda_k \leq d_k + d_{k-1}$.

2.2. The class $\mathcal{K}$ is invariant under the operation ϕ which removes corresponding rows and columns. This allows induction. The induction foundation $n = 1$ is obvious because the result holds for any 1×1 matrix with non-negative entries. For 2×2 matrices $K = \begin{bmatrix} d_1 & -t \\ -t & d_2 \end{bmatrix}$ we have with the trace $T = d_1 + d_2$ the eigenvalue $\lambda_2 = (T + \sqrt{T^2 + 4t^2 - 4d_1d_2})/2$ which is $\leq T = d_1 + d_2$ if $t \leq \sqrt{d_1 d_2}$ and especially if $t \leq d_1$.

2.3. The induction step uses the **Cauchy interlace theorem** or **Separation theorem** [20]: if μ_k are the eigenvalues of $\phi(K)$, then $\lambda_k \leq \mu_k \leq \lambda_{k+1}$. (The interlace theorem follows from the **Hermite interlace theorem** for real polynomials [21, 13]. If f is a monic polynomial of degree n with real roots $\lambda_1 \leq \dots \leq \lambda_n$ and g is a monic polynomial of degree $n-1$ with real roots $\mu_1 \leq \dots \leq \mu_{n-1}$ then g **interlaces** f if $\lambda_1 \leq \mu_1 \leq \lambda_2 \leq \dots \leq \mu_{n-1} \leq \lambda_n$. Equivalent for f and g to interlace is that the interpolation $tf + (1-t)g$ has real roots for all $t \in [0, 1]$.)

2.4. The interlace theorem does not catch the largest eigenvalue λ_n. This requires an upper bound for the **spectral radius**. This is where Anderson and Morley [1] come in. They realized that $K = F^*F$ is essentially isospectral to FF^*. The later is the adjacency matrix of the line graph but with the modification that all diagonal entries are 2. Since the row or column sum of FF^* is bound by $d_k(a) + d_k(b)$ for any edge (a, b), the upper bound holds. But we need to extend this estimate to $\mathcal{K}$.

Lemma 1 (Upgrade of Anderson and Morley)**.** *For any matrix in $\mathcal{K}$, the spectral radius satisfies $\lambda_n \leq d_n + d_{n-1}$.*

2.5. We can assume that after a coordinate change the diagonal entries of $K \in \mathcal{K}$ are ordered. This simply requires to order the vertices compatible with the order of the d_j. [1] estimate $\lambda_n \leq d_n + d_{n-1}$ for Kirchhoff matrices and even show that $\lambda_n \leq \max_{(a,b)\in E(G)} d(a) + d(b)$. We now verify that this extends to $\mathcal{K}$.

2.6. We have already seen the induction assumption for $n = 1$ and $n = 2$. Let K be a $n \times n$ matrix in $\mathcal{K}$ and assume we know the answer already for all $(n-1) \times (n-1)$ matrices in $\mathcal{K}$. When taking a principal submatrix of K by deleting the first row and first column, we do not change d_n nor d_{n-1}. The reason is that decoupling the lowest degree vertex does not change the largest two diagonal elements. The upper bound $d_n + d_{n-1}$ is therefore not affected.

2.7. Let $\mu_1 \leq \mu_2 \leq \cdots \leq \mu_{n-1}$ be the eigenvalues of the principal submatrix where the first row and column are deleted. The Cauchy interlacing result gives $\lambda_{n-1} \leq \mu_{n-1} \leq \lambda_n$ The largest eigenvalue μ_{n-1} of the deformed matrix is smaller or equal than than the largest eigenvalue λ_n and so smaller or equal than $d_n + d_{n-1}$. The inequality $\mu_{n-1} \leq d_n + d_{n-1}$ is what we wanted to show.

2.8. One could also explicitly track how the maximal eigenvalue decreases if all the non-diagonal entries in the first row and column is multiplied by t. If v is the normalized eigenvector to the largest eigenvalue λ_n, then since the matrices are symmetric, v is perpendicular to $[1, 1, \dots, 1, 1]$ the eigenvector to $\lambda_1 = 0$. This implies $\sum_{k=1}^{n-1} v_k = -v_1$. Let now E be the matrix in which the first row and first column except E_{11} contains only 1 and everything else is zero. We need to understand how $K - tE$ changes the largest eigenvalue λ. The **first Hadamard deformation formula** gives $\lambda(t)' = v^T E v = v_1^2 > 0$. The **second Hadamard deformation formula** would even show $\lambda(t)'' > 0$, illustrating **eigenvalue repulsion**. In any case, the largest eigenvalue increases under the deformation. Since at $t = 1$, the end of the deformation, we have $\lambda_n \leq d_n + d_{n-1}$ this is also the case for $t = 0$, where the connections to the weak vertex link have all been capped.

3. Remarks

3.1. Similarly than the Schur-Horn inequality $\sum_{j=1}^k \lambda_j \leq \sum_{j=1}^k d_j$ which is true for any symmetric matrix with diagonal entries d_j, Theorem (1) controls how close the ordered eigenvalue sequence is to the ordered vertex degree sequence. But it is different. For example, if the eigenvalues increase exponentially like $\lambda_k = 6^k$, then the inequality $\lambda_k \leq 2d_k$ implies on a logarithmic scale $\log(\lambda_k) \leq \log(2) + \log(d_k)$. Schur-Horn does not provide that. As for the **Gershgorin circle theorem**, it would only establish $\log(\lambda) \leq \log(2) + \log(d_n)$, where d_n is the largest entry because the theorem assures only that in each Gershgorin circle, there is at least one eigenvalue.

3.2. Anderson and Morley [1] have the better bound $\max_{(x,y)\in E} d(x) + d(y)$ and Theorem (1) could be improved in that $d_k + d_{k-1}$ can be replaced by $\max_{(x,y)\in E} d_k + d_j$. Any general better upper bound of the spectral radius leads to better results. The Anderson-Morley estimate as an early use of a **McKean-Singer super symmetry** [32] (see [22] for graphs). in a simple case where one has only 0-forms and 1-forms. There, it reduces to the statment that $K = F^* F$ is essentially isospectral to FF^* which is true for all matrices. It uses that the Laplacian K is of the form $F^* F = \text{divgrad}$, where $F = \text{grad}$ is the incidence matrix $Ff((a,b)) = f(b) - f(a)$ for functions f on vertices (0-forms) leading to functions on oriented edges (1-form).

3.3. There is much work on the spectral radius of the Kirchhoff Laplacian. It is bounded above by the spectral radius of the **signless Kirchhoff Laplacian** $|K|$ in which one takes the absolute values for each entry. This matrix is a non-negative matrix in the connected case has a power $|K|^n$ with all positive entries so that by the Perron-Frobenius theorem, the maximal eigenvalue is unique. (The Kirchhoff matrix itself of course can have multiple maximal eigenvalues like for the case of the complete graph). Also, unlike K which is never invertible $|K|$ is invertible if G is not bipartite. If we treat a graph as a one-dimensional simplicial complex (ignoring 2 and higher dimensional simplices in the graph), and denote d the exterior derivative of this skeleton complex, then $(d + d^*)^2 = K_0 + K_1$ where $K = K_0 = d^* d$ is the Kirchhoff matrix and $K_1 = dd^*$ is the one-form matrix with the same spectral radius. This leads to [1]. Much work has gone in improving this [6, 39, 31, 43, 12, 37, 29]. We have used that an identity coming from connection matrices [27].

3.4. We stumbled on the theorem when looking for bounds on the **tail distribution** $\mu([x,\infty))$ of the **limiting density of states** μ of the Barycentric limit $\lim_{n\to\infty} G_n$ of a finite simple graph $G = G_0$, where G_n is the Barycentric refinement of G_{n-1} in which the complete subgraphs of G_{n-1} are the vertices and two are connected if one is contained in the other [25, 26]. We wanted a **potential** $U(z) = \int_0^\infty \log(z-w)\, d\mu(w)$ because $U(-1)$ measures the exponential growth of rooted spanning forests while $U(0)$ measures the exponential growth of the rooted spanning trees.
The connection is that in general, the **pseudo determinant** [24] $\mathrm{Det}(K) = \prod_{\lambda\neq 0}\lambda$ is the number of **rooted spanning trees** in G by the **Kirchhoff matrix tree theorem** and $\det(1+K)$ is the number of rooted spanning forests in G by the **Chebotarev-Shamis matrix forest theorem** [33, 34, 23]. All these relations follow directly from the **generalized Cauchy-Binet theorem** that states that for any $n\times m$ matrices F, G, one has the pseudo determinant version $\mathrm{Det}(F^TG) = \sum_{|P|=k}\det(F_P)\det(G_P)$ with k depends on F, G and $\det(1+xF^TG) = \sum_P x^{|P|}\det(F_P)\det(G_P)$. **Pythagorean identities** like $\mathrm{Det}(F^TF) = \sum_{|P|=k}\det^2(F_P)$ and $\det(1+F^TF) = \sum_P \det^2(F_P)$ follow for an arbitrary $n\times m$ matrix F. Applied to the **incidence matrix** F of a connected graph, where $k(A) = n-1$ is the rank of $K = F^TF$, the first identity counts on the right spanning trees and the second identity counts on the right the number of spanning forests

3.5. Having noticed that the **tree-forest ratio** $\tau(G) = \mathrm{Det}(1+K)/\mathrm{Det}(K) = \prod_{\lambda\neq 0}(1+1/\lambda)$ has a Barycentric limit $\lim_{n\to\infty}(1/|G_n|)\log(\tau(G_n))$, we interpreted this as $U(-1)-U(0)$ requiring the normalized potential to exist. By the way, for complete graphs $G = K_n$ the tree-forest ratio is $(1+1/n)^{n-1}$ and converges to the **Euler number** e. For triangle-free graphs, $\log(\tau(G_n))/|V(G_n)|$ converges to $\log(\phi^2)$, where ϕ is the **golden ratio**. For example, for $G = C_n$, where $\mathrm{Det}(K) = n^2$ and the number of rooted spanning forests is the alternate **Lucas number** recursively given by $L(n+1) = 3L(n) - L(n-1) + 2, L(0) = 0, L(1) = 1$. We proved in general that $\log(\tau(G_n))/|V(G_n))|$ converges under **Barycentric refinements** $G_0 \to G_1 \to G_2 \dots$ for arbitrary graphs to a universal constant that only depends on the maximal dimension of $G = G_0$.

3.6. Theorem (1) needs to be placed in the context of the spectral graph literature like [3, 11, 15, 5, 8, 9, 38] or articles like [19, 40, 36]. Most research work in this area has focused on small eigenvalues like λ_2 or large eigenvalues like the spectral radius λ_n. For λ_2, there is a **Cheeger estimate** $h^2/(2d_n) \leq \lambda_2 \leq h$ for the eigenvalue λ_2 and Cheeger constant $h = h(G)$ [7] first defined for Riemannian manifolds, meaning in the graph case that one needs remove $h|H|$ edges to spearate a subgraph H from G. For the largest eigenvalue λ_n the Anderson-Morley bound has produced an industry of results.

3.7. Let us look at some example. Figure (1) shows more visually what happens in some examples of graphs with $n = 10$ vertices.
a) For the cyclic graph C_4, the Kirchhoff eigenvalues are $\lambda_1 = 0, \lambda_2 = 2, \lambda_3 = 2, \lambda_4 = 4$ and the edge degrees are $d_1 = d_2 = d_3 = d_4 = 2$.
b) For the star graph with $n-1$ spikes, the eigenvalues are $\lambda_1 = 0, \lambda_2 = \cdots \lambda_{n-1} = 1, \lambda_n = n$ while the degree sequence is $d_1 = \cdots = d_{n-1} = 1, d_n = n$.
c) For a complete bipartite graph $K_{n,m}$ with $m \leq m$, we have $0 \leq m \leq \cdots \leq m \leq n \cdots \leq n$

with $m-1$ eigenvalues m and $n-1$ eigenvalues n. The degree sequence has $m \leq m \leq \cdots \leq m \leq n \leq \cdots \leq n$ with m entries m and n entries n.

3.8. From all the 38 isomorphism classes of connected graphs with 4 vertices, there are only 3, for which equality holds in Theorem (1) and 7 for which $\lambda_k = 2d_k$. From the 728 isomorphism classes of connected graphs with 5 vertices, there are none for Theorem (1) and 5 for $\lambda_k = 2d_k$. From the 26704 isomorphism classes of connected graphs with 6 vertices, there are 70 for which Theorem (1) has equality and 76 for which $\lambda_k = 2d_k$. It is always only the largest eigenvalue, where we have seen equality $\lambda_n = 2d_n$ to hold.

3.9. The theorem implies $\sum_{j=1}^k \lambda_j \leq 2\sum_{j=1}^k d_j$ which is weaker than the Schur-Horn inequality $\sum_{j=1}^k \lambda_j \leq \sum_{j=1}^k d_j$. The later result is of wide interest. It can be seen in the context of partial traces [41] $\sum_{j=1}^k \lambda_j = \inf_{dim(V)=k} \text{tr}(A|V)$ and is special case of the **Atiyah-Guillemin-Sternberg convexity theorem** [2, 17]. The Schur inequality has been sharpened a bit for Kirchhoff matrices to $\sum_{j=1}^k \lambda_j \leq \sum_{j=1}^k d_j - 1$ [5] Proposition 3.10.1.

3.10. There is a general lower bound $\lambda_k \geq d_k - (n-k) + 1$ which had been conjectured of Guo [18] and is now a theorem [4] (see also [5] Proposition 3.10.2.). This Brouwer-Haemers estimate from 2008 generalizes $\lambda_n \geq d_n + 1$ [16] $\lambda_{n-1} \geq d_{n-1}$ ([30] and $\lambda_{n-2} \geq d_{n-2} - 1$ [18]. It follows also from $K = -A + B$ with $B = \text{Diag}(d_1, \cdots d_n)$ positive semi definite that $\lambda_k(K) \geq \lambda_k(-A)$ [20] (Corollary 4.3.12).

3.11. Unlike the Schur-Horn inequality, Theorem (1) does not extend to general symmetric matrices. Already for $A = \begin{bmatrix} 1 & 3 \\ 3 & 1 \end{bmatrix}$ which has eigenvalues $\lambda_1 = -2, \lambda_2 = 4$ and with $d_1 = 1, d_2 = 1$, the inequality $\lambda_2 \leq 2d_2$ fails. It also does not extend to symmetric matrices with non-negative eigenvalues, but also this does not work as $A = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix}$ shows, as this matrix has eigenvalues $0, 0, 3$ and diagonal entries $1, 1, 1$. The case of $n \times n$ matrices with constant entries 1 is an example with eigenvalues 0 and n showing that no estimate $\lambda_n \leq Cd_n$ is in general possible for symmetric matrices even when asking the diagonal entry to dominate the other entries.

4. Open ends

4.1. Theorem (1) also would follow from the statement

$$\sum_{j=1}^k d_j - \sum_{j=1}^k \lambda_j \leq d_k \tag{1}$$

which would be of independent interest as it estimates the **Schur-Horn error**. Indeed, the Schur-Horn gives together with such a hypothetical error bound $0 \leq \sum_{j=1}^k d_j - \sum_{j=1}^k \lambda_j + d_{k+1} - \lambda_{k+1} \leq d_k + d_{k+1} - \lambda_{k+1}$, which is $\lambda_k \leq d_k + d_{k+1}$. Can we prove the above Schur-Horn error estimate (1)? We do not know yet but our experiments indicate:

Conjecture A: [Schur-Horn error] Estimate (1) holds for all finite simple graphs

4.2. We have mentioned the Brouwer-Haemers bound $\lambda_k \geq d_k - (n-k) + 1$ which is very good for large k but far from optimal for smaller k. (Note that part of the graph theory literature labels the eigenvalues in decreasing order. We use an ordering more familiar in the manifold case, where one has no largest eigenvalue and which also appears in the earlier literature like [20].) The guess $d_{k-1}/2 \leq \lambda_k$ assuming $d_{-1} = 0$ is a **rule of thumb**, as it fails only in rare cases. The next thing to try is $d_{k-2}/2 \leq \lambda_k$ and this is still wrong in general but there are even less counter examples. We can try $d_{k-2}/3$ for which we have not found a counter example yet but it might just need to look for larger networks to find a counter example. We still believe that there is an affine lower bound. This is based only on limited experiments like for $A = 1/3$ where it already looks good.

Conjecture B: [Affine Brouwer-Haemers bound] There exist constants $0 < A < 1$ and B such that for all graphs and $1 \leq k \leq n$ we have $Ad_k - B \leq \lambda_k$.

4.3. We see for many Erdös-Rényi graphs that an upper bound $\lambda_k \leq Cd_k$ holds for most graphs for any $C > 1$, if the graphs are large. A possible conjecture is that

Conjecture C: [Linear bound for Erdoes-Renyi] For all $C > 1$ and all $p \in [0, 1]$, the probability of the set of graphs in the Erdös-Rényi probability space $E(n, p)$ with $\lambda_k \leq Cd_k$ for all $1 \leq k \leq n$ goes to 1 for $n \to \infty$.

5. Illustration

5.1. Here are a few examples of spectra with known upper and lower bounds:

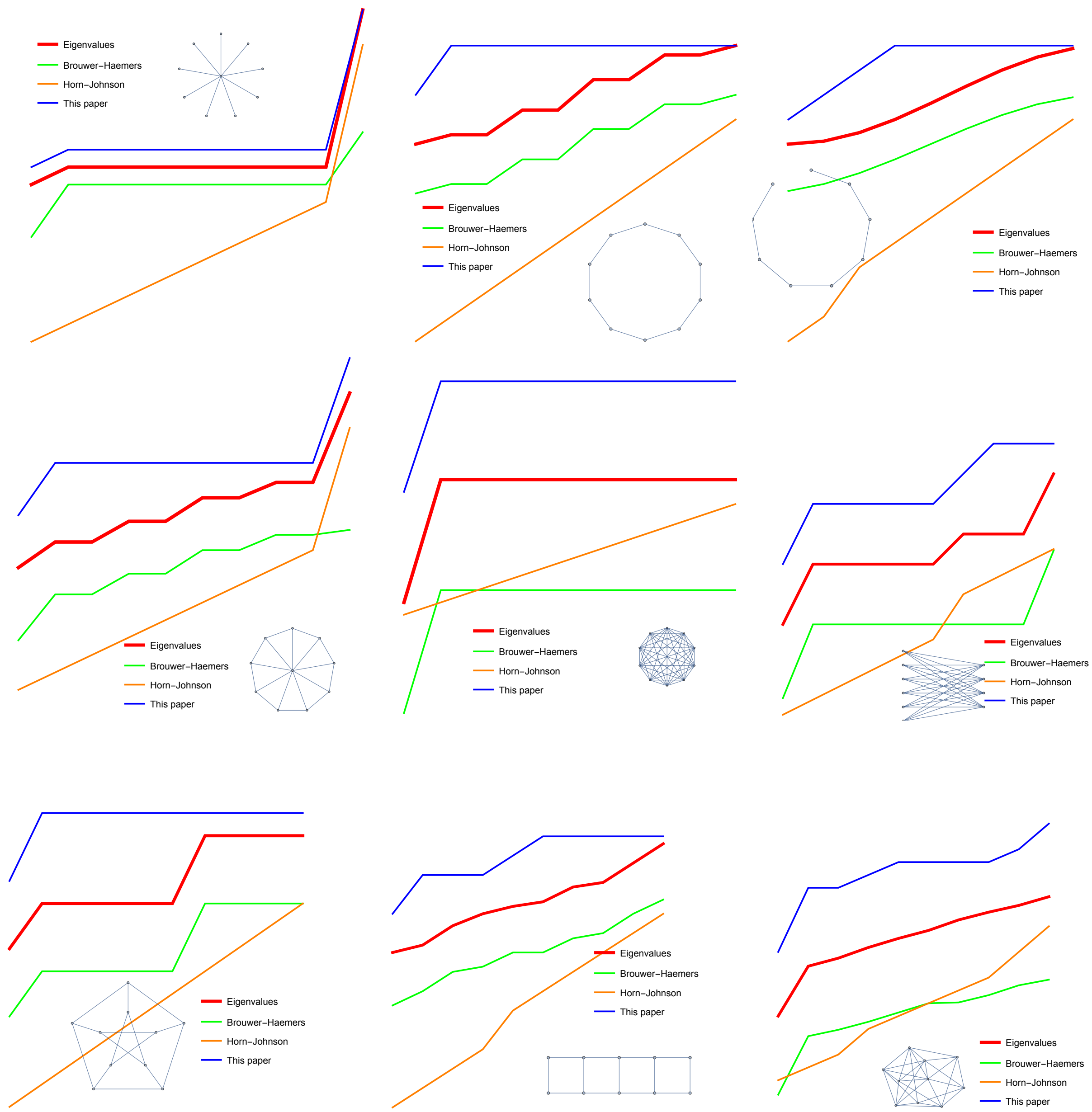

FIGURE 1. This figure shows examples of spectra and compares them with known upper and lower bounds. We see first the **Star, Cycle and Path graph**, then the **Wheel, Complete, Bipartite graph**, and finally the **Petersen, Grid and Random graph**, all with 10 vertices. The eigenvalues are outlined thick (in red). Above we see the upper bound (in blue) as proven in the present paper. Then there are the Brouwer-Haemers and Horn-Johnson lower bounds which, as the examples show, do not always compete but complement each other.

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