SOME RESULTS CONCERNING SPARSE ERDŐS-RÉNYI GRAPH ADJACENCY SPECTRA

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1. Introduction and Definitions

The first half of this paper is a very quick overview of the literature on the general subject of sparse graphs and their spectra. The second part makes some headway in finding the lowest positive eigenvalue for trees of a given size (alternatively: quantifying the decay of a sparse graph's limit spectrum near zero).

The paper builds on my Princeton University senior thesis. [1] Sections 3 and 5.3 were taken with a few changes from the thesis. Most of the other text was written from scratch. Section 5 consists primarily of new results and ideas: Proposition 5.2, Corollary 5.5, Proposition 5.7, Corollary 5.8, and Corollary 5.9 did not exist in the thesis.

1.1. Random graphs.

Definition 1.1. An *Erdős-Rényi graph* (further, *E-R graph*) with parameter p is a random graph on n vertices labeled by elements of $[n]$. For any two vertices i, j, the probability of an edge between them is $\frac{p}{n}$, independent of the other edges. The ensemble of such graphs will be called $G(n, p)$.

This object was introduced around 1960 in a series of papers by Paul Erdős and Alfréd Rényi. [2] They studied the random graphs in the limit $n \to \infty$, establishing many of their essential properties for a range of values of p.

Here, it's helpful to note that in the limit, the $G(n, p)$ model is equivalent to the so-called $G(n, m)$ model. In this model, we take n vertices, and select uniformly at random a graph with m edges. Algorithmically, a graph can be drawn from $G(n, m)$ as follows: first, create a $G(n, 0)$ graph with no edges. To get a $i+1$-edge graph from a $G(n, i)$ graph, we add a random edge from the remaining $\binom{n}{2} - i$ edges to the graph. It's clear that the resulting graph is again, uniformly drawn from all $i+1$-edge graphs, and so is a $G(n, i+1)$ graph. This inductive construction of $G(n, m)$ gives an intuitive way of thinking about $G(n, p)$ as p grows: we're just adding new edges at random.

So, we'd like to know what happens to a given graph property as the graph evolves by acquiring more and more edges. What follows is an informal summary of E-R's results on the component composition of the graph. There are three basic density regimes: $p = o(1)$ as $n \to \infty$, p constant in the limit, and p unbounded as $n \to \infty$.

For $p = o(1)$, almost all (in the probabilistic, not colloquial sense) vertices in the graph come from components that are small trees. Specifically, for $\frac{p}{n} < n^{\frac{k-1}{k-2}}$, almost no vertices come from trees of size k or larger (and trees of size k appear at

that threshold). As p grows closer and closer to a constant, the graph changes by acquiring progressively larger trees.

For p constant, trees of all sizes occur, with the following distribution. Let p_n be some function of n, and T_k be the number of components of $G(n, np_n)$ that are trees on k vertices. (So, $p = 1$ corresponds to $p_n = \frac{1}{n}$.) Then, we have the following result due to Barbour [3]:

Theorem 1.2. *For fixed $k \geq 2$, any n and p_n, let*

$$\lambda_n = \mathrm{E}\, T_k = n^k \frac{k^{k-2}}{k!} p_n^{k-1} (1-p_n)^{nk} (1 + O\left(\frac{1}{n}, p_n\right))$$

$$\sigma_n^2 = \mathrm{Var}\, T_k = \lambda_n \left(1 + \lambda_n k^2 (p_n + \frac{1}{n})\right) + O\,(1)$$

Then $\exists C(k)$, constant in n, such that,

$$\sup_{x \in \Re} \left| P\{\frac{T_k - \lambda_n}{\sigma_n} \leq x\} \right| \leq \frac{C(k)}{\sigma_n}$$

holds uniformly.

This theorem is quite general, and applies to the case $p = o(1)$ and p unbounded as well. Notice that $k = 1$ is missing. Barbour has a similar theorem which covers $k = 1$, and holds for $p_n \sim \frac{c}{n}$. Note, in particular, that the expected number of trees of size k decreases quite rapidly with k.

For $p < 1$, almost all vertices are on trees. At $p = 1$, this is still the case, but there appears a giant component containing $O(n^{\frac{2}{3}})$ of the vertices. For $p > 1$, the giant component contains cn of the vertices, but the remaining $(1-c)n$ of the vertices are still on trees.

As p grows, the graph becomes more and more connected, and the trees get absobed into the giant component. When p becomes unbounded as $n \to \infty$, almost all vertices are in the giant component. For $p_n > \frac{\log n}{n}$, almost every graph is completely connected in the limit.

1.2. **Spectrum considerations.** This paper is focused on the adjacency spectrum of graphs. That is, we take a graph (e.g. an E-R random graph as above), construct its adjacency matrix, and consider its eigenvalues. They are all real, because an adjacency matrix is real symmetric.

For E-R random graphs, we're interested in the limit spectrum – that is, what distribution, if any, do the eigenvalues of $G(n, p)$ approach as $n \to \infty$? The spectrum of a multi-component graph is the union of the spectra of its components. Hence, for $p < 1$ (including $p = o(1)$), the spectrum is the union of tree spectra, weighed according to Theorem 1.2. So, if the limit spectrum exists (more on that in Section 2), then for $p = o(1)$ it can be computed explicitly (just calculate the spectrum of all trees up to the desired size, and add them together, normalized by frequency of occurrence). For $p = o(1)$, it consists of a finite number of δ-functions, and hence is bounded.

For p constant, $p < 1$, the spectrum can be approximated arbitrarily well by computing spectra of smaller trees, and weighing them accordingly. The decay of $\mathrm{E}\, T_k$ is slowest for for $p = 1$, and even in that case trees of size ≤ 50 account for roughly 88% of the spectrum density (calculated from Theorem 1.2). The limit

spectrum is unbounded: for example, a non-zero fraction of the components are k-stars (for any k), which have eigenvalues $\pm\sqrt{k}, 0$. The asymptotics of the fraction of the limit spectrum above λ were determined by Rodgers and Bray [4] using physical methods. They determined that the probability of a tail eigenvalue (above λ, or below $-\lambda$) is $\sim \left(\frac{\lambda^2}{ep}\right)^{-\lambda^2}$. Unfortunately, their method is likely not mathematically rigorous. In my senior thesis, I an upper bound on the moments of the spectrum to show that the asymptotic decay is faster than $\left(\frac{\lambda^2}{Ce}\right)^{-\frac{\lambda^2}{Ce}}$, for an explicit constant depending on p. I also proved a lower bound on the moments of the spectrum, from which it should be straightforward to derive an analogous lower bound for the decay.

For $p > 1$, a fraction of the spectrum is still accounted for by trees. This tree spectrum we can compute approximately, as for $p < 1$, and all the observations above apply to it. As far as the giant component's spectrum, Semerjian and Cugliandolo [8] derived physical approximations that are empirically quite good for large constant p. For p unbounded, Rodgers and Bray proved in the same paper [4] that the limiting spectrum, properly normalized, approaches the Wigner semicircle. For references on Wigner's semicircle law see [11]. However, it's not obvious what rigorous techniques can be applied to the giant component's spectrum, in the constant p regime. Numerical estimates for its spectrum produce a very complicated picture for small $n > 1$. For this reason, the rest of the paper concerns primarily the tree spectrum. To do this, it's enough to understand the spectra of finite trees. This lends itself, at least partially, to combinatorial approaches.

2. Existence of the Spectral Limit

In the introduction, I talk about a limiting spectrum, although it isn't obvious that one exists. For instance, in the unbounded case, like in the standard Wigner semicircle law, normalization is required to obtain a limiting spectrum. This section shows that for constant p this is not the case, and the limit spectrum does exist.

In my senior thesis [1], I analyze the limits M_k as $n \to \infty$ of the moments $M_{k,n}$ of a $G(n,p)$ graph. I show that the limits of these moments exist, are finite, and give upper and lower bounds. I also show that, in the limit, the variance of M_k is zero (hence, a large enough matrix approximates the spectral limit). See A094149 in Sloane's encyclopedia [5] for the first few M_k.

To show that the spectral limit exists, all we need is that the M_k exist and are finite, and an upper bound (which, from [1], is $M_{2k} \leq \frac{4^k A_k}{(k+1)\sqrt{\pi k}}$, where A_k is the k-th Bell number). Then, we apply Carleman's criterion for the moment problem (see [10]): a distribution with the given moments exists and is unique if

$$\sum_{k=1}^{\infty} M_{2k}^{-\frac{1}{2k}} = \infty.$$

Using a rough asymptotic bound for the Bell numbers, we have $M_{2k} \leq 4^k k^k$. This gives

$$\sum_{k=1}^{\infty} M_{2k}^{-\frac{1}{2k}} \geq \sum_{k=1}^{\infty} \frac{1}{\sqrt{4k}} = \infty,$$

so the limiting distribution does exist.

As a side note, I also proved that $M_{2k+1} = 0$, so the spectral limit has an even symmetry about the origin. The tree spectrum alone also has even symmetry. That's because trees are bipartite graphs; the adjacency matrix of a bipartite graph can be written in block form thus:

$$\begin{pmatrix} 0 & A \\ A^T & 0 \end{pmatrix},$$

which means that if $\begin{pmatrix} \overrightarrow{x} \\ \overrightarrow{y} \end{pmatrix}$,with the same block boundaries, is an eigenvector with eigenvalue λ, then so is $\begin{pmatrix} \overrightarrow{x} \\ -\overrightarrow{y} \end{pmatrix}$, with eigenvalue $-\lambda$. Hence, the giant component's spectrum is even as well.

3. The $\delta-$function at Zero

Outside of the $p = o(1)$ regime, I do not know how to calculate the exact density of a generic δ-function in the tree spectrum (e.g. for $\lambda = \frac{1+\sqrt{5}}{2}$). However, the height of the zero δ-function can be computed thanks to the following clever result.

In [7], Bauer and Golinelli derive an explicit formula, a generating function and an asymptotic approximation for z_k – the number of zero eigenvalues (with multiplicity) in all trees of size k. Their approach uses two methods. First, they characterize the number of zero eigenvalues $Z(F)$ in a given forest F using a specialization of the recursion in 5.1. Then, they use this characterization to cleverly rewrite $Z(F)$ as a sum of a simple quantity over induced subtrees of the forest. Armed with that identity, the rest of the paper uses standard techniques from enumerative combinatorics to produce its results.

According to this paper, the expected multiplicity of the zero eigenvalue in a tree of size k is $\mathrm{E}\, Z_k = (2x_* - 1)k + \frac{x_*^2(x_*+2)}{(x_*+1)^3} + O\left(\frac{1}{k}\right)$. The expected number of tree components of size k in $G(n, \frac{p}{n})$ is $n\frac{k^{k-2}p^{k-1}e^{-kp}}{k!}$. So, the asymptotic (in k) contribution of trees of size k to the δ-function at zero is $(2x_* - 1)\frac{k^{k-1}p^{k-1}e^{-kp}}{k!} + \frac{x_*^2(x_*+2)}{(x_*+1)^3} + O\left(\frac{1}{k}\right)$. Using the weighting from Theorem 1.2, that yields the exact density of the zero δ-function.

4. Numerics

To give some context for the discussion that follows, here are some pictures from simulations.

The pictures of random 800-vertex graph spectra are a reasonable reflection of the spectral limit in these various regimes. For $p = 0.5$ and $p = 1.0$ we have pure tree spectra. Observe the rapid decline in density near zero. The spectrum of all trees of size 20 illustrates the source of this decay. The δ-functions comprising the spectrum of 20-vertex trees are packed quite tightly, except for a large gap near zero. This gap closes, slowly, as the trees get bigger, but big trees contribute very little of a sparse graph's spectrum. Of course, there is a similar root repulsion phenomenon going on around every other δ-function in the spectrum, but those are less appealing because:

(1) The repulsion is much weaker.

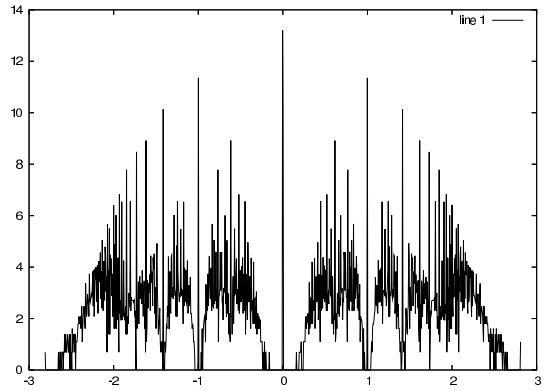


FIGURE 1. A histogram of all eigenvalues of 1100 sparse random graphs with parameter $p = 0.5$ and 800 vertices; the y axis is the natural log of the eigenvalue count plus 1.

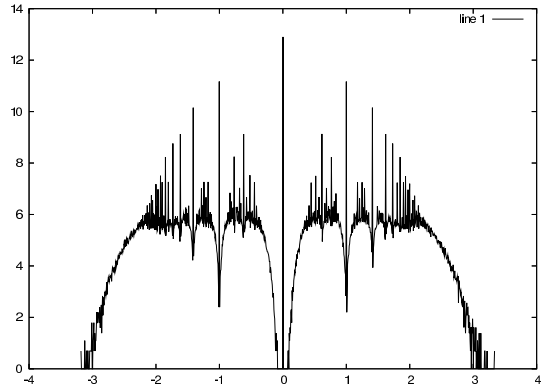


FIGURE 2. A histogram of all eigenvalues of 1100 sparse random graphs with parameter $p = 1.0$ and 800 vertices; the y axis is the natural log of the eigenvalue count plus 1.

(2) The largest positive eigenvalue of graphs, a well-studied object [6], specifies the *fastest growth* mode for a vector being acted on by the adjacency operator. On the other hand, the lowest positive eigenvalue specifies the *fastest decay* mode. But, practically nothing is known about it.
(3) Understanding the root repulsion rate generically (to handle e.g. ± 1,$\pm\sqrt{2}$, $\pm\sqrt{3}, \ldots$) is likely much harder than understanding the special case of zero.

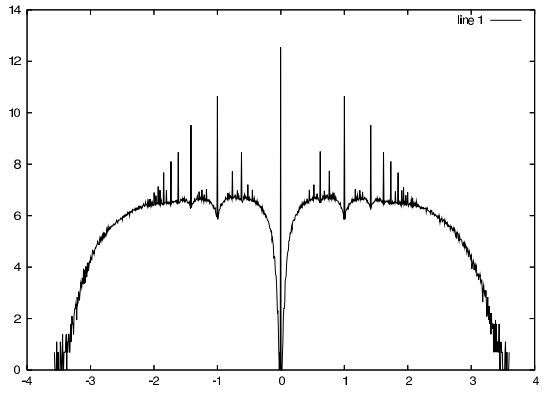


FIGURE 3. A histogram of all eigenvalues of 1100 sparse random graphs with parameter $p = 1.5$ and 800 vertices; the y axis is the natural log of the eigenvalue count plus 1.

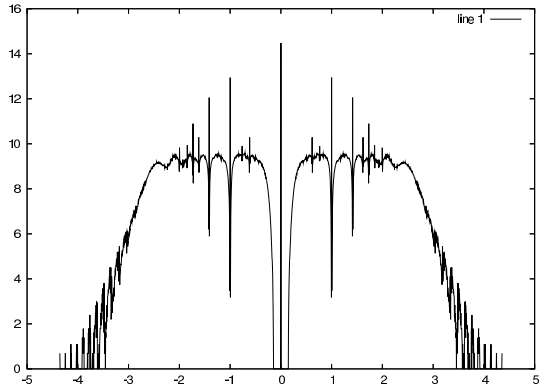


FIGURE 4. A histogram of all eigenvalues of trees on 20 vertices; the y axis is the natural log of the eigenvalue count plus 1.

5. Decay near Zero

From numerical experiments, it appears that the probability of an eigenvalue falling on a non-zero value near zero is quite low (see, e.g., Figure 1 on page 5). We'd like to compute for the limiting spectrum an upper bound on $p_A = P\{0 < \lambda < A\} = \frac{1}{2}P\{-A < \lambda < A, \lambda \neq 0\}$ as $A \to 0^+$. We'll use the following idea to produce an estimate. There are finitely many trees of size $\leq k$, and so they have a minimal positive eigenvalue $\lambda_{k,\min}$. Moreover, a positive fraction $W_k = \sum_{i=1}^{k} T_i$ of the whole spectrum comes from those trees. So, $p_{\lambda_{k,\min}} < 1 - W_k$. We know the

behavior of W_k, so we only need to find a lower bound for $\lambda_{k,\min}$ to produce an upper bound for p_A.

There's a very crude, but straightforward way to estimate $\lambda_{k,\min}$. Namely: all eigenvalues of trees of size $\leq k$ are roots of integer polynomials of degree $\leq k$ with bounded coefficients. The coefficients are bounded because we're taking the characteristic polynomial of a zero-one $k \times k$ matrix. Thus, any coefficient is at most $k!$.

Given these two constraints, the polynomial with a root closest to zero is $1 - k!(x + x^2 + \cdots + x^k)$. To see this, consider another polynomial $p(x)$. If $p(0) = 0$, then we can divide through by x, and effectively reduce the maximum allowed degree. Thus, we may assume $p(0) \neq 0$. Multiplying by -1, and reflecting around the y axis if necessary, we may assume that $p(0) > 0$ and that the minimum root is positive. To have a low root, the function must get down to zero as quickly as possible. Setting the constant term to 1 always helps, as does setting each of the other coefficients to $-n!$.

So, we get

$$x + x^2 + \cdots + x^k = \frac{1}{k!}$$

Rather than solve the above polynomial, observe that the right-hand side is ≤ 1 because $k \geq 1$, and so the left-hand side is always smaller than kx. Consequently, the polynomial's smallest positive root is $\geq \frac{1}{k!k}$. This is very far from the truth: experimentally, up to $k = 25$, the lowest positive eigenvalue (LPE) is roughly inversely proportional to k. I took a lot of shortcuts in the above calculations, but the fundamental problem is the use of a single upper bound for all coefficients.

The solution should lie in exploiting the fact that we're dealing with a tree's adjacency matrix. Below, I present some facts that could be helpful in finding the exact LPE for trees of size k.

The rest of this section contains a collection of facts that should be useful in proving the following conjecture:

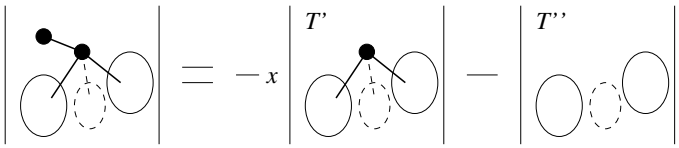
Conjecture 5.1. *The LPE on trees of size $2k$ occurs on the $2k$-path.*

***Bonus**: The LPE on trees of size $2k+1$ occurs on the forked $2k$-path (for $k = 4$, it looks like this: $---<$).*

5.1. **Coefficients of a tree's characteristic polynomial.** The first observation is that one can easily compute the characteristic polynomial of trees in a recursive way. The characteristic polynomial is the following kind of determinant:

$$\begin{vmatrix} -x & 1 & 0 & \dots & 0 \\ 1 & -x & & & \vdots \\ 0 & & \ddots & & \\ \vdots & & & \ddots & \vdots \\ 0 & \dots & & \dots & -x \end{vmatrix},$$

where the order of the vertices was chosen to make the first row/column a leaf, and the second – the leaf's neighbor. Now, we can do row expansion along the first row. Pictorially speaking, we get:



The first term is clear: it's just the principal minor we get when we expand on the the $(1,1)$-th element. For the second term, we expand along the $(1,2)$-th element, which leaves a single 1 in the first column. We then expand by this 1 (formerly, the $(2,1)$-th element) to get the principal minor with the first two elements removed.

With this, one can compute the polynomials for trees of up to, say, size 8, by hand. This is enough to notice the following pattern:

Proposition 5.2. *The characteristic polynomial of a k-vertex tree has the form*

$$(-\lambda)^k - a_1(-\lambda)^{k-2} + a_2(-\lambda)^{k-4} - a_2(-\lambda)^{k-6} + \cdots + (-1)^{\lfloor \frac{k}{2} \rfloor} a_{\lfloor \frac{k}{2} \rfloor}(-\lambda)^k \mod 2 = \\ = \sum_{i=0}^{\lfloor \frac{k}{2} \rfloor} a_i (-1)^{k-i} \lambda^{k-2i},$$

where a_i is the number of matchings of size i in the tree (and $a_0 = 1$).

Proof. We can just work by induction, using the rule above. For the base case, it's easy to see that the 1-vertex tree has characteristic polynomial $-\lambda$, and the 2-vertex tree has characteristic polynomial $(-\lambda)^2 + (-\lambda)$. Now, take a tree, and delete its leaf as in our recursive rule. The matchings in the original tree are of two types: there are some which contain the leaf's edge, and some that don't.

Ones that do, do not contain any of the edges coming out of the leaf's neighbor either, so such matchings correspond to the matchings of T'', the tree with both the leaf and its neighbor deleted (the right-hand term in the recursion). Let $f''(\lambda)$ be the characteristic polynomial of T''; by induction, its $(k-2)-2i$th degree term coefficient is the number of i-sized matchings in the subgraph. These correspond to $(i+1)$-sized matchings in T. The corresponding monomial's degree is the same in T: $k-2(i+1) = (k-2)-2i$, but the sign adjustment is different: $(-1)^{k-2-i}$ versus $(-1)^{k-(i+1)}$. Hence, the matchings in T containing our leaf's edge are enumerated by $-f''(\lambda)$.

Similarly, let's work with matchings that don't contain the leaf's edge. These may contain any of the remaining edges, so they correspond to i-sized matchings of T'. Let $f'(\lambda)$ be its characteristic polynomial. Again, by induction, the $(k-1)-2i$th degree term coefficient is the number of i-sized matchings, while the i-sized matching terms in $f(\lambda)$ have degree $k-2i$. The corresponding sign in f' is $(-1)^{k-1-i}$, but $(-1)^{k-i}$ in f. Hence, the matchings that don't contain our leaf's edge are enumerated by $-\lambda f'(\lambda)$.

So, we get that $f(\lambda) = -\lambda f'(\lambda) - f''(\lambda)$, counts the number of matchings in T as claimed. □

Here are some useful consequences:

Corollary 5.3. *If the multiplicity of the zero eigenvalue is j, then $\frac{k-j}{2}$ is the size of the largest matching in the tree.*

Corollary 5.4. *For k even, $a_{\frac{k}{2}}$ is either 0 or 1.*

Proof. In other words, there's at most one full matching. If a matching exists, start at a leaf, it is matched uniquely. Delete the leaf and win by induction. □

Corollary 5.5. *The maximal a_i is achieved for the k-path. Hence, the maximal $a_i = \binom{k-i}{i}$.*

Proof. Expand the claim to include forests on k vertices as well. We'll work by induction on the number of vertices k; the base case $k = 1$ is obvious. Let's compare the number of matchings of size i between the k-path and another tree. To do this, pick a leaf in each. In each tree, there are matchings that include this edge, and matchings that do not. To count those that do, we we delete the edge and its two vertices, and count $(i-1)$-matchings in what remains. The k-path turns into a $(k-2)$-path, while the other tree turns into some $(k-2)$-forest. To count those matchings that don't contain the edge, we count i-matchings after deleting the leaf and the edge. The path becomes a $(k-1)$-path, and the forest – some other forest. In both cases, by induction, the number of matchings of the path is at least that of the forest, which proves the claim.

The number of i-matchings in the k-path is just $\binom{k-i}{i}$, via the obvious bijection. □

5.2. **Sufficient to compute $\lambda_{k,\min}$ for k even.** The conjecture for the odd case is marked as "Bonus" above, because it turns out that $\lambda_{2k+1,\min} > \lambda_{2k,\min}$. Therefore, our bound on the decay rate near zero is specified entirely by even trees k. I can prove this fact without proving the conjecture.

For this, I need the following eigenvalue interlacing theorem, due to Cauchy (see, e.g. [9] for a proof).

Theorem 5.6 (Cauchy's Interlacing Theorem)**.** *If A is a Hermitian matrix with eigenvalues $\lambda_1 \le \lambda_2 \le \cdots \le \lambda_n$, and A' is any $n-1 \times n-1$ principal minor with eigenvalues $\mu_1 \le \mu_2 \le \cdots \le \mu_{n-1}$, then*

$$\lambda_1 \le \mu_1 \le \lambda_2 \le \mu_2 \le \lambda_3 \le \cdots \le \mu_{n-1} \le \lambda_n.$$

Proposition 5.7. *If the tree T of size $k > 1$ has LPE λ_T and at least one zero eigenvalue, there exists a tree T' of size $k-1$ with LPE $\lambda_{T'} \le \lambda_T$.*

Proof. Consider a tree T on k vertices with i zero eigenvalues. Then, it has a matching of size $\frac{k-i}{2}$; in particular, there is at least one vertex not included in the matching. Suppose, for the moment, that this vertex is a leaf. We will delete this vertex to get a graph T' on $k-1$ vertices which still has a matching of size $\frac{k-i}{2}$. Its matrix will be a principal minor, so the eigenvalues of T' interlace. Let's suppose the LPE of T is a; then, interlacing gives us b, an eigenvalue of T', like this:

$$\cdots \le -a \le -b \le 0 \le \cdots \le 0 \le b \le a \le \ldots$$

In particular, $b \neq 0$ by Corollary 5.3. Thus, the LPE of T' is at most that of T.

Above, we assumed that the vertex being deleted is a leaf. There are two way to deal with this. One way is to drop the assumption, and potentially end up with a forest. The spectrum of a forest is the union of its components' spectra, so its LPE comes from a tree of substantially smaller size (slight modification to the claim). It's not hard to check that all the proofs in this section carry through for forests as well as trees.

The other way is to find a matching with a missing leaf. To do that, suppose that only non-leaf vertices are excluded. Look at the path from an unmatched vertex

to a fixed leaf. If the rest of the path is not completely matched, we'll consider the last unmatched vertex instead of the current one. We can then invert the matching: $(- = - = - =) \Rightarrow (= - = - = -)$. The result remains is a matching because the initial vertex was not in the matching. This shows that there exists a matching with an unmatched leaf, and concludes the proof. □

There are two nice corollaries of this result. One was already stated:

Corollary 5.8. *For all $k \geq 1$, $\lambda_{2k+1,\min} \geq \lambda_{2_k,\min}$.*

Proof. By symmetry of a tree's spectrum (or because a matching covers an even number of vertices), every odd T has a zero eigenvalue. Proposition 5.7 tells us that every odd T is beaten by a smaller even tree, and the result follows. □

Furthermore, it follows that it's enough to prove Conjecture 5.1 for a subset of even trees.

Corollary 5.9. *If the $2k$-path has the LPE among all $2k$ trees with full matchings (of size k, that is), then Conjecture 5.1 holds.*

Proof. Start with a tree T of size $2k$. Since it's not full-matching, it has a zero eigenvalue. Apply Proposition 5.7 to get T' of size $2k-1$ (which has a zero eigenvalue by oddness), so apply Proposition 5.7 again to get T'' of size $2(k-1)$. If the result is a full-matching tree — stop, otherwise repeat these two steps, until a full-matching $2(k-i)$-tree $T^{(2i)}$ is obtained. Since the 2-tree has a full matching, the procedure does stop eventually. Proposition 5.7 says that $\mathrm{LPE}\left(T^{(2i)}\right) \leq \mathrm{LPE}\left(T^{(2i-1)}\right) \leq \cdots \leq \mathrm{LPE}\left(T\right)$. Moreover, if we denote the l-path by P_l, $\mathrm{LPE}\left(P_{2(k-i)}\right) \leq \mathrm{LPE}\left(T^{(2i)}\right)$, and, by Proposition 5.10, $\mathrm{LPE}\left(P_{2k}\right) < \mathrm{LPE}\left(P_{2(k-i)}\right)$. It follows that $\mathrm{LPE}\left(P_{2k}\right) < \mathrm{LPE}\left(T\right)$, as desired. □

This characterization may be helpful, for the following heuristic reason. For λ very small, we can approximate the characteristic polynomial by $a - b\lambda$, because all higher powers of λ become negligibly small. Since the coefficients of the higher powers are quite high, this isn't actually the case. However, the higher powers are sign-alternating, and we might assume that they cancel out to something small. So, assuming that a linear approximation makes sense, the LPE of a tree is just $\frac{a}{b}$. By Corollary 5.4, $a = 1$ for all fully-matched trees. By Corollary 5.5, b is maximal for the path. Hence, the LPE of all fully-matched trees should occur on the path.

To make the above heuristic argument work, we'd need rather tight bounds on the effects of higher-order terms. So far, I haven't been able to do it. This may not even be a good approach.

5.3. **Eigenvalues of the path and forked path.** Although it's not proved that the LPE occurs on paths or forked paths, it still makes sense to calculate their eigenvalues. Corollary 5.5 suggests that the characteristic polynomial of the path is closely related to the Chebyshev polynomial. Indeed, its roots have the same form and are quite easy to calculate.

Proposition 5.10. *The $2n$-path has eigenvalues: $\pm 2\cos(\frac{\pi k}{2n+1}), k = 1 \ldots n$. Its LPE is $2\cos(\frac{\pi n}{2n+1})$.*

Proof. Let $b_1, \ldots, b_{2n}$ be an eigenfunction of the eigenvalue λ for the $2n$-path. Then, $\lambda b_{k-1} = b_k + b_{k-2}$ with the constraint that $b_2 = \lambda b_1$ and $b_{2n-1} = \lambda b_{2n}$.

Suppose $\lambda = 0$; then, $b_2 = 0$, so $0 \cdot b_3 = b_2 + b_4 \Rightarrow b_4 = 0, \ldots, b_{2n} = 0$. But, then $b_{2n-1} = 0$ as well, and, propagating backwards: $0 \cdot b_{2n-2} = b_{2n-3} + b_{2n-1} \Rightarrow b_{2n-3} = 0, \ldots, b_1 = 0$. So, 0 is not an eigenvalue. We also want to show that $b_1 \neq 0$. Suppose otherwise; then $b_2 = 0$, so $\lambda \cdot 0 = 0 + b_3 \Rightarrow b_3 = 0$, etc. Thus, we can renormalize all our eigenfunctions to have $b_1 = 1$, and $b_2 = \lambda$.

Finally, suppose $\lambda = 2$; then $b_2 = 2$, $2 \cdot 2 = 1 + b_3 \Rightarrow b_3 = 3$; inductively, $2 \cdot (i-1) = (i-2) + b_i \Rightarrow b_i = i$. But, then $b_{2n-1} = 2 \cdot b_{2n} \Rightarrow 2n - 1 - 4n = 0 \Rightarrow n = -\frac{1}{2}$, which is absurd. Analogously, if $\lambda = -2$, $b_i = i(-1)^{i+1}$, so we get $n = \frac{1}{6}$.

Now, we solve the recursion relation $b_k - \lambda b_{k-1} + b_{k-2} = 0$. The corresponding polynomial equation $x^2 - \lambda x + 1 = 0$ has roots

$$x_1 = \frac{\lambda + \sqrt{\lambda^2 - 4}}{2}, x_2 = \frac{\lambda - \sqrt{\lambda^2 - 4}}{2}.$$

Consequently, the general solution to the recurrence is $b_k = c_1 x_1^k + c_2 x_2^k$, and in particular $c_1 x_1 + c_2 x_2 = 1$, $c_1 x_1^2 + c_2 x_2^2 = \lambda$. Writing these out, we get:

$$(c_1 + c_2)\lambda + (c_1 - c_2)\sqrt{\lambda^2 - 4} = 2$$

$$c_1(\lambda^2 + 2\lambda\sqrt{\lambda^2 - 4} + \lambda^2 - 4) + c_2(\lambda^2 - 2\lambda\sqrt{\lambda^2 - 4} + \lambda^2 - 4) = 4\lambda$$
$$\Rightarrow 2\lambda\left((c_1 + c_2)\lambda + (c_1 - c_2)\sqrt{\lambda^2 - 4}\right) - 4(c_1 + c_2) = 4\lambda$$

Simplifying, we get $c_1 = -c_2 = -c$. We must also have $\lambda c(x_1^{2n} - x_2^{2n}) = \lambda b_{2n} = b_{2n+1} = c(x_1^{2n-1} - x_2^{2n-1})$; rewriting, we have $x_1^{2n-1}(\lambda x_1 - 1) - x_2^{2n-1}(\lambda x_2 - 1) = 0$.

Recall that $x_1 + x_2 = \lambda$, and $x_1 x_2 = 1$. We can then write $\lambda x_1 - 1 = (x_1 + x_2)x_1 - 1 = x_1^2 + x_1 x_2 - 1 = x_1^2$, and the same for x_2. The final constraint is $x_1^{2n+1} + x_2^{2n+1} = 0$, which is equivalent to $x_2 = \gamma x_1$, where γ is a $2n+1$st root of unity (excluding 1, which would lead to $x_1 = x_2 = 0$, which is impossible). Also, $x_1 x_2 = x_1^2 \gamma = 1 \Rightarrow x_1^2 = \gamma^{2n}$. So, $x_1 = \pm\gamma^n$ and $x_2 = \pm\gamma^{n+1}$. This gives us all the eigenvalues: $\lambda = \pm(\gamma + \overline{\gamma}) = 2\operatorname{Re}\gamma = \pm 2\cos(\frac{\pi k}{2n+1})$, for $k = 1..n$. Cosine is closest to zero near $\frac{\pi}{2}$, so we want $\frac{k}{2n+1} \approx \frac{1}{2}$; it follows that the LPE is $2\cos(\frac{\pi n}{2n+1})$. □

The following can be proved by a more tedious calculation.

Proposition 5.11. *A forked path ($-\cdots-<$) with $2n+1$ vertices has eigenvalues: $0, \pm 2\cos(\frac{\pi(2k-1)}{4n}), k = 1 \ldots n$. Its LPE is $2\cos(\frac{\pi(2n-1)}{4n})$.*

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