3 Graph polynomials

Significant part of the algebraic graph theory of graphs revolves around studying polynomials whose definition is based on the graph. Coefficients or evaluations of such polynomials typically count things associated to the graph, but algebraic properties of them and of their roots also tend to bring interesting considerations about the graph.

One motivation to define polynomials for graphs is the hope that a given polynomial would be efficiently computable and at the same time completely identify the graph up to isomorphism. No such polynomial is known in general (otherwise graph isomorphism would be an easier problem). Another motivation possibly come (historically as well) from the famous Reconstruction Conjecture. In the next section, we will see a third and very recent relevant application of graph polynomials.

We start our section with a brief introduction to the Reconstruction Conjecture.

3.1 Reconstruction — an interlude

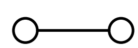
Given a graph G on n vertices, the set of n subgraphs obtained from G upon deleting each one of its vertices is called the *deck of G*. If G and its deck are presented with labelled vertices, then there is not much to ask or wonder. A totally more interesting question rises when one simply erases (or arbitrarily mixes up) the labels — we shall hence assume all graphs in this section are of such form.

Conjecture 1 (Kelly-Ulam). *For any graph G on $n > 2$ vertices, G is completely determined by its deck.*

The hypothesis on $n > 2$ is necessary because the two subgraphs

 and 

could have been obtained from either of the following graphs,

 or 

but these are the only known case of such phenomenon. Several graph theorists have worked on this conjecture for the past decades, and yet a complete answer seems to be far from being found.

Partial results usually have two flavours: either one determines that graphs belonging to a certain class are reconstructible (from their deck), or one determines which properties or invariants of a graph are reconstructible. For the remainder of this section, we will mostly focus on the second type of question. But in this brief interlude, we prove the following results.

Let $\nu(H, G)$ denote the number of subgraphs of G isomorphic to H. It is not too surprising that this parameter is reconstructible.

Lemma 3.1 (Kelly). *For any graphs G and H,*

$$(|V(G)| - |V(H)|)\ \nu(H,G) = \sum_{a \in V(G)} \nu(H, G\backslash a)$$

Proof. The result is trivial if $|V(H)| \geq |V(G)|$. Assume otherwise. We shall count the number of pairs (H', a) where H' is a copy of H in G, $a \in V(G)$ but $a \notin V(H')$. By choosing H' first, there are $(|V(G)| - |V(H)|)\ \nu(H,G)$ such pairs. By choosing a first, the number of copies of H not using a is precisely $\nu(H, G\backslash a)$. The result thus follows. □

Corollary 3.2. *If G has more than two vertices, the parameter $|E(G)|$ is reconstructible from the deck of G.*

Corollary 3.3. *The degree sequence of G (that is, the sequence of numbers listing the degrees of the vertices of G) is reconstructible.*

Exercise 3.4. Using Kelly's lemma, prove both corollaries above.

Theorem 3.5. *If G is a regular graph on more than 2 vertices, then G is reconstructible.*

Proof. From the degree sequence, decide whether G is regular. If it is, examine any of the graphs in its deck, and add a missing vertex so that it becomes regular. This graph will be equal to G. □

3.2 Walks

For any graph G, define $\phi_G(x)$ to be

$$\phi_G(x) = \det(x\mathbf{I} - \mathbf{A}).$$

The characteristic polynomial of a graph and of its subgraphs interplay nicely with walk counts and eigenvectors of the graph. Over the next few results, we shall make this relationship clearer.

Lemma 3.6. *If G is disconnected, and G_1 and G_2 are disjoint subgraphs of G with $G_1 \cup G_2 = G$, then*

$$\phi_G = \phi_{G_1} \cdot \phi_{G_2}.$$

This above is immediate from the block expansion of a determinant.

We now write a generating function whose coefficients are matrices:

$$W_G(x) = \sum_{k \geq 0} (\mathbf{A})^k x^k.$$

This is known as the walk generating function of G — the ij entry of the coefficient multiplying x^k counts the number of walks of length k from i to j. Rules for formal power series apply (existence of multiplicative inverses, substitutions, Laurent power series, etc.), and so we have

$$W_G(x) = \frac{1}{(\mathbf{I} - x\mathbf{A})}.$$

Notice that we are working with matrices whose coefficients are over $\mathbb{R}((x))$, but that shall mean no harm. In fact, properties about the determinant that you can prove exploring its Laplace expansion still hold true, in particular, for any $\mathbf{M}$ matrix with coefficients which are power series in x,

$$\mathbf{M} \cdot \operatorname{adj}(\mathbf{M}) = \det(\mathbf{M})\mathbf{I}. \tag{4}$$

Recall now that $\operatorname{adj}(\mathbf{M})$ is the matrix defined as

$$(\operatorname{adj} \mathbf{M})_{ij} = (-1)^{i+j} \det \mathbf{M}[j, i],$$

where $\mathbf{M}[j, i]$ stands for the matrix $\mathbf{M}$ removed of row j and column i.

Specifically, we are interested in what happens when $\mathbf{M} = (\mathbf{I} - x\mathbf{A})$. Equation (4) becomes

$$W_G(x) = \frac{\operatorname{adj}(\mathbf{I} - x\mathbf{A})}{\det(\mathbf{I} - x\mathbf{A})} = \frac{\operatorname{adj}(\mathbf{I} - x\mathbf{A})}{\det(\mathbf{I} - x\mathbf{A})}. \tag{5}$$

Corollary 3.7. *The generating function for the number of closed walks around a vertex a in the variable x is*

$$W_G(x)_{aa} = \frac{\phi_{G\backslash a}(x^{-1})}{x \cdot \phi_G(x^{-1})}.$$

Proof. Follows immediately from

$$W_G(x) = \frac{\operatorname{adj}(\mathbf{I} - x\mathbf{A})}{\det(\mathbf{I} - x\mathbf{A})} = \frac{x^{n-1} \operatorname{adj}(x^{-1}\mathbf{I} - \mathbf{A})}{x^n \det(x^{-1}\mathbf{I} - \mathbf{A})},$$

and the definition of the adjugate. □

We would also appreciate to have an expression for $W_G(x)_{ab}$. For that, we make use of an old trick due to Jacobi to arrive at an expression. For any matrix $\mathbf{M}$ with rows and columns indexed by a set V, let $\mathbf{M}_D$ stand for the submatrix with rows and columns indexed by $D \subseteq V$. The following theorem is the correct generalization of Corollary 3.7.

Theorem 3.8. *Let D be a subset of $V(G)$ (assume without loss of generality that the rows and columns indexed by D are the first). Then*

$$\det[W_G(x)]_D = \frac{1}{x^{|D|}} \frac{\phi_{G\backslash D}(x^{-1})}{\phi_G(x^{-1})}.$$

Proof. Let $\mathbf{C}$ be the matrix obtained from $\mathbf{I}$ upon replacing its first $|D|$ columns by the first $|D|$ columns of $\operatorname{adj}(\mathbf{I} - x\mathbf{A})$. Hence

$$(\mathbf{I} - x\mathbf{A}) \cdot \mathbf{C} = \begin{pmatrix} \det(\mathbf{I} - x\mathbf{A})\mathbf{I}_{|D|} & ? \\ \mathbf{0} & (\mathbf{I} - x\mathbf{A})_{\overline{D}} \end{pmatrix}.$$

Note that

$$\det \mathbf{C} = \det \operatorname{adj}(\mathbf{I} - x\mathbf{A})_D = \det[W_G(x)]_D \cdot (\det(\mathbf{I} - x\mathbf{A})^{|D|}).$$

Thus

$$\det[W_G(x)]_D = \frac{\det[(\mathbf{I} - x\mathbf{A})_{\overline{D}}]}{\det(\mathbf{I} - x\mathbf{A})} = \frac{x^{n-|D|} \det(x^{-1}\mathbf{I} - \mathbf{A})_{\overline{D}}}{x^n \det(x^{-1}\mathbf{I} - \mathbf{A})},$$

which yields the result. □

If $D = \{a, b\}$, then

$$W_G(x)_{aa} W_G(x)_{bb} - W_G(x)_{ab}^2 = \frac{1}{x^2} \frac{\phi_{G\backslash ab}(x^{-1})}{\phi_G(x^{-1})},$$

therefore

$$W_G(x)_{ab} = \frac{1}{x} \frac{\sqrt{\phi_{G\backslash a}(x^{-1})\phi_{G\backslash b}(x^{-1}) - \phi_G(x^{-1})\phi_{G\backslash ab}(x^{-1})}}{\phi_G(x^{-1})}.$$

Notice in particular, from Equation (5), and replacing $y = x^{-1}$, that

$$\sqrt{\phi_{G\backslash a}(y)\phi_{G\backslash b}(y) - \phi_G(y)\phi_{G\backslash ab}(y)} = \operatorname{adj}(y\mathbf{I} - \mathbf{A})_{ab},$$

which is a polynomial (meaning: a power series with finite terms), and therefore the term inside the square root must be a perfect square (a fact that is not at all immediate at first sight).

Exercise 3.9. Let $\mathcal{P}_{ab}$ be the set of all paths from a to b. Prove that

$$\sqrt{\phi_{G\backslash a}(y)\phi_{G\backslash b}(y) - \phi_G(y)\phi_{G\backslash ab}(y)} = \sum_{P \in \mathcal{P}_{ab}} \phi_{G\backslash P}(y).$$

Hints:

(i) This will be a proof by induction.

(ii) Define $N_G(y)_{ab}$ to be the generating function for the walks that start at a, never return to it, and end at b. Find a relation between W_{ab}, N_{ab} and W_{aa}.

(iii) Find a relation between N_{ab} and W_{cb} (in $G\backslash a$), where c runs over the neighbours of a.

(iv) Apply induction.

3.3 Spectral decomposition

Say $\mathbf{A} = \sum_{r=0}^{d} \theta_r \mathbf{E}_r$. From the walk generating function $W_G(x) = \sum_{k\geq 0}(\mathbf{A})^k x^k = (\mathbf{I} - x\mathbf{A})^{-1}$, we have

$$W_G(x) = \sum_{r=0}^{d} \frac{1}{1 - x\theta_r} E_r. \tag{6}$$

Thus,

$$W_G(x^{-1}) = \sum_{r=0}^{d} \frac{x}{x - \theta_r} E_r.$$

If we focus on the diagonal entries, we have

$$\frac{x\phi_{G\backslash a}(x)}{\phi_G(x)} = W_G(x^{-1})_{aa} = \sum_{r=0}^{d} \frac{x}{x - \theta_r} (E_r)_{aa},$$

thus, multiplying both sides by $(x - \theta_r)$ and evaluating at $x = \theta_r$, yields

$$(E_r)_{aa} = \left. \frac{(x - \theta_r)\phi_{G\backslash a}(x)}{\phi_G(x)} \right|_{x=\theta_r}$$

For off-diagonal entries, we obtain

$$(E_r)_{ab} = \left. \frac{(x - \theta_r)\sqrt{\phi_{G\backslash a}(x)\phi_{G\backslash b}(x) - \phi_G(x)\phi_{G\backslash ab}(x)}}{\phi_G(x)} \right|_{x=\theta_r}.$$

Exercise 3.10. Show that if θ_r is an eigenvalue of $\mathbf{A}(G)$ with multiplicity m_r, then, for any $a \in V(G)$, its multiplicity in $\mathbf{A}(G\backslash a)$ is at least $m_r - 1$. Prove that equality holds if and only if there is at least one eigenvector for θ_r whose entry corresponding to a is non-zero.

Exercise 3.11. The goal of this exercise is to show that for any two matrices $\mathbf{M}$ and $\mathbf{N}$ so that $\mathbf{MN}$ and $\mathbf{NM}$ are defined, the following identity holds

$$\det(\mathbf{I} - \mathbf{MN}) = \det(\mathbf{I} - \mathbf{NM}).$$

To achieve this, find the two matrices that make both products below true, and finish the exercise.

$$\begin{pmatrix} \mathbf{I} & -\mathbf{M} \\ \mathbf{N} & \mathbf{I} \end{pmatrix} = \begin{pmatrix} \mathbf{I} & -\mathbf{M} \\ \mathbf{0} & \mathbf{I} \end{pmatrix} \begin{pmatrix} ? & ? \\ ? & ? \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} \mathbf{I} & -\mathbf{M} \\ \mathbf{N} & \mathbf{I} \end{pmatrix} = \begin{pmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{N} & \mathbf{I} \end{pmatrix} \begin{pmatrix} ? & ? \\ ? & ? \end{pmatrix}$$

Exercise 3.12. Let $w(x)$ be the generating function whose coefficient of x^k count the total amount of all walks in the graph of length k. The goal of this exercise is to show that

$$w(x) = \frac{1}{x}\left(\frac{(-1)^n \phi_{\overline{G}}(-1 - x^{-1})}{\phi_G(x^{-1})} - 1 \right).$$

Recall that $\mathbf{A}(\overline{G}) = \mathbf{J} - \mathbf{I} - \mathbf{A}(G)$. You will use that $w(x) = \mathbf{1}^T W_G(x)\mathbf{1}$, that $\mathbf{J} = \mathbf{1}\mathbf{1}^T$, and finally the past exercise.

3.4 Reconstructing

In this section, we will show that the characteristic polynomial is reconstructible from the deck of the graph — that is, if the conjecture is false, then any counterexamples will have to be graphs with the same spectrum.

We would like to be able to reduce $\phi_G(x)$ somehow to an expression depending on the vertex-deleted subgraphs of G. Our best chance is then to look at Corollary 3.7, and take the trace in Equation (6). First, answer the exercise.

Exercise 3.13. Explain why $\operatorname{tr} E_r = m_r$, the multiplicity of θ_r as an eigenvalue.

Now we shall have

$$\frac{1}{\phi_G(x)} \left(\sum_{a \in V(G)} \phi_{G\backslash a}(x) \right) = \operatorname{tr}\left[x^{-1} W_G(x^{-1})\right] = \sum_{r=0}^{d} \frac{m_r}{x - \theta_r}.$$

Hence

$$\sum_{a \in V(G)} \phi_{G\backslash a}(x) = \sum_{r=0}^{d} \left(m_r (x - \theta_r)^{m_r - 1} \right) \prod_{s \neq r} (x - \theta_s)^{m_s} = \phi_G(x)'.$$

This shows that we need only the characteristic polynomial of the graphs in the deck of G to recover the characteristic polynomial of G, except for its constant term. This actually will prove itself a considerably harder task, to which we devote the remaining of this subsection.

We start by actually finding a combinatorial expansion for the coefficients of $\phi(x)$, which in its own self is interesting and relevant. A *sesquivalent* subgraph H of G is a subgraph satisfying

(i) $|V(H)| = |V(G)|$.

(ii) Every connected component of H is either an isolated vertex, or an edge, or a cycle.

For each sesquivalent subgraph H of G, let $v(H)$, $e(H)$ and $c(H)$ denote the number of connected components which are, respectively, isolated vertices, edges and cycles.

Theorem 3.14 (Harary, Sachs)**.** *Let G be a simple graph, and $\mathcal{H}$ the set of all sesquivalent subgraphs of G. Then*

$$\phi_G(x) = \sum_{H \in \mathcal{H}} (-1)^{e(H)} (-2)^{c(H)} x^{v(H)}.$$

Proof. Leibniz formula for the determinant gives

$$\phi_G(x) = \det(x\mathbf{I} - \mathbf{A}) = \sum_{\sigma \in S_n} (-1)^{\epsilon(\sigma)} \prod_{i=1}^{n} (x\mathbf{I} - \mathbf{A})_{i\sigma(i)}.$$

(The sum runs over all permutations of $\{1, ..., n\}$, and $\epsilon(\sigma)$ is the number of cycles of even length in the decomposition of σ as a product of disjoint cycles.)

Consider the set of all permutations fixing precisely the points belonging to the subset $D \subseteq V(G)$. The sum of the terms corresponding to these permutations will therefore be

$$x^{|D|}(-1)^{n-|D|} \det(\mathbf{A}(G\backslash D)).$$

Each permutation of $V(G)\backslash D$ with fixed points contributes nothing to the determinant of $\mathbf{A}(G\backslash D)$. Those without will contain cycles of length two, or longer. Note that the support of the cycle structure of a permutation is a sesquivalent subgraph of $G\backslash D$. The cycles of length 2 are edges. The longer ones are the cycles of the graph. Each of the longer cycles of σ could have their orders reversed, yielding a permutation corresponding to the same sesquivalent subgraph H. Thus the total number of permutations corresponding to the sesquivalent subgraph H is $2^{c(H)}$.

Say the permutation σ corresponds to sesquivalent subgraph H. The quantity of cycles of odd length in σ has the same parity as $n - |D|$. If this is even, then total number of cycles, which is $e(H) + c(H)$, has the same parity as the number of even cycles, which is $\epsilon(\sigma)$. Otherwise, total number of cycles has opposite parity. Thus, if σ corresponds to the sesquivalent subgraph H with no isolated vertices, then

$$(-1)^{n-|D|}(-1)^{\epsilon(\sigma)} = (-1)^{e(H)+c(H)}.$$

Therefore the sum of the terms corresponding to the permutations fixing the set D will be

$$x^{|D|}(-1)^{n-|D|}\det(\mathbf{A}(G\backslash D)) = x^{|D|}\sum_H (-1)^{e(H)+c(H)}2^{c(H)}.$$

where the sum runs over the sesquivalent subgraphs of $G\backslash D$ with no isolated vertices. Varying the set D over all subsets of G will yield the desired expressions of the theorem. □

The constant term in $\phi_G(x)$, which is $(-1)^n \det(\mathbf{A}(G))$, is, according to the theorem above, equal to

$$\sum_H (-1)^{e(H)}(-2)^{c(H)}$$

where the sum runs over the sesquivalent subgraphs H of G with no isolated vertices.

Recall Kelly's lemma, which is useful to count copies of a subgraph H with $|V(H)| < |V(G)|$.

Lemma 3.15. *For any graphs G and H,*

$$(|V(G)| - |V(H)|)\ \nu(H,G) = \sum_{a\in V(G)} \nu(H, G\backslash a).$$

With a little more work, we have the following. Recall that a graph homomorphism from G_1 to G_2 is a function from $V(G_1)$ to $V(G_2)$ that preserves adjacency (but not necessarily non-adjacency).

Lemma 3.16. *G on n vertices, and H a disconnected graph on n vertices. Then $\nu(H,G)$ is reconstructible.*

Proof. Let H_1 and H_2 be disjoint subgraphs whose union is H. There are $\nu(H_1,G)\nu(H_2,G)$ homomorphisms from H to G which are injective on H_1 and H_2. Several of those however overlay images of vertices from H_1 and H_2. But we can count those. For each F on fewer than n vertices, there are $\nu(F,G)$ copies of F in G, and we can count the number of surjective homomorphisms from H to F which are injective in both H_1 and H_2. We multiply both things, and sum this for all F. We then subtract the total from $\nu(H_1,G)\nu(H_2,G)$ to recover $\nu(H,G)$. □

The result above allows us to compute the sum

$$\sum_H (-1)^{e(H)}(-2)^{c(H)}$$

for all disconnected H. The only thing remaining now to account for are the connected H.

A graph has vertex connectivity 1 if it is connected and contains a vertex whose removal disconnects the graph (a cut-vertex). A block is a maximal subgraph that does not contain a cut-vertex. For example, a tree contains $n-1$ blocks (each corresponding to an edge). The number of blocks in a 1-connected subgraph is the number of cut-vertices added by 1.

Lemma 3.17. *Let H be a 1-connected graph, on n vertices. The number of subgraphs of G with n vertices that contain the same collection of blocks of H is reconstructible.*

Proof. Assume H contains exactly two blocks H_1 and H_2 (thus $|V(H_1)| + |V(H_2)| = n+1$). Consider all homomorphisms from $H_1 \cup H_2$ to G which are injective in both H_1 and H_2. There are $\nu(H_1, G)\nu(H_2, G)$ such homomorphisms. The number of such mappings whose image is contained in a vertex deleted subgraph of G is reconstructible (see lemma above and Kelly's lemma). Thus the number of those whose image is G, obtained from overlaying only one vertex of H_1 with one of H_2, is reconstructible. These will correspond precisely to the spanning subgraphs of G which have H_1 and H_2 as their blocks. Now we can simply apply induction on the number of blocks of H to account for when H has any number of blocks. □

Using both lemmas above, one can show that:

Corollary 3.18. *If G is disconnected, then G is reconstructible. If G is a tree, then G is reconstructible.*

Exercise 3.19. Write the details proving the corollary above.

Corollary 3.20. *The number of Hamilton cycles of G can be reconstructed from the deck.*

Proof. The number of edges of G is reconstructible, so we can count the number of subgraphs of G with precisely n edges. We can also count how many of those are in vertex-deleted subgraphs, thus we can recover how many spanning subgraphs of G have precisely n edges. Out of these, we can count those which are disconnected and those which contain a cut-vertex, because they will contain a unique cycle of length $k < n$. The remaining graphs in the count will be Hamilton cycles. □

Clearly the implicit algorithm in the proof above is extremely inefficient, but there was no hope of providing an efficient algorithm that counts the number of Hamilton cycles in a graph anyway (deciding whether one exists is already itself a hard task).

Theorem 3.21. *The characteristic polynomial of G is reconstructible from the deck.*

Proof. We proved that

$$\phi_G(x)' = \sum_{a \in V(G)} \phi_{G \backslash a}(x).$$

The constant term of $\phi_G(x)$ is

$$\sum_H (-1)^{e(H)}(-2)^{c(H)}$$

where the sum runs over the sesquivalent subgraphs H of G with no isolated vertices. Those which are disconnected can be dealt with Lemma 3.16. Those which are connected correspond precisely to the Hamilton cycles of G, and this number can be reconstructed from Corollary 3.20. □

Recall the we proved that

$$\phi_{G \backslash a}(y)\phi_{G \backslash b}(y) - \phi_G(y)\phi_{G \backslash ab}(y)$$

is a perfect square of a polynomial, say $q_{ab}(y)$. If $\phi_G(y)$ is irreducible over the rationals, that it is easy to show that $\phi_{G\backslash ab}(y)$ is completely determined by $\phi_G(y)$, $\phi_{G\backslash a}(y)$, and $\phi_{G\backslash b}(y)$.

Having the eigenvalues of $G\backslash ab$, we can recover its number of edges. So we know the number of edges in G, $G\backslash a$, $G\backslash b$ and $G\backslash ab$. Hence we can find whether there is an edge between a and b in G. As a consequence:

Theorem 3.22 (Tutte)**.** *If characteristic polynomial of G is irreducible over the rationals, then G itself is reconstructible.* □

We list two open questions related to our work in this chapter.

Problem 3.1. *Can you reconstruct of the characteristic polynomial of the Laplacian matrix from the deck?*

Problem 3.2. *Instead of the deck of G, assume you have access only to the characteristic polynomials of the graphs in the deck. Can you reconstruct $\phi_G(x)$? (It is known that this is possible if you have the characteristic polynomials of the graphs in the deck and their complement.)*

Define now the three-variable polynomial

$$\Phi_G(y, z, x) = \sum_{H \in \mathcal{H}} y^{e(H)} z^{c(H)} x^{v(H)}.$$

Note that $\phi_G(x) = \Phi_G(-1, -2, x)$.

Exercise 3.23. Prove that

$$\frac{\partial}{\partial x}\Phi_G(y, z, x) = \sum_{a \in V(G)} \Phi_{G\backslash a}(y, z, x).$$

Find expressions for

$$\frac{\partial}{\partial y}\Phi_G(y, z, x) \text{ and } \frac{\partial}{\partial z}\Phi_G(y, z, x).$$

Exercise 3.24. Verify that $\Phi_G(y, z, x)$ is reconstructible from the deck of G.

Exercise 3.25. Find a recurrence for Φ assuming G contains a cut-edge (meaning: write Φ_G in terms of Φ for some subgraphs of G.) Try the same exercise assuming G contains a cut-vertex.

Exercise 3.26. Let $\mathcal{C}_a$ be the set of cycles containing a vertex a. Explain why

$$\Phi_G = x\Phi_{G\backslash a} + y\sum_{b \sim a} \Phi_{G\backslash ab} + z\sum_{C \in \mathcal{C}_a} \Phi_{G\backslash C}.$$

Exercise 3.27. Assume all cycles of G have the same length, say c. Find a partial differential equation satisfied by Φ.

3.5 The matching polynomial of a graph

Let $\mathcal{M}(G)$ be the set of all spanning subgraphs of G whose connected components are either isolated vertices or isolated edges. The matching polynomial of a graph is defined as

$$\mu_G(x) = \sum_{M \in \mathcal{M}(G)} (-1)^{e(M)} x^{v(M)}.$$

Note that it is precisely equal to the evaluation $\Phi(-1, 0, x)$ of the polynomial $\Phi(y, z, x)$ defined in the past subsection. In fact,

Theorem 3.28. *Given a graph connected G,*

$$\mu_G(x) = \phi_G(x)$$

if and only if G is a tree.

Proof. One direction is obvious from the formula of Φ. The other I leave as a challenging exercise. □

Exercise 3.29. Verify that

$$\mu_G(x)' = \sum_{a \in V(G)} \mu_{G \setminus a}(x),$$

and, prove that, if $e = \{u, v\}$ is an edge of G, then

$$\mu_G(x) = \mu_{G \setminus e}(x) - \mu_{G \setminus uv}(x).$$

Exercise 3.30. Find recurrences for $\mu_{P_n}(x)$, $\mu_{K_n}(x)$ and $\mu_{C_n}(x)$ based on the matching polynomials of smaller graphs in each of the families. (Hint: use Exercise 3.26).

The recurrences you found in the past exercise show that matching polynomials in each of those families of graphs form what is a known as a sequence of orthogonal polynomials. We will not get into details of the theory of orthogonal polynomials, but over the next few results we will see some glimpse of it. Given polynomials $p(x)$ and $q(x)$, we define an inner product by

$$\langle p, q \rangle = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \mathrm{e}^{-x^2/2} p(x) q(x) \mathrm{d}x.$$

Do not get scared. Just bear with me. But maybe now it would be a good time to remember that

$$1 = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \mathrm{e}^{-x^2/2} \mathrm{d}x \quad \text{and} \quad 0 = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} x\mathrm{e}^{-x^2/2} \mathrm{d}x.$$

Exercise 3.31. Prove these equalities. Hint: one of them is easy. For the other, write its square, and change variables to polar coordinates.

Lemma 3.32. *Let*

$$M(n) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \mathrm{e}^{-x^2/2} x^n \, dx.$$

The number of perfect matchings in K_n is equal to $M(n)$.

Proof. Integration by parts implies

$$M(n) = \frac{1}{\sqrt{2\pi}} \left[\frac{x^{n+1}}{n+1} \mathrm{e}^{-x^2/2} \right]_{-\infty}^{+\infty} + \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \frac{x^{n+2}}{n+1} \mathrm{e}^{-x^2/2} \mathrm{d}x.$$

The first term is 0. So it follows that $M(n) = M(n+2)/(n+1)$. As seen above, $M(1) = 0$ and $M(0) = 1$. Hence $M(\text{odd}) = 0$ and

$$M(2m) = (2m-1)!!$$

as we wanted to show. □

Recall that $(-1)^{n/2}\mu_G(0)$ is the number of perfect matchings in G. Denote this number by $\mathrm{pm}(G)$.

Theorem 3.33. *For any G, we have*

$$\mathrm{pm}(\overline{G}) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \mathrm{e}^{-x^2/2} \mu_G(x)\, dx$$

sketch. The proof is by induction on the number of edges in G. If G has no edges, this falls precisely in the statement of the lemma. If G has one edge, then both sides satisfy the same recursion given by the second part of Exercise 3.29. □

Exercise 3.34. Prove that

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \mathrm{e}^{-x^2/2} \mu_{K_n}(x) \mu_{K_m}(x) \mathrm{d}x = \begin{cases} m!, & \text{if } m = n; \\ 0, & \text{otherwise.} \end{cases}$$

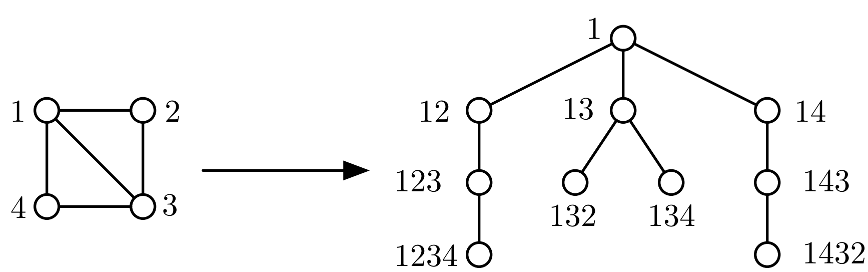
Hint: look at $K_n \cup K_m$, its complement, and the past exercise.

The conclusion from the result above is that the family $\{\mu_{K_n}(x)\}_{n \geq 0}$ is a family of orthogonal polynomials according to the inner product defined in this subsection.

3.6 Real roots

Our goal here is to show that the matching polynomial of any graph has only real roots.

Given a graph G and a vertex u in G, the *path tree* of G with respect to u is a rooted tree whose vertices correspond to the paths of G that start at u, and a the children of a vertex corresponding to path P are those vertices corresponding to paths obtained from one further edge at the end of P. For example



Theorem 3.35. *Let G be a graph, $u \in V(G)$. Let $T = T(G, u)$ be the path tree of G with respect to u. Then*

$$\mu_T(x)\mu_{G\backslash u}(x) = \mu_G(x)\mu_{T\backslash u}(x),$$

and $\mu_G(x)$ divides $\mu_T(x)$.

Proof. If G itself is already a tree, then there is nothing to prove, as $G = T$. We may assume the results holds true for vertex-deleted subgraphs of G. Thus

$$\mu_G(x) = x\mu_{G\backslash u} - \sum_{v\sim u} \mu_{G\backslash uv}(x).$$

Thus, applying induction, we have

$$\frac{\mu_G(x)}{\mu_{G\backslash u}(x)} = x - \sum_{v\sim u} \frac{\mu_{T(G\backslash u,v)\backslash v}(x)}{\mu_{T(G\backslash u,v)}(x)}.$$

Now, $T(G\backslash u, v)$ is isomorphic to the branch of $T(G, u)$ attached to u that starts at the vertex corresponding to the path uv. Thus

$$\frac{\mu_{T(G\backslash u,v)\backslash v}(x)}{\mu_{T(G\backslash u,v)}(x)} = \frac{\mu_{T(G,u)\backslash\{u,uv\}}(x)}{\mu_{T(G,u)\backslash u}(x)}.$$

Therefore

$$\frac{\mu_G(x)}{\mu_{G\backslash u}(x)} = \frac{x\mu_{T(G,u)\backslash u}(x) - \sum_{v\sim u} \mu_{T(G,u)\backslash\{u,uv\}}(x)}{\mu_{T(G,u)\backslash u}(x)} = \frac{\mu_{T(G,u)}(x)}{\mu_{T(G,u)\backslash u}(x)},$$

as wanted. For the second assertion, by induction, it follows that $\mu_{G\backslash u}(x)$ divides $\mu_{T(G\backslash u,v)}(x)$. As $T(G\backslash u, v)$ is a branch of $T(G, u)\backslash u$, it follows that $\mu_{T(G\backslash u,v)}(x)$ divides $\mu_{T(G,u)\backslash u}(x)$, so $\mu_{G\backslash u}(x)$ itself divides $\mu_{T(G,u)\backslash u}(x)$. Hence $\mu_G(x)$ divides $\mu_T(x)$. □

Corollary 3.36. *The roots of $\mu_G(x)$ are real, for any G. Moreover, they are symmetrically distributed around the origin.*

Proof. The polynomial $\mu_G(x)$ divides $\mu_T(x)$, which is equal to $\phi_T(x)$. This is the characteristic polynomial of a symmetric matrix, hence its roots are real. Therefore the roots of $\mu_G(x)$ are real.

The second part follows immediately from the fact that all exponents of x in $\mu_G(x)$ are either all odd or all even. □

Exercise 3.37. Prove that the zeros of $\mu_{G\backslash u}$ interlace those of μ_G. If G is connected, prove that the largest zero of μ_G is simple, and strictly larger than that of $\mu_{G\backslash u}$. Hint: use Theorem 3.35.

We can also bound the largest eigenvalue of μ relatively well.

Exercise 3.38. Show (again) that the largest eigenvalue of a non-negative matrix is upper bounded by its largest row sum.

Exercise 3.39. Extend the result above to argue that the largest eigenvalue of a non-negative matrix $\mathbf{M}$ is upper bounded by the largest row sum of $\mathbf{DMD}^{-1}$ for any positive diagonal matrix $\mathbf{D}$.

Exercise 3.40. Let T_Δ be a tree so that all vertices have degree $\Delta > 2$ or 1. Prove that its largest eigenvalue is upper bounded by $2\sqrt{\Delta - 1}$. Hint: Fix a vertex of degree Δ to call the root, and conjugate $\mathbf{A}(T_\Delta)$ by the diagonal matrix defined as $\mathbf{D}_{aa} = \sqrt{\Delta - 1}^{d(a)}$, where $d(a)$ is the distance from a to the root. Use the exercises above.

Exercise 3.41. Argue that any tree of maximum degree $\Delta > 1$ has its largest eigenvalue small or equal than $2\sqrt{\Delta - 1}$.

Exercise 3.42. Let G be a graph with $\Delta(G) > 1$. Show that the largest root λ of $\mu_G(x)$ satisfies

$$\sqrt{\Delta(G)} \leq \lambda \leq 2\sqrt{\Delta(G) - 1}.$$

(The upper bound should follow easily from the exercises above. The lower bound is your job to find.)

3.7 Number of matchings

The fact that the roots of $\mu_G(x)$ are real brings a combinatorial consequence. A sequence of numbers $(a_i)_{i\geq 0}$ is log-concave if $a_i^2 \geq a_{i-1}a_{i+1}$ for all $i \geq 1$. If the numbers are positive, then this is equivalent to having $(a_{i+1}/a_i)_{i\geq 0}$ non-increasing. Thus, a log-concave sequence of positive numbers is unimodal, meaning, it first increases, then stays constant, then decreases.

The binomial coefficients $\binom{n}{k}$, $k = 0, ..., n$, form a (finite) log-concave sequence. Clearly, if (a_i) and (b_i) are log-concave, so is $(a_i b_i)$.

Lemma 3.43. *If $p(x) = \sum_i a_i x^i$ is a polynomial of degree n with real roots only, then $(a_i/\binom{n}{i})$ form a log-concave sequence.*

Proof. This follows from writing

$$\frac{\mathrm{d}^{n-i-2}}{\mathrm{d}^{n-i-2}x} x^{n-i} \frac{\mathrm{d}^i}{\mathrm{d}^i x} p(x^{-1}) = \frac{1}{2} n! \left(\frac{a_i}{\binom{n}{i}} x^2 + \frac{a_{i+1}}{\binom{n}{i+1}} 2x + \frac{a_{i+2}}{\binom{n}{i+2}} \right).$$

(Fill in the details). $\square$

Let m_k be the number of matchings in G with k edges. Note that

$$\mu_G(x) = \sum_{k\geq 0} (-1)^k m_k x^{n-2k}.$$

Corollary 3.44. *The sequence $(m_k)_{k\geq 0}$ is log-concave (and therefore unimodal).*

Proof. Assume n is even. Then $\mu_G(x) = q(x^2)$. Note that

$$p(x) = \sum_{k\geq 0} m_k x^k = x^{n/2} q(-x^{-1}),$$

which also has real roots. Similar argument for n odd. It follows then from Lemma that $(m_k)_{k\geq 0}$ is a log-concave sequence. $\square$

3.8 Average

In this final section about the matching polynomial, we prove a remarkable result connecting $\mu(x)$ and $\phi(x)$.

Theorem 3.45. *Let G be a graph with m edges. Then*

$$\mu_G(x) = \frac{1}{2^m} \sum_F \phi_F(x),$$

where the sum runs over all 2^m signed graphs F whose underlying edges are exactly those of G.

To be a clear, $\mathbf{A}(F)$ is precisely $\mathbf{A}(G)$, except that certain symmetric off-diagonal entries have been changed to -1.

Proof. We have

$$\frac{1}{2^m} \sum_F \phi_F(x) = \frac{1}{2^m} \sum_F \sum_{\sigma \in S_n} (-1)^{\epsilon(\sigma)} \prod_{i=1}^{n} (x\mathbf{I} - \mathbf{A}(F))_{i\sigma(i)},$$

then

$$\frac{1}{2^m} \sum_F \phi_F(x) = \frac{1}{2^m} \sum_{\sigma \in S_n} (-1)^{\epsilon(\sigma)} \sum_F \prod_{i=1}^{n} (x\mathbf{I} - \mathbf{A}(F))_{i\sigma(i)},$$

Note that if σ contains a cycle with more than two vertices, then

$$\sum_F \prod_{i=1}^{n} (x\mathbf{I} - \mathbf{A}(F))_{i\sigma(i)} = 0,$$

as we can sum over all possible signings of this cycle having the rest constant, and later vary the rest, but the sum over all possible signings of a cycle of length larger than 2 is 0.

Thus the only permutations that contribute are those with transpositions and fixed points only, and for those the signing is irrelevant. The sum over all such permutations coincides with the matching polynomial of the graph. Therefore

$$\frac{1}{2^m} \sum_F \phi_F(x) = \frac{1}{2^m} \sum_F \sum_{M \in \mathcal{M}(G)} (-1)^{e(M)} x^{v(M)} = \frac{1}{2^m} 2^m \mu_G(x),$$

as we wished. □

Exercise 3.46. Let G be a graph, and F be obtained from G upon signing some of the edges. What exactly can be said about

$$\phi_G(x) + \phi_F(x) \quad ?$$

Exercise 3.47. Assume G is a graph with the property that every cycle of G contains at least one edge that belongs to no other cycle. Show how to compute μ_G efficiently.

3.9 References

Here is the set of references used to write the past few pages.

The main reference for this section is the book of Godsil, wherein references for all the results about the characteristic and matching polynomials can be found (Chapters 1, 2, 4 and 6).

(a) Chris D Godsil. *Algebraic Combinatorics*. Chapman & Hall, New York, 1993

(b) Chris Godsil and Gordon Royle. *Algebraic Graph Theory*. Springer-Verlag, New York, 2001

Elias Hagos proved that the characteristic polynomial is reconstructible from the characteristic polynomials of the graphs in the deck and their complements (if they are correctly paired up).

(c) Elias M Hagos. The characteristic polynomial of a graph is reconstructible from the characteristic polynomials of its vertex-deleted subgraphs and their complements. *The Electronic Journal of Combinatorics*, 7(1):12, 2000