Graph Polynomials and Spectral Gaps

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Abstract

These notes are mainly based on a paper by McKay [4] on the eigenvalues of large regular graphs, one by Sokal [5] on bounds of zeros of chromatic polynomials, and another by Sarnak [3], found in sections 4, 8 and 6 respectively. It turns out that the eigenvalues of large regular graphs follow with high probability a distribution depending only the degree and that for cubic graphs, for any $x \neq 3$ there exists a sequence of graphs such that their spectra avoid x (i.e. x can be *gapped*). In addition, the zeros of the chromatic polynomial of a regular graph is bounded linearly by its degree. Sections 1, 2 and 7 give some background on algebraic graph theory, mostly taken from Biggs [1]. Section 3, on the process of generating random regular graphs, is due to Bollobás [2].

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1 The spectrum of a graph

Definition 1.1. The *adjacency matrix* of G is the $n \times n$ matrix $\mathbf{A} = \mathbf{A}(G)$ where

$$a_{i,j} = \begin{cases} 1 & v_i \text{ and } v_j \text{ are adjacent;} \\ 0 & \text{otherwise.} \end{cases}$$

By definition, $\mathbf{A}$ is real symmetric and has trace 0. Since the ordering of rows and columns of $\mathbf{A}$ was arbitrary, we will be interested in permutation-invariant properties of $\mathbf{A}$, mainly its spectral properties.

Definition 1.2. The *spectrum* of G is the set of eigenvalues of $\mathbf{A}(G)$ with their multiplicities. If $\lambda_0 > \lambda_1 > \cdots > \lambda_{s-1}$ are eigenvalues with multiplicity $m(\lambda_0), \ldots, m(\lambda_{s-1})$ respectively, then we write

$$\operatorname{Spec} G = \begin{pmatrix} \lambda_0 & \lambda_1 & \cdots & \lambda_{s-1} \\ m(\lambda_0) & m(\lambda_1) & \cdots & m(\lambda_{s-1}) \end{pmatrix}.$$

These eigenvalues correspond precisely to the roots of the *characteristic polynomial*, with their multiplicity equal to the multiplicity of these roots.

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Definition 1.3. The *characteristic polynomial* of G is

$$\chi_G(x) = \det(x\mathbf{I} - \mathbf{A}) = x^n + c_1 x^{n-1} + \cdots + c_n.$$

Note that c_i is the sum of all $i \times i$ *principal minors* of $\mathbf{A}$, which is the determinant of a submatrix of $\mathbf{A}$ that takes i rows and *the same* set of columns, since c_i comes from expanding along the diagonal $n - i$ times, which always leaves such a matrix behind.

Proposition 1.4. *The coefficients of χ_G satisfy*

1. $c_1 = 0$;
2. $-c_2 = |E|$;
3. $-c_3$ *is twice the number of triangles of* G.

Proof. Essentially follows from the fact that those c_i are summed from principal minors.

1. All 1×1 principal minors of $\mathbf{A}$ are 0;
2. A 2×2 principal minor of $\mathbf{A}$ at i, j is non-zero if and only if the submatrix is $\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$, in which case the principal minor is -1, and we have such a submatrix if and only if v_i and v_j are adjacent;
3. A 3×3 principal minor of $\mathbf{A}$ at i, j, k is 0 unless all non-diagonal entries are 1, which is true if and only if v_i, v_j and v_k form a triangle. In this case, the principal minor is $\begin{vmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{vmatrix} = 2$. □

This shows that algebraic properties of $\mathbf{A}(G)$ have profound implications on graph-theoretical properties of G and vice-versa. Here we apply them to find $\operatorname{Spec} K_4$.

Example 1.5. For $G = K_4$, note

$$\mathbf{A} = \begin{bmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{bmatrix} \implies \mathbf{A} \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 3 \\ 3 \\ 3 \\ 3 \end{bmatrix}$$

so we see that 3 is an eigenvalue. We can use 1.4 to derive all but the last coefficient of χ, which is simply $\det \mathbf{A} = -3$. Thus

$$\chi_{K_4}(x) = x^4 - 6x^2 - 8x - 3 = (x-3)(x^3 + 3x^2 + 3x + 1) = (x-3)(x+1)^3$$
$$\implies \operatorname{Spec} K_4 = \begin{pmatrix} 3 & -1 \\ 1 & 3 \end{pmatrix}.$$

Later, in 2.6, we will see a general description of $\operatorname{Spec} K_n$.

Another interesting algebraic object is the *adjacency algebra*:

Definition 1.6. The *adjacency algebra* of G is the algebra generated by polynomials of $\mathbf{A} = \mathbf{A}(G)$, with the usual matrix addition and multiplication. We denote the adjacency algebra by $\mathcal{A}(G)$.

Since $\chi_G(G) = 0$, $\dim \mathcal{A}(G) \leq n$. We can derive a lower bound for $\dim \mathcal{A}(G)$ via graph-theoretical properties of G. We start by associating powers of $\mathbf{A}$ to graph-theoretical properties.

Definition 1.7. A *walk* from v_i to v_j of *length* ℓ is a sequence of vertices $v_i = v_0, v_1, \ldots, v_\ell = v_j$ such that v_{k-1} and v_k are adjacent for all $1 \leq k \leq \ell$.

Lemma 1.8. *The number of walks of length ℓ from v_i to v_j is precisely the entry (i, j) in $\mathbf{A}^\ell$.*

Proof. We prove this by induction. $\ell = 0$ is true since $\mathbf{A}^0 = \mathbf{I}$. Suppose this is true for $\ell = L$. Note that for each distinct walk from v_i to v_j of length $L+1$, there is a distinct walk of length L from v_i to some v_k adjacent to v_j and vice-versa. Thus the number of walks from v_i to v_j of length $L+1$ is precisely the sum of the number of walks of length L from v_i to each v_k adjacent to v_j, i.e. $(\mathbf{A}^L)_{ik}$. And the (i, j) entry of $\mathbf{A}^{L+1}$ is precisely

$$(\mathbf{A}^{L+1})_{ij} = \sum_{k=1}^{n} (\mathbf{A}^L)_{ik} a_{kj} = \sum_{(v_k, v_j) \in E} (\mathbf{A}^L)_{ik}.$$

□

Definition 1.9. We call G *connected* if there exists a walk from each v_i to each v_j. When there exists a walk from v_i to v_j, the length of the shortest walk is called the *distance* from v_i to v_j on G, denoted $\partial(v_i, v_j)$. The maximum distance on a connected G is called its *diameter*.

Proposition 1.10. *Let G be connected with diameter d. Then $\dim \mathcal{A}(G) \geq d + 1$.*

Proof. Let $x, y \in V$ be such that $\partial(x, y) = d$. Let $x = v_0, \ldots, v_d = y$ be a walk of length d. Then there are no walks from x to v_ℓ that are shorter than ℓ, so that entry in $\mathbf{A}^k$ is 0 for all $k < \ell$ so $\mathbf{A}^\ell$ is independent from $\{\mathbf{I}, \ldots, \mathbf{A}^{\ell-1}\}$ and this is true for all $0 \leq \ell \leq d$ so $\{\mathbf{I}, \ldots, \mathbf{A}^d\}$ are linearly independent, i.e. $\dim \mathcal{A}(G) \geq d + 1$. □

Since the dimension of $\mathcal{A}(G)$ corresponds directly to the degree of the minimal polynomial, which corresponds to the number of distinct eigenvalues of G, we have the following corollary:

Corollary 1.11. *A connected graph with diameter d has at least $d + 1$ distinct eigenvalues.*

Exercise 1.1. If G_i denotes the induced subgraph of $V \setminus v_i$, then

$$\chi'_G = \sum_{i=1}^{n} \chi_{G_i}.$$

Proof. Let $\mathbf{X}(x)$ be the diagonal matrix with $x_i(x)$ at the i-th row, where $x_i : x \mapsto x$ and let $\mathbf{X}_i(x)$ be $\mathbf{X}$ with the i-th row and column removed. Now we view χ_G as

$$\chi_G(x) = \det(x\mathbf{I} - \mathbf{A}(G)) = \det(\mathbf{X}(x) - \mathbf{A}(G)).$$

Then by chain rule (g_i denotes the part of $\det(\mathbf{X}(x) - \mathbf{A}(G))$ expanded at the i-th row that does not depend on x_i)

$$\begin{aligned}\frac{\partial \chi_G}{\partial x}(x) &= \sum_{i=1}^{n} \frac{\partial \chi_G}{\partial x_i}(x) \cdot \frac{\partial x_i}{\partial x}(x) = \sum_{i=1}^{n} \frac{\partial}{\partial x_i} \det(\mathbf{X}(x) - \mathbf{A}(G)) \\ &= \sum_{i=1}^{n} \frac{\partial}{\partial x_i}(x_i \det(\mathbf{X}_i(x) - \mathbf{A}(G_i)) - g_i(x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_n)) \\ &= \sum_{i=1}^{n} \det(\mathbf{X}_i(x) - \mathbf{A}(G_i)) = \sum_{i=1}^{n} \chi_{G_i}.\end{aligned}$$

□

Exercise 1.2. Let $g_{ij}(r)$ be the number of walks of length r from v_i to v_j in G. Let $\mathbf{G}(z)$ be the matrix where

$$(\mathbf{G}(z))_{ij} = \sum_{r=0}^{\infty} g_{ij}(r) z^r \tag{1.1}$$

under the assumption that (1.1) is absolutely convergent for all i, j. Then $\mathbf{G}(z) = (\mathbf{I} - z\mathbf{A})^{-1}$ (so in particular $\frac{1}{z} \notin \operatorname{Spec} G$).

Proof. We prove $\mathbf{G}(z) = \mathbf{G}(z)z\mathbf{A} + \mathbf{I}$. Indeed we have

$$(\mathbf{G}(z)z\mathbf{A})_{ij} = z \sum_{k=1}^{n} (\mathbf{G}(z))_{ik} a_{kj} = z \sum_{k=1}^{n} \sum_{r=0}^{\infty} g_{ik}(r) z^r a_{kj} = \sum_{r=0}^{\infty} z^{r+1} \sum_{k=1}^{n} g_{ik}(r) a_{kj}.$$

Recall from the proof of 1.8 we have $\sum_{k=1}^{n} g_{ik}(r) a_{kj} = g_{ij}(r+1)$, thus

$$(\mathbf{G}(z)z\mathbf{A})_{ij} = \sum_{r=0}^{\infty} z^{r+1} g_{ij}(r+1) = \sum_{r=1}^{\infty} z^r g_{ij}(r).$$

If $i \neq j$ then $g_{ij}(0) = 0$ so $(\mathbf{G}(z)z\mathbf{A})_{ij} = (\mathbf{G}(z))_{ij}$. If $i = j$ then $z^0 g_{ij}(0) = 1$ so $(\mathbf{G}(z)z\mathbf{A})_{ij} + 1 = (\mathbf{G}(z))_{ij}$. Thus $\mathbf{G}(z) = \mathbf{G}(z)z\mathbf{A} + \mathbf{I}$. □

2 Regular graphs

We will see in this section that combinatorial regularity can have consequences on spectra of graphs. The class of graphs possessing the most simple kind of regularity are *k-regular* graphs, or graphs in which every vertex has degree k. This property has direct consequences on the graphs' eigenvalues.

Proposition 2.1. *Let G be k-regular. Then*

1. $k \in \operatorname{Spec} G$;

2. The multiplicity of $k \in \operatorname{Spec} G$ is 1 if G is connected;

3. For all $\lambda \in \operatorname{Spec} G$, $|\lambda| \leq k$.

Proof. 1. Take $\mathbf{x} = [1, \dots, 1]^\intercal \in \mathbb{R}^n$, then $(\mathbf{Ax})_i = \sum_{j=1}^n a_{ij} = k$ so $\mathbf{Ax} = k\mathbf{x}$.

2. Suppose $\mathbf{x} = [x_1, \dots, x_n]^\intercal$ satisfies $\mathbf{Ax} = k\mathbf{x}$. Let i be such that $x_i = \max_{1 \leq j \leq n}(x_j)$. Then

$$(\mathbf{Ax})_i = \sum_{j=1}^n a_{ij} x_j = k x_i$$

so $x_i = x_j$ for all x_j adjacent to x_i. Since now those $x_j = \max_{1 \leq j \leq n}(x_j)$ also, their neighbours are also equal to x_i and so forth. Since G is connected, we get that $x_i = x_j \forall i, j$ so $\mathbf{x} = x_1[1, \dots, 1]^\intercal$.

3. Suppose $\mathbf{x} = [x_1, \dots, x_n]^\intercal \neq 0$ satisfies $\mathbf{Ax} = \lambda\mathbf{x}$. Let i be such that $|x_i| = \max_{1 \leq j \leq n}(|x_j|)$. Then

$$|\lambda x_i| = |(\mathbf{Ax})_i| = \left| \sum_{j=1}^n a_{ij} x_j \right| \leq \sum_{j=1}^n a_{ij} |x_j| \leq \sum_{j=1}^n a_{ij} |x_i| = k|x_i| \implies |\lambda| \leq k. \qquad \square$$

In particular, 2.1 gives us a way to characterize regular connected graphs from its adjacency algebra. Let $\mathbf{J}$ denote the matrix whose entries are all 1.

Proposition 2.2. *G is regular and connected if and only if $\mathbf{J} \in \mathcal{A}(G)$.*

Proof. Suppose $\mathbf{J} \in \mathcal{A}(G)$. Then for each (i, j) there exists r such that $(\mathbf{A}^r)_{ij} \neq 0$ so by 1.8 G is connected. Since $\mathbf{J}$ is a polynomial of $\mathbf{A}$, $\mathbf{JA} = \mathbf{AJ}$ so we have

$$(\mathbf{JA})_{ij} = \sum_{k=1}^n a_{kj} = (\mathbf{AJ})_{ij} = \sum_{k=1}^n a_{ik}$$

i.e. $\deg(v_j) = \deg(v_i)$ and this is for all $v_i, v_j \in V$ so G is regular.

Conversely suppose G is k-regular and connected. Let p be the minimal polynomial of G. Then by 2.1 $p(x) = (x - k)q(x)$ for some polynomial q. Note $p(\mathbf{A}) = 0 = (\mathbf{A} - k\mathbf{I})q(\mathbf{A}) \implies \mathbf{A}q(\mathbf{A}) = kq(\mathbf{A})$. In particular, this means that every column vector of $q(\mathbf{A})$ is a k-eigenvector of $\mathbf{A}$. Since A is connected, by 2.1 the columns of $q(\mathbf{A})$ are multiples of $[1, \dots, 1]^\intercal$. Since $(q(\mathbf{A}))^\intercal = q(\mathbf{A})$, $q(\mathbf{A})$ is a multiple of $\mathbf{J}$. $\square$

Note that the polynomial q used in 2.2 is simply $q(x) = \prod_{i=1}^{s-1}(x - \lambda_i)$, where λ_i are the distinct eigenvalues of G that are smaller than k. The following is an explicit construction of $\mathbf{J}$ from q (i.e. from $\operatorname{Spec} G$) given a connected k-regular G.

Corollary 2.3. *Let G be connected and k-regular and let q be as in the proof of 2.2. Then*

$$\mathbf{J} = \left(\frac{n}{q(k)} \right) q(\mathbf{A}).$$

Proof. From the proof of 2.2, $q(\mathbf{A}) = \alpha\mathbf{J}$ for some α. Let $\mathbf{x} = [1, \ldots, 1]^\intercal \in \mathbb{R}^n$. Note that $\alpha\mathbf{J}\mathbf{x} = n\alpha\mathbf{x}$. However since $\mathbf{A}\mathbf{x} = k\mathbf{x}$ we must have $q(\mathbf{A})\mathbf{x} = q(k)\mathbf{x}$ (since $\mathbf{A}^r\mathbf{x} = k^r\mathbf{x}$). Thus $\alpha = \frac{q(k)}{n}$ so $\mathbf{J} = \frac{1}{\alpha}q(\mathbf{A}) = (\frac{n}{q(k)})q(\mathbf{A})$. □

This shows that knowing Spec G can be particularly powerful. The following builds the linear algebraic theory for a special class of regular graphs for which we can compute Spec G explicitly.

Definition 2.4. An $n \times n$ matrix $\mathbf{M}$ is *circulant* if $m_{ij} = m_{1,(j-i+1)_n}$ for $i > 1$. A graph G is *circulant* if $\mathbf{A}(G)$ is circulant.

In other words, $\mathbf{M}$ is circulant if the i-th row of M is its first row slid right $i-1$ places. Let $\mathbf{W}$ be the $n \times n$ circulant matrix where the first row is $[0, 1, 0, \ldots, 0]$. Then if the first row of $\mathbf{M}$ is $[m_1, \ldots, m_n]$, we have

$$\mathbf{M} = \sum_{j=1}^{n} m_j \mathbf{W}^{j-1}$$

(since $\mathbf{W}^{j-1}$ is a circulant matrix where the first row has 1 at the j-th column and 0 elsewhere).

Suppose $\mathbf{x} = [x_1, \ldots, x_n]^\intercal$ is a non-zero eigenvector of $\mathbf{W}$, then note

$$\mathbf{W}\mathbf{x} = [x_2, \ldots, x_n, x_1]^\intercal = \lambda\mathbf{x} \iff \lambda x_j = x_{j+1} \forall 1 \le j < n \land \lambda x_n = x_1 \iff \lambda^n = 1 \land x_j = \lambda^{j-1}x_1.$$

In other words, the eigenvalues of $\mathbf{W}$ are precisely the n-th roots of 1, i.e. $1, \omega, \ldots, \omega^{n-1}$ where $\omega = \exp(2\pi i/n)$. It follows that the eigenvalues of $\mathbf{M}$, which is a polynomial of $\mathbf{W}$, are

$$\lambda_r = \sum_{j=1}^{n} m_j \omega^{(j-1)r}, 0 \le r \le n-1.$$

This gives us the following result:

Proposition 2.5. *Suppose that $[0, a_2, \ldots, a_n]$ is the first row of $\mathbf{A}(G)$ for G circulant, then the eigenvalues of G are*

$$\lambda_r = \sum_{j=2}^{n} a_j \omega^{(j-1)r}, 0 \le r \le n-1.$$

We remark that these n eigenvalues are not necessarily distinct. We will give three applications of 2.5.

Example 2.6. K_n is circulant, with the first row of $\mathbf{A}(K_n)$ being $[0, 1, \ldots, 1]$. Note $\sum_{j=1}^{n} \omega^{(j-1)r} = 0$ for $1 \le r \le n-1$, so in these cases

$$\lambda_r = \sum_{j=2}^{n} a_j \omega^{(j-1)r} = -1.$$

For $r = 0$, $\omega^{(j-1)r} = 1 \forall 1 \le j \le n$ so

$$\lambda_0 = \sum_{j=2}^{n} a_j \omega^{(j-1)r} = n-1.$$

Thus

$$\operatorname{Spec} K_n = \begin{pmatrix} n-1 & -1 \\ 1 & n-1 \end{pmatrix}.$$

Example 2.7. C_n is circulant, with the first row of $\mathbf{A}(C_n)$ being $[0, 1, 0, \dots, 0, 1]$ (so v_i is adjacent to v_{i-1} and v_{i+1} and v_1 is adjacent to v_n). Then

$$\lambda_r = \sum_{j=2}^{n} a_j \omega^{(j-1)r} = \omega^r + \omega^{(n-1)r} = \cos(2\pi r/n) + \cos(-2\pi r/n) + i(\sin(2\pi r/n) + \sin(-2\pi r/n)) = 2\cos(2\pi r/n).$$

However note that $2\cos(2\pi r/n) = 2\cos(2\pi(n-r)/n)$ so if n is odd then for all $1 \le r \le \frac{n-1}{2}$ there is a distinct $\frac{n+1}{2} \le r' \le n-1$ such that $n - r = r'$, thus

$$\operatorname{Spec} C_n = \begin{pmatrix} 2 & 2\cos(2\pi r/n) \forall 1 \le r \le \frac{n-1}{2} \\ 1 & 2 \end{pmatrix}.$$

On the other hand if n is even then for all $1 \le r \le \frac{n}{2} - 1$ there exists a distinct $\frac{n}{2} + 1 \le r' \le n-1$ such that $n - r = r'$ and $2\cos(2\pi(n/2)/n) = 2\cos\pi = -2$, thus

$$\operatorname{Spec} C_n = \begin{pmatrix} 2 & 2\cos(2\pi r/n) \forall 1 \le r \le \frac{n-2}{2} & -2 \\ 1 & 2 & 1 \end{pmatrix}.$$

Example 2.8. For K_{2s}, separate V into V_1, V_2 with $V_1 \cup V_2 = V$ and $|V_1| = |V_2| = s$ and pair V_1 and V_2 bijectively. Define H_s, called the *hyperoctahedral graph*, to be the subgraph of K_{2s} with the edges between those paired vertices removed. We now order $V(H_s)$ such that $(v_i, v_{i+s}) \notin E(H_s) \forall 1 \le i \le s$ (i.e. each $v_i \in V_1$ was paired to $v_{i+s} \in V_2$). Then we note that $\mathbf{A}(H_s)$ is circulant with the first row being all 1s except at the first and the $s+1$-th positions. Again due to $\sum_{j=1}^{2s} \omega^{(j-1)r} = 0$ for $1 \le r \le 2s-1$, in these cases

$$\lambda_r = \sum_{j=2}^{2s} a_j \omega^{(j-1)r} = -1 - \omega^{sr} = -1 - (-1)^r = \begin{cases} 0 & r = 2k-1, 1 \le k \le s; \\ -2 & r = 2k, 1 \le k \le s-1. \end{cases}$$

When $r = 0$, $\omega^{(j-1)r} = 1 \forall 2 \le j \le 2s$ so $\lambda_0 = 2s - 2$. Thus

$$\operatorname{Spec} H_s = \begin{pmatrix} 2s-2 & 0 & -2 \\ 1 & s & s-1 \end{pmatrix}.$$

3 Random Regular Graphs

A commonly used method to generate a *random* graph on n vertices[2] is $G(n, 1/2)$, where we take a graph with n vertices and each pair of vertices have independently a probability of $1/2$ to be adjacent. Under this model, all $2^{\binom{n}{2}}$ graphs have an equal chance of being chosen. It is also an effective algorithm for generating random graphs. Here, we define another algorithm for generating *regular* graphs because, as we will see later, a random graph is, with high probability, *not* regular.

Definition 3.1. Given $n > k$ natural numbers with nk being even, we define a *random k-regular graph on n vertices generated by the Bollobás model* as follows:

- Take nk balls grouped into n sets of k balls;
- Uniformly randomly take a perfect matching on those balls. If two balls from the same set matched, or if there are two or more matches between balls from the same pair of sets, then we say the generation *failed* and take a new matching;
- For each set of balls, we define a vertex. Two vertices are adjacent if there is a matching between balls of their corresponding set.

Suppose for each matching, we label all sets and all balls. For each regular graph, we label all vertices and label each edge by a 2-tuple corresponding to its two ends, such that the set of tuple values on edges out of any given vertex form exactly some k-element set (in Figure 1, $\{a, b, c\}$). Then it is clear that there is a bijection between labeled graphs and labeled matchings.

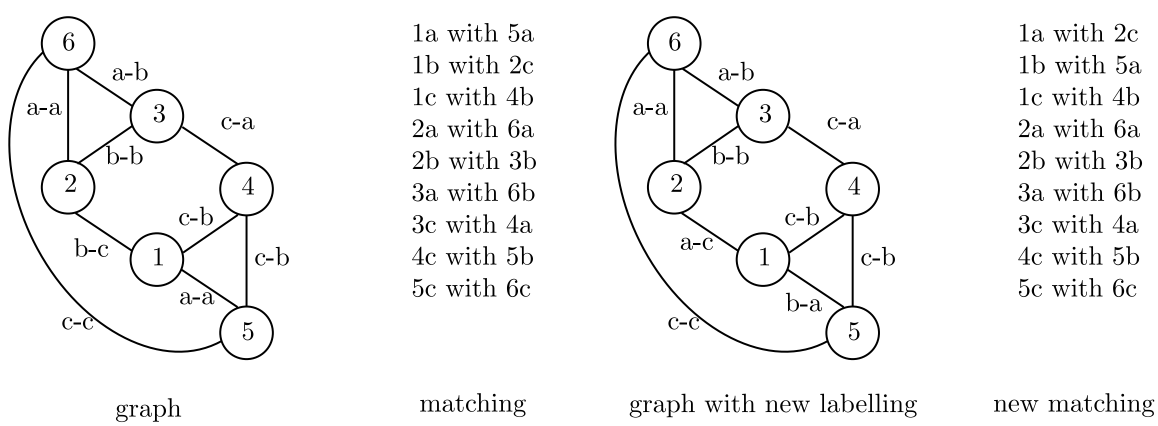

Figure 1: Two ways of labelling a 4-regular graph on 6 vertices and its corresponding matching.

The assignment of a labelling to matchings is clearly uniform by simply labelling the balls before matching. For a given vertex labelling (there are $n!$ ways to vertex label a graph), a permutation in the way any vertex labels its incident edges will result in a different graph labelling, so there are exactly $n^{k!}$ ways to edge label a graph given a vertex labelling. Thus all k-regular graphs are equally likely to be obtained from a random matching, giving us the following:

[2] We always assume the vertices to be labeled, i.e. distinct, so G_1 and G_2 could be isomorphic but not equal.

Proposition 3.2. *The Bollobás model generates all k-regular graphs on n vertices with equal probability.*

We note that the Bollobás model gives us an algorithm for generating random k-regular graphs. Now we prove that a random graph is not k-regular w.h.p.

Proposition 3.3. *$G(n, 1/2)$ is not k-regular w.h.p.*

Proof. There are $2^{\binom{n}{2}}$ graphs on n labeled vertices. Given n groups of k balls, there are $\binom{nk}{nk/2}$ ways to bipartition the balls and $(nk/2)!$ ways to make a matching. However, flipping any pair of matched balls will be counted as a new matching in this system, so each matching is actually counted $2^{nk/2}$ times. Thus there are $\frac{(nk)!}{(nk/2)!2^{nk/2}}$ matchings. As noted above, each k-regular graph can be produced from $n^{k!}$ matchings, so there are $\frac{(nk)!}{(nk/2)!2^{nk/2}n^{k!}}$ k-regular graphs on n labeled vertices. Finally for $n \geq k/2$

$$\frac{(nk)!}{(nk/2)!2^{nk/2}n^{k!}} \leq \left(\frac{k}{2}\right)^{nk/2} \cdot n^{nk/2-k!} \leq n^{nk} \lll 2^{\binom{n}{2}} = (\sqrt{2})^{n^2-n}. \qquad \square$$

4 Distribution of eigenvalues of a large regular graph

This section will be notes on a paper by McKay 1981.

4.1 Introduction

Given G (proper) k-regular graph, let $n(G)$ denote its number of vertices and $c_r(G)$ its number of cycles of length r. Let $F_G(x)$ denote the discrete CDF of its eigenvalues (i.e. each eigenvalue λ is assigned $p(\lambda) = \frac{m(\lambda)}{n(G)}$ where $m(\lambda)$ is its multiplicity). Then by basic probability

1. $F_G(x) = 0$ if $x < -k$;
2. $F_G(x) = 1$ if $x \geq k$;
3. $F_G(x)$ is increasing and right-continuous on $\mathbb{R}$.

Now we state the main result of the McKay paper:

Theorem 4.1. *Let $G_1, G_2, \ldots$ be a sequence of k-regular graphs satisfying the following:*

- *$n(G_i) \to \infty$ as $i \to \infty$;*
- *For each $r \geq 3$,*

$$c_r(G_i)/n(G_i) \xrightarrow{i\to\infty} 0. \tag{4.1}$$

Then, $F_{G_i}(x) \to F(x)$ for $x \in \mathbb{R}$ as $i \to \infty$, where $F(x)$ is the function defined as follows:

1. *$F(x) = 0$ if $x \leq -2\sqrt{k-1}$;*

2. *If* $-2\sqrt{k-1} < x < 2\sqrt{k-1}$,

$$F(x) = \int_{-2\sqrt{k-1}}^{x} \frac{k\sqrt{4(k-1)-t^2}}{2\pi(k^2-t^2)}dt = \frac{1}{2} + \frac{k}{2\pi}\left[\arcsin\frac{x}{2\sqrt{k-1}} - \frac{k-1}{k}\arctan\frac{(k-2)x}{k\sqrt{4(k-1)-x^2}}\right];$$

3. $F(x) = 1$ *if* $x \geq 2\sqrt{k-1}$.

Conversely, if $F_{G_i}(x)$ *does not converge to* $F(x)$ *for some* x*, then* (4.1) *fails for some* $r \geq 3$.

All graphs in this section take the assumptions of 4.1. We start with a short lemma or remark:

Lemma 4.2. *Let* $c(G_i)$ *denote the number of connected components in* G_i*. Then* $c(G_i)/n(G_i) \to 0$ *as* $i \to \infty$.

Proof. For contradiction suppose $\limsup_{i\to\infty} c(G_i)/n(G_i) = c > 0$, so by taking a subsequence of G_i, we can WLOG assume that $c(G_i)/n(G_i) \to c$. Fix $\min(c/2, 1) > \epsilon > 0$. Let $N \in \mathbb{N}$ be such that, for all $2(1/c+\epsilon) \leq r \leq 3$, $c_r(G_i)/n(G_i) < \epsilon$, $|n(G_i)/c(G_i) - 1/c| < \epsilon$ and $|c(G_i)/n(G_i) - c| < \epsilon$ for all $i \geq N$.

Now fix $i \geq N$. Note that since each component in G_i has on average at most $1/c + \epsilon$ vertices, at least $c(G_i)/2$ components have at most $2(1/c+\epsilon)$ vertices. Note that each such component contains at least one cycle of length $2(1/c+\epsilon) \leq r \leq 3$ (due to acyclic graphs being trees, which always have vertices of degree 1 or 0 so not k-regular). Thus each such cycle appears on average at least $c(G_i)/(4(1/c+\epsilon))$ times, so there must exist some $2(1/c+\epsilon) \leq r \leq 3$ such that

$$c_r(G_i) \geq c(G_i)/(4(1/c+\epsilon)) \implies \epsilon > \frac{c_r(G_i)}{n(G_i)} \geq \frac{c(G_i)}{4(1/c+\epsilon)n(G_i)} > \frac{c-\epsilon}{4(1/c+\epsilon)} > \frac{c}{8(1/c+1)}$$

which clearly does not hold as $\epsilon \to 0$. □

Corollary 4.3. *For all* $M \in \mathbb{N}$ *and* $c > 0$*, there exists* $N \in \mathbb{N}$ *such that for all* $i \geq N$*, components of* G_i *with less than* M *vertices have in total at most* $n(G_i)/c$ *vertices.*

Proof. Components with less than M vertices have in total at most $Mc(G_i)$ vertices, and

$$Mc(G_i) \leq n(G_i)/c \iff Mc(G_i)/n(G_i) \leq 1/c.$$

Thus we can simply apply 4.2 with $\epsilon \leq \frac{1}{cM}$. □

Example 4.4. When $k = 2$, G_i are all cycles $C_{r(i)}$ where $r(i) = n(G_i) \to \infty$ and for $-2 < x < 2$,

$$F(x) = \int_{-2}^{x} \frac{2\sqrt{4-t^2}}{2\pi(4-t^2)}dt = \int_{-2}^{x} \frac{1}{\pi\sqrt{4-t^2}}dt = \frac{1}{\pi}\left(\arcsin\frac{x}{2} + \frac{\pi}{2}\right) = \frac{1}{\pi}\arccos\frac{x}{2}.$$

If $X \sim \mathcal{U}(0,1)$ and $Y = 2\cos(\pi X) = 2\cos(2\pi X)$, then $F(x)$ is exactly the CDF of Y. It is known that each component of G_i must be a cycle. For each $r \geq 3$, let F_r denote the distribution of eigenvalues of C_r. Then by 2.7 we see that $F_r(x) \to F(x)$ for all $x \in \mathbb{R}$. 4.3 allows us to assume that at least $(1-1/c)n(G_i)$ eigenvalues are from cycles of size at least M, for large enough i, so it is clear that $F_{G_i}(x)$ is between $F_M(x) - 1/c$ and $\max(F(x), F_M(x)) + 1/c$ for each x, so with $M \to \infty$ and $c \to 0$ we have $F_{G_i}(x) \to F(x)$.

4.2 Existence and uniqueness of $F(x)$

We first prove a counting result related to Catalan numbers.

Lemma 4.5. *Fix $n, k \in \mathbb{N}, k \leq n$. Assume we have $\mathbf{x} = (x_1, \ldots, x_{2n})$ where $x_i \in \{-1, 1\}$ such that the following are satisfied:*

- $\sum_{i=1}^{2n} x_i = 0$ *and* $\sum_{i=1}^{j} x_i \geq 0 \forall 1 \leq j \leq 2n$ *(note that these are the same as for Catalan numbers);*
- $|\{1 \leq j \leq 2n : \sum_{i=1}^{j} x_i = 0\}| = k.$

Then there are

$$\binom{2n-k}{n} \frac{k}{2n-k}$$

possibilities for $\mathbf{x}$.

Proof. Let $N(n, k)$ denote the number of possibilities for $\mathbf{x}$ and let $P(n, k) = \binom{n+k-1}{k-1}$ denote the number of ways of putting n indistinguishable balls into k labeled baskets (equivalent to choosing $k-1$ positions out of $n+k-1$ to be cutoffs between baskets, with the rest being balls in each basket). Let $\mathbf{x}'$ be defined from $\mathbf{x}$ according to the following:

- For each $1 < j < 2n$ where $\sum_{i=1}^{j} x_i = 0$, remove x_j and x_{j+1} (note that $x_j = -1$ and $x_{j+1} = 1$ always);
- Remove x_1 and x_{2n} ($x_1 = 1$ and $x_{2n} = -1$ always).

Then $\mathbf{x}'$ satisfies the assumptions with $n-k$ and some ℓ as its parameters ($1 \leq \ell \leq n-k$). However, given $\mathbf{x}'$, there are $P(k-1, \ell+1)$ possible $\mathbf{x}$ (since there are $k-1$ "zeros" to be put into $\ell+1$ potential positions). Thus we have

$$N(n, k) = \sum_{\ell=1}^{n-k} N(n-k, \ell) P(k-1, \ell+1) = \sum_{\ell=1}^{n-k} \binom{\ell+k-1}{\ell} N(n-k, \ell).$$

We now prove by induction on $n-k$ that $N(n,k) = \binom{2n-k}{n}\frac{k}{2n-k}$. If $n = k$ then $N(n,k) = 1$. Now assume the proposition is true for all n, k such that $n - k < M$ ($M \in \mathbb{N}$) and now assume $n - k = M$. By IH (note $n - k - \ell < M$)

$$\begin{aligned}
N(n,k) &= \sum_{\ell=1}^{M} \binom{\ell+k-1}{\ell} N(M, \ell) = \sum_{\ell=1}^{M} \binom{\ell+k-1}{\ell} \binom{2M-\ell}{M} \frac{\ell}{2M-\ell} \\
&= \sum_{\ell=1}^{M} \frac{(\ell+k-1)!}{\ell!(k-1)!} \cdot \frac{(M+n-k-\ell)!}{(n-k)!(M-\ell)!} \cdot \frac{\ell}{M+n-k-\ell} \\
&= \frac{(2n-k)!}{n!(n-k)!} \frac{k}{2n-k} \sum_{\ell=1}^{M} \frac{(\ell+k-1)!(M-\ell+n-k-1)!n!}{(\ell-1)!k!(M-\ell)!(M+n-1)!}.
\end{aligned}$$

Note

$$\frac{(\ell+k-1)!(M-\ell+n-k-1)!M!}{(\ell-1)!k!(M-\ell)!(M+n-1)!} = \frac{\binom{\ell+k-1}{\ell-1}(M-\ell+n-k-1)!n!(M-1)!}{(M-\ell)!(M+n-1)!(n-k-1)!}$$
$$= \frac{\binom{\ell+k-1}{\ell-1}\binom{M-\ell+n-k-1}{M-\ell}}{\binom{M+n-1}{n}}$$
$$= \frac{P(\ell-1,k+1)P(M-\ell,n-k)}{P(M-1,n+1)}$$

which is the probability that when putting $M-1$ balls uniformly and independently randomly into $n+1$ baskets, there are $\ell-1$ balls inside $k+1$ specific baskets and the remaining $n-\ell$ balls inside the remaining $n-k$ baskets. Summing over ℓ from 1 to M, this covers all possible number of balls ending into those $k+1$ specific baskets (i.e. 0 to $M-1$), so this sums up to 1 over $1 \leq \ell \leq M$ and we are done. □

Note that we can use the above result to count the number of closed walks in an acyclic regular graph:

Lemma 4.6. *Suppose G is k-regular. Let $v_0 \in V(G)$ and suppose the subgraph of G induced by vertices at distance at most $r/2$ from v_0 is acyclic (i.e. a tree rooted at v_0). Then the number of closed walks of length r in X starting at v_0 is $\theta(r)$, where $\theta(r) = 0$ if r is odd, $\theta(0) = 1$ and otherwise*

$$\theta(2s) = \sum_{i=1}^{s} \binom{2s-i}{s} \frac{i}{2s-i} k^i (k-1)^{s-i}$$
$$= k \sum_{i=0}^{s-1} \binom{2s}{i} \frac{s-i}{s} (k-1)^i$$
$$= \sum_{i=1}^{s} \binom{2s}{i} \frac{2s-2i+1}{2s-i+1} (k-1)^i.$$

Proof. Let $\mathbf{v} = v_0, \ldots, v_r$ be a closed walk of length r. Corresponding to $\mathbf{v}$ we have a sequence of nonnegative integers $\mathbf{d} = d_0, \ldots, d_r$, where d_i is the distance from v_0 to v_i in G. Then $|d_i - d_{i-1}| = 1$ for $r \geq i \geq 1$ and $d_r - d_0 = \sum_{i=1}^{r}(d_i - d_{i-1}) = |\{i : d_i - d_{i-1} = 1\}| - |\{i : d_i - d_{i-1} = -1\}| = 0$ so r is even so let $s = r/2$ where $s > 0$.

It is proven in 4.5 (to see that it applies here, note $d_j = \sum_{i=1}^{j} x_i$) that the number of possible $\mathbf{d}$ with i d_j (for $1 \leq j \leq r$) being 0 ($i \geq 0$) (we say $\mathbf{d}$ has i zeros) is

$$\binom{2s-i}{s} \frac{i}{2s-i}.$$

Fix $\mathbf{d}$ with i zeros. Note that this fixes a sequence of moving away or towards v_0, starting at v_0 for the walk. Every move towards v_0 is predetermined. Since we start at v_0 i times throughout the walk and each time has k possibilities so those account for k^i possibilities in total. All the $s-i$ other times we need to move away from v_0 so those account for $(k-1)^{s-i}$ possibilities, thus each $\mathbf{d}$ accounts for $k^i(k-1)^{s-i}$ closed walks, giving us the first expression. The other equalities are by algebra. □

We then determine that $\theta(r)$ holds asymptotically without the acyclic assumption:

Lemma 4.7. *For $r \geq 0$, $i \geq 1$ let $\phi_r(G_i)$ denote the total number of closed walks of length r in G_i. Then for each r, $\phi_r(G_i)/n(G_i) \to \theta(r)$ as $i \to \infty$.*

Proof. Let $n_r(G_i)$ denote the number of vertices in G_i that satisfy the assumptions of 4.6 regarding v_0. Given $v_0 \in V(G_i)$, call the subgraph used in 4.6 $H_r(v_0) \subseteq G_i$. Then note $n_r(G_i)/n(G_i) \to 1$ as $i \to \infty$, since otherwise $n(G_i) - n_r(G_i)$ would not be $o(n(G_i))$, and since the number of v such that $V(H_r(v)) \cap V(H_r(v_0)) \neq \varnothing$ is upper bounded[3] regardless of G_i, the number of cycles that are in some $H_r(v)$, i.e. of size at most $k(k-1)^{r/2-1}+1$ (upper bound of the size of $H_r(v)$), is not $o(n(G_i))$, so there must be some r_0 at most $k(k-1)^{r/2-1}+1$ such that $c_{r_0}(G_i)$ is not $o(n(G_i))$, a contradiction to (4.1).

Note that for any $v \in V(G)$, the number of closed walks of length r is trivially upper bounded by k^{r-1}, thus by squeeze theorem

$$\frac{n_r(G_i)\theta(r)}{n(G_i)} \leq \frac{\phi_r(G_i)}{n(G_i)} \leq \frac{n_r(G_i)\theta(r) + (n(G_i) - n_r(G_i))k^{r-1}}{n(G_i)} \implies \frac{\phi_r(G_i)}{n(G_i)} \xrightarrow{i\to\infty} \theta(r). \qquad \square$$

We can rewrite ϕ_r/n as a Lebesgue-Stieltjes integral with respect to $F_{G_i}(x)$:

Lemma 4.8. *For each $r \geq 0$,*

$$\int x^r dF_{G_i}(x) \xrightarrow{i\to\infty} \theta(r).$$

Proof. By definition of F_G and 1.8,

$$\int x^r dF_{G_i}(x) = \sum_{\lambda \in \operatorname{Spec} G_i} \lambda^r p(\lambda) = \frac{1}{n(G_i)} \sum_{j=1}^{n(G_i)} \lambda_j^r = \frac{1}{n(G_i)} \operatorname{Tr}(A^r) = \frac{\phi_r(G_i)}{n(G_i)} \forall r \geq 0. \qquad \square$$

Now we arrive at the existence and uniqueness of $F(x)$.

Theorem 4.9. *There is a unique $F(x)$ increasing and right-continuous such that*

$$\int x^r dF = \theta(r) \forall r \geq 0.$$

Furthermore, $F_{G_i}(x) \to F(x)$ as $i \to \infty$ for every x where F is continuous.

To prove this, we state 3 standard results in analysis. Let $I = [\alpha, \beta]$ and for each $M \geq 0$, define $\operatorname{RBV}(I, M)$ to be the set of all real $f(x)$ such that

1. $f(x) = 0$ if $x < \alpha$ and $f(x)$ is constant if $x > \beta$;
2. f is right-continuous;
3. the total variation of f is at most M.

[3] By at most $(k(k-1)^{r/2-1}+1)^2$ since $u \in V(H_r(v)) \iff v \in V(H_r(u))$ and each $H_r(v)$ has at most $k(k-1)^{r/2-1}+1$ nodes, so $|v : V(H_r(v)) \cap V(H_r(v_0)) \neq \varnothing| = |\{v : v \in V(H_r(u)) : u \in V(H_r(v_0))\}| \leq (k(k-1)^{r/2-1}+1)^2$.

Lemma 4.10. *If $f \in \mathrm{RBV}(I, M)$ and $\int x^r df = 0 \forall r \geq 0$, then $f(x) = 0$ a.e.*

Lemma 4.11 (Helley-Bray)**.** *Let $f_1, f_2, \ldots$ be a sequence in $\mathrm{RBV}(I, M)$ such that $f_n(x) \to f(x)$ as $i \to \infty$ for some $f \in \mathrm{RBV}(I, M)$ at every x where f is continuous. Then $\int x^r df_i \to \int x^r df$ as $i \to \infty$ for each $r \geq 0$.*

Lemma 4.12 (Helley selection)**.** *Let $f_1, f_2, \ldots$ be a sequence in $\mathrm{RBV}(I, M)$. Then there exists a subsequence $f_{n_1}, f_{n_2}, \ldots$ and $f \in \mathrm{RBV}(I, M)$ such that $f_{n_k}(x) \to f(x)$ as $k \to \infty$ at every x where f is continuous.*

We use the above to prove the following:

Theorem 4.13. *Let $f_1, f_2, \ldots$ be a sequence in $\mathrm{RBV}(I, M)$ such that $\int x^r df_i \to \mu_r$ as $i \to \infty$ for each $r \geq 0$, where $\mu_r \in \mathbb{R} \forall r \geq 0$. Then there exists a unique (up to being equal a.e.) $f \in \mathrm{RBV}(I, M)$ such that $\int x^r df = \mu_r \forall r \geq 0$. Furthermore $f_n(x) \to f(x)$ wherever $f(x)$ is continuous.*

Proof. Suppose $f, g \in \mathrm{RBV}(I, M)$ satisfy $\int x^r df = \int x^r dg = \mu_r \forall r \geq 0$, then $f - g \in \mathrm{RBV}(I, 2M)$ satisfies $\int x^r d(f - g) = \int x^r df - \int x^r dg = 0 \forall r \geq 0$ so by 4.10 $f - g \equiv 0$ a.e.

We know by 4.12 that any subsequence of f_n has itself a subsequence $\mathbf{x}$ that converge to some $f_{\mathbf{x}} \in \mathrm{RBV}(I, M)$ wherever $f_{\mathbf{x}}$ is continuous. By 4.11, all such $f_{\mathbf{x}}$ satisfy $\int x^r df_{\mathbf{x}} = \mu_r$ so there is a unique $f_{\mathbf{x}} \equiv f \forall \mathbf{x}$.

It suffices now to prove that $f_n(x) \to f(x)$ wherever $f(x)$ is continuous. Suppose there exists x_0 where f is continuous, but $f_n(x_0)$ does *not* converge to $f(x_0)$. Then there must exist ϵ and a subsequence f_{n_k} such that

$$|f_n(x_0) - f_{n_k}(x_0)| \geq \epsilon \forall k \geq 1.$$

By 4.12 f_{n_k} has a subsequence $\mathbf{x} = f_{n_{k_j}}$ where $f_{n_k}(x) \to f_{\mathbf{x}}(x) = f(x)$ wherever $f(x)$ is continuous. However $f_{n_{k_j}}(x_0)$ cannot converge to $f(x_0)$ so f is not continuous at x_0, a contradiction. □

Then our result 4.9 is a direct corollary:

Proof of 4.9. 4.13 applies with $M = 1$ (since F_{G_i} are CDFs) and $I = [-k, k]$. It suffices to show that we have a unique, increasing and right-continuous F.

Let $X \subseteq \mathrm{RBV}(I, M)$ be the set of all f obtainable from 4.13 with F_{G_i}. For any $f \in X$, since $f \in \mathrm{RBV}(I, M)$, f is continuous a.e. Call the set on which f is continuous $A_f \subseteq \mathbb{R}$ and let $A = \bigcup_{f \in X} A_f$. Then $F_{G_i}(x)$ converges in A. Since F_{G_i} are increasing, $f|_A$. Let F be such that $F(x) = \lim_{i \to \infty} F_{G_i}(x) \forall x \in A$ and for every $x_0 \notin A$, $F(x_0) = \inf_{x \in A, x \geq x_0} F(x)$. Then F since F agrees with any $f \in X$ on A_f, F agrees with f a.e. so $F \in X$. F is unique and increasing, so the only discontinuity is of the first kind, so by its definition F is right-continuous. □

4.3 Derivations of $F(x)$

This section deals with the derivation of $F(x)$ from 4.9 and 4.6 and is quite technical so only an outline will be given. We start with an asymptotic expression for $\theta(2s)$:

Lemma 4.14. *As $s \to \infty$,*

$$\theta(2s) \sim \frac{4^s k(k-1)^{s+1}}{s(k-2)^2\sqrt{\pi s}}.$$

Outline of proof. By taking $z = 1/(k-1)$, the second form for $\theta(2s)$ from 4.6 can be written as (let $i' = s - i$)

$$\begin{aligned}
\theta(2s) &= k \sum_{i=0}^{s-1} \binom{2s}{i} \frac{s-i}{s} (k-1)^i \\
&= \frac{k(k-1)^{s-1}}{s} \sum_{i=0}^{s-1} \binom{2s}{i} (s-i)(k-1)^{i-s+1} \\
&= \frac{k(k-1)^{s-1}}{s} \sum_{i'=1}^{s} \binom{2s}{s-i'} i' z^{i'-1} \\
&= \frac{k(k-1)^{s-1}}{s} \binom{2s}{s-1} \left(\sum_{i'=1}^{s} i' z^{i'-1} - \varepsilon(s) \right)
\end{aligned}$$

where

$$\varepsilon(s) = \sum_{i=1}^{s} \left(1 - \frac{\binom{2s}{s-i}}{\binom{2s}{s-1}} \right) i z^{i-1}.$$

It can be shown that $\varepsilon(s) \to 0$ as $s \to \infty$, and it can also be shown that

$$\theta(2s) \sim \frac{k(k-1)^{s-1}}{s} \binom{2s}{s-1} \sum_{i'=1}^{s} i' z^{i'-1} \sim \frac{4^s k(k-1)^{s+1}}{s(k-2)^2\sqrt{\pi s}}.$$

□

Lemma 4.15. *Define $\omega = \sup\{|x| \mid 0 < F(x) < 1\}$. Then $\omega = 2\sqrt{k-1}$.*

Outline of proof. For any s, note that $x^2 \le \omega^2 \implies x^{2s+2} \le \omega^2 x^{2s}$ wherever $\frac{d}{dx}F(x) > 0$ by definition of ω so $\int x^{2s+2} dF \le \omega^2 \int x^{2s} dF$. Thus

$$\limsup_{s\to\infty} \frac{\int x^{2s+2} dF}{\int x^{2s} dF} \le \omega^2.$$

For any $0 < \beta < \omega$, we can find (details omitted)

$$\liminf_{s\to\infty} \frac{\int x^{2s+2} dF}{\int x^{2s} dF} \ge \beta^2.$$

Thus letting $\beta \to \omega$, we get $\lim_{s\to\infty} \frac{\int x^{2s+2} dF}{\int x^{2s} dF} = \lim_{s\to\infty} \frac{\theta(2(s+1))}{\theta(2s)} \to \omega^2$ as $s \to \infty$. Thus by 4.14 $\omega^2 = 4(k-1) \implies \omega = 2\sqrt{k-1}$. □

Lemma 4.16. *$F(x)$ is continuous at $x = \pm\omega$.*

The proof is based on examining the jump at $x = \pm\omega$ and is omitted.

Finally some further analysis involving Tchebyshev polynomials was used to prove 4.1.

4.4 Application to random regular graphs

Let $k \geq 2$ and $n_1 < n_2 < \dots$ be the sequence of number of vertices on which k-regular graphs are possible.[4] For each i define R_i to be the set of all labeled k-regular graphs on n_i vertices. Define $F_i(x)$ to be the average of $F_G(x)$ with G taken over all $G \in R_i$, i.e. $F_i(x) = \frac{1}{n_i}\sum_{G\in R_i} F_G(x)$. F_i can be seen as the *expected* eigenvalue distribution of k-regular graphs on n_i vertices. We will state the following lemma without proof:

Lemma 4.17. *For each $r \geq 3$ define $c_{r,i}$ to be the average number of r-cycles in one member of R_i. Then $c_{r,i} \to (k-1)^r/2r$ as $i \to \infty$.*

For our purposes, we actually only need a weaker result, which will be proven:

Lemma 4.18.

$$c_{r,i} \xrightarrow{i\to\infty} M_r < \infty.$$

Proof. Uniformly randomly take $G \in R_i$ and $v \in V(G)$. For the subgraph H induced by the set of all vertices with distance at most $m = \lceil r/2 \rceil$ from v, if H is acyclic then v is not part of any r-cycle. There are at most $\binom{n_i-1}{k}\binom{n_i-1}{k-1}^{k(k-1)^{m-1}}$ possibilities for H (the set of all H is the subset of all trees where each child of u is sampled from $V(G)\setminus\{u\}$: there are $\binom{n_i-1}{k}$ possibilities for children of v and $\binom{n_i-1}{k-1}$ possibilities for the children of $u \neq v$). Out of these, there are at least $\binom{n_i-1}{k}\binom{n_i-1-k(k-1)^{m-1}}{k-1}^{k(k-1)^{m-1}}$ possibilities where H is acyclic (since there are never less than $n_i - 1 - k(k-1)^{m-1}$ options to chose from for each node).

Let $t = k(k-1)^{m-1}$, then the probability that H is acyclic is at least $\prod_{j=0}^{k-2} \frac{n_i-1-t-i}{n_i-1-i} \geq (\frac{n_i-t-k+1}{n_i-k+1})^{k-1}$. Thus the expected number of $v \in V(G)$ whose H is acyclic is at least $n_i(\frac{n_i-t-k+1}{n_i-k+1})^{k-1}$, so the expected number of r-cycles is at most[5]

$$\frac{n_i}{r}\left(1-\left(\frac{n_i-t-k+1}{n_i-k+1}\right)^{k-1}\right) = \frac{n_i}{r}\left(1-\left(1-\frac{t}{n_i-k+1}\right)^{k-1}\right) \leq \frac{(k-1)^2 n_i t}{r(n_i-k+1)} = O(1).$$

□

Theorem 4.19.

$$F_i(x) \xrightarrow{i\to\infty} F(x).$$

[4] $n_1 = k+1$ and $n_{i+1} = n_i + 2$ if k is odd; otherwise $n_{i+1} = n_i + 1$

[5] Note $(a+\epsilon)^k$ (where $\epsilon \to 0$ and $a \geq 0$ constant) is upper bounded by $a^k + k^2 a^{k-1}\epsilon$, since the i-th term after $ka^{k-1}\epsilon$ in the binomial expansion is exactly $\frac{\epsilon^i\binom{k}{i+1}}{ka^i} \xrightarrow{\epsilon\to 0} 0$ multiplied onto $ka^{k-1}\epsilon$. $a = 1 - \frac{t}{n_i-k+1} \leq 1$ and $\epsilon = \frac{t}{n_i-k+1}$.

Proof. Define graph Y_i to be the graph consisting of all graphs in R_i put together in disjoint union. Then $F_{Y_i} \equiv F_i$. Now it suffices to show that Y_i satisfies the assumptions in 4.1. Indeed since by 4.18 there are on average at most $M_r + \epsilon$ r-cycles per member of R_i (true for i large enough),

$$c_r(Y_i) \leq |R_i|(M_r + \epsilon)$$

Since $n(Y_i) = |R_i|n_i$,

$$\frac{c_r(Y_i)}{n(Y_i)} \leq \frac{M_r + \epsilon}{n_i} \xrightarrow{i\to\infty} 0.$$

□

5 Vertex replacement on regular graphs

Let $\mathcal{F}_k$ be the set of k-regular graphs ($k \geq 2$ across this section). For a given k we will define a map from $\mathcal{F}_k$ onto itself that will help us generate k-regular graphs, via vertex replacement.

Definition 5.1. Let G be a graph. $D(G) = D_G$ (called the *subdivision graph* of G) is defined to be the graph created from subdividing every edge in $E(G)$. Formally, $V(D_G) = E(G) \cup V(G)$ and $E(D_G) = \{(e, v) : e \in E(G), v \in V(G), e \text{ incident to } v\}$.

Remark. For $x \in V(D_G)$, if $x \in V(G)$ then $\deg_{D_G}(x) = \deg_G(x)$ and if $x \in E(G)$ then $\deg_G(x) = 2$.

We start with a representation of the adjacency matrix of D_G.

Lemma 5.2. *Let G have n vertices and ℓ edges. Let $\mathbf{X}_{n\times\ell} = \mathbf{X}(G)$ be the undirected incidence matrix of G ($\mathbf{X}_{ve} = 1$ if and only if e incident to v). Then*

$$\mathbf{A}(D_G) = \begin{pmatrix} 0_{\ell\times\ell} & \mathbf{X}(G)^\intercal \\ \mathbf{X}(G) & 0_{n\times n} \end{pmatrix}.$$

Proof. The first ℓ rows and columns of $\mathbf{A}(D_G)$ represent $E(G)$ and the following n represent $V(G)$. $\mathbf{A}_{ij} = 0$ if $i, j \in V(G)$ or $i, j \in E(G)$ and $\mathbf{A}_{ij} = 1$ if and only if $\mathbf{X}(G)_{ij} = 1$ (if $i \in V(G)$ and $j \in E(G)$) or $\mathbf{X}(G)_{ji} = 1$ (if $i \in E(G)$ and $j \in V(G)$). □

Definition 5.3. Let G be a graph. $L(G) = L_G$ the *line graph* of G is defined where $V(L_G) = E(G)$ and $(e, f) \in E(L_G)$ if and only if e, f are incident to the same vertex in G.

Lemma 5.4. *For each $v \in V(G)$, if it is incident to $e_1, \dots, e_d \in E(G)$, then we can identify it with $H_v \subseteq L_G$, where $V(H_v)$ is the induced subgraph of $\{e_1, \dots, e_d\}$, H_v is isomorphic to K_d and $H_v \cap H_u \neq \varnothing$ if and only if $(u, v) \in E(G)$, in which case $H_v \cap H_u = \{(u, v)\}$.*

Proof. H_v is isomorphic to K_d since every $e, f \in V(H_v)$ are neighbours (they are all incident to v). The intersection property follows $V(H_v \cap H_u) = V(H_v) \cap V(H_u)$. □

Lemma 5.5. *For $e = (v, u) \in V(L_G)$ (where $v, u \in V(G)$ were neighbours in G), $\deg_{L_G}(e) = \deg_G(v) + \deg_G(u) - 2$.*

Proof. e is only neighbours with $f \in E(G)$ where $f \neq e$ incident to v or to u, and there are $\deg_G(v) + \deg_G(u) - 2$ of those. □

Proposition 5.6. *Let $G \in \mathcal{F}_k$ be k-regular.*

$$\phi : \mathcal{F}_k \to \mathcal{F}_k, G \mapsto L(D(G))$$

is a mapping where every $v \in V(G)$ can be identified to $H_v \subseteq \phi(G)$ whose vertex set are edges incident to v in G. H_v is isomorphic to K_k and H_v is joined by an edge to H_u if and only if $(u, v) \in E(G)$.

Remark. ϕ indeed maps into $\mathcal{F}_k$ by 5.5, since every $e \in E(D_G)$ joins a vertex of degree k (from $V(G)$) and one of degree 2 (from $E(G) \subseteq V(D_G)$). So $e \in V(\phi(G))$ would have degree $k + 2 - 2 = k$.

Proof. Since $V(G) \subseteq V(D(G))$ and the degrees stay unchanged, we use H_v from 5.4 to get that they are isomorphic to K_k and that they share a vertex with each of H_e, where $e \in E(G)$ was added by the subdivisions and e is incident to v and some u neighbour of v. But this means H_e also shares a vertex with H_u (and $H_u \cap H_v = \varnothing$ since $u, v \in V(G)$ can never be neighbours in D_G), which means H_v shares an edge with H_u.

By the degree of every $x \in V(H_v)$, since they have $k - 1$ degrees inside H_v, they must have precisely one degree out of H_v, hence the *only if*. □

Definition 5.7. $\phi(G)$ (from 5.6) is called the *para-line graph* of G.

In order to study the relationship between $\operatorname{Spec} G$ and $\operatorname{Spec} \phi(G)$ for $G \in \mathcal{F}_k$, we will use two well-known results from linear algebra, as well as one result that applies to graphs in general.

Lemma 5.8. *If $\mathbf{M}$ is invertible and $\mathbf{T}$ is square,*

$$\det \begin{pmatrix} \mathbf{M} & \mathbf{X} \\ \mathbf{Y} & \mathbf{T} \end{pmatrix} = \det \mathbf{M} \det(\mathbf{T} - \mathbf{Y}\mathbf{M}^{-1}\mathbf{X}).$$

Proof. Note (assume $\mathbf{M}_{\ell \times \ell}$ and $\mathbf{T}_{n \times n}$)

$$\begin{pmatrix} \mathbf{M}^{-1} & 0_{\ell \times n} \\ 0_{n \times \ell} & \mathbf{I}_n \end{pmatrix} \begin{pmatrix} \mathbf{I}_\ell & -\mathbf{X} \\ 0_{n \times \ell} & \mathbf{I}_n \end{pmatrix} = \begin{pmatrix} \mathbf{M}^{-1} & -\mathbf{M}^{-1}\mathbf{X} \\ 0_{n \times \ell} & \mathbf{I}_n \end{pmatrix}$$

is precisely the product of column operations that eliminate $\mathbf{M}$ and $\mathbf{X}$. Then

$$\begin{pmatrix}\mathbf{M} & \mathbf{X}\\ \mathbf{Y} & \mathbf{T}\end{pmatrix}\begin{pmatrix}\mathbf{M}^{-1} & -\mathbf{M}^{-1}\mathbf{X}\\ 0_{n\times\ell} & \mathbf{I}_n\end{pmatrix} = \begin{pmatrix}\mathbf{I}_\ell & 0_{\ell\times n}\\ \mathbf{Y}\mathbf{M}^{-1} & \mathbf{T}-\mathbf{Y}\mathbf{M}^{-1}\mathbf{X}\end{pmatrix}$$
$$\implies \det\begin{pmatrix}\mathbf{M} & \mathbf{X}\\ \mathbf{Y} & \mathbf{T}\end{pmatrix}(\det\mathbf{M})^{-1} = \det(\mathbf{T}-\mathbf{Y}\mathbf{M}^{-1}\mathbf{X}). \qquad \square$$

Lemma 5.9. *If $\mathbf{X}_{m\times n}$, $\mathbf{Y}_{n\times m}$ are matrices and $\chi_{\mathbf{A}}$ denotes the characteristic polynomial of a square matrix $\mathbf{A}$, then*

$$\lambda^n\chi_{\mathbf{XY}}(\lambda) = \lambda^m\chi_{\mathbf{YX}}(\lambda).$$

Proof. We start by the case where $\mathbf{X}, \mathbf{Y}$ are $n\times n$, and $\mathbf{X}$ is invertible. Then

$$\mathbf{X}(\mathbf{YX})\mathbf{X}^{-1} = \mathbf{XY} \implies \det(\lambda\mathbf{I}_n - \mathbf{XY}) = \det(\mathbf{X}(\lambda\mathbf{I}_n - \mathbf{YX})\mathbf{X}^{-1}) = \det(\lambda\mathbf{I}_n - \mathbf{YX}).$$

For $\mathbf{X}, \mathbf{Y}$ both singular, for fixed $\lambda\in\mathbb{R}$, if we consider

$$\psi_\lambda : \mathbb{R}^{2n^2}\to\mathbb{R}, (\mathbf{X},\mathbf{Y})\mapsto\chi_{\mathbf{XY}}(\lambda);\ \ \phi_\lambda : \mathbb{R}^{2n^2}\to\mathbb{R}, (\mathbf{X},\mathbf{Y})\mapsto\chi_{\mathbf{YX}}(\lambda)$$

then $\psi_\lambda = \phi_\lambda$ almost everywhere (wherever one of $\mathbf{X}, \mathbf{Y}$ is invertible), so since ψ_λ and ϕ_λ are analytic, $\psi_\lambda = \phi_\lambda$ everywhere. Thus $\chi_{\mathbf{XY}} = \chi_{\mathbf{YX}}$ whenever $\mathbf{X}, \mathbf{Y}$ are square.

Given $n > m$, we write (note $\mathbf{X}'_{n\times n}$ and $\mathbf{Y}'_{n\times n}$)

$$\mathbf{X}'\mathbf{Y}' = \begin{pmatrix}\mathbf{X}\\ 0_{(n-m)\times n}\end{pmatrix}\begin{pmatrix}\mathbf{Y} & 0_{n\times(n-m)}\end{pmatrix} = \begin{pmatrix}\mathbf{XY} & 0_{m\times(n-m)}\\ 0_{(n-m)\times m} & 0_{(n-m)\times(n-m)}\end{pmatrix}$$
$$\implies \chi_{\mathbf{X}'\mathbf{Y}'}(\lambda) = \det\begin{pmatrix}\lambda\mathbf{I}_m - \mathbf{XY} & 0_{m\times(n-m)}\\ 0_{(n-m)\times m} & \lambda\mathbf{I}_{n-m}\end{pmatrix} = \lambda^{n-m}\chi_{\mathbf{XY}}(\lambda) = \chi_{\mathbf{Y}'\mathbf{X}'}(\lambda).$$

and

$$\mathbf{Y}'\mathbf{X}' = \begin{pmatrix}\mathbf{Y} & 0_{n\times(n-m)}\end{pmatrix}\begin{pmatrix}\mathbf{X}\\ 0_{(n-m)\times n}\end{pmatrix} = \mathbf{YX} \implies \lambda^{n-m}\chi_{\mathbf{XY}}(\lambda) = \chi_{\mathbf{Y}'\mathbf{X}'}(\lambda) = \chi_{\mathbf{YX}}(\lambda). \qquad \square$$

Lemma 5.10. *Let G be a graph with n vertices, ℓ edges, degree matrix $\mathbf{D}$ and adjacency matrix $\mathbf{A}$. Then*

$$\chi_{L_G}(\lambda-2) = \lambda^{\ell-n}\det(\lambda\mathbf{I}_n - \mathbf{A} - \mathbf{D}).$$

Proof. Note $\mathbf{A}(L_G) + 2\mathbf{I}_\ell = \mathbf{X}(G)^\intercal\mathbf{X}(G)$. Indeed for $i\neq j$, $\mathbf{A}(L_G)_{ij} = 1$ if and only if i and j are incident to the same vertex, which is precisely when the i-th and j-th columns of $\mathbf{X}(G)$ have a 1 at the same position. For $i = j$, the i-th column of $\mathbf{X}(G)$ always has precisely two 1s, so $(\mathbf{X}(G)^\intercal\mathbf{X}(G))_{ii} = 2$. This implies

$$\chi_{L_G}(\lambda-2) = \det(\lambda\mathbf{I}_\ell - 2\mathbf{I}_\ell - \mathbf{A}(L_G)) = \chi_{\mathbf{X}(G)^\intercal\mathbf{X}(G)}(\lambda).$$

On the other hand $\mathbf{X}(G)\mathbf{X}(G)^\intercal = \mathbf{A}+\mathbf{D}$. Indeed for $i\neq j$, $\mathbf{A}_{ij} = 1$ if and only if i and j are incident to the same edge, which is when i is adjacent to j. If $i = j$ then $(\mathbf{X}(G)\mathbf{X}(G))_{ii} = \deg(i) = \mathbf{D}_{ii}$. The result then follows from 5.9:

$$\chi_{L_G}(\lambda-2) = \chi_{\mathbf{X}(G)^\intercal\mathbf{X}(G)}(\lambda) = \lambda^{\ell-n}\chi_{\mathbf{X}(G)\mathbf{X}(G)^\intercal}(\lambda) = \lambda^{\ell-n}\chi_{\mathbf{A}+\mathbf{D}}(\lambda) = \lambda^{\ell-n}\det(\lambda\mathbf{I}_n - \mathbf{A} - \mathbf{D}). \qquad \square$$

Now we are ready to state a result due to Cvetković to study the eigenvalues of $\phi(G)$.

Theorem 5.11. *Let $G \in \mathcal{F}_k$ have n vertices and $\ell = nk/2$ edges. Then*

$$\chi_{\phi(G)}(\lambda) = (\lambda(\lambda+2))^{\ell-n}\chi_G(\lambda^2 + (2-k)\lambda - k).$$

Proof. Recall

$$\mathbf{A}(D_G) = \begin{pmatrix} 0_{\ell\times\ell} & \mathbf{X}(G)^\intercal \\ \mathbf{X}(G) & 0_{n\times n} \end{pmatrix}, \ \mathbf{D}(D_G) = \begin{pmatrix} 2\mathbf{I}_\ell & 0_{\ell\times n} \\ 0_{n\times\ell} & k\mathbf{I}_n \end{pmatrix}.$$

By 5.10

$$\chi_{\phi(G)}(\lambda) = (\lambda+2)^{\ell-n}\det((\lambda+2)\mathbf{I}_{\ell+n} - \mathbf{A}(D_G) - \mathbf{D}(D_G)).$$

Then by 5.8

$$(\lambda+2)\mathbf{I}_{\ell+n} - \mathbf{A}(D_G) - \mathbf{D}(D_G) = \begin{pmatrix} (\lambda+2-2)\mathbf{I}_\ell & -\mathbf{X}(G)^\intercal \\ -\mathbf{X}(G) & (\lambda+2-k)\mathbf{I}_n \end{pmatrix} = \begin{pmatrix} \lambda\mathbf{I}_\ell & -\mathbf{X}(G)^\intercal \\ -\mathbf{X}(G) & (\lambda-k+2)\mathbf{I}_n \end{pmatrix}$$

$$\begin{aligned} \implies \det\begin{pmatrix} \lambda\mathbf{I}_\ell & -\mathbf{X}(G)^\intercal \\ -\mathbf{X}(G) & (\lambda-k+2)\mathbf{I}_n \end{pmatrix} &= \lambda^\ell \det((\lambda-k+2)\mathbf{I}_n - \lambda^{-1}\mathbf{X}(G)\mathbf{X}(G)^\intercal) \\ &= \lambda^{\ell-n}\det((\lambda(\lambda-k+2)-k)\mathbf{I}_n - \mathbf{A}(G)) = \lambda^{\ell-n}\chi_G(\lambda(\lambda-k+2)-k) \\ \implies \chi_{\phi(G)}(\lambda) &= (\lambda(\lambda+2))^{\ell-n}\chi_G(\lambda(\lambda-k+2)-k). \end{aligned}$$

□

Corollary 5.12. *Let $G \in \mathcal{F}_k$ have n vertices and $\ell = nk/2$ edges and let $f(\lambda) = \lambda^2 + (2-k)\lambda - k$. Then*

$$\operatorname{Spec}\phi(G) = \{0\}^{(\ell-n)} \cup \{-2\}^{(\ell-n)} \cup f^{-1}(\operatorname{Spec} G).$$

where $\operatorname{Spec} G$ and $\operatorname{Spec}\phi(G)$ are understood to be multisets (and $\{x\}^{(\ell-n)}$ denotes the multiset with x having multiplicity $\ell - n$) .

Proof. Everything follows 5.11: if $\lambda = 0$ or -2 then $\chi_{\phi(G)}(\lambda) = 0$; If $\lambda \in f^{-1}(\operatorname{Spec} G)$ then $f(\lambda) \in \operatorname{Spec} G$ so $\chi_G(f(\lambda)) = 0$ so $\chi_{\phi(G)}(\lambda) = 0$. The multiplicities follow from the multiplicity of λ as root of $\chi_{\phi(G)}$. □

Now we use the notation

$$f_k(\lambda) = \lambda^2 + (2-k)\lambda - k.$$

Denote

$$\Gamma_k = \bigcap_{j=0}^{\infty} f_k^{-j}([-k,k]).$$

We are looking for a set $A_k \subseteq [-k,k]$ such that

$$\operatorname{Spec} G \subseteq A_k \implies \operatorname{Spec}\phi(G) = f_k^{-1}(\operatorname{Spec} G) \cup \{0,2\} \subseteq A_k. \tag{5.1}$$

Note that if $f_k^{-j}(A_k \cup \{0,-2\}) \subseteq A_k$, $\forall j \geq 0$ then A_k would satisfy (5.1). We will proceed to show that $A_k = \Gamma_k \cup \bigcup_{j=0}^{\infty} f_k^{-j}(\{0\})$ has the desired property.

Lemma 5.13. *For $x \notin [-k,k]$, $f_k(x) \notin [-k,k]$. In particular, $x \notin f_k^{-1}[-k,k] \supseteq \Gamma_k$ and $f_k^j(x) \neq 0$, $\forall j \geq 0$.*

Proof. Assume $x > k$ i.e. $x = k + \epsilon$. Then

$$f_k(x) = (k+\epsilon)^2 + (2-k)(k+\epsilon) - k = (k+\epsilon)(\epsilon+2) - k > (k+\epsilon)(\epsilon+2) - k - \epsilon = (k+\epsilon)(\epsilon+1) > k.$$

Now assume $x < -k$ i.e. $x = -k - \epsilon$. Then (recall $k \geq 2$ so $2k - 3 \geq 1$)

$$f_k(x) = (-k-\epsilon)^2 + (k-2)(k+\epsilon) - k > (k+\epsilon)(k+\epsilon+k-2) - k - \epsilon = (k+\epsilon)(2k+\epsilon-3) > k. \qquad \square$$

Theorem 5.14. *Let $A_k = \Gamma_k \cup \bigcup_{j=0}^{\infty} f_k^{-j}(\{0\})$. Then $f_k^{-j}(A_k \cup \{0,-2\}) \subseteq A_k \subseteq [-k,k]$, $\forall j \geq 0$. In other words, A_k satisfies (5.1)*

Proof. By 5.13, $\Gamma_k \subseteq [-k,k]$ and $\bigcup_{j=0}^{\infty} f_k^{-j}(\{0\}) \subseteq [-k,k]$ so $A_k \subseteq [-k,k]$. Note

$$f_k^{-j}(A_k \cup \{0,-2\}) = f_k^{-j}(\Gamma_k \cup \{-2\}) \cup \bigcup_{i=0}^{\infty} f_k^{-(i+j)}(\{0\}), \forall j \geq 0.$$

Clearly $\bigcup_{i=0}^{\infty} f_k^{-(i+j)}(\{0\}) \subseteq A_k$ by definition. Furthermore, $f_k(-2) = (-2)^2 + (2-k)(-2) - k = k$ and $f_k^2(-2) = f_k(k) = k^2 + (2-k)k - k = k$ so $f_k^j(-2) \in [-k,k]$ for all $j \geq 0$ so $-2 \in f_k^{-j}([-k,k])$, $\forall j \in \mathbb{N}$ i.e. $-2 \in \Gamma_k$ so $\Gamma_k \cup \{-2\} = \Gamma_k$. Thus it would be sufficient if we can show that $f_k^{-j}(\Gamma_k) \subseteq \Gamma_k$, $\forall j \geq 0$.

Via induction this is equivalent to saying that $f_k^{-1}(\Gamma_k) \subseteq \Gamma_k$. If $x \in f_k^{-1}(\Gamma_k)$ i.e. $f_k(x) \in \Gamma_k$ so $f_k(x) \in f_k^{-j}([-k,k]) \implies x \in f_k^{-(j+1)}([-k,k])$, $\forall j \geq 0$. Now we only need $x \in [-k,k]$, but this follows 5.13: $x \notin [-k,k] \implies f_k(x) \notin [-k,k] \supseteq \Gamma_k$. $\square$

What we showed is that suppose we are given $G \in \mathcal{F}_k$ such that $\operatorname{Spec} G \subseteq A_k$, define $\{G_j = \phi^j(G) : j \geq 0\}$. Then $\operatorname{Spec} G_j \subseteq A_k$, $\forall j \geq 0$.

Example 5.15. Recall that

$$\operatorname{Spec} K_{k+1} = \begin{pmatrix} k & -1 \\ 1 & k \end{pmatrix}.$$

Note $f_k(-1) = 1 - 2 + k - k = -1$ is a fixed point so $-1 \in \Gamma_k \subseteq A_k$. So let $G = K_{k+1}$. Then $\{G_j = \phi^j(G) : j \geq 0\}$ has $\operatorname{Spec} G_j \subseteq A_k$, $\forall j \geq 0$.

5.1 Spectral gaps

One major application of studying spectra of graphs is the study of *mixing times* of random walks.

Definition 5.16. Let $G \in \mathcal{F}_k$. Then $\mathbf{M}_G = \frac{1}{k}\mathbf{A}_G$ is the *random walk matrix* on G.

The idea of random walk matrices is that $\mathbf{M}_G(i,j)$ is the probability of walking to node j in 1 step, if one starts at node i (namely $\frac{1}{k}$ for $G \in \mathcal{F}_k$).

Proposition 5.17. *Let* $\mathbf{M}$ *be a random walk matrix on* G*. Let* $p_{i,j}^{(m)}$ *denote the probability of going to node* j *in* $m \in \mathbb{N}$ *steps, starting at node* i*. Then* $p_{i,j}^{(m)} = (\mathbf{M}^m)_{i,j}$*.*

Proof. We do induction on m. $m = 1$ follows the definition. □

6 Gap sets for the spectra of cubic graphs

This section is an outline of a paper by Kollár and Sarnak.

Throughout this section, we will only study *cubic* graphs, i.e. 3-regular connected, simple graphs (unless noted otherwise), and the set of all such graphs will be denoted $\mathbf{X}$ and its planar subset, $\mathbf{X}_{\mathbf{Planar}}$. Recall that the *spectrum* of $G \in \mathbf{X}$, $\operatorname{Spec} G$, is a subset of $[-3, 3]$ and $3 \in \operatorname{Spec} G$.

Definition 6.1. A closed $K \subseteq [-3, 3]$ is called *spectral* if there exists infinitely many $\{G_n\}_{n\in\mathbb{N}} \subseteq \mathbf{X}$ such that $\operatorname{Spec} G_n \subseteq K \forall n \in \mathbb{N}$. $A = [-3, 3] \setminus K$ is then called a *gap set* and each $x \in A$ is said to be *gapped* by $\{G_n\}$.

Note that trivially $\overline{\bigcup_{n\in\mathbb{N}} \operatorname{Spec} G_n}$ is spectral. Since any closed superset of a spectral set is spectral, we are interested in *minimal* spectral sets (or equivalently maximal gap sets) in particular, i.e. spectral sets for which no proper subset is spectral.

Gap sets are always open in $[-3, 3]$ and 3 is never gapped. As such any $x \in [-3, 3)$ that is gapped must also have a neighbourhood around it within $[-3, 3)$ in which every point is gapped. The following is one of the main results of the paper:

Theorem 6.2. *Every point in* $[-3, 3)$ *is planar gapped.*

The proof of 6.2 will, in particular, make use of the *triangle map* $\mathcal{T}$, defined as follows:

Definition 6.3. The *triangle map* $\mathcal{T} : \mathbf{X} \to \mathbf{X}$ is defined by replacing every vertex in G by a triangle and joining them according to adjacency in G.

Explicitly, we first take a subdivision of G by adding a vertex on every edge, then take the edge dual of that graph, such that every vertex that was in $V(G)$ becomes K_3 and every added vertex becomes K_2 joining the K_3 together.

It turns out that the spectrum for G and $\mathcal{T}(G)$ are linked by the function

$$f(x) = x^2 - x - 3.$$

In fact, it can be shown that $\operatorname{Spec} G$ relates to $\operatorname{Spec} \mathcal{T}(G)$ via the following:

$$\operatorname{Spec} \mathcal{T}(G) = f^{-1}(\operatorname{Spec} G) \cup \{0\} \cup \{-2\} \tag{6.1}$$

with the multiplicities preserved in $f^{-1}(\operatorname{Spec} G)$ and with 0 and 2 having multiplicity $|V(G)|/2$ (on top of the multiplicity of 0 and 2 from $f^{-1}(\operatorname{Spec} G)$). This makes the iterative properties of f important. Consider

$$\Lambda = \bigcap_{m=0}^{\infty} f^{-m}([-3, 3]). \tag{6.2}$$

We will start by proving some general facts about sets invariant under some function. Let $g : \mathbb{R} \to \mathbb{R}$ and C non-empty bounded subset of $\mathbb{R}$ be such that for $x \notin C$, $g^n(x) \notin C$ and is unbounded as $n \to \infty$. Let

$$K = \bigcap_{m=0}^{\infty} g^{-m}(C).$$

Proposition 6.4. *K is the unique largest bounded set closed under g (meaning $g(K) \subseteq K$). Furthermore if $C \subseteq g(\mathbb{R})$ and is closed, then K is non-empty.*

Proof. Clearly no bounded g-closed set can contain any $x \notin C$. As a consequence, no bounded g-closed set can contain any x where $g^n(x) \notin C$. Thus suppose K' is some bounded set where $g(K') \subseteq K'$, then $K' \subseteq K$. Now it suffices to prove that K is indeed g-closed, i.e. $g(x) \in K$ for $x \in K$, but this is clear from the definition of K (since $g^n(g(x)) = g^{n+1}(x) \in C$). Since $g^m(x) \notin C \implies g^{m+1} \notin C$, $g^{-m-1}(C) \subseteq g^{-m}(C)$ which means that if $C \subseteq g(\mathbb{R})$, then $g^{-m+1}(C) \subseteq g(\mathbb{R})$ so $g^{-m}(C)$ is non-empty for $m \in \mathbb{N}$ and compact, so $K \neq \varnothing$. □

Corollary 6.5. *K is the unique largest bounded set invariant under g (meaning $g(K) = K$)*

Proof. Since any g-invariant set is necessarily g-closed, by 6.4 it suffices to prove that K itself is g-invariant. Note that we already have $g(K) \subseteq K \iff K \subseteq g^{-1}(K)$. For any $x \in g^{-1}(K)$, note $g(x) \in K \subseteq g^{-1}(K)$, so $g^{-1}(K)$ is g-closed, so $g^{-1}(K) \subseteq K$ and we are done. □

Now we take $g = f$, $C = [-3, 3]$ and $K = \Lambda$. Then it suffices to show that $x \notin [-3, 3]$ has $f(x) \notin [-3, 3]$ and $f^n(x) \to \infty$. Note that for $\epsilon > 0$, we have

$$f(3 + \epsilon) = (3 + \epsilon)^2 - 6 - \epsilon = 3 + 5\epsilon + \epsilon^2$$

so taking $5\epsilon + \epsilon^2$ as the new ϵ, since $5(5^n\epsilon + \epsilon^2) > 5^{n+1}\epsilon$ we inductively have $f^n(3 + \epsilon) > 3 + 5^n\epsilon \xrightarrow{n\to\infty} \infty$. For any $x < -3$, note $f(x) > x^2$ so $f^n(x) > x^{2n} \to \infty$ (and obviously $f(x) > 3$). Thus 6.4 and 6.5 apply to f and Λ.

In fact, taking $C = [-2, 3]$ would produce the same Λ, since

$$f(-2 - \epsilon) = (-2 - \epsilon)^2 - 1 + \epsilon = 3 + 5\epsilon + \epsilon^2$$

so $f(-2 - \epsilon) > 3$ so by the above, we have $f^n(-2 - \epsilon) \to \infty$ and everything applies. Now we show some properties of Λ.

Proposition 6.6. *Let $C_n = f^{-n}([-2, 3])$ be the n-th step in the construction of Λ ($n \geq 0$). Then C_n is made of 2^n disjoint (non-singleton) intervals. Furthermore, each endpoint x in C_n is also an endpoint in C_{n+1}.*

Proof. Note that since the minimum of f is $f(1/2) = -3 - 1/4$ which is smaller than all our intervals, each interval has two intervals as pre-images (and disjoint sets have disjoint pre-images) so C_n consists of precisely 2^n intervals.

Any interval $[a, b]$ *in* C_n, $n \geq 1$ (meaning $[a, b] \subseteq C_n$ and $a - \epsilon, b + \epsilon \notin C_n$ for all ϵ small enough) must have $f([a, b])$ being an interval in C_{n-1}, since $f([a, b]) \subseteq C_{n-1}$ and $f(a) \pm \epsilon \in C_{n-1} \implies a \pm \delta \in C_n$ for δ small enough (analogous for $f(b)$), and $f([a, b])$ is an actual interval since f is monotonic on $[a, b]$.

Thus if x were an endpoint of some interval in C_n, then $f^m(x)$ is an endpoint in C_{n-m} so $x \in \Lambda$, since $f^n(x) \in \{-2, 3\}$ so $f^m(x) = 3$ for $m > n$. This means $x \in C_{n+1}$, which forces x to be an endpoint, since $C_{n+1} \subseteq C_n$. □

Corollary 6.7. *Λ is uncountable.*

Proof. 6.6 showed that, since $C_{n+1} \subseteq C_n$ and has twice as many intervals, with one of the endpoints of each interval matching with endpoints of intervals in C_n and all the intervals in C_{n+1} being subsets of those in C_n, each interval in C_n must have been split into two intervals in C_{n+1}. The proof of uncountability then is exactly the same as the one for the Cantor set. □

7 The chromatic polynomial

In this section, we deal with general graphs rather than simple graphs. By an *r-color partition* of G, we mean a partitioning of $V(G)$ into $\{V_1, \ldots, V_r\}$ such that no $v \in V_i$ and $u \in V_j$ are adjacent for $i \neq j$. In other words, an r-color partition can define an r-coloring of G.

Definition 7.1. Given G (general) graph on n vertices and given $u \in \mathbb{C}$, for each $r \in \mathbb{N}$ let $m_r(G)$ denote the number of r-color partitions of G and let $u_{(r)}$ denote $u(u-1)(u-2)\cdots(u-r+1)$. We define the *chromatic polynomial* of G to be

$$C_G(u) = \sum_{r=1}^{n} m_r(G) u_{(r)}.$$

Proposition 7.2. *If $s \in \mathbb{N}$, then $C_G(s)$ is the number of colorings of G using at most s colors.*

Proof. We claim that $m_r(G)s_{(r)}$ is precisely the number of s-colorings of G after an r-color partition (i.e. using precisely r colors). If $r > s$ then there are no s-colorings allowed, and indeed $s_{(r)} = 0$ if and only if $s \in \mathbb{N}$ and $s < r$. If $r \leq s$ then $s_{(r)} = \binom{s}{r} r!$ and indeed, for each r-color partition, we have $\binom{s}{r}$ ways of choosing r colors out of s options, and then $r!$ ways of permuting r colors across the color classes. □

Arguably the simplest graph to compute the chromatic polynomial on is the complete graph.

Example 7.3. Since K_n has no color partition using less than n color classes, $m_1(K_n) = \cdots = m_{n-1}(K_n) = 0$ and $m_n(K_n) = 1$, thus

$$C_{K_n}(u) = u(u-1)\cdots(u-n+1)$$

and we can observe that this is indeed the number of ways to assign n colors out of u options to color K_n.

Note that the chromatic polynomial is indeed a polynomial since each $u_{(r)}$ is a polynomial. Its degree is no more than n. Since $m_n(G) = 1$, C_G is monic.

For G disconnected with components G_1 and G_2, for each way to color G_1 in $s \in \mathbb{N}$ colors or less paired with each way to s-color G_2, we have a distinct way to color G and vice versa. Thus we have, by 7.2,

$$C_G(s) = C_{G_1}(s) C_{G_2}(s).$$

Since a polynomial is uniquely determined by its values on $\mathbb{N}$, we have

$$C_G = C_{G_1} C_{G_2}.$$

Since u is a factor in $u_{(r)}$ for all $r \geq 1$, we have $C_G(0) = 0$ for any G (i.e. the coefficient of $1 = u^0$ is 0). If G has c components, then the coefficients of $u^0, u^1, \ldots, u^{c-1}$ are all 0 due to $C_G = \prod_{i=1}^{c} C_{G_i}$ where each C_{G_i} has coefficient 0 on u^0. Finally, if $E(G) \neq \varnothing$ then $m_1(G) = 0$ and $C_G(1) = 0$ and $u - 1$ is a factor of C_G.

Note that the problem of finding zeros of C_G encompasses the problem of finding the *chromatic number* of G, $\chi(G)$, since the smallest natural number that is not a zero of C_G *is* $\chi(G)$.

Now we discuss some techniques of calculating chromatic polynomials.

Definition 7.4. Suppose $e \in E(G)$ is not a loop. We define $G^{(e)}$ to be the graph with $V(G^{(e)}) = V(G)$ and $E(G^{(e)}) = E(G) \setminus e$ and say that $G^{(e)}$ is obtained from G by *deleting* e. We define $G_{(e)}$ to be the graph with e removed and with the two vertices incident to e identified as one vertex and say that $G_{(e)}$ is obtained from G by *contracting* e.

Note that $G^{(e)}$ has one edge fewer than G and $G_{(e)}$ has one edge and one vertex fewer than G. Thus the following proposition provides a method to compute the chromatic polynomial by repeated reduction to smaller graphs. This is known as the *deletion-contraction* method.

Proposition 7.5.

$$C_G = C_{G^{(e)}} - C_{G_{(e)}}.$$

Proof. We show $C_{G^{(e)}} = C_G + C_{G_{(e)}}$. Indeed for each way of coloring $G^{(e)}$, either the vertices incident to e in G are *not* colored the same, thus corresponding to a coloring of G, or they *are*, thus corresponding to a coloring of $G_{(e)}$. Thus $C_{G^{(e)}}(s) = C_G(s) + C_{G_{(e)}}(s)$ on $s \in \mathbb{N}$ and the general equality follows. □

We use 7.5 to obtain the general formula for C_T when T is a tree:

Corollary 7.6. *If T is a tree with n vertices, then*

$$C_T(u) = u(u-1)^{n-1}.$$

Proof. We use induction on n to prove $C_T(u) = u(u-1)^{n-1}$. $n = 1$ is trivial since there are s ways to s-color one vertex. Assume it is true for $n = N$ and let T be a tree with $N+1$ vertices. It is known that T has at least one vertex of degree 1 (in fact, at least two vertices) so call it v. Let e be the edge attaching v to the rest of T. Let $T' = \langle V(T) \setminus \{v\} \rangle$ and note that T' is a tree with N vertices, so by IH $C_{T'}(u) = u(u-1)^{N-1}$. Then note $T_{(e)} = T'$ so

$$C_{T_{(e)}}(u) = C_{T'}(u) = u(u-1)^{N-1}.$$

$T^{(e)}$ has disconnected components $\langle \{v\} \rangle$ and T' so

$$C_{T^{(e)}}(u) = C_{\langle \{v\} \rangle}(u) C_{T'}(u) = u(u(u-1)^{N-1}).$$

Thus by 7.5

$$C_T = C_{T^{(e)}} - C_{T_{(e)}} = u(u-1)^{N-1}(u-1) = u(u-1)^N.$$

□

We can apply 7.5 and 7.6 together to obtain the general formula for C_{C_n}.

Example 7.7. $C_{C_1} \equiv 0$. When $n \geq 2$, let $e \in E(C_n)$, then $C_{n,(e)} = C_{n-1}$ and $C_n^{(e)} = P_n$ so

$$\begin{aligned} C_{C_n}(u) &= C_{C_n^{(e)}}(u) - C_{C_{n,(e)}}(u) = C_{P_n}(u) - C_{C_{n-1}}(u) = u(u-1)^{n-1} - C_{C_{n-1}}(u) \\ &= (u-1)^n - (C_{C_{n-1}}(u) - (u-1)^{n-1}). \end{aligned}$$

We note that $C_{C_n}(u) - (u-1)^n = -(C_{C_{n-1}}(u) - (u-1)^{n-1}) \forall n \geq 2$ so we know

$$C_{C_n}(u) = (u-1)^n + (-1)^n f(u)$$

for some $f(u)$ independent of n. Since the base case is $C_{C_1} = 0 = u - 1 + (-1)(u-1)$, we know $f(u) = u - 1$ so

$$C_{C_n}(u) = (u-1)^n + (-1)^n (u-1).$$

Now we describe two additional methods of calculating chromatic polynomials. The first is based on a *join* operation for graphs:

Definition 7.8. Let G_1, G_2 be graphs (with $V(G_1) \cap V(G_2) = \varnothing$). We define their *join* $G_1 + G_2$ to be the graph with

$$V(G_1 + G_2) = V(G_1) \cup V(G_2)$$

and

$$E(G_1 + G_2) = E(G_1) \cup E(G_2) \cup \{(u, v) : u \in V(G_1), v \in V(G_2)\}.$$

In other words, $G_1 + G_2$ contains G_1 and G_2 as disjoint subgraphs and edges joining all vertices between them, and nothing else.

Proposition 7.9. *Suppose $G = G_1 + G_2$, then*

$$m_r(G) = \sum_{i+j=r} m_i(G_1) m_j(G_2).$$

Proof. For each r-color partition of G, the colors used on G_1 and G_2 must be disjoint, so G_1 must have an i-color partition and G_2 a j-color partition such that $i + j = r$ and conversely any such pair indeed gives an r-color partition of G. □

This directly give us the following formula for computing chromatic polynomials of joins:

Corollary 7.10. *Define*

$$\sum_{r=1}^{n} m(r) u_{(r)} \circ \sum_{s=1}^{\ell} m(s) u_{(s)} = \sum_{r=1}^{n} \sum_{s=1}^{\ell} m(r) m(s) u_{(r+s)} = \sum_{t=1}^{m+n} \sum_{r+s=t} m(r) m(s) u_{(t)}.$$

Then

$$C_{G_1+G_2} = C_{G_1} \circ C_{G_2}.$$

Here use 7.10 to derive $C_{K_{3,3}}$:

Example 7.11. Note that $K_{3,3} = N_3 + N_3$, where N_k defines a graph with k vertices and no edges. Since there are 3 ways to partition a set of 3 elements into 2 classes, note

$$C_{N_3}(u) = u_{(1)} + 3u_{(2)} + u_{(3)}.$$

Thus

$$\begin{aligned} C_{K_{3,3}}(u) = C_{N_3}(u) \circ C_{N_3}(u) &= (u_{(1)} + 3u_{(2)} + u_{(3)}) \circ (u_{(1)} + 3u_{(2)} + u_{(3)}) \\ &= u_{(2)} + 3u_{(3)} + u_{(4)} + 3u_{(3)} + 9u_{(4)} + 3u_{(5)} + u_{(4)} + 3u_{(5)} + u_{(6)} \\ &= u_{(2)} + 6u_{(3)} + 11u_{(4)} + 6u_{(5)} + u_{(6)}. \end{aligned}$$

Theoretically, we can apply the same argument to all $K_{n,m}$ and algorithmically find its chromatic polynomial. However note that there is no known closed-form expression for the number of ways to partition k elements into r classes, so we cannot obtain a closed-form $C_{K_{n,m}}$ this way for all $n, m \in \mathbb{N}$.

Another application of 7.10 relates the chromatic polynomial of G with that of $N_1 + G$, called the *cone* of G and denoted $c(G)$, and $N_2 + G$, called the *suspension* of G and denoted $s(G)$.

Proposition 7.12. *The chromatic polynomial of a cone and a suspension are given by*

$$C_{c(G)}(u) = uC_G(u-1), \tag{7.1}$$
$$C_{s(G)}(u) = u(u-1)C_G(u-2) + uC_G(u-1). \tag{7.2}$$

Proof. Note $C_{N_1} = u_{(1)}$ and $C_{N_2} = u_{(1)} + u_{(2)}$. (7.1) is due to 7.10 and the fact that $u_{(r+1)} = u(u-1)_{(r)}$, so

$$C_{c(G)}(u) = u_{(1)} \circ C_G(u) = uC_G(u-1).$$

(7.2) is similar, using $u_{(r+2)} = u(u-1)(u-2)_{(r)}$, so

$$C_{s(G)}(u) = (u_{(1)} + u_{(2)}) \circ C_{s(G)}(u) = u(u-1)C_G(u-2) + uC_G(u-1).$$ □

The second technique applies to graphs described as follows:

Definition 7.13. The (general) graph G is *quasi-separable* if there is $K \subseteq V(G)$ such that the induced subgraph $\langle K \rangle$ is complete but $\langle V(G) \setminus K \rangle$ is disconnected. G is *separable* if $|K| \leq 1$; in this case either $K = \varnothing$ so G is in fact disconnected, or $|K| = 1$, in which case we call $v \in K$ a *cut-vertex*.

It follows that by taking each of the disconnected components and unioning each with K, we can get $V_1, V_2 \subseteq V(G)$ such that $V_1 \cup V_2 = V(G)$, $V_1 \cap V_2 = K$ and there are no edges between $V_1 \setminus K$ and $V_2 \setminus K$. We call (V_1, V_2) a *quasi-separation*, or a *separation* if $|K| \leq 1$.

The following reduces the chromatic polynomial of a graph with quasi-separation (V_1, V_2) to the chromatic polynomials of $\langle V_1 \rangle$, $\langle V_2 \rangle$ and $\langle V_1 \cap V_2 \rangle$:

Proposition 7.14. *If G has quasi-separation (V_1, V_2), then*

$$C_G = \frac{C_{\langle V_1 \rangle} C_{\langle V_2 \rangle}}{C_{\langle V_1 \cap V_2 \rangle}}$$

with the convention that $C_{\langle \varnothing \rangle}(u) = 1$.

Proof. If $V_1 \cap V_2 = \varnothing$, then G is disjoint and the result follows a previous remark about 7.2. Suppose that $\langle K \rangle = \langle V_1 \cap V_2 \rangle \cong K_t$ with $t \geq 1$. Let $s \in \mathbb{N}$.

Due to the fact that all colorings on $\langle K_t \rangle$ are isomorphic (i.e. one can bijectively map each color to some other color to go from one coloring to another), each coloring on $\langle K \rangle$ can be extended in $C_G(s)/s_{(t)}$ ways to a coloring in G (because there exists a bijection between extensions starting from different colorings of $\langle K \rangle$). Since $K_t \subseteq \langle V_1 \rangle, \langle V_2 \rangle$, the same argument applies to $C_{\langle V_1 \rangle}(s)/s_{(t)}$ and $C_{\langle V_2 \rangle}(s)/s_{(t)}$.

Because $\langle V_1 \setminus K \rangle$ and $\langle V_2 \setminus K \rangle$ have no edges between them, extensions for $\langle V_1 \rangle$ and $\langle V_2 \rangle$ starting from the same coloring on K_t are independent, hence

$$\begin{aligned}
\frac{C_G(s)}{s_{(t)}} &= \frac{C_{\langle V_1 \rangle}(s)}{s_{(t)}} \frac{C_{\langle V_1 \rangle}(s)}{s_{(t)}} \\
\implies C_G(s) &= \frac{C_{\langle V_1 \rangle}(s) C_{\langle V_1 \rangle}(s)}{s_{(t)}} = \frac{C_{\langle V_1 \rangle}(s) C_{\langle V_1 \rangle}(s)}{C_{\langle V_1 \cap V_2 \rangle}(s)} \\
\implies C_G &= \frac{C_{\langle V_1 \rangle} C_{\langle V_2 \rangle}}{C_{\langle V_1 \cap V_2 \rangle}}.
\end{aligned}$$

□

7.14 is often useful for finding chromatic polynomials of small graphs for which the subgraphs induced by the quasi-separation are well-known. The following is an example:

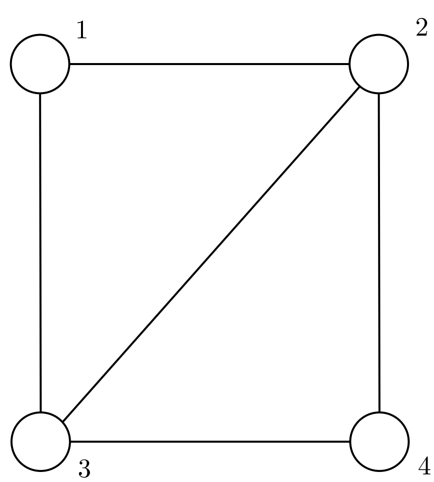

Figure 2: G separable with $V_1 = \{1, 2, 3\}$ and $V_2 = \{2, 3, 4\}$

Example 7.15. Consider the graph in Figure 2. Under the given separation and using the fact that $\langle V_1\rangle \cong \langle V_2\rangle \cong K_3$ while $\langle V_1 \cap V_2\rangle \cong K_2$, we get

$$C_G(u) = \frac{C_{\langle V_1\rangle}(u)C_{\langle V_2\rangle}(u)}{C_{\langle V_1\cap V_2\rangle}(u)} = \frac{(u(u-1)(u-2))^2}{u(u-1)} = u(u-1)(u-2)^2.$$

Note that there are other ways to compute C_G. For example, G can also be viewed as cP_3, in other words $N_1 + P_3$ where $V(N_1) = \{3\}$ and $V(P_3) = \{1,2,4\}$, in which case

$$C_G(u) = uC_{P_3}(u-1) = u(u-1)(u-2)^2.$$

8 Bounds on the complex zeros of chromatic polynomials

This section consists of notes on a paper by Sokal 2000.

8.1 Introduction

We have previously introduced (in 7) the chromatic polynomial for (general) graph G. For each $e \in E$ let $v_e \in \mathbb{C}$. Then we define (let $s \in \mathbb{N}$, $x_e, y_e \in V$ be the two endpoints of e, $\mathbf{1}$ denote the indicator function, and product over the empty set understood to give 1)

$$Z_G(s, \{v_e\}) = \sum_{\sigma: V\to\{1,\dots,s\}} \prod_{e\in E} \left[1 + v_e\mathbf{1}\{\sigma(x_e) = \sigma(y_e)\}\right]. \tag{8.1}$$

We will show below (8.1) that (8.1) is the restriction of a polynomial to $\mathbb{N}\times\mathbb{C}^{|E|}$. If one takes $v_e = -1 \forall e \in E$, then

$$\prod_{e\in E} \left[1 - \mathbf{1}\{\sigma(x_e) = \sigma(y_e)\}\right] = \mathbf{1}\{\sigma(x_e) \neq \sigma(y_e) \forall e \in E\} = \mathbf{1}\{\sigma \text{ is an } s\text{-coloring of } V\}$$

so $Z_G(s, -1, \dots, -1) = C_G(s)$ is precisely the chromatic polynomial. If one takes $v_e = v \forall e \in E$ then the two-variable $Z_G(s, v)$ is called, up to some trivial transformation (see 8.2), the *dichromatic polynomial* or the *Tutte polynomial*.

Proposition 8.1. *$Z_G(s, \{v_e\})$ is a polynomial in its arguments with 1 as the only non-zero coefficient.*

Proof. First we expand the multiplication in (8.1) (E' is taken over all subsets of E):

$$\begin{aligned}
Z_G(s, \{v_e\}) &= \sum_\sigma \prod_{e\in E} \left[1 + v_e\mathbf{1}\{\sigma(x_e) = \sigma(y_e)\}\right] \\
&= \sum_\sigma \sum_{E'\subseteq E} \prod_{e\in E'} v_e\mathbf{1}\{\sigma(x_e) = \sigma(y_e)\} \\
&= \sum_\sigma \sum_{E'\subseteq E} \mathbf{1}\{\sigma(x_e) = \sigma(y_e) \forall e \in E'\} \prod_{e\in E'} v_e \\
&= \sum_{E'\subseteq E} |\{\sigma : \sigma(x_e) = \sigma(y_e) \forall e \in E'\}| \prod_{e\in E'} v_e.
\end{aligned}$$

Fix $E' \subseteq E$. For any σ, note that $\sigma(x_e) = \sigma(y_e) \forall e \in E'$ if and only if all components of the subgraph induced by E' are colored in the same color. Since each component would have s choices of colors, let $c(E')$ denote the number of components in the said subgraph, then there are $s^{c(E')}$ possibilities of σ for a given $E' \subseteq E$. Thus

$$Z_G(s, \{v_e\}) = \sum_{E' \subseteq E} s^{c(E')} \prod_{e \in E'} v_e. \tag{8.2}$$

□

Since (8.1) was only defined for $s \in \mathbb{N}$, we take (8.2) to be the *definition* of $Z_G(s, \{v_e\})$ for $s, \{v_e\} \in \mathbb{C}$. We now show the relationship between the two-variable $Z_G(s, v)$ (i.e. $v_e = v \forall e \in E$) and the conventional Tutte polynomial $T_G(x, y)$.

Corollary 8.2. *Define*

$$T_G(x, y) = \sum_{E' \subseteq E} (x-1)^{c(E')-c(E)} (y-1)^{|E'|+c(E')-|V|}.$$

Then

$$T_G(x, y) = (x-1)^{-c(E)} (y-1)^{-|V|} Z_G((x-1)(y-1), y-1).$$

Proof.

$$Z_G((x-1)(y-1), y-1) = \sum_{E' \subseteq E} (x-1)^{c(E')} (y-1)^{|E'|+c(E')}.$$

□

In the context of statistical mechanics, (8.1) is known as the *partition function* of the *s-state Potts model*[6]. In this model, each site $x \in V$ can exist in any of the $s \in \mathbb{N}$ different 'states' (e.g. spins). The energy of $e \in E$ is 0 if the states of the end points are unequal and $-J_e$ if they are equal, and we sum over all $e \in E$ to get $H(\sigma)$, the *energy* of a given configuration σ. The *Boltzmann weight* of σ is then $e^{-\beta H(\sigma)}$, where $\beta \geq 0$ is the inverse temperature[7]. The *partition function* is the sum of Boltzmann weights over all σ. It is easy to see that by taking $v_e = e^{\beta J_e} - 1 \forall e \in E$, the partition function is equivalent to (8.1). An *interaction* $e \in E$ is called *ferromagnetic* if $J_e > 0 \iff v_e > 0$, *antiferromagnetic* if $-\infty \leq J_e < 0 \iff -1 \leq v_e < 0$, and otherwise the ends of e are *non-interacting* (i.e. $J_e = 0 \iff v_e = 0$, equivalent to e being removed).

We remark that the partition function (provided it is non-zero) serves as a normalizing constant for the Boltzmann weights, such that

$$f_{G,s,\{v_e\}}(\sigma) = \frac{e^{-\beta H(\sigma)}}{Z_G(s, \{v_e\})}$$

is a probability distribution (called an *ensemble* in statistical mechanics) over possible configurations σ. In fact, complex zeros of Z_G are often particular interest, as explained below.

Often, one would want to study *phase transitions*, i.e. points where some physical quantities (e.g. energy) depend nonanalytically (or even discontinuously) on the parameters of the system (e.g. temperature or the magnetic field, i.e. J_e). Such points are impossible in (8.1) for any finite G, but they could arise in an *infinite-volume limit*, i.e. some limit G_∞ of increasing graphs G_i with $n(G_i) \to \infty$. Regular lattices such as the d-dimensional integer lattice are typical examples. It can then be shown (under modest assumptions on G_i) that the *(limiting) free energy per unit volume*

$$f_{G_\infty}(s, v) = \lim_{i \to \infty} |n(G_i)|^{-1} \log Z_{G_i}(s, v)$$

[6] The $s = 2$ case is known as the *Ising model*.

[7] $\beta = 1/(k_B T)$ where k_B is the *Boltzmann constant* and T is the temperature.

exists for all *nondegenerate physical*[8] values of the parameters, namely either

1. $s \in \mathbb{N}$ and $-1 < v < \infty$ (using (8.1)), or
2. $s > 0$ and $0 \leq v < \infty$ (using (8.2)).

The limit f_{G_∞} is in general continuous in v, but can fail to be real-analytic in v, because complex singularities of $\log Z_{G_i}$, i.e. complex zeros of Z_{G_i}, can approach the real axis as $i \to \infty$. Therefore the real limits of such zeros are precisely the points of interest when studying phase transitions, so theorems on the location of the zeros of the partition function are very important.[9]

The purpose of the paper was to give an upper bound on complex zeros of Z_G for v_e in the 'complex antiferromagnetic regime' $A = \{v \in \mathbb{C} : |1+v| \leq 1\}$, i.e. $|1+v_e| \leq 1$. This bound can be valid for infinite families of G, if some local conditions on v_e hold. A corollary is an upper bound on the zeros of the chromatic polynomial based on the maximum degree of G: for each $r \geq 0$, there exists $C(r)$ such that for any loopless G with maximum degree r, the zeros of $C_G(u)$ lie in $|u| < C(r)$. It is also proven that $C(r)$ grows at most linearly in r. Note that $C(r)$ grows at *least* linearly because $r+1$ is a root of $C_{K_{r+1}}$. An explicit bound of $C(r) \leq 7.963907r$ was given. Finally, with *one* vertex of degree exceeding r, the zeros of $C_G(u)$ are bounded by $|u| < C(r)+1$. It is known that the roots of C_G are unbounded when there are two such vertices.

These notes will discuss the bound on the zeros of Z_G for a fixed G under $|1+v_e| \leq 1$ as well as the corollary on C_G. We will also show that $C(r)$ grows at most linearly, but with a worse bound than the one given.

8.2 Transformation of the Potts-model partition function to a polymer gas

Let $G = (V, E)$ have complex edge weights $\{v_e\}_{e \in E}$. If e is a loop then by (8.1) its presence simply multiplies Z_G by $(1+v_e)$, thus WLOG we assume G is loopless.[10] For each $E' \subseteq E$, if we decompose (V, E') into connected components $S_1, \ldots, S_N$, note that $c(E') = \sum_{i=1}^N (1 + |S_i| - |S_i|) = |V| - \sum_{i=1}^N (|S_i| - 1)$.

Proposition 8.3. *Let $G = (V, E)$ be loopless with edge weights $\{v_e\}_{e \in E}$. Then*

$$Z_G(s, \{v_e\}) = s^{|V|} Z_{\text{polymer}, G}(s, \{v_e\}), \tag{8.3}$$

where

$$Z_{\text{polymer},G}(s, \{v_e\}) = \sum_{N=0}^{\infty} \frac{1}{N!} \sum_{\bigsqcup_{i=1}^N S_i \subseteq V} \prod_{i=1}^N w(S_i) \tag{8.4}$$

and where

$$w(S) = \begin{cases} s^{-(|S|-1)} \sum_{E' \subseteq E_S,\, (S,E') \text{ connected}} \prod_{e \in E'} v_e & |S| \geq 2 \\ 0 & |S| \leq 1 \end{cases} \tag{8.5}$$

In particular note $w(S) = 0$ if (S, E_S) is not connected, i.e. if S is not the subset of a connected component.

[8] 'nondegenerate' excludes cases $v = -1$ (using (8.1)), which causes some σ to have weight 0, and $s = 0$ (using (8.2)); 'physical' means that v is such that there are no negative terms in the outmost summation, allowing a probability distribution to exist

[9] In particular, theorems that guarantee a certain complex region is free of zeros are known as *Lee-Yang theorems*.

[10] A similar argument can be made for parallel edges $e_1, \ldots, e_n$, which can be replaced by a single edge e with weight $\prod_{i=1}^n (1 + v_{e_i}) - 1$ and get the same Z_G. However this does not simplify much so we will not be assuming there be no parallel edges.

Proof. Clearly we only need to consider $\bigsqcup_{i=1}^{N} S_i = S \subseteq V$ where each (S_i, E_{S_i}) is connected and where each $|S_i| > 1$, due to which $E_{S_i} \neq \varnothing$. In that case

$$\prod_{i=1}^{N} w(S_i) = \prod_{i=1}^{N} s^{-(|S_i|-1)} \sum_{\substack{E' \subseteq E_{S_i}, \\ (S_i, E') \text{ connected}}} \prod_{e \in E'} v_e = \sum_{\substack{E' = \bigsqcup_{i=1}^{N} E'_i : \\ E'_i \subseteq E_{S_i}, \\ (S_i, E'_i) \text{ connected}}} s^{-\sum_{i=1}^{N}(|S_i|-1)} \prod_{e \in E'} v_e.$$

Note that since $|S| - \sum_{i=1}^{N}(|S_i|-1) = N$ which is the number of components in (S, E'), and there are precisely $|V| - |S|$ more components in (V, E') than in (S, E'), we have $c(E') = |V| - \sum_{i=1}^{N}(|S_i| - 1)$. Thus (8.3) is

$$s^{|V|} Z_{\text{polymer}, G}(s, \{v_e\}) = \sum_{N=0}^{\infty} \frac{1}{N!} \sum_{\bigsqcup_{i=1}^{N} S_i = S \subseteq V} \sum_{\substack{E' = \bigsqcup_{i=1}^{N} E'_i : \\ E'_i \subseteq E_{S_i}, \\ (S_i, E'_i) \text{ connected}}} s^{c(E')} \prod_{e \in E'} v_e. \tag{8.6}$$

For each $E' \subseteq E$ such that (V, E') has N components $S_1, \ldots, S_N$ where each $|S_i| > 1$, there are precisely $N!$ possible ways to permute those S_i such that $S_1, \ldots, S_N$ are still the connected components of (S, E'), so such E' appears throughout the summation in (8.6) exactly $N!$ times. By summing across all N, we taking into account every possible $E' \subseteq E$ so

$$s^{|V|} Z_{\text{polymer}, G}(s, \{v_e\}) = \sum_{E' \subseteq E} s^{c(E')} \prod_{e \in E'} v_e = Z_G(s, \{v_e\}). \qquad \square$$

The 'polymer model' (8.4) has the form of a *grand-canonical gas* (8.4)

$$Z_{\text{polymer},G}(s, \{v_e\}) = \sum_{N=0}^{\infty} \frac{1}{N!} \sum_{S_1, \ldots, S_N \subseteq V} \prod_{i=1}^{N} w(S_i) \prod_{1 \leq i,j \leq N} \mathbf{1}\{S_i \cap S_j = \varnothing\} \tag{8.7}$$

with *single-particle state space* $\mathscr{P}_*(V)$ (non-empty subsets of V, or, equivalently, due to how $w(S)$ was defined, $S \subseteq V$ with $|S| \geq 2$ and connected (S, E_S)), *fugacities* $w(S)$ and *two-particle Boltzmann factor* $\mathbf{1}\{S_i \cap S_j = \varnothing\}$.

If we define an *exponential generating function* (EGF) in M variables w.r.t. sequence $\{a(n_1, \ldots, n_M)\}_{n_i \in \mathbb{N}}$ as

$$G(\{a_n\}, x_1, \ldots, x_M) = \sum_{N=0}^{\infty} \frac{1}{N!} \sum_{\sum_{m=1}^{M} n_m = N} a(n_1, \ldots, n_M) \prod_{m=1}^{M} x_m^{n_m}, \tag{8.8}$$

then (8.7) is precisely (8.8) with $M = |\mathscr{P}_*(V)|$ with each m associated to some $S \in \mathscr{P}_*(V)$, $x_S = w(S) \forall S \in \mathscr{P}_*(V)$ and $a(\{n_S\}_{S \in \mathscr{P}_*(V)})$ is an indicator function for the following: $n_S = 1$ or $n_S = 0$ for each S, and $S \cap S' = \varnothing$ for each S, S' where $n_S, n_{S'} = 1$. (8.7) is thus the generating function for independent sets in the intersection graph constructed from $\mathscr{P}_*(V)$ with variables $w(S)$.

We remark that since $-(|S| - 1) \leq -1$ when $w(S) \neq 0$, $w(S)$ decreases in s. Thus if the sum over E' can be controlled, one can expect an exponential decay of $w(S)$ in $|S|$ provided s is large enough so that the exponential decay overshadows the increase in the sum over E'. Thus as we show that $Z_{\text{polymer},G}$ does not vanish for small enough $w(S)$, we have reason to believe that the same is true for large enough s. This essentially outlines the following sections, but in the opposite order.

8.3 Dobrushin and Kotechý-Preiss conditions for the nonvanishing of Z

Definition 8.4. A *grand-canonical gas* is defined by a *single-particle state space* X (here finite), a *fugacity vector* $\mathbf{w} = \{w_x\}_{x\in X} \in \mathbb{C}^{|X|}$ and a symmetric *two-particle Boltzmann factor* $W : X \times X \to \mathbb{C}$. The (grand) partition function $z(\mathbf{w}, W)$ is then defined to be the sum over ways of placing $N \geq 0$ *particles* on *sites* $x_1, \ldots, x_N \in X$, with each configuration given a *Boltzmann weight*, which is the product over all w_{x_i} and $W(x_i, x_j)$ (for $i \neq j$):

$$Z(\mathbf{w}, W) = \sum_{N=0}^{\infty} \frac{1}{N!} \sum_{x_1,\ldots,x_N \in X} \prod_{i=1}^{N} w_{x_i} \prod_{1\leq i<j\leq N} W(x_i, x_j). \tag{8.9}$$

Under weak assumptions on W (e.g. $|W(x, y)| \leq 1$ like in (8.7)) $Z(\mathbf{w}, W)$ is analytic in $\mathbf{w}$. We want to find a sufficient condition for $Z(\mathbf{w}, W)$ to be nonvanishing in a polydisc $D_R = \{\mathbf{w} : |w_x| < R_x\}$. This would imply in particular that $\log Z(\mathbf{w}, W)$ is analytic in D_R.

Note that if W were *hard-core self-repulsive*, i.e. $W(x, x) = 0 \forall x \in X$, then we only need to consider summation over distinct x_i, i.e. (8.9) would be equivalent to summing over subsets:

$$Z(\mathbf{w}, W) = \sum_{X'\subseteq X} \prod_{x\in X'} w_x \prod_{\{x,y\}\subseteq X'} W(x, y).$$

Under this assumption, we introduce the notation where, for each $\Lambda \subseteq X$, we write[11]

$$Z_\Lambda(\mathbf{w}, W) = \sum_{X'\subseteq \Lambda} \prod_{x\in X'} w_x \prod_{\{x,y\}\in X'} W(x, y). \tag{8.10}$$

Now we give an extension of a theorem due to Dobrushin:

Theorem 8.5 (Extension to Dobrushin)**.** *Let X be finite and let W satisfy*

1. $0 \leq W(x, y) \leq 1 \forall x, y \in X$;
2. $W(x, x) = 0 \forall x \in X$).

Suppose for each $x \in X$, there exists $R_x \geq 0$ and $0 \leq K_x < 1/R_x$ satisfying

$$K_x \geq \prod_{y\in X: y\neq x} \frac{1 - W(x, y)K_y R_y}{1 - K_y R_y}. \tag{8.11}$$

Then, for each $\Lambda \subseteq X$, $Z_\Lambda(\mathbf{w}, W)$ is nonvanishing in the closed polydisc $\overline{D_R} = \{\mathbf{w} \in \mathbb{C}^{|X|} : |w_x| \leq R_x\}$ and satisfies in $\overline{D_R}$

$$\left|\frac{\partial \log Z_\Lambda(\mathbf{w}, W)}{\partial w_x}\right| \leq \begin{cases} \frac{K_x}{1-K_x|w_x|} & x \in \Lambda, \\ 0 & x \in X \setminus \Lambda. \end{cases} \tag{8.12}$$

Moreover, given $\mathbf{w}, \mathbf{w}' \in \overline{D}_R$ such that $\mathbf{w}'_x/\mathbf{w}_x \in [0, \infty] \forall x \in X$, by integration, one can get[12]

$$\left|\log \frac{Z_\Lambda(\mathbf{w}', W)}{Z_\Lambda(\mathbf{w}, W)}\right| \leq \sum_{x\in\Lambda} \left|\log \frac{1 - K_x|w'_x|}{1 - K_x|w_x|}\right|. \tag{8.13}$$

[11] Note that this is equivalent to setting $w_x = 0$ for $x \notin \Lambda$.

We remark that since $W(x,y)K_yR_y \le K_yR_y$, by (8.11) we have $K_x \ge 1$ and thus $R_x < 1$.

Proof. On any Λ, (8.12) implies (8.13) because let $\mathbf{w}(t) : [0,1] \to \mathbb{C}^{|X|}, t \mapsto \mathbf{w}(1-t) + \mathbf{w}'t$, then $\mathbf{w}(0) = \mathbf{w}$ and $\mathbf{w}(1) = \mathbf{w}'$ and note $|\frac{\partial w_x}{t}| = |w'_x - w_x| = ||w'_x| - |w_x|| = |\frac{\partial |w_x|}{\partial t}|$, thus

$$\begin{aligned}
\left|\frac{\partial}{\partial t}\log Z_\Lambda(\mathbf{w}(t), W)\right| &= \left|\sum_{x\in X}\frac{\partial \log Z_\Lambda(\mathbf{w}, W)}{\partial w_x}\frac{\partial w_x}{\partial t}\right| \le \sum_{x\in X}\left|\frac{\partial \log Z_\Lambda(\mathbf{w}, W)}{\partial w_x}\frac{\partial w_x}{\partial t}\right| \\
&\le \sum_{x\in X}\frac{K_x}{1-K_x|w_x|}\left|\frac{\partial |w_x|}{\partial t}\right| = \sum_{x\in X}\left|\frac{\partial}{\partial t}\log(1-K_x|w_x(t)|)\right| \\
\implies \left|\int_0^1 \frac{\partial}{\partial t}\log Z_\Lambda(\mathbf{w}(t), W)dt\right| &\le \sum_{x\in X}\int_0^1\left|\frac{\partial}{\partial t}\log(1-K_x|w_x(t)|)\right|dt \\
\implies \left|\log\frac{Z_\Lambda(\mathbf{w}', W)}{Z_\Lambda(\mathbf{w}, W)}\right| &\le \sum_{x\in\Lambda}\left|\log\frac{1-K_x|w'_x|}{1-K_x|w_x|}\right|.
\end{aligned}$$

The rest of the proof is by induction on the cardinality Λ. The claim is vacuously true for $\Lambda = \varnothing$. Assume (8.12) (and thus (8.13)) hold for all sets with cardinality less than $n \in \mathbb{N}$ and let $|\Lambda| = n$. Let $X \in \Lambda$ and let $\Lambda' = \Lambda \setminus \{x\}$. Then from (8.10), by breaking down the summation over $X' \subseteq \Lambda$ into X' containing x and those that do not, we get

$$Z_\Lambda(\mathbf{w}, W) = w_x Z_{\Lambda'}(\tilde{\mathbf{w}}, W) + Z_{\Lambda'}(\mathbf{w}, W) \tag{8.14}$$

where $\tilde{w}_y = W(x,y)w_y$, so

$$w_x Z_{\Lambda'}(\tilde{\mathbf{w}}, W) = \sum_{X':x\notin X'} w_x \prod_{y\in X'} w_y W(x,y) \prod_{\{y,y'\}\in X'} W(y,y') = \sum_{X':x\in X'}\prod_{y\in X'} w_y \prod_{\{y,y'\in X'\}} W(y,y').$$

We note $\tilde{\mathbf{w}} \in \overline{D_R}$ since $|W(x,y)| \le 1$. From (8.14) we directly get

$$\frac{\partial}{\partial w_x}\log Z_\Lambda(\mathbf{w}, W) = \frac{Z_{\Lambda'}(\tilde{\mathbf{w}}, W)}{w_x Z_{\Lambda'}(\tilde{\mathbf{w}}, W) + Z_{\Lambda'}(\mathbf{w}, W)} = \frac{k(w)}{k(w)w_x + 1}$$

where $k(w) = \frac{Z_{\Lambda'}(\tilde{\mathbf{w}}, W)}{Z_{\Lambda'}(\mathbf{w}, W)}$. Finally since $\tilde{w}_y/w_y = W(x,y) \ge 0$, by IH we can apply (8.13) to bound $|k(w)|$ with

$$|k(w)| \le \prod_{y\in\Lambda'}\frac{1-K_y|\tilde{w}_y|}{1-K_y|w_y|} = \prod_{y\in\Lambda'}\frac{1-K_yW(x,y)|w_y|}{1-K_y|w_y|} \le \prod_{y\in X\setminus x}\frac{1-K_yW(x,y)|w_y|}{1-K_y|w_y|}. \tag{8.15}$$

Note

$$\frac{1-K_yW(x,y)|w_y|}{1-K_y|w_y|} \le \frac{1-K_yW(x,y)R_y}{1-K_yR_y} \iff -K_yR_y \le -K_y|w_y|$$

which is true so by (8.11) $|k(w)| \le K_x$. Note $\frac{|k(w)|}{|k(w)w_x+1|} \le \frac{|k(w)|}{1-|k(w)||w_x|}$ and similarly to the above

$$\frac{|k(w)|}{1-|k(w)||w_x|} \le \frac{K_x}{1-K_x|w_x|} \iff |k(w)| \le K_x$$

so (8.12) is proven and we are done. ☐

[12] $\log z$ denotes the *principal value* of $z \neq 0$, i.e. the logarithm where $\operatorname{Im}\log z \in [-\pi, \pi]$, i.e. $\log(x+yi) = \log\sqrt{x^2+y^2} + i\,\mathrm{atan2}(x,y)\forall x, y \in \mathbb{R}, xy \neq 0$.

Now we restrict to W being a *hard-core* interaction, i.e. $W(x,y) \in \{0,1\} \forall x, y \in X$ (while still being hard-core self-repulsive). If $W(x,y) = 0$ (resp. 1), we say x and y are *incompatible* (resp. *compatible*) and write $x \not\sim y$ (resp. $x \sim y$). In particular $x \not\sim x$. The hypothesis of 8.5, (8.11), is then equivalent to

$$K_x \geq \prod_{y \sim x} \frac{1 - W(x,y)K_y R_y}{1 - K_y R_y} \prod_{y \neq x : y \not\sim x} \frac{1 - W(x,y)K_y R_y}{1 - K_y R_y} = \prod_{y \neq x : y \not\sim x} \frac{1}{1 - K_y R_y}$$
$$\iff \prod_{y \not\sim x} (1 - K_y R_y) \frac{K_x R_x}{1 - K_x R_x} = \prod_{y \not\sim x} (1 - K_y R_y) \left(\frac{1}{1 - K_x R_x} - 1 \right) \geq R_x.$$

Thus if $c_x = -\log(1 - K_x R_x) \geq 0 \forall x \in X$ then (8.11) is equivalent to finding $c_x \geq 0$ such that

$$\exp\left[-\sum_{y \not\sim x} c_y \right] (e^{c_x} - 1) \geq R_x \forall x \in X.$$

This is the *Dobrushin condition.* Since $e^{c_x} - 1 \geq c_x$, a stronger and more convenient to check condition is the *Kotechý-Preiss condition*:

$$\exp\left[-\sum_{y \not\sim x} c_y \right] c_x \geq R_x \forall x \in X. \tag{8.16}$$

Now we consider the special case where X can be partitioned into $X = \bigsqcup_{n=1}^{\infty} X_n$ and where there are suitable $\{A_n\}_{n \in \mathbb{N}}$ such that

$$\sum_{y \in X_n : y \not\sim x} R_y \leq A_n m \forall n \in \mathbb{N} \forall x \in X_m. \tag{8.17}$$

(8.17) typically arises when X is a set of subsets of some V, and $x \not\sim y \iff x \cap y \neq \varnothing$. Then we take X_n to be $\{x \in X : |x| = n\}$. Then if we showed that we can find $\{A_n\}$ such that

$$\sum_{y \in X_n : i \in y} R_y \leq A_n \forall n \in \mathbb{N} \forall i \in V, \tag{8.18}$$

then for fixed $x \in X_m$ and $i \in x$, A_n upper bounds summing R_y over $y \in X_n$ with $i \in x \cap y \implies x \not\sim y$, so summing over the m $i \in x$ we can get (8.17) to hold.

Suppose (8.17) holds and suppose we take $c_x = e^{\alpha m} R_x \forall x \in X_m$ for some suitable $\alpha > 0$. Then

$$\exp\left[-\sum_{y \not\sim x} c_y \right] c_x = \exp\left[-\sum_{n=1}^{\infty} \sum_{y \in X_n : y \not\sim x} e^{\alpha n} R_y \right] e^{\alpha m} R_x \geq \exp\left[-\sum_{n=1}^{\infty} e^{\alpha n} A_n m \right] e^{\alpha m} R_x$$
$$= \exp\left[\left(\alpha - \sum_{n=1}^{\infty} e^{\alpha n} A_n \right) m \right] R_x$$

and this upper bounds R_x if and only if

$$\alpha \geq \sum_{n=1}^{\infty} e^{\alpha n} A_n. \tag{8.19}$$

This proves the following proposition:

Proposition 8.6. *Suppose that $X = \bigsqcup_{n=1}^{\infty} X_n$ and there exists $\{A_n\}_{n\in\mathbb{N}}$ and $\alpha > 0$ such that*

1. $\sum_{y\in X_n : y\not\sim x} R_y \le A_n m$ *for all m, n and all $x \in X_m$ (8.17);*
2. $\sum_{n=1}^{\infty} e^{\alpha n} A_n \le \alpha$ (8.19).

Then the Kotechý-Preiss condition (8.16) (and thus 8.5) holds with $c_x = e^{\alpha m} R_x \forall x \in X_m$.

Note that since X is finite, only finitely many A_n are nonzero. However for the rest of this section we will 'forget' this fact and instead consider the general case where $\{A_n\}_{n\in\mathbb{N}}$ is simply an infinite sequence.

In this case, for the existence of $\alpha > 0$ such that $\sum_{n=1}^{\infty} e^{\alpha n} A_n \le \alpha$ to hold, it is necessary that A_n decays exponentially, i.e. there exists $c > 1$ such that $\limsup_{n\to\infty} c^n A_n = M < \infty$. However, since this would imply that $(\frac{c}{2})^n A_n \le (M+\epsilon)/2^n$ after finitely many terms, let N be such that $(\frac{c}{2})^n A_n \le (M+\epsilon)/2^n \forall n \ge N$ and $\sum_{n=N}^{\infty} (M+\epsilon)/2^n \le (\log c)/2$, then it suffices to modify the first $N-1$ A_n so that $\sum_{n=1}^{N-1} c^n A_n \le (\log c)/2$ for the desired $\alpha = \log c$ to exist. Thus *any* exponential decay on A_n is sufficient for α to exist, up to modifying finitely many A_n. In some applications it is thus important to estimate A_n for small n.

Let $\delta = \liminf_{n\to\infty} (-\log A_n)/n$ and let

$$F(\alpha) = \alpha^{-1} \sum_{n=1}^{\infty} e^{\alpha n} A_n.$$

Then since $(e^{\alpha})^n < A_n$ for large enough n as long as $0 < \alpha < \delta$, e^{α} is within the domain where $g(x) = \sum_{n=1}^{\infty} x^n A_n$ is analytic, so F is real-analytic in $0 < \alpha < \delta$ as a composition and then product of analytic functions. Furthermore, $F(\alpha) \to \infty$ as $\alpha \to \delta$ since $e^{((-\log A_n)/n - \epsilon)n} A_n = e^{-\epsilon n}$ can make the series grow arbitrarily large as $\epsilon \to 0$, so since the series is increasing in α, it diverges when $\alpha \ge \delta$ so in that case $F(\alpha) = \infty$. As $\alpha \to 0$, clearly since $e^{\alpha n} A_n \to A_n$ and $\alpha^{-1} \to \infty$ we have $F(\alpha) \to \infty$, thus by IVT the infimum of $F(\alpha)$ on $0 < \alpha < \delta$ is actually attained, making (8.19) equivalent to

$$\inf_{\alpha>0} \alpha^{-1} \sum_{n=1}^{\infty} e^{\alpha n} A_n \le 1.$$

8.4 Some combinatorial lemmas

8.4.1 Reduction to trees

In order to compute $w(S)$, we need to sum over all connected subgraphs $(S, E') \subseteq (S, E_S)$. However there are often 'too many' such (S, E') to upper bound. It is thus helpful that this sum can sometimes be bounded by simply a sum over *spanning trees*. This is where $|1 + v_e| \le 1 \forall e \in E$ comes into play.

Proposition 8.7. *Let $G = (V, E)$ be equipped with complex edge weights $\{v_e\}_{e\in E}$ satisfying $|1 + v_e| \le 1$ for all e. Then*

$$\left| \sum_{\substack{E' \subseteq E,\\ (V,E')\text{ connected}}} \prod_{e\in E'} v_e \right| \le \sum_{\substack{E' \subseteq E,\\ (V,E')\text{ tree}}} \prod_{e\in E'} |v_e|. \tag{8.20}$$

Outline of proof. WLOG G is connected since otherwise both sides are 0. It is known that there exists a map $\mathbf{R}$ from the set of spanning trees in G to its set of connected subgraphs such that $T \subseteq \mathbf{R}(T)$ and that for each connected subgraph $(V, E') \subseteq (V, E)$, there exists a unique tree T such that $E_T \subseteq E' \subseteq \mathbf{E}_{R(T)}$. Thus by factoring out $\prod_{e\in E_T} v_e$ for each such H on the left side of (8.20), we get

$$\begin{aligned}
\left|\sum_{\substack{E'\subseteq E,\\ (V,E')\text{ connected}}} \prod_{e\in E'} v_e\right| &= \left|\sum_{\substack{E_T\subseteq E,\\ (V,E_T)\text{ tree}}} \prod_{e\in E_T} v_e \sum_{\substack{E':\\ E_T\subseteq E'\subseteq E_{\mathbf{R}(T)}}} \prod_{e\in E'\setminus E_T} v_e\right| \\
&= \left|\sum_{\substack{E_T\subseteq E,\\ (V,E_T)\text{ tree}}} \prod_{e\in E_T} v_e \sum_{E':E'\subseteq E_{\mathbf{R}(T)}\setminus E_T} \prod_{e\in E'} v_e\right| \\
&= \left|\sum_{\substack{E_T\subseteq E,\\ (V,E_T)\text{ tree}}} \prod_{e\in E_T} v_e \prod_{e\in E_{\mathbf{R}(T)}\setminus E_T} (1+v_e)\right| \\
&\le \sum_{\substack{E_T\subseteq E,\\ (V,E_T)\text{ tree}}} \prod_{e\in E_T} |v_e| \prod_{e\in E_{\mathbf{R}(T)}\setminus E_T} |1+v_e| \le \sum_{\substack{E'\subseteq E,\\ (V,E')\text{ tree}}} \prod_{e\in E'} |v_e|. \qquad \square
\end{aligned}$$

8.4.2 Connected subgraphs containing a specified vertex

Definition 8.8. Let $G = (V, E)$ be finite or countably infinite equipped with edge weights $\{v_e\}_{e\in E}$ and let $x \in V$. Define the *weighted sum* (over connected subgraphs on n vertices and m edges)

$$C_{n,m}(G, \{v_e\}, x) = \sum_{\substack{(V',E')\subseteq G\text{ connected},\\ x\in V',|V'|=n,|E'|=m}} \prod_{e\in E'} |v_e|$$

with special cases *tree sum*

$$T_n(G, \{v_e\}, x) = C_{n,n-1}(G, \{v_e\}, x) = \sum_{\substack{(V',E')\subseteq G\text{ tree},\\ x\in V',|V'|=n}} \prod_{e\in E'} |v_e|$$

and *edge-counted sum*

$$C_{\bullet,m} = \sum_{n=1}^{m+1} C_{n,m}(G, \{v_e\}, x).$$

When the edge weights are all 1, we can omit them from the notation (i.e. $C_{n,m}(G, x) = C_{n,m}(G, 1, \dots, 1, x)$ etc.). For the *infinite r-regular tree* $\mathbf{T}_r$ containing vertex y, define the constant

$$t_n^{(r)} = T_n(\mathbf{T}_r, y).$$

Note that we trivially have

$$C_{n,m}(G,\{v_e\},x) \le C_{n,m}(G,x)\left(\sup_{e\in E}|v_e|\right)^m. \tag{8.21}$$

We actually as of now already have all we need to state and prove the main result. However, in this section we will first state some results that will improve our main theorem. The following was proven using the universal cover graph[13] for the first inequality, and generating functions and Lagrange's implicit function theorem for the closed form of $t_n^{(r)}$, but it is stated here without proof.

Proposition 8.9. *Let $G=(V,E)$ be finite or countably infinite of maximum degree r and equipped with edge weights $\{v_e\}_{e\in E}$. Let $x\in V$ and y be a vertex in $\mathbf{T}_r$. Then*

$$C_{\bullet,m}(G,x) \le C_{\bullet,m}(\mathbf{T}_r,y) = T_{m+1}(\mathbf{T}_r,y) = t_{m+1}^{(r)} = r\frac{((r-1)(m+1))!}{m!((r-2)m+3)!}.$$

In consequence (8.21)

$$C_{\bullet,m}(G,\{v_e\},x) \le t_{m+1}^{(r)}\left(\sup_{e\in E}|v_e|\right)^m,$$

a particular case of which is

$$T_n(G,\{v_e\},x) \le t_n^{(r)}\left(\sup_{e\in E}|v_e|\right)^{n-1}. \tag{8.22}$$

Another result, whose proof will be given, helps bound the expression 8.9 gives for $t_n^{(r)}$.

Proposition 8.10.

$$t_n^{(r)} = r\frac{((r-1)(n))!}{(n-1)!((r-2)n+2)!} \le \frac{(rn)^{n-1}}{n!}$$

Proof.

$$\frac{((r-1)(n))!}{((r-2)n+2)!} = \frac{(rn-n)!}{(rn-n-(n-2))!} \le (rn-n)^{n-2} \le (rn)^{n-2}.$$ □

8.5 The main results

This is the main theorem of the paper:

Theorem 8.11. *Let $G=(V,E)$ be loopless, finite and equipped with complex edge weights satisfying $\{v_e\}_{e\in E}$ satisfying $|1+v_e|\le 1 \forall e\in E$. Let $Q=Q(G,\{v_e\})>0$ be the smallest number satisfying*

$$\inf_{\alpha>0}\alpha^{-1}\sum_{n=2}^{\infty}e^{\alpha n}Q^{-(n-1)}\max_{x\in V}T_n(G,\{v_e\},x) \le 1. \tag{8.23}$$

[13] The universal cover graph U is a tree constructed from the set of all walks starting at x and that do not using any edge consecutively. U is a subgraph of $\mathbf{T}_r$ so $C_{\bullet,m}(U,x) \le C_{\bullet,m}(\mathbf{T}_r,y)$ is clear. However proving $C_{\bullet,m}(G,x) \le C_{\bullet,m}(U,x)$ requires more work and is omitted.

Then all zeros (in s) of $Z_G(s,\{v_e\})$ lie in $|s|<Q$.

Note that $Q<\infty$ since $T_n\equiv 0$ for $n>|V|$, so the series is finite.

Proof. First by 8.3 we view Z_G as a grand-canonical gas with $w_S=w(S)$ and $W(S_i,S_j)$ being the exclusion function $\mathbf{1}\{S_i\cap S_j=\varnothing\}$. Let $R_S=w(S)$ and let $A_n=\max_{x\in V}\sum_{S:x\in S,|S|=n}|w(S)|$. Note $A_1=0$ which is why the series in (8.23) starts at 2. Then using the partition of $\mathscr{P}_*(V)$ into $X_n=\{S\in\mathscr{P}_*(V):|S|=n\}$, we have

$$\sum_{S\in X_m:x\in S}R_S=\sum_{S:|S|=n,x\in S}R_S\le A_n\forall x\in V$$

i.e. (8.18) and in consequence the first condition of 8.6 hold.

Note that from 8.7 we have, for all S where $x\in S$ and $|S|=n$,

$$\begin{aligned}
&|w(S)|\le|s|^{-(|S|-1)}\sum_{\substack{E'\subseteq E_S,\\(S,E')\text{ tree}}}\prod_{e\in E'}|v_e|\\
\implies&\sum_{S:x\in S,|S|=n}|w(S)|\le|s|^{-(n-1)}\sum_{S:x\in S,|S|=n}\sum_{\substack{E'\subseteq E_S,\\(S,E')\text{ tree}}}\prod_{e\in E'}|v_e|=|s|^{-(n-1)}T_n(G,\{v_e\},x)\\
\implies&A_n=\max_{x\in V}\sum_{S:x\in S,|S|=n}|w(S)|\le|s|^{-(n-1)}\max_{x\in V}T_n(G,\{v_e\},x)\\
\implies&\alpha^{-1}\sum_{n=1}^{\infty}e^{\alpha n}A_n=\alpha^{-1}\sum_{n=2}^{\infty}e^{\alpha n}A_n\le\alpha^{-1}\sum_{n=2}^{\infty}e^{\alpha n}|s|^{-(n-1)}\max_{x\in V}T_n(G,\{v_e\},x)\\
\implies&\inf_{\alpha>0}\alpha^{-1}\sum_{n=2}^{\infty}e^{\alpha n}A_n\le\inf_{\alpha>0}\alpha^{-1}\sum_{n=2}^{\infty}e^{\alpha n}|s|^{-(n-1)}\max_{x\in V}T_n(G,\{v_e\},x)
\end{aligned}\tag{8.24}$$

Since the right hand side of (8.24) is decreasing in $|s|$ and the second condition of 8.6 would be satisfied with $|s|=Q$, it would also be satisfied with $|s|>Q$ so by 8.5 $Z_G(s,\{v_e\})$ is nonvanishing in $w_S\le R_S=w(S)$, thus $Z_G(s,\{v_e\})\ne 0\forall|s|>Q$. ☐

If, in addition, the degree of vertices in G is at most r, then let $C(r)$ be the smallest number such that

$$\inf_{\alpha>0}\alpha^{-1}\sum_{n=2}^{\infty}e^{\alpha n}(C(r))^{-(n-1)}t_n^{(r)}\le 1.$$

Then as a corollary to 8.11, directly from 8.9, we have

Corollary 8.12. *Let $G=(V,E)$ be loopless, finite, of maximum degree r and equipped with complex edge weights satisfying $\{v_e\}_{e\in E}$ satisfying $|1+v_e|\le 1\forall e\in E$. Let $v_{\max}=\max_{e\in E}|v_e|$. Then all zeros of $Z_G(s,\{v_e\})$ lie in $|s|<C(r)v_{\max}$.*

Recall that the chromatic polynomial $C_G(s)=Z_G(s,-1,\dots,-1)$. Thus directly from 8.12 we have

Corollary 8.13. *Let $G = (V, E)$ be loopless, finite, of maximum degree r. Then all zeros of $C_G(s)$ lie in $|s| < C(r)$.*

The following is a corollary of the bound on $t_n^{(r)}$ from 8.10.

Corollary 8.14.

$$C(r) = O(r).$$

Proof. Note $\log \frac{n^{n-1}}{n!} = (n-1)\log n - \sum_{i=1}^{n} \log n \leq (n-1)\log n - n\log n + n = n - \log n$ so $\frac{n^{n-1}}{n!} \leq \frac{e^n}{n} \leq e^n$. Thus if $C(r) \geq Mr$,

$$\begin{aligned}
\inf_{\alpha>0} \alpha^{-1} \sum_{n=2}^{\infty} e^{\alpha n} (C(r))^{-(n-1)} t_n^{(r)} &\leq \inf_{\alpha>0} \alpha^{-1} \sum_{n=2}^{\infty} e^{\alpha n} (C(r))^{-(n-1)} \frac{(rn)^{n-1}}{n!} \\
&= \inf_{\alpha>0} \alpha^{-1} \sum_{n=2}^{\infty} e^{\alpha n} \left(\frac{C(r)}{r}\right)^{-(n-1)} \frac{n^{n-1}}{n!} \\
&\leq \inf_{\alpha>0} \alpha^{-1} \sum_{n=2}^{\infty} e^{(\alpha+1)n} \left(\frac{C(r)}{r}\right)^{-(n-1)} \\
&\leq \inf_{\alpha>0} \alpha^{-1} M \sum_{n=2}^{\infty} \left(\frac{e^{\alpha+1}}{M}\right)^{n} = \inf_{\alpha>0} (M\alpha)^{-1} e^{2(\alpha+1)} \frac{1}{1 - e^{\alpha+1}/M}.
\end{aligned}$$

The above can be verified with $M = 45$ and $\alpha = 0.5$. □

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