A Combinatorial Proof of Ihara-Bass's Formula for the Zeta Function of Regular Graphs

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Abstract

We give an elementary combinatorial proof of Bass's determinant formula for the zeta function of a finite regular graph. This is done by expressing the number of non-backtracking cycles of a given length in terms of Chebyshev polynomials in the eigenvalues of the adjacency operator of the graph. A related observation of independent interest is that the Ramanujan property of a regular graph is equivalent to tight bounds on the number of non-backtracking cycles of every length.

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1 Introduction

1.1 Ramanujan graphs and Non-backtracking Cycles

For a fixed $d \geq 3$, a family G_n of d-regular n-vertex connected graphs is said to be an *expander* family if the second largest eigenvalues of the corresponding adjacency matrices are uniformly bounded away from d. It is easy to show (using a simple application of the probabilistic method) that a random d-regular graph family is an expander family with high probability. The question as to how small the second largest eigenvalue can get is answered by the Alon-Bopanna bound [16]: For fixed $d \geq 3$, the second largest eigenvalue, in absolute value, is at least $2\sqrt{d-1} - o_n(1)$. The occurrence of the term $2\sqrt{d-1}$ in this setting is related to it being the spectral radius of (the adjacency operator of) the *universal cover* of a d-regular graph (which is the infinite d-regular tree).

▶ **Definition 1.** For $d \geq 3$, a finite connected d-regular graph G is said to be *Ramanujan* if every eigenvalue $\mu \in \mathbb{R}$ of the adjacency matrix A of G with $|\mu| \neq d$ satisfies

$$|\mu| \leq 2\sqrt{d-1}$$

In other words, a family of Ramanujan graphs is the "optimal" expander family in light of the Alon-Bopanna lower bound. Ramanujan graphs were defined and explicitly constructed by Lubotzky, Phillips and Sarnak [11] for $d-1$ being a prime, and extended by Morgenstern [14] for $d-1$ being a prime power. Their constructions used deep results from modern number theory (in particular a conjecture of Ramanujan which was later settled by Deligne et al). However, the existence (leave alone explicit constructions) of Ramanujan graph families for general $d \geq 3$ remained open for a long time until Marcus, Spielman and Srivastava [13] used the method of interlacing polynomials to establish the existence of bipartite Ramanujan families for every $d \geq 3$. For a broad survey of Ramanujan graphs, expander families and

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their applications, the reader is referred to Murty's monograph [15] and the survey by Hoory, Linial and Wigderson [6].

The Ramanujan property (or more generally, the spectrum of the adjacency matrix) of a graph is reflected in the error term in the number of closed walks on the graph of a given length. More precisely, suppose $d = \mu_0 \geq \mu_1 \geq \cdots \geq \mu_{n-1} \geq -d$ are the n eigenvalues of an n-vertex d-regular graph. Then we know that for every $k \geq 1$, $Tr(A^k) = d^k + \sum_{j=1}^{n-1} \mu_j^k$ is precisely the number of closed walks of length k on G. We can express this succinctly using Jacobi's identity:

$$\frac{1}{det(I - At)} = \prod_{j=0}^{n-1} \frac{1}{1 - \mu_j t} = exp\left(\sum_{k=1}^{\infty} Tr(A^k) \frac{t^k}{k}\right)$$

Now if $|\mu_j| \leq 2\sqrt{d-1}$ for every $1 \leq j \leq n-1$, then the number of closed walks of length k in G is d^k (or roughly a $1/n$ fraction of the total number nd^k of walks of length k), and with a small error term of $O(n 2^k d^{k/2})$.
As we shall soon see in more detail, a stronger connection between the Ramanujan property and closed walks on the graph reveals itself when we restrict the closed walks to be *non-backtracking*. An instance of backtracking is said to occur in a walk when a traversed edge is followed immediately by its reversal. Let N_k denote the number of non-backtracking cycles of length k on G. We can construct an analogous generating function for $\{N_k\}_{k \geq 1}$ as:

$$exp\left(\sum_{k=1}^{\infty} N_k \frac{t^k}{k}\right)$$

As it so happens, the above formal series can also be expressed as the inverse of a polynomial $det(I - Ht)$ where H is the Hashimoto non-backtracking walk matrix of G, which is the adjacency matrix of the oriented line digraph of G. This formal series is called the *Ihara zeta function* of the graph, denoted $\zeta_G(t)$.

1.2 Zeta functions and Riemann Hypotheses

In the 158 years since Bernard Riemann published his seminal work "On the Number of Primes Less Than a Given Magnitude", there have been several generalizations of the Riemann zeta function in various settings. Broadly speaking, a zeta function is a complex function which when expressed as an appropriate series, yields a coefficient sequence that counts "objects" of a given "weight" assembled from an underlying set of building blocks or "primes". For instance, the Riemann zeta function corresponds to a Dirichlet series where the coefficient of $1/k^s$ counts the number of positive integers (constructed using the primes of $\mathbb{Z}$ as building blocks) of absolute value k (which in this case is trivially 1 for every $k \in \mathbb{N}$). The utility of a zeta function arises from the fact that many interesting properties of the underlying structure can be inferred from the zeros and poles of the corresponding zeta function.

The precursor to the zeta function of a graph, as we know it today, is the Selberg zeta function of a Riemannian manifold. For a hyperbolic surface $M = \Gamma/H$, the Selberg zeta function $\gamma_M(s)$ is an Euler product over the set of all primitive closed geodesics of M. The zeros and poles of the Selberg zeta function appear in the Selberg trace formula, which relates the distribution of primes with the spectrum of the Laplace-Beltrami operator of the surface. This line of study was further extended by Ihara [7] to obtain a p-adic analogue of the Selberg trace formula, opening up further avenues for the study of geodesic zeta functions in discrete settings. The idea of considering closed geodesics as primes inspired the work of Hashimoto [5], Hyman Bass [2], Kotani and Sunada [9] to study the analogous notion in the discrete setting of a finite graph, using the prime cycle classes of the graph in place of primitive geodesics. We shall construct the zeta function of a graph in this way in section 2. Just like the Selberg zeta function is related to the spectrum of the Laplace-Beltrami operator of the surface, it is natural to ask if its discrete analogue, the Ihara zeta function of a graph, is related to the spectrum of the Laplacian matrix of the graph. This is precisely the result of Bass [2] who gives an elegant expression for the Ihara zeta function of a graph $G = (V, E)$ as follows:

▶ **Theorem 2** (Bass)**.** *For a finite connected graph $G = (V, E)$,*

$$\zeta_G(t) = \frac{1}{(1-t^2)^{|E|-|V|}det(I - tA + (D - I)t^2)}$$

where A is the adjacency matrix of G and D is the diagonal matrix of degrees of the vertices of G, or in other words, $D = diag(A\vec{1})$.

In particular, if G is a d-regular connected graph, then

$$\zeta_G(t) = \frac{1}{(1-t^2)^{|E|-|V|}det(I - tA + (d - 1)t^2)}$$

This immediately tells us what the poles of the Ihara zeta function are. The significance of these poles arises from a surprising analogue of the classical Riemann hypothesis in our present context. The classical Riemann hypothesis for the Riemann zeta function $\zeta(t)$ states that every non-trivial zero of $\zeta(t)$ lies on the line $Re(z) = 1/2$ in the complex plane. Analogues of the Riemann hypothesis can be formulated for other zeta functions too. For instance, the Riemann hypothesis for curves over finite fields states that every zero of the Hasse-Weil zeta function for a projective curve over a finite field $\mathbb{F}_q$ is of absolute value exactly $1/\sqrt{q}$. It is interesting to note that while the classical Riemann hypothesis remains elusive, the Riemann hypothesis for finite fields has been proved, and is one of the crowning achievements of twentieth-century mathematics.

It is natural to ask if there is an appropriate formulation of a Riemann hypothesis for the Ihara zeta function, and what it means for the graph. Recall that a d-regular graph G is *Ramanujan* if for every eigenvalue $\mu \in \mathbb{R}$ of the adjacency matrix of G with $|\mu| \neq d$ satisfies $|\mu| \leq 2\sqrt{d-1}$. Combining this with Bass's determinant formula for the zeta function of G, if can be easily shown [15] that

▶ **Lemma 3** (Riemann Hypothesis for graphs)**.** *A d-regular graph G is Ramanujan iff every pole $\lambda \in \mathbb{C}$ of $\zeta_G(t)$ such that $|\lambda| \neq 1$ and $|\lambda| \neq (d-1)^{-1}$ satisfies*

$$|\lambda| = \frac{1}{\sqrt{d-1}}$$

1.3 Proof Sketch

There exist several proofs [9] [17] of theorem 2, and most proofs start by expressing the zeta function in terms of not the adjacency matrix A of G, but the adjacency matrix H of the oriented line digraph of G (the Hashimoto non-backtracking walk matrix). After all, $\zeta_G(t)^{-1} = det(I - Ht)$, and so the problem reduces to expressing $det(I - Ht)$ in terms of the adjacency matrix A. We shall briefly sketch the standard proof in the next section once we have the preliminaries in place. There also exists another purely combinatorial proof by Foata and Zeilberger [4] employing the algebra of Lyndon words.

In this paper, we shall see an elementary proof of theorem 2 for the special case when G is d-regular. While the assumption of regularity is certainly a limitation, it allows for a more transparent combinatorial proof. The basic idea is outlined as follows:

- We use the fact that the zeta function $\zeta_G(t)$ has an expansion of the form

$$\zeta_G(t) = exp\left(\sum_{k=1}^{\infty} N_k \frac{t^k}{k}\right)$$

  where for $k \in \mathbb{N}$, N_k is the number of non-backtracking cycles in G of length k. This is explored in section 2.
- While an expression for N_k is not immediate, a natural starting point is the study of non-backtracking walks on G. We can construct the family $\{A_k\}_{k\in\mathbb{Z}_{\geq 0}}$ of $n \times n$ matrices such that for every $k \in \mathbb{Z}_{\geq 0}$ and every $v, w \in V$, $(A_k)_{v,w}$ is the number of non-backtracking walks on G of length k from v to w. We shall discuss the construction of these non-backtracking walk matrices in section 3.
- While it might be tempting to claim that $N_k = Tr(A_k)$, unfortunately that is not the case! However, while they may not be equal, they are indeed precisely related. In section 4, we develop a combinatorial lemma to relate N_k and $Tr(A_k)$. This expression, while simple, could prove useful and is of independent interest.
- The combinatorial lemma greatly simplifies the problem since $Tr(A_k)$ is well-understood in terms of the eigenvalues of A and a family of orthogonal polynomials called the Chebyshev polynomials. We shall put these ingredients together in section 5 to arrive at Bass's determinant formula.

Essentially, the main contribution of this paper is a proof of following lemma:

▶ **Lemma 4.** *Let G be a finite, connected d-regular graph on n vertices, and suppose $d = \mu_0 \geq \mu_1 \geq \cdots \geq \mu_{n-1} \geq -d$ are the n real eigenvalues of its adjacency matrix A. Let N_k be the number of non-backtracking cycles of length k on G. Then*

$$N_k = \begin{cases} \sum\limits_{j=0}^{n-1} 2(d-1)^{k/2} T_k\left(\frac{\mu_j}{2\sqrt{d-1}}\right) & \text{if } k \text{ is odd} \\ n(d-2) + \sum\limits_{j=0}^{n-1} 2(d-1)^{k/2} T_k\left(\frac{\mu_j}{2\sqrt{d-1}}\right) & \text{if } k \text{ is even} \end{cases}$$

where T_k is the k-th Chebyshev polynomial of the first kind.

While the above expression is easy to derive given Bass's determinant formula for the zeta function, our proof proceeds in the other direction: by establishing this expression first and then using it to derive Bass's determinant formula using the generating function for Chebyshev polynomials of the first kind.

An interesting consequence of the above formula for N_k is an interpretation of the summand corresponding to the trivial eigenvalue d of G. Using a standard explicit formula for the polynomial T_k given by

$$T_k(x) = \begin{cases} \cos(k \arccos x) & \text{if } |x| \leq 1 \\ \frac{1}{2}(x - \sqrt{x^2-1})^k + \frac{1}{2}(x + \sqrt{x^2-1})^k & \text{if } |x| > 1 \end{cases}$$

we can compute $T_k(d/2\sqrt{d-1})$ to get

$$T_k\left(\frac{d}{2\sqrt{d-1}}\right) = (d-1)^k + 1$$

So if G is non-bipartite, we get

$$N_k = \begin{cases} (d-1)^k + 1 + \sum_{j=1}^{n-1} 2(d-1)^{k/2} T_k\left(\frac{\mu_j}{2\sqrt{d-1}}\right) & \text{if k is odd} \\ (d-1)^k + 1 + (d-2) + \sum_{j=1}^{n-1} \left((d-2) + 2(d-1)^{k/2} T_k\left(\frac{\mu_j}{2\sqrt{d-1}}\right)\right) & \text{if k is even} \end{cases}$$

In particular, when G is Ramanujan,

$$N_k = \begin{cases} (d-1)^k + 1 + O(nd^{k/2}) & \text{if k is odd} \\ (d-1)^k + 1 + (d-2) + O(nd^{k/2}) & \text{if k is even} \end{cases}$$

It is known that T_k is an odd function when k is odd, and an even function when k is even. So when G is bipartite,

$$N_k = \begin{cases} 0 & \text{if k is odd} \\ 2(d-1)^k + 2 + 2(d-2) + \sum_{j=1}^{n-2} \left((d-2) + 2(d-1)^{k/2} T_k\left(\frac{\mu_j}{2\sqrt{d-1}}\right)\right) & \text{if k is even} \end{cases}$$

and in particular when G is a bipartite Ramanujan graph,

$$N_k = \begin{cases} 0 & \text{if k is odd} \\ 2(d-1)^k + 2 + 2(d-2) + O(nd^{k/2}) & \text{if k is even} \end{cases}$$

It is interesting to ask what these dominant terms represent. It is known [12] that the number of *cyclically reduced words* of length k in a free group of rank m is exactly $(2m-1)^k + 1$ when k is odd, and $(2m-1)^k + 2m - 1$ when k is even. So if G were a Cayley graph of a group Γ and a symmetric generating set S (without involutive elements) of size d, then consider the walks on G corresponding to a choice of root and a cyclically reduced word over S of length k. The total number of such walks is $n\left((d-1)^k + 1\right)$ if k is odd, and $n\left((d-1)^k + 1 + (d-2)\right)$ if k is odd. If G is non-bipartite, we would expect a $1/n$ fraction of these walks to return to the root (that is, become non-backtracking cycles). If G is bipartite, then for even k, we would expect a $2/n$ fraction of these walks to be non-backtracking cycles (as there are now only $n/2$ candidates for the end vertex). These quantities are precisely the ones that appear as the dominant terms in the expressions for N_k.
So the Ramanujan property (or the graph Riemann hypothesis) implies that the number N_k of non-backtracking cycles is close to the expected value, with optimally tight error term.

2 Preliminaries

2.1 Non-backtracking cycles and the Ihara Zeta Function

For an integer $d \geq 2$, let $G = (V, E)$ be a finite d-regular undirected graph with adjacency matrix A. A *walk* on the graph G is a sequence $v_0 v_1 \dots v_k$ where $v_0, v_1, \dots, v_k$ are (not necessarily distinct) vertices in V, and for every $0 \leq i \leq k-1$, $(v_i, v_{i+1}) \in E$. The vertex v_0 is referred to as the *root* (or origin) of the above walk, v_k is the terminus of the walk, and the walk is said to have length k.

It is often useful to equivalently define a walk as a sequence of directed or oriented edges. Associate each edge $e = (v, w) \in E$ with two directed edges (or rays) denoted

$$\vec{e} = (v \to w) \text{ and } \vec{e}^{-1} = (w \to v)$$

Note that the origin $org(\vec{e})$ is the vertex v and its terminus $ter(\vec{e})$ is the vertex w. Similarly, the origin $org(\vec{e}^{-1})$ is the vertex w and its terminus $ter(\vec{e})$ is the vertex v. Let $\vec{E}$ denote the set of $m = nd$ directed edges of G. So a walk of length k can equivalently be described as a sequence $\vec{e}_1\vec{e}_2 \dots \vec{e}_k$ of k (not necessarily distinct) oriented edges in $\vec{E}$ such that for every $1 \le i \le k-1$, $ter(\vec{e}_i) = org(\vec{e}_{i+1})$. This is a walk that starts at $org(\vec{e}_1)$ and ends at $ter(\vec{e}_k)$. It is easy to show that for any $k \in \mathbb{N}$, the number of walks of length k between vertices $u, v \in V$ is exactly $(A^k)_{u,v}$. In particular, the total number of closed walks of length k in G is exactly $Tr(A^k)$.

▶ **Definition 5.** A *non-backtracking walk* of length k from $v_0 \in V$ to $v_k \in V$ is a walk $v_0v_1 \dots v_k$ such that for every $1 \le i \le k-1$, $v_{i-1} \neq v_{i+1}$. Equivalently, a non-backtracking walk of length k from $v \in V$ to $w \in V$ is a walk $\vec{e}_1\vec{e}_2 \dots \vec{e}_k$ such that $org(\vec{e}_1) = v$, $ter(\vec{e}_k) = w$ and for every $1 \le i \le k-1$, $\vec{e}_{k+1} \neq \vec{e}_k^{-1}$.

▶ **Definition 6.** A *non-backtracking cycle* of length k with root v is a non-backtracking closed walk $v, v_1, v_2, \dots, v_{k-1}, v$ with the additional boundary constraint that $v_1 \neq v_{k-1}$.

Non-backtracking random walks (NBRW) on graphs have been studied in the context of mixing time [1], cut-offs [10], and exhibit more useful statistical properties than simple random walks (SRW).

Let $\mathcal{C}$ denote the set of all non-backtracking cycles in G, and for $C \in \mathcal{C}$, let $|C|$ denote the length of the cycle C. There are two elementary constructions we can carry out to generate more elements of $\mathcal{C}$ from a given cycle C:

- *Powering*: Given a non-backtracking cycle $C \in \mathcal{C}$ of length k of the form $C = \vec{e}_1\vec{e}_2 \dots \vec{e}_k$ and $m \ge 1$, define the power

  $$C^m = \underbrace{\vec{e}_1 \dots \vec{e}_k.\vec{e}_1 \dots \vec{e}_k \dots \vec{e}_1 \dots \vec{e}_k}_{\text{m times}}$$

  which is the concatenation of the string of edges corresponding to the walk C with itself m times. Note that C^m is also a non-backtracking cycle in G of length mk. Essentially, C^m represents the walk obtained by repeating or winding the walk C m times. Also note that C and C^m are both rooted at the same vertex. A cycle $P \in \mathcal{C}$ shall be called a *prime* cycle if there exists no element $C \in \mathcal{C}$ and $m \ge 2$ such that $P = C^m$. Essentially, a prime cycle in $\mathcal{C}$ is one that is not a repeated winding of a simpler cycle in $\mathcal{C}$. Note that every element of $\mathcal{C}$ is either a prime or a prime power.
- *Cycle Equivalence*: Given a non-backtracking cycle $C \in \mathcal{C}$ of length k of the form $C = \vec{e}_1\vec{e}_2 \dots \vec{e}_k$, we can form another walk $C^{(2)} = \vec{e}_2\vec{e}_3 \dots \vec{e}_k\vec{e}_1$ which is also a non-backtracking cycle in G of length k, but now rooted at the origin of the directed edge $\vec{e}_2$ (or the terminus of $\vec{e}_1$). More generally, for $1 \le j \le k$, define

  $$C^{(j)} = \vec{e}_j\vec{e}_{j+1} \dots \vec{e}_k\vec{e}_1\vec{e}_2 \dots \vec{e}_{j-1}$$

  which is a cyclic permutation of the walk C obtained by choosing a different root. So given a cycle $C \in \mathcal{C}$ of length k, we get $k-1$ additional cycles in $\mathcal{C}$ of length k for free this way. In fact, this defines an equivalence class $\sim$ on $\mathcal{C}$, and the set $[C] = \{C^{(1)}, C^{(2)}, \dots, C^{(k)}\}$ is called the equivalence class of C. An element $[C] \in \mathcal{C}/\sim$ represents a non-backtracking cycle modulo a choice of root.

We can now formally define the zeta function of the graph G. For simplicity, let us assume that G is connected and does not have any leaves (or vertices of degree 1).

▶ **Definition 7.** Let $\mathcal{P}$ denote the set of equivalence classes of prime non-backtracking cycles in G. The Euler product

$$\prod_{[P]\in\mathcal{P}} \frac{1}{1-t^{|P|}}$$

is called the *Ihara zeta function* of the graph G, denoted $\zeta_G(t)$.

Let N_k denote the number of non-backtracking cycles in G of length k. Then observe that

$$\sum_{k=1}^{\infty} N_k \frac{t^k}{k} = \sum_{\text{prime } P} \frac{1}{|P|}\left(\sum_{m=1}^{\infty} \frac{t^{m|P|}}{m}\right) = -\sum_{[P]\in\mathcal{P}} \log\left(1-t^{|P|}\right)$$

Thus,

$$\zeta_G(t) = \prod_{[P]\in\mathcal{P}} \frac{1}{1-t^{|P|}} = exp\left(\sum_{k=1}^{\infty} N_k \frac{t^k}{k}\right)$$

Just like the number of cycles in G of length k is $Tr(A^k)$, we can describe the number N_k of non-backtracking cycles in G of length k as the trace of the matrix H^k where H is the *Hashimoto non-backtracking walk matrix* of G defined as follows: $H \in \mathbb{C}^{dn\times dn}$ with

$$H_{i,j} = \begin{cases} 1 & \text{if } \vec{e}_j \neq \vec{e}_i^{\,-1} \text{ and } ter(\vec{e}_i) = org(\vec{e}_j) \\ 0 & \text{otherwise} \end{cases}$$

In other words, the entry $H_{i,j}$ is an indicator for whether the oriented edge $\vec{e}_i$ feeds into the oriented edge $\vec{e}_j$ allowing us to form a non-backtracking walk $\vec{e}_i\vec{e}_j$ of length 2. Note that unlike A, the Hashimoto matrix H is *not* a symmetric matrix, and hence it need not have all real eigenvalues and an associated orthonormal eigenbasis. The interested reader is referred to [10] where the authors work out the precise eigendecomposition of the Hashimoto matrix H.

It is clear that for every $k \in \mathcal{N}$,

$$N_k = Tr(H^k)$$

and so

$$\zeta_G(t) = exp\left(\sum_{k=1}^{\infty} Tr(H^k)\frac{t^k}{k}\right) = exp\left(-Tr\left(\log\left(I-tH\right)\right)\right)$$

By Jacobi's formula relating the trace of the logarithm of a matrix to the logarithm of its determinant, we get

$$\zeta_G(t) = \frac{1}{det(I-Ht)}$$

In particular, this establishes the rationality of the Ihara zeta function of a regular graph, and further implies that the reciprocal $\zeta_G(t)^{-1}$ is a polynomial in t over $\mathbb{Z}$ of degree at most $m = nd$. However, it is not immediate what the spectrum of H is. Thus, in a sense, Bass's determinant formula for regular graphs can be interpreted as a way to determine the spectrum of the Hashimoto matrix H in terms of the spectrum of the adjacency matrix A. Now that we have defined the Hashimoto non-backtracking walk matrix H, we shall briefly sketch a previous proof of Bass's determinant formula (from [8]) involving expressing both the matrix H and the adjacency matrix A in terms of two directed edge incidence matrices S and T and a backtracking matrix B defined as follows: For a directed edge $(u \to v)$ and a vertex $w \in V$, define

$$S_{w,(u\to v)} = \begin{cases} 1 & \text{if } u = w \\ 0 & \text{otherwise} \end{cases} \qquad T_{(u\to v),w} = \begin{cases} 1 & \text{if } v = w \\ 0 & \text{otherwise} \end{cases}$$

Note that S is an $n \times dn$ edge incidence matrix that indicates the origin or starting vertex of the directed edge, while T is a $dn \times n$ edge incidence matrix that indicates the terminating vertex of the directed edge. It can be checked that

$$A = ST$$

$$H = TS - B$$

$$SBT = dI$$

where B is a $dn \times dn$ backtracking indicator matrix defined as

$$B_{(u\to v),(w\to z)} = \begin{cases} 1 & \text{if } v = w \text{ and } u = z \\ 0 & \text{otherwise} \end{cases}$$

Now that A and H are related through S, T and B, standard matrix manipulation would suffice to show that

$$det(I - Ht) = (1 - t^2)^{\frac{dn}{2} - n} det\left(I - At + (d-1)t^2\right)$$

In fact, this proof works even when the graph G is not regular. However, the linear-algebraic calculations, though simple, tend to mask the underlying combinatorial structure.

2.2 Non-backtracking Walks and Chebyshev Polynomials

Just like $(A^k)_{v,w}$ counts the total number of walks on G from v to w (with backtrackings) of length k, we can construct a family

$$A_0, A_1, A_2, A_3, \ldots$$

of $n \times n$ matrices over $\mathbb{C}$ such that the value $(A_k)_{v,w}$ is the number of non-backtracking walks on G from v to w of length k. This family $\{A_k\}_{k\in\mathbb{N}}$ can be inductively defined using powers of A as follows:

- $A_0 = I$ and $A_1 = A$
- $A_2 = A^2 - dI$
- For $k \geq 3$,

$$A_k = A_{k-1}A - (d-1)A_{k-2}$$

The recurrence relation above can be used to easily show that the ordinary (matrix) generating function for the above sequence, with some mild abuse of notation, is

$$\sum_{k=0}^{\infty} t^k A_k = \frac{1 - t^2}{I - At + (d-1)t^2}$$

The generating function above is closely related to the generating function of a well-studied family of orthogonal polynomials. Consider the family of Chebyshev polynomials $\{U_k\}_{k\geq 0}$ of the second kind, which are univariate complex polynomials defined by the recurrence

$$U_0(x) = 1 \text{ and } U_1(x) = 2x$$

and for $k \geq 2$,

$$U_k(x) = 2xU_{k-1}(x) - U_{k-2}(x)$$

and with generating function

$$\sum_{k=0}^{\infty} U_k(x)t^k = \frac{1}{1-2xt+t^2}$$

It can be shown [3] that for every $k \geq 2$,

$$\sum_{0\leq j\leq k/2} A_{k-2j} = (d-1)^{k/2} U_k\left(\frac{A}{2\sqrt{d-1}}\right)$$

and so by taking trace on both sides we get

$$\sum_{0\leq j\leq k/2} Tr(A_{k-2j}) = (d-1)^{k/2} \sum_{j=0}^{n-1} U_k\left(\frac{\mu_j}{2\sqrt{d-1}}\right)$$

where

$$d = \mu_0 \geq \mu_1 \geq \cdots \geq \mu_{n-1} \geq -d$$

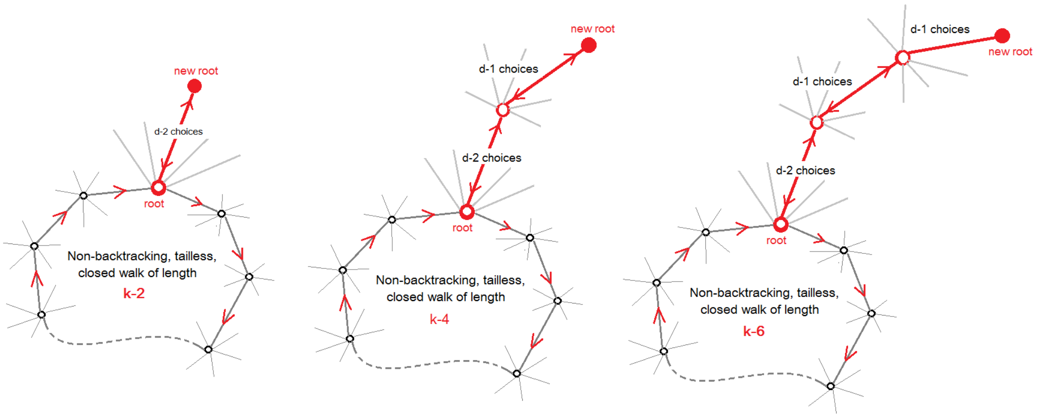
are the n eigenvalues of the adjacency matrix A. Thus we have an expression for the trace of A_k as a polynomial in the eigenvalues of A. This approach is used in the seminal work of Lubotzky, Phillips and Sarnak in their construction of Ramanujan graphs [11], and for a more detailed exposition of Chebyshev polynomials and non-backtracking walks on regular graphs, the reader is referred to the monograph by Davidoff, Sarnak and Valette [3].

While $(A_k)_{v,w}$ counts the number of walks on G from vertex v to vertex w without backtracking, observe that the diagonal element $(A_k)_{v,v}$ does *not* count the number of non-backtracking cycles of length k rooted at v. This is because $(A_k)_{v,v}$ also counts walks of the form $\vec{e}_1\vec{e}_2\ldots\vec{e}_k$ where $\vec{e}_{i+1} \neq \overleftarrow{e_i}^{1}$ for any $1 \leq i \leq k-1$ but $\vec{e}_k = \overleftarrow{e_1}^{1}$. That is, $\vec{e}_1\vec{e}_2\ldots\vec{e}_k$ is non-backtracking as a walk from v to v, but when considered as a closed walk, the two end edges form a backtracking and is hence not a non-backtracking cycle! Such an instance of a backtracking that gets overlooked in $Tr(A_k)$ shall be referred to as a *tail*.
So $Tr(A_k)$ counts the number of closed walks of length k that could have at most 1 tail (and hence does *not* count the non-backtracking cycles of length k). Denote $Tr(A_k)$ by M_k. In the following section, we shall establish a simple but useful combinatorial lemma relating M_k with N_k.

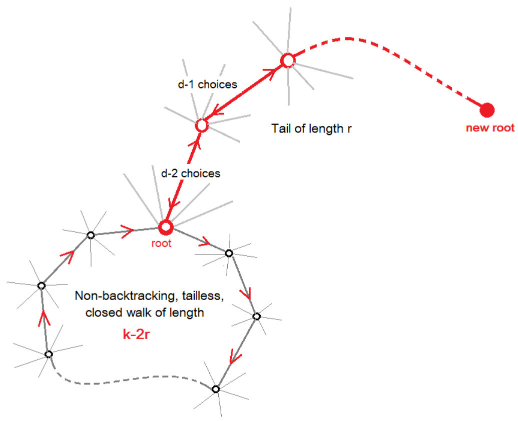
3 The Combinatorial Lemma

Firstly it is clear that $N_1 = N_2 = 0$. For $k \geq 3$, we can count the number M_k of *tailed* non-backtracking, closed walks of length k based on the length of the tail as illustrated below:

- A tailless, non-backtracking closed walk of length k, and there are N_k of them.
- A tailless, non-backtracking closed walks of length $k-2$ and a tail of length 1. Since the root is fixed and there are $d-2$ choices for the tail (and consequently, the new root), the number of non-backtracking closed walks of length k with a tail of length 1 is $(d-2)N_{k-2}$.
- A tailless, non-backtracking closed walks of length $k-4$ and a tail of length 2. In this case the first vertex of the tail can be chosen in $d-2$ ways, and the next vertex (the new root) can be chosen in $d-1$ ways. So the number of non-backtracking closed walks of length k with a tail of length 2 is $(d-1)(d-2)N_{k-4}$.



More generally, for $2 \le r \le \lfloor k/2 \rfloor$, the number of non-backtracking closed walks of length k with a tail of length r is $(d-1)^{r-1}(d-2)N_{k-2r}$.



Thus for every $k \ge 3$,

$$\begin{aligned} M_k =& N_k + (d-2)N_{k-2} + (d-2)(d-1)N_{k-4} + (d-2)(d-1)^2 N_{k-6} \\ &+ \cdots + (d-2)(d-1)^{\lfloor \frac{k-1}{2} \rfloor - 1} N_{k-2\lfloor \frac{k-1}{2} \rfloor} \end{aligned}$$

While this expression looks cumbersome, observe that

$$M_k - N_k = (d-2)\left(N_{k-2} + (d-1)N_{k-4} + \cdots + (d-1)^{\lfloor \frac{k-1}{2} \rfloor - 1} N_{k-2\lfloor \frac{k-1}{2} \rfloor}\right)$$

and a straightforward summation shows that

$$\sum_{j=1}^{\lfloor \frac{k-1}{2} \rfloor} M_{k-2j} = N_{k-2} + (d-1)N_{k-4} + \cdots + (d-1)^{\lfloor \frac{k-1}{2} \rfloor - 1} N_{k-2\lfloor \frac{k-1}{2} \rfloor}$$

▶ **Lemma 8.** *For every $k \geq 3$,*

$$N_k = \begin{cases} M_k - (d-2)(M_{k-2} + M_{k-4} + \cdots + M_1) & \textit{if } k \textit{ is odd} \\ M_k - (d-2)(M_{k-2} + M_{k-4} + \cdots + M_2) & \textit{if } k \textit{ is even} \end{cases}$$

4 The Bass Determinant Formula

From the combinatorial lemma established in the previous section and the linearity of trace, we get

$$N_k = \begin{cases} Tr\left(A_k - (d-2)(A_{k-2} + A_{k-4} + \cdots + A_1)\right) & \text{if k is odd} \\ Tr\left(A_k - (d-2)(A_{k-2} + A_{k-4} + \cdots + A_2)\right) & \text{if k is even} \end{cases}$$

Recall that

$$\sum_{0 \leq j \leq k/2} A_{k-2j} = (d-1)^{k/2} U_k\left(\frac{A}{2\sqrt{d-1}}\right)$$

So for odd k

$$\begin{aligned} &A_k - (d-2)(A_{k-2} + A_{k-4} + \cdots + A_1) \\ &= (A_k + A_{k-2} + \cdots + A_1) - (d-1)(A_{k-2} + A_{k-4} + \cdots + A_1) \\ &= (d-1)^{k/2} U_k\left(\frac{A}{2\sqrt{d-1}}\right) - (d-1)^{k/2} U_{k-2}\left(\frac{A}{2\sqrt{d-1}}\right) \end{aligned}$$

Similarly for even k,

$$\begin{aligned} &A_k - (d-2)(A_{k-2} + A_{k-4} + \cdots + A_2) \\ &= (A_k + A_{k-2} + \cdots + A_2) - (d-1)(A_{k-2} + A_{k-4} + \cdots + A_2) \\ &= (d-1)^{k/2} U_k\left(\frac{A}{2\sqrt{d-1}}\right) - (d-1)^{k/2} U_{k-2}\left(\frac{A}{2\sqrt{d-1}}\right) + (d-2)I \end{aligned}$$

As it so happens, the polynomial

$$U_k(x) - U_{k-2}(x) = 2T_k(x)$$

where $T_k(x)$ is called the *Chebyshev polynomial of the first kind* of order k. The Chebyshev polynomials of the first kind are defined in a way very similar to the Chebyshev polynomials of the second kind:

$$T_0(x) = 1$$

$$T_1(x) = x$$

and for $k \geq 2$,

$$T_k(x) = 2xT_{k-1}(x) - T_{k-2}(x)$$

It is easy to show that $T_k(x)$ has a generating function

$$\sum_{k=0}^{\infty} T_k(x) t^k = \frac{1 - xt}{1 - 2xt + t^2}$$

It is convenient to express N_k in terms of Chebyshev polynomials of the first kind as follows:

$$N_k = \begin{cases} Tr\left(2(d-1)^{k/2}T_k\left(\frac{A}{2\sqrt{d-1}}\right)\right) & \text{if k is odd} \\ Tr\left(2(d-1)^{k/2}T_k\left(\frac{A}{2\sqrt{d-1}}\right) + (d-2)I\right) & \text{if k is even} \end{cases}$$

This simplifies to

$$N_k = \begin{cases} \sum_{j=0}^{n-1} 2(d-1)^{k/2}T_k\left(\frac{\mu_j}{2\sqrt{d-1}}\right) & \text{if k is odd} \\ n(d-2) + \sum_{j=0}^{n-1} 2(d-1)^{k/2}T_k\left(\frac{\mu_j}{2\sqrt{d-1}}\right) & \text{if k is even} \end{cases}$$

The generating function for N_k is given by

$$\begin{aligned} \sum_{k=1}^{\infty} N_k t^k &= n(d-2)(t^2+t^4+t^6+\dots) + \sum_{k=1}^{\infty} t^k \left(\sum_{j=0}^{n-1} 2(d-1)^{k/2}T_k\left(\frac{\mu_j}{2\sqrt{d-1}}\right)\right) \\ &= n(d-2)(t^2+t^4+t^6+\dots) + \sum_{j=0}^{n-1}\left(\frac{2-\mu_j t}{1-\mu_j t+(d-1)t^2} - 2\right) \\ &= n(d-2)\frac{t^2}{1-t^2} + \sum_{j=0}^{n-1} \frac{\mu_j t - 2(d-1)t^2}{1-\mu_j t+(d-1)t^2} \end{aligned}$$

Thus,

$$N_1 + N_2 t + N_3 t^2 + \dots = n(d-2)\frac{t}{1-t^2} + \sum_{j=0}^{n-1} \frac{\mu_j - 2(d-1)t}{1-\mu_j t+(d-1)t^2}$$

While this expression does not seem very elegant stated this way, observe that the derivative of $1-t^2$ is $-2t$, and the derivative of $1-\mu_j t+(d-1)t^2$ is $-\mu_j + 2(d-1)t$. Rewriting the above expression to highlight this observation,

$$N_1 + N_2 t + N_3 t^2 + \dots = -\frac{n(d-2)}{2}\frac{-2t}{1-t^2} - \sum_{j=0}^{n-1} \frac{-\mu_j + 2(d-1)t}{1-\mu_j t+(d-1)t^2}$$

This suggests that we could integrate both sides to obtain

$$\begin{aligned} N_1 t + N_2\frac{t^2}{2} + N_3\frac{t^3}{3} + \dots &= -\frac{n(d-2)}{2}\log(1-t^2) - \sum_{j=0}^{n-1}\log(1-\mu_j t+(d-1)t^2) \\ &= -\left(\frac{nd}{2} - n\right)\log(1-t^2) - \log\left(\prod_{j=0}^{n-1} 1-\mu_j t+(d-1)t^2\right) \\ &= -(|E|-|V|)\log(1-t^2) - \log\left(det(I-At+(d-1)t^2)\right) \end{aligned}$$

Now since we know that the Ihara zeta function $\zeta_G(t)$ has the expression

$$\zeta_G = exp\left(N_1 t + N_2\frac{t^2}{2} + N_3\frac{t^3}{3} + \dots\right)$$

we now have the familiar determinant formula for the zeta function in terms of the adjacency matrix:

► **Theorem 9** (Bass's determinant formula)**.** *Let $d \geq 3$ and $G = (V, E)$ be a d-regular connected graph with adjacency matrix A. Then*

$$\zeta_G(t) = \frac{(1-t^2)^{|V|-|E|}}{det(I-At+(d-1)t^2)}$$

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