Expander Graphs

by

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Abstract

In this thesis, we investigate the expansion properties of regular graphs. By definition, an (α, β, k, n)-expander is a k-regular graph where any subset of size at most αn is adjacent to at least βn vertices. The expansion of a subset is the ratio of the size of its set of neighbors to its own size. Expander graphs are extensively used in Computer Science, in areas ranging from parallel and distributed computation to complexity theory and cryptography.

Random graphs are known to be good expanders; the expansion of their linear-sized subsets is roughly $k-1$. The explicit construction of graphs with provably good expansion turns out to be a much more difficult problem, however.

The best currently known techniques for bounding the expansion from below is by analyzing the spectrum of the adjacency matrix of the graph. The best previously known lower bound on the expansion of linear-sized subsets of k-regular graphs based on this approach was roughly $k/4$. This bound was attained by Ramanujan graphs, which have asymptotically optimal second eigenvalue. Ramanujan graphs are the best known explicit expanders, and have been constructed explicitly by Lubotzky, Phillips, and Sarnak, and independently by Margulis.

We improve the lower bound on the expansion of Ramanujan graphs to approximately $k/2$. Moreover, we construct a family of k-regular graphs with asymptotically optimal second eigenvalue and linear expansion equal to $k/2$. This shows that $k/2$ is the best bound one can obtain using the second eigenvalue method. The bound $k/2$ coincides with an important combinatorial property: if a subset has expansion greater than $k/2$, a constant fraction of its nodes have unique neighbors. This property was required in some applications, such as the construction of non-blocking networks. We also show that the provable expansion (in polynomial time) of random k-regular graphs is at least $k/2 - O(k^{3/4}\log^{1/2} k)$. We establish that subsets of sublinear size of the LPS-M graphs have expansion greater than $k/2$.

We also analyze the relation between the second eigenvalue and other combinatorial properties, such as average degree of induced subgraphs and diameter. In the first case, we show an upper bound of roughly $1+\sqrt{k-1}$ on the average degree of linear-sized induced subgraphs of Ramanujan graphs. This compares positively with the classical bound $2\sqrt{k-1}$. In the second case, we show that the classical bound $2\log_{k-1} n$ cannot be improved using the spectral method. We also study the relation between the diameter, girth, and subsequent eigenvalues of a graph.

Given a graph H, we exhibit a necessary and sufficient condition for the existence of a family of k-regular graphs with a given asymptotic bound on the second largest eigenvalue and that contain H as an induced subgraph.

As a byproduct of our techniques, we establish improved bounds on random walks on expanders. We also obtain explicit constructions of selection networks of asymptotic size $3n\log_2 n$. This compares positively with the previous bound $6n\log_2 n$. We show that Ramanujan graphs of degree at least 7 are extrovert graphs. This improves the previously known bound 15. From any family of k-regular Ramanujan graphs with high girth, we show how to construct a family of $k(k-1)^t$-regular non-Ramanujan graphs with linear expansion at least $k(k-2)(k-1)^{t-1}/2$, for any integer $t \geq 1$.

We also give bounds on the chromatic polynomial and the number of acyclic orientations of a graph. The number of acyclic orientations arises in various decision and sorting problems, and is

equal to the absolute value of the chromatic polynomial evaluated at -1. We obtain upper bounds in terms of the eigenvalues of the Laplacian, and lower bounds in terms of the degree sequence. We show that the number of acyclic orientations of graphs with girth at least 5 is larger than what was previously known.

Section 5.3 is joint work with Noga Alon, and Chapter 6 is joint work with Leonard Schulman.

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Contents

1 Introduction **1**

1.1 Previous work 2

1.2 Classification of expanders 5

1.3 Our main results 6

1.4 Bounds on the chromatic polynomial and the number of acyclic orientations of a graph 8

1.5 Outline of thesis 9

2 Intuition and Basic Ideas **11**

2.1 Notation, definitions, and background 11

2.2 A proof of Tanner's result 13

2.3 Improved Expansion 14

3 Bounds on the Expansion **19**

3.1 Main lemma 19

3.2 Lower bounds on the expansion and on the average degree 26

3.3 Lower bounds on the expansion of $N(X)$ and on $|N^t(X)|$, for $t \geq 2$. 28

3.4 A family of almost Ramanujan graphs with expansion $k/2$ 31

3.5 Expansion of subsets of sublinear size 40

4 Other results and Applications **43**

4.1 Random walks and bounds on the spectrum of induced subgraphs 44

4.2 Spectrum of collapsed graphs 46

4.3 Examples and applications 49

5 Diameter and Eigenvalues **51**

5.1 Bounds on the distance between two subsets 51

5.2 Relation with subsequent eigenvalues 54

5.3 Tightness of bounds 56

6 Bounds on the Chromatic Polynomial and on the Number of Acyclic Orientations of a Graph **61**

6.1 Acyclic Orientations and Spanning Trees 62

6.2 Estimates on the Determinant of the Kirchhoff Matrix 64

6.2.1 Regular Graphs 64

6.2.2 General Graphs 66

6.3 Example 67

6.4 Bounds on the Chromatic Polynomial at Negative Values 69

6.4.1 Upper Bound on $\bar{\chi}_G$ 69

6.4.2 Lower Bound on $\bar{\chi}_G$ 70

6.5 Improved Lower Bound for degree 3, girth ≥ 5 72

Chapter 1

Introduction

Expander graphs are widely used in Computer Science, in areas ranging from parallel computation [1, 8, 42, 55, 66] to complexity theory and cryptography [2, 9, 32, 67]. Given an undirected k-regular graph $G = (V, E)$ and a subset X of V, the expansion of X is defined to be the ratio $|N(X)|/|X|$, where $N(X) = \{w \in V : \exists v \in X,\ (v, w) \in E\}$ is the set of neighbors of X. An (α, β, k, n)-expander is a k-regular graph on n nodes such that every subset of size at most αn has expansion at least β. The range of the subsets whose expansion is relevant and the magnitude of the expansion needed depends on the nature of the application.

It is known that random regular graphs are good expanders. For example, it is not hard to show that for any $\beta < k - 1$, there exists a constant α such that, with high probability, all the subsets of a random k-regular graph of size at most αn have expansion at least β. However, the explicit construction of expander graphs is much more difficult. Moreover, the provable expansion properties of the best known explicit expanders fall behind the expansion properties of random graphs. Finally, although some of the explicit constructions are simple to describe, little is known about the combinatorial structure of these graphs.

In this thesis, we improve the known lower bounds for the expansion of small subsets of the best known explicit expanders, and the provable expansion (in polynomial time) of random regular graphs. Also, we show that the bound we get cannot be substantially improved by using the best known technique for lower bounding the expansion, namely the spectral method. We also study other graph theoretic properties of expander graphs, such as the diameter and the degree of induced subgraphs on small subsets. A part of the thesis will be devoted to the related problem of bounding the number of acyclic orientations and the chromatic polynomial of a graph.

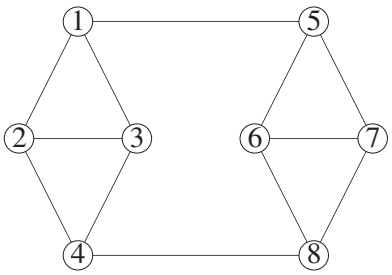


Figure 1-1: An $(1/2, 3/2, 3, 8)$-expander. The set of neighbors of $X = \{2, 3, 8\}$ is $\{1, 2, 3, 4, 6, 7\}$. The expansion of X is 2.

1.1 Previous work

The first explicit construction of an infinite family of expanders was discovered by Margulis [48] in 1973. He proved a lower bound on the expansion that exceeds 1 by an undetermined but positive factor. He used bipartite 5-regular graphs, where the set of inputs and the set of outputs are copies of $(Z/mZ)^2$, and an input node (u, v) is connected to the output nodes (u, v), $(u + 1, v)$, $(u, v + 1)$, $(u, u + v)$ and $(-v, u)$. (Since these graphs are bipartite, the expansion of the subset consisting of one side of the partition is 1, although its size is half the total number of nodes. Generally, in the bipartite case, we are interested in the expansion of subsets lying in one side of the partition, whose size is usually denoted by n. Bipartite expanders are sometimes called magnifiers. It is easy to construct magnifiers from expanders with the same expansion properties; we limit our discussion to expanders in this thesis.) The proof that these graphs are expanders is based on deep results in group representation theory. In 1981, Gabber and Galil [30] constructed similar graphs and gave an estimate of their expansion coefficient using techniques from harmonic analysis. Their results were improved in [5, 37] using techniques from linear algebra.

The best currently known method to calculate lower bounds on the expansion in polynomial time relies on analyzing the second eigenvalue of the graph. Since the adjacency matrix A is symmetric, all its eigenvalues are real and will be denoted by $\lambda_0 \geq \lambda_1 \geq \ldots \lambda_{n-1}$. We remind the reader that the adjacency matrix is the $0-1$ $n \times n$ matrix indexed by the vertices of the graph and whose entry (i, j) is equal to 1 if and only if (i, j) is an edge.

The largest eigenvalue is $\lambda_0 = k$ because the graph is k-regular. Since G is connected, we know that k is a simple eigenvalue and that $-k$ is an eigenvalue if and only if the graph is bipartite. Tanner [64] proved that for any subset X of V,

$$|N(X)| \geq \frac{k^2|X|}{\lambda^2 + (k^2 - \lambda^2)|X|/n}, \tag{1.1}$$

where $\lambda = \max(\lambda_1, |\lambda_{n-1}|)$ is the second largest eigenvalue in absolute value. Therefore, in order

$$A = \begin{pmatrix} 0 & 1 & 1 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 1 & 1 & 0 \end{pmatrix}$$

Eigenvalues of A: $\{3, \sqrt{5}, 1, -1, -1, -1, -1, -\sqrt{5}\}$

Figure 1-2: The adjacency matrix A of G and its eigenvalues.

to get high expansion, we want to find graphs with λ as small as possible. However, there is a limitation to this method. Indeed, Alon and Boppana [3] (see [45, 53] for the proof) showed that, for any sequence $G_{n,k}$ of k-regular graphs on n vertices, $\liminf \lambda(G_{n,k}) \geq 2\sqrt{k-1}$ as n goes to infinity. Therefore, even for sparse sets, the best expansion coefficient we can obtain by applying Tanner's result is $\frac{k^2}{4(k-1)} \approx k/4$. This bound is achieved by graphs for which $\lambda \leq 2\sqrt{k-1}$. These graphs, called Ramanujan graphs, have been explicitly constructed by [45, 49] for many pairs (k, n). Note that if the graph is bipartite, Eq. 1.1 reduces to $|N(X)| \geq |X|$ since $\lambda = k$. However, using Tanner's original result, it can be shown that in the bipartite case Eq. 1.1 remains valid if λ is replaced by λ_1 and n is replaced by $n/2$.

By definition, a Ramanujan graph is a connected k-regular graph whose eigenvalues $\neq \pm k$ are at most $2\sqrt{k-1}$ in absolute value. Alon [3] conjectured in 1986 that the second largest eigenvalue of a random k-regular graph is $2\sqrt{k-1} + o(1)$ with high probability as the number of nodes goes to infinity. This conjecture was partially solved by Friedman [29, 27] who showed that $\lambda(G) \leq 2\sqrt{k-1} + O(\log k)$ with high probability. (In fact, experimental results [28] show that "most" regular graphs are Ramanujan.) Tanner's result then implies that, for most k-regular graphs, we can check in polynomial time that the expansion is at least $k/4 - O(\sqrt{k}\log k)$. The relationship between the eigenvalues of the adjacency matrix and the expansion coefficient has also been investigated in [3, 5, 6, 19], but the bound they get, when applied to non-bipartite Ramanujan graphs and for sufficiently large k, is no better than Tanner's bound. Fig. 1.1 represents an $(1/2, 3/2, 3, 8)$-expander. This graph is Ramanujan since its second largest eigenvalue $\sqrt{5}$ is less than $2\sqrt{2}$ (Fig. 1.2).

Ramanujan graphs are quite easy to construct. We describe below [45] a class of non-bipartite Ramanujan graphs $Y_{p,q}$ on $q+1$ vertices, each of degree degree $p+1$, where p and q are primes congruent to 1 modulo 4. From elementary number theory, we know the existence of $p+1$ vectors

$a = (a_0, a_1, a_2, a_3) \in (2\mathcal{N}+1) \times (2\mathcal{Z})^3$ such that $||a||^2 = a_0^2 + a_1^2 + a_2^2 + a_3^2 = p$. Let γ_a be the matrix

$$\gamma_a = \begin{pmatrix} a_0 + ia_1 & a_2 + ia_3 \\ -a_2 + ia_3 & a_0 - ia_1 \end{pmatrix},$$

where i is an integer such that $i^2 \equiv -1 \pmod{q}$. The $p+1$ matrices γ_a's act on $P^1(F_q) = \{0, 1, \ldots, q-1, \infty\}$ in the usual way:

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} z = \frac{az+b}{cz+d} \pmod{q}.$$

Define the graphs $Y_{p,q}$ on $P^1(F_q)$ by joining each z to $\gamma_a(z)$. The proof that these graphs are Ramanujan graphs relies on a theorem that approximates the number $r_m(n)$ of ways to represent an integer n as $n = x_0^2 + mx_1^2 + mx_2^2 + mx_3^2$, where m is a fixed positive integer and the x_i's are integers. More precisely, we have [45]

$$r_m(n) = c_m \sum_{d|n} d + \beta_m(n),$$

where $\beta_m(n)$ is an "error" term. The Ramanujan conjecture, proved in [25], states that $\beta_m(n) = O(n^{1/2+\epsilon})$, for any $\epsilon > 0$. The proof of this conjecture uses very sophisticated mathematical techniques and has lead to extensions considered a crowning achievement in Mathematics. Morgenstern [51] constructed explicit Ramanujan graphs of degree $s+1$, where s is any prime power.

The Ramanujan graphs constructed independently by Margulis [49] and Lubotzky, Phillips and Sarnak [45] have other extremal properties. For example, in the bipartite case, it can be shown [12, 49] that $c(G) = (4/3 + o(1)) \log_{k-1} n$, where $c(G)$ is the *girth* of G, i.e. the length of its shortest cycle. This bound beats all the previous bounds, except for the cubic sextet graphs [13, 69]. It even beats the lower bound $\log_{k-1} n - O(1)$ on the girth obtained by Erdös and Sacks [34] using a non-constructive method. Note that the girth of any k-regular graph is at most about $2\log_{k-1} n$. It can also be shown that the diameter of Ramanujan graphs is at most $2\log_{k-1} n + O(1)$. It is not difficult to show that the diameter of any k-regular graph is at least $\log_{k-1} n - O(1)$. As was observed by Pippenger, Ramanujan graphs can be used to construct acyclic superconcentrators of density 64, which is the smallest known density obtained by explicit constructions. Recall that a superconcentrator of density k is a graph with n inputs and n outputs and at most kn edges such that any subset of inputs can be connected to any subset of outpus of equal size in an edge disjoint fashion.

Alon [3] showed that a k-regular graph is an expander if and only if there is a gap between k and the second largest eigenvalue. More precisely, if for any subset X of size at most $n/2$, we have

$|N(X)-X| \geq c|X|$, then $k-\lambda_1 \geq c^2/(4+2c^2)$. Conversely, for any subset X of size at most $n/2$, we have $|N(X)-X| \geq c|X|$, where $c = 2(k-\lambda_1)/(k+2(k-\lambda_1))$. An excellent survey on expanders is found in [10]. Chung [21] proved that graphs with small λ have small diameter. The recent books by Sarnak [58] and Lubotzky [44] give a mathematical background on the construction of Ramanujan graphs. Other results about graph spectra are contained in [11, 23, 24].

1.2 Classification of expanders

The amount of expansion needed depends on the application where the expanders are used. Following Pippenger [56], we classify expanders into three categories depending on the expansion needed and the restriction on the size of expanding subsets.

- Grade 1. Sufficiently small subsets must have expansion at least c, where c is a constant greater than 1 depending on the application. In some cases, the expanding subsets could be as large as almost half the size of the expander [30].

- Grade 2. Linear-sized subsets have expansion greater than $c\sqrt{k}$, where c is a constant that depends on the application. Token distribution is an example [18, 54].

- Grade 3. Linear-sized subsets have expansion at least ck, where c is constant greater than $1/2$. An example is the initial construction of non-blocking networks [8].

Random regular graphs have sufficient expansion for all the applications of expanders that we know of. The first explicit constructions [30, 37, 48] are (at least provably) of grade 1.

Ramanujan graphs [45, 49] are expanders of grade 2. We don't know of explicit constructions of expanders of grade 3. We explain briefly why some applications required an expansion greater than $k/2$ of linear-sized subsets. Indeed, if the expansion of a subset X is greater than $k/2$, a constant fraction its nodes have *unique neighbors*, i.e. neighbors adjacent to only one node in X. This allows the construction of a matching between X and $N(X)$ in a logarithmic number of steps and using only *local computations*. This can be done by matching the nodes having unique neighbors to their neighbors, then eliminating the matched nodes from X and recursing.

Recently, Kelsen [41] designed a randomized local algorithm for finding such a matching in a logarithmic number of steps provided that the expansion is $\Omega(\sqrt{k \log k})$. Pippenger [56] found a general framework to show that expanders of grade 1 are sufficient in applications where expanders of degree 2 or 3 were required.

We note that in many applications in complexity theory and cryptography, the properties of expanders used are related to random walks and are directly deduced from the spectrum of the graph rather than its expansion properties.

In a recent work, Nisan and Zuckerman [70] construct explicit expanders beating the eigenvalue bounds. They are interested in the expansion of subsets of sublinear size, and the expanders they construct have non-constant degree. We also mention the explicit construction by Morgenstern [52] of natural expanders with a set of input nodes and a set of output nodes, where the number of input nodes exceeds the number of output nodes by a small multiplicative factor.

1.3 Our main results

We define the linear expansion of a family of k-regular graphs G_n on n vertices to be the best lower bound on the expansion of subsets of size up to αn, where α is an arbitrary small positive constant, that is

$$\sup_{\alpha>0} \inf_{n} \inf_{X} \frac{|N(X)|}{|X|},$$

where X ranges over the subsets of G_n of size at most αn. Our aim is to calculate the best linear expansion one can prove using the second eigenvalue technique. We saw in Section 1.2 why an expansion greater than $k/2$ was required in some applications. We show that if (G_n) is a family of k-regular graphs whose second largest eigenvalue is upper bounded by $\tilde{\lambda}$, the linear expansion of (G_n) is at least $(k/2)\left(1-\sqrt{1-(4k-4)/\tilde{\lambda}^2}\right)$. In particular, the expansion of linear-sized subsets of Ramanujan graphs is lower bounded by a factor arbitrary close to $k/2$. More precisely, for any $\beta < k/2$, there exists $\alpha > 0$ such that any k-regular Ramanujan graph on n nodes is an (α, β, k, n)-expander. On the other hand, for any integer k such that $k-1$ is a prime congruent to 1 modulo 4, and for any function m of n such that $m = o(n)$, we explicitly construct an infinite family of k-regular graphs G_n on n vertices such that $\lambda(G_n) \leq (2+o(1))\sqrt{k-1}$ and G_n contains a subset of size $2m$ with expansion $k/2$. Since such a family has asymptotically optimal second eigenvalue, this shows that $k/2$ is essentially the best lower bound on the linear expansion one can obtain by the second eigenvalue method. However, it is still an open question whether there exists a family of Ramanujan graphs with linear expansion at most $k/2$. Our results provide an efficient way to test that the expansion of linear sized subsets of random graphs is at least $k/2 - O(k^{3/4}\log^{1/2} k)$.

We also analyze the *edge expansion* of subsets of k-regular graphs, defined as the ratio of the number of edges leaving the subset to its size. Our results are best expressed in terms of the average degree of the induced subgraph. The two quantities, edge expansion and average degree, obviously sum up to k. We show that the average degree of the induced subgraphs on linear-sized subsets of a k-regular graph G is upper bounded by a factor arbitrary close to $1 + \tilde{\lambda}/2 + \sqrt{\tilde{\lambda}^2/4 - (k-1)}$, where $\tilde{\lambda} = \max(\lambda, 2\sqrt{k-1})$. This bound is equal to $1+\sqrt{k-1}$ in the case of Ramanujan graphs, improving upon the previously known bound [4] of $2\sqrt{k-1}$. Our method gives lower bounds on the size of $N^t(X)$, the set of nodes at distance t from X, for integer $t \geq 2$. In particular, we show that the size of $N^t(X)$ is at least $(k-1)^t|X|/2$. We also establish that if X is a linear-sized subset of a

Ramanujan graph, the expansion of $N(X)$ is at least $2k/3 - O(1)$. We also study the expansion of subsets of sublinear size. Using the fact that the known explicit Ramanujan graphs have high girth, we show that subsets of sublinear size of these graphs have expansion greater than $k/2$.

Our main tool is a lemma that describes small subsets of an expander. More precisely, given a graph H, we exhibit an asymptotic necessary and sufficient condition for the existence of a family of k-regular graphs that have a given bound on the second eigenvalue and that contain H as an induced subgraph. Most of our results mentioned above follow by applying this lemma to the expanding subset X itself, or to its union with its set of neighbors, or to the set of nodes at distance at most t from X.

As an application of the improved expansion of Ramanujan graphs, we can build explicit selection networks of asymptotic size $(3+o(1))n\log_2 n$, improving on the bound $6n\log_2 n$ that was previously known. As defined in [55], a selection network is a network of comparators that classifies a set of n numbers, where n is even, into two subsets of $n/2$ numbers such that any element in the first set is smaller than any element in the second set. Our results also show that Ramanujan graphs of degree at least 7 are extrovert graphs. We say that a graph is extrovert if all its linear-sized subsets contain a constant fraction of extrovert nodes; a node is extrovert with respect to a subset if more than half of its neighbors are outside the subset. Such graphs have been used [18] to solve the token distribution problem. Classical results [4] require the degree to be at least 15. As a byproduct of our techniques, we obtain improved results on random walks on expanders. Finally, we show how to construct, from any family of k-regular Ramanujan graphs with high girth, a family of $k(k-1)^t$-regular non-Ramanujan graphs with linear expansion at least $k(k-2)(k-1)^{t-1}/2$, for any integer $t \geq 1$.

We use Chebychev polynomials to give lower bounds on the size of $N^t(X)$, the set of nodes reachable from X by a path of length t. This leads us to study the relation between the diameter $D(G)$ of a graph and its second largest eigenvalue. This problem has already been studied in [6, 21, 22, 45, 57, 58]. It is known that [22, 57, 58]

$$D(G) \leq \left\lfloor \frac{\cosh^{-1}(n-1)}{\cosh^{-1}(k/\lambda)} \right\rfloor + 1 \tag{1.2}$$

For fixed n and k, the right-hand side is an increasing function of λ. When $\lambda = 2\sqrt{k-1}$, it is roughly $2\log_{k-1} n$. We show that Eq. 1.2 is tight by exhibiting, for many integers k, an infinite family of graphs on n nodes with diameter $(2+o(1))\log_{k-1} n$ and $\lambda \leq (2+o(1))\sqrt{k-1}$. This essentially shows that the bound $(2+o(1))\log_{k-1} n$ is the best one can obtain by the second eigenvalue method. We generalize Eq. 1.2 by giving an upper bound on the distance between subsets of arbitrary size. This gives a simple proof of a recent result by Quenell [57] relating diameter, second eigenvalue, and girth of a graph. We also establish a tight relation between the diameter and subsequent eigenvalues of

a graph. To our knowledge, this is the first isoperimetric inequality that involves the subsequent eigenvalues and does not depend on the second eigenvalue.

1.4 Bounds on the chromatic polynomial and the number of acyclic orientations of a graph

We successfully apply algebraic and probabilistic techniques to study another graph theoretical problem: bounding the chromatic polynomial and the number of acyclic orientations of a graph. The chromatic polynomial of a graph is the polynomial which, when evaluated at an integer point m, counts the number of ways to color the graph with at most m colors. The importance of the chromatic polynomial, introduced by Birkhoff [14] in 1932, is related to the fact that its exact determination allows the calculation of the chromatic number of a graph.

We comment on the relation between expanders and the number of acyclic orientations of a graph. It should be intuitively clear that graphs with high girth have many acyclic orientations. Also, expander graphs tend to have high girth. Therefore, the existence of a bound on the number of acyclic orientations in terms of the eigenvalues of the Laplacian is not surprising. Given an undirected graph G, the number of acyclic orientations of G, $\alpha(G)$, is the number of ways in which all of its arcs can be directed without introducing directed cycles. number of acyclic orientations was first considered by Stanley [60] in 1973, who pointed out a remarkable characterization of this number as the value at -1 of the chromatic polynomial of the graph. Since then interest has arisen in $\alpha(G)$ in computer science, because $\log \alpha(G)$ is a lower bound on the computational complexity of various decision and sorting problems [31, 46].

However Stanley's result does not provide an effective indication of the magnitude of $\alpha(G)$. In fact Linial has shown that the problem of exact determination of the number of acyclic orientations of a graph is complete for the complexity class #P [43]. (More generally Jaeger, Vertigan and Welsh [26] have shown that evaluation of the Tutte polynomial of the cycle matroid of a graph is #P complete at all but nine special points; $\alpha(G)$ is the value of the Tutte polynomial at a non-special point.) This hardness result suggests that effective exact expressions for $\alpha(G)$ are an unlikely prospect, and provides additional motivation for obtaining bounds on this number. The problem of finding a fully polynomial approximation scheme for counting the number of acyclic orientations of a graph remains open despite many efforts.

The first bound on $\alpha(G)$, due to Fredman [33] and to Manber and Tompa [46], was the upper bound $\alpha(G) \leq \prod_{v \in G}(d_v + 1)$, where d_v represents the degree of vertex v. As noted in [31], this bound is sometimes close to the truth, as for the case of $G = K(a, b)$ with $b >> a$. In this case $\alpha(G) \sim a!(a+1)^b$. The second such result was the following lower bound, also in terms of the degree sequence of the graph [31]. Let $f(x) = (x!)^{1/x}$. Then $\alpha(G) \geq \prod_{v \in G} f(d_v + 1)$. This bound is tight in

the case of the complete graph. The gap between these two bounds can be estimated using Stirling's formula, and is bounded by about e^n, where n is the number of vertices in G.

We present a new upper bound on the number of acyclic orientations of a graph. We show that the degree bound $\prod_{v \in G}(d_v + 1)$ can be replaced by a spectral bound $\prod_{i=1}^{n}(\mu_i + 1)$ where $\{\mu_i\}$ are the eigenvalues of the Laplacian of the graph. Thus the bound is the determinant of the sum of the Laplacian of the graph and the identity matrix; or, the Kirchhoff matrix of the graph. We then show that this bound always improves upon the degree bound of [46]. For k-regular graphs, we prove that the determinant of the Kirchhoff matrix is asymptotically bounded by roughly $(k + 1/2)^n$; and that for the LPS-M graphs [45, 49], this is a nearly tight estimate of the Kirchhoff determinant. We also give an asymptotic bound, in terms of the degree sequence, on the Kirchhoff determinant in general graphs. As an example we bound the number of acyclic orientations of the hypercube from above and below.

We also present a new approach to giving lower bounds on the number of acyclic orientations of a graph, using the probabilistic method.

We extend our study of acyclic orientations to the study of χ_G at arbitrary negative values. We show that the inequality between the number of acyclic orientations and the determinant of the Kirchoff matrix extends to an inequality between $\det(Q + wI)$ and $(-1)^n \chi_G(-w)$ for $w \geq 0$, where Q is the Laplacian of a graph and χ is its chromatic polynomial. We provide a simple probabilistic proof of the aforementioned lower bound on $\alpha(G)$ for arbitrary graphs. We also show how this proof extends to give a lower bound on $(-1)^n \chi_G(-w)$ for arbitrary positive w.

We show how to use the probabilistic lower bound method to take advantage of a structural assumption on the graph, namely that it has no 3-cycles or 4-cycles (i.e. girth ≥ 5). In this case we can prove lower bounds for $\alpha(G)$ and for the chromatic polynomial that are strictly stronger than those possible for an arbitrary graph.

1.5 Outline of thesis

In Chapter 2, we give some intuition behind our proofs. Chapter 3 contains our main results on expanders. Some of the work in this chapter has appeared in extended abstract form [38, 39]. In Chapter 4, we present applications to our results, and we establish general results in algebraic graph theory. In Chapter 5, we analyze the relation between eigenvalues and diameter. This chapter contains joint work with Noga Alon. Chapter 6 contains our results on the chromatic polynomial and number of acyclic orientations of a graph. This chapter is joint work with Leonard Schulman, and is based on [40].

Chapter 2

Intuition and Basic Ideas

The main object of this chapter is to familiarize the reader with the main tools for bounding the expansion from below. In Section 2.1, we give some definitions and basic results on the adjacency matrix. We also state elementary facts in linear algebra, whose proof can be found in introductory books in linear algebra, such as [47, 62]. In Section 2.2, we give a proof of Tanner's result which is basically the same as the original proof. In Section 2.3, we show how to improve Tanner's result to get a better bound on the expansion. In particular, we get a lower bound of $5k/16 - O(1)$ on the expansion of small subsets of Ramanujan graphs, which already beats the bound $k/4$ that follows from Tanner's result. Our method illustrates a key idea that we will use in the next chapter: it is possible to get better bounds on the expansion by considering the set of nodes at distance t from X, for $t \geq 1$.

2.1 Notation, definitions, and background

Throughout the thesis, $G = (V, E)$ will denote an undirected graph on a set V of vertices. Let $L^2(V)$ denote the set of real valued functions on V and $L_0^2(V) = \{f \in L^2(V);\ \sum_{v \in V} f(v) = 0\}$. As usual, we define the scalar product of two vectors f and g of $L^2(V)$ by

$$f \cdot g = \sum_{v \in V} f(v)g(v),$$

and the euclidean norm of a vector f by $||f|| = \sqrt{f \cdot f}$. We denote the adjacency matrix of G by A_G, or simply by A if there is no risk of confusion. The matrix A is the 0-1 $n \times n$ matrix whose (i, j) entry is equal to 1 if and only $(i, j) \in E$. It defines a linear operator in $L^2(V)$ that maps every

vector $f \in L^2(V)$ to the vector Af defined by

$$(Af)(v) = \sum_{(v,w)\in E} f(w). \tag{2.1}$$

This operator is selfadjoint since $\forall f, g \in L^2(V)$ we have

$$(Af) \cdot g = f \cdot (Ag) = \sum_{(v,w)\in E} f(v)g(w). \tag{2.2}$$

We remind the reader that an operator B in a vector space H is said to be selfadjoint if for all vectors f and g in H, $Bf \cdot g = f \cdot Bg$. For any subset W of V, we denote by χ_W the characteristic vector of W:

$$\chi_W(v) = \begin{cases} 1 & \text{if } v \in W \\ 0 & \text{otherwise} \end{cases}$$

The support of a vector $f \in L^2(V)$ is defined to be the set of nodes v for which $f(v) \neq 0$. For any matrix M with real eigenvalues, we denote by $\lambda_i(M)$ the i-th largest eigenvalue of M. Since the adjacency matrix of any graph G is real and symmetric, all its eigenvalues are real. We will denote $\lambda_i(A_G)$ by $\lambda_i(G)$, or simply by λ_i. The same remark holds for $\lambda(G) = \max(\lambda_1(G), |\lambda_{n-1}(G)|)$. For the rest of the chapter, we assume that G is connected and k-regular.

Fact 2.1 *For any vector $g \in L^2(V)$, the sum of the coordinates of Ag is equal to k times the sum of the coordinates of g.*

Proof This follows simply by summing the two sides of Eq. 2.1 for all vertices v. Each term $f(w)$ in the right-hand side will be counted k times. ■

Fact 2.2 *[35, page 314] A selfadjoint operator in a finite dimensional space is diagonalizable in an orthonormal basis.* ■

Fact 2.3 *The vector space $L_0^2(V)$ is invariant under A.* ■

Clearly, the vector χ_V is an eigenvector of A with eigenvalue k. This eigenvalue is simple and is the largest in absolute value [11, page 14]. Denote by $A_{|L_0^2(V)}$ the restriction of A to $L_0^2(V)$, i.e. the operator in $L_0^2(V)$ that coincides with A on $L_0^2(V)$. The operator $A_{|L_0^2(V)}$ is diagonalizable since it is selfadjoint (Fact 2.2), and so the eigenvalues of A consist of k and the eigenvalues of $A_{|L_0^2(V)}$. This is because the eigenvectors of the restriction of an operator B to a vector subspace are also eigenvectors of B with the same eigenvalues. Therefore, the eigenvalues of $A_{|L_0^2(V)}$ are $\lambda_1, \ldots, \lambda_{n-1}$. In particular,

Fact 2.4 *The largest eigenvalue in absolute value of $A_{|L_0^2(V)}$ is λ.* ■

Fact 2.5 *If L is a vector space and B is a selfadjoint operator in L whose largest eigenvalue in absolute value is γ, then $||Bg|| \leq \gamma ||g||$ for any $g \in L$.*

Proof Since B is selfadjoint, it is diagonalizable (Fact 2.2) in an orthonormal basis $(e_0, e_1, \ldots, e_{l-1})$, where $l = \dim L$. Let $g = \sum_{i=0}^{l-1} c_i e_i$ be the decomposition of g in this basis. Then $Bg = \sum_{i=0}^{l-1} \mu_i c_i e_i$, where μ_i is the eigenvalue corresponding to e_i. The square of the norm of g is equal to the sum of the squares of its coordinates in the orthonormal basis $(e_0, e_1, \ldots, e_{l-1})$, that is

$$||g||^2 = \sum_{i=0}^{l-1} {c_i}^2.$$

Similarly,

$$||Bg||^2 = \sum_{i=0}^{l-1} {\mu_i}^2 {c_i}^2.$$

Since ${\mu_i}^2 \leq \gamma^2$, it follows that $||Bg||^2 \leq \gamma^2 ||g||^2$. This concludes the proof. ■

Combining Facts 2.4 and 2.5 yields:

Fact 2.6 *For any $g \in L_0^2(V)$, we have $||Ag|| \leq \lambda ||g||$.* ■

We will often use the following elementary results:

Fact 2.7 (Pythagorean theorem) *If g and h are two orthogonal vectors, then $||g+h||^2 = ||g||^2 + ||h||^2$.* ■

Fact 2.8 (Cauchy-Schwartz inequality) *[35, page 277] For any two vectors g and h, we have $|g \cdot h| \leq ||g||\ ||h||$.* ■

We remind the reader of the O notation. Following [65], we say that $\psi = O(\phi)$ if $|\psi(x)| \leq c\phi(x)$ near some limit, for some positive constant c. In particular, we do not make any assumptions about the sign of ψ.

2.2 A proof of Tanner's result

Let X be a subset of V, and $f = \chi_X$. To get a lower bound on $|N(X)|$, we show that it is sufficient to bound $||Af||$ from above. Then we derive the upper bound on $||Af||$ in terms of λ and $|X|$.

To prove our first claim, we note that the vector Af has support $N(X)$. Moreover, its sum of coordinates is $k|X|$ by Fact 2.1. By convexity of the square function, it follows that its norm is minimal if all of its non-zero coordinates are equal to $k|X|/|N(X)|$. Hence

$$||Af||^2 \geq |N(X)| \frac{k^2|X|^2}{|N(X)|^2} = \frac{k^2|X|^2}{|N(X)|}. \tag{2.3}$$

An alternative way to derive Eq. 2.3 is to apply the Cauchy-Schwartz inequality to the vectors Af and $\chi_{N(X)}$. The scalar product of the vectors Af and $\chi_{N(X)}$ is equal to the the sum of coordinates of Af, which is $k|X|$. On the other hand,

$$|Af \cdot \chi_{N(X)}|^2 \leq ||Af||^2 \, |\chi_{N(X)}|^2 = |N(X)| \, ||Af||^2.$$

Replacing $Af \cdot \chi_{N(X)}$ by $k|X|$ yields Eq. 2.3.

Our next step is to get an upper bound on $||Af||$. Using Fact 2.5 and the fact that k is the largest eigenvalue of A, we have $||Af|| \leq k||f||$. By combining this inequality with Eq. 2.3 and noting that $||f||^2 = |X|$, we get the bound $|N(X)| \geq |X|$, which can be derived directly by combinatorial arguments. In order to get a better bound, we will use the second largest eigenvalue of A. Let $\overline{f}$ and f_0 be the orthogonal projections of f on $\mathcal{R}\chi_V$ (the vector subspace generated by χ_V) and $L_0^2(V)$ respectively. Then $f = \overline{f} + f_0$, since $L_0^2(V)$ is the orthogonal complement of $\mathcal{R}\chi_V$. By linearity, we have $Af = A\overline{f} + Af_0 = k\overline{f} + Af_0$. But $Af_0 \in L_0^2(V)$ by Fact 2.3, and so it is orthogonal to $\overline{f}$. By the Pythagorean theorem, it follows that

$$\begin{aligned} ||Af||^2 &= k^2||\overline{f}||^2 + ||Af_0||^2 \\ &\leq k^2||\overline{f}||^2 + \lambda^2||f_0||^2 \\ &= k^2||\overline{f}||^2 + \lambda^2(||f||^2 - ||\overline{f}||^2) \\ &= \lambda^2||f||^2 + (k^2 - \lambda^2)||\overline{f}||^2 \\ &= \lambda^2|X| + (k^2 - \lambda^2)\frac{|X|^2}{n}. \end{aligned} \tag{2.4}$$

The second equation follows from Fact 2.6. The third equation follows from the Pythagorean theorem applied to f_0 and $\overline{f}$. The last equality follows from the fact that, since $f - \overline{f} \in L_0^2(V)$, the vectors f and $\overline{f}$ have the same sum of coordinates, and so each coordinate of $\overline{f}$ is $|X|/n$. By combining Eqs. 2.3 and 2.4, we get Eq. 1.1. ■

Note that the lower bound on the expansion that follows from Tanner's result increases as the size of X decreases. To explain this, we observe that the smaller $|X|$ is, the larger is the norm of f_0 compared to the norm of $f = \chi_X$. Informally, when $|X|$ is small, the vector f is almost orthogonal to χ_V, and so $||Af||$ is upper bounded by a term close to $\lambda||f||$.

2.3 Improved Expansion

There are two sources of slack in the preceding proof. The first one comes from Eq. 2.3. This inequality is tight only if all the non-zero coordinates of Af are equal. We will construct in the next chapter "nearly Ramanujan" graphs containing a subset X of two vertices and expansion $k/2$, and

such that Eq. 2.3 is tight. Therefore, there exists apparently no way to solve our primary goal (to get an expansion greater than $k/2$) by improving this inequality. It is however possible to improve the lower bound on the expansion that follows from Tanner's result, if this lower bound does not divide k. Indeed, if Eq. 1.1 were tight in this case, Eq. 2.3 would also be tight, and so all the non-zero values of Af would be equal to $k|X|/|N(X)|$, which is not an integer, leading to a contradiction. A similar observation has been used in [19] to improve of Tanner's result in special cases. This improvement seems to be small in almost all interesting cases, however. For example, Tanner's result implies a lower bound close to $k/4$ on the expansion of linear-sized subsets of Ramanujan graphs. This bound divides k, and so it cannot be improved by the aforementioned observation.

The second source of slack is the inequality in Eq. 2.4. This inequality is tight only if $||Af_0|| = \lambda||f_0||$. But the proof of Fact 2.5 shows that this equality holds if and only if f_0 is the sum of an eigenvector of A with eigenvalue λ and eigenvector of A with eigenvalue $-\lambda$. Assume this is the case. Both such eigenvectors are eigenvectors of A^2 with eigenvalue λ^2, and so $A^2 f_0 = \lambda^2 f_0$. By linearity, it follows that

$$A^2 f = A^2 f_0 + A^2 \overline{f} = \lambda^2 f_0 + k^2 \overline{f} = \lambda^2 f + (k^2 - \lambda^2)\overline{f}.$$

But this cannot happen if X is sufficiently small, because the support of the leftmost term is $N^2(X)$, whereas the support of the rightmost term is V. Therefore, the inequality $||Af_0|| \leq \lambda||f_0||$ is strict if $|X|$ is small. By bounding from below the norm of the difference of the squares of the two sides, we will be able to get a quantitative improvement of Tanner's result.

Theorem 2.1 *If $G = (V, E)$ is k-regular, for any subset X of V, we have*

$$\frac{|N(X)|}{|X|} \geq \frac{k^2 + (k^2 - \lambda^2)^2/\lambda^2 k}{\lambda^2 + k^2(k^2 - \lambda^2)|X|/(\lambda^2 n)}$$

In particular, if G is a Ramanujan graph, any subset of size $O(k^{-3}n)$ has expansion at least $5k/16 - O(1)$.

Proof We start by showing a lower bound on the difference $\lambda^2||f_0||^2 - ||Af_0||^2$ in terms of $||A^2 f_0 - \lambda^2 f_0||$.

Claim 2.1

$$\lambda^2||f_0||^2 - ||Af_0||^2 \geq \frac{||A^2 f_0 - \lambda^2 f_0||^2}{\lambda^2}.$$

Proof By bilinearity of the scalar product and Eq. 2.2, we have

$$\begin{aligned} ||A^2 f_0 - \lambda^2 f_0||^2 &= (A^2 f_0 - \lambda^2 f_0) \cdot (A^2 f_0 - \lambda^2 f_0) \\ &= ||A^2 f_0||^2 - 2\lambda^2 A^2 f_0 \cdot f_0 + \lambda^4 ||f_0||^2 \end{aligned}$$

$$= \quad ||A^2 f_0||^2 - 2\lambda^2 ||Af_0||^2 + \lambda^4 ||f_0||^2.$$

Thus our claim reduces to show $||A^2 f_0|| \leq \lambda ||Af_0||$. But this follows from Fact 2.6 since $Af_0 \in L_0^2(V)$. ■

Therefore, in order to get a lower bound on $\lambda^2||f_0||^2 - ||Af_0||^2$, it is sufficient to get a lower bound on the norm of $A^2 f_0 - \lambda^2 f_0$, which we do next. By linearity, we have

$$A^2 f - \lambda^2 f = (A^2 f_0 - \lambda^2 f_0) + (A^2 \overline{f} - \lambda^2 \overline{f}) = (A^2 f_0 - \lambda^2 f_0) + (k^2 - \lambda^2)\overline{f}.$$

But $(A^2 f_0 - \lambda^2 f_0) \in L_0^2(V)$, and so the two vectors $A^2 f_0 - \lambda^2 f_0$ and $(k^2 - \lambda^2)\overline{f}$ are orthogonal. It follows from the Pythagorean theorem that

$$\begin{aligned} ||A^2 f - \lambda^2 f||^2 &= ||A^2 f_0 - \lambda^2 f_0||^2 + (k^2 - \lambda^2)^2 ||\overline{f}||^2 \\ &= ||A^2 f_0 - \lambda^2 f_0||^2 + (k^2 - \lambda^2)^2 \frac{|X|^2}{n} \end{aligned} \tag{2.5}$$

But the vector $A^2 f - \lambda^2 f$ is supported in $N^2(X)$ and, by Fact 2.1, the sum of its coordinates is equal to $(k^2 - \lambda^2)|X|$. Therefore, by a calculation similar to Section 2.2,

$$||A^2 f - \lambda^2 f||^2 \geq (k^2 - \lambda^2)^2 \frac{|X|^2}{|N^2(X)|}.$$

Combining this with Eq. 2.5 yields

$$||A^2 f_0 - \lambda^2 f_0||^2 \geq (k^2 - \lambda^2)^2 \frac{|X|^2}{|N^2(X)|} - (k^2 - \lambda^2)^2 \frac{|X|^2}{n}.$$

Together with Claim 2.1, this implies

$$\lambda^2 ||f_0||^2 - ||Af_0||^2 \geq \frac{(k^2 - \lambda^2)^2}{\lambda^2} \frac{|X|^2}{|N^2(X)|} - \frac{(k^2 - \lambda^2)^2}{\lambda^2} \frac{|X|^2}{n}. \tag{2.6}$$

Eq. 2.6 gives a stronger bound than the inequality $||Af_0|| \leq \lambda ||f_0||$ that we used in Section 2.2 to establish Tanner's result. The rest of the proof is almost identical to the proof in Section 2.2. By using Eq. 2.6 and a calculation similar to Eq. 2.4, it follows that

$$||Af||^2 \leq \lambda^2 |X| + (k^2 - \lambda^2)\frac{|X|^2}{n} - \frac{(k^2 - \lambda^2)^2}{\lambda^2} \frac{|X|^2}{|N^2(X)|} + \frac{(k^2 - \lambda^2)^2}{\lambda^2} \frac{|X|^2}{n}.$$

Using Eq. 2.3 and after some simplifications, we get

$$k^2 \frac{|X|}{|N(X)|} \leq \lambda^2 - \frac{(k^2-\lambda^2)^2}{\lambda^2} \frac{|X|}{|N^2(X)|} + \frac{k^2(k^2-\lambda^2)}{\lambda^2} \frac{|X|}{n}.$$

Note that the smaller the size of $N^2(X)$, the better lower bound on the expansion we get. By upper bounding $|N^2(X)|$ by $k|N(X)|$, we get the first part of the theorem. The second part follows immediately. ■

It is possible to improve Theorem 2.1 by a more careful treatment of the inequalities involved. In particular, one can show that for Ramanujan graphs, any subset of size at most $k^{-3}n$ has expansion at least $k/3 - O(1)$. We omit the proof, which can be found in [38]. This bound seems to be the best (up to an additive constant) one can obtain by considering only the set $N^2(X)$. We will get an even better bound on the expansion in the next chapter by using a different approach and considering the sets $N^t(X)$, for $t \geq 3$.

Chapter 3

Bounds on the Expansion

This chapter contains our main results: getting the best possible expansion for linear-sized subsets using the spectral method. Our approach to lower bounding the expansion is to use the second largest eigenvalue to derive information on the structure of subgraphs induced on linear-sized subsets. Roughly speaking, we show that the largest eigenvalue of a matrix associated with an induced subgraph is upper bounded by the second largest eigenvalue of the graph. We prove this result in Section 3.1. We then use it in Section 3.2 to derive a lower bound on the expansion of X and an upper bound on its average degree. We use it again in Section 3.3 to bound from below the expansion of $N(X)$ and the size of $N^t(X)$, for integer $t \geq 2$, where $N^t(X)$ is the set of nodes that can be reached from X by a path of length t, that is,

$$\underbrace{N(N(\ldots N(}_{t \text{ times}} X))\ldots).$$

In Section 3.4, we construct k-regular graphs with linear expansion $k/2$ and asymptotically optimal second largest eigenvalue, for any integer k such that $k-1$ is a prime congruent to 1 modulo 4. We generalize this result as follows: given a graph H, we exhibit an asymptotic necessary and sufficient condition for the existence of a family of k-regular graphs that contains H as an induced subgraph, and whose second largest eigenvalue does not exceed a given bound. In Section 3.5, we study the expansion properties of subsets of sublinear size of the LPS-M graphs. In particular, we show that the expansion of subsets of size at most n^γ is at least $k-2$, if $\gamma = \gamma(k)$ is sufficiently small.

3.1 Main lemma

We start by stating basic facts that we will use throughout the chapter. We then prove the main lemma (Theorem 3.1) that we will use later to derive lower bounds on the expansion. We first fix

some notations that we will use throughout this chapter. Given a subset W of nodes of a graph $G = (V, E)$, we will denote the adjacency matrix of the graph induced on W by A_W, the real number $\lambda_i(A_W)$ by $\lambda_i(W)$, and the set of nodes at distance at most l from W by $B_l(W)$.

Fact 3.1 *If B is a selfadjoint operator in a vector space L, then*

$$\lambda_0(B) = \max_{g \in L - \{0\}} \frac{g \cdot Bg}{||g||^2}.$$

Proof We can show that $g \cdot Bg \leq \lambda_0(B)||g||^2$ by decomposing g in an orthonormal basis of eigenvectors of B, as in the proof of Fact 2.5. The maximum is attained when g is an eigenvector of B corresponding to the eigenvalue $\lambda_0(B)$. ■

Fact 3.2 *For any $g \in L_0^2(V)$, we have $g \cdot Ag \leq \lambda_1(G)||g||^2$.*

Proof The proof is similar to Facts 2.4 and 2.5. ■

Fact 3.3 *The eigenvalues of a graph are the union of the eigenvalues of its connected components.*

Proof The eigenvectors of each component can be easily extended to form an independent set of eigenvectors of the graph. ■

The following three results follow from the classic theory of matrices with nonnegative entries [59]. For simplicity, we state them in the symmetric case. For two column vectors g and h, we say that $g \leq h$ if every coordinate of g is at most its corresponding coordinate in h. We say that a matrix B with nonnegative entries is irreducible if its underlying (weighted) graph is connected.

Fact 3.4 *[59, page 28, ex. 1.12] If a real symmetric matrix has only nonnegative entries, its largest eigenvalue is nonnegative and has a corresponding eigenvector with nonnegative components. This eigenvalue is largest in absolute value.* ■

Fact 3.5 *[59, page 22] If a real symmetric matrix with nonnegative entries is irreducible, then its largest eigenvalue is positive and has a corresponding eigenvector with positive components.* ■

Fact 3.6 *If a real symmetric matrix B has only nonnegative entries, and s is a vector with positive components such that $Bs \leq \gamma s$, then the largest eigenvalue of B is at most γ. This property still holds if only the off-diagonal entries of B are assumed to be nonnegative [28].*

Proof The first part is known if B is irreducible [59, page 27, ex. 1.6]. We can reduce to this case by considering the irreducible components of B. If only the off-diagonal entries of B are assumed to be nonnegative, we can reduce to the previous case by adding a sufficiently large multiple of the identity, as in [28]. ■

Fact 3.7 *The average degree of a graph is no greater than its largest eigenvalue.*

Proof By Fact 3.1, we have $\chi_V \cdot A\chi_V / ||\chi_V||^2 \leq \lambda_0(A)$, where V is the vertex set of the graph and A is its adjacency matrix. The left-hand side is equal to the average degree. ■

Fact 3.8 *The largest eigenvalue of a graph is no less than the largest eigenvalue of any induced subgraph [16, page 156].* ■

Fact 3.9 *The function that associates to a symmetric matrix its largest eigenvalue is subadditive.*

Proof This follows immediately from Fact 3.1. ■

Given a graph H, the *cover graph* H' of H is the graph defined on $V' = V \times \{0,1\}$ and where $((u,l),(v,m)) \in V' \times V'$ is an edge if and only $(u,v) \in E$ and $l \neq m$.

Fact 3.10 *The eigenvalues of H' consist of the eigenvalues of H and their negated values.*

Proof Let $(e_0, \ldots, e_{n-1})$ be a basis of orthonormal eigenvectors of H corresponding to the eigenvalues $\lambda_0, \ldots, \lambda_{n-1}$, where n is the number of vertices of H. For $0 \leq i \leq n-1$, let f_i be the vector of H' defined by $f_i(u,l) = e_i(u)$. The vector f_i is an eigenvector of H' with eigenvalue λ_i. Similarly, the vector g_i defined by $g_i(u,l) = (2l-1)e_i(u)$ is an eigenvector of H' with eigenvalue $-\lambda_i$. A simple calculation shows that the vectors f_i and g_j, for $0 \leq i \leq n-1$ and $0 \leq j \leq n-1$, are orthogonal, and so they form a basis of $A_{H'}$. Hence the eigenvalues of H' are $\lambda_0, \ldots, \lambda_{n-1}, -\lambda_0, \ldots, -\lambda_{n-1}$. ■

Lemma 3.1 *If $G = (V,E)$ is k-regular on n vertices, then for any $f \in L^2(V)$, we have*

$$f \cdot Af \leq \lambda_1(G)||f||^2 + \frac{k - \lambda_1(G)}{n}\Big(\sum_{v \in V} f(v)\Big)^2$$

Proof First note that Lemma 3.1 reduces to Fact 3.2 if $f \in L_0^2(V)$. To prove that it holds for any f, we decompose f as the sum of a constant vector and a vector in $L_0^2(V)$, as we did in Chapter 2.

Let $\overline{f} = (f \cdot \chi_V / n)\chi_V$ be the orthogonal projection of f on the subspace spanned by the constant vector χ_V. Then $f_0 = f - \overline{f}$ is the orthogonal projection of f on $L_0^2(V)$. By linearity, $Af = A\overline{f} + Af_0 = k\overline{f} + Af_0$, and so $f \cdot Af = k||\overline{f}||^2 + f_0 \cdot Af_0$ since $\overline{f} \cdot Af_0 = A\overline{f} \cdot f_0 = k\overline{f} \cdot f_0 = 0$. By Fact 3.2 and the Pythagorean theorem, we have

$$f_0 \cdot Af_0 \leq \lambda_1(G)||f_0||^2 = \lambda_1(G)(||f||^2 - ||\overline{f}||^2).$$

Therefore, $f \cdot Af \leq \lambda_1(G)||f||^2 + (k - \lambda_1(G))||\overline{f}||^2$. We conclude the proof by noting that

$$||\overline{f}||^2 = \frac{(f \cdot \chi_V)^2}{n^2}||\chi_V||^2 = \Big(\sum_{v \in V} f(v)\Big)^2 / n.$$

■

Lemma 3.2 *For any subset W of a k-regular graph G, we have $\lambda_0(W) \leq \lambda_1(G)+(k-\lambda_1(G))|W|/n$.*

Proof Let g be any element of $L^2(W)$. Consider the vector $f \in L^2(V)$ that coincides with g on $L^2(W)$ and is null on $V - W$. By Eq. 2.2, we see that $g \cdot A_W g = f \cdot A_G f$. By applying Lemma 3.1 to f and using the fact that g and f have the same norm and the same sum of coordinates, we have

$$g \cdot A_W g \leq \lambda_1(G)||g||^2 + \frac{k-\lambda_1(G)}{n}\big(\sum_{v \in W} g(v)\big)^2 \tag{3.1}$$

On the other hand, using the Cauchy-Schwartz inequality,

$$\big(\sum_{v \in W} g(v)\big)^2 = |\chi_W \cdot g|^2 \leq |W|\ ||g||^2$$

Combining this with Eq. 3.1 shows that $g \cdot A_W g \leq (\lambda_1(G) + (k - \lambda_1(G))|W|/n)||g||^2$. We conclude using Fact 3.1. ■

Section 4.1 contains a generalization of Lemma 3.2. Lemma 3.2 shows that the largest eigenvalue of subgraphs induced on small linear-sized subsets is upper bounded by about $\lambda_1(G)$. This bound is optimal for Ramanujan graphs, even for subsets of sublinear size. Lemma 3.2 already gives a restriction on the structure of induced subgraphs. Together with Fact 3.7, it implies that the average degree of the induced subgraph on W is at most $\lambda_1(G) + (k - \lambda_1(G))|W|/n$, which is roughly $\lambda_1(G)$ for small linear-sized subsets, or for subsets of sublinear size. To obtain a stronger restriction on the induced subgraph on a linear-sized subset X, we will apply Lemma 3.2 to the set $B_l(X)$. We start by comparing the largest eigenvalue of the subgraph induced on $B_l(X)$ to the matrix of a weighted graph associated with X.

Let Δ_X be the diagonal matrix indexed by the vertices of X and whose entry (v, v) is equal to the degree of v in the subgraph induced on X. We will simply denote by $\Delta_X(v)$ the diagonal entry $\Delta_X(v, v)$. For $\theta' > 0$ and integer l, let

$$M_X^{\theta',l} = A_X + \frac{1}{\sqrt{k-1}}\frac{\sinh(l\theta')}{\sinh((l+1)\theta')}(kI - \Delta_X).$$

The matrix $M_X^{\theta',l}$ can be regarded as the matrix of the weighted graph that is induced on X and has in addition a loop of weight $(k-1)^{-1/2}(\sinh(l\theta')/\sinh((l+1)\theta'))(k - \Delta_X(v))$ on each node v of X.

Lemma 3.3 *Suppose $G = (V, E)$ is k-regular. Let l be a positive integer, X a non-empty subset of V, θ' a positive real number, and $\lambda' = 2\sqrt{k-1}\cosh\theta'$. If $\lambda_0(B_l(X)) \leq \lambda'$, then $\lambda_0(M_X^{\theta',l}) \leq \lambda'$.*

Proof Let $W = B_l(X)$. The idea behind the proof is as follows: given an eigenvector of $M_X^{\theta',l}$ corresponding to its largest eigenvalue, we will extend it to W so that it becomes roughly an

eigenvector of A_W. If the largest eigenvalue of M_X^θ were too big, we would get a large eigenvalue for A_W, contradicting the fact that $\lambda_0(W) \leq \lambda'$.

We define the sequence r_i as follows:

$$r_i = \frac{\sinh((l+1-i)\theta')(k-1)^{-i/2}}{\sinh((l+1)\theta')}.$$

The sequence r_i is strictly positive and decreasing for $0 \leq i \leq l$, and

$$\lambda' r_i = r_{i-1} + (k-1) r_{i+1} \tag{3.2}$$

$$\lambda' r_l = r_{l-1}, \tag{3.3}$$

Eq. 3.3 follows from Eq. 3.2 and the equality $r_{l+1} = 0$. Note that the sequence r_i behaves like $e^{-\theta' i}(k-1)^{-i/2}$ for $0 \leq i \leq l+1$, but it vanishes at $l+1$. Let $f \in L^2(X)$ be an eigenvector of the matrix $M_X^{\theta',l}$ corresponding to its largest eigenvalue. Since all the entries of $M_X^{\theta',l}$ are nonnegative, we can assume that all the entries of f are nonnegative (Fact 3.4.) We extend the vector f to W by setting

$$f(v) = \max_{u \in X}(f(u) r_{d(v,u)}),$$

for $v \in W - X$, where $d(v,u)$ denote the distance (length of shortest path) between node v and node u. Note that f is positive on W since every node in W is at distance at most l from some node in X.

Claim 3.1 *For any $v \in W - X$, we have $(A_W f)(v) \geq \lambda' f(v)$.*

Proof Let $u \in X$ be such that $f(v) = f(u) r_{d(v,u)}$. Note that $i = d(v,u)$ is at most l since f is positive and $r_j \leq 0$ for $j \geq l+1$. Let v_1 be the first node on a shortest path from v to u. Since the distance between v_1 and u is $i-1$, we have $v_1 \in W$ and

$$f(v_1) \geq f(u) r_{i-1}. \tag{3.4}$$

We now distinguish two cases:

- **Case 1.** $i = l$. Combining Eqs. 3.4 and 3.3, we get in this case

  $$(A_W f)(v) \geq f(v_1) \geq f(u) r_{l-1} = \lambda' f(u) r_l = \lambda' f(v),$$

  as required. The first equation is a consequence of the positivity of f.

- **Case 2.** $i < l$. In this case, the k neighbors of v are at distance at most $i+1 \leq l$ from u. In particular, all these neighbors belong to W. Moreover, by monotonicity of the sequence r, it

follows that the value of f on each of these neighbors is at least $f(u)r_{i+1}$. Using again Eq. 3.4, we have

$$\begin{aligned}(A_W f)(v) &\geq f(v_1) + (k-1)f(u)r_{i+1} \\ &\geq f(u)(r_{i-1} + (k-1)r_{i+1}) \\ &= \lambda' f(u) r_i \\ &= \lambda' f(v).\end{aligned}$$

■

We now establish a lower bound on $(A_W f)(v)$, for $v \in X$.

Claim 3.2 *For any $v \in X$, we have $(A_W f)(v) \geq \lambda_0(M_X^{\theta',l})f(v)$.*

Proof It follows from the definition of f that for any $v \in X$, the value of f on each of the $k - \Delta_X(v)$ neighbors of v in $W - X$ is at least $f(v)r(1)$. Therefore,

$$(A_W f)(v) \geq (A_X f)(v) + (k - \Delta_X(v))f(v)r(1) = (M_X^{\theta',l} f)(v) = \lambda_0(M_X^{\theta',l})f(v).$$

The second equation follows from the expression of $r(1)$ and definition of $M_X^{\theta',l}$. ■

Since $\lambda_0(W) \leq \lambda'$, we have $(A_W f) \cdot f \leq \lambda' ||f||^2$, by Fact 3.1. Assume for contradiction that $\lambda' < \lambda_0(M_X^{\theta',l})$. By considering a node in X where f is nonzero and using Claim 3.1, Claim 3.2 and the fact that f is nonnegative, we conclude that $(A_W f) \cdot f > \lambda' ||f||^2$, leading to a contradiction. This concludes the proof. ■

For $\theta \geq 0$, define

$$M_X^\theta = A_X + \frac{1}{\sqrt{k-1}e^\theta}(kI - \Delta_X).$$

The matrix M_X^θ can be regarded as the matrix of the weighted graph that is induced on X and has in addition a loop of weight $(k-1)^{-1/2}e^{-\theta}(k - \Delta_X(v))$ on each node v of X. For any graph H, we can define the matrix M_H^θ similarly to the definition of M_X^θ.

Theorem 3.1 *Suppose $G = (V, E)$ is k-regular, and let $\tilde{\lambda} = \max(\lambda_1(G), 2\sqrt{k-1}) = 2\sqrt{k-1}\cosh\theta$, where $\theta \geq 0$. For any non-empty subset X of V of size at most $k^{-1/\epsilon}|V|$, we have*

$$\lambda_0(M_X^\theta) \leq \tilde{\lambda}(1 + O(\epsilon)),$$

where the constant behind the O is a small absolute constant.

Proof Let $l = \lfloor 1/2\epsilon \rfloor$ and let W be the set of nodes at distance at most l from X. A simple calculation shows that $|W| \leq 3k^l|X| \leq 3k^{-1/(2\epsilon)}n$. It follows from Lemma 3.2 that $\lambda_0(W) \leq \lambda'$, where $\lambda' = \tilde{\lambda} + 3k^{1-1/(2\epsilon)} = 2\sqrt{k-1}\cosh\theta'$ and $\theta' > \theta \geq 0$. A straightforward calculation shows that $\lambda' = \tilde{\lambda}(1 + O(\epsilon))$ and $\cosh\theta' - \cosh\theta = O(k^{1/2-1/(2\epsilon)}) = O(\epsilon^2)$. We will use the following results to show that the matrix $M_X^{\theta',l}$ is approximated by M_X^{θ}.

Claim 3.3 *For $x \geq y \geq 0$, we have $(x-y)^2 \leq 2(\cosh x - \cosh y)$.*

Proof We apply Taylor's expansion formula. Since the derivative of $\cosh x$ is $\sinh x$ and vice-versa, we have

$$\cosh x = \cosh y + (x-y)\sinh y + \frac{(x-y)^2}{2}\cosh\gamma,$$

where $y \leq \gamma \leq x$. The claim follows immediately. ■

Claim 3.4

$$\frac{l}{l+1}e^{-\theta'} \leq \frac{\sinh(l\theta')}{\sinh((l+1)\theta')} \leq e^{-\theta'} \tag{3.5}$$

Proof Since $\sinh((l+1)\theta') \geq (l+1)\sinh\theta'$, we have

$$e^{-\theta'} - \frac{\sinh(l\theta')}{\sinh((l+1)\theta')} = \frac{e^{-l\theta'} - e^{-(l+2)\theta'}}{e^{(l+1)\theta'} - e^{-(l+1)\theta'}} = e^{-(l+1)\theta'}\frac{\sinh\theta'}{\sinh((l+1)\theta')} \leq \frac{e^{-\theta'}}{l+1}.$$

■

It follows from Claim 3.3 that $\theta' - \theta = O(\epsilon)$. On the other hand, Eq. 3.5 implies that

$$\frac{\sinh(l\theta')}{\sinh((l+1)\theta')} = e^{-\theta'}(1 + O(1/l)) = e^{-\theta}(1 + O(\epsilon)).$$

Therefore, all entries of the matrix $M_X^{\theta} - M_X^{\theta',l}$ are $O(\sqrt{k-1}\epsilon)$. Since it is diagonal, it follows that its largest eigenvalue is $O(\sqrt{k-1}\epsilon)$. By Fact 3.9 and Lemma 3.3, we have

$$\begin{aligned}
\lambda_0(M_X^{\theta}) &\leq \lambda_0(M_X^{\theta',l}) + O(\sqrt{k-1}\epsilon) \\
&\leq \lambda' + O(\tilde{\lambda}\epsilon) \\
&= \tilde{\lambda}(1 + O(\epsilon))
\end{aligned}$$

■

Remark 3.1 The only place where we used in the proof the fact that $\lambda_1(G)$ is the second eigenvalue of G was in conjunction with Lemma 3.2 to upper bound $\lambda_0(W)$. In particular, if λ^* is a real number such that for any subset W of V, we have $\lambda_0(W) \leq \lambda^* + 2k|W|/|V|$, then Theorem 3.1 remains valid if $\lambda_1(G)$ is replaced by λ^*.

3.2 Lower bounds on the expansion and on the average degree

We will derive lower bounds on the expansion by applying Theorem 3.1 to the union of X and $N(X)$, after reducing to the case where the graph is bipartite and X is on one side of the partition. The idea is that if the expansion of X is small, a node in $N(X)$ will be adjacent to many nodes in X, in average. This implies that the largest eigenvalue of the weighted matrix associated to the subgraph induced on $X \cup N(X)$ is large, contradicting with Theorem 3.1. We also use Theorem 3.1 to derive upper bounds on the average degree of induced subgraphs.

Theorem 3.2 *If $G = (V, E)$ is k-regular and $\tilde{\lambda} = \max(\lambda_1(G), 2\sqrt{k-1})$, then for any non-empty subset X of V of size at most $k^{-1/\epsilon}|V|$,*

$$\frac{|N(X)|}{|X|} \geq \frac{k}{2}\left(1 - \sqrt{1 - \frac{4k-4}{\tilde{\lambda}^2}}\right)(1 - O(\epsilon)),$$

where the constant behind the O is a small absolute constant.

Proof We first show how to reduce the problem to the case where the graph G is bipartite and X is on one side of the partition. Consider the cover graph G' of G, as defined in Section 3.1. We will show that Remark 3.1 applies to $\lambda^* = \lambda_1(G)$. Indeed, let W be a subset of V', let $W_p \subseteq V$ be its projection on V, i.e. the set of nodes u of V such that $(u, 0) \in W$ or $(u, 1) \in W$. Let $W^* = W_p \times \{0, 1\}$. Since $W \subseteq W^*$, it follows from Fact 3.8 that $\lambda_0(W) \leq \lambda_0(W^*)$. (We remind the reader that $\lambda_0(W)$ (resp. $\lambda_0(W^*)$) is the largest eigenvalue of the subgraph of G' induced on W (resp. W^*), and $\lambda_0(W_p)$ is the largest eigenvalue of the subgraph of G induced on W_p.)

On the other hand, the subgraph of G' induced on W^* is the graph cover of the subgraph of G induced on W_p. It follows from Fact 3.10 that $\lambda_0(W^*)$ is the largest eigenvalue in absolute value of the subgraph of G induced on W_p. Hence, by Fact 3.4, we have $\lambda_0(W^*) = \lambda_0(W_p)$. Using Lemma 3.2, it follows that

$$\lambda_0(W) \leq \lambda_0(W_p) \leq \lambda_1(G) + k\frac{|W_p|}{|V|} \leq \lambda_1(G) + 2k\frac{|W|}{|V'|},$$

as required by Remark 3.1. Note that we cannot apply directly Theorem 3.1 because, by Fact 3.10, we have $\lambda_1(G') = \lambda(G)$, which may be different from $\lambda_1(G)$.

Let Y be the subset of V' equal to $X \times \{0\}$. Denote the adjacency matrix of G' by A', and the set of neighbors of Y in G' by $N'(Y)$. Note that $|Y| = |X|$ and $|N'(Y)| = |N(X)|$.

By applying Remark 3.1 to the graph G', the set of vertices $Y \cup N'(Y)$, and $\epsilon' = 2\epsilon$, we see that the largest eigenvalue of the matrix $M' = M^{\theta}_{Y \cup N'(Y)}$ is at most $\tilde{\lambda}(1 + O(\epsilon))$ ($M' = M^{\theta}_H$, where H is the subgraph of G' induced on $Y \cup N'(Y)$.) Now, consider the function $f \in L^2(Y \cup N'(Y))$ defined

by $f = k\chi_Y + \tilde{\lambda}\chi_{N'(Y)}$. We have (Fact 3.1)

$$M'f \cdot f \leq \tilde{\lambda}(1 + O(\epsilon))||f||^2. \tag{3.6}$$

The left-hand side is the sum of two terms. The first is equal to $A'f \cdot f$, and the second corresponds to the weighted self-loops. By Eq. 2.2, and since the two sets Y and $N'(Y)$ are independent in G' and there are $k|Y|$ undirected edges between Y and $N'(Y)$, we have $A'f \cdot f = 2\tilde{\lambda}k^2|Y|$. To calculate the second term, we observe that the loops have no weight on Y and have average weight $e^{-\theta}(k-1)^{-1/2}(k - k|Y|/|N'(Y)|)$ on $N'(Y)$. This is because a vertex in $N'(Y)$ has in average $k|Y|/|N'(Y)|$ neighbors in Y. Hence, the second term is equal to $e^{-\theta}(k-1)^{-1/2}(k|N'(Y)| - k|Y|)\tilde{\lambda}^2$.

By expanding the two sides of Eq. 3.6, we see that it reduces to

$$2\tilde{\lambda}k^2|Y| + \frac{\tilde{\lambda}^2}{\sqrt{k-1}e^{\theta}}k(|N'(Y)| - |Y|) \leq \tilde{\lambda}(1 + O(\epsilon))(k^2|Y| + \tilde{\lambda}^2|N'(Y)|).$$

By dividing the two sides by $\tilde{\lambda}$ and replacing $|Y|$ by $|X|$, $|N'(Y)|$ by $|N(X)|$, and $\tilde{\lambda}$ by $2\sqrt{k-1}\cosh\theta$ in the left-hand side, we get

$$k|X|(k(1 - O(\epsilon)) - 2e^{-\theta}\cosh\theta) \leq |N(X)|(\tilde{\lambda}^2 - 2ke^{-\theta}\cosh\theta)(1 + O(\epsilon)). \tag{3.7}$$

The factor $1 - O(\epsilon)$ in the left-hand side gets absorbed in the right-hand side since $e^{-\theta}\cosh\theta \leq 1$. On the other hand,

$$\begin{aligned}
\tilde{\lambda}^2 - 2ke^{-\theta}\cosh\theta &= 2((2k-2)\cosh\theta - ke^{-\theta})\cosh\theta \\
&= 2(k(2\cosh\theta - e^{-\theta}) - 2\cosh\theta)\cosh\theta \\
&= 2(ke^{\theta} - 2\cosh\theta)\cosh\theta.
\end{aligned}$$

Eq. 3.7 therefore reduces to:

$$\frac{|N(X)|}{|X|} \geq \frac{k}{2e^{\theta}\cosh\theta}(1 - O(\epsilon)).$$

It remains to replace the terms in θ with a function of $\tilde{\lambda}$. We do this using the formula $e^{-\theta} = \cosh\theta - \sqrt{\cosh^2\theta - 1}$, which leads to

$$\frac{1}{e^{\theta}\cosh\theta} = \frac{e^{-\theta}}{\cosh\theta} = 1 - \sqrt{1 - \frac{1}{\cosh^2\theta}} = 1 - \sqrt{1 - \frac{4k-4}{\tilde{\lambda}^2}}.$$

This concludes the proof. ■

Theorem 3.3 *If $G = (V, E)$ is k-regular and $\tilde{\lambda} = \max(\lambda_1(G), 2\sqrt{k-1})$, then for any non-empty subset X of V of size at most $k^{-1/\epsilon}|V|$, the average degree σ of the subgraph of G induced on X is*

at most

$$\left(1+\frac{\tilde{\lambda}}{2}+\sqrt{\frac{\tilde{\lambda}^2}{4}-(k-1)}\right)(1+O(\epsilon)),$$

where the constant behind the O is a small absolute constant.

Proof We use the same notations as in Theorem 3.1. As noted before, the matrix M_X^θ can be regarded as the matrix of the weighted graph on X that is induced on X and has in addition a loop of weight $(k-1)^{-1/2}e^{-\theta}(k-\Delta_X(v))$ on each node v of X. By applying Theorem 3.1 and Fact 3.7 to this graph, we get

$$\sigma+\frac{k-\sigma}{\sqrt{k-1}e^\theta}\leq 2\sqrt{k-1}(1+O(\epsilon))\cosh\theta,$$

which implies

$$\begin{aligned}\sigma &\leq \frac{2(k-1)e^\theta\cosh\theta-k}{\sqrt{k-1}e^\theta-1}(1+O(\epsilon))\\ &= \left(\sqrt{k-1}e^\theta+1\right)(1+O(\epsilon)).\end{aligned}$$

We conclude by noting that $e^\theta=\cosh\theta+\sinh\theta=\cosh\theta+\sqrt{\cosh^2\theta-1}$. ■

3.3 Lower bounds on the expansion of $N(X)$ and on $|N^t(X)|$, for $t\geq 2$.

We again apply the same techniques as in Section 3.2 to get lower bounds on the size of $N^t(X)$, for $t\geq 2$, and on the expansion of $N(X)$. We start with the case $t=2$.

Theorem 3.4 *If $G=(V,E)$ is a k-regular graph such that $\lambda_1(G)\leq 2\sqrt{k-1}$, then for any non-empty subset X of V of size at most $k^{-1/\epsilon}|V|$,*

$$\frac{|N^2(X)|}{|X|}\geq(1+k(k-2)/2)(1-O(\epsilon)),$$

where the constant behind the O is a small absolute constant.

Proof As in the proof of Theorem 3.2, we can assume without loss of generality that G is bipartite and that X is on one side of the partition. Let $f\in L^2(N(X)\cup N^2(X))$ be the function defined by $f=k\chi_X+2\sqrt{k-1}\chi_{N(X)}+2\chi_{N^2(X)-X}$. By applying Remark 3.1 to the set $N(X)\cup N^2(X)$, we have

$$M'f\cdot f\leq 2\sqrt{k-1}(1+O(\epsilon))||f||^2, \tag{3.8}$$

where $M'=M^0_{N(X)\cup N^2(X)}$. As in Section 3.2, we can calculate $M'f\cdot f$ by using Eq. 2.2 and the fact that there are $k|X|$ edges between X and $N(X)$, and $k|N(X)|-k|X|$ edges between $N(X)$ and

$N^2(X) - X$. This yields

$$M'f \cdot f = 4k^2\sqrt{k-1}|X| + 8k\sqrt{k-1}(|N(X)| - |X|) + \frac{4k}{\sqrt{k-1}}(|N^2(X)| - |N(X)|). \tag{3.9}$$

On the other hand,

$$||f||^2 = k^2|X| + 4(k-1)|N(X)| + 4(|N^2(X)| - |X|). \tag{3.10}$$

By combining Eqs. 3.8, 3.9 and 3.10, and after some simplifications and factoring out the term $k-2$, we get

$$(k-1)(k-2)|X| + 2|N(X)| \leq 2|N^2(X)|(1 + O(\epsilon)). \tag{3.11}$$

(A technical point: the expansion coefficients of X and of $N(X)$ are both $\Theta(k)$, as can be seen directly using Theorem 3.2. Therefore, the three terms in the expression of $M'f \cdot f$ are proportional to each other. The same holds for $||f||^2$. This allows us to make simplifications without worrying about the multiplicative term $1 + O(\epsilon)$.)

Using again the inequality $|N(X)| \geq k|X|(1 - O(\epsilon))/2$ and combining it with Eq. 3.11 yields the desired lower bound on $|N^2(X)|$. ■

Theorem 3.4 can be generalized as follows:

Theorem 3.5 *If $G = (V, E)$ is a k-regular graph such that $\lambda_1(G) \leq 2\sqrt{k-1}$, then for any integer $t \geq 2$ and any non-empty subset X of V of size at most $k^{-t-1/\epsilon}|V|$,*

$$\frac{|N^t(X) - N^{t-2}(X)|}{|X|} \geq \frac{k(k-2)(k-1)^{t-2}}{2}(1 - O(t\epsilon)),$$

where the constant behind the O is a small absolute constant.

Proof Since $N^{t-2}(X) \subseteq N^t(X)$, we have $|N^t(X) - N^{t-2}(X)| = |N^t(X)| - |N^{t-2}(X)|$. Hence, as before, we can reduce the problem to the case where the graph is bipartite and X is on one side of the partition. Let $M' = M^0_{N^{t-1}(X) \cup N^t(X)}$, and $f \in L^2(N^{t-1}(X) \cup N^t(X))$ be the function defined by

$$f = k\chi_X + 2\sqrt{k-1}\chi_{N(X)} + 2\sum_{i=2}^{t}(k-1)^{1-i/2}\chi_{N^i(X) - N^{i-2}(X)}.$$

As before,

$$M'f \cdot f \leq 2\sqrt{k-1}(1 + O(\epsilon))||f||^2.$$

There are $k|N^t(X)| - k|N^{t-1}(X)|$ edges between $N^t(X) - N^{t-2}(X)$ and $N^{t+1}(X) - N^{t-1}(X)$. Indeed, if $e(A, B) = |E| \cap (A \times B)$ is the number of edges whose first endpoint is in A and second endpoint

in B, then

$$\begin{aligned} e(N^t(X) - N^{t-2}(X), N^{t+1}(X) - N^{t-1}(X)) &= e(N^t(X), N^{t+1}(X) - N^{t-1}(X)) \\ &= e(N^t(X), N^{t+1}(X)) - e(N^t(X), N^{t-1}(X)) \\ &= k|N^t(X)| - k|N^{t-1}(X)|, \end{aligned}$$

as required. As a consequence,

$$M'f \cdot f = 2\sqrt{k-1}\left(2k^2|X| + 4k\sum_{i=1}^{t-1}\frac{|N^i(X)| - |N^{i-1}(X)|}{(k-1)^{i-1}} + \frac{2k}{(k-1)^{t-1}}(|N^t(X)| - |N^{t-1}(X)|)\right),$$

and

$$||f||^2 = k^2|X| + 4(k-1)|N(X)| + 4\sum_{i=2}^{t}\frac{|N^i(X)| - |N^{i-2}(X)|}{(k-1)^{i-2}}.$$

But

$$\begin{aligned} \sum_{i=2}^{t}\frac{|N^i(X)| - |N^{i-2}(X)|}{(k-1)^{i-2}} &= \sum_{i=2}^{t}\frac{|N^i(X)| - |N^{i-1}(X)|}{(k-1)^{i-2}} + \sum_{i=1}^{t-1}\frac{|N^i(X)| - |N^{i-1}(X)|}{(k-1)^{i-1}} \\ &= \frac{|N^t(X)| - |N^{t-1}(X)|}{(k-1)^{t-2}} + |N(X)| - |X| + k\sum_{i=2}^{t-1}\frac{|N^i(X)| - |N^{i-1}(X)|}{(k-1)^{i-1}}, \end{aligned}$$

and so

$$|f||^2 = (k^2-4)|X| + 4k|N(X)| + 4\frac{|N^t(X)| - |N^{t-1}(X)|}{(k-1)^{t-2}} + 4k\sum_{i=2}^{t-1}\frac{|N^i(X)| - |N^{i-1}(X)|}{(k-1)^{i-1}}.$$

After some simplifications, we conclude that

$$(k-2)(k-1)^{t-1}|X| + 2|N^{t-1}(X)| \leq 2|N^t(X)|(1 + O(t\epsilon)). \tag{3.12}$$

The same inequality holds if t is replaced by $t-1$. Theorem 3.5 follows immediately. By applying Eq. 3.12 for $t, t-1, \ldots, 2$, we see that $|N^t(X)| \geq ((k-1)^t + 1)(1 - O(t^2\epsilon))|X|/2$. ■

Theorem 3.6 *If $G = (V, E)$ is a k-regular graph such that $\lambda_1(G) \leq 2\sqrt{k-1}$, then for any non-empty subset X of V of size at most $k^{-1/\epsilon}|V|$,*

$$\frac{|N^2(X)|}{|N(X)|} \geq (2k/3 + O(1))(1 + O(\epsilon)),$$

where the constants behind the O are small absolute constants.

Proof We use the same notations and similar techniques as in Theorem 3.4, but we use the function $f \in L^2(N(X) \cup N^2(X))$ defined $f = k\chi_X + 2\sqrt{k}\chi_{N(X)} + 3\chi_{N^2(X)-X}$. We have

$$M'f \cdot f \leq 2\sqrt{k-1}(1 + O(\epsilon))||f||^2. \tag{3.13}$$

A simple calculation shows that

$$\begin{aligned} M'f \cdot f &= 4k^{5/2}|X| + 12k^{3/2}(|N(X)| - |X|) + \frac{9k}{\sqrt{k-1}}(|N^2(X)| - |N(X)|) \\ &= (4k^{5/2}|X| + 12k^{3/2}|N(X| + 9\sqrt{k}|N^2(X)|)(1 + O(1/k)). \end{aligned}$$

The last equality follows from the fact that the expansion coefficients of X and of $N(X)$ are both $\Theta(k)$, as can be seen directly using Theorem 3.2. On the other hand,

$$||f||^2 = k^2|X| + 4k|N(X)| + 9(|N^2(X)| - |X|).$$

By combining Eqs. 3.13 with the last equations and doing some simplifications, we get

$$2k^2|X| + 4k|N(X)| \leq 9(1 + O(1/k))(1 + O(\epsilon))|N^2(X)|.$$

We conclude by noting that $|N(X)| \leq k|X|$. ■

3.4 A family of almost Ramanujan graphs with expansion $k/2$

In this section, we show that no technique based on the second eigenvalue method can yield a lower bound on the expansion better than $k/2$. We do so by constructing an explicit family of k-regular graphs G_n containing subsets of sublinear size having expansion $k/2$, and such that $\lambda(G_n) = (2 + o(1))\sqrt{k-1}$. This leads us to study the following question: given a graph H and real number $\overline{\lambda}$, is there an infinite family of graphs containing H as a subgraph and whose second eigenvalue is at most $\overline{\lambda}(1 + o(1))$? We give a necessary and sufficient condition on H for the existence of such a family. We start with a lemma that will be used throughout this section.

Lemma 3.4 *Consider a graph on a vertex set W, a subset X of W, and $s \in L^2(W)$. Let X_i be the set of nodes at distance i from X. Assume the following conditions hold:*

1. *For $h - 1 \leq i, j \leq h$, all nodes in X_i have the same number of neighbors in X_j.*
2. *The vector s is constant on X_{h-1} and X_h.*

3. s has positive components and $As \leq \mu s$ on $B_{h-1}(X)$, where μ is a positive real number.

Then for any $g \in L^2(W)$ such that $|Ag(u)| = \mu|g(u)|$ for $u \in B_{h-1}(X)$, we have

$$\frac{\sum_{v \in X_h} g(v)^2}{\sum_{v \in X_h} s(v)^2} \geq \frac{\sum_{v \in X_{h-1}} g(v)^2}{\sum_{v \in X_{h-1}} s(v)^2}.$$

Proof Let P, P_{h-1} and P_h be the projections on the sets $B_{h-1}(X), X_{h-1}$ and X_h respectively. We need to show that $||P_h g||^2/||P_h s||^2 \geq ||P_{h-1} g||^2/||P_{h-1} s||^2$. Let $A_h = (P + P_h)A(P + P_h)$. The operator A_h corresponds in some sense to the adjacency matrix of the subgraph induced on $B_h(X)$, but it acts on $L^2(W)$. By Conditions 1 and 2, there exist positive coefficients α, β and γ such that $P_h A_h s = \gamma P_h s$ and $A_h P_h s = \alpha P_h s + \beta P_{h-1} s$. By hypothesis, we have $A_h s \leq \mu P s + \gamma P_h s$. Premultiplying both sides of this equation by P and A_h yields successively

$$\begin{aligned} PA_h s &\leq \mu P s \\ &= \mu s - \mu P_h s, \\ A_h P A_h s &\leq \mu A_h s - \mu(\alpha P_h s + \beta P_{h-1} s) \\ &\leq \mu^2 P s + \mu(\gamma - \alpha) P_h s - \mu\beta P_{h-1} s. \end{aligned}$$

But the matrix $A_h P A_h - \mu^2 P - \mu(\gamma - \alpha)P_h + \mu\beta P_{h-1}$ has only nonnegative entries off its diagonal, and so its largest eigenvalue is 0 since s is positive (Fact 3.6.) The quadratic form associated to this matrix is therefore semi-definite negative (Fact 3.1), and so

$$A_h P A_h g \cdot g \leq \mu^2 P g \cdot g + \mu(\gamma - \alpha) P_h g \cdot g - \mu\beta P_{h-1} g \cdot g. \tag{3.14}$$

Since both A_h and P are selfadjoint and since $P^2 = P$, the left-hand side of Eq. 3.14 is equal to $||PA_h g||^2$. We can rewrite Eq. 3.14 as follows:

$$||PA_h g||^2 \leq \mu^2 ||Pg||^2 + \mu(\gamma - \alpha)||P_h g||^2 - \mu\beta||P_{h-1} g||^2.$$

But $||PA_h g|| = \mu||Pg||$ by hypothesis, and so

$$(\gamma - \alpha)||P_h g||^2 \geq \beta||P_{h-1} g||^2. \tag{3.15}$$

On the other hand, since A_h and P_h are selfadjoint, we have $A_h P_h s \cdot s = P_h A_h s \cdot s$, and so $\alpha||P_h s||^2 + \beta||P_{h-1} s||^2 = \gamma||P_h s||^2$. Comparing this with Eq. 3.15 concludes the proof. ■

Remark 3.2 The only time where we used Conditions 1 and 2 in the lemma was to prove the existence of α, β and γ such that $P_h A_h s = \gamma P_h s$ and $A_h P_h s = \alpha P_h s + \beta P_{h-1} s$. Therefore, the

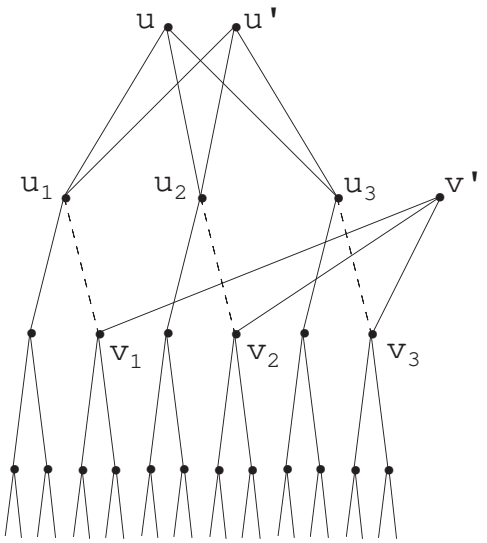


Figure 3-1: The graph G_{n+2} in the neighborhood of u in the case $k = 3$. The dotted edges are those belonging to $E - E'$.

conclusion of Lemma 3.4 still holds if Conditions 1 and 2 are replaced by the existence of α, β and γ satisfying the above equations.

Theorem 3.7 *For any integer k such that $k-1$ is prime, we can explicitly construct an infinite family of k-regular graphs G_n on n vertices whose linear expansion is $k/2$ and such that $\lambda_1(G_n) \leq 2\sqrt{k-1}(1 + 2\log^2 \log n / \log_k^2 n)$.*

Proof We construct the family (G_n) by altering the known constructions of explicit Ramanujan graphs, so that the expansion of (G_n) is $k/2$. Roughly speaking, we show that an eigenvector of G_n associated to a large eigenvalue corresponds to an eigenvector of the original graph with the same eigenvalue, and thereby conclude that G_n is almost Ramanujan.

From [45] and [49], we know that we can explicitly construct an infinite family of bipartite Ramanujan graphs (F_n) on n vertices whose girth is $(4/3 + o(1)) \log_{k-1} n$. Let $F_n = (V, E)$ be an element of the family, $u \in V$ a vertex of F_n and $l = \lfloor c(F_n)/2 \rfloor - 2$. Let $u_1, \ldots, u_k$ be the neighbors of u and let $v_1, \ldots, v_k$ be k vertices at distance two from u such that $(u_i, v_i) \in E$. The subgraph of F_n induced on $B_{l+1}(\{u\})$ is a tree rooted at u since it is connected and contains no cycle. Let u' and v' be two elements not belonging to V. Consider the k-regular graph $G_{n+2} = (V', E')$, where $V' = V \cup \{u', v'\}$ and $E' = E \cup \bigcup_{i=1}^{k} \{(u', u_i), (u_i, u'), (v', v_i), (v_i, v')\} - \bigcup_{i=1}^{k} \{(u_i, v_i), (v_i, u_i)\}$. Fig. 3-1 shows the graph G_{n+2} in the neighborhood of u in the case $k = 3$. For shorthand, we denote A_{F_n} by A, $A_{G_{n+2}}$ by A' and $\lambda_1(A')$ by λ'. We need to show that $\lambda' \leq (2 + o(1))\sqrt{k-1}$. Assume that $\lambda' > 2\sqrt{k-1}$ (otherwise we are done), and let $\lambda' = 2\sqrt{k-1}\cosh\theta'$, with $\theta' > 0$. Let $g \in L_0^2(V')$ be an eigenvector corresponding to λ'.

We outline informally the basic ideas of the proof. Roughly speaking, we will show that the values that g takes on the nodes u', v', u_i, v_i are small compared to $||g||$. Since $g \in L_0^2(V')$, we conclude that g almost belongs to $L_0^2(V)$. Fact 3.2 then implies that $g \cdot Ag \leq (2+o(1))\sqrt{k-1}||g||^2$. But, since $g(u')$, $g(v')$, $g(u_i)$ and $g(v_i)$ are small, the scalar product $g \cdot Ag$ is close to $g \cdot A'g = \lambda'||g||^2$, and so $\lambda' \leq (2+o(1))\sqrt{k-1}$.

Since u and u' have the same neighbors in G_{n+2} and $\lambda' \neq 0$, we have $g(u) = g(u')$. Let f be the element of $L^2(V)$ that coincides with g on V. By Eq. 2.2, we have

$$\begin{aligned} \lambda'||g||^2 &= g \cdot A'g \\ &= f \cdot Af - 2\sum_{i=1}^{k} g(u_i)g(v_i) + 2\sum_{i=1}^{k} g(u')g(u_i) + 2\sum_{i=1}^{k} g(v')g(v_i). \end{aligned} \tag{3.16}$$

We upper bound $-2g(u_i)g(v_i)$ by $g(u_i)^2 + g(v_i)^2$. On the other hand, using the Cauchy-Schwartz inequality and the equality $(A'g)(u') = \lambda' g(u')$, we have

$$\sum_{i=1}^{k} g(u')g(u_i) = \lambda' g(u')^2 = \frac{1}{\lambda'}\Big(\sum_{i=1}^{k} g(u_i)\Big)^2 \leq \frac{k}{\lambda'}\sum_{i=1}^{k} g(u_i)^2.$$

A similar relation holds for v'. Combining this with Eq. 3.16, we get

$$\lambda'||g||^2 \leq f \cdot Af + (1 + \frac{2k}{\lambda'})\sum_{i=1}^{k}(g(u_i)^2 + g(v_i)^2). \tag{3.17}$$

Next, we bound the term $f \cdot Af$. Note that $\sum_{w \in V} f(w) = -g(u') - g(v')$ since $g \in L_0^2(V')$. Using Lemma 3.1, we get

$$\begin{aligned} f \cdot Af &\leq \lambda_1(A)||f||^2 + \frac{k}{n}(g(u') + g(v'))^2 \\ &\leq 2\sqrt{k-1}(||g||^2 - g(u')^2 - g(v')^2) + \frac{2k}{n}(g(u')^2 + g(v')^2) \\ &\leq 2\sqrt{k-1}||g||^2, \end{aligned}$$

for sufficiently large n. Combining this with Eq. 3.17 and noting that $1 + 2k/\lambda' \leq 4\sqrt{k-1}$, we obtain

$$\lambda'||g||^2 \leq 2\sqrt{k-1}\big(||g||^2 + 2\sum_{i=1}^{k}(g(u_i)^2 + g(v_i)^2)\big). \tag{3.18}$$

We now compare $g(u_i)$ and $g(v_i)$ to $||g||$. Let s be the function on V' defined by $s(u) = s(u') = k$ and, for $v \in V' - \{u, u'\}$ at distance i from u,

$$s(v) = 2(k-1)^{1-i/2}\cosh i\theta'.$$

An easy calculation shows that the function s verifies the conditions of Lemma 3.4 for the graph G', with $X = \{u, u'\}$, $\mu = \lambda'$, and for any integer h between 1 and $l+1$. Therefore, the sequence $||P_h g||^2/||P_h s||^2$ is an increasing function of h. Hence

$$\begin{aligned} ||g||^2 &\geq \sum_{v \in X_{l+1}} g(v)^2 \\ &\geq \frac{\sum_{v \in X_{l+1}} s(v)^2}{\sum_{v \in X_1} s(v)^2} \sum_{v \in X_1} g(v)^2 \\ &= \frac{k-2}{k-1} \frac{\cosh^2(l+1)\theta'}{\cosh^2 \theta'} \sum_{i=1}^{k} g(u_i)^2 \\ &\geq \frac{1}{2} \cosh^2(l\theta') \sum_{i=1}^{k} g(u_i)^2, \end{aligned}$$

The last equation follows from the inequality $\cosh(l+1)\theta' \geq \cosh\theta' \cosh l\theta'$. Similarly, we can prove the inequality $||g||^2 \geq \frac{1}{2}\cosh^2(l\theta') \sum_{i=1}^{k} g(v_i)^2$. Combining this with Eq. 3.18 yields

$$\cosh\theta' \leq 1 + \frac{8}{\cosh^2 l\theta'}. \tag{3.19}$$

Using the inequalities $\cosh\theta' \geq 1 + \theta'^2/2$ and $\cosh l\theta' \geq e^{l\theta'}/2$, we see from Eq. 3.19 that $\theta' = O(e^{-l\theta'})$, and so $\log\theta' \leq -l\theta' + O(1)$. Hence $\theta' \leq (\log l)/l$ for sufficiently large n. Finally,

$$\lambda' = 2\sqrt{k-1}\cosh\theta' = 2\sqrt{k-1}(1 + \frac{\theta'^2}{2}(1+o(1))) \leq 2\sqrt{k-1}(1 + 2\frac{\log^2 \log n}{\log_k^2 n}),$$

since $l \geq (2/3 - o(1)) \log_k n$. Theorem 3.2 implies that the linear expansion of the family (G_n) is at least $k/2$. Since the subset $\{u, u'\}$ has k neighbors, this bound is tight. ■

If $k-1$ is a prime congruent to 1 modulo 4, we know from [45] that there exists an infinite family of non-bipartite k-regular Ramanujan graphs with girth at least $(2/3 + o(1)) \log_{k-1} n$. By doing the same construction as in Theorem 3.7, we obtain k-regular graphs whose second largest eigenvalue *in absolute value* is $(2 + o(1))\sqrt{k-1}$ and linear expansion $k/2$. Moreover, by adjoining nodes at regions of the graph at sufficiently large distance from each other, we can construct for any $m = m(n) = o(n)$ a family of k-regular graphs whose second largest eigenvalue in absolute value is $(2 + o(1))\sqrt{k-1}$ and containing a subset of size $2m$ with expansion $k/2$. The proofs of these two statements are very similar to the proof of Theorem 3.7. The following theorem generalizes Theorem 3.7.

Theorem 3.8 *Let k be an integer such that $k-1$ is a prime congruent to 1 modulo 4, and $\overline{\lambda}$ a real number no smaller than $2\sqrt{k-1}$. Let $\overline{\lambda} = 2\sqrt{k-1}\cosh\theta$, where $\theta \geq 0$. Consider a graph H of maximum degree at most k and such that $\lambda_0(M_H^\theta) \leq \overline{\lambda}$. There exists an explicitly constructible*

infinite family G_n of k-regular graphs containing H as an induced subgraph and such that $\lambda(G_n) \leq (1 + o(1))\overline{\lambda}$.

Proof The proof is similar to the proof of Theorem 3.7. Let X be the vertex set of H. Consider an explicit family of non-bipartite Ramanujan [45] graphs (F_n) on n vertices whose girth is $(2/3 + o(1))\log_{k-1} n$. Let $F_n = (V, E)$ be an element of the family. Consider a set of $|X|$ vertices of F_n at distance at least $l + 4$ from each other, where $l = 1 + (\log_{k-1}(n/|X|))/4$. We can find such set greedily if n is large enough. Identify the vertices of H with this set of vertices. For each such vertex v, delete $\Delta_H(v)$ edges of E adjacent to it. Since $\sum_{v \in H} \Delta_H(v)$ is even, we obtain an even number of vertices of degree $k-1$ as a result of the edge deletion process. We add a perfect matching between these vertices. The graph G_n we obtain after these operations is k-regular and has V as vertex set. The subgraph of G_n induced on X is identical to H. Moreover, the subgraph of G_n induced on $B_{l+1}(X)$ has no loops other than those inside X. Denote by E' be the set of edges of G_n, by A' its adjacency matrix, and by A the adjacency matrix of F_n. Without loss of generality, we will assume that the second largest eigenvalue in absolute value of G_n is positive (the case where it is negative can be treated similarly) and greater than $\overline{\lambda}$. We denote it by $\lambda' = 2\sqrt{k-1}\cosh\theta'$, with $\theta' > \theta$. Let $g \in L_0^2(V)$ be an eigenvector of A' corresponding to λ'. As before, we need to show that the value of g on the set of vertices adjacent to edges in $E \Delta E'$ is small compared to $||g||$. We have

$$\begin{aligned} \lambda'||g||^2 &= g \cdot A'g \\ &= g \cdot Ag + \sum_{(u,v)\in E'-E} g(u)g(v) - \sum_{(u,v)\in E-E'} g(u)g(v) \\ &\leq 2\sqrt{k-1}||g||^2 + \frac{1}{2}\sum_{(u,v)\in E\Delta E'} (g(u)^2 + g(v)^2). \end{aligned} \tag{3.20}$$

Using Remark 3.2, we will show that the second term in the last equation is small compared to $||g||^2$. Assume for the moment that H is connected. Let $s \in L^2(X)$ be an eigenvector of the matrix M_H^θ corresponding to its largest eigenvalue. We can assume without loss of generality that s takes only positive values (Fact 3.5). For $v \in B_{l+1}(X) - X$ (the set of nodes in $V - X$ at distance at most $l+1$ from X in G_n), there exists a unique point u in X that minimizes the distance (in G_n) $d(u, v)$. We extend the domain of s to $B_{l+1}(X) - X$ by setting $s(v) = \alpha_i s(u)$, where $i = d(u, v)$ and

$$\alpha_i = (k-1)^{-i/2}(e^{(i-1)\theta'}(e^{-\theta} - e^{-\theta'}) + e^{-i\theta'}).$$

We assign to s an arbitrary positive value on $V - B_{l+1}(X)$. Let us now verify that the conditions of Remark 3.2 apply for the graph G_n, the set X, $\mu = \lambda'$ and any h between 2 and $l+1$. First, we verify the existence of α, β and γ as defined in Remark 3.2. Using the same notations as in Remark 3.2, we have $P_h A_h s = (\alpha_{h-1}/\alpha_h)P_h s$. This is because any node v in X_h has a unique

neighbor v' in X_{h-1}, and $s(v') = (\alpha_{h-1}/\alpha_h)s(v)$. Similarly, $A_h P_h s = (k-1)(\alpha_h/\alpha_{h-1})P_{h-1}s$. It remains to verify that $A's \leq \lambda' s$. Observe that the sequence α_i satisfies the following equations:

$$\begin{aligned} \alpha_0 &\geq 1 && (3.21)\\ \alpha_1 &= (k-1)^{-1/2}e^{-\theta} && (3.22)\\ \lambda'\alpha_i &= \alpha_{i-1} + (k-1)\alpha_{i+1}, \quad \text{for } i \geq 1. && (3.23) \end{aligned}$$

If $v \in X$, we have

$$\begin{aligned} (A's)(v) &= (A_X s)(v) + (k - \Delta_X(v))s(v)\alpha_1 && (3.24)\\ &= (M_X^\theta s)(v)\\ &= \overline{\lambda} s(v)\\ &\leq \lambda' s(v). \end{aligned}$$

The inequality $(A's)(v) \leq \lambda' s(v)$ for $v \in B_l(X) - X$ follows from Eqs. 3.21 and 3.23. Indeed, if $v \in X_1 = N(X) - X$, and u its neighbor in X, we have

$$\begin{aligned} (A's)(v) &= s(u) + (k-1)s(u)\alpha_2\\ &\leq (\alpha_0 + (k-1)\alpha_2)s(u)\\ &= \lambda'\alpha_1 s(u)\\ &= \lambda' s(v). \end{aligned}$$

A similar calculation shows that $(A's)(v) = \lambda' s(v)$ for $v \in B_l(X) - (X \cup N(X))$.

By applying Remark 3.2 for $2 \leq h \leq l+1$, we get

$$\begin{aligned} ||g||^2 &\geq \frac{\sum_{v \in X_{l+1}} s(v)^2}{\sum_{v \in X_1} s(v)^2} \sum_{v \in X_1} g(v)^2 && (3.25)\\ &= (k-1)^l \frac{{\alpha_{l+1}}^2}{{\alpha_1}^2} \sum_{v \in X_1} g(v)^2\\ &\geq (k-1)^l \frac{(k-1)^{-(l+1)} e^{2l\theta'}(e^{-\theta} - e^{-\theta'})^2}{(k-1)^{-1}e^{-2\theta}} \sum_{v \in X_1} g(v)^2\\ &= e^{2l\theta'}(1 - e^{\theta - \theta'})^2 \sum_{v \in X_1} g(v)^2\\ &\geq e^{2(l-1)\theta'}(\theta' - \theta)^2 \sum_{v \in X_1} g(v)^2. \end{aligned}$$

The last equation follows from the inequality $e^{\theta'} - e^{\theta} \geq (\theta' - \theta)$, whose proof is similar to the proof of Claim 3.3.

We now need to show that $g(v)^2$ is upper bounded by $\sum_{v \in X_1} g(v)^2$ times a multiplicative constant, for any $v \in X$. We proceed by induction on the distance from v to X_1. As in Lemma 3.4, we denote by P the projection on X, by P_1 the projection on X_1, and by A_1 the matrix $(P+P_1)A'(P+P_1)$. Let $s' = (P + P_1)s$ be the projection of s on $X \cup N(X)$. We have

$$A_1 s' \leq \overline{\lambda} s'. \tag{3.26}$$

Indeed, for $v \in X$, we have $(A_1 s')(v) = (A's')(v) = \overline{\lambda} s'(v)$ by Eq. 3.24. On the other hand, for $v \in X_1$, we have $(A_1 s')(v) = s'(v)/\alpha_1 = \sqrt{k-1} e^{\theta} s'(v) \leq \overline{\lambda} s'(v)$, since $e^{\theta} \leq 2\cosh\theta$. Premultiplying both sides of Eq. 3.26 by P and A_1 yields successively:

$$\begin{aligned} PA_1 s' &\leq \overline{\lambda} s' - \overline{\lambda} P_1 s' \\ A_1 P A_1 s' &\leq \overline{\lambda}^2 s' - \overline{\lambda} A_1 P_1 s'. \end{aligned}$$

Therefore, $\overline{\lambda}^2 s' - A_1 P A_1 s' \geq \overline{\lambda} A_1 P_1 s' \geq P_{N(X_1) \cap X} s'$, where $P_{N(X_1)\cap X}$ is the projection on the set of vertices in X adjacent to X_1. To prove the last inequality, consider a node u in $N(X_1) \cap X$, and let $v \in N(\{u\}) \cap X_1$. Then $(P_{N(X_1)\cap X} s')(u) = s'(u)$, and

$$(A_1 P_1 s')(u) = \sum_{(u,w) \in E} (P_1 s')(w) \geq (P_1 s')(v) = s'(v) = \alpha_1 s'(u).$$

Finally, $\overline{\lambda}\alpha_1 \geq 1$. Hence

$$\overline{\lambda}^2 (P + P_1)s - A_1 P A_1 s \geq P_{N(X_1)\cap X} s.$$

As in Lemma 3.4, we conclude that

$$\begin{aligned} ||P_{N(X_1)\cap X} g||^2 &\leq \overline{\lambda}^2 ||(P + P_1)g||^2 - ||PA_1 g||^2 \\ &= \overline{\lambda}^2 ||Pg||^2 + \overline{\lambda}^2 ||P_1 g||^2 - \lambda'^2 ||Pg||^2 \\ &\leq \overline{\lambda}^2 ||P_1 g||^2 \\ &= \overline{\lambda}^2 \sum_{v \in X_1} g(v)^2. \end{aligned}$$

Now, let us consider the set of nodes in X at distance i from X_1, for $2 \leq i \leq \log_{k-1} |X|$. By a similar reasoning, we can show that the ratio of the norms of the restriction of g to two successive levels is at most $\overline{\lambda}$. Therefore, the squared norm of the restriction of g to level i is at most

$$\overline{\lambda}^{2i} \sum_{v \in X_1} g(v)^2 \leq |X|^{2\log_{k-1}\overline{\lambda}} \sum_{v \in X_1} g(v)^2 \leq |X|^4 \sum_{v \in X_1} g(v)^2.$$

Combining this with Eq. 3.25 shows that, for all $u \in X$,

$$||g||^2|X|^4 \geq e^{2(l-1)\theta'}(\theta' - \theta)^2 g(u)^2. \tag{3.27}$$

The same relation holds for any vertex in the graph. We have assumed so far that H is connected. If it is not, then each of its components H_i satisfies the condition $\lambda_0(M^\theta_{H_i}) \leq \overline{\lambda}$, by Fact 3.3. Therefore, Eq. 3.27 still holds if X is replaced by the vertex set of H_i, for each vertex of H_i. But this gives an even stronger relation than Eq. 3.27.

Combining Eq. 3.27 with Eq. 3.20 and noting that $E\Delta E'$ contains at most $2k|X|$ undirected edges yields

$$\lambda' ||g||^2 \leq 2\sqrt{k-1}||g||^2 + \frac{2k|X|^5 e^{-2(l-1)\theta'}}{(\theta' - \theta)^2}||g||^2,$$

from which we deduce that

$$\cosh\theta' \leq 1 + \frac{e^{-2(l-1)\theta'}}{(\theta' - \theta)^2} k|X|^5.$$

Assume now that $\theta > 0$. Using the relations $\cosh\theta' \geq 1 + \theta'^2/2 \geq 1 + \theta^2/2$, we conclude that

$$\theta' - \theta \leq 2k|X|^3 e^{-(l-1)\theta'}/\theta \leq 2k|X|^3 e^{-(l-1)\theta}/\theta.$$

This implies that $\theta' \leq \theta + o(1)$ as n goes to infinity, and therefore $\lambda' \leq \overline{\lambda}(1 + o(1))$. We can get a more precise on the upper bound as follows: since $\cosh\theta' \leq \cosh\theta + 2(\theta' - \theta)\sinh\theta$ for $\theta' \approx \theta$, we deduce after some calculations that $\lambda' \leq \overline{\lambda}(1 + 4e^{-(l-1)\theta} k|X|^3(\tanh\theta)/\theta)$. Replacing l by its value, we get

$$\lambda' \leq \overline{\lambda}(1 + 2\frac{\tanh\theta}{\theta} k|X|(|X|/n)^{\theta/(4\log(k-1))}). \tag{3.28}$$

This achieves the proof in the case $\theta > 0$. Suppose now that $\theta = 0$. For any $\epsilon > 0$, we have $\lambda_0(M^\epsilon_H) \leq \overline{\lambda} = 2\sqrt{k-1}\cosh\epsilon$. Therefore, by the above results, we have $\lambda' \leq \overline{\lambda}(1+\epsilon) = 2(1+\epsilon)\sqrt{k-1}\cosh\epsilon$, for sufficiently large n. Hence, $\lambda' \leq (2 + o(1))\sqrt{k-1}$ as n goes to infinity, as required.

■

We now combine Theorems 3.1 and 3.8 to get the following result:

Theorem 3.9 *Let H be a graph, k an integer such that $k-1$ is a prime congruent to 1 modulo 4, and $\overline{\lambda}$ a real number no smaller than $2\sqrt{k-1}$. Let $\overline{\lambda} = 2\sqrt{k-1}\cosh\theta$, where $\theta \geq 0$. The following conditions are equivalent:*

1. *There exists an infinite family G_n of k-regular graphs containing H as an induced subgraph and such that $\lambda(G_n) \leq (1 + o(1))\overline{\lambda}$.*
2. *There exists an infinite family G_n of k-regular graphs containing H as an induced subgraph and such that $\lambda_1(G_n) \leq (1 + o(1))\overline{\lambda}$.*

3. The maximum degree of H is at most k, and $\lambda_0(M_H^\theta) \leq \overline{\lambda}$.

Proof Condition 1 clearly implies Condition 2. Condition 2 implies Condition 3 by Theorem 3.1. Indeed, it implies that $\lambda_0(M_H^{(1+o(1))\theta}) \leq (1+o(1))\overline{\lambda}$. As n goes to infinity, we get Condition 3 by continuity. Condition 3 implies Condition 1 by Theorem 3.8. ■

3.5 Expansion of subsets of sublinear size

The graphs constructed in [45, 49] besides being Ramanujan, have other properties such as high girth. In particular, the bipartite Ramanujan graphs constructed in [45, 49] have girth $(4/3-o(1))\log_{k-1} n$. We will use this property to get high expansion for subsets of sublinear size.

Proposition 3.1 *Let $G = (V, E)$ be a k-regular graph of girth $(4/3 + o(1))\log_{k-1} n$. For any subset X of V of size at most n^α, the average degree of the subgraph induced on X is at most $2 + 2(k-1)^{(3+o(1))\alpha/2}$.*

Proof Let σ be the average degree of the subgraph induced on X. A classical result in graph theory [15, p. 126] shows that the girth of this subgraph is at most $2\lceil \log_{\lfloor \sigma/2 \rfloor} |X| \rceil + 1 \leq 2\lceil \alpha \log_{\lfloor \sigma/2 \rfloor} n \rceil + 1$. On the other hand, it is at least $(4/3 + o(1))\log_{k-1} n$. Comparing these two inequalities yields the desired bound on σ. ■

Note that α must be less than $1/3$ for the bound in Proposition 3.5 to beat the bound in Theorem 3.3, when the graph is Ramanujan.

Theorem 3.10 *Let $G = (V, E)$ be a k-regular graph of girth $(4/3 + o(1))\log_{k-1} n$. For any subset X of V of size at most n^α,*

$$\frac{|N(X)|}{|X|} \geq \lfloor k - (k-1)^{(3+o(1))\alpha} \rfloor.$$

Proof Let Y be a minimal nonempty subset of X having expansion at most $\beta = |N(X)|/|X|$. If $\beta = k$, we are done. Otherwise Y is not a singleton, and for any element v of Y, the expansion of the subset $Y - \{v\}$ is greater than β. In other words,

$$|N(Y - \{v\})| > \beta |Y - \{v\}| = \beta |Y| - \beta \geq |N(Y)| - \beta.$$

Therefore, the vertex v has less than β neighbors in the complement of $N(Y - \{v\})$, and so it has at least $k - \lceil \beta \rceil + 1$ neighbors in $N(Y - \{v\})$. Hence, there are at least $k - \lceil \beta \rceil + 1$ vertices in Y at distance 2 from v. More generally, for $l < c(G)/4$, there are at least $(k - \lceil \beta \rceil + 1)(k - \lceil \beta \rceil)^{l-1}$ vertices in Y at distance $2l$ from v. This implies a strict lower bound of $(k - \lceil \beta \rceil)^l$ on the size of Y, and so

$$(k - \lceil \beta \rceil)^{(1/3+o(1))(\log_{k-1} n)} < n^\alpha.$$

Solving this inequality yields the desired bound on β. ■

As a consequence of Theorem 3.10, if α is a constant less than 1/3, subsets of size at most n^α have expansion at least $k(1 - O(k^{3\alpha-1}))$, which is greater than $k/2$ for sufficiently large k.

Chapter 4

Other results and Applications

In this chapter, we describe applications of the results obtained in Chapter 3. We also generalize some of the results obtained Chapter 3, and prove general results in algebraic graph theory that have been used in the first proof [39] of Theorem 3.2.

In Section 4.1, we give an upper bound on the probability that a random walk stays inside a given subset of an expander. This property is often used in complexity theory and cryptography. Several papers [2, 32, 36] have addressed this problem, but our result is stronger. We also give an upper bound on the eigenvalues of induced subgraphs. In Section 4.2, we give bounds on the spectrum of *collapsed graphs*. For a given a graph G and a partition $(Z_0, Z_1, \ldots, Z_t)$ of the vertices, we define the collapsed graph associated to this partition as the weighted graph having $t+1$ nodes, each corresponding to a subset Z_i, and such that the weight of the edge (Z_i, Z_j) is equal to the number of neighbors in Z_j that a node in Z_i has in average. The spectrum of collapsed graphs has been studied [16, page 158] under strong regularity conditions. In Section 4.3, we describe applications of Theorems 3.2, 3.3 and 3.4 to the construction of selection networks, extrovert graphs, and highly expanding non-Ramanujan graphs.

We start by stating some general facts in linear algebra.

Fact 4.1 *If B is a selfadjoint operator in a vector space L, then*

$$\lambda_{n-1}(B) = \min_{g \in L - \{0\}} \frac{g \cdot Bg}{||g||^2}$$

Proof Follows from Fact 3.1 applied to the operator $-B$. ■

Fact 4.2 *Two vector subspaces whose sum of dimensions exceeds the dimension of the entire vector space have a nonzero intersection.* ■

Fact 4.3 (Rayleigh quotient principle) *If B is a selfadjoint operator in a vector space L, then*

$$\lambda_i(B) = \max_H \min_{g \in H - \{0\}} \frac{g \cdot Bg}{||g||^2}, \tag{4.1}$$

where H ranges over the vector subspaces of L of dimension $i+1$.

Proof If H is a vector subspace of L of dimension $i+1$, it has a nonzero common vector g with the subspace spanned by the eigenvectors associated to the $n-i$ smallest eigenvalues. Hence $g \cdot Bg \leq \lambda_i ||g||^2$ by Fact 3.1. It follows that the right-hand side is at most the left-hand side. There is equality when H is equal to the subspace spanned by the eigenvectors associated to the $i+1$ largest eigenvalues, by Fact 4.1. ■

Fact 4.4 *For any operator B and any polynomial P, the eigenvalues of the operator $P(B)$ are the images by P of the eigenvalues of B.*

Proof There exists a basis (over the field of complex numbers) where the matrix of B is upper triangular. The eigenvalues of B consist of the diagonal elements. The matrix of $P(B)$ in the same basis is upper triangular, and its diagonal elements are the images by P of the diagonal elements of B. ■

4.1 Random walks and bounds on the spectrum of induced subgraphs

We start by showing that the probability that a walk stays inside a given set has an exponential decay in the length of the walk. We show that our bound is optimal in some cases. Then we provide a generalization of Lemma 3.2.

Corollary 4.1 *If $G = (V, E)$ is k-regular and W a subset of V, the fraction of walks in G of length l whose all vertices belong to W is at most $\mu\ (\alpha + \mu - \alpha\mu)^l$, where $\alpha = \lambda_1/k$ and $\mu = |W|/n$.*

Proof The number of walks of length l in W is equal to the sum of entries of ${A_W}^l$. Hence, the fraction of walks of length l in W is equal to $((A_W)^l \chi_W \cdot \chi_W)/(k^l n)$. On the other hand, Fact 3.4 shows that $\lambda_0(A_W)$ is the largest eigenvalue of A_W *in absolute value*. Therefore (Fact 4.4), the largest eigenvalue of ${A_W}^l$ is $(\lambda_0(A_W))^l$. Using Lemma 3.2 and Fact 3.1, we conclude that

$$({A_W}^l \chi_W) \cdot \chi_W \leq (\lambda_0(A_W))^l ||\chi_W||^2 \leq \mu n\ (\lambda_1 + k\mu - \lambda_1\mu)^l.$$

■

Define the density of a subset of vertices to be the ratio of its size to the total number of vertices. Corollary 4.1 is optimal in the following sense: for any rational $\alpha \in [1/2, 1]$ and any rational $\mu \in [0, 1]$, there exists an arbitrary large graph k-regular graph G and a subset W of G of density μ such that $\lambda_1(G) = \alpha k$ and, for any integer l, the fraction of walks in W of length l is equal to $\mu\ (\alpha + \mu - \alpha\mu)^l$. Indeed, let $G = K_{a+2} \times K_b$, where $b = a(1-\alpha)/\alpha$ and $K_{a+2} \times K_b$ is the graph on $V = \{1, \ldots, a+2\} \times \{1, \ldots, b\}$, with $((i,j),(i',j')) \in E$ if and only if $i = i'$ XOR $j = j'$. The graph G is the cartesian product of the complete graphs K_{a+2} and K_b, and so [6] its eigenvalues are equal to the sum of the eigenvalues of K_{a+2} and K_b. Since the eigenvalues of K_{a+2} and K_b are respectively $a+1, -1$ and $b-1, -1$, the eigenvalues of G are $a+b, a, b-2$ and -2. The graph G is regular of degree $a+b$, and $\lambda_1(H) = a = \alpha(a+b)$. Let $W = \{1, \ldots, a+2\} \times \{1, \ldots, \mu b\}$. The set W has density μ in V; the subgraph induced on W is isomorphic to $K_{a+2} \times K_{\mu b}$, and so it is regular of degree $a + \mu b$. Therefore, the fraction of walks in W of length l is equal to $\mu(a+\mu b)^l/(a+b)^l$, which is equal to the value given by Claim 4.1.

Lemma 3.2 can be generalized as follows:

Lemma 4.1 *If G is a k-regular graph, and W a subset of V, then $\lambda_i(W) \leq \lambda_{i+1}(G) + k\mu - \lambda_{i+1}(G)\mu$. Also, $\lambda_0(W) \geq \lambda_{n-1}(G) + k\mu - \lambda_{n-1}(G)\mu$.*

Proof It follows from Fact 4.3 that

$$\lambda_i(W) = \max_H \min_{g \in H - \{0\}} \frac{g \cdot (A_W g)}{||g||^2},$$

where H ranges over the subspaces of $L^2(W)$ of dimension $i+1$. Let H be a subspace where the maximum is attained. For any vector g in H, we associate the vector $\phi(g)$ in $L^2(V)$ that coincides with g on W, and is null on $V - W$. The map ϕ is linear, and its image H' is a vector subspace of $L^2(V)$. Let $e_0, e_1, \ldots, e_{n-1}$ be a set of eigenvectors of A_G corresponding to $\lambda_0(G), \lambda_1(G), \ldots, \lambda_{n-1}(G)$. Since $\dim \mathrm{Vect}(e_0, e_{i+1}, e_{i+2}, \ldots, e_{n-1}) = n - i$ and $\dim H' = \dim H = i + 1$, there exists (Fact 4.2.) a nonzero vector $f' = \phi(f)$ in $H' \cap \mathrm{Vect}(e_0, e_{i+1}, e_{i+2}, \ldots, e_{n-1})$. Let $f' = \bar{f}' + h$, with $\bar{f}' \in \mathcal{R}e_0$ and $h \in \mathrm{Vect}(e_{i+1}, e_{i+2}, \ldots, e_{n-1})$. Since e_0 is orthogonal to $\mathrm{Vect}(e_{i+1}, e_{i+2}, \ldots, e_{n-1})$, the vector $\bar{f}'$ is the orthogonal projection of f' on $\mathcal{R}e_0$. Denote $\lambda_{i+1}(G)$ by λ_{i+1}. By a calculation similar to Lemma 3.1, we have

$$\begin{aligned} f \cdot A_W f &= f' \cdot A f' \qquad (4.2) \\ &= k||\bar{f}'||^2 + h \cdot Ah \\ &\leq k||\bar{f}'||^2 + \lambda_{i+1}||h||^2 \\ &= (k - \lambda_{i+1})||\bar{f}'||^2 + \lambda_{i+1}||f'||^2 \\ &\leq (k - \lambda_{i+1})\mu||f'||^2 + \lambda_{i+1}||f'||^2 \end{aligned}$$

$$= \quad (k - \lambda_{i+1})\mu||f||^2 + \lambda_{i+1}||f||^2.$$

The third equation follows from Fact 3.1. Hence,

$$\min_{g \in H - \{0\}} \frac{g \cdot A_W g}{||g||^2} \leq \frac{f \cdot A_W f}{||f||^2} \leq \lambda_{i+1} + k\mu - \lambda_{i+1}\mu.$$

Since the left-hand side is equal to $\lambda_i(W)$, the first part of Lemma 4.1 follows.

To prove the second part of the Lemma 4.1, it is sufficient (Fact 3.1) to show that $\chi_W \cdot A_W \chi_W \geq (k\mu - \lambda_{i+1}\mu + \lambda_{i+1})|W|$. This calculation is similar to Eq. 4.3, except that we use Fact 4.1 to lower bound $h \cdot Ah$ by $\lambda_{n-1}||h||^2$ in the third equation. ■

Corollary 4.2 *The size of the largest independent set of G is at most $|\lambda_{n-1}|n/(1 + |\lambda_{n-1}|)$.*

Proof This follows from the fact that the adjacency matrix of an independent set is null, and so $\lambda_{n-1} + \mu - \lambda_{n-1}\mu \leq 0$. ■

The bound of Corollary 4.2 is slightly better than the one derived in [45].

4.2 Spectrum of collapsed graphs

If X and Y are two subsets of a graph $G = (V, E)$, let $e(X, Y) = |(X \times Y) \cap E\}|$ be the number of edges whose first endpoint is in X and second endpoint in Y. If $Z_0, \ldots, Z_t$ is a sequence of non-empty subsets of V, we denote by $R^{\{Z_0, Z_1, \ldots, Z_t\}}$ the set of real valued functions on the set $\{Z_0, Z_1, \ldots, Z_t\}$. We define $\Phi(Z_0, Z_1, \ldots, Z_t)$ to be the linear mapping in $R^{\{Z_0, Z_1, \ldots, Z_t\}}$ whose matrix in the canonical basis $(\chi_{\{Z_0\}}, \ldots, \chi_{\{Z_t\}})$ is the $(t+1, t+1)$ matrix whose entry (i, j) equal to $e(Z_i, Z_j)/|Z_i|$. The matrix of $\Phi(Z_0, Z_1, \ldots, Z_t)$ can be viewed as the adjacency matrix of the weighted directed graph on the set $\{Z_0, Z_1, \ldots, Z_t\}$ where the weight of the edge (Z_i, Z_j) is equal to the average number of neighbors that a node in Z_i has in Z_j. Note that the sum of the $(i+1)$-st row is equal to the average degree in G of the vertices of Z_i.

Lemma 4.2 *Let $G = (V, E)$ be a graph and let $Z_0, \ldots, Z_t$ be a sequence of non-empty disjoint subsets of V. For $0 \leq i \leq t$, we have $\lambda_i(G) \geq \lambda_i(\Phi)$, and $\lambda_{n-1-i}(G) \leq \lambda_{t-i}(\Phi)$, where $\Phi = \Phi(Z_0, Z_1, \ldots, Z_t)$.*

Proof We prove only the first inequality. The proof of the second inequality is very similar. The idea behind the proof is to realize an injective embedding from $R^{\{Z_0, \ldots, Z_t\}}$ into $L^2(V)$.

Define the scalar product $<,>$ on $R^{\{Z_0, \ldots, Z_t\}}$ by

$$< r, s >= \sum_{i=0}^{t} |Z_i| r(Z_i) s(Z_i).$$

Let ψ be the linear mapping from $R^{\{Z_0,\ldots,Z_t\}}$ to $L^2(V)$ that maps $\chi_{\{Z_i\}}$ to χ_{Z_i}.

Claim 4.1 *For any $r, s \in R^{\{Z_0,\ldots,Z_t\}}$, we have $\psi(r) \cdot \psi(s) = < r, s >$.*

Proof Since both sides of the above equality are bilinear in r and s, it suffices to show that the equality holds when r and s are elements of the canonical basis of $R^{\{Z_0,\ldots,Z_t\}}$. But

$$\begin{aligned} \psi(\chi_{\{Z_i\}}) \cdot \psi(\chi_{\{Z_j\}}) &= \chi_{Z_i} \cdot \chi_{Z_j} \\ &= \delta_{i,j}|Z_i| \\ &= < \chi_{\{Z_i\}}, \chi_{\{Z_j\}} > . \end{aligned}$$

■

Claim 4.2 *For any $r, s \in R^{\{Z_0,\ldots,Z_t\}}$, we have $\psi(r) \cdot A\psi(s) = < r, \Phi s >$.*

Proof The claim follows from bilinearity and the equalities

$$\begin{aligned} \psi(\chi_{\{Z_i\}}) \cdot A\psi(\chi_{\{Z_j\}}) &= \chi_{Z_i} \cdot A\chi_{Z_j} \\ &= e(Z_i, Z_j) \\ &= < \chi_{\{Z_i\}}, \Phi\chi_{\{Z_j\}} > . \end{aligned}$$

■

Claim 4.2 implies in particular that Φ defines a self-adjoint operator with respect to the product $<,>$ and so the eigenvalues of Φ are real. Using Fact 4.3 and the injectivity of ψ, it follows that

$$\begin{aligned} \lambda_i(\Phi) &= \max_H \min_{r \in H - \{0\}} \frac{< r, \Phi r >}{< r, r >} \\ &= \max_H \min_{f \in \psi(H) - \{0\}} \frac{f \cdot Af}{||f||^2} \\ &\leq \max_{H'} \min_{f \in H' - \{0\}} \frac{f \cdot Af}{||f||^2} \\ &= \lambda_i(G), \end{aligned}$$

where H and H' range respectively over the subspaces of $R^{\{Z_0,\ldots,Z_t\}}$ and $L^2(V)$ of dimension $i+1$.

■

Lemma 4.3 *Let $G = (V, E)$ be a graph and $X_{-1} = \emptyset, X_0, X_1, \ldots, X_t$ be a sequence of subsets of V such that, for $0 \leq i \leq t-1$, the degree of any element of X_i is equal to k, $N(X_i) \subseteq X_{i+1}$ and $|X_{i-1}| < |X_i|$. If the eigenvalues of the adjacency matrix of G are $\delta_0, \delta_1, \ldots, \delta_t$, with $|\delta_0| \geq |\delta_1| \geq \cdots \geq |\delta_t|$,*

then $|\delta_i|$ is no smaller than the i-th largest eigenvalue of the matrix $R_{t+1}(k;\rho_0,\rho_1,\ldots,\rho_{t-1})$ equal to

$$\begin{pmatrix} 0 & k & 0 & 0 & \ldots & 0 \\ \rho_0 & 0 & k-\rho_0 & 0 & \ldots & 0 \\ 0 & \rho_1 & 0 & k-\rho_1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ 0 & \ldots & 0 & \rho_{t-2} & 0 & k-\rho_{t-2} \\ 0 & 0 & \ldots & 0 & \rho_{t-1} & 0 \end{pmatrix},$$

where

$$\rho_i = k\frac{|X_i|-|X_{i-1}|}{|X_{i+1}|-|X_{i-1}|}.$$

Proof Note that $X_i \subseteq N^2(X_i) \subseteq X_{i+2}$. We remind the reader that the cover graph G' of G is the graph defined on $V' = V \times \{0,1\}$, and where $((u,l),(v,m)) \in V' \times V'$ is an edge if and only if $(u,v) \in E$ and $l \neq m$. By Fact 3.10, the eigenvalues of G' consist of $\lambda_0,\ldots,\lambda_{n-1}$ and $-\lambda_0,\ldots,-\lambda_{n-1}$. Hence $\lambda_i(G') = |\delta_i|$ for $0 \leq i \leq n-1$. For $0 \leq i \leq t$, let Y_i be the subset of V' defined by $Y_i = X_i \times \{(i \bmod 2)\}$. Then, for $0 \leq i \leq t-1$, we have $N_{G'}(Y_i) \subseteq Y_{i+1}$ and $Y_{i-1} \neq Y_{i+1}$. Now, we apply Lemma 4.2 to G' and the subsets $Z_i = Y_i - Y_{i-2}$, for $0 \leq i \leq t$. The subsets Z_i's are clearly nonempty and disjoint. Note that $|Y_i| = |X_i|$ and $|Z_i| = |X_i| - |X_{i-2}|$.

Let us calculate the entries of the matrix $\Phi(Z_0,Z_1,\ldots,Z_t)$. For $0 \leq i \leq t-1$, we have

$$\begin{aligned} e(Z_i,Z_{i+1}) &= e(Y_i - Y_{i-2}, Y_{i+1} - Y_{i-1}) \\ &= e(Y_i, Y_{i+1} - Y_{i-1}) - e(Y_{i-2}, Y_{i+1} - Y_{i-1}) \\ &= e(Y_i,Y_{i+1}) - e(Y_i,Y_{i-1}) \\ &= k|Y_i| - k|Y_{i-1}| \\ &= k(|X_i| - |X_{i-1}|). \end{aligned}$$

The third equation follows from the fact that, since $N(Y_{i-2}) \subseteq Y_{i-1}$, there are no edges between Y_{i-2} and $Y_{i+1} - Y_{i-1}$. Therefore, the entry $(i+2,i+1)$ of $\Phi(Z_0,Z_1,\ldots,Z_t)$ is equal to ρ_i. On the other hand, there are no edges between Z_i and Z_j if $|i-j| \neq 1$. This is because $N(Z_i) \subseteq Z_{i+1} \cup Z_{i-1}$. Indeed, if a vertex v is adjacent to Z_i, it belongs to $N(Y_i) \subseteq Y_{i+1}$. If $v \notin Y_{i-1}$, then $v \in Z_{i+1} = Y_{i+1} - Y_{i-1}$. If $v \in Y_{i-1}$, then $v \in Z_{i-1}$. Indeed, since $v \in N(Z_i)$, then $v \notin Y_{i-3}$, as we observed earlier. Hence, $N(Z_i) \subseteq Z_{i+1} \cup Z_{i-1}$, as required. Moreover, since the degree of any element of Y_i is equal to k, for $0 \leq i \leq t-1$, the sum of the $(i+1)$-st row of $\Phi(Z_0,Z_1,\ldots,Z_t)$ is equal to k. We conclude that $\Phi(Z_0,Z_1,\ldots,Z_t) = R_{t+1}(k;\rho_0,\rho_1,\ldots,\rho_{t-1})$. This achieves the proof. ■

4.3 Examples and applications

We list two examples illustrating Lemmas 4.2 and 4.3, and four applications of Ths. 3.2, 3.3 and 3.4.

1. **Number of edges in an induced subgraph.** Let $G = (V, E)$ be a k-regular graph on n vertices and Z_0 a proper subset of V. We apply Lemma 4.2 with $t = 1$ and $Z_1 = V - Z_0$. Since the row sum of ϕ is equal to k, we have $\lambda_0(G) = \lambda_0(\Phi) = k$. An easy (but dull) calculation shows that $|Z_0||Z_1|\lambda_1(\Phi) = ne(Z_0, Z_0) - k|Z_0|^2$. The inequality $|\lambda_1(\Phi)| \leq \lambda$ then becomes $|e(Z_0, Z_0) - k|Z_0|^2/n| \leq \lambda|Z_0|(1 - |Z_0|/n)$. Note that this inequality is also true in the case $Z_0 = \emptyset$ or $Z_0 = V$. This result has already been established in [4].

2. **Tanner's inequality.** Again, we assume that $G = (V, E)$ is a k-regular graph on n vertices. Let X be a proper subset of V. We apply Lemma 4.3 with $t = 3$, $X_0 = X$, $X_1 = N(X)$ and $X_2 = X_3 = V$. We have $\rho_0 = k|X|/|X_1|$, $\rho_1 = k(|X_1| - |X|)/(|V| - |X|)$, and $\rho_2 = k$. As before, k is an eigenvalue of $R_4(k; \rho_0, \rho_1, k)$. Since the (i, j) entry of this matrix is null if $i \equiv j \pmod 2$, the other eigenvalues of $R_4(k; \rho_0, \rho_1, k)$ are $\{\sigma, -\sigma, -k\}$. But $\det(R_4(k; \rho_0, \rho_1, k)) = k^2\rho_0(k - \rho_1) = k^2\sigma^2$. Since $|\sigma| \leq \lambda$ by lemma 4.3, we have $\rho_0(k - \rho_1) \leq \lambda(G)^2$. Eq. 1.1 follows by a simple calculation. Note that we have implicitly assumed that $N(X)$ is a proper subset of V. However, we can directly check that Eq. 1.1 holds if $N(X) = V$ or $X = \emptyset$.

3. **Random regular graphs.** In [27], it was shown that, if k is even, then for a random k-regular graphs G, we have $\lambda_1(G) \leq 2\sqrt{k-1} + O(\log k)$ with high probability. Using Theorem 3.2, we deduce that for a random regular graphs, we can prove with high probability *in polynomial time* that linear sized subsets (of size at most $k^{-1/\epsilon}$, where $\epsilon = k^{-1/4}$) have expansion at least

$$\frac{k}{2}\left(1 - \sqrt{1 - \frac{4k-4}{(2\sqrt{k-1} + O(\log k))^2}}\right)(1 + O(k^{-1/4})) = \frac{k}{2} - O(k^{3/4}\log^{1/2} k).$$

4. **Selection networks.** We can use Theorem 3.2 to build explicit selection networks of small size. A selection network is a network of comparators that classifies a set of n numbers, where n is even, into two subsets of $n/2$ numbers such that any element in the first set is smaller than any element in the second set. In [55], a probabilistic construction of a selection network is given using an asymptotic upper bound of $2n\log_2 n$ comparators. Also, an upper bound slightly less than $6n\log_2 n$ is shown by a deterministic construction. Using Theorem 3.2, we can construct selection networks of asymptotic size $(3 + o(1))n\log_2 n$. Indeed, it is shown in [55] how to construct selection networks of size $(2+o(1))n\log_2 n$ from expanders of degree 4 having linear expansion at least 3. The construction can be easily generalized to build selection networks of size $k(1/2 + o(1))n\log_2 n$ from expanders of degree k having linear expansion at least 3. Theorem 3.2 shows that the linear expansion of k-regular Ramanujan graphs is at least

$k/2$, and thus we can build explicit selection networks of size $(3+o(1))n\log_2 n$ using 6-regular Ramanujan graphs.

5. **Extrovert graphs.** Given a graph $G=(V,E)$ and a subset X of V, an element of X is said to be extrovert if at least half of its neighbors are outside X. A family of graphs is called extrovert if all linear-sized subsets contain a constant fraction of extrovert nodes. Theorem 3.3 shows that the average degree of the nodes of a linear-sized induced subgraph of a k-regular Ramanujan graph is upper bounded by roughly $1+\sqrt{k-1}$, which is less than $k/2$ for $k \geq 7$. This shows that Ramanujan graphs of degree at least 7 are extrovert graphs.

6. **Highly expanding non-Ramanujan graphs.** Let G be a k-regular Ramanujan graph, and t an integer greater than 1. We define the graph G^t on the same vertex set as G by joining two vertices with an edge if their distance in G is t. The graph G^t has maximum degree at most $k(k-1)^{t-1}$. The set of neighbors in G^t of a subset X contains $N_G^t(X) - N_G^{t-2}(X)$. Hence, by Theorem 3.5, subsets of G^t of size at most $k^{-t-1/\epsilon}|V|$ have expansion at least $k(k-2)(k-1)^{t-2}(1-O(t\epsilon))/2$. Assume now that the girth of G^t is greater than $2t$. Then G^t is regular of degree $k(k-1)^{t-1}$. As in [45, 27], we see that the adjacency matrix of G^t satisfies the equality $A_{G^t} = A_G A_{G^{t-1}} - (k-1)A_{G^{t-2}}$, for $t \geq 3$. Consider the sequence r_i given by $r_i = \lambda(G)r_{i-1} - (k-1)r_{i-2}$, with $r_1 = \lambda(G)$ and $r_2 = \lambda(G)^2 - k$. An eigenvector of A_G corresponding to the eigenvalue $\lambda(G)$ is also an eigenvector of G^t with eigenvalue r_t. It follows that $\lambda(G^t) \geq r_t$. Since $\lambda(G) = 2\sqrt{k-1}(1-o(1))$, it follows that $\lambda(G^t) \geq (k-1)^{t/2-1}(t(k-2)+k)(1-o(1))$, as $|V|$ goes to infinity. The graph G^t is far from being Ramanujan if $|V|$ is large enough. Hence, from any family of k-regular Ramanujan graphs G_n with high girth, we can construct a family of $k(k-1)^t$-regular graphs whose linear expansion is at least $k(k-2)(k-1)^{t-1}$.

   Note that by considering two disjoint copies of G_n, we get a family of k-regular non-Ramanujan graphs with the same linear expansion as (G_n). However, the expansion of some subsets containing half the nodes is null. Moreover, all the eigenvalues of any element of this family, except the largest two, satisfy the Ramanujan condition. In contrast, it can be shown that a linear number of eigenvalues of G^t violate the Ramanujan condition.

Chapter 5

Diameter and Eigenvalues

In this chapter, we establish some isoperimetric inequalities related to the spectrum of the graph. We prove new results and give simpler proofs of known results relating the eigenvalues of a graph to its diameter and girth. Our method is based on elementary linear algebra, the use of Chebychev polynomials, and some of the techniques developed in the previous chapters. In Section 5.1, we establish a lower bound on the size of $N^t(X)$, where X is a set of vertices and $N^t(X)$ is the set of nodes that can be reached from X by a path of length t, that is,

$$\underbrace{N(N(\ldots N(}_{t \text{ times}} X))\ldots).$$

The lower bound is a function of the size of X and of the second eigenvalue in absolute value λ of the graph. As a first corollary, we obtain an upper bound on the distance between two subsets of given size. As a second corollary, we get a simple proof of a recent result [57] relating the diameter, the girth, and λ. In Section 5.2, we exhibit a relation between the diameter of a graph and its subsequent eigenvalues. In Section 5.3, we show that these bounds are tight. In particular, we exhibit k-regular graphs with $\lambda = (2+o(1))\sqrt{k-1}$ and diameter $(2+o(1))\log_{k-1} n$, thereby showing that the bound $2\log_{k-1} n$ is the best one can obtain using the second eigenvalue method.

5.1 Bounds on the distance between two subsets

Let P_t be the Chebychev polynomial of degree t. It is the unique polynomial satisfying the equation

$$P_t(\cos y) = \cos(ty), \tag{5.1}$$

for any complex number y. The Chebychev polynomials have already been used in [45] in the study of expanders. The following facts follow easily from Eq. 5.1:

Fact 5.1 *For any complex number z, we have $P_t(-z) = (-1)^t P_t(z)$.*

Proof Replacing y by $y + \pi$ in Eq. 5.1, and since $\cos(ty + t\pi) = (-1)^t \cos(ty)$, we deduce that $P_t(-z) = (-1)^t P_t(z)$ for infinitely many values of z, and therefore for all values of z, since the two sides are polynomial in z. ■

Fact 5.2 *For any real number s between -1 and 1, we have $|P_t(s)| \leq 1$*

Proof Since $s = \cos y$, for some real number y, we have $P_t(s) = \cos(ty)$, and so it is between -1 and 1. ■

Fact 5.3 *For any complex number z, we have $P_t(\cosh z) = \cosh(tz)$.*

Proof This follows by replacing y by iz in Eq. 5.1, where i is the usual square root of -1. ■

The L^1 norm $||h||_1$ of a vector h is defined to be $\sum_{v \in V} |h(v)|$.

Fact 5.4 *For any $h \in L^2(V)$, we have*

$$||h|| \leq ||h||_1 \leq \sqrt{n}||h||.$$

Proof The first inequality follows by squaring the two sides. The second follows from the Cauchy-Schwartz inequality. ■

Theorem 5.1 *Let $G = (V, E)$ be a k-regular graph and let λ be its second largest eigenvalue in absolute value. For any subset X of V and any integer $t \geq 1$, we have*

$$|N^t(X)| \geq \frac{{P_t}^2(k/\lambda)|X|}{1 + ({P_t}^2(k/\lambda) - 1)|X|/|V|} \tag{5.2}$$

If G is a non-bipartite Ramanujan graph of degree k, then

$$\frac{|N^t(X)|}{|X|} \geq \frac{((k-1)^t + 1)^2}{4(k-1)^t + ((k-1)^t - 1)^2|X|/|V|} \geq \frac{(k-1)^t}{4 + (k-1)^t|X|/|V|}$$

In particular, if $|X|/|V|$ is at most $4(k-1)^{-t-1}$, then $|N^t(X)| \geq (k-2)(k-1)^{t-1}|X|/4$.

Proof Denote by f be the characteristic vector of X. Let $f = \bar{f} + f_0$, where $\bar{f}$ is a constant vector and $f_0 \in L_0^2(V)$. The parity property of the polynomial P_t shows that it is of the form $P_t(s) = c_t s^t + c_{t-2} s^{t-2} + \cdots$, and so $P_t(\lambda^{-1}A)\ f = c_t \lambda^{-t} A^t f + c_{t-2} \lambda^{-(t-2)} A^{t-2} f + \ldots$. This implies that the support of the vector $g = P_t(\lambda^{-1}A)\ f$ is a subset of $N^t(X)$. This is because the support of the vector $A^l f$ is $N^l(X)$, and $N^t(X) \supseteq N^{t-2}(X) \supseteq \ldots$. We will obtain a lower bound on the size of

$N^t(X)$ by comparing the norm of g and its sum of coordinates, as we did in the proof of Tanner's result. Since $A\bar{f} = k\bar{f}$, we have

$$g = P_t(\lambda^{-1}A)\ \bar{f} + P_t(\lambda^{-1}A)\ f_0 = P_t(k/\lambda)\ \bar{f} + P_t(\lambda^{-1}A)\ f_0$$

We note that $P_t(\lambda^{-1}A)\ f_0 \in L_0^2(V)$ since $L_0^2(V)$ is invariant under A. Therefore,

$$||g||^2 = {P_t}^2(k/\lambda)||\bar{f}||^2 + ||P_t(\lambda^{-1}A)\ f_0||^2 \leq {P_t}^2(k/\lambda)||\bar{f}||^2 + ||f_0||^2$$

The second inequality follows from the fact that the operator $P_t(\lambda^{-1}A_{|L_0^2(V)})$ is selfadjoint and its eigenvalues $P_t(\lambda_i/\lambda)$, $1 \leq i \leq n-1$, are at most 1 in absolute value (Facts 4.4, 5.2 and 2.5.) It follows from the Cauchy-Schwartz inequality that

$$\begin{aligned} |\chi_{N^t(X)} \cdot g|^2 &\leq |N^t(X)|\ ({P_t}^2(k/\lambda)||\bar{f}||^2 + ||f_0||^2) \\ &= |N^t(X)|\ ({P_t}^2(k/\lambda)||\bar{f}||^2 + |X| - ||\bar{f}||^2) \end{aligned} \tag{5.3}$$

Since the operator $P_t(\lambda^{-1}A)$ is selfadjoint and the support of g is a subset of $N^t(X)$, we have

$$\begin{aligned} \chi_{N^t(X)} \cdot g &= \chi_V \cdot (P_t(\lambda^{-1}A)\ f) \\ &= (P_t(\lambda^{-1}A)\ \chi_V) \cdot f \\ &= P_t(k/\lambda)\ \chi_V \cdot f \\ &= P_t(k/\lambda)|X| \end{aligned}$$

By replacing the terms $\chi_{N^t(X)} \cdot g$ and $||\bar{f}||$ by their values in Eq. 5.3, we get

$$\frac{|X|}{|N^t(X)|} \leq \frac{|X|}{|V|} + \frac{1 - |X|/|V|}{{P_t}^2(k/\lambda)} \tag{5.4}$$

Eq. 5.2 follows from this inequality.

If G is a non-bipartite Ramanujan graph, we can replace λ by $2\sqrt{k-1}$ in Eq 5.2. We have

$$\begin{aligned} P_t(\frac{k}{2\sqrt{k-1}}) &= P_t(\cosh(\frac{\ln(k-1)}{2})) \\ &= \cosh(t\frac{\ln(k-1)}{2}) \\ &= \frac{(k-1)^{t/2} + (k-1)^{-t/2}}{2}. \end{aligned}$$

The rest of the theorem follows by an easy calculation. ■

Corollary 5.1 *If X and Y are two subsets of V of cardinality xn and yn respectively,*

$$d(X,Y) \leq \left\lfloor \frac{\cosh^{-1}\sqrt{(x^{-1}-1)(y^{-1}-1)}}{\cosh^{-1}(k/\lambda)} \right\rfloor + 1.$$

Proof If t is an integer such that the right-hand side of Eq. 5.4 is less than $|X|/(n-|Y|)$, then $|N^t(X)| > n-|Y|$, and so the distance between X and Y is at most t. Let $\theta = \cosh^{-1}(k/\lambda)$, so that $P_t(k/\lambda) = \cosh(t\theta)$. We want t to be such that

$$x + \frac{1-x}{\cosh^2(t\theta)} < \frac{x}{1-y},$$

which is equivalent to

$$\cosh^2(t\theta) > \frac{(1-x)(1-y)}{xy}$$

Solving for t yields the desired bound on $d(X,Y)$. ■

By applying Corollary 5.1 to any pair of subsets consisting of single vertices, we obtain Eq. 1.2, which has already been established in [22, 58].

Corollary 5.2 ([57])

$$D(G) \leq \left\lfloor \frac{\cosh^{-1}\left(\frac{n}{k(k-1)^{r-1}} - 1\right)}{\cosh^{-1}(k/\lambda)} \right\rfloor + 2r + 1,$$

where $r = \lfloor (c(G)-1)/2 \rfloor$ is the injectivity radius *of G.*

Proof We remind the reader that $c(G)$ is the girth of G. Consider any pair of vertices u and v. The subsets $N^r(\{u\})$ and $N^r(\{v\})$ have size $k(k-1)^{r-1}$. By applying Corollary 5.1 to these subsets, we get

$$d(N^r(\{u\}, N^r(\{v\}) \leq \left\lfloor \frac{\cosh^{-1}\left(\frac{n}{k(k-1)^{r-1}} - 1\right)}{\cosh^{-1}(k/\lambda)} \right\rfloor + 1.$$

Corollary 5.2 follows immediately. ■

Corollary 5.2 has first been established by Quenell [57], who argued that it always gives a better bound than Eq. 1.2.

5.2 Relation with subsequent eigenvalues

We generalize Corollary 5.1 as follows:

Theorem 5.2 *If the eigenvalues of the adjacency matrix of G are $\delta_0, \delta_1, \ldots, \delta_{n-1}$, with $|\delta_0| \geq |\delta_1| \geq \cdots \geq |\delta_{n-1}|$, then for any set S of $i+1$ vertices of V,*

$$\min_{\{u,v\} \subset S, u \neq v} \leq \left\lfloor \frac{\cosh^{-1}(n-1)}{\cosh^{-1}(k/|\delta_i|)} \right\rfloor + 2.$$

Proof Let e_j be an eigenvector of A corresponding to the eigenvalue δ_j, and let $f \in L^2(V)$ be a nonzero function nul on $V - S$, and such that f belongs to the vector space E_i spanned by $e_i, e_{i+1}, \ldots, e_{n-1}$. The existence of f follows from the fact that $\dim L^2(S) = i+1$ and $\dim E_i = n-i$ (Fact 4.2.) Given an integer t, let $g = P_t(|\delta_i|^{-1}A)f$. The vector space E_i is invariant under A, and the eigenvalues of the restriction of A to E_i are δ_h, for $i \leq h \leq n-1$. By a similar reasoning to the proof of Theorem 5.1, we know that the eigenvalues $P_t(\delta_h/|\delta_i|)$, for $i \leq h \leq n-1$, of the restriction of the operator $P_t(|\delta_i|^{-1}A)$ to E are at most 1 in absolute value, and so $||g|| \leq ||f||$. Assume now that $\min_{\{u,v\} \subset S, u \neq v} d(u,v) > 2t$. Then the vectors $P_t(|\delta_i|^{-1}A)\chi_{\{u\}}$, for $u \in S$, have disjoint supports, and so

$$\begin{aligned}
||g||_1 &= ||\sum_{u \in S} f(u)\ P_t(|\delta_i|^{-1}A)\chi_{\{u\}}||_1 \qquad (5.5)\\
&= \sum_{u \in S} |f(u)|\ ||P_t(|\delta_i|^{-1}A)\chi_{\{u\}}||_1 \\
&\geq \sum_{u \in S} |f(u)|\ (P_t(|\delta_i|^{-1}A)\chi_{\{u\}}) \cdot \chi_V \\
&= \sum_{u \in S} |f(u)|\ (P_t(|\delta_i|^{-1}A)\chi_V) \cdot \chi_{\{u\}} \\
&= \sum_{u \in S} |f(u)| P_t(k/|\delta_i|) \\
&= P_t(k/|\delta_i|)||f||_1
\end{aligned}$$

On the other hand,

$$\begin{aligned}
||g||_1 &\leq \sqrt{n}||g|| \qquad (5.6)\\
&\leq \sqrt{n}||f|| \qquad (5.7)\\
&\leq \sqrt{n/2}||f||_1. \qquad (5.8)
\end{aligned}$$

The first inequality follows from Fact 5.4. The last inequality is valid because $f \in L^2_0(V)$. Indeed,

$$\begin{aligned}
||f||^2 &= ||f^+||^2 + ||f^-||^2 \\
&\leq ||f^+||_1^2 + ||f^-||_1^2 \\
&= \frac{||f||_1^2}{2},
\end{aligned}$$

where $f^+ = \max(f, 0)$ and $f^- = \min(f, 0)$.

Comparing Eq. 5.5 and Eq. 5.6 shows that $P_t(k/|\delta_i|) \leq \sqrt{n/2}$. If

$$t = \left\lfloor \frac{\cosh^{-1}\sqrt{n/2}}{\cosh^{-1}(k/|\delta_i|)} \right\rfloor + 1,$$

the above inequality does not hold, and so $\min_{\{u,v\}\subset S, u\neq v} \leq 2t$. The lemma follows by noting that $2\cosh^{-1}\sqrt{n/2} = \cosh^{-1}(n-1)$. ■

Theorem 5.2 can be easily generalized as follows:

Theorem 5.3 *If $X_1, X_2, \ldots, X_{i+1}$ are $i+1$ subsets of V of same cardinality xn, then*

$$\min_{1\leq j<h\leq i+1} d(X_j, X_h) \leq \left\lfloor \frac{\cosh^{-1}(x^{-1}-1)}{\cosh^{-1}(k/|\delta_i|)} \right\rfloor + 2.$$

Proof The proof is almost identical to the proof of Theorem 5.2. The main difference is that we consider a function f in $L^2(\cup_{j=1}^{i+1} X_j)$ which is constant on each X_j. ■

Theorem 5.4 *If the eigenvalues of the adjacency matrix of G are $\delta_0, \delta_1, \ldots, \delta_t$, with $|\delta_0| \geq |\delta_1| \geq \cdots \geq |\delta_t|$, then for any integer i between 1 and $n-1$,*

$$D(G) \leq i \left\lfloor \frac{\cosh^{-1}(n-1)}{\cosh^{-1}(k/|\delta_i|)} \right\rfloor + 3i - 1. \tag{5.9}$$

If r is the injectivity radius of G, then for any integer i between 1 and $n-1$,

$$D(G) \leq i \left\lfloor \frac{\cosh^{-1}(\frac{n}{k(k-1)^{r-1}}-1)}{\cosh^{-1}(k/|\delta_i|)} \right\rfloor + 2ir + 3i - 1.$$

Proof Let u and v be two vertices at maximal distance in G. Consider a shortest path between u and v. There exists a sequence of $i+1$ vertices $u_0 = u, u_1, \ldots, u_i = v$ on this path at distance at least $\lfloor D(G)/i \rfloor$ from each other. By applying Theorem 5.2 to the set $\{u_0, u_1, \ldots, u_i\}$, we get the first bound on $D(G) = d(u, v)$.

The second bound can be established similarly by applying Theorem 5.3 to the subsets $N^r(\{u_j\})$.

■

5.3 Tightness of bounds

We use techniques similar to Section 3.4 to prove that the inequality Eq. 5.9 is asymptotically tight, for any fixed i. We start with the case $i = 1$.

Theorem 5.5 *For any integer k such that $k-1$ is prime congruent to 1 modulo 4, there exists an infinite family of k-regular graphs G_n on n vertices with $\lambda(G_n) = (2+o(1))\sqrt{k-1}$ and diameter $(2+o(1))\log_{k-1} n$.*

Proof We start with a k-regular Ramanujan graph H on n' vertices, and we form two identical trees T and T' of depth $l = \lfloor \log_{k-1} m - 2 \rfloor$, where $m = \lfloor n'/\log n' \rfloor$, and whose internal nodes have degree k. All leaves in T and T' have the same depth. Consider a set E^r of edges in H at distance $r = \Omega(\log_{k-1}(n'/m))$ from each other and having the same cardinality as the number of leaves in T. For each edge in E^r, identify one of its endpoints to a leaf in T and the other endpoint to a leaf in T', so that the leaves of T and T' are identified to distinct vertices in H. By deleting the edges in E^r, we obtain a k-regular graph $G = G_n$. The diameter of G is at least twice the depth of T, which is $(1+o(1))\log_{k-1} n$. Using similar techniques to the proof of Theorem 3.7, we will show that $\lambda(G) = (2+o(1))\sqrt{k-1}$. Eq. 1.2 then implies that the diameter of G is equal to $(2+o(1))\log_{k-1} n$. Let A be the adjacency matrix of H, A' the adjacency matrix of G, and $\lambda' = \lambda(G)$. We assume that $\lambda' > 2\sqrt{k-1}$ (otherwise, we are done), and let $\lambda' = 2\sqrt{k-1}\cosh\theta'$, with $\theta' > 0$. We also assume that $\lambda' = \lambda_1(G)$. The case $\lambda' = -\lambda_{n-1}(G)$ can be treated similarly. Denote by $V(G)$, $V(H)$, $V(T)$ and $V(T')$ the vertex sets of G, H, T and T', respectively.

Let $g \in L^2(V(G))$ be an eigenvector of A' corresponding to λ', and let $f \in L^2(V(H))$ be the vector of $L^2(H)$ that coincides with g on H. By Eq. 2.2, we have

$$\begin{aligned} \lambda'||g||^2 &= g \cdot A'g \\ &= f \cdot Af - \sum_{(u,v)\in E^r} g(u)g(v) + \sum_{(u,v)\in E(T)} g(u)g(v) + \sum_{(u,v)\in E(T')} g(u)g(v) \\ &\leq f \cdot Af + (2\sqrt{k-1}+1) \sum_{v\in V(T)\cup V(T')} g(v)^2. \end{aligned} \tag{5.10}$$

The third equation follows from the fact that the largest eigenvalue of T is at most $2\sqrt{k-1}$ and the largest eigenvalue of the edge-subgraph E^r is 1. Since $g \in L_0^2(V(G))$,

$$\sum_{w\in V(H)} f(w) = -\sum_{w\in (V(T)\cup V(T'))-V(H)} g(w).$$

Using Lemma 3.1, we get

$$\begin{aligned} f \cdot Af &\leq \lambda_1(A)||f||^2 + \frac{k}{n}\Big(\sum_{w\in (V(T)\cup V(T'))-V(H)} g(w)\Big)^2 \\ &\leq 2\sqrt{k-1}(||g||^2 - \sum_{w\in (V(T)\cup V(T'))-V(H)} g(w)^2) + \frac{2km}{n} \sum_{w\in (V(T)\cup V(T'))-V(H)} g(w)^2 \\ &\leq 2\sqrt{k-1}||g||^2, \end{aligned}$$

for sufficiently large n. Combining this with Eq. 5.10 yields

$$\lambda' ||g||^2 \leq 2\sqrt{k-1}(||g||^2 + 2 \sum_{v \in V(T) \cup V(T')} g(v)^2). \tag{5.11}$$

Next, we show that $\sum_{v \in V(T) \cup V(T')} g(v)^2$ is small compared to $||g||^2$. We use the following lemma:

Lemma 5.1 *Let $G = (V, E)$ be a k-regular graph and g an eigenvector of G corresponding to the eigenvalue $2\sqrt{k-1}\cosh\theta$, with $\theta > 0$. If l and l' are two nonegative integers with $l < l'$, and u is a node of G such that the subgraph induced on $B_{l'}(\{u\})$ is a tree, then*

$$\frac{\sum_{v \in V : d(u,v) = l'} g(v)^2}{\sum_{v \in V : d(u,v) = l} g(v)^2} \geq e^{2(l'-l)\theta}.$$

Proof We apply Lemma 3.4 with $s(v) = (k-1)^{-d(u,v)/2} e^{d(u,v)\theta}$. The calculations are similar to the proof of Theorem 3.7. ■

By applying Lemma 5.1 in the case where u is the root of T and $l' = l + r$, we see that

$$||g||^2 \geq e^{2r\theta'} \sum_{v \in V : d(u,v) = l} g(v)^2.$$

By applying the lemma to $l-1, l-2, \ldots, 0$, we see that

$$||g||^2 \geq e^{2r\theta'}(1 - e^{-2\theta'}) \sum_{v \in T} g(v)^2.$$

Combining this Eq. 5.11 yields

$$\cosh\theta' \leq 1 + 2\frac{e^{-2r\theta'}}{1 - e^{-2\theta'}}.$$

As a consequence, $\theta' \leq 3(\log r)/(2r)$, for large n, and so $\lambda' \leq (2 + o(1))\sqrt{k-1}$. On the other hand [3, 45, 53], $\lambda' \geq (2 + o(1))\sqrt{k-1}$ for any family of k-regular graphs, as the number of vertices goes to infinity. ■

For any graph G, let $\delta_i(G)$ denote the $(i+1)$-st largest eigenvalue of G in absolute value, i.e. $|\delta_0(G)| \geq |\delta_1(G)| \geq \ldots \geq |\delta_{n-1}(G)|$.

Theorem 5.6 *If $k-1$ is a prime congruent to 1 modulo 4 and i is an integer, there exists an infinite family of k-regular graphs G_n on n vertices of diameter $(2 + o(1))i\log_{k-1} n$ and such that $\delta_j(G_n) = k - O(1/n)$, for $0 \leq j \leq i-1$, and $|\delta_i(G_n)| = (2 + o(1))\sqrt{k-1}\log n$.*

Proof Consider a family (F_n) of k-regular graphs satisfying the conditions of Theorem 5.5. We construct the graphs G_n (for n multiple of i and such that $F_{n/i}$ exists) as follows: consider i distinct copies of $F_{n/i}$, denoted by $F^j_{n/i}$, for $1 \leq j \leq i$. Let (u_j, v_j) be a pair of vertices in $F^j_{n/i}$ at maximal

distance from each other, and let u'_j (resp. v'_j) be a vertex of $F^j_{n/i}$ adjacent to u_j (resp. v_j). We form the graph G_n by connecting v_j (resp. v'_j) to u_{j+1} (resp. u'_{j+1}), for $1 \leq j \leq i-1$, and deleting the edge between u_j and u'_j, for $2 \leq j \leq i$, and the edge between v_j and v'_j, for $1 \leq j \leq i-1$. Clearly, the diameter of G_n is $(2+o(1))i \log_{k-1} n$.

The eigenvalues of the union of the $F_{n/i}$ satisfy the conditions of Theorem 5.6. Indeed, by Fact 3.3, the first i eigenvalues are equal to k, and the $(i+1)$-st largest eigenvalue in absolute value is, in absolute value, equal to $\lambda(F_{n/i}) \leq (2+o(1))\sqrt{k-1}$. We will show that the $i+1$ largest eigenvalues of G_n are close to the largest $i+1$ eigenvalues of the union of the $F_{n/i}$.

Let A (resp. A') be the adjacency matrix of the union of the $F_{n/i}$ (resp. G_n.) Let V_j be the vertex set of $F^j_{n/i}$, and V the vertex set of G_n. By a calculation similar to the proof of Theorem 3.7, it follows that for any $f \in L^2(V)$,

$$\begin{aligned} |A'f \cdot f - Af \cdot f| &= 2\Big|\sum_{j=1}^{i-1} (f(v_j)f(u_{j+1}) + f(v'_j)f(u'_{j+1}) - f(u_{j+1})f(u'_{j+1}) - f(v_j)f(v'_j))\Big| \quad (5.12) \\ &\leq 2\sum_{j=1}^{i} (f(u_j)^2 + f(u'_j)^2 + f(v_j)^2 + f(v'_j)^2). \end{aligned}$$

Denote by H be the subspace of $L^2(V)$ of vectors constant on each V_j. Eq. 5.12 shows that, for each $f \in H$, we have $A'f \cdot f \geq (k - 8i/n)||f||^2$. Since $\dim H = i$, it follows from Fact 4.3 that λ_{i-1} is lower bounded by $k - 8i/n$, and so are $|\delta_0|, |\delta_1|, \ldots, |\delta_{i-1}|$.

We now show how to approximate δ_i. Let r be the injectivity radius of G_n. It is at least equal to the injectivity radius of $F_{n/i}$, which is $\Omega(\log_{k-1} \log n)$. If $|\delta_i| \leq 2\sqrt{k-1}$, we are done. So we will assume in the rest of the proof that $\delta_i > 2\sqrt{k-1}$ (the case where $\delta_i < -2\sqrt{k-1}$ can be treated similarly.) Let $\delta_i = 2\sqrt{k-1}\cosh\theta$, with $\theta > 0$. Let e_h be an eigenvector of A' corresponding to δ_h, for $0 \leq h \leq i$. Since $|\delta_h| \geq \delta_i$, it follows from Lemma 5.1 that $e^{r\theta}|e_h(u_j)| \leq ||e_h||$, for $0 \leq j \leq i$. Using the Cauchy-Schwartz inequality and the orthogonality of the vectors e_h, this implies that for any vector $g \in \mathrm{Vect}(e_0, e_1, \ldots, e_i)$,

$$e^{r\theta}|g(u_j)| \leq \sqrt{i+1}||g||. \quad (5.13)$$

Indeed, if $g = \sum_{h=0}^{i} c_h e_h$, then

$$\begin{aligned} g(u_j)^2 &\leq (i+1)\sum_{h=0}^{i} {c_h}^2 e_h(u_j)^2 \\ &\leq \frac{i+1}{e^{2r\theta}} \sum_{h=0}^{i} {c_h}^2 ||e_h||^2 \\ &= \frac{i+1}{e^{2r\theta}} ||g||^2. \end{aligned}$$

Eq. 5.13 remains valid if u_j is replaced by u'_j, v_j or v'_j. Since the vector space $\mathrm{Vect}(e_0, e_1, \ldots, e_i)$ has greater dimension than H, it intersects $H^\perp - \{0\}$ (Fact 4.2.) Let g be an element of this intersection. Since the restriction of g to each V_j belongs to $L^2_0(V_j)$, it follows from Fact 3.1 that

$$Ag \cdot g \leq \lambda(F_{n/i})||g||^2 \leq (2 + o(1))\sqrt{k-1}||g||^2.$$

Combining this with Eqs. 5.12 and 5.13 yields

$$A'g \cdot g \leq (2 + o(1))\sqrt{k-1}||g||^2 + \frac{8i}{e^{2r\theta}}||g||^2. \tag{5.14}$$

But, since $g \in \mathrm{Vect}(e_0, e_1, \ldots, e_i)$, we have $A'g \cdot g \geq \delta_i||g||^2$ (Fact 4.1.) Combining this with Eq. 5.14 shows that

$$\cosh\theta \leq 1 + o(1) + \frac{4i}{\sqrt{k-1}e^{2r\theta}},$$

from which we deduce that $\theta = o(1)$, as in the proof of Theorem 3.7. By replacing δ_i by its value, we conclude that $|\delta_i| \leq (2 + o(1))\sqrt{k-1}$. On the other hand [28], $|\delta_i| \geq (2 + o(1))\sqrt{k-1}$ for any family of k-regular graphs, as the number of vertices goes to infinity. ■

Chapter 6

Bounds on the Chromatic Polynomial and on the Number of Acyclic Orientations of a Graph

In this chapter, we discuss various techniques for bounding the number of acyclic orientations and the chromatic polynomial of a graph. As pointed out in the introduction, the number of acyclic orientations is equal to the absolute value of the chromatic polynomal evaluated at -1. We use mainly algebraic techniques to derive our upper bounds, and probabilistic techniques to derive our lower bound. Most of our results are not restricted to the class of regular graphs, which were the focus of our attention in the previous chapters,

We start by bounding the number of acyclic orientations, denoted by $\alpha(G)$. In Section 6.1 we show how to bound from above the number of acyclic orientations of a graph by the number of spanning trees in a closely related graph; the latter quantity is in turn expressed in terms of the spectrum of the Kirchhoff matrix of the original graph, via the matrix-tree theorem. We conclude that $\alpha(G)$ is upper bounded by the determinant of the the Kirchhoff matrix. By elementary linear algebra, we show that this bound is no worse than the degree bound [46] of $\prod_{v \in G}(d_v + 1)$, where d_v represents the degree of vertex v.

In Section 6.2 we provide estimates on the determinant of the Kirchhoff matrix. We show that for d-regular graphs, it is asymptotically upper bounded by about $(d + 1/2)^n$; and that for graphs with high girth, such as the LPS-M graphs, this is a nearly tight estimate of the Kirchhoff determinant. We also give a bound on the Kirchhoff determinant in general graphs in terms of the degree sequence. In Section 6.3 we provide bounds on the number of acyclic orientations of the hypercube.

In Section 6.4 we consider the problem of bounding χ_G at arbitrary negative values. In Subsec-

tion 6.4.1 we show how to extend the inequality between number of acyclic orientations and number of spanning trees to an inequality between $\det(Q + wI)$ and $(-1)^n \chi_G(-w)$ for $w \geq 0$, where Q is the Laplacian of a graph and χ is its chromatic polynomial. In Subsection 6.4.2 we provide a simple probabilistic proof of the known [31] lower bound $\alpha(G) \geq \prod_{v \in G} f(d_v + 1)$, where $f(x) = (x!)^{1/x}$. We extend this proof to give a lower bound on $(-1)^n \chi_G(-w)$ for arbitrary positive w.

In Section 6.5 we study the relation between the number of acyclic orientations and the girth of the graph. In the case where the girth is at least 5, we can prove lower bounds for $\alpha(G)$ and for the chromatic polynomial that are strictly stronger than those possible for an arbitrary graph. Our improvement is most significant for small-degree graphs, and we calculate the case of degree 3 in detail.

6.1 Acyclic Orientations and Spanning Trees

It will be convenient to view an acyclic orientation as the Hasse diagram of a partial order, and speak of one vertex dominating another if it precedes it in the orientation.

Form the undirected graph G' from G by adjoining a new vertex u which is connected to all the vertices of G. Let $\tau(G')$ denote the number of spanning trees of G' rooted at u (equivalently, the number of spanning trees of G'). We show that:

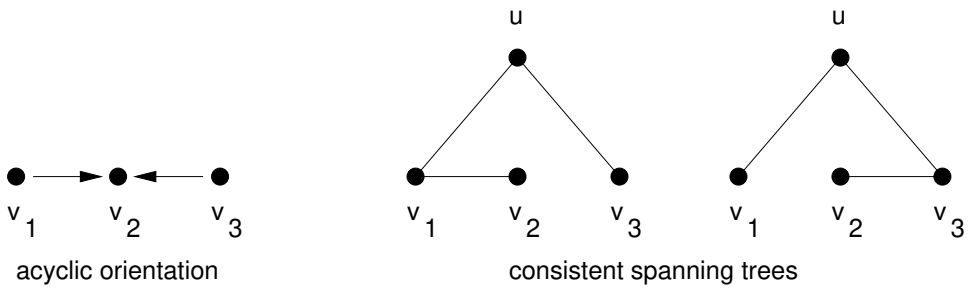
Lemma 1 *$\alpha(G) \leq \tau(G')$.*

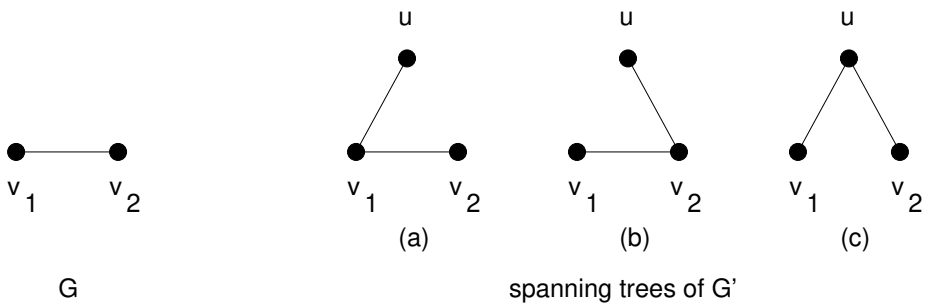
Proof The argument is by injection from acyclic orientations to spanning trees rooted at u. We construct the tree associated with an orientation level by level, beginning with u at level 0. In the first stage we connect every maximal vertex of the orientation to u, thus obtaining level 1 of the tree. In general at stage i we select all as yet unplaced vertices of G which are dominated only by vertices that are already in the spanning tree; and we place these vertices in level i of the tree by connecting them to a neighboring vertex which is at level $i - 1$. Such a neighbor must exist else we would have placed the current vertex in the tree at an earlier stage.

Observe that if one vertex precedes another in the acyclic orientation then it will be placed at a lower level of the tree. Any pair of distinct acyclic orientations disagree on some edge vw and so their associated trees will differ as to which of the two vertices is lower. Hence no two orientations are carried to the same tree. ■

We comment that for two reasons this inequality is not tight. First, there are arbitrary choices in the tree construction whenever a vertex may be connected to one of several vertices at the preceding level (see Fig. 6.1). The proof demonstrates that the sets of trees which can be formed from different orientations are disjoint; our bound might be tightened with the help of estimates on the sizes of these sets. Second, not all spanning trees can be formed by the construction: e.g. (c) in Fig. 6.1.

The spanning trees which can be formed are precisely those in which every level of the tree is an independent set in the graph.





We can now relate the number of acyclic orientations to the graph spectrum. The Laplacian $Q(H)$ of an undirected graph H is the symmetric matrix which for $i \neq j$, has a 0 in entry $Q(H)_{ij}$ if vertices i and j are not connected, and a -1 if they are connected; while on the diagonal, the degrees of the vertices appear in the corresponding order. Kirchhoff's matrix-tree theorem [17] establishes that the number of spanning trees of a graph is equal to the determinant of a minor of the Laplacian in which the row and column corresponding to any vertex are omitted.

The Kirchhoff matrix $K(H)$ of an undirected graph H is defined as $Q(H) + I$, where I is the identity. Observe that the spectrum of the Kirchhoff matrix is simply shifted by 1 from that of the Laplacian. Applying the matrix-tree theorem to G' by omitting the row and column corresponding to the introduced vertex u, we obtain a bound on acyclic orientations directly in terms of the spectrum of G: $\alpha(G) \leq \det(K(G))$. Namely

Theorem 1 *The number of acyclic orientations of an undirected graph is no greater than the determinant of its Kirchhoff matrix.* ■

Comparison with the Degree Bound

We now show that the bound given by Theorem 1 on the number of acyclic orientations of a graph improves upon the degree bound. In the next section we give estimates on the improvement achieved.

Let d_v be the degree of vertex v.

Lemma 2 *The determinant of the Kirchhoff matrix of a graph G is at most $\prod_{v \in G}(d_v + 1)$.*

Proof The Laplacian of G is a positive semidefinite matrix, and its Kirchhoff matrix is positive definite. A classical result in linear algebra [47, page 114] shows that the determinant of a positive semidefinite matrix is no greater than the product of its diagonal elements. The proof follows by applying this result to $K(G)$ and noting that the diagonal element of $K(G)$ indexed by vertex v is $d_v + 1$. ■

6.2 Estimates on the Determinant of the Kirchhoff Matrix

We will obtain bounds on the determinant of the Kirchhoff matrix. In the case of regular graphs of degree d, these bounds will be of the form $(d+1)^n e^{-(1/2d+O(1/d^2))n}$, which is roughly $(d+1/2)^n$. We then study the case of arbitrary graphs.

6.2.1 Regular Graphs

In this section we consider the case of a regular graph G of degree d. Let $\beta = d/2(d-1)$ and $\psi_d(z) = \sqrt{1-4(d-1)z^2}$.

Theorem 2 *The determinant of the Kirchhoff matrix of a d-regular graph on n vertices is at most $(d+1)^n \exp(-\phi(d)n)$, for a function ϕ of the form $\phi(d) = \frac{1}{2d} - \frac{1}{2d^2} + \frac{1}{12d^3} - \frac{1}{4d^4} + O(d^{-5})$.*

Proof Let A be the adjacency matrix of G and $f(z) = \det(I - zA)$. Since $K(G) = (d+1)I - A$, we have $\det(K(G)) = (d+1)^n f(1/(d+1))$. In order to get the desired bound on the determinant of $K(G)$, we are going to bound $f(1/(d+1))$. A classical result [61, pages 242–243] shows that

$$\frac{f'(z)}{f(z)} = -\frac{1}{z}\sum_{l \geq 1} \mathrm{tr}(A^l) z^l. \tag{6.1}$$

From the definition we see that the radius of convergence of this generating function is the inverse of the largest eigenvalue of A in absolute value, which in this case is d. Note that $\mathrm{tr}(A^l)$ is the number of closed walks in G of length l. Let T^d be the infinite d-regular tree. T^d can be mapped into G in a manner that preserves edges and carries the neighbors of any vertex in T^d to distinct vertices in G. As observed in [45], it follows that $\mathrm{tr}(A^l) \geq n\rho(l)$, where $\rho(l)$ is the number of closed walks of length l in T^d starting from any vertex x. (Let $\rho(0) = 1$.) By standard generating function methods [68],

$$\sum_{l \geq 0} \rho(l) z^l = \frac{1}{1 - \beta + \beta\psi_d(z)}. \tag{6.2}$$

Combining Eqs. 6.1 and 6.2 and integrating, we have

$$\begin{aligned}\log(f(\frac{1}{d+1})) &\leq -n\int_0^{1/(d+1)} \frac{du}{u}\left(\frac{1}{1-\beta+\beta\psi_d(u)}-1\right)\\ &= -\frac{n}{2\beta-1}\left[(1-\beta)\log\left(1-\beta+\beta\psi_d(u)\right)-\beta\log\left(\frac{1+\psi_d(u)}{2}\right)\right]_0^{1/(d+1)}\\ &= -n\phi(d),\end{aligned}$$

where ϕ is defined by

$$\phi(d) = \frac{d-2}{2}\log\left(\frac{d-2+d\psi_d(\frac{1}{d+1})}{2(d-1)}\right) - \frac{d}{2}\log\left(\frac{1+\psi_d(\frac{1}{d+1})}{2}\right) \ .$$

Change variables to $s = 1/d$ and note that the resulting function of s is analytic at $s = 0$, with power series

$$\frac{s}{2} - \frac{s^2}{2} + \frac{s^3}{12} - \frac{s^4}{4} + O(s^5)$$

(hence the expansion of ϕ given in the theorem). Thus $f(\frac{1}{d+1}) \leq \exp(-n\phi(d))$ as desired.

It follows that $\phi(d) \sim 1/2d$ as d goes to infinity. It can also be shown that $\phi(d) \geq 1/2d - 1/2d^2$ for $d \geq 2$. (Calculation shows $\rho(2) = d$, $\rho(4) = 2d^2 - d$, $\rho(6) = d(5d^2 - 6d + 2)$. As a consequence, $\phi(d) \geq 1/2d - 1/2d^2$ for $d \geq 18$. It can be checked directly that $\phi(d) \geq 1/2d - 1/2d^2$ for any integer d, $2 \leq d \leq 18$.) ■

Theorem 2 is for some graphs a nearly tight bound on the determinant of the Kirchhoff matrix. For example: note that $\phi(2) = -\log\left(\frac{3+\sqrt{5}}{6}\right)$, and so in the case of the n-cycle, the bound of the theorem is $\left(\frac{3+\sqrt{5}}{2}\right)^n$. This differs from the exact value $\left(\frac{3+\sqrt{5}}{2}\right)^n + \left(\frac{3-\sqrt{5}}{2}\right)^n - 2$ only by a constant. There are also graphs of high degree for which the bound is nearly tight:

Theorem 3 *For any integer $d \geq 2$, there exists a family of d-regular graphs G_n on n vertices such that* $\det(K(G_n)) = (d+1)^n \exp\left(-(\phi(d) + o(1))n\right)$.

Proof The girth of a graph is defined as the length of its shortest cycle. Let G_n be a family of d-regular graphs such that the girth g of G_n is at least $(1 + o(1)) \log_{d-1} n$. The existence of such a family was shown in [34]. With notation as in the proof of Theorem 2, for A the adjacency matrix of G_n, we have

$$\frac{f'(z)}{f(z)} = -\frac{1}{z}\sum_{l\geq 1} \mathrm{tr}(A^l)z^l.$$

For $l \leq g - 1$ we have $\mathrm{tr}(A^l) = n\rho(l)$ since any cycle in the graph has length greater than l. On the other hand, for any l, we have $\mathrm{tr}(A^l) \leq nd^l$. Therefore, for $0 \leq z \leq 1/(d+1)$,

$$\frac{f'(z)}{f(z)} \geq -\frac{1}{z}(n\sum_{l\geq 1}\rho(l)z^l + n\sum_{l\geq g} d^l z^l),$$

from which we deduce that

$$\log(f(\frac{1}{d+1})) \geq -n\phi(d) - nd\left(\frac{d}{d+1}\right)^{g-1} \geq -n\phi(d) - n^{1-1/(d+1)\log(d-1)+o(1)}.$$

■

Observe that if $d-1$ is prime, there exists a family of bipartite d-regular Ramanujan graphs [45, 49] of girth $(4/3+o(1))\log_{d-1} n$. Since $\mathrm{tr}(A^l) \leq 2d^l + (n-2)(2\sqrt{d-1})^l$ for any nonnegative integer l, we obtain a tighter lower bound on the determinant of the Kirchhoff matrices of these graphs from the equation

$$\begin{aligned}\log(f(\frac{1}{d+1})) &\geq -n\phi(d) - \exp\left(\left(1 - \frac{4\log\left(\frac{d+1}{2\sqrt{d-1}}\right)}{3\log(d-1)} + o(1)\right)\log n\right) \\ &\geq -n\phi(d) - n^{1/3+(4\log 2)/(3\log(d-1))+o(1)}.\end{aligned}$$

The problem of estimating the determinant of the Kirchoff matrix is related to the problem of counting the number of spanning trees of d-regular graphs. McKay [50] showed that for any family G_n of d-regular graphs,

$$\lim_{n\to\infty} \sup(\kappa(G_n))^{1/n} \leq \frac{(d-1)^{d-1}}{(d^2-2d)^{d/2-1}}, \tag{6.3}$$

where $\kappa(G_n)$ is the number of spanning trees in G_n. He also showed the existence of a family of d-regular graphs for which this bound is tight. Note that the right-hand side of Eq. 6.3 is equal to $d - 1/2 + O(1/d)$.

6.2.2 General Graphs

The notation (v, w) refers to an ordered pair of vertices.

Theorem 4 *The determinant of the Kirchhoff matrix of a graph G is no greater than $\prod_{v\in G}(d_v + 1)\prod_{(v,w)\in E(G)} \exp(-1/2(d_v+1)(d_w+1))$.*

Proof Let Δ be the diagonal matrix indexed by the vertices of G and whose diagonal consists of the degrees of the vertices. Since $K(G) = (\Delta + I) - A$, we have $\det K(G) = \det(\Delta + I)\det(I - M)$, where $M = (\Delta + I)^{-1}A$. To prove the theorem, we need to show that $\det(I - M) \leq \prod_{(v,w)\in E(G)} \exp(-1/2(d_v+1)(d_w+1))$.

In order to bound $\det(I - M)$ we introduce the function $h(z) = \det(I - zM)$; of course $h(1) = \det(I - M)$. As before, we have

$$\frac{-zh'(z)}{h(z)} = \sum_{l\geq 1} \mathrm{tr}(M^l)z^l. \tag{6.4}$$

Observing that $\mathrm{tr}(M) = 0$, we lower bound this expression by $\mathrm{tr}(M^2)z^2$. The largest eigenvalue of M is less than one in norm since the sum of the absolute values of the entries in each row is less than one. (Specifically, the sum is $d_v/(d_v+1)$ in the row corresponding to vertex v). Therefore, the radius of convergence of the generating function in Eq. 6.4 is greater than one. Hence, for $0 \leq z \leq 1$, we have $-h'(z)/h(z) \geq \mathrm{tr}(M^2)z$, and so by integration of h'/h from 0 to 1, we find that $h(1) \leq \exp(-\mathrm{tr}(M^2)/2)$. But $h(1) = \det(I - M)$; and by inspecting M we see that

$$\mathrm{tr}(M^2) = \sum_{(v,w)\in E(G)} \frac{1}{(d_v+1)(d_w+1)}.$$

■

By imitating the proof of Theorem 2, it is possible to get a bound on the determinant of the Kirchhoff matrix in terms of the maximum degree and the degree of each node. However, this bound is too complicated to merit inclusion here. It coincides with the bound given by Theorem 2 when the graph is regular, but it is incomparable with the bound given by Theorem 4 in general.

6.3 Example

We give an estimate of the Kirchoff determinant of the hypercube. We also give a lower bound on the number of acylic orientations of the hypercube.

Theorem 5 *The determinant of the Kirchhoff matrix of the d-dimensional hypercube is no greater than* $(d+1)^{2^d} \exp\left(-2^d(\frac{1}{2d} - \frac{1}{4d^2} + O(d^{-3}))\right)$.

Proof The eigenvalues of the adjacency matrix of the d-dimensional hypercube $\mathcal{H}_d$ are $d-2k$ with multiplicity $\binom{d}{k}$, for $0 \leq k \leq d$. The eigenvalues of the Kirchhoff matrix are therefore $2k+1$, with multiplicity $\binom{d}{k}$, for $0 \leq k \leq d$. Hence,

$$\begin{aligned}
\log(\det(K(\mathcal{H}_d))) &= \sum_{k=0}^{d} \binom{d}{k} \log(2k+1) \\
&= 2^d \mathrm{E}\left[\log(d+1+Y)\right] \\
&= 2^d \log(d+1) + 2^d \mathrm{E}\left[\log\left(1+\frac{Y}{d+1}\right)\right],
\end{aligned}$$

where Y is the sum of d mutually independent random variables that take values 1 or -1, each with probability one half. But, by linearity of expectation,

$$\mathrm{E}\left[\log\left(1+\frac{Y}{d+1}\right)\right] = \sum_{i\geq 1} \frac{(-1)^{i+1}}{i} \mathrm{E}\left[\left(\frac{Y}{d+1}\right)^i\right]$$

$$= \quad - \sum_{i \geq 2,\ i \text{ even}} \frac{\mathrm{E}\left[Y^i\right]}{i(d+1)^i}.$$

The second equality follows from the fact that the expectation of odd powers of Y is equal to 0. Thus, we can get approximate upper bounds on the determinant of the Kirchhoff matrix simply by calculating the expectation of the powers of Y. In particular, using the equalities $\mathrm{E}\left[Y^2\right] = d$ and $\mathrm{E}\left[Y^4\right] = 3d^2 - 2d$, we obtain

$$\mathrm{E}\left[\log\left(1 + \frac{Y}{d+1}\right)\right] < -\frac{d}{2(d+1)^2} - \frac{3d^2 - 2d}{4(d+1)^4} = -\frac{1}{2d} + \frac{1}{4d^2} + O(d^{-3})$$

Combining this with the preceding equations gives the proof. ■

Note that the bound given in Theorem 5 is better than the bound given in Theorem 2. This is due to the fact that the hypercube has many cycles of length 4, which implies that $\mathrm{tr}(A^l) > \rho(l)$ for even l greater than or equal to 4.

Theorem 6 *The number of acyclic orientations of the d-dimensional hypercube is lower bounded by* $(d/2+1)^{2^d} \exp\left(-2^d(\frac{1}{2d} + O(d^{-2}))\right)$.

Proof We use the following lemma, implicit in [31].

Lemma 3 *Let an acyclic orientation of a graph G be given, and for each vertex v let $\delta(v)$ denote the out-degree of vertex v. Then $\alpha(G) \geq \prod_{i=1}^{n}(\delta(v_i)+1)$.* ■

To apply the lemma we partially order the vertices of the hypercube according to the Hamming distance from the origin $(0, \ldots, 0)$. Note that $\delta(v)$ is equal to the number of ones in the binary representation of vertex v. Therefore:

$$\alpha(\mathcal{H}_d) \geq \prod_{k=0}^{d} (k+1)^{\binom{d}{k}}.$$

By calculations similar to those in the proof of Theorem 5, we can write

$$\begin{aligned} \log \alpha(\mathcal{H}_d) &\geq \sum_{k=0}^{d} \binom{d}{k} \log(k+1) \\ &= 2^d \log\left(\frac{d}{2}+1\right) + 2^d \mathrm{E}\left[\log\left(1 + \frac{Y}{d+2}\right)\right], \end{aligned}$$

and

$$\mathrm{E}\left[\log\left(1 + \frac{Y}{d+2}\right)\right] = - \sum_{i \geq 2,\ i \text{ even}} \frac{\mathrm{E}\left[Y^i\right]}{i(d+2)^i}.$$

Using classical results about large deviations [20], we have for even i,

$$\begin{aligned} \mathrm{E}[Y^i] &\leq \Pr\left[Y \geq \sqrt{d}\log d\right] d^i + \left(\sqrt{d}\log d\right)^i \\ &\leq e^{-(\log^2 d)/2} d^i + (\log d)^i d^{i/2} \end{aligned}$$

Therefore,

$$\sum_{i\geq 6,\ i \text{ even}} \frac{\mathrm{E}\left[Y^i\right]}{i(d+2)^i} \leq e^{-(\log^2 d)/2} \sum_{i\geq 6,\ i \text{ even}} \left(\frac{d}{d+2}\right)^i + \sum_{i\geq 6,\ i \text{ even}} \frac{(\log d)^i}{d^{i/2}} = O(d^{-2})$$

Using the equalities $\mathrm{E}\left[Y^2\right] = d$ and $\mathrm{E}\left[Y^4\right] = O(d^2)$, we conclude that

$$\mathrm{E}\left[\log\left(1 + \frac{Y}{d+2}\right)\right] = -\frac{1}{2d} + O(d^{-2}).$$

■

Corollary 1 *For any integer $d \geq 3$, there exists a family of d-regular graphs on n vertices having at least $(d/2 + 3/4 + O(d^{-1}))^n$ acyclic orientations.*

Proof Any disjoint union of hypercubes of dimension d satisfies this condition since the number of acyclic orientations of a disjoint union of graphs is equal to the product of the number of acyclic orientations of each graph. ■

6.4 Bounds on the Chromatic Polynomial at Negative Values

In this section we bound χ_G from above and below along the negative real axis. The results of this section are stated most naturally in terms of the function $\bar{\chi}_G(w) = (-1)^n \chi_G(-w)$ (where χ_G is the chromatic polynomial of G), which we therefore study along the positive real axis. Note in particular that $\bar{\chi}_G(1) = \alpha(G)$.

6.4.1 Upper Bound on $\bar{\chi}_G$

The matrix-tree theorem extends to the case in which edges are assigned arbitrary weights. If, in the construction of Section 6.1, we assign weight w (rather than 1) to all the edges incident to the new vertex u, we find that the coefficient of w^{n-j} in the polynomial $\det(Q + wI)$ is equal to the number of rooted spanning forests of G with j edges. It is known that the coefficient of w^{n-j} in $\bar{\chi}_G(w)$ is equal to the number of j-edge subgraphs which contain no "broken circuits"; the latter is a condition

which, in particular, implies that the subgraphs are forests [11, page 69]. Hence for nonnegative w, all the terms of $\det(Q+wI)$ and $\bar{\chi}_G(w)$ are nonnegative, and each term in $\det(Q+wI)$ is at least as large as the corresponding term in $\bar{\chi}_G(w)$. Therefore we have the following extension of Theorem 1:

Theorem 7 *For all $w \geq 0$, $\bar{\chi}_G(w) \leq \det(Q+wI)$.*

■

There are two sources of slack in each of the inequalities on the coefficients, which give rise to the above theorem. The first is that the coefficient in the chromatic polynomial enumerates only certain kinds of j-edge forests; the second is that it enumerates unrooted forests, whereas $\det(Q+wI)$ enumerates rooted forests. The latter consideration introduces a factor of at least $j+1$ (typically more) into the coefficient inequality. In particular a sharper inequality on $\bar{\chi}_G(w)$ is $\bar{\chi}_G(w) \leq \sum a_j w^j$, where a_j is the number of j-edge spanning forests of G.

No effective expression is known for the $\{a_j\}$. In fact, calculating their sum is #P-complete, since the number of spanning forests in a graph is equal to the value of the Tutte polynomial at the point $(2,1)$, which is not one of the special points mentioned in the introduction. (In the case of the complete graph Takács has given an exact expression for the number of spanning forests [63].) However these numbers do have the following interesting interpretation:

For each acyclic orientation σ of G, define $h(\sigma) = (h(v_1), h(v_2), \ldots, h(v_n))$, where the v_i's are the vertices of G and $h(v_i)$ is the outdegree of vertex v_i. Let P be the convex hull in $\mathcal{R}^n$ of the vectors $h(\sigma)$, where σ ranges over the acyclic orientations of G. The number of spanning forests of G is the number of integer points in P. More generally [61, Exercise 4.32], the number of spanning forests with j edges is the coefficient of w^j in the Ehrhart polynomial $i(P,w)$.

The inequality noted above can therefore be expressed as $\bar{\chi}_G(w) \leq i(P,w)$.

Recently, Annan [7] gave a fully polynomial randomised approximation scheme for calculating the number of forests in a dense graph.

6.4.2 Lower Bound on $\bar{\chi}_G$

We begin by showing a new, simpler proof of the lower bound of [31] for the number of acyclic orientations in a graph. Then we show how an extension of this proof technique bounds $\bar{\chi}_G$ from below anywhere on the positive real axis.

Let G be an arbitrary graph; let $f(x) = (x!)^{1/x}$ (as defined previously); and given any acyclic orientation of G, let the function δ give the out-degree of a vertex, as in Lemma 3.

Theorem 8 ([31]) $\alpha(G) \geq \prod_{v \in G} f(d_v + 1)$.

Proof If a permutation of the vertices of G is chosen uniformly at random among all permutations, and the acyclic orientation on G is induced from this permutation, then for each vertex v, $\delta(v)$ is

uniformly distributed in the set $\{0, 1, \ldots, d_v\}$. Therefore,

$$\begin{aligned} \mathrm{E}\left[\log\left(\prod_{v\in G}(\delta(v)+1)\right)\right] &= \sum_{v\in G}\mathrm{E}\left[\log(\delta(v)+1)\right] \\ &= \sum_{v\in G}\frac{1}{d_v+1}\sum_{j=0}^{d_v}\log(j+1) \\ &= \sum_{v\in G}\log(f(d_v+1)) \\ &= \log\left(\prod_{v\in G}f(d_v+1)\right) \end{aligned}$$

Hence there exists an acyclic orientation for which $\prod_{v\in G}(\delta(v)+1) \geq \prod_{v\in G} f(d_v+1)$.

■

We now extend this proof to $\bar{\chi}_G$. For arbitrary $x > 0$ and nonnegative integer k, let $F(x,k) = (x\cdot(x+1)\cdots(x+k-1))^{\frac{1}{k}}$.

Theorem 9 *For all $w > 0$, $\bar{\chi}_G(w) \geq \prod_{v\in G} F(w, d_v+1)$.*

Proof Let v be a vertex of G, and (v,w) be an edge of G. By $G-v$ we denote the graph remaining after v and all incident edges have been deleted; by $G-(v,w)$ we denote the graph remaining after the edge (v,w) has been deleted; and by $G/(v,w)$ we denote the contraction of G by (v,w), i.e. the graph in which v and w have been identified into a single vertex whose neighborhood is the union of their neighborhoods in G.

Our proof relies upon the following:

Lemma 4 *For all $w \geq 0$, $\bar{\chi}_G(w) \geq (d_v+w)\bar{\chi}_{G-v}(w)$.*

Proof For any edge e in G, $\bar{\chi}_G$ satisfies the contraction-deletion identity [60]

$$\bar{\chi}_G = \bar{\chi}_{G/e} + \bar{\chi}_{G-e}. \tag{6.5}$$

If $e_1, \ldots, e_{d_v}$ are the edges incident to vertex v, then we can expand this identity to obtain

$$\begin{aligned} \bar{\chi}_G = \bar{\chi}_{G/e_1} + \bar{\chi}_{(G-e_1)/e_2} + \bar{\chi}_{(G-e_1-e_2)/e_3} + \cdots + \bar{\chi}_{(G-e_1-e_2-\cdots-e_{d_v-1})/e_{d_v}} \\ + \bar{\chi}_{G-e_1-e_2-\cdots-e_{d_v}}. \end{aligned} \tag{6.6}$$

Now we make two observations. First, if u is an isolated vertex of a graph H, then $\bar{\chi}_H = w\bar{\chi}_{H-u}$. Hence in particular for the last term of (6.6) we have $\bar{\chi}_{G-e_1-e_2-\cdots-e_{d_v}} = w\bar{\chi}_{G-v}$.

Second, $\bar{\chi}_G$ is, for positive w, monotone in the edges of the graph. (This can for instance be seen from the identity (6.5) and from the positivity of $\bar{\chi}_G$ for positive w.) Therefore each of the terms

$\bar{\chi}_{G/e_1}$, $\bar{\chi}_{(G-e_1)/e_2}, \ldots, \bar{\chi}_{(G-e_1-e_2-\cdots-e_{d_v-1})/e_{d_v}}$ in (6.6) is at least as great as $\bar{\chi}_{G-v}$.

Combining these observations we find that $\bar{\chi}_G \geq (d_v + w)\bar{\chi}_{G-v}$.

■

As a result, if an acyclic orientation of the vertices of G is given and the $\{\delta(v)\}$ are as defined above, then $\bar{\chi}_G(w) \geq \prod_v(\delta(v) + w)$. The remainder of the proof now proceeds just as for the case of acyclic orientations, by considering the expectation of $\log \prod_v(\delta(v) + w)$ over uniformly selected permutations of the vertices.

■

Note that both the upper and lower bounds on $\bar{\chi}_G(w)$ given in theorems 7 and 9 are asymptotically equivalent to w^n as w goes to infinity.

6.5 Improved Lower Bound for degree 3, girth ≥ 5

We show that in certain cases it is possible to improve the lower bound on the chromatic polynomial of a graph along the negative real axis (and in particular, the number of acyclic orientations), by modifying the probabilistic argument given in the previous section.

In a complete graph the analysis of that argument is tight, and there is no variation in the random variable $\sum_v \log(\delta(v) + 1)$ used to lower bound $\alpha(G)$ (or more generally in the random variable $\sum_v \log(\delta(v)+w)$ used to lower bound $\bar{\chi}_G$); but in other graphs there will be some variation and the inequality based on the expectation of this variable, will be strict. Hence under suitable assumptions on G, improvement in the bound can be sought. In this section we show how the absence of small cycles in the graph is enough to provide a stronger lower bound. Unfortunately the improvement provided by this method degrades for large degree graphs, so we restrict ourselves to describing the method for degree 3 graphs, where the improvement is substantial.

If, given a graph, we could exhibit the existence of an acyclic orientation in which most of its vertices had approximately balanced in-degrees and out-degrees, then using Lemma 3 we could demonstrate a strong lower bound on $\bar{\chi}_G$ and on the number of acyclic orientations of the graph. (As in Section 6.3, in the case of the hypercube.) In general however we do not know how to do this, and instead describe a method of sampling acyclic orientations, which tends to produce orientations with more balanced in-degrees and out-degrees, than result from the straightforward method of Section 6.4.2 in which we sampled uniformly among linear orders.

It may be possible to improve our application of this method, and, under suitable assumptions on the girth or other parameters of the graph, show lower bounds on $\alpha(G)$ approaching $(d/2+1)^n$. This would be very desirable, even keeping in mind that there are some graphs (e.g. $K(a, b)$ with $b >> a$, as mentioned earlier) for which the truth is closer to $(d + 1)^n$.

Theorem 10 *Let G be a 3-regular graph G on n vertices, without 3-cycles or 4-cycles (i.e. of girth ≥ 5). Let $w \geq 0$. Then*

$$\bar{\chi}_G(w) \geq (w^{1/8}(w+1)^{3/8}(w+2)^{3/8}(w+3)^{1/8})^n.$$

In particular

$$\alpha(G) \geq (2^{3/8}3^{3/8}4^{1/8})^n \cong 2.328^n$$

In comparison the lower bound of Section 6.4.2 is $\alpha(G) \geq (2^{1/4}3^{1/4}4^{1/4})^n \cong 2.213^n$.

Proof Denote the neighbors of v by v_1, v_2, v_3; and denote the remaining neighbors of v_1 by $v_{1,1}, v_{1,2}$, the remaining neighbors of v_2 by $v_{2,1}, v_{2,2}$, and the remaining neighbors of v_3 by $v_{3,1}, v_{3,2}$.

At each vertex v select a random variable x_v independently, uniformly in $[0,1]$. Let $y_v = x_v + \sum_{(w,v)} x_w/2$. (Where (w,v) is an edge.) The values $\{y_v\}$ induce an order on the vertices of G. (Observe that if we used the values $\{x_v\}$ to induce the order, then the distribution on orders would be uniform, as in Section 6.4.2.) Now

$$y_v > y_{v_1} \iff x_v + x_{v_2} + x_{v_3} - x_{v_1} - x_{v_{1,1}} - x_{v_{1,2}} > 0$$

$$y_v > y_{v_2} \iff x_v + x_{v_1} + x_{v_3} - x_{v_2} - x_{v_{2,1}} - x_{v_{2,2}} > 0$$

$$y_v > y_{v_3} \iff x_v + x_{v_1} + x_{v_2} - x_{v_3} - x_{v_{3,1}} - x_{v_{3,2}} > 0$$

Observe by symmetry that $P(y_v > y_{v_1}) = P(y_v > y_{v_2}) = P(y_v > y_{v_3}) = 1/2$. Further observe by symmetry that

(a) The probabilities $P(y_v > y_{v_1}, y_{v_2}, y_{v_3})$ and $P(y_v < y_{v_1}, y_{v_2}, y_{v_3})$ are equal. Denote this quantity a.

(b) All of the probabilities $P(y_{v_i} > y_v > y_{v_j}, y_{v_k})$ and $P(y_{v_i}, y_{v_j} > y_v > y_{v_k})$ (for i,j,k ranging over all permutations of $1,2,3$) are equal. Denote this quantity b.

Therefore $2a + 6b = 1$.

Note that $P(y_v > y_{v_2}, y_{v_3}) = a + b$, while $P(y_{v_2} > y_v > y_{v_3}) = 2b$. We will exhibit an isometry of the portion of the sample space corresponding to the event $y_v > y_{v_2}, y_{v_3}$, with the portion corresponding to the event $y_{v_2} > y_v > y_{v_3}$; it will then follow that $a = b$, and consequently that $a = b = 1/8$.

Thus, in fact, the events $\{y_v > y_{v_i}\}_i$ are independent. (Locally, as if the process oriented the edges of the graph independently at random.)

The isometry is given by the following map:

$$\begin{pmatrix} x'_0 \\ x'_1 \\ x'_2 \\ x'_3 \\ x'_{2,1} \\ x'_{2,2} \\ x'_{3,1} \\ x'_{3,2} \end{pmatrix} = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \\ x_{2,1} \\ x_{2,2} \\ x_{3,1} \\ x_{3,2} \end{pmatrix}$$

It is readily verified that this map is an isometry of the regions described.

Hence:

$$P(\text{rank}(y_v) \in \{y_v, y_{v_1}, y_{v_2}, y_{v_3}\} = 1) = 1/8$$

$$P(\text{rank}(y_v) \in \{y_v, y_{v_1}, y_{v_2}, y_{v_3}\} = 2) = 3/8$$

$$P(\text{rank}(y_v) \in \{y_v, y_{v_1}, y_{v_2}, y_{v_3}\} = 3) = 3/8$$

$$P(\text{rank}(y_v) \in \{y_v, y_{v_1}, y_{v_2}, y_{v_3}\} = 4) = 1/8$$

The theorem now follows by substituting these probabilities in place of $1/4 = 1/(d_v + 1)$ in the proof of Section 6.4.2. ■

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