Spectral Graph Theory

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Chapter 1

Expander Graphs

In this chapter, we assume all graphs are undirected, contain no loops, nor have any duplicate edges.

Given a graph G containing some vertex v, we let $N(v)$ denote the set of all vertices in G connected to v by an immediate edge, and we call this set the **neighbourhood** of v in G. One can study the properties of the neighbourhood function via the **adjacency operator** $A : \mathbf{C}^V \to \mathbf{C}^V$ given by

$$(Af)(v) = \sum_{w \in N(v)} f(w)$$

With respect to the basis induced by the characteristic functions over the vertices of the graph, A is represented in matrix form by the adjacency matrix of its graph.

A graph isomorphism replaces an adjacency with a similar matrix, so the properties of the operator A invariant under basis changes are isomorphism invariant. We shall find that in particular, the eigenvalues of A give useful information about the graph G, especially if G is a regular graph. As G is undirected, A is a self-adjoint operator, and therefore is diagonalizable, with n real eigenvalues $\lambda_1 \geqslant \cdots \geqslant \lambda_n$. We will write $\lambda_i(G)$ if the graph is not specified. The study of the relationship between a graph G and the eigenvalues of the operator A form the core study of spectral graph theory.

Example. *The invariant subspaces of A correspond to the components of G. That is, if H is a connected component of G, then the subspace of functions* *vanishing outside of H is invariant under the action of A. On the other hand, if G is a connected graph, then all the invariant subspaces of A are trivial.*

Proposition 1.1. *If $\Delta(G)$ denotes the maximum degree in a graph G, and $\delta(G)$ the minimum degree, then for any function $f \in \mathbf{C}^G$ with $L_0 \leqslant f \leqslant L_1$,*

$$\delta(G)L_0 \leqslant Af \leqslant \Delta(G)L_1$$

Proof. We find that for any vertex v

$$\sum_{w \in N(v)} f(w) \leqslant \sum_{w \in N(v)} L_1 = |N(v)|L_1 \leqslant \Delta(G)L_1$$

and the reverse direction gives

$$\sum_{w \in N(v)} f(w) \geqslant \sum_{w \in N(v)} L_0 = |N(v)|L_0 \geqslant \delta(G)L_0$$

This gives the required inequality. □

Corollary 1.2. *For any eigenvalue λ of A, $|\lambda| \leqslant \max(\delta(G), \Delta(G))$.*

Proof. The spectral radius of A is bounded by any of the matrix norms giving the space of operators a Banach algebra structure. In particular, the spectral radius is bounded by $\|A\|_\infty$, and the theorem above bounds the values of $\|A\|_\infty$ as required. □

Example. *As a particular example of this, we find that for K regular graphs, we find $-K \leqslant \lambda_n \leqslant \lambda_1 \leqslant K$, and we actually have $\lambda_1 = K$, because A operates on constant functions by multiplication by K.*

Proposition 1.3. *On a K regular graph, $\lambda_2 = K$ iff G is disconnected.*

Proof. If we break G into two connected components H_0 and H_1, then the functions vanishing outside of H_0 and the functions outside of H_1 form two complementary invariant subspaces of G, and both of these subspaces contain eigenfunctions of eigenvalue 1. On the other hand, we show that if G is connected, then every eigenfunction f of eigenvalue K is constant. Let v^* maximize f over all vertices in v. Then

$$Kf(v^*) = \sum_{w \in N(v^*)} f(w) \leqslant Kf(v^*)$$

If $f(w) \neq f(v^*)$ for some $w \in N(v^*)$, the inequality above is strict, which is impossible. Thus if v^* maximizes f, then all its neighbours maximize f. Since G is connected, we conclude that f is constant on G. □

Lemma 1.4. *If f is an eigenfunction of a K regular graph with eigenvalue $\lambda \neq K$, then $\sum f(v) = 0$.*

Proof. If $\sum f(v) \neq 0$, we may assume without loss of generality that $\sum f(v) = 1$. Then, if we take the sum of the adjacency of the operator over all vertices, we sum over each vertex K times, and so

$$K = K \sum_v f(v) = \sum_v \sum_{w \in N(v)} f(w) = \sum_v \lambda f(v) = \lambda$$

and this gives the required equality. □

Example. *If G is a K regular graph, then $\lambda_n = -K$ if and only if G has a bipartite connected component. Because of our discussion, we might as well assume G is connected, because invariant subspaces contain all the eigenfunctions of an operator. If $G = H_0 \cup H_1$ is bipartite, the function $\chi_{H_0} - \chi_{H_1}$ has eigenvalue $-K$. On the other hand, if f is an eigenfunction of A with eigenvalue $-K$, we claim that f must cycle over two distinct values, which are negations of each other. Let v^* maximize f, and let v_* minimize the function. We know that $f(v_*) < 0 < f(v^*)$. Since*

$$-Kf(v^*) = \sum_{w \in N(v^*)} f(w) \geqslant Kf(v_*)$$

We conclude that $f(v_*) \leqslant -f(v^*)$. The same argument applied to the neighbours of v_* gives $-f(v_*) \leqslant f(v^*)$. Putting these two inequalities together gives $-f(v_*) = f(v^*)$. If $f(w) \neq f(v_*)$ for $w \in N(v^*)$, then the inequality above is strict, which is impossible. Similarily, we conclude that $f(w) = f(v^*)$ for each $w \in N(v_*)$. Since v_* and v^* were arbitrary vertices minimizing and maximizing f, every vertex takes one of these two values, and adjacent vertices have opposite values, so these two values give a bipartite structure on the given graph.

A K regular graph G is said to be an ε **expander** (one sided) if $\lambda_2 \leqslant (1-\varepsilon)K$, and a *two sided* ε expander if one also has $\lambda_n \geqslant -(1-\varepsilon)K$. Every connected graph is an ε expander for some ε, and a non bipartite graph is a two sided expander for some ε. Thus unless we want to perform analysis parameterized by ε, we are forced to look at 'limits' of graphs which control their eigenvalues. A sequence of K regular graphs is said to be an expander family if there is a ε such that eventually the graphs are all ε expanders.

Theorem 1.5. *Let G be a K regular graph on n vertices. Then*

- $\sum \lambda_i = 0$.
- $\sum \lambda_i^2 = nK$.
- $\max(|\lambda_2|, |\lambda_n|) \geqslant \sqrt{K} - o_K(1)$.

where $o_K(1)$ denotes a quantity tending to zero at a rate dependant on K.

Proof. In its adjacency matrix representation, the adjacency operator A has no loops, hence its diagonal vanishes and so it has trace zero. It follows that the sum of the eigenvalues of A is equal to zero. The sum of the squares of the eigenvalues is equal to the trace of A^2, which corresponds to a kind of 'second order' adjacency operator. Since we have no multiedges,

$$(A^2\chi_v)(v) = \sum_{w \in N(v)} \sum_{u \in N(w)} \chi_v(u) = K$$

Hence, with respect to the canonical basis on the graph, A^2 has diagonal entries K, and hence has trace Kn. Finally, this shows that

$$nK = \sum \lambda_i^2 = \sum |\lambda_i|^2 \leqslant 1 + (n-1)\max(|\lambda_2|^2, |\lambda_n|^2)$$

and therefore that

$$\max(|\lambda_2|, |\lambda_n|) = \sqrt{\max(|\lambda_2|^2, |\lambda_n|^2)} \geqslant \sqrt{\frac{nK-1}{n-1}}$$

and the last term is $\sqrt{K} - \sqrt{K}O(1/n) + K^2 O(1/n^2)$. □

This result places an upper bound on the rate of a two sided expansion for large graphs. A more sophisticated result sharpens the inequality to obtain the improvement

$$\max(|\lambda_2|, |\lambda_n|) \geqslant 2\sqrt{K-1} - o_K(1)$$

Graphs with $\max(|\lambda_2|, |\lambda_n|) \leqslant 2\sqrt{K-1}$ are known as Ramanujan graphs, and have connections to number theory.

Example. *For each n, let G_n be the 2-regular graph whose vertex set is $\mathbf{Z}_n$, and such that the neighbours of k are $k+1$ and $k-1$. Then the adjacency operator A_n is really just the combination of shifts $L_1 + L_{-1}$ in disguise. Now if $\chi_1, \dots, \chi_n$ are the basis of n characters on $\mathbf{Z}_n$, with $\chi_m(1) = e^{2i\pi m/n}$, then*

$$\begin{aligned} A_n(\chi_m)(k) &= \chi_m(k+1) + \chi_m(k-1) \\ &= (\chi_m(1) + \chi_m(-1))\chi_m(k) \\ &= \cos(2\pi m/n)\chi_m(k) \end{aligned}$$

As $n \to \infty$, the space of eigenvalues of A_n becomes dense in $[-1,1]$, so this sequence of graphs cannot be an expander family for any ε.

Example. *The complete graph C_n on n vertices, which is an $n-1$ regular graph, is an excellent example of an expander graph family. If f is an eigenfunction of A_n with eigenvalue $\lambda_i \neq n-1$, then $\sum f(v) = 0$, and so*

$$\lambda_i f(v) = \sum_{w \neq v} f(v) = -f(v)$$

so $\lambda_i = -1$, and the sequence of eigenvalues for A_n is $1, -1, \dots, -1$. This shows that C_n is a one-sided $1 + 1/(n-1)$ expander, and a $1 - 1/(n-1)$ two sided expander. The goal of the theory of expander graphs is to find sparse graphs with similar properties to complete graphs, and so we desire sparse expander graphs.

Example. *If G is a K regular graph on n edges, then the complement graph G^c is an $n-K-1$ regular graph. If A is the adjacency operator corresponding to G, and B the operator corresponding to G^c, then $(A+B)(f)(v) = \sum f(w) - f(v)$. In particular, if f is an eigenvector for A with eigenvalue $\lambda_i \neq K$, then $\sum f(w) = 0$, and so $Bf = -(1+A)f = -(1+\lambda_i)f$. If we assume G is connected, then the sequence $K \neq \lambda_2 \geqslant \dots \geqslant \lambda_n$ gives the eigenvalues $-(1+\lambda_2) \leqslant \dots \leqslant -(1+\lambda_n)$. Since none of the eigenfunctions f corresponding to the eigenvalues $\lambda_2, \dots, \lambda_n$ are constant, we find that B has the additional eigenvalue $n-K-1$ corresponding to the constant function.*

Example. *Let G be the complete bipartite graph between two sets of n vertices. Then $\lambda_{2n} = -n$, because G is bipartite. Note that for any function f, Af is a function which is constant on each side of the bipartition, so for any eigenfunction f with a nonzero eigenvalue λ, f is constant on each side of the bipartition. But this means that if f takes the value x on one side of the bipartition, and y*

on the other side, then $\lambda x = ny$, and $\lambda y = nx$. If $x = 0$, we find that $y = 0$. If $x \neq 0$, then $\lambda = ny/x$, and also $ny^2/x = nx$, so $y^2 = x^2$ implying that $y = \pm x$. These give the two eigenfunctions corresponding to the constant function with eigenvalue n and the bipartite eigenfunction with eigenvalue $-n$. This tells us that the remaining eigenvalues $\lambda_2, \dots, \lambda_{2n-1}$ are all equal to zero.

Viewing a graph as the discrete version of a K regular graph, and f is a function on the graph, we can define the **discrete gradient magnitude**

$$|\nabla f|(v) = \sqrt{\sum_{w \in N(v)} |f(w) - f(v)|^2}$$

The classical Poincaré inequality in Euclidean space says that $\|f\|_2 \leqslant C\|\nabla f\|_2$. This inequality is actually connected to the theory of expanders, because a graph G is a one sided ε expander if and only if

$$\|\nabla f\|_2^2 \geqslant 2K\varepsilon\|f\|_2^2$$

for any mean zero function f. We may assume that G is a connected graph to prove this theorem, for if G is not connected it is not an expander for any $\varepsilon > 0$. We can write

$$\begin{aligned}
\sum_v \sum_{w \in N(v)} |f(w) - f(v)|^2 &= \sum_v \sum_{w \in N(v)} |f(w)|^2 + |f(v)|^2 - 2\mathfrak{Re}[\overline{f}(v) f(w)] \\
&= 2K\|f\|_2^2 - 2\mathfrak{Re}\left(\sum_v \overline{f(v)}(Af)(v)\right) \\
&= 2K\|f\|_2^2 - 2\mathfrak{Re}\langle f, Af\rangle
\end{aligned}$$

If f has mean zero, then we can write $f = \sum f_j$ for the decomposition of f into the j'th eigenspace. Since A is self adjoint, these eigenspaces are orthogonal, and so

$$\langle f, Af\rangle = \sum \lambda_j \|f_j\|_2^2$$

Since $\sum_v f_j(v) = 0$ for all $j > 1$, we find $0 = \sum_v f(v) = \mu_1 \sum_v f_1(v)$. Since $\sum_v f_1(v) \neq 0$, we find $\mu_1 = 0$. This means that

$$\sum \lambda_i \|f_i\|_2^2 \leqslant \sum \lambda_2 \|f_i\|_2^2 = \lambda_2 \|f\|_2^2$$

and this shows that

$$\|\nabla f\|_2^2 \geqslant 2(K - \lambda_2)\|f\|_2^2$$

and $K - \lambda_2$ gives the maximal value of ε for which G is a ε expander.

1.1 Expanders and Edge Expansion

We now make the intuition about expander graphs having good 'expansion properties' precise. Given two disjoint sets of vertices V and W, we let $E(V,W)$ denote the set of edges between the two vertex sets. We find that

$$|E(V,W)| = \langle A\chi_V, \chi_W \rangle$$

Given a vertex set V, we let $\delta(V)$ denote the set of edges leaving V. We define the **edge expansion ratio**

$$h(G) = \min_{|V| \leqslant n/2} \frac{|\delta(V)|}{|V|} = \min_{|V| \leqslant n/2} \frac{\langle A\chi_V, 1-\chi_V \rangle}{|V|}$$

The choice that $|V| \leqslant n/2$ is done to avoid trivial values where we let V be the set of all vertices in the graph, so that $\delta(V) = \emptyset$. The edge expansion ratio can be seen as a discrete isoperimetry bound for the graph, and as such it is often called the **Cheeger constant** of the graph.

Proposition 1.6. *$h(G) \neq 0$ if and only if G is connected, and more generally, a family of K regular graphs G_i is an expander family if $h(G_i)$ is lower bounded.*

Proof. We may assume each graph is connected. Fix $\varepsilon > 0$ such that eventually $\lambda_2 \leqslant (1-\varepsilon)K$. For any subset V of edges in G_i, the projection of χ_V onto the first eigenspace is $|V|/n$, and so

$$\langle A\chi_V, \chi_V \rangle \leqslant \frac{1}{n} K|V|^2 + (1-\varepsilon)K \left\| \chi_V - \frac{|V|}{n} \right\|^2$$

And

$$\begin{aligned} \left\| \chi_V - \frac{|V|}{n} \right\|^2 &= |V| \left(1 - \frac{|V|}{n}\right)^2 + [n - |V|] \left(\frac{|V|}{n}\right)^2 \\ &= |V| - \frac{1}{n}|V|^2 \end{aligned}$$

Hence

$$\frac{1}{n}K|V|^2 + (1-\varepsilon)K \left\| \chi_V - \frac{|V|}{n} \right\|^2 \leqslant (1-\varepsilon)K|V| - \frac{\varepsilon K |V|^2}{n} \leqslant (1-\varepsilon/2)K|V|$$

Since $\langle A\chi_V, 1\rangle = K|V|$, this shows that

$$\begin{aligned} h(G) &= \min_{|V| \leqslant n/2} \frac{|\delta(V)|}{|V|} = \min_{|V| \leqslant n/2} \frac{\langle A\chi_V, 1-\chi_V\rangle}{|V|} \\ &= \min_{|V| \leqslant n/2} \frac{\langle A\chi_V, 1\rangle}{|V|} - \frac{\langle A\chi_V, \chi_V\rangle}{|V|} \\ &\geqslant \min_{|V| \leqslant n/2} K - (1-\varepsilon/2)K = (\varepsilon/2)K \end{aligned}$$

Another way to see this is that $\langle A\chi_V, \chi_V\rangle$ counts the number of edges between vertices in V, and since each vertex in V is adjacent to exactly K vertices, we conclude that the total number of edges leaving V is exactly $K|V| - \langle A\chi_V, \chi_V\rangle$, which we have bounded below by $(\varepsilon/2)K|V|$.

The other direction is harder. The difficulty is that the lower bound $h(G) \geqslant c$ enables us to conclude that $\langle A\chi_V, \chi_V\rangle \leqslant (K-c)|V|$ for all vertex sets with $|V| \leqslant n/2$, whereas proving that G is an expander requires us to understand $\langle Af, f\rangle$ for all functions f, because we know

$$\lambda_2 = \sup_{\sum f(v)=0} \frac{\langle Af, f\rangle}{\|f\|_2^2}$$

so it suffices to show $\langle Af, f\rangle \leqslant (1-\varepsilon)K$ for all functions f with mean zero and with $\|f\|_2 = 1$, for some ε depending only on K and c. Since A is real, we may assume that f is real. We will prove that if f is non-negative, and is supported on a set of cardinality $n/2$, then $\langle Af, f\rangle \leqslant (1-c)K\|f\|_2^2$. To see how this implies the main inequality, note that if we write $f = f_+ - f_-$, then

$$\langle Af, f\rangle \leqslant \langle Af_+, f_+\rangle + \langle Af_-, f_-\rangle$$

and $1 = \|f_+\|_2^2 + \|f_-\|_2^2$. Either f_+ or f_- is supported on a set of size less than or equal to $n/2$, and by symmetry we may assume this is f_-. Consider a small value σ, to be fixed later. If $\|f_-\|_2^2 \geqslant \sigma^2$, then applying the trivial bound $\langle Af_+, f_+\rangle \leqslant K\|f_+\|_2^2$

$$\langle Af_+, f_+\rangle + \langle Af_-, f_-\rangle \leqslant K\|f_+\|_2^2 + (1-c)K\|f_-\|_2^2 \leqslant K(1-\sigma^2)\|f\|_2^2$$

TODO: FINISH BOUNDS LATER. □

Example. *On the graph defined on* $\mathbf{Z}_n$ *we considered before, for* $n > 2$*, the set of points* $\{1, \dots, n/2\}$ *has two boundary edges, between* 0 *and* 1*, and between*

$n/2$ and $n/2+1$. It follows that $h(G_n) \leqslant 4/n$, and this is an equality, because if $|V| \leqslant n/2$, then $\delta(V)$ contains at least two edges, so $\delta(V) \geqslant 2 \geqslant 4|V|/n$. This is another way to think about why the graphs are not a family of expander graphs.

Example. *Every 2 regular graphs breaks down into connected components, which form loops in the graph. It follows that if G is connected, it is isomorphic to $\mathbf{Z}_n$, and any family of such graphs which form an expander family must have bounded size.*

A more precise relationship between the best value ε that makes G into a one sided expander and it's Cheeger constant. Namely,

$$\frac{\varepsilon K}{2} \leqslant h(G) \leqslant \sqrt{2\varepsilon} K$$

proved in the 1980s by Dodzuik and Alon-Milman.

TODO: EXERCISES

1.2 Random Walks

We now discuss how the theory of expanders connects to the theory of convergence rates of random walks on graphs. Given a graph G and an initial vertex v_0 (which can be randomly chosen), the random walk $v_0, v_1, v_2, \dots$ is chosen such that v_{i+1} is obtained from v_i by choosing a neighbour uniformly at random. We will let μ_i be the function on the vertices of G such that $\mu_i(v) = \mathbf{P}(v_i = v)$. Then arguing by conditional probabilities, we find that $\mu_{i+1} = (A\mu_i)/K$. Provided our graph is connected and aperiodic, the corresponding Markov chain is ergodic, and the distributions μ_i will converge pointwise to an eigenfunction for the adjacency operator of highest eigenvalue. In particular, over a K regular connected graph the distribution will eventually be indistinguishable from the uniform distribution.

We can measure how fast μ_i converges to a constant distribution by quantifying $\|\mu_i - 1/n\|_2$. It is decreasing in i, because one calculates

$$\begin{aligned} \|A\mu_i/K - 1/n\|_2^2 - \|\mu_i - 1/n\|_2^2 &= \left[\frac{\|A\mu_i\|_2^2}{K^2} - \frac{1}{n} \right] - \left[\|\mu_i\|_2^2 - \frac{1}{n} \right] \\ &= \frac{\|A\mu_i\|_2^2}{K^2} - \|\mu_i\|_2^2 \end{aligned}$$

If μ_i has a decomposition as $\sum \mu_{ij}$ via its eigenspaces, then $\mu_{i1} = 1/n$, because $\sum \mu_i(v) = 1$, and so

$$\|A\mu_i\|_2^2 \geqslant K^2 \|\mu_{i1}\|_2^2 = K^2$$

Yet $\|\mu_i\|_2^2 = \sum \mu_i(v)^2 \leqslant \sum \mu_i(v) = 1$, so

$$\frac{\|A\mu_i\|_2^2}{K^2} - \|\mu_i\|_2^2 \geqslant 1 - 1 = 0$$

This is an equality only when $\mu_i = 1/n$, so the function is decreasing everywhere else. The expansion properties are intricately tied to the expansion properties of the graphs.

Theorem 1.7. *Fix $\alpha > 1/2$. A sequence of K regular graphs G_n with m_n vertices is a two-sided expander family if and only if there is $C > 0$ independent of n such that for sufficiently large n, $\|\mu_i - m_n^{-1}\|_2 \leqslant m_n^{-\alpha}$ for all $i \geqslant C \log m_n$, and all choices of initial vertices v_0.*

Note that the theorem holds for any initial probability distribution by an easy application of the Minkowski inequality. Thus from a dynamical systems point of view, the uniform distribution is a very strong attractor in the space of all probability distributions. Essentially, this theorem says that two sided expanders are those graphs such that random walks become close to uniform in $O(\log n)$ steps. On the other hand, the central limit theorem only implies that the walks $\mathbf{Z}_n$ become close to uniformly mixing only at time beyond n^2, as indicated by the central limit theorem (TODO: WHY?). This theorem is useful for generating near random distributions using little work by taking a random walk on some basic combinatorial structure.