Bipartite and neighborhood graphs and the spectrum of the normalized graph Laplacian

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Abstract

We study the spectrum of the normalized Laplace operator of a connected graph $\Gamma$. As is well known, the smallest nontrivial eigenvalue measures how difficult it is to decompose $\Gamma$ into two large pieces, whereas the largest eigenvalue controls how close $\Gamma$ is to being bipartite. The smallest eigenvalue can be controlled by the Cheeger constant, and we establish a dual construction that controls the largest eigenvalue. Moreover, we find that the neighborhood graphs $\Gamma[l]$ of order $l \geq 2$ encode important spectral information about $\Gamma$ itself which we systematically explore. In particular, we can derive new estimates for the smallest nontrivial eigenvalue that improve the Cheeger estimate for certain graphs, as well as an explicit estimate for the largest eigenvalue from above and below. As applications of such spectral estimates, we provide a criterion for the synchronizability of coupled map lattices, and an estimate for the convergence rate of random walks on graphs.

Keywords: Laplacian spectrum of graphs, graph Laplacian, largest eigenvalue, Cheeger constant, neighborhood graph, coupled map lattice.

1 Introduction

A general principle in geometry tells us that the spectrum of a Laplace operator encodes important geometric information about the underlying space. This principle has been particularly fertile in Riemannian geometry. One of the key questions has been the control from below of the first nonzero eigenvalue of the Laplace-Beltrami operator in terms of the geometry of the underlying Riemannian manifold (assumed to be compact here for simplicity of exposition). The Lichnerowicz bound estimates the first eigenvalue from below in terms of a lower bound for the Ricci curvature. In contrast, the Cheeger estimate controls the first eigenvalue from below in terms of a global quantity that expresses how difficult it is to cut the manifold into two large pieces \cite{5}. In this way,
the first eigenvalue could be related to the fundamental analytic constants of a Riemannian manifold, like the isoperimetric or Sobolev constants. The work of Li and Yau [18] utilized gradient bounds for eigenfunctions in order to control the first eigenvalue from below in terms of the diameter and Ricci bounds of the Riemannian manifold. More generally, their famous Harnack inequality for the heat kernel [19] then allowed for a systematic control of all eigenvalues of a Riemannian manifold, with the optimal asymptotics as given by Weyl’s law. See for instance [4] for a systematic treatment of eigenvalues in Riemannian geometry.

In graph theory, the algebraic graph Laplacian has been explored for a long time, see for example [20]. More recently, F.Chung and S.T.Yau, see e.g. [9, 8, 10] and the monograph [7], systematically investigated the normalized graph Laplace operator $\Delta$ of an unweighted and undirected graph. This operator, which is different from the algebraic graph Laplace operator, underlies random walks and diffusion processes with conservation laws on graphs. The normalized graph Laplace operator is related to the Laplace-Beltrami operator for a Riemannian manifold. Thus, in order to study the spectrum of $\Delta$, one can systematically apply methods developed in Riemannian geometry for the investigation of the spectrum of the Laplace-Beltrami operator and this led to many remarkable insights, see the works just cited and the references therein.

In particular, the smallest nontrivial eigenvalue can be well controlled in terms of the Cheeger constant $h$ [7]. (In a graph-theoretical setting, such constants can already be found in earlier work by Polyá and Szegö [21].)

In contrast to a Riemannian manifold, on a graph, the spectrum of the normalized Laplacian is always bounded from above. In fact, the upper bound 2 is achieved if and only if the graph is bipartite. (We recall that a graph is bipartite if its vertex set consists of two classes such that edges are only permitted between two vertices from opposite classes.) Therefore, it is a natural question how to control the largest eigenvalue for graphs that are not bipartite. The original goal of this article was to derive bounds for the largest eigenvalue of $\Delta$ from above and below. These bounds reflect how different the graph in question is from a bipartite one resp. how close it is to such a graph.

In fact, however, these estimates led us to discover more general structures that go beyond our original goal. First of all, we construct a dual version $\bar{h}$ of the Cheeger constant $h$ and derive bounds for the largest eigenvalue from above and below in terms of $\bar{h}$. We find interesting relations between $h$ and $\bar{h}$, and the combination of these two constants tells us more about the graph than either of them does individually. Moreover, we find that the neighborhood graphs $\Gamma[2]$, of order $l \geq 2$, of a graph $\Gamma$ also encode important spectral information about $\Gamma$ itself. For concreteness let $l = 2$ for the moment. The idea then is that $\Gamma[2]$ is a weighted graph with the same vertices as $\Gamma$ itself, and two vertices are connected in $\Gamma[2]$ when they share at least one neighbor in $\Gamma$, with higher weights for more shared neighbors. More precisely, let $\Gamma$ be a weighted graph, with the weight of the edge between the vertices $i$ and $j$ denoted by $w_{ij}$ (which is 0 unless $i$ and $j$ are neighbors), and the degree of $i$ being $d_i = \sum_j w_{ij}$. For the neighborhood graph $\Gamma[2]$, the weight of the edge $e[2] = (i, j)$ in $\Gamma[2]$ then
is given by \( w_{ij}[2] = \sum_k \frac{1}{d_k} w_{ik} w_{kj} \). Consequently, \( i \) and \( j \) are neighbors in \( \Gamma[2] \) if \( i \) and \( j \) have at least one common neighbor in \( \Gamma \), i.e. there exists a path of length 2 between \( i \) and \( j \) in \( \Gamma \). Note that the weights of \( \Gamma[2] \) are normalized in such a manner that every vertex \( i \) has the same degree in both \( \Gamma \) and \( \Gamma[2] \). It turns out that the eigenvalues of \( \Gamma[2] \) are given by \( \lambda(2 - \lambda) \) when \( \lambda \) stands for the eigenvalues of \( \Gamma \). This well suits our purpose because controlling the highest eigenvalue \( \lambda_{\text{max}} \) from above is equivalent to controlling \( 2 - \lambda_{\text{max}} \) from below. Thus, lower spectral bounds on \( \Gamma[2] \) yield lower and upper spectral bounds for \( \Gamma \). For certain graphs, these new lower bounds improve the Cheeger estimate for the smallest nonzero eigenvalue. We not only utilize this principle to derive such bounds, but we also explore the relation between the spectra of \( \Gamma \) and \( \Gamma[2] \) in more general terms. Naturally, the construction of the neighborhood graph \( \Gamma[l] \) can be generalized to higher order neighborhood graphs, i.e. \( i \) and \( j \) are neighbors in \( \Gamma[l] \) if there exists a path of length \( l \) between \( i \) and \( j \) in \( \Gamma \). Again, the weights of \( \Gamma[l] \) are normalized in such a way that every vertex has the same degree in both \( \Gamma \) and \( \Gamma[l] \). In the present paper, we also explore the spectra of the higher order neighborhood graphs \( \Gamma[l] \) and their relations to the spectrum of \( \Gamma \). The concept of the neighborhood graph is quite general, and can also be used to investigate the spectrum of the normalized graph Laplacian defined on directed or infinite graphs.

In the last two sections, we will apply our new eigenvalue bounds to two concrete problems - the convergence of random walks on graphs, and the synchronization for coupled map lattices, that is, a dynamical system supported on the vertices of a graph and coupled according to the interaction structure given by the edges of the graph. Again, the principle is that eigenvalue estimates control how different the graph in question is from the two extremes of a disconnected or a bipartite graph. On a disconnected or a bipartite graph, for different reasons, the random walk does not converge to a stationary distribution, and the coupled map lattice does not synchronize.

### 2 The graph Laplacian and its basic properties

In this paper, \( \Gamma \) is an undirected, weighted, connected, finite, simple graph of \( N \) vertices. We do not exclude loops, i.e., edges connecting a vertex with itself. The vertices are denoted by \( i, j, \ldots \). \( V \) denotes the vertex and \( E \) the edge set of \( \Gamma \), respectively. When the vertices \( i \) and \( j \) are connected by an edge, they are called neighbors, in symbols \( i \sim j \). The associated weight function \( w : V \times V \to \mathbb{R} \) satisfies \( w_{ij} = w_{ji} \) and \( w_{ij} > 0 \) whenever \( i \sim j \) and \( w_{ij} = 0 \) iff \( i \sim j \). For a vertex \( i \), its degree \( d_i \) is given by \( d_i := \sum_j w_{ij} \). When \( w_{ij} = 1 \) whenever \( i \sim j \), we shall speak of an unweighted graph.

The clustering coefficient \( C \) of an unweighted graph \( \Gamma \) is defined as

\[
C := \frac{3 \times \text{number of triangles}}{\text{number of connected triples of vertices}},
\]

where a triangle is a triple of mutually connected vertices. The clustering co-
efficient measures how many connections there exist between the neighbors of a node. \( C \) becomes maximal if \( \Gamma \) is a fully connected graph. In contrast, \( C \) vanishes when \( \Gamma \) is a bipartite graph, that is, consists of two classes \( V_1, V_2 \) of vertices such that no vertices in the same class are connected by an edge. In particular, there are no loops in a bipartite graph. Equivalently, a graph is bipartite iff it has no cycles of odd length, and thus in particular no triangles.

We now recall the definition of the normalized graph Laplace operator and state its basic properties.

**Definition 2.1.** For a graph \( \Gamma = (V, E) \) we define the scalar product
\[
(u, v)_\Gamma := \sum_{i \in V} d_i u(i) v(i).
\]
The space \( \ell^2(\Gamma) \) is then given by
\[
\ell^2(\Gamma) = \{ u : V \to \mathbb{R} \mid (u, u)_\Gamma < \infty \}.
\]
We study the normalized graph Laplacian
\[
\Delta : \ell^2(\Gamma) \to \ell^2(\Gamma)
\]
\[
\Delta v(i) := \frac{1}{d_i} \left( \sum_j w_{ij} (v(i) - v(j)) \right). \tag{2}
\]
This shows that, the Laplacian \( \Delta \) is given by \( \Delta = I - P \), where \( I \) denotes the identity and \( P \) is transition probability operator, respectively. We note that the Laplacian underlies random walks on graphs. We should point our here that the normalized graph Laplacian \( \Delta \) is not exactly the one studied by Fan Chung [7]. However, both Laplacians are unitarily equivalent and therefore in particular have the same spectrum. We recall the following basic properties:

1. \( \Delta \) is selfadjoint w.r.t. \((.,.)_\Gamma\), i.e.
\[
(u, \Delta v)_\Gamma = (\Delta u, v)_\Gamma \tag{3}
\]
   for all \( u, v \in \ell^2(\Gamma) \). This follows from the symmetric weight function, i.e. \( w_{ij} = w_{ji} \) for all \( i \) and \( j \).

   Moreover,

   2. \( \Delta \) is nonnegative, i.e.
\[
(\Delta u, u)_\Gamma \geq 0 \tag{4}
\]
   for all \( u \in \ell^2(\Gamma) \). This follows from the Cauchy-Schwarz inequality.

   3. \( \Delta u = 0 \) iff \( u \) is constant.

   Clearly, \( \Delta u = 0 \) if \( u \) is constant. Let \( \Delta u = 0 \) and assume that \( u \) is not constant. Then there exists a vertex, say \( i \), with \( u(i) \geq u(j) \) for all \( j \sim i \).
with strict inequality for at least one such \( j \). Thus there exists a nontrivial local maximum. This is a contradiction since \( \Delta u(i) = 0 \) implies that the value \( u(i) \) is the average of the values at the neighbors of \( i \). Since \( \Gamma \) is connected, \( u \) then has to be a constant. (When \( \Gamma \) is not connected, a solution of \( \Delta u = 0 \) is constant on every connected component of \( \Gamma \).)

We say that \( \lambda \) is an eigenvalue of \( \Delta \) if there exists some \( u \not= 0 \) with

\[
\Delta u = \lambda u. \tag{5}
\]

The preceding properties have consequences for the eigenvalues of \( \Delta \):

- By 1, the eigenvalues are real.
- By 2, they are nonnegative, i.e. \( \lambda_k \geq 0 \) for all \( k \).
- By 3, the smallest eigenvalue is \( \lambda_0 = 0 \). Since \( \Gamma \) is connected, this eigenvalue is simple, i.e.

\[
\lambda_k > 0 \tag{6}
\]

for \( k > 0 \) where the eigenvalues are ordered as

\[
\lambda_0 = 0 < \lambda_1 \leq \ldots \leq \lambda_{N-1}.
\]

For neighbors \( i, j \), we also consider

\[
Du(i, j) := (w_{ij})^{1/2}(u(i) - u(j)) \tag{7}
\]

and introduce the product

\[
(Du, Dv)_{\Gamma} := \sum_{e=(i,j)} w_{ij} (u(i) - u(j))(v(i) - v(j)). \tag{8}
\]

We have

\[
(Du, Dv)_{\Gamma} = \frac{1}{2} \left( \sum_{i,j} w_{ij} u(i)v(i) + \sum_{i,j} w_{ij} u(j)v(j) - 2 \sum_{i,j} w_{ij} u(i)v(j) \right)
\]

\[
= \sum_i d_i u(i) \left( v(i) - \frac{1}{d_i} \sum_j w_{ij} v(j) \right)
\]

\[
= (u, \Delta v)_{\Gamma}. \tag{9}
\]

Consequently,

\[
\Delta = D^* D. \tag{10}
\]

\( D^* \) can be considered as a boundary operator mapping 1-chains defined on edges to 0-chains defined on vertices. \( D \) is the corresponding coboundary operator.

An orthonormal basis of \( \ell^2(\Gamma) \) consisting of eigenfunctions of \( \Delta \),

\[
u_k, \; k = 0, \ldots, N - 1
\]
can be constructed in the standard way which we now recall. Let $H_0 := H := \ell^2(\Gamma)$ be the Hilbert space of all real-valued functions on $\Gamma$ with the scalar product $(\cdot, \cdot)_\Gamma$. We iteratively define

$$H_k := \{ v \in H : (v, u_i)_\Gamma = 0 \text{ for } i \leq k - 1 \},$$

starting with a constant function $u_0$ as the eigenfunction for the eigenvalue $\lambda_0 = 0$. Then the $k$th eigenvalue is given by

$$\lambda_k = \inf_{u \in H_k - \{0\}} \frac{(Du, Du)_\Gamma}{(u, u)_\Gamma},$$

and the corresponding eigenfunction $u_k$ realizes this infimum. By way of contrast, the highest eigenvalue is also given by

$$\lambda_{N-1} = \sup_{u \neq 0} \frac{(Du, Du)_\Gamma}{(u, u)_\Gamma}.$$  

In particular, for any eigenfunction $u$ for some eigenvalue $\lambda$, we then have

$$\lambda = \frac{(Du, Du)_\Gamma}{(u, u)_\Gamma}.$$  

All different eigenfunctions are orthogonal to each other. In particular the eigenfunctions $u_1, \ldots, u_{N-1}$ are orthogonal to $u_0$, the eigenfunction for the eigenvalue $\lambda_0 = 0$. This implies that

$$\sum_i d_i u_k(i) = 0$$

for $k = 1, \ldots, N - 1$, since $u_0(i)$ is constant for all $i$.

The largest eigenvalue satisfies

$$\lambda_{N-1} \leq 2$$

with equality if and only if $\Gamma$ is bipartite. A corresponding eigenfunction equals a positive constant $c$ on one class and $-c$ on the other class of vertices. In contrast, for loopless graphs, the highest eigenvalue $\lambda_{N-1}$ becomes smallest on a complete graph $K_N^1$, namely

$$\lambda_{N-1} = \frac{N}{N - 1}.$$  

By considering the trace of $\Delta$ we obtain

$$\sum_i \lambda_i = N - \sum_i \frac{w_{ii}}{d_i}.$$  

Altogether, the eigenvalues satisfy

$$0 = \lambda_0 < \lambda_1 \leq \frac{N - \sum_i \frac{w_{ii}}{d_i}}{N - 1} \leq \lambda_{N-1} \leq 2.$$  

\footnote{$K_N$ denotes an unweighted complete loopless graph on $N$ vertices.}
Similarly to (17), the first eigenvalue $\lambda_1$ is largest for the complete graph $K_N$, achieving the bound in (19), that is
\[
\lambda_1 = \frac{N}{N - 1}.
\] (20)
For any other unweighted graph, we have in fact
\[
\lambda_1 \leq 1.
\] (21)

3 The Cheeger constant and its dual and eigenvalue estimates

Our starting point are the estimates for the first eigenvalue $\lambda_1$ in terms of the (Polya-)Cheeger constant, as obtained by Chung [6, 7]. The (Polya-)Cheeger constant [21] of an unweighted graph is defined as
\[
h := \min_{U} \frac{|E(U, \overline{U})|}{\min\{\text{vol}(U), \text{vol}(\overline{U})\}} = \min_{U \subset V: \frac{1}{2}\text{vol}(V)} \frac{|E(U, \overline{U})|}{\text{vol}(U)},
\] (22)
where $U$ and $\overline{U} = V \setminus U$ yield a partition of the vertex set $V$ and $U, \overline{U}$ are both nonempty. Here the volume of $U$ is given by $\text{vol}(U) := \sum_{i \in U} d_i$, $E(U, \overline{U}) \subseteq E$ is the subset of all edges with one vertex in $U$ and one vertex in $\overline{U}$, and $|E(U, \overline{U})| := \sum_{k \in U, l \in \overline{U}} w_{kl}$ is the sum of the weights of all edges in $E(U, \overline{U})$. In general we have $h \leq 1$. This follows from the definition of $h$, since $|E(U, \overline{U})| \leq |E(U, \overline{U})| + |E(U, U)| = \text{vol}(U)$ and $|E(U, \overline{U})| \leq |E(U, \overline{U})| + |E(\overline{U}, \overline{U})| = \text{vol}(\overline{U})$.

If, for example, $\Gamma$ is given by $K_2$ or $K_3$ then the estimate $h \leq 1$ is sharp. Let us first recall [6, 7] how $h$ can bound $\lambda_1$ from above. We use the variational characterization (12), observing that $H_1$ is the set of all functions $v$ with the normalization $\sum_{i \in V} d_i v(i) = 0$. Let the edge set $E(U, \overline{U})$ divide the graph into the two disjoint sets $U, \overline{U}$ of nodes, and let $U$ be the one with the smaller volume $\text{vol}(U) = \sum_{i \in U} d_i$. We consider a function $v$ that is $= 1$ on all the nodes in $U$ and $= -\alpha$ for some positive $\alpha$ on $\overline{U}$. $\alpha$ is chosen so that the normalization $\sum_{i \in V} d_i v(i) = 0$ holds, that is, $\sum_{i \in U} d_i - \sum_{i \in \overline{U}} d_i \alpha = 0$. Since $\overline{U}$ is the subset with the larger volume $\sum_{i \in \overline{U}} d_i$, we have $\alpha \leq 1$. Thus, for our choice of $v$, the quotient in (12) becomes
\[
\lambda_1 \leq 2h.
\] (23)
In fact, this estimate holds under rather general conditions, and an appropriate version is also true for the algebraic (non-normalized) graph Laplacian. In contrast, the lower bound
\[
\lambda_1 \geq \frac{1}{2} h^2.
\] (24)

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crucially needs the normalization. It is actually possible to improve the lower bound slightly, i.e.

$$\lambda_1 \geq 1 - \sqrt{1 - h^2}. \quad (25)$$

The crucial point in the proof of (25) is the following lemma which we recall here, because we will make use of it in the sequel. Our proof is mainly based on [12] and uses some generalizations that can be found in [7].

**Lemma 3.1.** Let $g \in \ell^2(\Gamma)$ with $S(g) := \{i \in V : g(i) > 0\} \neq \emptyset$, put

$$h(g) := \min_{\emptyset \neq S \subseteq S(g)} \frac{|E(S, \overline{S})|}{\text{vol}(S)}$$

and let $g_+$ be the positive part of $g$, i.e.

$$g_+(i) = \begin{cases} g(i) & \text{if } g(i) > 0 \\ 0 & \text{else.} \end{cases}$$

Then

$$1 + \sqrt{1 - h^2(g)} \geq \frac{\sum_{e=(i,j)} w_{ij} (g_+(i) - g_+(j))^2}{\sum_i d_i g_+(i)^2} \geq 1 - \sqrt{1 - h^2(g)}.$$

**Proof.** First, we write

$$W := \frac{\sum_{e=(i,j)} w_{ij} (g_+(i) - g_+(j))^2}{\sum_i d_i g_+(i)^2} = \frac{\sum_{e=(i,j)} w_{ij} (g_+(i) - g_+(j))^2 \sum_{e=(i,j)} w_{ij} (g_+(i) + g_+(j))^2}{\sum_i d_i g_+(i)^2 \sum_{e=(i,j)} w_{ij} (g_+(i) + g_+(j))^2} =: \frac{I}{II}.$$ 

Using the Cauchy-Schwarz inequality we obtain

$$I \geq \left( \sum_{e=(i,j)} w_{ij} |g_+(i)^2 - g_+(j)^2| \right)^2.$$ 

Now we have

$$I \geq \sum_{e=(i,j)} w_{ij} |g_+(i)^2 - g_+(j)^2|$$

$$= \sum_{e=(i,j): g_+(i) \geq g_+(j)} w_{ij} (g_+(i)^2 - g_+(j)^2)$$

$$= 2 \sum_{e=(i,j): g_+(i) \geq g_+(j)} w_{ij} \int_{g_+(j)}^{g_+(i)} t \, dt$$

$$= 2 \int_0^\infty \sum_{e=(i,j): g_+(j) \leq t \leq g_+(i)} w_{ij} t \, dt.$$
Note that \( \sum_{e=(i,j): g_+(j) \leq t \leq g_+(i)} w_{ij} = E(S_t, \overline{S_t}) \) where \( S_t := \{ i : g_+(i) > t \} \). Thus,

\[
I^2 \geq 2h(g) \int_0^\infty \text{vol}(S_t) t dt \\
= 2h(g) \int_0^\infty \sum_{i: g_+(i) > t} d_i t dt \\
= 2h(g) \sum_{i \in V} d_i \int_0^{g_+(i)} t dt \\
= h(g) \sum_{i} d_i g_+(i)^2
\]

and so we obtain

\[
I \geq h^2(g)(\sum_{i} d_i g_+(i)^2)^2.
\]

\[
II = \sum_{i} d_i g_+(i)^2 \sum_{e=(i,j)} w_{ij} (g_+(i) + g_+(j))^2 \\
= \sum_{i} d_i g_+(i)^2 \left( \sum_{i} d_i g_+(i)^2 + 2 \sum_{e=(i,j)} w_{ij} g_+(i)g_+(j) \right) \\
= \sum_{i} d_i g_+(i)^2 \left( 2 \sum_{i} d_i g_+(i)^2 - \sum_{e=(i,j)} w_{ij} (g_+(i) - g_+(j))^2 \right) \\
= (2 - W) (\sum_{i} d_i g_+(i)^2)^2.
\]

Combining everything we obtain,

\[
W \geq \frac{h^2(g)}{2 - W}
\]

and consequently

\[
1 + \sqrt{1 - h^2(g)} \geq W \geq 1 - \sqrt{1 - h^2(g)}.
\]

The second observation that we need to prove the Cheeger inequality is the following lemma:

**Lemma 3.2.** For every non-negative real number \( \lambda \) and \( g \in \ell^2(\Gamma) \) we have

\[
\lambda \geq \frac{\sum_{e=(i,j)} w_{ij} (g_+(i) - g_+(j))^2}{\sum_{i} d_i g_+(i)^2} = W
\]

if \( \Delta g \leq \lambda g \) on \( S(g) \).
Proof. We have

\[(\Delta g, g_+) = \sum_i d_i \Delta g(i) g_+(i) \leq \lambda \sum_i d_i g(i) g_+(i) = \lambda \sum_i d_i g(i) g_+(i)\]

and

\[(\Delta g, g_+) = (Dg, Dg_+) = \sum_{e=\{i,j\}} w_{ij} (g(i) - g(j)) (g_+(i) - g_+(j)) \geq \sum_{e=\{i,j\}} w_{ij} (g_+(i) - g_+(j))^2\]

The Cheeger inequality now follows from the last two Lemmata by taking \(\lambda = \lambda_1\) and \(g = u_1\) an eigenfunction for \(\lambda_1\). Since \((u_1, 1) = 0\) we have \(S(u_1) \neq 0\), and \(T(u_1) = \{i \in V : u_1(i) < 0\} \neq 0\). Thus it is always possible to choose \(u_1\) such that \(\text{vol}(S(u_1)) \leq \text{vol}(S(u_1))\) (if \(\text{vol}(S(u_1)) \geq \text{vol}(S(u_1))\) take \(-u_1\) instead of \(u_1\)) and thus \(h(u_1) \geq h\).

In any case, in qualitative terms, the Cheeger inequalities (23) and (25) simply say that \(\lambda_1\) becomes small when the graph can be easily (that is, by cutting only few edges) decomposed into two large parts. Thus, \(\lambda_1\) is small, that is, close to its minimal value 0, when \(\Gamma\) is similar to a disconnected graph, with equality iff \(\Gamma\) is disconnected itself. Similarly, and this brings us to our topic, the largest eigenvalue is large, that is, close to its maximal value 2, when \(\Gamma\) is close to a bipartite graph, with equality iff \(\Gamma\) is bipartite itself.

The main purpose of this section then is a dual version of (23) and (25) for the largest eigenvalue \(\lambda_{N-1}\). More precisely, we shall obtain an estimate for \(\lambda_{N-1}\) in terms of a dual version of the Cheeger constant which we now introduce. Let \(V_1, V_2\), and \(V_1 \cup V_2 \cup V_3\) be a partition of the vertex set \(V\) into three disjoint sets such that \(V_2\) and \(V_3\) are nonempty. It is helpful to think of \(V_1 \cup V_2\) as the (almost) bipartite part of \(\Gamma\) and \(V_3\) as the part of \(\Gamma\) that contains many cycles of odd length, i.e. \(V_3\) is not bipartite.

For a partition \(V_1, V_2, V_3\) of the vertex set \(V\) we define:

\[
\overline{h} := \max_{V_1, V_2} \frac{2|E(V_1, V_2)|}{\text{vol}(V_1) + \text{vol}(V_2)},
\]

where the volume of \(V_k\) is given by \(\text{vol}(V_k) := \sum_{i \in V_k} d_i\) and \(|E(V_i, V_j)| := \sum_{k \in V_i, l \in V_j} w_{kl}|\).

The next theorem shows that \(\overline{h}\) characterizes bipartite graphs.

Theorem 3.1. \(\overline{h} \leq 1\), and \(\overline{h} = 1\) if and only if \(\Gamma\) is bipartite.

Proof. First, note that, for a partition \(V_1, V_2\) and \(V_3\) of \(V\), the volume of \(V_1\) can also be written in the form

\[
\text{vol}(V_1) = \sum_{j=1}^3 |E(V_i, V_j)|
\]
Consequently, $\bar{h}$ is given by
\[
\bar{h} = \max_{V_1, V_2} \frac{2|E(V_1, V_2)|}{\sum_{j=1}^{3} |E(V_1, V_j)| + \sum_{j=1}^{3} |E(V_2, V_j)|}.
\] (28)

Thus, clearly,
\[
\bar{h} \leq 1.
\] (29)

Assume that $\Gamma$ is bipartite. Then there exists a partition $V_1, V_2, V_3$ of $V$ such that $V_3 = \emptyset$ and there are no edges within the subsets $V_1$ and $V_2$. Thus, $|E(V_1, V_3)| = |E(V_2, V_3)| = |E(V_1, V_1)| = |E(V_2, V_2)| = 0$. By (28) we have $\bar{h} \geq 1$. Together with (28) it follows that $\bar{h} = 1$.

Now assume that $\bar{h} = 1$. Equation (28) implies that there exists a partition $V_1, V_2, V_3$ of $V$ such that $|E(V_1, V_3)| = |E(V_2, V_3)| = |E(V_1, V_1)| = |E(V_2, V_2)| = 0$. Since $\Gamma$ is connected $V_3 = \emptyset$. Thus $\Gamma$ is bipartite.

As an illustration, let us consider loopless Erdős-Renyi random graphs, i.e. we start with a given vertex set and add edges between two vertices with a fixed probability $p$. If we start with $p = 1$ then we obtain a complete graph and thus $\bar{h} \approx 1/2$, as will be shown in Example 4.1. Now if we decrease $p$ we decrease the number of edges in the graph. This will lead to an increase in the local bipartite subgraph and thus $\bar{h}$ will be increased. If we decrease $p$ further we finally have $|E| \approx |V|$, i.e. the graph will be approximately a tree (we assume that the random graphs are connected) thus $\bar{h} \approx 1$. Thus, for random graphs $\bar{h}$ is a function of $p$. More details are revealed by numerical simulations.

**Proposition 3.1.** For a loopless graph $\Gamma$,

\[
\frac{1}{2} \leq \bar{h}.
\]

**Proof.** If there exists a partition $V_1, V_2$ and $V_3 = \emptyset$ of the vertex set $V$ such that
\[
|E(V_1, V_2)| \geq \max_{i=1,2} |E(V_i, V_1)|
\] (30)

then we can conclude that
\[
\bar{h} \geq \max_{V_1, V_2, V_3 = \emptyset} \frac{2|E(V_1, V_2)|}{2|E(V_1, V_2)| + |E(V_1, V_1)| + |E(V_2, V_2)|} = \frac{1}{2}.
\]

Thus, it is sufficient to find a partition that satisfies (30).

In the sequel we will construct such a partition. Start with an arbitrarily partition $V_1, V_2$ and $V_3 = \emptyset$ of $V$. If (30) is satisfied we are done. Otherwise, assume w.l.o.g. that $|E(V_1, V_1)| > |E(V_1, V_2)|$, i.e.
\[
\sum_{i \in V_1} \sum_{j \in V_1} w_{ij} > \sum_{i \in V_1} \sum_{j \in V_2} w_{ij}.
\]
Thus there exists a vertex \( i \) in \( V_1 \) such that

\[
\sum_{j \in V_1} w_{ij} > \sum_{j \in V_2} w_{ij}.
\]

Remove the vertex \( i \) from \( V_1 \) and add it to \( V_2 \). Thus, \(|E(V_1, V_2)|\) is increased by \( \sum_{j \in V_1} w_{ij} - \sum_{j \in V_2} w_{ij} > 0 \), \(|E(V_1, V_1)|\) is decreased by \( \sum_{j \in V_1} w_{ij} \), and \(|E(V_2, V_2)|\) is increased by \( \sum_{j \in V_2} w_{ij} \). If (30) is still not satisfied, continue this procedure several times. Eventually, (30) holds since \(|E(V_1, V_2)|\) strictly monotonically increases.

From Example 4.1 it follows that for complete graphs \( K_N \), \( \overline{\theta}(K_N) \to \frac{1}{2} \) as \( N \to \infty \). Clearly, the proof of Proposition 3.1 can not be extended to graphs with loops. In fact, Proposition 3.1 only holds for loopless graphs, as can be seen from the example of a graph with \( \sum_i w_{ii} > N - 1 \). In that case, such an estimate would lead to a contradiction of Theorem 3.2 since

\[ 1 \leq 2\overline{\theta} \leq \lambda_{N-1} < 1. \]

The last inequality follows from (18).

We now have a counterpart of the Cheeger inequality (23) and (25).

**Theorem 3.2.** The largest eigenvalue \( \lambda_{N-1} \) of the graph Laplacian \( \Delta \) satisfies

\[ 2\overline{\theta} \leq \lambda_{N-1} \leq 1 + \sqrt{1 - (1 - \overline{\theta})^2}. \]  

(31)

**Proof.** First, we prove that \( 2\overline{\theta} \leq \lambda_{N-1} \). The largest eigenvalue \( \lambda_{N-1} \) of \( \Delta \) is given by \( \langle u, \Delta u \rangle \). Let \( V_1, V_2, V_3 \) be a partition that achieves \( \overline{\theta} \). We consider the following function \( u \):

\[
u(i) = \begin{cases} 
\frac{1}{\text{vol}(V_1)} & \text{if } i \in V_1 \\
\frac{1}{\text{vol}(V_2)} & \text{if } i \in V_2 \\
0 & \text{else.}
\end{cases}
\]

Substituting \( u \) in (13) yields:

\[
\lambda_{N-1} = \sup_{v \neq 0} \frac{(Dv, Dv)_\Gamma}{(v, v)_\Gamma} = \sup_{v \neq 0} \frac{\sum_{e=(i,j)} w_{ij} (v(i) - v(j))^2}{\sum_i d_i v(i)^2} \geq \left( \frac{1}{\text{vol}(V_1)} + \frac{1}{\text{vol}(V_2)} \right)^2 E(V_1, V_2) + \left( \frac{1}{\text{vol}(V_1)} \right)^2 E(V_1, V_3) + \left( \frac{1}{\text{vol}(V_2)} \right)^2 E(V_2, V_3)
\geq \left( \frac{\text{vol}(V_1) + \text{vol}(V_2)}{2\text{vol}(V_1)\text{vol}(V_2)} \right) \frac{2E(V_1, V_2)}{\text{vol}(V_1) + \text{vol}(V_2)} + \frac{\text{min}(\text{vol}(V_1), \text{vol}(V_2))}{\text{max}(\text{vol}(V_1), \text{vol}(V_2))} E(V_1 \cup V_2, V_3)
\geq 2\overline{\theta} + \frac{\text{min}(\text{vol}(V_1), \text{vol}(V_2))}{\text{max}(\text{vol}(V_1), \text{vol}(V_2))} E(V_1 \cup V_2, V_3)
\geq 2\overline{\theta},
\]

where the last inequality follows from (18).
where we used the simple inequality \( \frac{(a+b)^2}{2ab} \geq 2 \) for \( a, b \in \mathbb{R} \).

Now we prove the remaining inequality \( \lambda_{N-1} \leq 1 + \sqrt{1 - (1 - h)^2} \). For technical reasons we consider the operator \( L = I + P \) instead of the graph Laplacian \( \Delta = I - P \). Clearly, if \( \lambda \) is an eigenvalue of \( \Delta \) and corresponding eigenfunction \( u \) then \( u \) is also an eigenfunction for \( L \) and corresponding eigenvalue \( \mu = 2 - \lambda \). Thus, controlling the largest eigenvalue \( \lambda_{N-1} \) of \( \Delta \) from above is equivalent to controlling the smallest eigenvalue \( \mu_0 \) of \( L \) from below. The smallest eigenvalue \( \mu_0 \) of \( L \) is given by

\[
\mu_0 = \inf_{u \neq 0} \frac{\frac{1}{2} \sum_{i,j} w_{ij} (u(i) + u(j))^2}{\sum_{i} d_i u(i)^2}
= \inf_{u \neq 0} \frac{\sum_{e=(i,j) \in E} \mu_{ij} (u(i) + u(j))^2}{\sum_{i} d_i u(i)^2}
\]

where \( \mu_{ij} = w_{ij} \) for all \( i \neq j \) and \( \mu_{ii} = \frac{1}{2} w_{ii} \) for all \( i \in V \). This simply follows from the standard minmax characterization of eigenvalues

\[
\mu_0 = \inf_{u \neq 0} \frac{(Lu, u)}{(u, u)}.
\]

We have for all \( u, v \in \ell^2(\Gamma) \)

\[
(Lu, v) = \sum_i d_i Lu(i)v(i) = \sum_i \sum_j w_{ij} (u(i) + u(j))v(i)
= \sum_j \sum_i w_{ji} (u(j) + u(i))v(j)
\]

where we just exchanged \( i \) and \( j \). Adding the last two lines and setting \( u = v \) yields

\[
(Lu, u) = \frac{1}{2} \sum_{i,j} w_{ij} (u(i) + u(j))^2.
\]

In order to prove the lower bound for \( \mu_0 \) we will use a technique developed in [11]. The idea is the following: Construct a graph \( \Gamma' \) out of \( \Gamma \) s.t. the quantity \( h'(g) \) in Lemma 3.1 for the new graph \( \Gamma' \) can be controlled by the quantity \( 1 - \overline{h} \) of the original graph.

Let \( u \) be an eigenfunction for the eigenvalue \( \mu_0 \) and define as above \( S(u) = \{ i \in V : u(i) > 0 \} \) and \( T(u) = \{ i \in V : u(i) < 0 \} \). Since \( u \) is also an eigenfunction for \( \lambda_{N-1} \) of \( \Delta \) we know that \( (u, 1) = 0 \) and thus \( S(u), T(u) \neq \emptyset \). Then the new graph \( \Gamma' = (V', E') \) is constructed from \( \Gamma \) in the following way. Duplicate all vertices in \( S(u) \cup T(u) \) and denote the copies by a prime, e.g. if \( i \in S(u) \) then the copy of \( i \) is denoted by \( i' \). The copies of \( S(u) \) and \( T(u) \) are denoted by \( S'(u) \) and \( T'(u) \) respectively. The vertex set \( V' \) of \( \Gamma' \) is given by \( V' = V \cup S'(u) \cup T'(u) \). Every edge \( (i, j) \in E(S(u), S(u)) \) in \( \Gamma \) is replaced by two edges \( (i, j') \) and \( (j, i') \) in \( \Gamma' \) s.t. \( w_{ij} = w_{ij'} = w_{ji'} \). The same is done...
with edges in \(E(T(u), T(u))\). All other edges are unchanged, i.e. if \((k, l) \in E \setminus (E(S(u), S(u)) \cup E(T(u), T(u)))\) then \((k, l) \in E'\) and \(w_{kl} = w'_{kl}\).

Consider the function \(g : V' \to \mathbb{R}\),

\[
g(i) = \begin{cases} |u(i)| & \text{if } i \in S(u) \cup T(u) \\ 0 & \text{else.} \end{cases}
\]

It can easily be checked that the construction of \(\Gamma'\) leads to

\[
\mu_0 = \frac{\sum_{e=(i,j) \in E} \mu_{ij}(u(i) + u(j))^2}{\sum_{i \in V} d_i u(i)^2} \geq \frac{\sum_{e'=(i,j) \in E'} w'_{ij}(g(i) - g(j))^2}{\sum_{i \in V'} d_i g(i)^2} \geq 1 - \sqrt{1 - (h'(g))^2}
\]

where we used Lemma 3.1 to obtain the last inequality. For any non-empty subset \(W \subseteq S(g) = S(u) \cup T(u)\) we define \(S_1 = W \cap S(u)\) and \(T_1 = W \cap T(u)\). Let \(\emptyset \neq U \subseteq S(g)\) the subset that realizes the infimum, i.e.

\[
h'(g) = \inf_{\emptyset \neq W \subseteq S(g)} \frac{|E'(W, W)|}{\text{vol}(W)} = \frac{|E'(U, U)|}{\text{vol}(U)}
\]

\[
= \frac{2|E(S_1, S_1)| + 2|E(T_1, T_1)| + |E(S_1 \cup T_1, S_1 \cup T_1)|}{\text{vol}(S_1) + \text{vol}(T_1)} \geq \frac{|E(S_1, S_1)| + |E(T_1, T_1)| + |E(S_1 \cup T_1, S_1 \cup T_1)|}{\text{vol}(S_1) + \text{vol}(T_1)}
\]

\[
= 1 - \frac{2|E(S_1, T_1)|}{\text{vol}(S_1) + \text{vol}(T_1)} \geq 1 - \tilde{h}
\]

Thus we have

\[
2 - \lambda_{N-1} = \mu_0 \geq 1 - \sqrt{1 - (1 - \tilde{h})^2}
\]

and so

\[
\lambda_{N-1} \leq 1 + \sqrt{1 - (1 - \tilde{h})^2}.
\]

For example, the lower estimate for \(\lambda_{N-1}\) in (31) is sharp if \(\Gamma\) is a bipartite (by Theorem 3.1) or if \(\Gamma\) is a complete graph \(K_N\), if \(N\) is even (by Example 4.1). In both examples the partition that achieves \(\tilde{h}\) satisfies \(V_3 = \emptyset\). In fact, the proof of Theorem 3.2 shows that the estimate (31) can only be sharp if \(V_3 = \emptyset\). However, if the volume of \(V_3\) is sufficiently large, we can improve the estimate given in (31) and estimate the eigenvalue \(\lambda_{N-1}\) from below by using both the Cheeger constant \(h\) and its dual \(\tilde{h}\).
Corollary 3.1. Assume that $V_1, V_2$ and $V_3$ is a partition of $V$ that achieves $\overline{h}$. If
$$\text{vol}(V_1 \cup V_2) \leq \text{vol}(V_3),$$
then
$$\lambda_{N-1} \geq 2\overline{h} + \mathcal{R}(V_1, V_2) h,$$
where we define for the partition $V_1, V_2, V_3$ of the vertex set $V$
$$\mathcal{R}(V_1, V_2) := \frac{\text{min}(\text{vol}(V_1), \text{vol}(V_2))}{\text{max}(\text{vol}(V_1), \text{vol}(V_2))}.$$
(32)

Proof. The proof of Theorem 3.2 shows that
$$\lambda_{N-1} \geq \frac{2\overline{h} + \mathcal{R}(V_1, V_2) |E(V_1 \cup V_2, V_3)|}{\text{vol}(V_1) + \text{vol}(V_2)} \geq 2\overline{h} + \mathcal{R}(V_1, V_2) h$$

Corollary 3.2. Let $u$ be the eigenfunction for the largest eigenvalue of $\Delta$. If the eigenfunction is sufficiently localized, i.e.
$$\sum_{i: u(i) \neq 0} d_i = \text{vol}(S(u) \cup T(u)) \leq \text{vol}(S(u) \cup \overline{T(u)}) = \sum_{i: u(i) = 0} d_i$$
where $S(u)$ and $T(u)$ are defined as above then
$$\lambda_{N-1} \leq 1 + \sqrt{1 - h^2}.$$ 

Proof. Again we consider the smallest eigenvalue $\mu_0$ of the operator $L = I + P$. Since $u$ is an eigenfunction for the eigenvalue $\mu_0$ we have
$$\mu_0 = \frac{\sum_{e=(i,j)} \mu_{ij} (u(i) + u(j))^2}{\sum_i d_i u(i)^2} \geq \frac{\sum_{e=(i,j)} w_{ij} |u(i)| - |u(j)|^2}{\sum_i d_i |u(i)|^2} \geq 1 - \sqrt{1 - h^2(|u|)}$$
where we used the triangle inequality and Lemma 3.1. Since $\text{vol}(S(u) \cup T(u)) \leq \text{vol}(S(u) \cup \overline{T(u)})$ we have $h(|u|) \geq \overline{h}$ and thus
$$2 - \lambda_{N-1} = \mu_0 \geq 1 - \sqrt{1 - h^2}.$$
Proposition 3.2. Let \( u \) be a normalized eigenfunction for the largest eigenvalue of \( \Delta \), s.t. \( \max_i |u(i)| = 1 \) then
\[
\lambda_{N-1} \leq 2 - \frac{\min_{i,j} w_{ij} (1 - \min_i |u(i)|)^2}{D \ vol(V)}
\]
where \( D \) is the diameter of the graph. In particular, if there exists a vertex \( i \) such that \( u(i) = 0 \) then
\[
\lambda_{N-1} \leq 2 - \frac{\min_{i,j} w_{ij}}{D \ vol(V)}.
\]

Proof. Again, we consider the smallest eigenvalue \( \mu_0 \) of \( L = I + P \) instead of the largest eigenvalue \( \lambda_{N-1} \) of \( \Delta \). Let \( i_k, k = 1, \ldots, n \) be the shortest path connecting the vertices that satisfy \( \max_i |u(i)| = |u(i_1)| = 1 \) and \( \min_i |u(i)| = |u(i_n)| \). Then
\[
\mu_0 = \frac{\sum_{e=(i,j)} \mu_{ij} (u(i) + u(j))^2}{\sum_i d_i |u(i)|^2} \geq \frac{\sum_{e=(i,j)} w_{ij} ||u(i)| - |u(j)||^2}{\sum_i d_i |u(i)|^2} \geq \frac{\min_{i,j} w_{ij} \sum_{k=1}^n (|u(i_k)| - |u(i_{k+1})|)^2}{\vol(V)} \geq \frac{\min_{i,j} w_{ij} (\sum_{k=1}^n |u(i_k)| - |u(i_{k+1})|)^2}{n \vol(V)} \geq \frac{\min_{i,j} w_{ij} (1 - \min_i |u(i)|)^2}{D \ vol(V)}
\]
where we used the Cauchy-Schwarz inequality and the fact that the length of a shortest path connecting any two vertices is less or equal to \( D \). Since \( 2 - \lambda_{N-1} = \mu_0 \) the proof is complete. 

In particular, the estimate in Proposition 3.2 is sharp for bipartite graphs. Let \( u_{N-1} \) be the eigenfunction for the largest eigenvalue \( \lambda_{N-1} \). If \( |u_{N-1}(i)| \) is not constant for all \( i \) then Proposition 3.2 always yields non-trivial estimates. This should hold for all graphs that are not bipartite.

Jerrum and Sinclair have shown how one can bound the Cheeger constant \( h \) by using canonical paths [22, 23]. Similarly, we can derive a upper bound for the dual Cheeger constant \( \bar{h} \) by considering a suitable collection of paths. Let \( \sigma_i \) be a path from vertex \( i \) to vertex \( i \) with an odd number of edges and let \( \Sigma \) be the collection of all paths (one for each vertex).

Theorem 3.3. We have
\[
\bar{h} \leq 1 - \frac{1}{\xi},
\]
where
\[
\xi := \max_{e=(k,l)} \frac{1}{w_{kl}} \sum_{i: \sigma: e=(k,l)} d_i.
\]
The sum is over all \( i \) for which the path \( \sigma_i \) contains the edge \( e = (k, l) \).

**Proof.** For simplicity we define the subset \( \Omega \subset E \) as \( \Omega := E(V_1, V_1) \cup E(V_1, V_3) \cup E(V_2, V_2) \cup E(V_2, V_3) \). Now observe that any path \( \sigma_i \) with an odd number of edges contains at least one edge in \( \Omega \). Thus we have for any partition \( V_1, V_2, V_3 \) of the vertex set \( V \)

\[
\text{vol}(V_1) + \text{vol}(V_2) = \sum_{i \in V_1 \cup V_2} d_i \\
\leq \sum_{e=(k,l) \in \Omega \cap \sigma_i} \sum_{i \in V_1 \cup V_2} d_i \\
\leq \sum_{e=(k,l) \in \Omega} \sum_{i \in V_1 \cup V_2} \frac{w_{kl}}{w_{kl}} d_i \\
\leq \xi \sum_{e=(k,l) \in \Omega} w_{kl} \leq \xi |\Omega|.
\]

Since this holds for all partitions, we have for the partition \( V_1, V_2 \) and \( V_3 \) that achieves \( \overline{h} \)

\[
1 - \overline{h} = \frac{|\Omega|}{\text{vol}(V_1) + \text{vol}(V_2)} \geq \frac{1}{\xi}.
\]

\[\square\]

**Corollary 3.3.**

\[
\xi \leq d_\Gamma w_\Gamma b_\Gamma,
\]

where \( d_\Gamma = \max_i d_i \), \( w_\Gamma = \frac{1}{\min_{i,j} w_{ij}} \) and \( b_\Gamma = \max_e \# \{ \sigma \in \Sigma : e \in \sigma \} \) and thus,

\[
\lambda_{N-1} \leq 1 + \sqrt{1 - \left( \frac{1}{d_\Gamma w_\Gamma b_\Gamma} \right)^2}.
\]  \hspace{1cm} (34)

**Remark.** Diaconis and Stroock show in [12], by using a discrete analog of the Poincare inequality, that the largest eigenvalue satisfies

\[
\lambda_{N-1} \leq 2 - \frac{2}{d_\Gamma w_\Gamma b_\Gamma \sigma_\Gamma}
\]  \hspace{1cm} (35)

where \( \sigma_\Gamma \) is the maximum number of edges in any \( \sigma \in \Sigma \). Thus, the estimate (34) obtained from the dual Cheeger inequality is better that the estimate (35) obtained from the Poincare inequality iff

\[
d_\Gamma w_\Gamma b_\Gamma < \frac{1}{\sigma_\Gamma} + \frac{\sigma_\Gamma}{4}.
\]

In general, it is not clear which of these estimates is better.
4 Relations between \( h \) and \( \overline{h} \)

By looking at the definitions of \( h \) and \( \overline{h} \) it is apparent that there is a connection between those two quantities. We shall explore this now in more detail.

Similarly to (33) we define:

**Definition 4.1.** For any partition \( U, \overline{U} \) of the vertex set \( V \) we define

\[
\mathcal{R}(U) := \frac{\min(\text{vol}(U), \text{vol}(\overline{U}))}{\max(\text{vol}(U), \text{vol}(\overline{U}))}.
\]

Furthermore,

\[
\mathcal{R} := \max_{U} \mathcal{R}(U).
\]

First, we will restrict ourselves to unweighted graphs. Later on we will prove similar results for weighted graphs.

4.1 Unweighted graphs

**Lemma 4.1.** Let \( \Gamma \) be an unweighted graph with \( N \) vertices, then

\[
\frac{N - 1}{N + 1} \leq \mathcal{R} \leq 1.
\]

Equality holds on the left hand side if and only if \( \Gamma \) is a regular graph and \( N \) is odd.

**Proof.** Order the vertices w.r.t. their degree, i.e. \( d_1 \geq d_2 \geq \ldots \geq d_N \). We construct a partition \( U, \overline{U} \) of \( V \) that satisfies \( \frac{N - 1}{N + 1} \leq \mathcal{R}(U) \). We begin with two empty sets \( U_0, \overline{U}_0 \). After the partition of \( K \) vertices we denote the subsets by \( U_K, \overline{U}_K \). Having started with vertex 1 as one of largest degree, we iteratively partition the vertices into two subsets such that vertex \( K + 1 \) is then added to the subset \( U_K, \overline{U}_K \) that has the smaller volume. We continue this procedure until we obtain a complete partition \( U, \overline{U} := U_N, \overline{U}_N \) of the graph. Let \( M \leq N \) be such that

\[
\text{vol}(U_{M-1}) \geq \text{vol}(\overline{U}_{M-1})
\]

and

\[
\text{vol}(\overline{U}_K) \geq \text{vol}(U_K)\quad \text{for } M \leq K \leq N.
\]

For simplicity we define

\[
\text{vol}(U_K) + \text{vol}(\overline{U}_K) =: \text{vol}(V_K)\quad \text{for } 1 \leq K \leq N.
\]

Then we have

\[
\text{vol}(\overline{U}_M) - \text{vol}(U_M) \leq d_M \leq \frac{\text{vol}(U_M) + \text{vol}(\overline{U}_M)}{M} = \frac{\text{vol}(V_M)}{M}. \]
Equality holds on the left hand side if and only if \( \text{vol}(U_{M-1}) = \text{vol}(\overline{U}_{M-1}) \) and equality holds on the right hand side if and only if \( d_1 = d_2 = \ldots = d_M \). For the final partition \( U_N, \overline{U}_N \) we obtain

\[
\text{vol}(\overline{U}_N) - \text{vol}(U_N) = \text{vol}(\overline{U}_M) - (\text{vol}(U_M) + \text{vol}(V_N) - \text{vol}(V_M)) \\
\leq \frac{\text{vol}(V_M)}{M} - \text{vol}(V_N) + \text{vol}(V_M) \\
\leq \frac{\text{vol}(V_N)}{N}.
\]

The last inequality follows from

\[
\frac{\text{vol}(V_N)}{N} + \text{vol}(V_N) - \text{vol}(V_M) - \frac{\text{vol}(V_M)}{M} \\
= \frac{1}{NM} [M(1+N)\text{vol}(V_N) - N(1+M)\text{vol}(V_M)] \\
= \frac{1}{NM} [M(1+N)(\text{vol}(V_N) - \text{vol}(V_M)) + (M - N)\text{vol}(V_M)] \\
\geq \frac{1}{NM} [M(1+N)(N-M) + (M - N)MN] \\
= \frac{(N-M)}{N} \geq 0
\]

Thus, we constructed a partition that satisfies

\[
\max(\text{vol}(U_N), \text{vol}(\overline{U}_N)) - \min(\text{vol}(U_N), \text{vol}(\overline{U}_N)) \leq \frac{\text{vol}(V_N)}{N}.
\]

Since

\[
\frac{\text{vol}(V_N)}{N} = \frac{\max(\text{vol}(U_N), \text{vol}(\overline{U}_N)) + \min(\text{vol}(U_N), \text{vol}(\overline{U}_N))}{N},
\]

this yields

\[
\frac{N-1}{N+1} \leq \mathcal{R}(U) \leq \mathcal{R}.
\]

From the proof we see that equality holds iff \( N = M \), the graph is regular, and \( \text{vol}(U_{M-1}) = \text{vol}(\overline{U}_{M-1}) \). Thus, equality holds iff \( \Gamma \) is regular and \( N \) is odd. \( \square \)

The last lemma shows that for large graphs, i.e. \( N \) large, it is always possible to partition \( V \) into two subsets of almost equal volume.

**Corollary 4.1.** In particular we have for unweighted graphs,

\[
\frac{1}{2} \leq \mathcal{R} \leq 1
\]

and equality holds on the left hand side iff \( \Gamma \) is a triangle.
Proof. The proof follows from Lemma 4.1 since there exists only one connected graph on 2 vertices for which we have $R = 1$ and the only regular graph on 3 vertices is the triangle. □

Theorem 4.1. For unweighted graphs we have

$$\frac{N - 1}{N} h \leq \frac{2R}{1 + R} h \leq \overline{h} \leq 1. \quad (40)$$

Equality holds on the l.h.s. iff $\Gamma$ is a regular graph and $N$ is odd.

Proof. By (26),

$$h \leq \frac{|E(U, \overline{U})|}{\min(\text{vol}(U), \text{vol}(\overline{U}))}. \quad (41)$$

For the partition $V_1 = U$, $V_2 = \overline{U}$ and $V_3 = \emptyset$ we obtain

$$\overline{h} \geq \frac{2|E(U, \overline{U})|}{\text{vol}(U) + \text{vol}(\overline{U})}. \quad (42)$$

Since this holds for all partitions $U, \overline{U}$, we get

$$h \leq \overline{h} \frac{\text{vol}(U) + \text{vol}(\overline{U})}{2\min(\text{vol}(U), \text{vol}(\overline{U}))} = \overline{h} \left( \frac{1}{2} + \frac{1}{2R} \right) \leq \overline{h} \frac{N}{N - 1}$$

where we used Lemma 4.1. The remaining inequality follow from Theorem 3.1. □

Corollary 4.2. Let $\Gamma$ be an unweighted graph. If there exists a partition $U, \overline{U}$ of the vertex set $V$ such that $\text{vol}(U) = \text{vol}(\overline{U})$ then

$$h \leq \overline{h} \leq 1. \quad (43)$$

If $\Gamma = K_2$, we even have equality in (43), i.e. $h = \overline{h} = 1$. Note that, in general there does not exist a partition $U, \overline{U}$ of $V$ such that $\text{vol}(U) = \text{vol}(\overline{U})$. Some counterexamples are regular graphs if $N$ is odd and so-called wheel graphs $W_N$ with $N$ vertices and degree sequence $\pi = \{N - 1, 3, \ldots, 3\}$ if $N - 1$ is not a multiple of 3.

Example 4.1. For a complete graph $K_N$ on $N$ vertices we have

$$h = \begin{cases} \frac{N}{2(N + 1)} & N \text{ even} \\ \frac{N}{2(N - 1)} & N \text{ odd} \end{cases} \quad (44)$$

and

$$\overline{h} = \begin{cases} \frac{N}{2(N - 1)} & N \text{ even} \\ \frac{N}{2(N + 1)} & N \text{ odd} \end{cases} \quad (45)$$
Figure 1: For sufficiently small weights $c$ this graph shows that Lemma 4.1 cannot hold for weighted graphs.

Using Theorem 4.1, Corollary 4.2 and (45) we obtain the following upper bound for $h$ in terms of $\frac{1}{N}$:

$$h \leq \begin{cases} \frac{N}{N-1} \frac{1}{N} & N \text{ even} \\ \frac{2(N+1)}{2(N+1)} & N \text{ odd} \end{cases}$$

(46)

Thus, the upper bound is sharp for complete graphs. From

$$\lambda_1 \leq 2h \leq \begin{cases} \frac{2N}{N+1} & N \text{ even} \\ \frac{N}{N+1} & N \text{ odd} \end{cases}$$

and (45) we obtain

$$\lambda_1 \leq \begin{cases} \frac{N}{N+1} & N \text{ even} \\ \frac{(N+1)(N-1)}{(N-1)} & N \text{ odd} \end{cases}$$

(47)

This shows that the estimate is sharp if $N$ is even and almost sharp if $N$ is odd and large. Clearly, we can also use $h$ in order to bound $\frac{1}{N}$ from below. Applying Theorem 3.2 then yields a lower bound for the largest eigenvalue from below in terms of $h$.

### 4.2 Weighted graphs

Lemma 4.1 does not hold for weighted graphs. This can be seen by considering sufficiently small weights $c$ in figure 1. In particular, it turns out that inequality (39) does not hold for weighted graphs. However, we have the following result for weighted graphs.

**Lemma 4.2.** Let $\Gamma$ be a weighted graph with $N$ vertices and let $M \leq N$ be defined as in (37), then

$$\frac{M-1}{M+1} \leq R \leq 1.$$  

(48)

**Proof.** Using the notation from the proof of Lemma 4.1 we conclude from (38):

$$\text{vol}(U_N) - \text{vol}(U_M) = \text{vol}(U_M) - \text{vol}(U_M)$$

$$\leq \frac{\text{vol}(U_M) + \text{vol}(U_M)}{M}$$

$$= \frac{\text{vol}(U_M) + \text{vol}(U_N)}{M}$$
This implies
\[
\frac{M - 1}{M + 1} \leq \frac{\text{vol}(U_M)}{\text{vol}(U_N)} \leq \frac{\text{vol}(U_N)}{\text{vol}(\overline{U_N})} \leq R.
\]

Note that figure 1 does not contradict Lemma 4.2 for all \( c > 0 \). Similarly to Theorem 4.1, we obtain for weighted graphs:

**Theorem 4.2.** Let \( \Gamma \) be a weighted graph and let \( M \) be defined as in (37), then
\[
\frac{M - 1}{M} h \leq \frac{2R}{1 + R} h \leq h \leq \bar{h} \leq 1.
\]

(49)

### 5 Neighborhood graphs

A common concept in spectral graph theory is to use geometric properties of the underlying graph in order to control the eigenvalues of the graph Laplacian. A well-known example is the Cheeger inequality (23) and (24) that controls the smallest nonzero eigenvalue. Similarly, we can control the largest eigenvalue of the graph Laplacian by geometric properties of the underlying graph, see Theorem 3.2 and Theorem 8.1.

In the sequel, we shall use a new, conceptually different approach in order to control the eigenvalues of the graph Laplacian. Instead of using the properties of \( \Gamma \) itself, we shall use the geometric properties of the neighborhood graph \( \Gamma[l] \), to be defined shortly, in order to control the eigenvalues of \( \Delta \) on \( \Gamma \).

As a motivation, consider the following result for infinite graphs [13, 17]:

**Theorem 5.1.** If \( \Gamma \) is an infinite graph, then
\[
1 - \sqrt{1 - \alpha^2(\Gamma)} \leq \inf \text{spec}(\Delta) \leq \sup \text{spec}(\Delta) \leq 1 + \sqrt{1 - \alpha^2(\Gamma)},
\]

(50)

where
\[
\alpha(\Gamma) = \inf_{W \subseteq V, |W| < \infty} \frac{E(W, \overline{W})}{\text{vol}(W)}
\]

(51)

is a version of the Cheeger constant for an infinite graph.

Thus, for infinite graphs, it is possible to control the supremum and the infimum of \( \text{spec}(\Delta) \) by the Cheeger constant \( \alpha(\Gamma) \). Clearly, this estimate is not useful for finite graphs as \( \alpha(\Gamma) = 0 \) in that case, because we may then simply take \( W = V \). However, if the eigenfunction that corresponds to the largest eigenvalue is sufficiently localized then we can prove a similar result, see Corollary 5.2. The point here is that \( \inf \text{spec}(\Delta) = \lambda_0 = 0 \) for finite graphs, but not necessarily for infinite graphs, and this is the content of the lower bound in Theorem 5.1 in qualitative terms. It is remarkable that the constant \( \alpha(\Gamma) \) at the same time may also yield a nontrivial upper spectral bound for an infinite graph.

We shall show (Corollary 5.1) in this section that it is possible to control the
maximal and the smallest nonzero eigenvalue of a finite graph in a similar way as in [10], if we use the Cheeger constant $h[l]$ of the neighborhood graph $\Gamma[l]$, if $l$ is even, instead of the Cheeger constant $h$ of the graph $\Gamma$ itself. These new lower bounds for the second smallest eigenvalue can improve the Cheeger estimate [25]; for a discussion and examples see the next section.

**Definition 5.1.** For a graph $\Gamma = (V,E)$ its neighborhood graph $\Gamma[l] = (V,E[l])$ of order $l \geq 1$ is the graph with the same vertex set $V$ and its edge set $E[l]$ is defined in the following way: The weight $w_{ij}[l]$ of the edge $c[l] = (i,j)$ in $\Gamma[l]$ is given by

$$w_{ij}[l] = \frac{1}{d_{k_1} \cdots d_{k_{l-1}}} w_{ik_1 k_2 \cdots k_{l-1} j}$$

if $l > 1$ and we set $w_{ij}[l] = w_{ij}$ if $l = 1$, i.e. $\Gamma[1] = \Gamma$. In particular, $i$ and $j$ are neighbors in $\Gamma[l]$ if there exists at least one path of length $l$ between $i$ and $j$ in $\Gamma$.

In order to become familiar with the concept of neighborhood graphs we consider the following examples:

**Example 5.1.** Consider the family of graphs in Figure 2 for $c \geq 0$. The weighted adjacency matrix $W$ of the graph in Figure 2 is given by

$$W = W[1] = \begin{pmatrix} 1 & c \\ c & 1 \end{pmatrix}.$$ 

If we go to higher order neighborhood graphs $\Gamma[l]$ of $\Gamma$, the topological structure remains the same and the weighted adjacency matrix $W[l]$, $l = 2, 3, 4, 5$, is given by

$$W[2] = \begin{pmatrix} \frac{2+4c}{2+c} & \frac{2c}{1+c} \\ \frac{2c}{1+c} & \frac{1+4c}{1+c} \end{pmatrix}, \quad W[3] = \begin{pmatrix} \frac{c^3+3c}{(1+c)^3} & \frac{3c^2+1}{(1+c)^2} \\ \frac{3c^2+1}{(1+c)^2} & \frac{c^3+3c}{(1+c)^3} \end{pmatrix},$$

$$W[4] = \begin{pmatrix} \frac{(c^2+1)^2+4c^2}{(1+c)^4} & \frac{c^3+4c^2}{(1+c)^3} \\ \frac{c^3+4c^2}{(1+c)^3} & \frac{(c^2+1)^2+4c^2}{(1+c)^4} \end{pmatrix}, \quad W[5] = \begin{pmatrix} \frac{c(5+10c^2+c^4)}{(1+c)^5} & \frac{1+10c^2+c^4}{(1+c)^4} \\ \frac{1+10c^2+c^4}{(1+c)^4} & \frac{(5+10c^2+c^4)}{(1+c)^5} \end{pmatrix}.$$

**Example 5.2.** As a second example we consider the family of graphs in Figure 3. We have

$$W = W[1] = \begin{pmatrix} 0 & c & c & 0 & 0 \\ c & 0 & c & 0 & 0 \\ c & c & 0 & 1 & 0 \\ 0 & 0 & 1 & c & c \\ 0 & 0 & 0 & c & 0 \\ 0 & 0 & 0 & c & 0 \end{pmatrix},$$

$$W[2] = \begin{pmatrix} c/2 + c^2/a & c^2/a & c/2 & c/a & 0 & 0 \\ c^2/a & c/2 + c^2/a & c/2 & c/a & 0 & 0 \\ c/2 & c/2 & 1/a + c & 0 & c/a & c/a \\ c/a & c/a & 0 & 1/a + c & c/2 & c/2 \\ 0 & 0 & c/a & c/2 & c/2 + c^2/a & c^2/a \\ 0 & 0 & c/a & c/2 & c^2/a & c/2 + c^2/a \end{pmatrix}.$$
where \( a := 1 + 2c \).

The neighborhood graphs \( \Gamma[l] \) have the following properties:

**Lemma 5.1.**

(i) \( d_i = d_i[l] \) for all \( i \in V \) and \( l \geq 1 \).

(ii) If \( \Gamma \) is connected and \( l \) is even, then \( \Gamma[l] \) consists of exactly two connected components iff \( \Gamma \) is bipartite.

(iii) If \( l \) is odd, then \( \Gamma[l] \) is bipartite iff \( \Gamma \) is bipartite. Furthermore, \( \Gamma[l] \) has the same number of connected components as \( \Gamma \). In particular, \( \Gamma[l] \) is connected iff \( \Gamma \) is connected.

**Proof.**

(i). We have

\[
\begin{align*}
d_i[l] &= \sum_j w_{ij}[l] = \sum_{k_1, \ldots, k_l-1} \frac{1}{d_{k_1}} \cdots \frac{1}{d_{k_l-1}} w_{ik_1} w_{k_1 k_2} \cdots w_{k_l-2 k_l-1} \sum_j w_{k_l-1 j} \\
&= \sum_{k_1, \ldots, k_l-2} \frac{1}{d_{k_1}} \cdots \frac{1}{d_{k_l-2}} w_{ik_1} w_{k_1 k_2} \cdots \sum_{k_{l-1}} w_{k_l-2 k_{l-1}} \\
&\vdots \\
&= \sum_{k_1} w_{ik_1} = d_i
\end{align*}
\]

(ii). From Theorem 5.2 we conclude that the eigenvalues \( \lambda[l][k] \) of \( \Delta[l] \) are given by \( \lambda[l][k] = 1 - (1 - \lambda_k)^l \) where \( \lambda_k \) are the eigenvalues of \( \Delta \). Thus, if \( l \) is even, \( \lambda_k[l] = 0 \) iff \( \lambda_k = 0 \) or \( \lambda_k = 2 \). Recall that the multiplicity of the zero eigenvalue is equal to the number of connected components of a graph and 2 is an eigenvalue iff the graph is bipartite. If \( \Gamma \) is connected, bipartite, and \( l \) is even, then \( \lambda[l] = 0 \) is twice in the spectrum of \( \Delta[l] \) since \( \lambda_0 = 0 \) and \( \lambda_{N-1} = 2 \) are in the spectrum of \( \Delta \). Consequently, \( \Gamma[l] \) consists of exactly two connected components. On the other hand if \( \Gamma[l] \) consists of exactly two connected components, \( \lambda[l] = 0 \) is
twice in the spectrum of $\Delta[l]$, and we know that either the eigenvalue $\lambda = 0$ is twice in the spectrum of $\Delta$ or $\lambda = 0$ and $\lambda = 2$ are both in the spectrum of $\Delta$. Since we assume that $\Gamma$ is connected, $\lambda = 0$ is a simple eigenvalue, and thus we can conclude that $2 \in \text{spec}(\Delta)$ and $\Gamma$ is bipartite.

(iii). If $l$ is odd, we observe that $0$ (respectively $2$) is an eigenvalue of $\Delta$ iff $0$ (respectively $2$) is an eigenvalue of $\Delta[l]$.

Remark. Lemma 5.1 (i) implies that $(\cdot, \cdot)_\Gamma = (\cdot, \cdot)_{\Gamma[l]}$ and thus $\ell^2(\Gamma) = \ell^2(\Gamma[l])$, as will be frequently utilized below. Lemma 5.1 (ii) indicates that, if $l$ is even, there exists a relationship between the smallest non-zero eigenvalue of $\Gamma[l]$ and the largest eigenvalue of $\Gamma$. This will be made more precise in the next Theorem. However, based on Lemma 5.1 (ii) we can already expect that, if $l$ is even, a lower bound for $\lambda_1[l]$ can also be used to derive an upper bound for $\lambda_{N-1}$ if $l$ is even. Theorem 5.3 will show that this is indeed the case.

Theorem 5.2. For any function $u \in \ell^2(\Gamma)$ we have

$$(I - (I - \Delta)^l)u = (I - P^l)u = \Delta[l]u,$$

where $P$ is the transition probability operator of $\Gamma$ and $\Delta[l]$ is the graph Laplacian on $\Gamma[l]$.

Proof. For any function $u \in \ell^2(\Gamma)$ we have

$$(I - P^l)u(i) = u(i) - \sum_j q_{ij}u(j),$$

where $q_{ij} := \sum_{k_1, \ldots, k_{l-1}} \frac{w_{ik_1}}{d_i} \cdots \frac{w_{k_{l-1}j}}{d_{k_{l-1}}} = ij$-th entry of $P^l$. Thus,

$$(I - P^l)u(i) = u(i) - \sum_j \sum_{k_1, \ldots, k_{l-1}} \frac{w_{ik_1}}{d_i} \cdots \frac{w_{k_{l-1}j}}{d_{k_{l-1}}} u(j).$$

Using the definition $w_{ij}[l] = \sum_{k_1, \ldots, k_{l-1}} \frac{1}{d_{k_1}} \cdots \frac{1}{d_{k_{l-1}}} w_{ik_1}w_{k_1k_2} \cdots w_{k_{l-1}j}$ and $d_i = d_i[l]$, this yields

$$(I - P^l)u(i) = \frac{1}{d_i[l]} \sum_j w_{ij}[l](u(i) - u(j)) = \Delta[l]u(i).$$

We note that $\Delta[l]$ is the operator that underlies random walks on graphs with stepsize $l$.

Lemma 5.2. Let $\Gamma$ be a graph and $\Gamma[l]$ its neighborhood graph of order $l$.

(i) The multiplicity $m_1$ of the eigenvalue one is an invariant for all neighborhood graphs, i.e. $m_1(\Delta) = m_1(\Delta[l])$ for all $l \geq 1$.  

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(ii) The eigenvalues of $\Delta[l]$ satisfy

$$0 = \lambda_1[l] \leq \ldots \lambda_{N-1}[l] \leq 1$$

if $l$ is even and

$$0 = \lambda_1[l] \leq \ldots \lambda_{N-1}[l] \leq 2$$

if $l$ is odd.

(iii) If $\lambda \neq 0,2$ then $\lambda[l] = 1 - (1 - \lambda)^l \to 1$ as $l \to \infty$.

Proof. $\Gamma$ and $\Gamma[l]$ have the same vertex set, thus both $\Delta$ and $\Delta[l] = (I - (I - \Delta)^l)$ have $N = |V|$ eigenvalues. Every eigenfunction $u_k$ for $\Delta$ and eigenvalue $\lambda_k$ is also an eigenfunction for $\Delta[l]$ and eigenvalue $1 - (1 - \lambda_k)^l$. (i). This follows from the observation that $1 - (1 - \lambda_k)^l = 1$ iff $\lambda_k = 1$. (ii). This holds since all eigenvalues $\lambda_k$ of $\Delta$ satisfy $\lambda_k \in [0,2]$ and thus $1 - (1 - \lambda_k)^l \in [0,1]$ if $l$ is even and $1 - (1 - \lambda_k)^l \in [0,2]$ if $l$ is odd. (iii). If $\lambda \neq 0,2$ is an eigenvalue of $\Delta$ then the corresponding eigenvalue $\mu$ of the transition probability matrix $P$ satisfies $|\mu| < 1$. Since $\Delta[l] = I - P^l$ we have $\lambda[l] = 1 - (1 - \lambda)^l = 1 - \mu^l \to 1$ as $l \to \infty$.

Remark. For $l$ even, all eigenvalues are less or equal to 1 and thus in particular $\lambda_{N-1} \leq 1$. From (19) we observe that this is only possible because $\Gamma[l]$, $l$ even, contains many (in fact $N$) loops. In contrast, for loopless graphs we have $1 < \frac{N}{N-1} \leq \lambda_{N-1}$.

Using Theorem 5.2 we can derive bounds for the eigenvalues of $\Delta$ on $\Gamma$ by using geometric properties of its neighborhood graphs $\Gamma[l]$.

**Theorem 5.3.** Let $\mathcal{A}[l]$ be a lower bound for the eigenvalue $\lambda_1[l]$ of $\Delta[l]$, i.e. $\mathcal{A}[l] \leq \lambda_1[l]$. Then,

$$1 - (1 - \mathcal{A}[l])^* \leq \lambda_1 \leq \ldots \leq \lambda_{N-1} \leq 1 + (1 - \mathcal{A}[l])^*,$$

(53)

if $l$ is even and

$$1 - (1 - \mathcal{A}[l])^* \leq \lambda_1$$

(54)

if $l$ is odd.

Proof. Let $u_k$, $k \neq 0$ be an eigenfunction of $\Delta$. Using (52) we obtain

$$1 - (1 - \lambda_k)^l = \frac{(u_k, (I - (I - \Delta)^l) u_k)_{\Gamma}}{(u_k, u_k)_{\Gamma}} = \frac{(u_k, \Delta[l] u_k)_{\Gamma[l]}}{(u_k, u_k)_{\Gamma[l]}} \geq \inf_{u \perp 1} \frac{(u, \Delta[l] u)_{\Gamma[l]}}{(u, u)_{\Gamma[l]}} = \lambda_1[l] \geq \mathcal{A}[l],$$

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since \( u_k \perp 1 \) w.r.t. \( (\cdot, \cdot)_\Gamma \) iff \( u_k \perp 1 \) w.r.t. \( (\cdot, \cdot)_{\Gamma[l]} \). Alternatively, since the eigenvalues of \( \Delta[l] \) are given by \( 1 - (1 - \lambda_k)^l \) if \( \lambda_k \) are the eigenvalues of \( \Delta \) we have

\[
1 - (1 - \lambda_k)^l \geq \min_{k \neq 0} 1 - (1 - \lambda_k)^l = \lambda_1[l] \geq A[l].
\]

This implies that for all \( k \neq 0 \)

\[
|1 - \lambda_k| \leq (1 - A[l])^{\frac{1}{l}}
\]

if \( l \) is even and

\[
1 - \lambda_k \leq (1 - A[l])^{\frac{1}{l}}
\]

if \( l \) is odd.

As a concrete example we use the Cheeger inequality \( (25) \), i.e. \( A[l] = 1 - \sqrt{1 - h^2[l]} \leq \lambda_1[l] \).

**Corollary 5.1.** All eigenvalues of \( \Delta(\Gamma) \) satisfy

\[
1 - (1 - h^2[l])^{\frac{1}{2l}} \leq \lambda_1 \leq \ldots \leq \lambda_{N-1} \leq 1 + (1 - h^2[l])^{\frac{1}{2l}}.
\]

(55)

if \( l \) is even and

\[
1 - (1 - h^2[l])^{\frac{1}{2l}} \leq \lambda_{N-1}
\]

(56)

if \( l \) is odd.

**Remark.** We remark here that some graph properties, e.g. the discrepancy and the expansion property of a graph, can be controlled by the quantity \( \rho = \max_{k \neq 0} |1 - \lambda_k| \). Consequently, Corollary 5.1 or more generally Theorem 5.3 can be used to derive explicit bounds for those quantities. As one particular application, we show in section 9 how Corollary 5.1 can be used to estimate the convergence of random walks on graphs.

**Remark.** For bipartite graphs \( \Gamma \) we have \( \lambda_{N-1} = 2 \). If \( l \) is even, then at the same time \( h[l] = 0 \) since by Lemma 5.1 the neighborhood graph \( \Gamma[l] \) of a bipartite graph is disconnected. Thus, for bipartite graphs the upper bound in \( (55) \) is sharp. On the other hand, if \( l \) is even and \( \Gamma \) is not bipartite or if \( l \) is odd then the lower bound in Corollary 5.1 yields only the trivial estimate \( 0 \leq \lambda_1 \). In contrast, if \( l \) is even and \( \Gamma \) is not bipartite or if \( l \) is odd then Corollary 5.1 always yields a non-trivial lower bound \( 0 < 1 - (1 - h^2[l])^{\frac{1}{2l}} \leq \lambda_1 \) for the second smallest eigenvalue. These new lower bounds for \( \lambda_1 \) can actually improve the Cheeger estimate \( (25) \). A more elaborate discussion of this issue, and two examples, are given in the next section.

**Theorem 5.4.** Let \( B[l] \) be any upper bound for \( \lambda_1[l] \), i.e. \( \lambda_1[l] \leq B[l] \). Then we have

\[
\lambda_1 \leq 1 - (1 - B[l])^{\frac{1}{l}}
\]

(57)

or

\[
\lambda_{N-1} \geq 1 + (1 - B[l])^{\frac{1}{l}}
\]

(58)
if $l$ is even and
\[ \lambda_1 \leq 1 - (1 - B[l])^\dagger \]
if $l$ is odd.

Proof. First note that, by Lemma 5.2, (57) and (58) are well defined, if $l$ is even, since we can assume w.l.o.g. that $B[l] \leq 1$. Using (52) we obtain $B[l] \geq \lambda_1[l] = \min_{k \neq 0} 1 - (1 - \lambda_k)^l$. This implies that for at least one eigenvalue $\lambda_i$, $i \neq 0$ we have
\[ (1 - B[l])^\dagger \leq |1 - \lambda_i| \]
if $l$ is even and
\[ (1 - B[l])^\dagger \leq 1 - \lambda_i \]
if $l$ is odd. \qed

Using the Cheeger inequality (23) for $\Gamma[l]$ we obtain:

Corollary 5.2. Assume that $2h[l] \leq 1$ and $l$ is even, then we have
\[ \lambda_1 \leq 1 - (1 - 2h[l])^\dagger \]  
(59)
or
\[ \lambda_{N-1} \geq 1 + (1 - 2h[l])^\dagger \]  
(60)
If $l$ is odd then we have
\[ \lambda_1 \leq 1 - (1 - 2h[l])^\dagger \]
We remark here that the estimate (59) for $\lambda_1$ can improve the Cheeger estimate (23), see the next section for a discussion.

Theorem 5.5. Let $C[l]$ be any lower bound for the largest eigenvalue $\lambda_{N-1}[l]$, i.e. $C[l] \leq \lambda_{N-1}[l]$. There exists at least one eigenvalue $\lambda_k$ in the interval
\[ \left[ 1 - (1 - C[l])^\dagger, 1 + (1 - C[l])^\dagger \right] \]  
(61)
if $l$ is even and
\[ \lambda_{N-1} \geq 1 + (1 - C[l])^\dagger \]
if $l$ is odd.

Proof. Again, by Lemma 5.2, (61) is well defined, if $l$ is even, since $C[l] \leq \lambda_{N-1}[l] \leq 1$. Using (52) we have $C[l] \leq \lambda_{N-1}[l] = \max_k (1 - (1 - \lambda_k)^l)$. Thus,
\[ \min_k |1 - \lambda_k| \leq (1 - C[l])^\dagger \]
if $l$ is even and
\[ \min_k (1 - \lambda_k) = 1 - \max_k \lambda_k \leq (1 - C[l])^\dagger \]
if $l$ is odd. \qed
In particular, we have from Theorem 3.2 and Theorem 5.5:

**Corollary 5.3.** Assume that $2h[l] \leq 1$ and $l$ is even then there exists at least one eigenvalue $\lambda_k$ in the interval

$$\left[ 1 - (1 - 2h[l])^{\frac{1}{l}}, 1 + (1 - 2h[l])^{\frac{1}{l}} \right].$$

(62)

If $l$ is odd then

$$\lambda_{N-1} \geq 1 + (1 - 2h[l])^{\frac{1}{l}}.$$  

We now turn to the gap phenomenon for eigenvalues, that is, find some interval that does not contain any eigenvalue.

**Theorem 5.6.** Let $D[l]$ be any upper bound for the largest eigenvalue, i.e. $\lambda_{N-1}[l] \leq D[l]$. Then all eigenvalues $\lambda_k$ of $\Delta(\Gamma)$ are contained in the union of intervals

$$\left[ 0, 1 - (1 - D[l])^{\frac{1}{l}} \right] \cup \left[ 1 + (1 - D[l])^{\frac{1}{l}}, 2 \right]$$

(63)

if $l$ is even and

$$\lambda_{N-1} \leq 1 - (1 - D[l])^{\frac{1}{l}}$$

if $l$ is odd.

The proof is similar to the proofs above so we omit it here. We only note that (63) is well defined if $l$ is even since, by Lemma 5.2, we can assume w.l.o.g. that $D[l] \leq 1$.

In other words: Let $l$ be even, then for any upper bound $D[l]$ none of the eigenvalues is contained in the interval $\left[ 1 - (1 - D[l])^{\frac{1}{l}}, 1 + (1 - D[l])^{\frac{1}{l}} \right]$. Thus, if $l$ is even, an upper bound $D[l]$ for $\lambda_{N-1}[l]$ of $\Delta(l)\Gamma$ can be used to bound all eigenvalues of $\Delta$ on $\Gamma$ away from 1. In particular, if $D[l] < 1$, $\Gamma$ then does not possess the eigenvalue 1, see also Lemma 5.2. In [1], it was observed that the eigenvalue 1 occurs in an unweighted graph whenever there are two nodes $i_1, i_2$ that are not neighbors themselves, but who possess the same neighbors, that is, for any $k$, we have $k \sim i_1$ iff $k \sim i_2$. Thus, a graph satisfying the assumptions of Theorem 5.6 cannot have any such pair of nodes if $D[l] < 1$ and $l$ is even.

In particular, we can apply the upper bound for the largest eigenvalue derived in Theorem 8.1 below (with the constant $H$ defined there) to obtain

**Corollary 5.4.** Assume that $H[l] \geq 1$ if $l$ is even, then all eigenvalues $\lambda_k$ of $\Delta$ on $\Gamma$ are contained in the union of intervals

$$\left[ 0, 1 - (H[l] - 1)^{\frac{1}{l}} \right] \cup \left[ 1 + (H[l] - 1)^{\frac{1}{l}}, 2 \right].$$

(64)

If $l$ is odd we have

$$\lambda_{N-1} \leq 1 - (H[l] - 1)^{\frac{1}{l}}.$$
From the dual Cheeger inequality (31) we only obtain an upper bound for \( \lambda_{N-1} \) if \( l \) is odd since
\[
1 + \sqrt{1 - (1 - \overline{h}(l))^2} \geq 1
\]
for all \( l \).

**Corollary 5.5.** If \( l \) is odd, then
\[
\lambda_{N-1} \leq 1 + (1 - (1 - \overline{h}(l))^2)^{\frac{1}{2l}}.
\]

6 Comparison of the Cheeger estimates with the new estimates obtained in the last section

In the sequel we compare the Cheeger estimates (23) and (25) with the new estimates obtained in Corollary 5.1 and Corollary 5.2. Recall that Corollary 5.1 and Corollary 5.2 were obtained by applying Theorem 3.2 to the neighborhood graph \( \Gamma[l] \) and then using the relationship between the Laplacian spectrum of \( \Gamma \) and its neighborhood graph \( \Gamma[l] \) which was established in Theorem 5.2. Thus, Corollary 5.1 and Corollary 5.2 are in some sense "indirect" estimates because they only indirectly use the geometrical properties of \( \Gamma \), i.e. only use geometric properties of the neighborhood graph \( \Gamma[l] \). In contrast, the Cheeger inequality (23) and (25) is a "direct" estimate since here we use directly the geometric properties of the graph \( \Gamma \).

In Corollary 5.1 we found new lower bounds for the second smallest eigenvalue \( \lambda_1 \) of a graph \( \Gamma \). This raises the question whether these new bounds improve the Cheeger estimate (25) for the second smallest eigenvalue. Comparing Corollary 5.1 with (25) reveals that our new estimates improve the Cheeger estimate (25) if
\[
h[l] \geq \sqrt{1 - (1 - h^2)^{l}}, \tag{65}
\]
for some \( l \geq 2 \). In general it is not clear for which graphs \( \Gamma \) and which \( l \) the equation (65) is satisfied. However, we can develop some qualitative intuition about (65).

We have to distinguish whether \( l \) is even or odd. Assume for the moment that \( l \) is even. Clearly, (65) is not satisfied whenever \( \Gamma \) is bipartite since then, by Lemma 5.1, \( \Gamma[l] \) is disconnected and thus \( h[l] = 0 \). In fact, Corollary 5.1 yields only the trivial estimate \( 0 \leq \lambda_1 \) for bipartite graphs. In contrast, for graphs that are not bipartite the estimate in (65) always yields a non-trivial lower bound \( 0 < 1 - (1 - h^2)^l \) for the second smallest eigenvalue \( \lambda_1 \).

Note, that a necessary condition for strict inequality in (65) is that \( h[l] > h \) if this is the case we can not expect that \( h[l] > h \) is satisfied, unless the Cheeger estimate on the graph \( \Gamma[l] \) is sharper (this will be made more precise in the next proposition) than the Cheeger estimate on the graph \( \Gamma \). In particular, we can not expect that (65) is satisfied. On the other hand if \( \lambda_1 < 2 - \lambda_{N-1} \) then \( \lambda_1[l] = 1 - (1 - \lambda_1)^l > \lambda_1 \) and so we can expect that the necessary condition \( h[l] > h \) is satisfied. Roughly
speaking, if $l$ is even, graphs that are closer to disconnected graphs than to bipartite graphs are good candidates for satisfying \( (65) \).

If $l$ is odd then Corollary 5.1 always yields non-trivial estimates and $\lambda_1[l] > \lambda_1$ is always satisfied. Thus we can expect that the necessary condition $h[l] > h$ is, in general, satisfied if $l$ is odd.

After all, we are mainly interested in the question when \( (65) \) is satisfied. We have the following sufficient condition for \( (65) \).

**Proposition 6.1.** Let $S[l] := \frac{1 - \sqrt{1 - h^2[l]}}{\lambda_1[l]}$ be the sharpness of the Cheeger estimate \( (25) \) on the graph $\Gamma[l]$, i.e. the closer $S[l]$ is to 1 the sharper is the Cheeger estimate. For simplicity, we set $S[1] := S$ and $h[1] := h$ on the graph $\Gamma$. If

$$S[l] \geq \frac{1 - (1 - h^2)^{\frac{1}{2}}}{1 - (1 - h^2)^{\frac{1}{2}}} \quad (66)$$

and in addition $\lambda_1 \leq 2 - \lambda_{N-1}$ if $l$ is even, then \( (65) \) is satisfied.

**Proof.** We have

$$S[l] = \frac{1 - \sqrt{1 - h^2[l]}}{\lambda_1[l]} = \frac{1 - \sqrt{1 - h^2[l]}}{1 - (1 - \lambda_1)^{\frac{1}{2}}} = \frac{1 - \sqrt{1 - h^2[l]}}{1 - (1 - h^2)^{\frac{1}{2}}}$$

A comparison with \( (66) \) yields

$$1 - \sqrt{1 - h^2[l]} \geq 1 - (1 - h^2)^{\frac{1}{2}}.$$

\[\Box\]

**Proposition 6.1** shows that if the Cheeger estimate \( (26) \) for graphs $\Gamma[l]$ is sufficiently good compared to the Cheeger estimate \( (25) \) for $\Gamma$ then \( (65) \) is satisfied.

As an example we consider again the family of graphs in Example 5.1. The corresponding Cheeger constants of the neighborhood graphs are given by $h[1] = \frac{1}{1+c}$, $h[2] = \frac{2c}{(2c+1)}$, $h[3] = \frac{3c^2+1}{(1+c)^2}$, $h[4] = \frac{1+10c^2+c^4}{(1+c)^4}$, and $h[5] = \frac{1+10c^2+c^4}{(1+c)^5}$. In Figure 4 we plot the lower bounds $1 - (1 - h[l]^2)^{\frac{1}{2}}$, for the second smallest eigenvalue $\lambda_1$, for different values of $l$. We observe that for $c < 2.2$ the Cheeger inequality $l = 1$ yields the best estimate for the second smallest eigenvalue $\lambda_1$ of the graph in Figure 2. However, if we increase $c$ the estimates for larger values of $l$ become better.

As a second example, we consider the family of graphs in Example 5.2. The Cheeger constants of the neighborhood graphs are given by $h[1] = \frac{1}{6c+1}$, $h[2] = \min\{\frac{4c}{(6c+1)(2c+1)}, \frac{3c^2+c^2}{(2c+1)^2}\}$, and $h[3] = \min\{\frac{12c^2+12c+7}{(1+2c)(1+6c)}, \frac{12c^2+12c+7}{\min\{8c, 4c+1\}}\}$. In Figure 5 the lower bounds $1 - (1 - h[l]^2)^{\frac{1}{2}}$, for the second smallest eigenvalue
Figure 4: Plot of different lower bounds $1 - (1 - h^2[1])^\frac{1}{2}$ for the second smallest eigenvalue $\lambda_1$ of the family of graphs in Figure 2. The Cheeger estimate ($l = 1$) is plotted in dark blue, and the red, yellow, green and light blue curves correspond to $l = 2, 3, 4,$ and $l = 5$ respectively.

Figure 5: Plot of different lower bounds $1 - (1 - h^2[l])^\frac{1}{2}$, for the second smallest eigenvalue of the family of graphs in Figure 3. The Cheeger estimate ($l = 1$) is plotted in blue, and the black, red curves correspond to $l = 2$, and $l = 3$ respectively.
Figure 6: Plot of different upper bounds $1 - (1 - 2h[l])^\frac{l}{2}$, for the second smallest eigenvalue of the family of graphs in Figure 3. The Cheeger estimate ($l = 1$) is plotted in blue, and the black, red curves correspond to $l = 2$, and $l = 3$ respectively. The dashed black line indicates that for $c \leq 0.5$ this is not an upper bound for $\lambda_1$ because in this case (60) holds and (59) is not satisfied.

$\lambda_1$, are plotted for $l = 1, 2, 3$. Again, for small $c$ the Cheeger estimate, $l = 1$ yields the best estimate. However, if $c > 0.8$ then the estimate for $l = 3$ improves the Cheeger estimate.

We can also compare the upper bound for $\lambda_1$ in Corollary 5.2 with the Cheeger inequality (23). We observe that the estimate in Corollary 5.2 improves (23) if $l$ is odd and

$$h[l] \leq \frac{1 - (1 - 2h[l])^l}{2}.$$  \hspace{1cm} (67)

If $l$ is even, Corollary 5.2 improves (23) if in addition $h[l] \leq \frac{1}{2}$ and $\lambda_1 \leq 2 - \lambda_{N-1}$. We have to assume that $\lambda_1 \leq 2 - \lambda_{N-1}$ if $l$ is even, because otherwise (60) holds instead of (59) and so we do not have an upper bound for $\lambda_1$. Similarly to Proposition 6.1 we obtain:

**Proposition 6.2.** Let $s[l] := \frac{\lambda_1[l]}{2\lambda[l]}$ be the sharpness of the upper Cheeger estimate for the second smallest eigenvalue $\lambda_1[l]$ of $\Gamma[l]$. If

$$s[l] \geq \frac{1 - (1 - s2h)^l}{1 - (1 - 2h)^l},$$  \hspace{1cm} (68)

where $s := s[1]$ and in addition $h[l] \leq \frac{1}{2}$ and $\lambda_1 \leq 2 - \lambda_{N-1}$ if $l$ is even then (67) is satisfied, i.e. the estimate in Corollary 5.2 improves the Cheeger estimate (23).

The proof is straightforward so we omit it here.

It turns out that, if we consider the family of graphs in Example 5.1, the different upper bounds $\lambda_1 \leq 1 - (1 - 2h[l])^\frac{l}{2}$ for the second smallest eigenvalue are
the same for all $l$. In contrast for the family of graphs in Example 5.2 the plot in Figure 6 shows that the estimate in Corollary 5.2 can improve the Cheeger estimate (23). For example if $c > 0.3$ the estimate for $l = 3$ improves the Cheeger estimate (23). Comparing Figure 5 and Figure 6 shows that the estimates in Corollary 5.1 and Corollary 5.2 improve both Cheeger estimates (23) and (25) at the same time if $c > 0.8$ and $l = 3$.

Finally we observe that if $h[l]$ is not contained in the interval $\left[\frac{1-(1-2h)^l}{2}, \sqrt{1-(1-h^2)^l}\right]$ (where the interval is the empty set if $\frac{1-(1-2h)^l}{2} > \sqrt{1-(1-h^2)^l}$) then at least one of the Cheeger estimates (23) and (25) is improved by the estimates in Corollary 5.1 and Corollary 5.2.

Similarly, one can also compare the Cheeger-like estimate for the largest eigenvalue in Theorem 3.2 with the estimate obtained in Corollary 5.5. We observe that, similarly to the Cheeger estimate, the indirect estimate in Corollary 5.5 can improve the "direct" estimate given by Theorem 3.2. As one such example we consider the family of graphs in Example 5.1. In Figure 7 we plot different upper bounds $1 + (1 - (\bar{h}[l])^2)^{\frac{1}{2}}$ for the largest eigenvalue $\lambda_{N-1}$. Clearly one can also derive similar results as (65) and Proposition 5.1 in the case of the largest eigenvalue $\lambda_{N-1}$. However, we do not want to go into further detail here because the calculations are exactly the same as before.

We conclude this section by noting that the concept of the neighborhood graph is very powerful because it may, at least for some graphs, improve any eigenvalue bound.
7 An example

As discussed above, the highest eigenvalue $\lambda_{N-1}$ of $\Delta$ becomes largest for bipartite and smallest for complete graphs, respectively. And a guiding question for this paper is what can we say about the highest eigenvalue of graphs that are neither bipartite nor complete, i.e., what structural properties of $\Gamma$ lead to a highest eigenvalue $\lambda_{N-1}$ close to 2, or very different from 2, respectively.

In order to develop some further intuition about the highest eigenvalue, we now consider the following example. Let $\Gamma_0$ be a bipartite graph with $N$ vertices. We consider a highest eigenfunction $\bar{u}$ that is +1 on one class and −1 on the other class of vertices, as described above. In particular by (14),

$$\frac{1}{2} \sum_k \sum_j w_{kj} (\bar{u}(j) - \bar{u}(k))^2 \sum_i d_i \bar{u}(i)^2 = 2.$$  \hfill (69)

By adding another vertex $i_0$ and connecting it to one of the vertices $i_1$ of $\Gamma_0$ we obtain a new bipartite graph $\Gamma_1$. We extend $\bar{u}$ by $\bar{u}(i_0) = 0$ to $\Gamma_1$. Thus, the numerator and the denominator of (69) are both increased by $w_{i_0i_1}$. Let $\Gamma_0$ be sufficiently large, i.e., $\sum_i d_i$ is sufficiently large, then we can achieve for $\Gamma_1$ that for any given small $\epsilon > 0$,

$$\frac{1}{2} \sum_k \sum_j w_{kj} (\bar{u}(j) - \bar{u}(k))^2 \sum_i d_i \bar{u}(i)^2 > 2 - \epsilon.$$  \hfill (70)

Now, this is not affected when we construct a graph $\Gamma$ by attaching another graph $\Gamma_2$ at $i_0$ and extend $\bar{u}$ by 0 to all of $\Gamma_2$. For instance, $\Gamma_2$ could be a complete graph $K_M$ with $M$ vertices, for any $M$. In particular, the difference $2 - \lambda_{N-1}$ which has to be smaller than $\epsilon$ by (13), is not very sensitive to the shape of $\Gamma_2$. This implies, for instance, that $2 - \lambda_{N-1}$ cannot reflect a global quantity like the clustering coefficient $C$ of (1) that expresses an averaged difference from a graph being bipartite. In fact, our construction of attaching a complete graph $K_M$ to a bipartite graph $\Gamma_0$ through a connecting node produces a graph with $C$ arbitrarily close to its maximal value 1 when $M$ is sufficiently large.

By extending this example, we can also see that we should have many eigenvalues $\lambda$ for which $2 - \lambda$ is small when the graph possesses several relatively large bipartite or almost bipartite parts that are only loosely connected with the rest. (By (52), the neighborhood graph $\Gamma[2]$ of such a graph contains several large components that are only loosely connected, i.e. many eigenvalues $\lambda_k[2]$ that are small.) This is analogous to the fact that a graph possesses several small eigenvalues when it has many relatively large components that are only loosely connected to the rest, that is, when the graph can be easily decomposed into several large clusters. Of course, for a nonconnected graph, that is, one with several components without links between them, the spectrum simply is the union of the spectra of the components. Therefore, by the continuity principle, a graph consisting of clusters that are only loosely connected to each other has its spectrum approximated by the spectra of these clusters, that is, by the one of the graph resulting from deleting the few links between the clusters.
8 Controlling the largest eigenvalue from above

In this section, we shall provide a more technical estimate from above for the highest eigenvalue $\lambda_{N-1}$. For that purpose, we shall first derive some general identity, for a function $u$ on the vertex set $V$ of $\Gamma$.

Lemma 8.1. Let $u$ be an eigenfunction of $\Delta$ for the eigenvalue $\lambda$. Then,

$$2 - \lambda = \frac{\sum_i \frac{1}{d_i} \sum_{j,k} w_{ij} w_{ik} (u(j) - u(k))^2}{\sum_i \sum_j w_{ij} (u(i) - u(j))^2}. \quad (71)$$

Remark. This identity follows from Theorem 5.2 for $l=2$ and (9) applied to the neighborhood graph. Here, as an alternative, we shall provide a direct proof.

Proof. \[ \sum_i \frac{1}{d_i} \sum_{j,k} w_{ij} w_{ik} (u(j) - u(k))^2 \]

\[ = \sum_i \frac{1}{d_i} \left( \sum_{j,k} w_{ik} w_{ij} u(j)^2 - 2 \sum_{j,k} w_{ij} w_{ik} u(j) u(k) + \sum_{j,k} w_{ij} w_{ik} u(k)^2 \right) \]

\[ = 2 \sum_i \left( \sum_j w_{ij} u(j)^2 - \frac{1}{d_i} \left( \sum_j w_{ij} u(j) \right)^2 \right) \]

\[ = 2 \sum_i \sum_j w_{ij} u(j)^2 - \sum_i 2d_i \left( \frac{1}{d_i} \sum_j w_{ij} u(j) \right)^2. \]

We now observe that we can replace $u$ by $u - u(i)$ in the first and hence also in all subsequent lines. This yields

\[ \sum_i \frac{1}{d_i} \sum_{j,k} w_{ij} w_{ik} (u(j) - u(k))^2 \]

\[ = 2 \sum_i \sum_j w_{ij} (u(j) - u(i))^2 - \sum_i 2d_i \left( \frac{1}{d_i} \sum_j w_{ij} (u(j) - u(i)) \right)^2 \]

\[ = 2 \sum_i \sum_j w_{ij} (u(j) - u(i))^2 - \sum_i 2d_i (\Delta u(i))^2. \]

Since $u$ is an eigenfunction, $\Delta u = \lambda u$ for some eigenvalue $\lambda$, then, recalling (14), we obtain

\[ \sum_i \frac{1}{d_i} \sum_{j,k} w_{ij} w_{ik} (u(j) - u(k))^2 = 2\lambda(2 - \lambda) \sum_i d_i u(i)^2. \quad (72) \]
Using (14) again, we can also reformulate this as

\[ 2 - \lambda = \frac{\sum_i \frac{1}{d_i} \sum_{j,k} w_{ij} w_{ik} (u(j) - u(k))^2}{\sum_i \sum_j w_{ij} (u(i) - u(j))^2}. \]

We also observe, by a reasoning similar to the one for Lemma 8.1:

**Lemma 8.2.** Let \( u \) be an eigenfunction of \( \Delta \) for the eigenvalue \( \lambda \). Then,

\[ 2 - \lambda = \frac{2 \sum_i \sum_k w_{ik} \left( \frac{1}{d_i} \sum_j w_{ij} (u(j) - u(k)) \right)^2}{\sum_i \sum_j w_{ij} (u(j) - u(i))^2}. \] \hspace{1cm} (73)

We now employ (71) to interpret \( 2 - \lambda_{N-1} \) as quantifying how much \( \Gamma \) is locally different from being bipartite. Recall that this quantity is 0 iff \( \Gamma \) happens to be bipartite. Note that (72) can also be used to estimate the local difference from being bipartite in terms of \( 2 - \lambda_{N-1} \).

As discussed above, the (global) clustering coefficient \( C \) is not an appropriate measure for the difference \( 2 - \lambda_{N-1} \). However, we shall see that it is possible to control \( 2 - \lambda_{N-1} \) by the following local clustering measure

\[ C_0 := \min_{e=(i,j)} \frac{\alpha_i + \alpha_j}{2}, \] \hspace{1cm} (74)

where

\[ \alpha_i := \frac{\sum_{i:\text{e}=(i,j)\in\Delta} w_{ij}}{d_i} \]

and \( e = (i, k) \in \Delta \) (\( i \in \Delta \)) denotes that the edge \( e = (i, k) \) (the vertex \( i \)) is contained in some triangle. Hence, \( \alpha_i \) is the fraction of weights \( w_{ij} \) for fixed \( i \) that are contained in some triangle. In particular, if \( i \notin \Delta \) then \( \alpha_i = 0 \). Again, \( C_0 = 0 \) for a bipartite and \( C_0 = 1 \) for a complete graph. Furthermore, we define

\[ W := \left( \min_{i \in \Delta} \min_{k \in \Delta} \sum_{L:(i,k,l)\in\Delta} \frac{d_i w_{il} w_{lk}}{d_i d_l} \right)^{1/2} \] \hspace{1cm} (75)

and

\[ d := \max_{i \in \Delta} d_i. \] \hspace{1cm} (76)

**Theorem 8.1.** The largest eigenvalue \( \lambda_{N-1} \) of \( \Delta \) can be controlled from above by

\[ 2 - \frac{1}{2d} C_0 \left( \frac{W}{1+W} \right)^2 =: 2 - H \geq \lambda_{N-1}. \] \hspace{1cm} (77)
Proof. First we rewrite (71) for the largest eigenvalue \( \lambda_{N-1} \) in the following form:

\[
2 - \lambda_{N-1} = \frac{\sum_{\varepsilon=(i,j)} \left( \frac{1}{d_i} \sum_k \mu_{ij} w_{ik}(u_{N-1}(j) - u_{N-1}(k))^2 + \frac{1}{d_j} \sum_k \mu_{ji} w_{jk}(u_{N-1}(i) - u_{N-1}(k))^2 \right)}{\sum_{\varepsilon=(i,j)} \mu_{ij}(u_{N-1}(i) - u_{N-1}(j))^2 + \mu_{ji}(u_{N-1}(j) - u_{N-1}(i))^2}
\]

(78)

where again \( \mu_{ij} = w_{ij} \) if \( i \neq j \) and \( \mu_{ij} = \frac{1}{4} w_{ij} \) if \( i = j \). In order to control \( 2 - \lambda_{N-1} \) from below we need to match any term \( \mu_{ij}(u_{N-1}(i) - u_{N-1}(j))^2 \) in the denominator by some term in the numerator of comparable magnitude. Since there is noting to match if \( i = j \) we can use the weights \( w_{ij} \) instead of \( \mu_{ij} \) throughout the proof. For ease of notation we will drop the index \( N-1 \) in the rest of the proof.

For simplicity, we first match the term \( w_{ij}(u(i) - u(j))^2 \) in the denominator with \( \frac{1}{d_i} \sum_k w_{ij} w_{ik}(u(j) - u(k))^2 \) in the numerator. Because of the symmetry in \( i \) and \( j \) the second term in the numerator and denominator can be treated in the same way.

Let \( K_1(i) \subset V \) be the set of all neighbors \( k \) of \( i \) for which \( e = (i, k) \in \Delta \) and

\[
(u(j) - u(k))^2 \geq \gamma_{ij}^2(u(i) - u(j))^2
\]

is satisfied. The constant \( \gamma_{ij} \) will be used later on to minimize our upper bound for \( \lambda_{N-1} \). Similarly, let \( K_2(i) \subset V \) be the set of all neighbors \( k \) of \( i \) which satisfy \( e = (i, k) \in \Delta \) and

\[
(u(j) - u(k))^2 < \gamma_{ij}^2(u(i) - u(j))^2.
\]

Clearly,

\[
\sum_{k \in K_1(i) \cup K_2(i)} w_{ik} = \sum_{k : e = (i, k) \in \Delta} w_{ik} = \alpha_i d_i.
\]

If \( i \notin \Delta \) then \( \alpha_i = 0 \) and \( K_1(i) = K_2(i) = \emptyset \). We distinguish the following two cases:

(i) Assume that \( \sum_{k \in K_1(i)} w_{ik} \geq \frac{\alpha_i d_i}{2} \) is satisfied for vertex \( i \). Consequently, there exists a term

\[
\frac{1}{d_i} \sum_k w_{ij} w_{ik}(u(j) - u(k))^2 \geq \frac{\alpha_i \gamma_{ij}^2}{2} w_{ij}(u(i) - u(j))^2
\]

(81)

in the numerator. Thus \( w_{ij}(u(i) - u(j))^2 \) is matched.

(ii) Now assume that \( \sum_{k \in K_2(i)} w_{ik} \geq \frac{\alpha_i d_i}{2} \) is satisfied for vertex \( i \). We can not directly match \( w_{ij}(u(i) - u(j))^2 \) by using (80) because it could happen that \( \frac{1}{d_i} \sum_k w_{ij} w_{ik}(u(j) - u(k))^2 = 0 \). However, Equation (80) can be used to find a term of comparable size in the numerator. (80) implies that

\[
(u(i) - u(k))^2 > (1 - \gamma_{ij}^2)(u(i) - u(j))^2.
\]

(82)
Now the idea is to use the terms in the numerator several times in order to match \( w_{ij}(u(i) - u(j))^2 \). Multiplying the numerator in (71) by \( w_{ij} \) yields

\[
\begin{align*}
  w_{ij} \sum_l \frac{1}{d_l} \sum_{m,k} w_{lm} w_{lk} (u(m) - u(k))^2 &= w_{ij} \sum_l \frac{1}{d_l} \sum_k w_{lk} (u(i) - u(k))^2 \\
  &\quad + w_{ij} \sum_l \frac{1}{d_l} \sum_{k,m \neq i} w_{lm} w_{lk} (u(m) - u(k))^2
\end{align*}
\]

Now we will only use the first term on the r.h.s. The second term can be used to match other terms in the denominator. The first term on the r.h.s. of (83) yields:

\[
\begin{align*}
  w_{ij} \sum_l \frac{1}{d_l} \sum_{k \in K_{2}(i)} w_{lk} (u(i) - u(k))^2 &\geq w_{ij} \sum_l \frac{1}{d_l} \sum_{k \in K_{2}(i)} \min_{k \in K_{2}(i)} w_{lk} (u(i) - u(k))^2 \\
  &\quad + \sum_l \frac{1}{d_l} \sum_{k,m \neq i} w_{lk} (u(m) - u(k))^2
\end{align*}
\]

Thus \( w_{ij}(u(i) - u(j))^2 \) is matched in the numerator. In order to match all other terms of the form \( w_{ip}(u(i) - u(p))^2 \) in the denominator for fixed \( i \) we need to use the terms in the numerator at most \( \sum p w_{ip} = d_i \) times. Note that we can use the second term on the r.h.s. of (83) in order to match other terms of the form \( w_{mp}(u(m) - u(p))^2 \) for \( m \neq i \). If some vertex \( q \) is not contained in a triangle we have \( \alpha_q = 0 \) and thus we do not need to match the terms \( w_{qp}(u(q) - u(p))^2 \) for fixed \( q \). We conclude that we used the terms in the numerator at most \( \max_{\triangle} d_i \) times. Because of the symmetry in \( i \) and \( j \) the second term in the numerator (78) can be treated in the same way. We obtain the following estimate:

\[
2 - \lambda_{N-1} \geq \frac{1}{2d} \min_{e=(i,j)} \max_{\gamma_{ij}} \{ a_{ij}, b_{ij}, c_{ij}, d_{ij} \}.
\]
where

\[ a_{ij} := \frac{\alpha_i + \alpha_j}{2} \gamma_{ij}, \]
\[ b_{ij} := \frac{\alpha_i}{2} \gamma_{ij}^2 + \frac{\alpha_j}{2} W^2 (1 - \gamma_{ij})^2, \]
\[ c_{ij} := \frac{\alpha_i}{2} W^2 (1 - \gamma_{ij})^2 + \frac{\alpha_j}{2} \gamma_{ij}^2, \]
\[ d_{ij} := \frac{\alpha_i}{2} W^2 (1 - \gamma_{ij})^2 + \frac{\alpha_j}{2} W^2 (1 - \gamma_{ij})^2, \]

and \( W^2 := \min_{i \in \Delta} A(i) \).

Choosing \( \gamma_{ij} = W \) yields

\[ 2 - \lambda_{N-1} \geq \frac{1}{2d} C_0 \left( \frac{W}{1+W} \right)^2. \]

(84)

With the scheme developed in this section, the control in the other direction, that is, estimating the largest eigenvalue from below, does not quite work, because of the following example. Consider a graph with many cycles of odd length, but all of them of length at least 5. Here, \( C_0(\Gamma) = 0 \) as there are no triangles, but \( 2 - \lambda_{N-1} \neq 0 \) because the graph is not bipartite as bipartite graphs can only have cycles of even length. However, we can control the largest eigenvalue from below in a different way, as we have seen in Section 3.

9 Random walks on graphs and the convergence to equilibrium

By the above considerations it is apparent that the techniques developed in section 3 and 5 can be applied to random walks on graphs. We recall the following theorem for the convergence of random walks on graphs [14, 7].

Theorem 9.1. For any function \( f \in \ell^2(\Gamma) \), set

\[ \overline{f} = \frac{1}{\text{vol}(V)} \sum_j d_j f(j). \]

Then for any positive integer \( t \), we have

\[ \| P^t f - \overline{f} \| \leq \rho^t \| f \|, \]

(85)

where \( \rho = \max_{k \neq 0} |1 - \lambda_k| = \max\{ |1 - \lambda_1|, |1 - \lambda_{N-1}| \} \) is the spectral radius of the transition probability matrix \( P \) and \( \| f \| = \sqrt{(f, f)_\Gamma} \). Consequently, if \( \Gamma \) is connected and not bipartite, then

\[ \| P^t f - \overline{f} \| \to 0 \]

as \( t \to \infty \), i.e. \( P^t f \) converges to the stationary distribution \( \overline{f} \) as \( t \to \infty \).
We define the equilibrium transition probability matrix as follows:

\[
\mathbf{P} := \begin{pmatrix}
d_1/\text{vol}(V) & \ldots & d_N/\text{vol}(V) \\
\vdots & \ddots & \vdots \\
d_1/\text{vol}(V) & \ldots & d_N/\text{vol}(V)
\end{pmatrix}
\]

Observe that \(\mathbf{P} f = f\) for all functions \(f \in \ell^2(\Gamma)\) and thus, by (85), \(P^t\) converges to \(\mathbf{P}\) as \(t \to \infty\), if \(\Gamma\) is not bipartite. As expected, the equilibrium transition probability for going from \(i\) to \(j\) only depends on the degree of vertex \(j\) (and the volume of the graph, i.e. the sum of all degrees). In addition, we define the equilibrium weighted adjacency matrix as

\[
\mathbf{W} := \mathbf{D} \mathbf{P},
\]

where \(\mathbf{D} = \text{diag}\{d_1, \ldots, d_N\}\) is the diagonal matrix of vertex degrees. Consequently, if \(\Gamma\) is not bipartite, then its neighborhood graph \(\Gamma[l]\) converges to the equilibrium graph \(\Gamma\), that has the weighted adjacency matrix \(\mathbf{W}\), as \(l \to \infty\). The equilibrium graphs of the families of graphs studied in Example 5.1 and Example 5.2 have the following equilibrium weighted adjacency matrices

\[
\mathbf{W} = \begin{pmatrix}
\frac{1+c}{2c} & \frac{1+c}{2c} \\
\frac{1+c}{2c} & \frac{1+c}{2c}
\end{pmatrix}
\]

and

\[
\mathbf{W} = \begin{pmatrix}
a_1 & a_2 & a_2 & a_1 & a_1 \\
a_1 & a_2 & a_2 & a_1 & a_1 \\
a_2 & a_2 & a_3 & a_3 & a_2 \\
a_2 & a_2 & a_3 & a_3 & a_2 \\
a_1 & a_1 & a_2 & a_2 & a_1 \\
a_1 & a_1 & a_2 & a_2 & a_1
\end{pmatrix},
\]

where \(a_1 = \frac{4c^2+2}{12c+2}\), \(a_2 = \frac{4c^2+2}{12c+2}\), and \(a_3 = \frac{4c^2+4c+1}{12c+2}\). If \(\Gamma\) is bipartite then \(\Gamma[l]\) does not converge as \(l \to \infty\). This can be seen from Lemma 5.1 since \(\Gamma[l]\) is then disconnected and not bipartite whenever \(l\) is even and \(\Gamma[l]\) is connected and bipartite whenever \(l\) is odd. However, for a bipartite graph \(\Gamma\), \(\Gamma[l]\) converges if \(l\) is even and \(l \to \infty\). The weighted adjacency matrix is then given by

\[
\mathbf{W}_{l, \text{even}} = \begin{pmatrix}
\mathbf{W}_1 & 0 \\
0 & \mathbf{W}_2
\end{pmatrix},
\]

where \((\mathbf{W}_k)_{i,j} = \frac{2d_i d_j}{\text{vol}(V)}\), for \(k = 1, 2\), if \(i\) and \(j\) belong to the same subset \(V_k\) and \(V_1, V_2\) yields a bipartite decomposition of the vertex set \(V\). Thus, \(\Gamma\) is the disjoint union of two complete graphs of size \(|V_1|\) and \(|V_2|\). Similarly, if \(\Gamma\) is bipartite, \(\Gamma[l]\) converges if \(l\) is odd and \(l \to \infty\). In this case the weighted adjacency matrix is given by

\[
\mathbf{W}_{l, \text{odd}} = \begin{pmatrix}
0 & \mathbf{W}_1 \\
\mathbf{W}_2 & 0
\end{pmatrix},
\]

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where $(W_k)_{i,j} = \frac{2d_id_j}{\text{vol}(V)}$, for $k = 1, 2$, if $i$ and $j$ belong to different subsets. Thus $\Gamma$ is the complete bipartite graph with the same bipartite decomposition $V_1, V_2$ of vertex set $V$ as $\Gamma$.

Note, that by (85) the spectral radius $\rho$ of the transition probability matrix $P$ controls the convergence of $P^t$ to the stationary distribution $\overline{f}$. Thus, we need to control $\rho$ from above in order to estimate the convergence to the stationary distribution. Our results in section 3 and 5 allow us to control $\rho$ in various different ways from above. As one such example we mention Corollary 5.1 from which we conclude that

$$\rho = \max_{k \neq 0} |1 - \lambda_k| \leq (1 - h^2[l])^{1/2},$$

if $l$ is even. Thus, (85) implies

**Theorem 9.2.**

$$\|P^tf - \overline{f}\| \leq (1 - h^2[l])^{1/2} \|f\|,$$

where we can use the Cheeger constant $h^2[l]$ for any even $l$.

**Remark.** Instead of considering the convergence in the $\ell^2$-norm, as in (85), one could also study stronger notions of convergence, e.g. the relative pointwise distance [24] or other measures of convergence as the mixing time [14, 24]. All these quantities can be bounded from above in terms of the spectral radius of the transition probability matrix $P$. Thus, by using the techniques developed in section 3 and 5 we can give explicit bounds for the convergence of a random walk on a graph using any of these measures of convergence.

## 10 Synchronization in coupled map lattices

In this section, we present another application of our eigenvalue estimates.

We consider a coupled map lattice supported by a graph $\Gamma$, that is, a dynamical system updated at discrete times $t \in \mathbb{N}$ and of the form

$$x_i(t + 1) = f(x_i(t)) + \frac{\epsilon}{d_i} \sum_j w_{ij} (f(x_j(t)) - f(x_i(t))), \quad (86)$$

where $\epsilon \geq 0$ is the overall coupling strength and $w_{ij}$ is the strength of the influence of unit $j$ on unit $i$. It was discovered by Kaneko [16] that the system (86) can (asymptotically) synchronize, i.e., $|x_i(t) - x_j(t)| \to 0$ for $t \to \infty$ and all $i, j$, even if the function $f$ displays chaotic behavior, i.e. its Lyapunov exponent $\mu(f)$ satisfies

$$\mu(f) = \lim_{T \to \infty} \frac{1}{T} \sum_{t=0}^{T-1} \ln |f'(s(t))| > 0. \quad (87)$$

Here $s(t)$ is a synchronous solution, i.e. $x_i(t) = s(t)$ for all $i$. 

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More precisely, the system (86) synchronizes under suitable conditions that will depend on $\mu(f)$, $\epsilon$, and the properties of $\Gamma$. In particular, we have the following criterion for the asymptotic stability of a synchronized state (which, when fulfilled, implies that (86) will asymptotically synchronize when its initial values are sufficiently close to that state).

**Theorem 10.1** ([15]). A synchronized state $s(t)$ of the coupled map lattice (87) is asymptotically stable if

$$\frac{1 - e^{-\mu(f)}}{\lambda_1} < \epsilon < \frac{1 + e^{-\mu(f)}}{\lambda_{N-1}}.$$  \hspace{1cm} (88)

Thus, there exists a range of values of $\epsilon$ for which we have asymptotic stability if

$$\frac{\lambda_{N-1}}{\lambda_1} < \frac{e^{\mu(f)} + 1}{e^{\mu(f)} - 1} \quad \text{and} \quad \mu(f) > 0$$  \hspace{1cm} (89)

or

$$\frac{\lambda_{N-1}}{\lambda_1} > \frac{e^{\mu(f)} + 1}{e^{\mu(f)} - 1} \quad \text{and} \quad \mu(f) < 0.$$  \hspace{1cm} (90)

The nontrivial case here is, of course, the one where $\mu(f) > 0$.

In order to apply this result, we need to control the ratio $\frac{\lambda_{N-1}}{\lambda_1}$. The above results imply

**Corollary 10.1.** For every graph we have:

$$\frac{h}{h} \leq \frac{\lambda_{N-1}}{\lambda_1} \leq \frac{\min_{l \in \mathbb{N}, \text{even}} 1 + (1 - h[l]^2)^{\frac{1}{2}}, \min_{l \in \mathbb{N}, \text{odd}} 1 + (1 - (1 - h[l])^2)^{\frac{1}{2}}}{\max_{l \in \mathbb{N}} (1 - (1 - h[l]^2)^{\frac{1}{2}})}.$$  \hspace{1cm} (91)

Thus, we can determine conditions under which system (86) synchronizes.

The main point of Theorem [10.1] is that the graph in question should be sufficiently different from both a disconnected graph (as characterized by $\lambda_1 = 0$) and a bipartite one (as characterized by $\lambda_{N-1} = 2$). A disconnected graph cannot synchronize dynamics because its components do not interact. Dynamics on a bipartite graph need not synchronize because the two classes can exchange their states every other period, that is, the bipartite graph can sustain nonsynchronized period 2 oscillations.

For a more general framework for synchronization of coupled dynamics, see [2].

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