Alcom-FT Technical Report Series
ALCOMFT-TR-03-145

On Spectral Bounds for the k-Partitioning of Graphs *

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Abstract

When executing processes on parallel computer systems they encounter as a major bottleneck inter-processor communication. One way to address this problem is to minimize the communication between processes that are mapped to different processors. This translates to the k-partitioning problem of the corresponding process graph, where k is the number of processors. The classical spectral lower bound of $\frac{|V|}{2k}\sum_{i=1}^{k}\lambda_i$ for the k-section width of a graph is well-known. We show new relations between the structure and the eigenvalues of a graph and present a new method to get tighter lower bounds on the k-section width. This method makes use of the level structure defined by the k-section. We define a global expansion property and prove that for graphs with the same k-section width the spectral lower bound increases with this global expansion. We also present examples of graphs for which our new bounds are tight up to a constant factor.

1 Introduction

The partitioning of a graph into several balanced parts has a wide range of applications, especially in the field of parallel computation. Large numerical simulations like e.g. crash-simulations are commonly executed on parallel processor systems using the *FEM* approach. For the parallel computation, the mesh is partitioned into k subdomains with k being the number of processors. In order not to affect the speed of computations, the assignment of the nodes should be as uniform as possible, and the data exchange between the processors should be minimized. Since the data dependencies are defined by adjacencies in the mesh,

*Partly supported by the DFG-Sonderforschungsbereich 376 Massive Parallelität: Algorithmen, Entwurfsmethoden, Anwendungen, and by the IST Programme of the EU under contract number IST-1999-14186 (ALCOM-FT). An extended abstract of these results has been presented at SPAA 2001.

the parallel algorithms only require communications on the edges between two vertices of different subdomains. Hence, the goal is to find a balanced k-partitioning of a given graph G with a minimal number of cut edges separating the sets from each other. This minimal number of cut edges of a balanced optimal k-partition is called the k-section width of the graph.

It is easy to find optimal k-sections only for "trivial" graphs as e.g. cycles, paths and complete graphs. The calculation of the k-section width for arbitrary graphs is *NP*-complete. This is already true for the bi-section problem [13], and it remains *NP*-complete by considering only d-regular graphs [6]. However, finding the k-section width is very difficult even for graphs for which computing the bi-section width is easy, as for hypercubes or grids [1, 3].

Many papers in the literature deal with the design of partition algorithms [10, 14] and the analysis of their optimality [7, 15], or with the complexity of partition problems. Different methods of calculating partitions of a graph have been proposed in the past by scientists from different fields like mathematics, computer science or engineering. There are also many software libraries available which include the most efficient graph partitioning approaches. For the evaluation of the quality of partition algorithms it is helpful to know good lower bounds for the k-section width.

There are only few approaches that are known for determining lower bounds on the k-section width of a graph. Leighton [18] proposes a lower bound of the bi-section width by calculating a routing scheme between all pairs of vertices such that the congestion is minimized. This technique can also be extended to the k-section width. Rendl and Wolkowicz get lower bounds using a different approach. They define the k-section problem as a semidefinite program and get the well known lower bound (1) stated below [12]. Furthermore they apply projection techniques from continuous optimization [16] to prove better lower bounds [20].

Lower bounds on the k-section width can also be derived from algebraic graph theory by relating the k-section problem to an eigenvalue problem. The well known lower bound on the k-section width $\nabla_k(G)$ of a graph $G = (V, E)$ with $n = |V|$ and the first k smallest eigenvalues $\lambda_1(G), \ldots, \lambda_k(G)$ of the Laplacian is (see section 2)

$$\nabla_k(G) \geq \sum_{i=1}^{k} \lambda_i(G) \cdot \frac{n}{2k}. \tag{1}$$

In [4] Bolla considers the spectra of hypergraphs and derives spectral bounds on the k-partitioning of them. In [5] Bolla and Tusnády also use spectral techniques to handle combinatorial problems concerning minimal k-cuts of weighted graphs. However, they do not require balanced partitioning sets.

In [2] the authors study relations between the second smallest eigenvalue and the bi-section width of graphs. They determine the case when the classical lower bound of the bi-section width of a graph is tight and derive new bounds in other cases. However, we need new ideas and further techniques to handle the relation between the structure of the k-section and the spectrum of a graph.

We show in the present paper that in (1) equality holds for a restricted number of graphs. In general, there is a large gap between this lower bound and the k-section width. For example, the first three smallest nonzero eigenvalues of a $\sqrt{n} \times \sqrt{n}$ torus are $\lambda_2 = \lambda_3 = \lambda_4 = 2 - 2\cos(\frac{2\pi}{\sqrt{n}}) \approx 4\pi^2/n$. Obviously, the 4-section width is $4\sqrt{n}$. However, the lower bound of inequality (1) does only result in a value of $\frac{3}{2}\pi^2$. According to Spielman and Teng, $\lambda_2 = O(\frac{1}{n})$ holds for bounded-degree planar graphs and two-dimensional meshes. Furthermore, $\lambda_2 = O(\frac{1}{n^{2/d}})$ for well-shaped d-dimensional meshes [21]. So there is a quadratic gap between the classical lower bound and the real value of the sum of the first k eigenvalues for a small k. Deriving new lower bounds which use $\sqrt{\sum_{i=1}^k \lambda_i}$ instead of $\sum_{i=1}^k \lambda_i$ for graphs with a grid-like structure, we close this quadratic gap up to a constant factor for this type of graphs.

To determine a new upper bound for $\sum_{i=1}^k \lambda_i$ we make use of the level structure of a k-section in which every level consists of all vertices which have the same distance to the cut. This leads to a generalized lower bound of (1) depending on the growth of the sizes of these levels in each section. Let $g : I\!N \to I\!N$ be a function. We will introduce the class of Level Structured graphs $LS(g, \nabla, k)$ which have a k-section with a cut size of ∇ and a level structure such that there are not more than $\nabla g(j)$ edges between vertices of distance j to the cut and vertices of distance $j+1$ to the cut. We get improved relations between the k-section width and $\sum_{i=1}^k \lambda_i$ for the graph class $LS(g, \nabla, k)$. These new relations differ from the classical bound (1) by a constant factor if the sum $\sum_{j=2}^{\infty} \frac{1}{g(j-1)}$ is bounded. In the other cases we prove that for $\frac{n}{\nabla} \to \infty$ there exists a constant δ with

$$\nabla \geq \delta \left(\sum_{i=1}^{k} \lambda_i \right)^{\beta} n(1 - o(1)), \tag{2}$$

where β is in the range $\frac{1}{2} \leq \beta < 1$. We also show that there are graphs for which the new bounds are tight up to a constant factor. These new bounds may also be used the other way around to get an upper bound of $\sum_{i=1}^k \lambda_i$ for any k-section with a cut size ∇ and a growth function g.

In general, the level structure of an optimal k-section is not known, but there are notable exceptions. If G is a graph of maximum degree d, then $G \in LS(g, \nabla, k)$ with $g(j) = (d-1)^j$. Thus, for $\frac{n}{\nabla} \to \infty$, we obtain a lower bound of

$$\nabla \geq \frac{k(d-2)+2}{k(d-2)} \cdot \frac{\sum_{i=1}^k \lambda_i(G) n}{2k}(1 - o(1)).$$

We expect that there exist further classes of graphs for which we can directly derive better lower bounds on the k-section width using the results of this work.

The contents of the paper are the following. Section 2 presents the basic relation of $\sum_{i=1}^k \lambda_i$ and the k-section width of graphs. In Section 3 we show a new relation between $\sum_{i=1}^k \lambda_i$ and the cut size ∇ of a k-section and demonstrate in section 4 that there are graphs for which the new bounds are tight up to a constant factor.

2 Theoretical Background

A k-partition of an undirected unweighted graph $G = (V, E)$ with $|V| = n$ and $k|n$ is a partition of $V = V_1 \uplus V_2 \uplus \ldots \uplus V_k$ such that $|V_i| = |V_j|$ for any $i, j \in \{1, \ldots, k\}$. Here $\uplus$ denotes the union of two disjoint sets. The number of edges connecting vertices from different partitioning sets V_i and V_j, $i, j \in \{1, \ldots, k\}$, $i \neq j$ is called the *cut size* of the k-partition. In the following we are interested in the minimum cut size among all partitions.

For a graph G, the $n \times n$ *Laplacian matrix* $L(G) = \{l_{v,w}\}$ is defined as

$$l_{v,w} = \begin{cases} \deg(v), & \text{if } v = w \\ -1, & \text{if } v \neq w \text{ and } \{v, w\} \in E \\ 0, & \text{otherwise} \end{cases}$$

It is known that all the eigenvalues of $L(G)$ are nonnegative. We denote them by $\lambda_1, \ldots, \lambda_n$ with $0 = \lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n$. They have the pairwise perpendicular eigenvectors $y_1, y_2, \ldots y_n$. The eigenvector with the eigenvalue 0 is $y_1 = \frac{1}{\sqrt{n}}(1, 1, 1, \ldots 1)$, and its multiplicity is equal to 1 since we consider connected graphs only (see e.g. [19]). Let $x = (x_1, x_2, \ldots, x_n)$ be a nonzero vector. It follows from the Courant-Fisher Theorem [23] that

$$\begin{aligned} \lambda_i(G) &= \max_{dim(U)=n-i+1} \left\{ \min_{x \in U} \left\{ \frac{x^t L x}{\|x\|^2} \right\} \right\} \\ &= \max_{dim(U)=n-i+1} \left\{ \min_{x \in U} \left\{ \frac{\sum\limits_{\{u,v\} \in E} (x_u - x_v)^2}{\sum\limits_{v \in V} {x_v}^2} \right\} \right\}. \end{aligned} \tag{3}$$

The well-known lower bound (1) on the k-section width was stated by Donath and Hoffman [11] using a modification of the famous Hoffman-Wielandt theorem [17].

A powerful tool for determining new lower bounds for the size of the optimal k-partitioning is the following Courant-Fischer-like inequality for the sum of the first k eigenvalues which generalizes the well-known upper bound of λ_2 over the Rayleigh-coefficient. This theorem can be derived immediately from the so-called Representation Theorem of [4]. We present a new proof using the result of [17].

Theorem 1 *Let $G = (V, E)$ be a graph and n, k two integers with $|V| = n$ and $k|n$. Let $\lambda_1, \lambda_2, \ldots, \lambda_k$ be the k smallest eigenvalues of $L(G)$. Then it holds*

$$\sum_{i=1}^{k} \lambda_i \leq \min_{x_1, \ldots, x_k} \left\{ \sum_{i=1}^{k} \frac{\sum_{(q,r) \in E} (x_{i,q} - x_{i,r})^2}{\sum_{q \in V} x_{i,q}^2} \;\middle|\; x_i \perp x_j \text{ for any } 1 \leq i, j \leq k,\ i \neq j \right\} \tag{4}$$

where $x_{i,q}$ denotes the q^{th} entry of the vector x_i.

Proof: Let N be a matrix with the elements $N_{i,j} = x_{\lfloor j/k \rfloor + 1, i}$. So, the first n/k columns contain the vector x_1, the next n/k columns contain the vector $x_2, \ldots$, the last n/k

columns contain the vector x_k. We consider now the trace of the matrix LNN^T. First we compute $L \cdot N$

$$(LN)_{1,1} = \cdots = (LN)_{1,n/k} = x_{1,1} deg_1 - \sum_{(1,j)\in E} x_{1,j},$$

where deg_1 denotes the degree of the vertex $1 \in V$. Moreover

$$(LN)_{1,r} = x_{\lfloor r/k \rfloor +1,1} \cdot deg_1 - \sum_{(1,j)\in E} x_{\lfloor r/k \rfloor +1,j}$$

for all $1 \le r \le n$. It also holds that

$$(LN)_{q,r} = x_{\lfloor r/k \rfloor +1,q} \cdot deg_q - \sum_{(q,j)\in E} x_{\lfloor r/k \rfloor +1,j}, \text{ with } q, r \in \{1, \ldots, n\}.$$

Again, deg_q denotes the degree of the vertex $q \in V$. Multiplying (LN) with N^T we obtain

$$\begin{aligned}(LNN^T)_{q,q} &= \frac{n}{k}\left(x_{1,q}^2 deg_q - \sum_{(q,j)\in E} x_{1,j}x_{1,q} + x_{2,q}^2 deg_q \right. \\ &\left. - \sum_{(q,j)\in E} x_{2,j}x_{2,q} + \cdots + x_{k,q}^2 deg_q - \sum_{(q,j)\in E} x_{k,j}x_{k,q} \right).\end{aligned}$$

Then

$$Tr(LNN^T) = \frac{n}{k} \sum_{i=1}^{k} \sum_{(q,r)\in E} (x_{i,q} - x_{i,r})^2.$$

On the other hand the spectrum of NN^T is the same as the spectrum of N^TN. Using the fact that x_i and x_j are perpendicular for each pair of i, j, $1 \le i, j \le k$ with $i \ne j$ we obtain that the eigenvalues of NN^T are $n - k$ times 0 and each $\frac{n}{k}\sum_{q\in V} x_{i,q}^2$ once, where $i \in \{1, \ldots, k\}$. Then we have

$$\sum_{i=1}^{k} \sum_{(q,r)\in E} (x_{i,q} - x_{i,r})^2 \ge \lambda_1 \sum_{q\in V} x_{1,q}^2 + \cdots + \lambda_k \sum_{q\in V} x_{k,q}^2$$

where $\sum_{q\in V} x_{1,q}^2 \ge \sum_{q\in V} x_{2,q}^2 \ge \cdots \ge \sum_{q\in V} x_{k,q}^2$. We obtain the theorem by normalizing the vectors $x_1, x_2, \ldots, x_k$. □

From Theorem 1 we obtain the classical lower bound for the size of the optimal k-partitioning in the following way. Let $V = V_1 \uplus V_2 \uplus \ldots \uplus V_k$ be the optimal k-partitioning of G. We consider the vectors $x_1, x_2, \ldots, x_k$ with the entries $x_{i,j} = 1$ whenever the vertex $j \in V_i$, and $x_{i,j} = 0$ otherwise. Using inequality (4) we obtain the inequality (1).

In the following theorem we determine the case when the classical lower bound is tight.

Theorem 2 *Let $G = (V, E)$ be a graph, and let $V = V_1 \uplus V_2 \uplus \ldots \uplus V_k$ be an optimal k-partitioning of G with a cut size ∇, where $|V| = n$ and $k|n$. Let $\lambda_1, \lambda_2, \ldots, \lambda_k$ be the first k smallest eigenvalues of $L(G)$ and let $x_1, x_2, \ldots, x_k$ be the corresponding eigenvectors. We represent with $x_{i,j}$ the j^{th} entry of x_i for any $1 \le i \le k$ and $1 \le j \le n$. Then the statement*

a. $\nabla = \frac{n}{2k} \sum_{i=1}^{k} \lambda_i$

implies that

b. if $q, r \in V_i$ for an $i \in \{1, \ldots, k\}$ then $x_{j,q} = x_{j,r}$ for any $j \in \{1, \ldots, k\}$;

and

c. for any $i, j \in \{1, \ldots, k\}$, $i \neq j$ and any two vertices $q, r \in V_i$ the number of adjacent vertices to q in V_j equals the number of adjacent vertices to r in V_j.

Proof: We prove that statement (a) implies (b) and (b) implies (c).

(a) → (b): The Courant-Fischer Theorem [23] implies that by adding an additional edge to a graph G there exists no eigenvalue λ_i, $i \in \{1, \ldots, |V|\}$, of $L(G)$ which decreases (see equation (3)). For simplicity we assume that all eigenvalues are simple. Let $\nabla = \frac{n}{2k} \sum_{i=1}^{k} \lambda_i$ and let $V = V_1 \uplus V_2 \uplus \ldots \uplus V_k$ be an optimal k-partition of G. Assume there exists $i, j \in \{1, \ldots, k\}$ and two vertices $q, r \in V_i$ such that $x_{j,q} \neq x_{j,r}$. (Note that x_j is the eigenvector of $L(G)$ with the eigenvalue λ_j.) We can assume w.l.o.g. that x_j is the eigenvector corresponding to the smallest eigenvalue with this property, so $x_{1,q} = x_{1,r}$, $x_{2,q} = x_{2,r}$, $\ldots$, $x_{j-1,q} = x_{j-1,r}$. If there is no edge between q and r, then equation (3) implies that if we add the edge (q, r) to the graph G then x_1, x_2, $\ldots$, x_{j-1} remain eigenvectors corresponding to the first $j-1$ eigenvalues of G with this new edge added to it, and λ_j increases without increasing the optimal cut of the k-partition. Thus we have a contradiction to inequality (1).

If there is an edge between q and r then we consider the cartesian product $G \times K_n$ of G with the complete graph K_n. We denote with $w_1, \ldots, w_n$ the vertices of K_n. Then the vertex (v, w_m) of $G \times K_n$ is adjacent to $(v', w_{m'})$ iff $(v, v') \in E$ and $w_m = w_{m'}$ or $v = v'$. The eigenvalues of $G \times K_n$ have the form $\lambda_i + \mu_j$ where μ_j are the eigenvalues of K_n [8]. Therefore the first k eigenvalues of $G \times K_n$ still remain $\lambda_1, \lambda_2, \ldots, \lambda_k$ and the classical lower bound will still be tight. Let y_j be the eigenvector of $G \times K_n$ with the eigenvalue λ_j, $j \in \{1, \ldots, k\}$. Furthermore $y_{j,l,m}$ represents the entry of y_j for the vertex (l, w_m) of $G \times K_n$. Then it also holds that $y_{j,l,m} = x_{j,l}$ for any $w_m \in \{1, \ldots, |V|\}$ and arbitrary j, l. Now, since we assumed that $x_{j,q} \neq x_{j,r}$ it follows that $y_{j,q,m} \neq y_{j,r,m'}$ for any $w_m, w_{m'} \in \{1, \ldots, |V|\}$. By adding the edge $((q, w_m), (r, w_{m'}))$ to the graph $G \times K_n$ we increase λ_j and this leads to a contradiction to inequality (1).

Similar arguments apply if there exist multiple eigenvalues.

(b) → (c): Assume that $x_{i,q} = x_{i,r}$ if $q, r \in V_j$ for any $i, j \in \{1, \ldots, k\}$. Let x_i^j be the entry of the eigenvector x_i for each vertex $v \in V_j$ (so, $x_{i,q} = x_{i,r} = x_i^j$). Consider the

system of linear equations

$$X \cdot z_j \;=\; b^j \tag{5}$$

where $X = (x_i^s)$, $b^j = (\lambda_i x_i^j)$, and $z_j = (z_{j,s})$, $1 \le j, s \le k$ (z_j is the vector of indeterminants). Let $e_j = (e_{j,s})_{1 \le s \le k}$ where $e_{j,s}$ is the number of vertices in V_s adjacent to the vertex $v \in V_j$ if $s \ne j$, and $e_{j,j} = -\sum_{1 \le s \le k, s \ne j} e_{j,s}$ otherwise. Obviously e_j is a solution of (5). Since $x_1, \ldots, x_k$ are pairwise perpendicular, X has full rank and thus e_j is unique. But the system of linear equations (5) also holds for all $u \in V_j, u \ne v$, and so (c) follows. □

Now, the question arises: Does *(c)* imply *(a)*? The answer is no. Consider for example the hypercube $Q(m)$ with $m \ge 4$, and let $k = 4$. The first three nonzero eigenvalues of $Q(m)$ are $\lambda_2 = \lambda_3 = \lambda_4 = 2$. The minimal cut of the 4-partition is 2^m and condition *(c)* of Theorem 2 is fulfilled. However, the lower bound of the inequality (1) is $2^m \frac{3}{4}$. Examples of graphs for which the bound in (1) is tight are the complete graph or the complete bipartite graph. However, if *(c)* of theorem 2 holds, then there exist some eigenvalues $\lambda_{i_1}, \ldots, \lambda_{i_k}$ (not necessarily the first k smallest) of G such that $\nabla = \frac{n}{2k} \sum_{j=1}^{k} \lambda_{i_j}$.

3 New Spectral Bounds using the Structure of Graphs

In Theorem 2 we showed that, if the lower bound in inequality (1) is tight, then any vertex of G must be incident to a cut edge. Now, we consider the case where this condition is not satisfied, and show that for such graphs the lower bound can be improved significantly. This new result holds for arbitrary structures of the k-section and does not depend on the number and the positions of the cut-edges.

In the following, we consider the level structure of a k-section. Each level of vertices consists of the vertices which have the same distance to the cut.

Definition 1 (Level Structure) *Let $V = V_1 \uplus V_2 \uplus \ldots \uplus V_k$ be a k-section of a graph $G = (V, E)$ with $n = |V|$ and assume that $k|n$. Define the subsets V_i^j of V_i, $i \in \{1, \ldots, k\}$ as follows. Let V_i^1 be the set of all vertices in V_i which are incident to a cut edge. Let V_i^j be the set of all vertices in V_i with distance $j-1$ to V_i^1. Furthermore, denote with E_i^j, $j \ge 1$, $i \in \{1, \ldots, k\}$, the edge sets which connect vertices between sets V_i^j and V_i^{j+1}.*

Let $g : \mathbb{N} \to \mathbb{N}$ be a function. We denote with $LS(g, \nabla, k)$ the class of graphs which have a k-section with a cut size ∇ and a level structure such that $|E_i^j| \le \nabla g(j)$ for all $j \ge 1$ and $i \in \{1, \ldots, k\}$.

In a certain sense the level structure can be viewed as k cones where the cone ends are connected by some edges. The function g represents their widths. For graphs with large width of the cone, information can flow more easily to the distant vertices and therefore we can view this as a global expansion property. In the following we show that for a fixed k-section width the spectral lower bound increases with the width of the cone.

In Lemma 1 we bound $\sum_{i=1}^{k} \lambda_i$ from above by some expression depending only on the growth function $g(j)$. This result will be used in Theorem 3 below.

Lemma 1 *Let $G \in LS(g, \nabla, k)$ and let $l \in I\!N$ be a number such that $n > k\nabla \sum_{j=1}^{l-1} g(j-1)$. Then*

$$\sum_{i=1}^{k} \lambda_i \leq \min_{1=a_1 \leq a_2 \leq \cdots \leq a_l} \frac{2\nabla a_1^2 + k\nabla \sum_{j=1}^{l-1} g(j)(a_j - a_{j+1})^2}{\nabla \sum_{j=1}^{l-1} a_j^2 g(j-1) + a_l^2 \left(\frac{n}{k} - \nabla \sum_{j=1}^{l-1} g(j-1)\right)}.$$

Proof: We define some vectors $x_1, \ldots, x_k$ which are pairwise perpendicular, so $x_i \perp x_j$ for any $1 \leq i, j \leq k$, $i \neq j$. We choose the vectors x_i with entries $x_{i,v}$ for $v \in V$ defined by

$$x_{i,v} = \begin{cases} a_j, & \text{if } v \in V_i^j \\ 0, & \text{otherwise} \end{cases} \tag{6}$$

with $1 = a_1 \leq a_2 \leq \cdots \leq a_l$. The upper bound of (4) from Theorem 1 now only depends on the a_j's. Denote by $A(x_i) := \sum_{\{u,v\} \in E} (x_{i,u} - x_{i,v})^2$ the numerators in (4). Let $Q_{i,m}$ be the number of edges separating V_i from V_m for $m \in \{1, \ldots, k\}$. One has

$$\begin{aligned} A(x_i) &= \sum_{m=1}^{k} Q_{i,m} a_1^2 + \sum_{j=1}^{l-1} |E_i^j| (a_j - a_{j+1})^2 \qquad (7) \\ &\leq \sum_{m=1}^{k} Q_{i,m} a_1^2 + \nabla \sum_{j=1}^{l-1} g(j)(a_j - a_{j+1})^2, \end{aligned}$$

where $Q_{i,i} = 0$. To estimate the denominators $B(x_i) := \sum_{v \in V} x_{i,v}^2$ of the inequality (4) from theorem 1, assume $|V_i^j| < |E_i^{j-1}|$ for some j, $1 \leq j < l$. Let $\tilde{x}_i$ be the corresponding vector for the level structure obtained by moving a vertex from V_i^l to V_i^j. One has $B(\tilde{x}_i) - B(x_i) = a_j^2 - a_l^2 < 0$. Therefore, $B(x_i)$ will not increase after this transformation. Since $|V_i^j| \leq |E_i^{j-1}|$, the minimum of $B(x_i)$ (for a fixed part V_i) is attained if $|V_i^j| = |E_i^{j-1}| \leq \nabla g(j-1)$ for $1 \leq j < l$. By summing $\frac{A(x_i)}{B(x_i)}$ over all $i \in \{1, \ldots, k\}$ we obtain

$$\sum_{i=1}^{k} \lambda_i \leq \sum_{i=1}^{k} \frac{A(x_i)}{B(x_i)} \leq \frac{2\nabla a_1^2 + k\nabla \sum_{j=1}^{l-1} g(j)(a_j - a_{j+1})^2}{\nabla \sum_{j=1}^{l-1} a_j^2 g(j-1) + a_l^2 \left(\frac{n}{k} - \nabla \sum_{j=1}^{l-1} g(j-1)\right)}.$$

□

Lemma 1 shows that the level structure of the k-section gives an upper bound on $\sum_{i=1}^{k} \lambda_i$. In fact, the proof of the lemma shows that the worst case occurs if $|V_i^j| = \nabla \cdot g(j-1)$ holds for any level j. We will use Lemma 1 in the following theorem to derive new relations between $\sum_{i=1}^{k} \lambda_i$ and the cut size ∇ of a k-section. These relations depend on the growth of the function g.

Theorem 3 *Let $G \in LS(g, \nabla, k)$. Then there exists a function $\gamma : I\!R^+ \to I\!R$ with $\gamma(x) \to 0$ for $x \to \infty$ such that*

- *If* $A := 1 + \frac{2}{k}\sum_{j=2}^{\infty}\frac{1}{g(j-1)}$ *and* $\sum_{j=2}^{\infty}\frac{j-1}{g(j-1)} < \infty$, *then*

$$\nabla \geq A\frac{\sum_{i=1}^{k}\lambda_i n}{2k}(1-\gamma(\frac{n}{\nabla})).$$

- *Let* $LambertW(x)$ *be the inverse function of* $x \cdot e^x$. *If* $g(j) = (j+1)$, *then*

$$\nabla \geq LambertW\left(\frac{4k}{\sum_{i=1}^{k}\lambda_i}\right) \cdot \frac{\sum_{i=1}^{k}\lambda_i n}{2k^2}(1-\gamma(\frac{n}{\nabla})),$$

- *If* $g(j) = (j+1)^{\alpha}$ *and* $0 \leq \alpha < 1$, *then there exists a constant* $\delta(\alpha)$, *such that*

$$\nabla \geq \delta(\alpha)(\sum_{i=1}^{k}\lambda_i)^{\frac{\alpha+1}{2}}n(1-\gamma(\frac{n}{\nabla})).$$

Proof: Let $l \in I\!N$ be defined by $k\nabla\sum_{j=1}^{l-1}g(j-1) < n \leq k\nabla\sum_{j=1}^{l}g(j-1)$. This, in particular, implies $\frac{n}{\nabla} \to \infty$ as $l \to \infty$. We apply lemma 1 with $a_j = 1 + \frac{2}{k}\sum_{m=2}^{j}\frac{1}{g(m-1)}$. Since $2a_1^2 + k\sum_{j=1}^{l-1}g(j)(a_j - a_{j+1})^2 = 2 + \frac{4}{k}\sum_{j=1}^{l-1}\frac{1}{g(j)} = 2a_l$ we obtain

$$\sum_{i=1}^{k}\lambda_i \leq \frac{2\nabla a_l}{\nabla\sum_{j=1}^{l-1}a_j^2 g(j-1) + a_l^2\left(\frac{n}{k} - \nabla\sum_{j=1}^{l-1}g(j-1)\right)} \leq \frac{2a_l}{\sum_{j=1}^{l-1}a_j^2 g(j-1)}. \quad (8)$$

In the following we use some functions γ_1, γ_2, γ_3 and γ_4 with the property described in the theorem for the function γ.

- $A := 1 + \frac{2}{k}\sum_{j=2}^{\infty}\frac{1}{g(j-1)} < \infty$: Set $r_j := A - a_j$, $1 \leq j \leq l$, with $r_j > 0$. The first inequality of (8) implies

$$\begin{aligned}\sum_{i=1}^{k}\lambda_i &\leq \frac{2\nabla(A-r_l)}{\nabla\sum_{j=1}^{l-1}(A-r_j)^2 g(j-1) + (A-r_l)^2\left(\frac{n}{k} - \nabla\sum_{j=1}^{l-1}g(j-1)\right)} \\ &\leq \frac{2\nabla(A-r_l)}{\nabla A^2\sum_{j=1}^{l-1}(1-\frac{2r_j}{A})g(j-1) + A^2(1-\frac{2r_l}{A})\left(\frac{n}{k} - \nabla\sum_{j=1}^{l-1}g(j-1)\right)}\end{aligned}$$

We know that $\lim_{l\to\infty}\frac{2r_l}{A} = 0$. Now we have to give an upper bound for $\lim_{l\to\infty}\sum_{j=1}^{l-1}\frac{2r_j}{A}g(j-1)$. Using the Chebishev inequalities we obtain

$$\sum_{j=1}^{l-1}\frac{2r_j}{A}g(j-1) \leq \frac{\sum_{j=1}^{l-1}2r_j \cdot \sum_{j=1}^{l-1}g(j-1)}{A \cdot l}.$$

Now, $\sum_{j=1}^{l-1} \frac{2r_j}{A} = \frac{2}{A}\sum_{j=1}^{l-1} \frac{j-1}{g(j-1)}$ and therefore there exists a γ_1 such that $\sum_{j=1}^{l-1} \frac{2r_j}{A} g(j-1) \le \gamma_1(l) \sum_{j=1}^{l-1} g(j-1)$. Then we have

$$\sum_{i=1}^{k} \lambda_i = \frac{2\nabla(A-r_l)}{\nabla A^2(1-\gamma_1(l))\sum\limits_{j=1}^{l-1} g(j-1) + A^2(1-\gamma_2(l))\left(\frac{n}{k} - \nabla\sum\limits_{j=1}^{l-1} g(j-1)\right)}.$$

Then it follows:

$$\sum_{i=1}^{k} \lambda_i \le \frac{2k\nabla}{A \cdot n(1-\gamma(l))}.$$

- $g(j) = (j+1)$: Note that $\ln(n+1) = \int_1^{n+1} \frac{1}{x} dx \le \sum_{j=1}^{n} \frac{1}{j} \le 1 + \int_1^n \frac{1}{x} dx = 1 + \ln(n)$. Therefore, the second inequality in (8) with $g(j) = j+1$ provides

$$\begin{aligned}\sum_{i=1}^{k} \lambda_i &\le \frac{2a_l}{\sum\limits_{j=1}^{l-1} j \cdot a_j^2} \le \frac{\frac{4}{k}\ln(l)(1+\gamma_1(l))}{1+\sum\limits_{j=2}^{l-1} j(\frac{2}{k}\ln(j+1) + \frac{k-2}{k})^2} \\ &\le \frac{\frac{4}{k}\ln(l)(1+\gamma_1(l))}{1+\int\limits_1^{l-1}(\frac{4}{k^2}x\ln^2(x+1)(1+\gamma_2(\frac{n}{\nabla})))dx} \\ &\le \frac{2k}{l^2\ln(l)(1-\gamma_3(\frac{n}{\nabla}))}.\end{aligned}$$

It follows from $n \le k\nabla\sum_{j=1}^{l} j = k\nabla\frac{l^2}{2}(1+\gamma_3(\frac{n}{\nabla}))$ that $l \ge \sqrt{\frac{2n}{k\nabla}(1+\gamma_3(\frac{n}{\nabla}))}$. This leads to $\sum_{i=1}^{k} \lambda_i \le \frac{k^2\nabla}{n\ln(\sqrt{2n/k\nabla})}(1+\gamma_3(\frac{n}{\nabla}))$. Solving this equation in ∇ we get the theorem.

- $g(j) = (j+1)^\alpha$ with $0 \le \alpha < 1$: Since $\sum_{j=1}^{l} j^\beta = \frac{l^{\beta+1}}{\beta+1}(1+\gamma_1(l))$ for $\beta > -1$, it holds

$$\begin{aligned}\sum_{i=1}^{2} \lambda_i &\le \frac{2a_l}{\sum\limits_{j=1}^{l-1} j^\alpha a_j^2} \le \frac{\frac{4}{k}\cdot\frac{l^{1-\alpha}}{1-\alpha}}{\sum\limits_{j=1}^{l-1} j^\alpha \frac{4}{k^2}(\frac{j^{1-\alpha}}{1-\alpha})^2(1-\gamma_1(\frac{n}{\nabla}))} \\ &= \frac{k(1-\alpha)l^{1-\alpha}}{\sum\limits_{j=1}^{l-1} j^{2-\alpha}(1-\gamma_1(\frac{n}{\nabla}))} \le \frac{k(1-\alpha)(3-\alpha)}{l^2(1-\gamma_2(\frac{n}{\nabla}))}.\end{aligned}$$

From $n \le k\nabla\sum_{j=1}^{l} j^\alpha = k\nabla\frac{l^{\alpha+1}}{\alpha+1}(1+\gamma_3(\frac{n}{\nabla}))$ it follows that $l \ge (\frac{n(\alpha+1)}{k\nabla(1+\gamma_3(\frac{n}{\nabla}))})^{\frac{1}{\alpha+1}}$. This leads to

$$\sum_{i=1}^{k} \lambda_i \le \frac{k(1-\alpha)(3-\alpha)}{(\frac{n(\alpha+1)}{k\nabla})^{\frac{2}{\alpha+1}}(1-\gamma_4(\frac{n}{\nabla}))} \quad \text{, i. e.}$$

$$\nabla \geq \frac{(1+\alpha) \cdot \left(\sum_{i=1}^{k} \lambda_i\right)^{\frac{\alpha+1}{2}} n}{k(k(1-\alpha)(3-\alpha))^{\frac{\alpha+1}{2}}} (1 - \gamma(\frac{n}{\nabla})).$$

□

As an important application of Theorem 3 we obtain the following corollary:

Corollary 1 *Let G be a graph of maximum degree d. Then $G \in LS(g, \nabla_k(G), k)$ with $g(j) = (d-1)^j$. Then we have*

$$\nabla_k(G) \geq \frac{k(d-2)+2}{k(d-2)} \cdot \frac{\sum_{i=1}^{k} \lambda_i n}{2k} (1 - o(1)), \text{ as } l \to \infty.$$

Proof: Theorem 3 implies

$$\begin{aligned} \nabla_k(G) &\geq A \frac{\sum_{i=1}^{k} \lambda_i n}{2k} (1 - o(1)) \\ &= \left(1 + \frac{2}{k} \left(\sum_{j=1}^{\infty} \frac{1}{(d-1)^j}\right)\right) \frac{\sum_{i=1}^{k} \lambda_i n}{2k} (1 - o(1)) \\ &= \frac{k(d-2)+2}{k(d-2)} \cdot \frac{\sum_{i=1}^{k} \lambda_i n}{2k} (1 - o(1)), \text{ as } l \to \infty. \end{aligned}$$

□

4 Graph Classes

Now we present examples for which the results of the previous section are asymptotically tight. Firstly, we introduce a new class of edge-weighted graphs. They belong to the class $LS(g, \nabla, k)$ with $g(j) = (j+1)^\alpha$. Secondly, we analyze the k-rooted trees as a more realistic example.

The Laplacian of a graph can also be generalized for edge weighted graphs, where the off-diagonal entries contain the negative values of the corresponding edge weight. The results of the previous sections and, especially, Theorem 3 can also easily be generalized to edge weighted graphs.

Definition 2 *Denote with $B_{l,k}^\alpha$, $\alpha \geq 0$ and $l \geq 1$, the edge-weighted graph obtained as follows. $B_{l,k}^\alpha$ consists of k isomorphic subgraphs. Each of these subgraphs consists of l levels of vertices with j^α vertices in level j, $1 \leq j \leq l$. Edges connect every pair of vertices in consecutive levels. Each edge between vertices in levels j and $j+1$ is weighted by $\frac{1}{j^\alpha}$. Moreover, the vertex on level 1 of each subgraph is connected to the vertices on level 1 of all other subgraphs by an edge of weight $\frac{2}{k}$.*

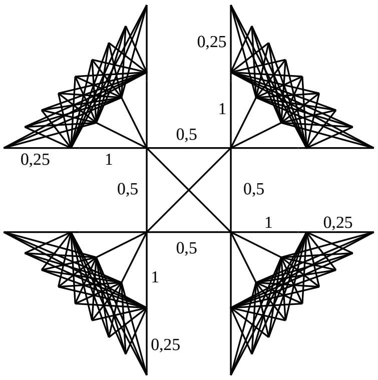

Figure 1: The structure of the graph $B^2_{3,4}$. The values indicate the weight of the edges.

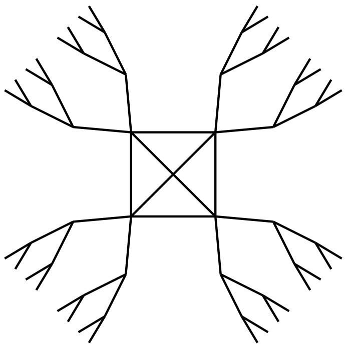

Figure 2: The structure of the graph $T_{3,4,4}$.

The graphs $B^{\alpha}_{l,k}$ belong to the class $LS(g, k-1, k)$ with $g(j) = (j+1)^{\alpha}$. An example with $\alpha = 2$, $l = 3$ and $k = 4$ is presented in Figure 1. In the following we compute the eigenvalues of such a graph.

Theorem 4 *Denoting by $\lambda_i(B^{\alpha}_{l,k})$, $1 \leq i \leq k$, the first k eigenvalues of the Laplacian of $B^{\alpha}_{l,k}$ there exist some constants $c_1(\alpha)$ and $c_2(\alpha)$ such that*

$$\lambda_i(B^{\alpha}_{l,k}) = \begin{cases} \frac{2k}{n(1+2\sum_{j=2}^{\infty}\frac{1}{g(j-1)})}(1+o(1)) & \text{if } \alpha > 1 \\ c_1(\alpha)\frac{1}{n\ln(n)}(1+o(1)) & \text{if } \alpha = 1 \\ c_2(\alpha)\left(\frac{1}{n}\right)^{\frac{2}{\alpha+1}}(1+o(1)) & \text{if } 0 \leq \alpha < 1. \end{cases}$$

Proof: To compute the eigenvalues $\lambda_i(B^{\alpha}_{l,k})$ we use the following observation. The eigenvalues of a square matrix of the form

$$\begin{bmatrix} A & C & C & \dots & C \\ C & A & C & \dots & C \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ C & C & C & \dots & C \\ C & C & C & \dots & A \end{bmatrix} \tag{9}$$

are the eigenvalues of the matrix

$$A + \sum_{j=1}^{k-1}(\sqrt[k]{1})^{(i-1)\cdot j}\cdot C = \begin{cases} A+(k-1)\cdot C & \text{if } i = 1 \\ A - C & \text{otherwise} \end{cases}$$

where $\sqrt[k]{1} = \cos(\frac{2\pi}{k}) + I\cdot\sin(\frac{2\pi}{k})$ (see [9]). Here A and C are square matrices. Then it follows that the eigenvalues of $A - C$ appear $k-1$ times as eigenvalues of the original matrix.

Now, the Laplacian of $B^{\alpha}_{l,k}$ has the form of the matrix in (9) where A represents one subgraph of $B^{\alpha}_{l,k}$ and C represents a single edge which separates one subgraph from another in $B^{\alpha}_{l,k}$. So $C_{1,1} = -\frac{2}{k}$, and all other entries of C are 0; furthermore A contains the Laplacian of a subgraph of $B^{\alpha}_{l,k}$ where we add the value $\frac{2(k-1)}{k}$ to $A_{1,1}$. Now the first k smallest eigenvalues of $B^{\alpha}_{l,k}$ are as follows: 0 appears once, and the smallest eigenvalue of $A - C$ appears $k-1$ times. But the smallest eigenvalue of the matrix $A - C$ is the second smallest eigenvalue of the Laplacian of the graph $B^{\alpha}_{l,2}$ which has been already computed (see theorem 4 and 5 in [2]). Hence, the theorem follows. □

The example of the graph $B^{\alpha}_{l,k}$ shows that the bounds calculated in Theorem 3 are tight up to a constant factor.

Let us analyze a $\sqrt{n} \times \sqrt{n}$ torus which belongs to the class $LS(g, 4 \cdot \sqrt{n}, 4)$ with $g(x) = 1$ which has to be partitioned into four parts. Figure 3 illustrates the optimal 4-section of an 8×8-torus. The sum of the first three nonzero eigenvalues is about $\frac{12\pi^2}{n}$ and the upper bound computed by Theorem 3 is $\frac{12 \cdot (16)^2}{n}$. They differ only by a constant factor.

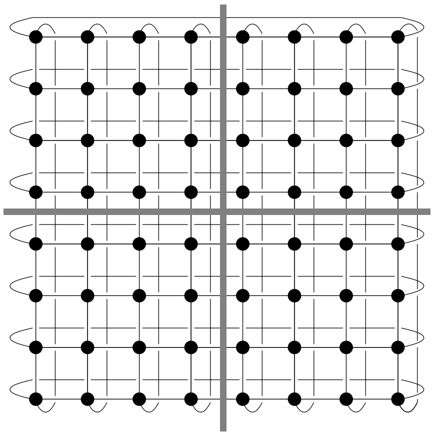

Figure 3: The optimal 4-section of an 8×8-torus.

As another example we define the k-rooted tree as follows (see Figure 2).

Definition 3 *The k-rooted tree $T_{d,l,k}$ consists of k complete $(d-1)$-ary subtrees, and every vertex of these subtrees at distance $1, 2, \ldots, l-2$ from the root has degree d. The vertices which are at distance $l-1$ from the root have degree 1. The roots of the trees are pairwise connected with each other, and therefore the degree of these roots equals $(k-1) + (d-1)$.*

Now we compute the smallest k eigenvalues of such a k-rooted tree and show that the spectral lower bound provided by Theorem 3 differs from the k-section width only by a small constant factor. Denote with $\lambda_1, \lambda_2, \ldots, \lambda_k$ the smallest k eigenvalues of the Laplacian of the k-rooted tree $T_{d,l,k}$. Furthermore, let $A(T_{d,l,k})$ be the adjacency matrix of a weighted k-rooted tree in which each leaf has a loop of weight $d-1$ and each root has a loop of weight $2-k$. Denoting with μ_i the eigenvalues of $A(T_{d,l,k})$ it follows that $\lambda_i = d - \mu_{n-i+1}$.

Therefore it is sufficient to concentrate on the computation of the eigenvalues of $A(T_{d,l,k})$. Using the techniques of theorem 4 we get $\mu_n = d$. Furthermore we obtain that $\mu_{n-1} = \ldots = \mu_{n-k+1}$ is the largest eigenvalue of the adjacency matrix of a weighted $d-1$-ary tree with height $l-1$ and with a loop of weight $1-k$ at the root and a loop of weight $d-1$ at the leaves. As shown in [22], the largest eigenvalue of such a matrix equals the largest eigenvalue of the adjacency matrix of a weighted path of length l with a loop of weight $1-k$ at one end and a loop of weight $d-1$ at the other end. The edges between two consecutive vertices have weight $\sqrt{d-1}$.

Denote with $Q(X)$ the characteristic polynomial of the adjacency matrix corresponding to such a weighted path. Then

$$Q(X) = (X + (k-1))P_{l-1}(X) - (d-1)P_{l-2}(X),$$

where $P_i(X)$ is the characteristic polynomial of the adjacency matrix corresponding to the weighted path of length i described above without the loop of weight $1-k$ at the one end. As described in [22] it can be easily checked that if we set $X = 2\sqrt{d-1}\cosh(\phi)$, then

$$P_l(X) = XP_{l-1}(X) - (d-1)P_{l-2}(X) = (d-1)^{l/2}\frac{\sinh((l+1)\phi) - \sqrt{d-1}\sinh(l\phi)}{\sinh(\phi)}. \quad (10)$$

Now we are ready to state the following theorem.

Theorem 5 *For large l the first $k-1$ nonzero eigenvalues of the Laplacian of the graph $T_{d,l,k}$ satisfy*

$$\lambda_i = \left(\frac{k(d-2)^2}{d+k-2} - o(1)\right)\frac{1}{(d-1)^l}.$$

Proof: Using equation (10) we obtain

$$\begin{aligned}
Q(X) &= XP_{l-1}(X) - (d-1)P_{l-2}(X) + (k-1)P_{l-1}(X) = P_l(X) + (k-1)P_{l-1}(X) \\
&= \frac{(d-1)^{l/2}}{\sinh(\phi)}\Big(\sqrt{d-1}\cdot\sinh((l+1)\phi) - (d-1)\sinh(l\phi) \\
&\quad + (k-1)\sinh(l\phi) - (k-1)\sqrt{d-1}\cdot\sinh((l-1)\phi)\Big) \\
&= \frac{(d-1)^{l/2}}{\sinh(\phi)}\Big(\sqrt{d-1}(\sinh(l\phi)\cosh(\phi) + \sinh(\phi)\cosh(l\phi)) \\
&\quad - (d-k)\sinh(l\phi) - (k-1)\sqrt{d-1}(\sinh(l\phi)\cosh(\phi) - \sinh(\phi)\cosh(l\phi))\Big) \\
&= \frac{(d-1)^{l/2}\cosh(l\phi)}{\sinh(\phi)}\Big(\sqrt{d-1}(\tanh(l\phi)\cosh(\phi) + \sinh(\phi)) \\
&\quad - (d-k)\tanh(l\phi) - (k-1)\sqrt{d-1}(\tanh(l\phi)\cosh(\phi) - \sinh(\phi))\Big) \\
&= \frac{(d-1)^{l/2}\cosh(l\phi)}{\sinh(\phi)}\Big(\sqrt{d-1}(2-k)\tanh(l\phi)\cosh(\phi) \\
&\quad - (d-k)\tanh(l\phi) + \sqrt{d-1}\cdot k\cdot\sinh(\phi)\Big).
\end{aligned}$$

Let $Q'(X)$ be defined by

$$Q(X) = \frac{(d-1)^{l/2}\cosh(l\phi)}{\sinh(\phi)} Q'(X).$$

Obviously $Q(X) = 0$ iff $Q'(X) = 0$. Theorem 3 implies that $2\sqrt{d-1}\cosh(\phi) = d - O(\frac{1}{(d-1)^l})$. Since $\lim_{x\to\infty} \tanh x = 1 - (2+o(1))e^{-2x}$, we get

$$\tanh(l\phi) = 1 - (2+o(1))(d-1+o(1))^{-l} = 1 - 2(d-1)^{-l} - o(1)(d-1)^l. \quad (11)$$

Using equation (11) and the fact that $\sinh(\phi) = \sqrt{\cosh^2(\phi) - 1}$, $Q'(X) = 0$ yields

$$\begin{aligned}\sqrt{d-1}\cdot k\sqrt{\cosh^2(\phi)-1} &= 2\left(\sqrt{d-1}(2-k)\frac{d}{2\sqrt{d-1}} - (d-k)\right)(d-1)^{-l} \\ &\quad +(d-k) - \sqrt{d-1}(2-k)\cosh(\phi) - o(1)(d-1)^{-l}.\end{aligned}$$

Squaring both sides leads to

$$\begin{aligned}(d-1)k^2(\cosh^2(\phi)-1) &= ((d-k) - \sqrt{d-1}(2-k)\cosh(\phi))^2 \\ &\quad +2((d-k) - \sqrt{d-1}(2-k)\cosh(\phi)) \\ &\quad \cdot(((2-k)d/2) - (d-k))\cdot 2(d-1)^{-l} - o(1)(d-1)^{-l}.\end{aligned}$$

Hence

$$\begin{aligned}0 &= 4(d-1)(k-1)\cosh^2(\phi) \\ &\quad -2\sqrt{d-1}(k-2)((d-k) - k(d-2)(d-1)^{-l})\cosh(\phi) \\ &\quad -(d(d-2k+k^2) - 2(d-k)k(d-2)(d-1)^{-l}) - o(1)(d-1)^{-l}.\end{aligned}$$

Calculating $\cosh(\phi)$ we get

$$\cosh(\phi) = \frac{d}{2\sqrt{d-1}} - \frac{k(d-2)^2}{2\sqrt{d-1}(d+k-2)}\cdot\frac{1}{(d-1)^l} + o(1)\frac{1}{(d-1)^l}.$$

Taking into account, that $\lambda_i = d - 2\sqrt{d-1}\cdot\cosh(\phi)$ for any $2 \le i \le k$, we obtain the theorem. $\square$

Note that $T_{d,l,k}$ belongs to the graph class $LS(g, k-1, k)$ with $g(j) = (d-1)^j$. Let $n = k\frac{(d-1)^l - 1}{d-2}$ denote the number of vertices of $T_{d,l,k}$. Using Theorem 3 we obtain that

$$\sum_{i=2}^{k} \lambda_i \le (k-1)k\frac{(d-2)k^2}{(k(d-2)+2)n(1+o(1))}.$$

There is a factor of $\frac{kd-2k+k^2}{kd-2k+2}$ in which the upper bound differs from the sum of the first k eigenvalues of $T_{d,l,k}$. This factor grows with an increasing number of partitions. However, if d is much larger than k, then this factor is nearly 1. The example $T_{d,l,k}$ also shows that if the growth of the function g defined in the previous section is smaller than the number of different partitions, then the gap between the new bound and the k-section width becomes larger.

5 Conclusion

Let us now summarize the results of the paper. We derived new relations between structural and spectral properties of graphs. For graphs with a certain structure these new relations allow us to find better spectral lower bounds on the k-section width. If the growth function $g(j)$ increases strongly, we can improve the old spectral lower bound by a constant factor. Otherwise the lower bound depends on $(\sum_{i=1}^{k} \lambda_i)^{\beta}$, $\frac{1}{2} \leq \beta < 1$ instead of $\sum_{i=1}^{k} \lambda_i$. Furthermore we gave a theoretical analysis for which classes of graphs the new bounds are tight.

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