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Tighter spectral bounds for the cut size, based on Laplacian eigenvectors

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ABSTRACT

The cut-set $\partial\mathcal{V}$ in a graph is defined as the set of all links between a set of nodes $\mathcal{V}$ and all other nodes in that graph. Finding bounds for the size of a cut-set $|\partial\mathcal{V}|$ is an important problem, and is related to mixing times, connectedness and spreading processes on networks. A standard way to bound the number of links in a cut-set $|\partial\mathcal{V}|$ relies on Laplacian eigenvalues, which approximate the largest and smallest possible cut-sets for a given size of the set $\mathcal{V}$. In this article, we extend the standard spectral approximations by including information about the Laplacian eigenvectors. This additional information leads to provably tighter bounds compared to the standard spectral bounds. We apply our new method to find improved spectral bounds for the well-known Cheeger constant, the Max Cut problem and the expander mixing lemma. We also apply our bounds to study cut sizes in the hypercube graph, and describe an application related to the spreading of epidemics on networks. We further illustrate the performance of our new bounds using simulations, revealing that a significant improvement over the standard bounds is possible.

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1. Introduction

In spectral graph theory [22], the eigenvalues and eigenvectors of matrix representations of graphs are studied and related to properties of the graph. This spectral methodology often enables a very concise characterization of a graph by relating complex combinatorial graph properties to simple expressions involving the graphs' eigenvalues. While other methods may provide tight algorithmic approximations to such combinatorial problems, for instance the famous Arora-Rao-Vazirani algorithm for finding sparse cuts [4], the added value of the spectral approach is that it provides analytical relations and bounds in terms of the graphs' spectral properties rather than numerical or algorithmic solutions.

The combinatorial property of interest in this work is related to the number of links between disjoint sets of nodes in a graph. If we select two such sets, then the cut-set is defined as the set of all links that connect nodes from one set to nodes from the other set. The number of links in the cut-set is then called the cut size. Given the number of nodes in each subset, one is often interested in the smallest and largest possible value of the cut size. Here, we propose new spectral bounds for the cut size. We start from the standard spectral approach, which we refer to as the *standard relaxation* method (SR), which yields spectral bounds by relaxing the combinatorial optimization problem of finding the smallest and largest cut-sets. By considering additional constraints based on Laplacian eigenvectors, our *constrained relaxation* method (CR) leads to a tighter relaxation of the combinatorial optimization problem, and tighter bounds on the cut size. While the SR bounds contain limited spectral information about the graph — in fact, only the largest or second-smallest eigenvalue of the Laplacian of the graph — the CR bounds include a larger number of eigenvalues, and additionally, some properties of the Laplacian eigenvectors. To illustrate the applicability of our new bounds, we relate the cut size to three well-studied problems in graph theory: the Cheeger inequalities, the Max Cut problem, and the expander mixing lemma [3], [14], [17, Lemma 2.5]. Numerical simulations of the new (CR) and existing (SR) bounds further illustrate the potential of our constrained relaxation approach. Finally, we apply our bounds to study cut sizes in the hypercube graph, and describe how bounding the cut size plays an important role in the study of epidemics on networks, where the cut size relates to the spreading velocity of a disease over a network [24].

In Section 2, we introduce some basic definitions from spectral graph theory and formally define the cut size. In Section 3, we derive the new cut size bounds starting from the definition of the largest and smallest cut size and the standard relaxation. We then compare all bounds, which results in a hierarchy of bounds. Section 4 describes the application of our constrained relaxation method to the Cheeger inequality, the Max

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Cut problem, the expander mixing lemma, cuts in the hypercube graph and epidemics on graphs. Finally, Section 5 concludes and summarizes the results.

2. Preliminaries

2.1. Graphs and the Laplacian matrix

We consider a connected and unweighted graph $G(\mathcal{N}, \mathcal{L})$ without self-loops, where $\mathcal{N}$ is the set of N nodes and $\mathcal{L}$ the set of L links. The structure of any such graph can be represented by a symmetric $N \times N$ Laplacian matrix Q with elements:

$$Q_{ij} = \begin{cases} d_i & \text{if } i = j \\ -1 & \text{if } (i,j) \in \mathcal{L} \\ 0 & \text{otherwise} \end{cases}$$

Here, the degree d_i is the number of nodes connected to node i, and $(i,j) \in \mathcal{L}$ represents the condition that there is a link between node i and node j. The quadratic form $x^T Q x$, for some vector $x \in \mathbb{R}^N$, can be written as a sum over the graph links:

$$x^T Q x = \sum_{(i,j)\in\mathcal{L}} (x_i - x_j)^2 \tag{1}$$

Furthermore, since the Laplacian matrix Q is a real and symmetric matrix, its eigendecomposition is [22]:

$$Q = \sum_{k=1}^{N} \mu_k z_k z_k^T,$$

where μ_k is the k^{th} real eigenvalue and z_k the corresponding eigenvector. Equation (1) shows that the Laplacian matrix is positive semi-definite and, additionally, a basic result from spectral graph theory states that the multiplicity of the zero eigenvalue equals the number of connected components [22, art. 80]. Since we are considering connected graphs, we can thus always define the ordered sequence of eigenvalues $\mu_1 \geq \mu_2 \geq \cdots > \mu_N = 0$. From the definition of the Laplacian matrix Q, we find that the eigenvector corresponding to the zero eigenvalue $\mu_N = 0$ equals $z_N = \frac{u}{\sqrt{N}}$, where $u = [1, 1, \ldots, 1]^T$ is the all-one vector. Furthermore, as the Laplacian is real and symmetric, we know that the set of all eigenvectors $\{z_1, z_2, \ldots, z_N\}$ forms an orthonormal basis of $\mathbb{R}^N$. In other words, we know that $z_i^T z_j = \delta_{ij}$, where δ_{ij} is the Kronecker delta, which is equal to $\delta_{ij} = 1$ if $i = j$, and $\delta_{ij} = 0$ otherwise. An important consequence of this orthonormality property is Plancherel's theorem:

$$\sum_{k=1}^{N} (z_k^T x)^2 = x^T x \quad \forall x \in \mathbb{R}^N. \tag{2}$$

2.2. Cut size: definition, quadratic form and constraints

Definition 1 *(Cut-set).* For two non-empty, disjoint node subsets $\mathcal{V}, \mathcal{S} \subset \mathcal{N}$ of a graph, the cut-set $\mathcal{C}(\mathcal{V}, \mathcal{S})$ is the set of all links that connect nodes in $\mathcal{V}$ to nodes in $\mathcal{S}$. In other words:

$$\mathcal{C}(\mathcal{V}, \mathcal{S}) = \{(i, j) \in \mathcal{L} \mid i \in \mathcal{V}, j \in \mathcal{S}\}$$

For a subset $\mathcal{V}$ and its complement $\overline{\mathcal{V}}$, this cut-set equals the edge boundary $\partial\mathcal{V}$ of the set $\mathcal{V}$:

$$\partial\mathcal{V} = \mathcal{C}(\mathcal{V}, \overline{\mathcal{V}})$$

In the remainder of this article, we will work with the edge boundary $\partial\mathcal{V}$, which is invariant when $\mathcal{V}$ and its complement $\overline{\mathcal{V}}$ are interchanged. The number of links in the edge boundary $\partial\mathcal{V}$ is called the *cut size* and is denoted by $|\partial\mathcal{V}|$. The number of nodes in $\mathcal{V}$ will be denoted by $V = |\mathcal{V}|$ and the fraction of nodes in $\mathcal{V}$ by $v = \frac{V}{N}$. Appendix E extends the results for $\partial\mathcal{V}$ to $\mathcal{C}(\mathcal{V}, \mathcal{S})$ in context of the expander mixing lemma, illustrating how the derivations and results for $\partial\mathcal{V}$ can be generalized.

The ability to find spectral bounds for the cut size follows from its algebraic representation as a quadratic form:

Definition 2 *(Quadratic and Spectral Form).* The cut size $|\partial\mathcal{V}|$ of a set $\mathcal{V}$ in a graph with Laplacian matrix Q can be written as:

$$|\partial\mathcal{V}| = w_{\mathcal{V}}^T Q w_{\mathcal{V}} = \sum_{k=1}^{N-1} (w_{\mathcal{V}}^T z_k)^2 \mu_k, \tag{3}$$

where $w_{\mathcal{V}} \in \{0, 1\}^N$ is the zero-one partition indicator vector specifying the nodes in $\mathcal{V}$ by $(w_{\mathcal{V}})_i = 1$ if $i \in \mathcal{V}$, and $(w_{\mathcal{V}})_i = 0$ otherwise.

The quadratic form for the cut size can be rewritten with (1) as

$$w_{\mathcal{V}}^T Q w_{\mathcal{V}} = \sum_{(i,j)\in\mathcal{L}} \left((w_{\mathcal{V}})_i - (w_{\mathcal{V}})_j\right)^2,$$

where the sum in the right-hand side runs over all links, and only links in the cut-set contribute a "+1" to the sum. Furthermore, based on Plancherel's theorem and on the specific form of $w_{\mathcal{V}}$ as a zero-one vector, we show in Appendix A that the projections $w_{\mathcal{V}}^T z_k$ obey the following constraints:

Property 1 *(Spectral Constraints). For any vector $w_{\mathcal{V}}$ representing a subset of V nodes, the projections $w_{\mathcal{V}}^T z_k$ on the Laplacian eigenvectors are constrained by:*

$$\begin{cases} \sum_{k=1}^{N-1} (w_{\mathcal{V}}^T z_k)^2 = Nv(1-v) & \text{(a)} \\ (w_{\mathcal{V}}^T z_k)^2 \leq s_k^2(v), & \text{(b)} \end{cases} \tag{4}$$

where we introduce

$$s_k^2(v) := \max \left\{ \left(\sum_{i=1}^{V} \left(z_k^{\downarrow} \right)_i \right)^2, \left(\sum_{i=1}^{N-V} \left(z_k^{\downarrow} \right)_i \right)^2 \right\}, \tag{5}$$

where $z_k^{\downarrow}$ *is the vector* z_k *with entries ordered by decreasing value, such that* $\left(z_k^{\downarrow}\right)_1 \geq \left(z_k^{\downarrow}\right)_2 \geq \cdots \geq \left(z_k^{\downarrow}\right)_N$.

Property (4a) follows from Plancherel's theorem applied to the partition indicator vector $w_{\mathcal{V}}$ and the eigenvectors of Q. Property (4b) follows from the fact that $w_{\mathcal{V}}$ is a zero-one vector with exactly V non-zero elements.

3. Deriving the constrained relaxation bounds

Our main result is the formulation of the constrained relaxation bounds in Theorem 2 and the hierarchy of bounds in Theorem 3, which proves that these new bounds are at least as tight the standard bounds.

Assuming that a graph $G(\mathcal{N}, \mathcal{L})$ is given and its eigendecomposition is either known or can be calculated, we propose a new upper-bound on the cut size $|\partial\mathcal{V}|$. First, we discuss the exact characterization of the cut size range (EX), then formulate the standard spectral approximation approach (SR) and finally discuss our constrained relaxation approach (CR), which improves these standard bounds.

3.1. The Exact Method

The tightest characterization for the range of the cut size $|\partial\mathcal{V}|$ for a given size of the set $\mathcal{V}$ is:

Definition 3 *(Exact Cut Size Bounds).* The cut size between a subset $\mathcal{V}^\star$ of V nodes and its complement is bounded by:

$$\min_{\substack{\mathcal{V}\subset\mathcal{N} \\ |\mathcal{V}|=V}} |\partial\mathcal{V}| \leq |\partial\mathcal{V}^\star| \leq \max_{\substack{\mathcal{V}\subset\mathcal{N} \\ |\mathcal{V}|=V}} |\partial\mathcal{V}|. \tag{6}$$

The lower and upper-bound are further abbreviated by $\theta_E(v)$ and $\Theta_E(v)$, respectively, where $v = \frac{V}{N}$.

While (6) is an explicit description for the tightest possible cut size range, finding the maximum and minimum over all possible sets $\mathcal{V}$ of size V is NP-hard[2] [17, Sec. 2.4], [6], [18], which motivates the pursuit to approximate the cut size bounds instead.

3.2. The Standard Relaxation Method

The standard relaxation method (SR) addresses the combinatorial difficulty of finding θ_E and Θ_E by writing the optimization objective in a spectral form, and by subsequently relaxing the optimization domain.

First, using the spectral form of the cut size (3), the exact upper-bound (6) can be written as[3]:

$$\Theta_E(v) = \max_{\substack{\mathcal{V}\subset\mathcal{N}\\ |\mathcal{V}|=V}} |\partial\mathcal{V}| = \max_{\substack{w_\mathcal{V}\in\{0,1\}^N\\ u^T w_\mathcal{V}=V}} \sum_{k=1}^{N-1} (z_k^T w_\mathcal{V})^2 \mu_k \tag{7}$$

Next, the combinatorial domain is relaxed from the zero-one partition indicator vector $w_\mathcal{V}$ to a real vector x, taking property (4a) into account:

$$\left\{ w_\mathcal{V} \in \{0,1\}^N \middle| \sum_{k=1}^{N} (w_\mathcal{V})_k = V \right\} \subset \left\{ x \in \mathbb{R}^N \middle| \sum_{k=1}^{N-1} (z_k^T x)^2 = Nv(1-v) \right\} \tag{SR relaxation}$$

Finally, after denoting the projection of x on the k^{th} Laplacian eigenvector by $y_k = (z_k^T x)^2$ and rewriting the sum using the all-one vector u, the SR optimization problem follows as:

Problem 1 *(SR Problem).*

$$\begin{aligned} \underset{y\in\mathbb{R}^{N-1}}{\text{maximize}} \quad & \sum_{k=1}^{N-1} y_k \mu_k \\ \text{subject to} \quad & 0 \le y_k, \\ & u^T y = Nv(1-v). \end{aligned} \tag{8}$$

This optimization problem is solved by the vector $y^\star$, with its first entry equal to $(y^\star)_1 = Nv(1-v)$ and all other entries equal to zero, leading to the SR bounds:

[2] The problem $\max_\mathcal{V} |\partial\mathcal{V}|$ is NP-hard (see also Section 4.2) and can be rewritten as $\max_V \max_{\mathcal{V},|\mathcal{V}|=V} |\partial\mathcal{V}|$, which implies that $\max_{\mathcal{V},|\mathcal{V}|=V} |\partial\mathcal{V}|$ is NP-hard for general V.

[3] We confine our derivation to the upper-bound, but the results for the lower-bound follow in direct analogy by replacing the matrix Q with eigenvalues μ_i and eigenvectors z_i by the matrix $\widehat{Q}$ with eigenvalues $(-\mu_i)$ and eigenvectors z_i.

Proposition 1 *(SR Bounds). The cut size between a subset $\mathcal{V}$ of V nodes and its complement is bounded by:*

$$\theta_S(v) \leq |\partial\mathcal{V}| \leq \Theta_S(v), \tag{9}$$

where the lower and upper-bound are defined as

$$\begin{cases} \theta_S(v) & = Nv(1-v)\mu_{N-1} \\ \Theta_S(v) & = Nv(1-v)\mu_1 \end{cases} \tag{10}$$

Since the SR bounds (9) solve the relaxed optimization problem (8), they are necessarily less tight than the exact bounds, which means that $\Theta_E(v) \leq \Theta_S(v)$ holds for all v.

3.3. The Constrained Relaxation Method

In order to improve the bounds obtained by the standard relaxation method, we further constrain the relaxed optimization domain. Starting from the exact formulation of the cut size upper-bound (7), the zero-one partition indicator vector $w_{\mathcal{V}}$ is relaxed to a real vector x taking both property (4a) and property (4b) into account:

$$\left\{ w_{\mathcal{V}} \in \{0,1\}^N \middle| \sum_{k=1}^{N} (w_{\mathcal{V}})_k = V \right\} \subset \left\{ x \in \mathbb{R}^N \middle| \sum_{k=1}^{N-1} (z_k^T x)^2 = Nv(1-v),\ (z_k^T x)^2 \leq s_k^2(v) \right\} \tag{CR relaxation}$$

Relying again on the notation $y_k = (z_k^T x)^2$, the relaxed problem can be written as:

$$\begin{aligned} \underset{y \in \mathbb{R}^{N-1}}{\text{maximize}} \quad & \sum_{k=1}^{N-1} y_k \mu_k \\ \text{subject to} \quad & 0 \leq y_k \leq s_k^2(v), \\ & u^T y = Nv(1-v). \end{aligned} \tag{11}$$

By explicitly incorporating the equality constraint, variable y_{N-1} can be eliminated as $y_{N-1} = Nv(1-v) - \sum_{k=1}^{N-2} y_k$. The problem can then be rewritten as:

Problem 2 *(CR* Problem).*

$$\begin{aligned} \underset{y \in \mathbb{R}^{N-2}}{\text{maximize}} \quad & \sum_{k=1}^{N-2} y_k(\mu_k - \mu_{N-1}) + Nv(1-v)\mu_{N-1} \\ \text{subject to} \quad & 0 \leq y_k \leq s_k^2(v), \\ & 0 \leq Nv(1-v) - u^T y \leq s_{N-1}^2(v). \end{aligned} \tag{12}$$

Since the CR* problem is a linear program, it can be solved efficiently in polynomial time, yielding numerical solutions $\theta_{C\star}(v)$ and $\Theta_{C\star}(v)$ for the cut size lower and upper-bound, respectively. In order to find closed-form bounds, we introduce further approximations.

We derive a set of bounds parametrized by $K \in \{1, 2, \ldots, N\}$, by upper-bounding the objective function of (11). For any K, the eigenvalue order dictates that $\mu_k \leq \mu_K$ for all $k \geq K$, and thus that $\sum_{k=1}^{N-1} y_k\mu_k \leq \sum_{k=1}^{K-1} y_k\mu_k + \mu_K \sum_{k=K}^{N-1} y_k$. Now, from property (4a), we have $\sum_{k=K}^{N-1} y_k = Nv(1-v) - \sum_{k=1}^{K-1} y_k$, by which the objective function of (11) can be upper-bounded by:

$$\sum_{k=1}^{N-1} y_k\mu_k \leq \sum_{k=1}^{K-1} y_k(\mu_k - \mu_K) + Nv(1-v)\mu_K, \tag{13}$$

for $y \in \mathbb{R}^{N-1}$ subject to the constraints in (11). Introducing the approximate objective function (13) for general values of K in problem (11) and translating the constraints leads to:

Problem 3 *(CR-K Problem).*

$$\begin{aligned} \underset{y\in\mathbb{R}^{K-1}}{\text{maximize}} \quad & \sum_{k=1}^{K-1} y_k(\mu_k - \mu_K) + Nv(1-v)\mu_K \\ \text{subject to} \quad & 0 \leq y_k \leq s_k^2(v), \\ & 0 \leq Nv(1-v) - u^T y \leq \sum_{k=1}^{K-1} s_{N-k}^2(v). \end{aligned} \tag{14}$$

We will show that there always exists some K (see later: this corresponds to $K = K_u(v)$ or $K = K_l(v)$) for which the second inequality constraint in (14) follows from the first inequality constraint. For this K, the exact solution $y^\star$ can be found, which has elements $(y^\star)_k = s_k^2(v)$. In Appendix B, this solution and approximate solutions for other values of K are derived, leading to the following bounds:

Theorem 2 *(CR-K Bounds). The cut size between a subset $\mathcal{V}$ of V nodes and its complement is bounded by:*

$$\theta_C(v, K) \leq |\partial\mathcal{V}| \leq \Theta_C(v, K) \quad \textit{for all } 1 \leq K \leq N \tag{15}$$

where the lower and upper-bound are defined as

$$\begin{cases} \theta_C(v,K) & = \sum_{k=1}^{K-1} s_{k'}^2(v)(\mu_{k'} - \mu_{K'}) + Nv(1-v)\mu_{K'} \\ \Theta_C(v,K) & = \sum_{k=1}^{K-1} s_k^2(v)(\mu_k - \mu_K) + Nv(1-v)\mu_K \end{cases} \tag{16}$$

with $k' = N - k$ and $K' = N - K$.

3.4. Comparison between bounds

When comparing the constrained relaxation bounds for different values of the parameter K, certain values of K are "special". In particular, the values $K_u(v)$ and $K_l(v)$, defined as

$$\begin{cases} K_u(v) &= \max\left\{1 \le K \le N \middle| \sum_{k=1}^{K-1} s_k^2(v) \le Nv(1-v)\right\} \\ K_l(v) &= \max\left\{1 \le K \le N \middle| \sum_{k=1}^{K-1} s_{k'}^2(v) \le Nv(1-v)\right\}, \end{cases} \tag{17}$$

are important since the CR-K bounds (15) are tightest at these values. This optimality of $K_u(v)$ and $K_l(v)$ is derived in Appendix C in context of a *hierarchy of bounds*:

Theorem 3 *(Hierarchy of Bounds). The cut size bounds are related by*

$$|\partial\mathcal{V}| \le \underbrace{\Theta_E(v)}_{NP\text{-}hard} \le \underbrace{\Theta_{C\star}(v)}_{Lin.Prog.} \le \underbrace{\Theta_C(v,K_u) \le \Theta_C(v,K)}_{new\ bounds} \le \underbrace{\Theta_S(v) \equiv \Theta_C(v,1)}_{standard\ bound} \tag{18}$$

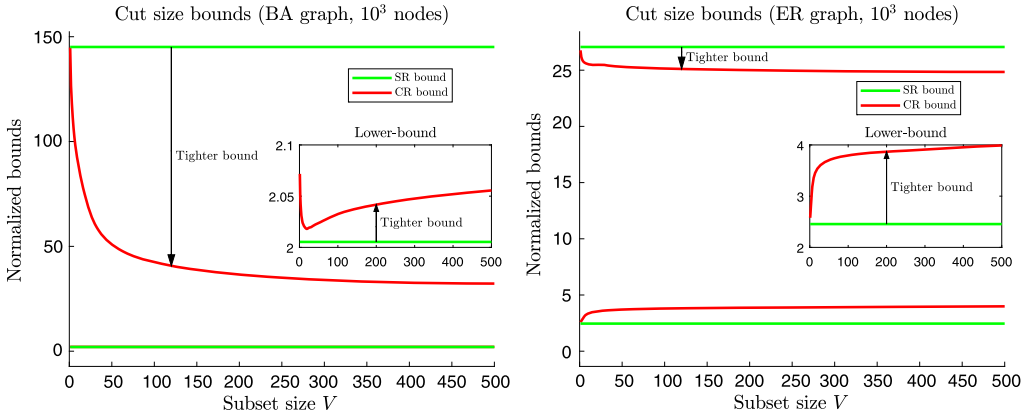
for all $K \le K_u$ and similarly for the lower bounds.

Theorem 3 thus states that amongst all CR-K bounds, the bound with $K = K_u(v)$ according to (17) is the tightest bound. Since the SR bound corresponds to the CR-K bound with $K = 1$, this implies that the CR-K bounds are at least as tight as the SR bound, and that the constrained relaxation method can yield strictly tighter bounds only if $K_u(v) > 1$ holds. More specifically, and taking the multiplicity of eigenvalues into account,[4] the following condition can be formulated:

Corollary 1. *The constrained relaxation method leads to tighter upper-bounds than the standard relaxation method, if and only if $K_u(v)$ is strictly larger than the multiplicity of the largest eigenvalue, in other words if $K_u(v) > \mathrm{mult}(\mu_1)$ holds. The same result holds for the lower-bound, with condition $K_l(v) > \mathrm{mult}(\mu_{N-1})$.*

Interestingly, a similar condition can be used as a criterion to determine in which graphs the SR bounds are achieved for some set $\mathcal{V}^\star$: *if $K_l(v) = 1$ for some v, then the set $\mathcal{V}^\star$ consisting of the V nodes with the largest elements of z_{N-1} corresponds to a cut size $|\partial\mathcal{V}^\star|$ which equals the SR lower-bound.* An example where the condition of Corollary 1 can be invoked to find when the constrained spectral bounds and standard spectral bounds coincide, is the hypercube graph (see Section 4.4).

[4] When an eigenvalue μ_k has multiplicity higher than one, say multiplicity m, then the corresponding eigenvectors $\mathcal{Z}_k = \{z_{k1}, z_{k2}, \ldots, z_{km}\}$ and thus also $s_{k1}^2, s_{k2}^2, \ldots, s_{km}^2$ are not uniquely defined. For any particular set of m vectors that spans $\mathcal{Z}_k$ all derivations still hold, and in some cases it might be desirable to consider specific choices of these m vectors.



(a) Cut size bounds for Barabási-Albert graph.

(b) Cut size bounds for Erdős-Rényi graph.

Fig. 1. Simulation of the SR and CR bounds for a Barabási-Albert and Erdős-Rényi random graph on $N = 10^3$ nodes. The bounds are normalized to $\frac{\Theta_S(v)}{Nv(1-v)}$ and $\frac{\Theta_C(v)}{Nv(1-v)}$, such that the standard bounds correspond to constant bounds μ_1 and μ_{N-1}. The lower bounds are magnified in the inset.

To further illustrate the discrepancy between the SR and the CR-K bounds, Figs. 1a and 1b show numerical simulations of the bounds for a randomly generated Barabási-Albert graph and a randomly generated Erdős-Rényi graph.[5] These simulations indicate that the improvements can be considerable, and hint towards "degree heterogeneity" as a property that leads to large differences between the SR and the CR methodology.

4. Applications of the improved bound

4.1. The Cheeger constant

In 1969, Jeff Cheeger [7] proved a relation between the smallest non-zero eigenvalue of the Laplace operator on a Riemannian manifold M, and a geometric characterization $\tilde{h}(M)$ of that manifold. Later, this inspired others to define the Cheeger constant for graphs:

Definition 4. The Cheeger constant $h(G)$ of a graph is defined as

$$h(G) = \min_{\substack{\mathcal{V}\subset\mathcal{N} \\ |\mathcal{V}|\leq\frac{N}{2}}} \frac{|\partial\mathcal{V}|}{|\mathcal{V}|} \tag{19}$$

In other words, the Cheeger constant, also called the edge expansion or the isoperimetric constant, is the smallest number $h(G)$ such that each partition of V nodes has a

[5] The Barabási-Albert graph was generated starting from a clique of 10 nodes and by adding degree four nodes that link to the existing nodes with probability proportional to their degree. For the Erdős-Rényi random graph, link density $p = 4p_c$ was chosen, with $p_c = \frac{\log(N)}{N} = \frac{3}{1000}$ the connectedness threshold for p.

cut size of at least $Vh(G)$ links. By this description, it is clear that the Cheeger constant is closely related to how well-connected a graph is. Similar to the spectral result of Jeff Cheeger for Riemannian manifolds, the Cheeger constant (19) for graphs can also be bounded by spectral properties of the Laplacian matrix Q [12,3,1,19]:

Theorem 4. *The Cheeger constant $h(G)$ of a graph can be bounded by:*

$$\frac{\mu_{N-1}}{2} \leq h(G) \leq \sqrt{\mu_{N-1}(2d_{\max} - \mu_{N-1})}, \tag{20}$$

where d_{max} is the largest degree.

Invoking the CR-K bounds (15) for the cut size, it is possible to find tighter lower-bounds for the Cheeger constant:

Corollary 2 *(Tighter Cheeger lower-bound). The Cheeger constant $h(G)$ of a graph is lower-bounded by*

$$\frac{\mu_{N-1}}{2} \leq \min_v \{\theta_C(v, K_l(v))\} \leq h(G) \tag{21}$$

The standard Cheeger inequality (20) is an important result in spectral graph theory, that highlights the relation between the second-smallest Laplacian eigenvalue μ_{N-1} and the connectedness of a graph. This fact was discovered earlier by Fiedler [13,9], who coined the appropriate name *algebraic connectivity* for μ_{N-1}. The constrained relaxation method and resulting tighter Cheeger lower-bound (21) provide additional information about the connectivity of a graph in terms of the other eigenvalues. Assume for simplicity that $K_l(v) > 1$ for all v, such that we can look at $\theta_C(v, 2)$ as a lower bound. The standard Cheeger inequality is based on $\min_v \{(1-v)\mu_{N-1}\} \leq h(G)$, which relates μ_{N-1} to the connectedness of a graph. The constrained relaxation (limited to $K = 2$) is then based on $\min_v \left\{(1-v)\mu_{N-2} + (\mu_{N-2} - \mu_{N-1})\frac{s^2_{N-2}(v)}{V}\right\} \leq h(G)$. This inequality shows that μ_{N-2} is related to the graph connectedness in a similar way as the algebraic connectivity μ_{N-1}, and that a large eigenvalue gap $(\mu_{N-2} - \mu_{N-1})$ contributes to a higher connectedness. The CR-K bounds for higher values of K thus provide relations between the K smallest Laplacian eigenvalues and the graph's connectedness.

4.2. The Max Cut problem

Finding the node subset $\mathcal{V}^\star$ with the largest cut size $|\partial\mathcal{V}^\star|$ in a graph was one of the original 21 NP-hard problems[6] identified by Karp [18]. This problem is commonly known as *the Max Cut problem*, and several approaches were developed to approximate

[6] More precisely, the following decision problem was shown to be NP-hard: "given a graph G and a positive integer k, is there a cut-set in G of at least k links?" Consequently, finding the largest cut size or the subset $\mathcal{V}^\star$ must be NP-hard as well.

the largest cut size, or to find subsets with large cut sizes. The spectral relaxation, corresponding to what we have called the SR methodology, was first invoked on the max cut problem by Mohar and Poljak [20], yielding the bound

$$\max_{\mathcal{V}\subset\mathcal{N}} |\partial\mathcal{V}| \leq \frac{N}{4}\mu_1. \tag{22}$$

It was shown that (22) is tight for a number of graph families, such as complete graphs, regular bipartite graphs and others [20]. Taking into account additional constraints, the CR methodology can be invoked to yield the new bound

$$\max_{\mathcal{V}\subset\mathcal{N}} |\partial\mathcal{V}| \leq \max_{v} \Theta_C(v, K_u) \tag{23}$$

with the CR bound $\Theta_C(v, K_u)$ as in Theorem 2. By the hierarchy of bounds (18), the CR max cut bound (23) is tighter than the SR max cut bound (22). A different eigenvalue-based bound was formulated by Delorme and Poljak [10], given by the optimization problem

Theorem 5 *(Delorme-Poljak max cut bound). The largest cut size in a graph is bounded by*

$$\max_{\mathcal{V}\subset\mathcal{N}} |\partial\mathcal{V}| \leq \frac{N}{4} \min_{\substack{c\in\mathbb{R}^N \\ c^T u=0}} \mu_{\max}\left(Q + \mathrm{diag}(c)\right), \tag{24}$$

with $\mu_{\max}(M)$ the largest eigenvalue of matrix M.

This spectral optimization problem (24) is solvable in polynomial time, and is tighter than the SR max cut bound (22), as (24) reduces to (22) for $c = 0$. In 1995, Goemans and Williamson [14] relaxed the max cut problem to a semidefinite program:

Theorem 6 *(Goemans-Williamson max cut bound). The largest cut size in a graph is bounded by*

$$\max_{\mathcal{V}\subset\mathcal{N}} |\partial\mathcal{V}| \leq \frac{1}{4} \max_{\substack{Y\in PSD \\ (Y)_{ii}=1\ \forall i}} \mathrm{tr}(QY), \tag{25}$$

where $Y \in PSD$ means that Y is a real, symmetric matrix with non-negative eigenvalues (positive semi-definite).

The Goemans-Williamson semidefinite optimization problem is the dual problem of the spectral optimization of Delorme and Poljak (see [14]), which means that (25) is a tighter max cut bound than (24) (with equality possible), and consequently is tighter than the SR max cut bound (22). The approach of Goemans and Williamson moreover leads to an elegant randomized construction of a set $\mathcal{V}_{GW}$, whose average cut

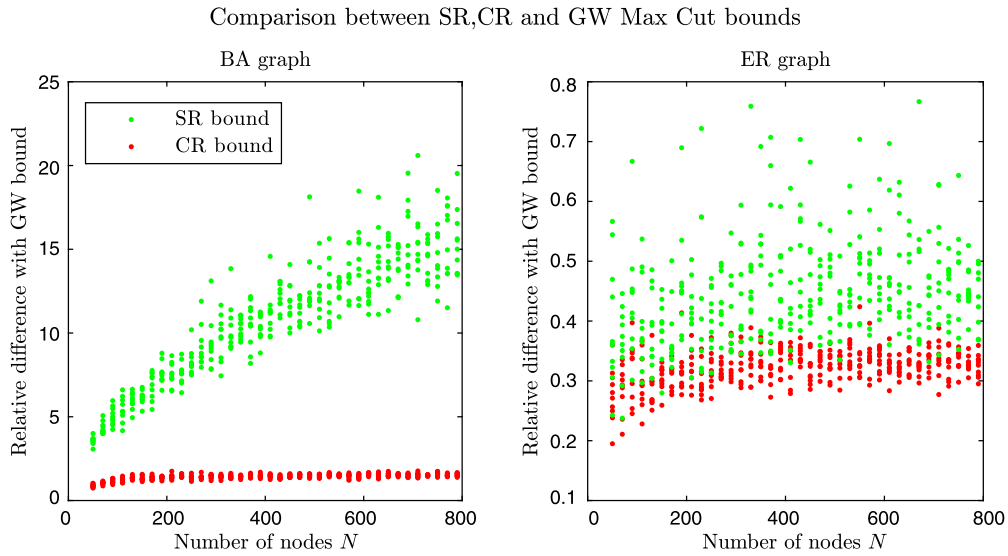


Fig. 2. Comparison between the standard (spectral) relaxation bounds (SR) (22), the constrained (spectral) relaxation bounds (CR) (23) and the Goemans-Williamson bound (GW) (25) for the largest cut size of a graph. The relative differences $\frac{SR-GW}{GW}$ and $\frac{CR-GW}{GW}$ are calculated for Erdős-Rényi and Barabási-Albert random graphs of size $N = 50, 70, 90, \ldots, 800$, and for each size 10 random graphs are sampled.

size is guaranteed to be within a constant factor $\alpha \approx 0.878$ of the max cut value, i.e. $\mathbf{E}\left(|\partial \mathcal{V}_{GW}|\right) \geq \alpha \max_{\mathcal{V} \subset \mathcal{N}} |\partial \mathcal{V}|$ (see [14]).

Fig. 2 above compares the different max cut bounds (22) and (23) to the GW max cut bound (25) for a number of Erdős-Rényi and Barabási-Albert random graphs[7] of increasing size N. The SDP problem in (25) is solved using CVX, a package for specifying and solving convex programs [15]. The positive relative differences $\frac{GW-SR}{GW}$ and $\frac{GW-CR}{GW}$ which are plotted in Fig. 2 show that the GW bound (25) clearly outperforms the spectral bounds (22), (23) for these random graphs. The relative difference for both SR and CR max cut bounds seems to be much smaller for Erdős-Rényi random graphs than for Barabási-Albert random graphs. However, the improvement of the CR bound over the SR bound is significantly larger for Barabási-Albert random graphs compared to the improvement for Erdős-Rényi random graphs, which was also the case in Fig. 1a. While the Goemans-Williamson bound seems to generally give a tighter bound than the spectral bounds, it yields a numerical solution rather than a closed-form expression in terms of properties of the Laplacian Q, such as Laplacian eigenvalues and eigenvectors. Hence, we believe that the interpretable expression of our constrained relaxation bound (23) has complementary value to the numerical solution of the GW bound, even if the latter might generally be tighter.

[7] The Barabási-Albert random graphs are generated starting from a clique of 10 nodes and adding degree four nodes with probability proportional to the existing degrees. The Erdős-Rényi random graphs have link density equal to $p = 4p_c$ with $p_c = \frac{\log(N)}{N}$, the connectedness threshold for p.

4.3. The Expander Mixing Lemma

The expander mixing lemma (EML) is a basic result in the study of expander graphs [2,17], which relates the expansion properties of a graph to the Laplacian spectrum. In context of the graph isoperimetric problem [5,8], the same inequality appears in a geometric context. While generally stated in terms of the cut-set $\mathcal{C}(\mathcal{V},\mathcal{S})$ between two disjoint sets $\mathcal{V}$ and $\mathcal{S}$ (see Appendix E), we focus here on the cut-set $\partial\mathcal{V}$ corresponding to $\mathcal{S}=\overline{\mathcal{V}}$. The expander mixing lemma is then stated as:

Lemma 1 *(Expander Mixing Lemma). In a graph $G(\mathcal{N},\mathcal{L})$, the difference between the cut size $|\partial\mathcal{V}|$ for any subset $\mathcal{V}$ of V nodes, and the average cut size $2Lv(1-v)$ is bounded by*

$$\left||\partial\mathcal{V}|-2Lv(1-v)\right|\leq\lambda Nv(1-v),$$

with $\lambda=\max\left\{|\mu_{N-1}-\frac{2L}{N}|,|\mu_1-\frac{2L}{N}|\right\}$.

The expander mixing lemma quantifies how far the cut size of a set with V nodes can possibly diverge from $2Lv(1-v)$, which is the expected cut size in a random graph with the same "link density" or average degree as G. Hence, rather than bounding the cut size range, EML bounds the variation of this range around a central value. In Appendix D, we show that the CR-K bounds naturally translate to the EML bounds:

Corollary 3 *(Tighter Expander Mixing Lemma). In a graph $G(\mathcal{N},\mathcal{L})$, the difference between the cut size $|\partial\mathcal{V}|$ for any subset $\mathcal{V}$ of V nodes, and the average cut size $2Lv(1-v)$ is bounded by*

$$\left||\partial\mathcal{V}|-2Lv(1-v)\right|\leq\max\left\{\left|\widetilde{\theta}_C(v,K_l(v))\right|,\left|\widetilde{\Theta}_C(v,K_u(v))\right|\right\}\leq\lambda Nv(1-v),$$

where $\widetilde{\Theta}_C(v,K)$ and $\widetilde{\theta}_C(v,K)$ are the CR-K bounds corresponding to the matrix $\widetilde{Q}=Q-\frac{2L}{N}(I-\frac{uu^T}{N})$.

The proof of Corollary 3 in Appendix D shows that the standard EML inequality corresponds to the least tight bound in the bound hierarchy of Theorem 3, for bounds calculated from the matrix $\widetilde{Q}=Q-\frac{2L}{N}(I-\frac{uu^T}{N})$. Appendix E further generalizes the result to cut-sets between any pair of disjoint subsets.

4.4. Spectral lower bounds in the hypercube graph $\mathcal{H}_d$

The hypercube graph is a graph where cuts and cut sizes have been thoroughly studied. The d-dimensional hypercube graph is the graph $\mathcal{H}_d=G(\mathcal{N},\mathcal{L})$ with $N=2^d$ nodes, and with links $\mathcal{L}$ determined by identifying each node $n\in\mathcal{N}$ with a unique d-length bit string $b(n)\in\{0,1\}^d$, and connecting two nodes with a link if their bit strings differ

in only one entry, i.e. $\mathcal{L} = \{(i,j) \mid \|b(i) - b(j)\|_1 = 1\}$. In 1964, Harper [16] proved the following result for the smallest cut size in the hypercube graph:

Theorem 7. *In the hypercube graph $\mathcal{H}_d$ the smallest cut size for a set of size V is achieved by the set of nodes $\mathcal{V}^\star$ containing the nodes with the V smallest bit strings, in other words*

$$\min_{\substack{\mathcal{V}\subset\mathcal{N}\\|\mathcal{V}|=V}} |\partial\mathcal{V}| = |\partial\mathcal{V}^\star| \text{ where } \mathcal{V}^\star = \left\{ n \in \mathcal{N} \;\middle|\; \sum_{i=1}^{d} (b(n))_i \, 2^{i-1} \leq V - 1 \right\}, \tag{26}$$

where $(b(n))_i$ is the i^{th} bit of the bit string $b(n)$.

Harper's result (26) does not give an explicit numerical result in terms of graph properties, and in practice the following approximate bound can be used [17, Example 4.2.1]:

$$\min_{\substack{\mathcal{V}\subset\mathcal{N}\\|\mathcal{V}|=V}} |\partial\mathcal{V}| \geq V \log_2\left(\frac{N}{V}\right), \tag{27}$$

which is tight when $V = 2^\ell$ for some integer ℓ. As the Laplacian eigenvalues and eigenvectors of the hypercube graph $\mathcal{H}_d$ are known, we can compare (26) and (27) to the CR bounds. The hypercube graph $\mathcal{H}_d$ has Laplacian eigenvalues $\mu_k = 2m$ with multiplicity $\binom{d}{m}$ for $0 \leq m \leq d$, and except for the eigenvector $z_N = \frac{u}{\sqrt{N}}$, all eigenvectors z_k contain exactly 2^{d-1} entries equal to $\frac{1}{\sqrt{2^d}}$ and 2^{d-1} entries equal to $\frac{-1}{\sqrt{2^d}}$. As a result, the ordered eigenvectors obey

$$\begin{cases} \left(z_k^{\downarrow}\right)_i &= \frac{1}{\sqrt{2^d}} \quad \text{for all } 1 \leq i \leq 2^{d-1} \\ \left(z_k^{\downarrow}\right)_i &= \frac{-1}{\sqrt{2^d}} \quad \text{for all } 2^{d-1}+1 \leq i \leq 2^d, \end{cases}$$

such that $s_k^2(v) = \frac{V^2}{N}$ is independent of k. Since $s_k^2(v)$ is constant, we find that $K_l(v) = \max\left\{ 1 \leq K \leq N \;\middle|\; \sum_{k=1}^{K} \frac{V^2}{N} \leq \frac{V(N-V)}{N} \right\} = \lfloor v^{-1} \rfloor$. By Corollary 1 and the fact that $\text{mult}(\mu_{N-1}) = d$, it thus follows that the CR bound can only be tighter than the SR bound when $\lfloor v^{-1} \rfloor \geq d$. More specifically, the CR bound will always equal the SR bound when $v \geq d^{-1}$. Fig. 3, comparing lower bounds for the cut size in the hypercube graph $\mathcal{H}_d$, shows that the CR bound is better than the SR bound for small cuts, i.e. when $v < d^{-1}$, but that both the SR and CR bounds are significantly less tight than Harper's bound (26) and its approximation (27). However, this difference can be expected as (26) and (27) are tailored to the hypercube $\mathcal{H}_d$ specifically, while the CR bound is valid for general graphs.

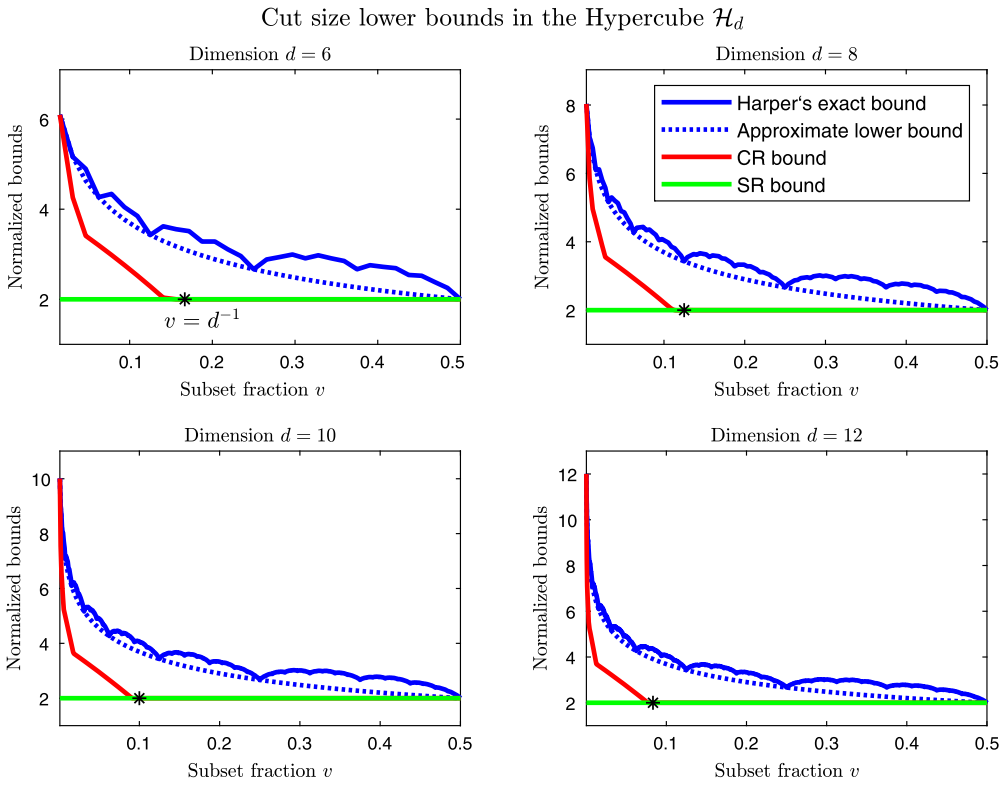


Fig. 3. Comparison between different bounds for the smallest cut size in the hypercube graph $\mathcal{H}_d$ of dimension d. All bounds are divided by $Nv(1-v)$ for normalization. This comparison indicates that the tightest bounds are, respectively: Harper's bound (26), the approximate lower bound (27), the CR bound and finally the SR bound. The black star indicates $v = d^{-1}$ from which point the CR bound is guaranteed to equal the SR bound.

4.5. Bounding the spread of epidemics and mean-field accuracy

In epidemics on networks, a disease spreads through the network, infecting new nodes via links between infected nodes and healthy nodes [21]. If all infected nodes at some time t are grouped in the set $\mathcal{V}(t)$, and all healthy nodes in the complementary set $\overline{\mathcal{V}}(t)$, then the cut-set $\partial\mathcal{V}(t)$ is the set of all "infectious links" at that time, i.e. links between healthy and infected nodes over which the disease can spread.

By modeling the spreading dynamics as independent Poisson processes, the epidemic process satisfies the Markov property [23] and the probability distribution $P_{\mathcal{V}^\star}(t) = \Pr[\mathcal{V}(t) = \mathcal{V}^\star]$ can be solved from the Kolmogorov equations. However, since this probability distribution is defined over all 2^N possible states $\mathcal{V}^\star \subseteq \mathcal{N}$, several methods have been developed to approximate the exact description. In [24], a compact differential equation for the average number of infected nodes in the SIS epidemic model is proposed:

$$\frac{d\mathbf{E}_{\mathcal{V}(t)}[|\mathcal{V}|]}{dt} = -\mathbf{E}_{\mathcal{V}(t)}[|\mathcal{V}|] + \tau\mathbf{E}_{\mathcal{V}(t)}[|\partial\mathcal{V}|] \tag{28}$$

where τ is the effective infection rate of the disease and $\mathbf{E}_{\mathcal{V}(t)}[.]$ the expected value with respect to $P_{\mathcal{V}^\star}(t)$. Since the second term contains the cut size, equation (28) is not self-contained and cannot be solved for $\mathbf{E}_{\mathcal{V}(t)}[|\mathcal{V}(t)|]$. However, using the CR-K bounds for $|\partial\mathcal{V}|$, we can write:

$$-\mathbf{E}_{\mathcal{V}(t)}[|\mathcal{V}|] + \tau \min_v \{\theta_C(v, K_l(v))\} \leq \frac{d\mathbf{E}_{\mathcal{V}(t)}[|\mathcal{V}|]}{dt} \leq -\mathbf{E}_{\mathcal{V}(t)}[|\mathcal{V}|] + \tau \max_v \{\Theta_C(v, K_u(v))\}$$

which shows how the best and worst-case SIS spreading behavior of a disease can be bounded, based on spectral information of the network over which the epidemic spreads.

More detailed approximations exist, ranging from approaches that incorporate the full topology of the graph, to mean-field approaches that coarse-grain the topological information. This variety of approaches is unified in [11] from the perspective of cut-set approximations. Specifically, the class of mean-field methods (MF) rely on approximations of the form:

$$\mathbf{E}_{\{\mathcal{V}(t)||\mathcal{V}|=V\}}\left[|\partial\mathcal{V}|\right] \xrightarrow{\text{MF approx.}} 2Lv(1-v) \tag{29}$$

where $\mathbf{E}_{\{\mathcal{V}(t)||\mathcal{V}|=V\}}[.]$ is the expectation with respect to the conditional probability distribution $\Pr[\mathcal{V}(t) = \mathcal{V}^\star \big| |\mathcal{V}(t)| = V]$, and similar results were found for general cut-sets $\mathcal{C}(\mathcal{V}, \mathcal{S})$. The main result in [11] was to show that the topological mean-field approximation (29) can be bounded using the isoperimetric inequality (equivalently, the expander mixing lemma). Since we provide tighter bounds for EML in Corollary 3, these bounds for the MF accuracy are also improved:

$$\begin{aligned}\left|\mathbf{E}_{\{\mathcal{V}(t)||\mathcal{V}|=V\}}\left[|\partial\mathcal{V}|\right] - 2Lv(1-v)\right| &\leq \underbrace{\max\left\{\left|\widetilde{\theta}_C(v, K_l(v))\right|, \left|\widetilde{\Theta}_C(v, K_u(v))\right|\right\}}_{\text{CR-K bounds}} \\ &\leq \underbrace{\lambda v(1-v)}_{\text{SR bounds [11]}},\end{aligned}$$

where $\lambda = \max\left\{\left|\mu_{N-1} - \frac{2L}{N}\right|, \left|\mu_1 - \frac{2L}{N}\right|\right\}$.

5. Conclusion

We formulate new spectral bounds for the cut size $|\partial\mathcal{V}|$ in general graphs. The bounds follow from a convex relaxation of the combinatorial (EX) problem $\max_{\mathcal{V}} |\partial\mathcal{V}|$ and, compared to the standard spectral relaxation approach (SR), additional constraints based on the Laplacian eigenvectors lead to a tighter relaxation of the problem (CR). The new bounds that follow from this constrained relaxation problem are given by Theorem 2, and as summarized in Theorem 3, these new bounds are at least as tight as the existing spectral bounds. Corollary 1 additionally specifies the condition that determines whether the CR bounds are strictly tighter than the SR bounds. The numerical results

in Figs. 1a–3 show that, indeed, the CR bounds are tighter than the SR bounds, and that the improvement can be significant.

We furthermore apply the constrained relaxation method to a number of problems in spectral graph theory. In particular, we show that the Cheeger inequality lower-bound, max cut bounds and the expander mixing lemma and related graph isoperimetric inequality [17,2] can be tightened using the constrained relaxation method. Finally, the conceptual importance of the cut-set in epidemics on networks is highlighted, and we show how our improved bounds provide a tighter characterization of best and worst-case spreading behavior, as well as improved bounds for the error of mean-field approximation methods.

Appendix A. Proof of spectral constraints

Proof of property (4a). From Plancherel's theorem applied to the Laplacian eigenvectors z_k (2), we know that for any vector $x \in \mathbb{R}^N$ the relation

$$\sum_{k=1}^{N} (z_k^T x)^2 = \sum_{k=1}^{N} (x_k)^2$$

holds. For the partition indicator vector $w_{\mathcal{V}}$ in particular, and using the fact that $z_N = \frac{u}{\sqrt{N}}$, this yields:

$$\sum_{k=1}^{N-1} (z_k^T w_{\mathcal{V}})^2 = Nv(1-v),$$

proving property (4a). □

Proof of property (4b). Since the partition indicator vector $w_{\mathcal{V}}$ is a zero-one vector, the projection $w_{\mathcal{V}}^T z_k$ can be written as

$$w_{\mathcal{V}}^T z_k = \sum_{i \in \mathcal{V}} (z_k)_i.$$

In other words, the projection is a sum of V entries of eigenvector z_k. This sum can be bounded by

$$\sum_{i \in \mathcal{V}_-} (z_k)_i \leq w_{\mathcal{V}}^T z_k \leq \sum_{i \in \mathcal{V}_+} (z_k)_i, \tag{30}$$

where $\mathcal{V}_+$ is the subset of $\mathcal{N}$ corresponding to the V nodes with the highest z_k values, and $\mathcal{V}_-$ the subset with the V lowest z_k values. Introducing the ordered vector $z_k^{\downarrow}$, with $\left(z_k^{\downarrow}\right)_1 \geq \left(z_k^{\downarrow}\right)_2 \geq \cdots \geq \left(z_k^{\downarrow}\right)_N$, allows inequality (30) to be written as

$$\sum_{i=N-V+1}^{N} \left(z_k^{\downarrow}\right)_i \leq w_{\mathcal{V}}^T z_k \leq \sum_{i=1}^{V} \left(z_k^{\downarrow}\right)_i .$$

Since all eigenvectors z_k, with $k \neq N$, are orthogonal to $z_N = \frac{u}{\sqrt{N}}$, which means that $\sum_{i=1}^{N}(z_k)_i = 0$ holds, we can write

$$-\sum_{i=1}^{N-V} \left(z_k^{\downarrow}\right)_i \leq w_{\mathcal{V}}^T z_k \leq \sum_{i=1}^{V} \left(z_k^{\downarrow}\right)_i .$$

Squaring leads to the inequality

$$(w_{\mathcal{V}}^T z_k)^2 \leq \max\left\{ \left(\sum_{i=1}^{V} \left(z_k^{\downarrow}\right)_i\right)^2, \left(\sum_{i=1}^{N-V} \left(z_k^{\downarrow}\right)_i\right)^2 \right\},$$

which proves property (4b). □

Appendix B. Derivation of constrained relaxation bounds

Proof of Theorem 2. From expression (3) and introducing the parameter $K \in \{1, 2, \ldots, N\}$, we know that the cut size can be written as

$$|\partial\mathcal{V}| = \sum_{k=1}^{N} (w_{\mathcal{V}}^T z_k)^2 \mu_k = \sum_{k=1}^{K-1} (w_{\mathcal{V}}^T z_k)^2 \mu_k + \sum_{k=K}^{N-1} (w_{\mathcal{V}}^T z_k)^2 \mu_k,$$

where the empty sums $\sum_{k=1}^{0}$ and $\sum_{k=N}^{N-1}$ are defined to be zero. By the ordering of the eigenvalues $\mu_K \geq \mu_k$ holds for all $k \geq K$. Replacing μ_k by μ_K in the second summation then yields the inequality:

$$|\partial\mathcal{V}| \leq \sum_{k=1}^{K-1} (w_{\mathcal{V}}^T z_k)^2 \mu_k + \mu_K \sum_{k=K}^{N-1} (w_{\mathcal{V}}^T z_k)^2$$

Invoking property (4a) as $\sum_{k=1}^{K-1}(w_{\mathcal{V}}^T z_K)^2 + \sum_{k=K}^{N-1}(w_{\mathcal{V}}^T z_K)^2 = Nv(1-v)$ then leads to

$$|\partial\mathcal{V}| \leq \sum_{k=1}^{K-1} (w_{\mathcal{V}}^T z_k)^2 (\mu_k - \mu_K) + Nv(1-v)\mu_K.$$

Finally, invoking property (4b), we can further bound the cut-set size as:

$$|\partial\mathcal{V}| \leq \sum_{k=1}^{K-1} s_k^2(v)(\mu_k - \mu_K) + Nv(1-v)\mu_K \quad \text{for any } 1 \leq K \leq N,$$

which proves that the CR-K bounds upper-bound the cut size. □

The lower-bound inequality follows similarly by replacing μ_k by $-\mu_k$ (turning maximization into minimization) and subsequently ordering the eigenvalues according to decreasing values, which leads to the index replacement $k \to k' = N - k$.

Appendix C. Hierarchy of bounds

We start by proving an additional Lemma, which relates the CR-K bounds for different values of K:

Lemma 2. *The constrained relaxation upper-bounds for different values of K satisfy*

$$\begin{cases} \Theta_C(v, K_1) \geq \Theta_C(v, K_2) & \text{for } 1 \leq K_1 \leq K_2 \leq K_u(v) \\ \Theta_C(v, K_3) \leq \Theta_C(v, K_4) & \text{for } K_u(v) \leq K_3 \leq K_4 \leq N, \end{cases}$$

and similarly for the lower-bounds.

Proof of Lemma 2. The difference between two consecutive bounds equals:

$$\Theta_C(v, K-1) - \Theta_C(v, K) = \underbrace{(\mu_K - \mu_{K-1})}_{\leq 0} \left(\sum_{k=1}^{K-1} s_k^2(v) - Nv(1-v) \right) \quad \text{for } 2 \leq K \leq N,$$

where the first factor is always negative or zero by the eigenvalue ordering. Hence, the sign of the second factor determines which of the consecutive bounds is tighter:

$$\begin{cases} \Theta_C(v, K-1) \geq \Theta_C(v, K) & \text{if } \sum_{k=1}^{K-1} s_k^2(v) \leq Nv(1-v) \\ \Theta_C(v, K-1) \leq \Theta_C(v, K) & \text{if } \sum_{k=1}^{K-1} s_k^2(v) \geq Nv(1-v) \end{cases}$$

from which Lemma 2 follows by definition of $K_u(v) = \max\left\{1 \leq K \leq N \middle| \sum_{k=1}^{K-1} s_k^2(v) \leq Nv(1-v)\right\}$ in (17), and by transitivity of "$\leq$" and "$\geq$". □

In order to prove the hierarchy of bounds (18), we start by proving pairwise inequalities of the form $\theta_1 \leq \theta_2$ and $\theta_2 \leq \theta_3$, which by transitivity of "$\leq$" over the real numbers also proves $\theta_1 \leq \theta_2 \leq \theta_3$.

Proof of Theorem 3. By definition, the exact bound satisfies:

$$|\partial \mathcal{V}| \leq \max_{\substack{\mathcal{V} \subset \mathcal{N} \\ |\mathcal{V}| = V}} |\partial \mathcal{V}| = \Theta_E(v) \tag{a}$$

Since the CR* bound is found by relaxing the exact optimization problem, the solution to the CR* problem (12) is less tight than the exact bound:

$$\Theta_E(v) \leq \Theta_{C\star}(v) \tag{b}$$

Next, the CR-K problem approximates the CR* problem by replacing $\mu_{k>K}$ by μ_K, which means that for all K and for $K_u(v)$ in particular, the inequality

$$\Theta_{C\star}(v) \leq \Theta_C(v, K_u(v)) \tag{c}$$

must hold. From Lemma 2, it follows that $K = K_u(v)$ achieves the tightest bound among all CR-K bounds:

$$\Theta_C(v, K_u(v)) \leq \Theta_C(v, K) \quad \text{for } 1 \leq K \leq K_u(v) \tag{d}$$

Finally, since the CR-K bound for $K = 1$ equals the SR bound, and invoking Lemma 2 leads to:

$$\Theta_C(v, K) \leq \Theta_C(v, 1) \equiv \Theta_S(v) \quad \text{for } 1 \leq K \leq K_u(v) \tag{e}$$

By transitivity, the inequalities (a)-(e) then lead to

$$|\partial\mathcal{V}| \overset{(a)}{\leq} \Theta_E(v) \overset{(b)}{\leq} \Theta_{C\star}(v) \overset{(c)}{\leq} \Theta_C(v, K_u(v)) \overset{(d)}{\leq} \Theta_C(v, K) \overset{(e)}{\leq} \Theta_S(v) \equiv \Theta_C(v, 1),$$

proving Theorem 3. □

Appendix D. Proof of Tighter Expander Mixing Lemma

We prove that the tighter expander mixing lemma follows as a corollary from Theorem 2, by rewriting the difference between the cut size $|\partial\mathcal{V}|$ and the average cut size $2Lv(1-v)$.

Proof of Corollary 3. Using the partition indicator vector $w_\mathcal{V}$, we can write the difference between the cut size $|\partial\mathcal{V}|$ and the average cut size $2Lv(1-v)$ as:

$$|\partial\mathcal{V}| - 2Lv(1-v) = w_\mathcal{V}^T Q w_\mathcal{V} - \frac{2L}{N} w_\mathcal{V}^T \left(I - \frac{uu^T}{N}\right) w_\mathcal{V},$$

with I the identity matrix. Since all Laplacian eigenvectors z_k that correspond to non-zero eigenvalues $\mu_k \neq 0$ satisfy $z_k^T u = 0$, and thus satisfy $\sum_{k=1}^{N-1} z_k z_k^T = I - \frac{uu^T}{N}$, this can be rewritten as:

$$|\partial\mathcal{V}| - 2Lv(1-v) = w_\mathcal{V}^T \left(\sum_{k=1}^{N-1} z_k z_k^T \left(\mu_k - \frac{2L}{N}\right)\right) w_\mathcal{V}.$$

Defining the matrix $\widetilde{Q} = \sum_{k=1}^{N-1} z_k z_k^T (\mu_k - \frac{2L}{N})$ leads to

$$|\partial\mathcal{V}| - 2Lv(1-v) = w_{\mathcal{V}}^T \widetilde{Q} w_{\mathcal{V}} = |\widetilde{\partial}\mathcal{V}|, \tag{31}$$

where $\widetilde{\partial}\mathcal{V}$ is the "cut-set" with respect to the matrix $\widetilde{Q}$. While in general this matrix $\widetilde{Q}$ is not a Laplacian matrix (since $\mu_k - \frac{2L}{N}$ can be negative for some k), the derivation of the CR-K bound still works for the matrix $\widetilde{Q}$, because $\widetilde{Q}$ has a single zero eigenvalue corresponding to the eigenvector $\frac{u}{\sqrt{N}}$. Hence, we can bound the cut size $|\widetilde{\partial}\mathcal{V}|$ by the CR-K bounds $\widetilde{\Theta}_C(v,K)$, which means equation (31) can be written as

$$\left|\widetilde{\theta}_C(v,K)\right| \leq |\partial\mathcal{V}| - 2Lv(1-v) \leq \left|\widetilde{\Theta}_C(v,K)\right|,$$

which proves Corollary 3 by taking the absolute value and using the tightest bounds $K = K_u(v)$ and $K = K_l(v)$ for the upper and lower-bound, respectively. □

Appendix E. The General Expander Mixing Lemma

Here, we prove an improvement of the general expander mixing lemma which is based on the cut-set $\mathcal{C}(\mathcal{V},\mathcal{S})$ between any pair of disjoint partitions [2,17]:

Lemma 3 *(General Expander Mixing Lemma). In a graph $G(\mathcal{N},\mathcal{L})$, the difference between the average cut size $2Lsv$ and the cut size $|\mathcal{C}(\mathcal{V},\mathcal{S})|$ between two disjoint partitions $\mathcal{V}$ and $\mathcal{S}$ is bounded by*

$$\left||\mathcal{C}(\mathcal{V},\mathcal{S})| - 2Lsv\right| \leq \lambda N\sqrt{v(1-v)s(1-s)},$$

with $\lambda = \max\{|\mu_{N-1} - \frac{2L}{N}|, |\mu_1 - \frac{2L}{N}|\}$, and $s = \frac{|\mathcal{S}|}{N}$ and $v = \frac{|\mathcal{V}|}{N}$.

As we show further, it is possible to upper-bound the cut size $|\mathcal{C}(\mathcal{V},\mathcal{S})|$ using the cut sizes $|\partial\mathcal{V}|$ and $|\partial\mathcal{S}|$, which allows the general expander mixing lemma to be improved using the constrained relaxation method:

Theorem 8 *(Tighter Expander Mixing Lemma). In a graph $G(\mathcal{N},\mathcal{L})$, the difference between the average cut size $2Lsv$ and the cut size $|\mathcal{C}(\mathcal{V},\mathcal{S})|$ between two disjoint partitions $\mathcal{V}$ and $\mathcal{S}$ is bounded by*

$$\left||\mathcal{C}(\mathcal{V},\mathcal{S})| - 2Lsv\right| \leq \sqrt{\widehat{\Theta}_C(v,K_u(v))\widehat{\Theta}_C(s,K_u(s))} \leq N\lambda\sqrt{v(1-v)s(1-s)}$$

where $\widehat{\Theta}_C(v,K)$ is the CR-K bound with respect to the matrix $\widehat{Q} = \left|Q - \frac{2L}{N}(I - \frac{uu^T}{N})\right|$.

Proof. Using the zero-one partition indication vectors $w_{\mathcal{V}}$ and $w_{\mathcal{S}}$ with $w_{\mathcal{V}}^T u = Nv$ and $w_{\mathcal{S}}^T u = Ns$ and the fact that $w_{\mathcal{V}}^T w_{\mathcal{S}} = 0$, we have:

$$\left||\mathcal{C}(\mathcal{V},\mathcal{S})| - 2Lvs\right| = \left|-w_{\mathcal{V}}^T Q w_{\mathcal{S}} + \frac{2L}{N} w_{\mathcal{V}}^T \left(I - \frac{uu^T}{N}\right) w_{\mathcal{S}}\right|.$$

Since all eigenvectors of the Laplacian Q that correspond to non-zero eigenvalues satisfy $z_k^T u = 0$ and thus satisfy $\sum_{k=1}^{N-1} z_k z_k^T = I - \frac{uu^T}{N}$, this can be written as:

$$\big||\mathcal{C}(\mathcal{V},\mathcal{S})| - 2Lsv\big| = \left|\sum_{k=1}^{N-1} (w_{\mathcal{V}}^T z_k)(w_{\mathcal{S}}^T z_k)(\mu_k - \frac{2L}{N})\right|.$$

Now we define $\hat{\mu}_k = |\mu_{i^\star} - \frac{2L}{N}|$ and $\hat{z}_k = z_{i^\star}$, where $i^\star$ is the index such that $\hat{\mu}_k$ is ordered according to descending values. Invoking the Cauchy-Schwarz inequality then leads to:

$$\big||\mathcal{C}(\mathcal{V},\mathcal{S})| - 2Lsv\big| \leq \sqrt{\sum_{k=1}^{N-1} (w_{\mathcal{V}}^T \hat{z}_k)^2 \hat{\mu}_k \sum_{i=1}^{N-1} (w_{\mathcal{S}}^T \hat{z}_k)^2 \hat{\mu}_k}.$$

If by $\widehat{\partial}$ we denote the "cut-set" with respect to the matrix $\widehat{Q} = \sum_{k=1}^{N-1} \tilde{z}_k \hat{z}_k^T \hat{\mu}_k$, then we can write:

$$\big||\mathcal{C}(\mathcal{V},\mathcal{S})| - 2Lsv\big| \leq \sqrt{|\widehat{\partial}\mathcal{V}||\widehat{\partial}\mathcal{S}|}.$$

By introducing the CR-K upper-bounds for $|\widehat{\partial}\mathcal{V}|$ and $|\widehat{\partial}\mathcal{S}|$ in this expression, we arrive at Corollary 3. □

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