On The Isoperimetric Spectrum of Graphs and Its Approximations

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Abstract

In this paper[2] we consider higher isoperimetric numbers of a (finite directed) graph. In this regard we focus on the nth mean isoperimetric constant of a directed graph as the minimum of the mean outgoing normalized flows from a given set of n disjoint subsets of the vertex set of the graph. We show that the second mean isoperimetric constant in this general setting, coincides with (the mean version of) the classical Cheeger constant of the graph, while for the rest of the spectrum we show that there is a fundamental difference between the nth isoperimetric constant and the number obtained by taking the minimum over all n-partitions. In this direction, we show that our definition is the correct one in the sense that it satisfies a Federer-Fleming-type theorem, and we also define and present examples for the concept of a *supergeometric graph* as a graph whose mean isoperimetric constants are attained on partitions at all levels.
Moreover, considering the **NP**-completeness of the isoperimetric problem on graphs, we address ourselves to the approximation problem where we prove general spectral inequalities that give rise to a general Cheeger-type inequality as well. On the other hand, we also consider some algorithmic aspects of the problem where we show connections to orthogonal representations of graphs and following J. Malik and J. Shi (2000) we study the close relationships to the well-known k-means algorithm and normalized cuts method.

Key words: Isoperimetric number, Connectivity, Graph, Markov chain.

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1 Introduction

1.1 Objectives and main results

The chapter on isoperimetric numbers and Cheeger-type inequalities is a classic in geometric analysis as well as spectral graph theory and has been considered from many different aspects

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and points of view [3, 7, 8, 22, 29, 36, 39]. The study of such concepts in the discrete case, although more recent, has also been a center of attention mainly because of its many diverse connections to important problems of the century, both applied and theoretical in nature (e.g. see [1, 6, 9, 12, 13, 14, 23, 28, 30, 32, 34, 38, 41, 42, 43]).
Let us recall (e.g. see [42]) the definition of the classical Cheeger constant of a Markov chain[3] K on a directed base-graph $G = (V(G), E(G))$, with a nowherezero stationary distribution π, as

$$\varsigma(K,\pi) \stackrel{\text{def}}{=} \min_{\pi(Q)\leq 1/2} \frac{\partial(Q)}{\pi(Q)} = \min_{Q\subseteq V(G)} \max\left\{\frac{\partial(Q)}{\pi(Q)}, \frac{\partial(Q)}{\pi(Q^c)}\right\},$$

where

$$\partial(Q) \stackrel{\text{def}}{=} \sum_{u\in Q \ \& \ v\notin Q} K(u,v)\pi(u),$$

and the not so common mean version as follows

$$\iota(K,\pi) \stackrel{\text{def}}{=} \min_{Q\subseteq V(G)} \frac{\partial(Q)}{2\pi(Q)(1-\pi(Q))}. \tag{1}$$

Our main objective in this paper is to analyze the *connectivity* of a (directed) finite graph through its isoperimetric spectrum and to consider the computational aspects of this problem. In this regard, we will show that the natural generalization of the classical definition to the nth level for $n > 2$ does not work if one takes the minimum over n-partitions of the vertex set and we propose a correct definition in the sense that it satisfies a coarea formula. We also show that this fundamental difference not only is important in the approximation problem of the isoperimetric spectrum but also can be quite discriminating in an algorithmic approach to applications.
In what follows we try to present a short overview of our approach in this article. Firstly, it should be noted that our main strategy is to transfer the problem to the symmetric base graph and then use the machinery that is already available through the theory of reversible Markov chains. Our basic *symmetrization* approach is adopted from some classical methods as presented in [26]. In this regard, in Section 2, on the one hand, we have tried to present this well-known setup in a unified and concise way accessible to graph theorist with an emphasis on concepts related to connectivity and flows on the base graph, where we have tried to keep our notations classic enough to be most natural for all communities involved. On the other hand, in this section we show that the standard symmetrization process that translates the connectivity parameters of a given (in general directed) graph to the connectivity of its symmetrized undirected base graph is natural in the sense that the stationary distribution and the total flow are preserved in this change of base (see Equation (2) and Lemma 2(a)).
Secondly, it also ought to be noted that computing the isoperimetric numbers of a graph is known to be a computationally hard problem (e.g. see [38] for the classic version. For the mean version see [24] or [43] where an **NP**-completeness result attributed to Papadimitrou (1997) is presented), when the eigenvalues and eigenfunctions of a finite graph are quite close at hand and can be computed effectively (essentially in polynomial time) through well-known methods of linear algebra.
In the sequel, we concentrate on the *mean* version of the isoperimetric number, and introduce its extensions to higher indices, as a set of constants called the (mean) *isoperimetric spectrum*, in juxtaposition to the classical spectrum consisting of the Laplacian eigenvalues. It is instructive to note that although the idea of using the maximum version of the higher isoperimetric numbers as

$$\varsigma_n(G,K) \stackrel{\text{def}}{=} \min_{\{Q_i\}_1^n} \max_{1\leq i\leq n} \left(\frac{\partial(Q_i)}{\pi(Q_i)}\right),$$

[3]By abuse of language we only refer to the kernel instead of the stochastic process itself.

can be traced back into some texts as [7], it seems that the subtle problem of choosing the suitable class of subsets $\{Q_i\}_1^n$ has not been discussed in detail.
The main reason for our shift of interest toward the mean version are manifold. On the one hand, we must note that most of our results are correct for both maximum and mean versions, however usually the proofs for the mean version are more involved. On the other hand, in our opinion, the *mean spectrum* of the Laplacian whose nth element is the (arithmetic) mean of the first n eigenvalues of the Laplacian operator, seems to be much more well-behaved than the classical spectrum because of the smoothing property of the mean operator (e.g. see [31] for the spectral approximations and a perturbation analysis). This may, in a way, present a fair chance of a better study/approximation of the spectrum and, in this regard, the generalized mean version of the isoperimetric constant plays the central role as the most natural L^1 counterpart.
Another important aspect of considering the mean version is the fact that it can be traced back into some important applications as clustering (e.g. see [24, 43] among many other references and Section 5.3) and as far as we could verify, it presents the most natural applied framework to generalize the isoperimetric constant. In this setup, what is in our opinion a bit of a *surprise*, is that the new definition seems to be well defined (e.g. in the sense that it satisfies a generalized co-area formula) only when it is defined as the minimum over *disjoint* subsets of the space (which does not necessarily constitute a *partition*). The difference between the two definitions based on taking the minimum over *partitions* or *disjoint* sets, although disguised in the case of the classical Cheeger constant (i.e. when we deal with 2-partitions; also, see Proposition 1), seems to be inherently nontrivial in general for both of mean and maximum versions. In Section 3 we introduce and investigate some basic properties of the generalized mean isoperimetric numbers, where in Section 4, we concentrate on some examples and special cases (specifically, in relation to Theorem 1 and the proceeding paragraph). In Section 4.1 we define the concept of a *supergeometric* graph as a graph for which all parameters involved are equivalent, and we provide some examples of such graphs. We believe that supergeometric graphs possess interesting properties that ought to be investigated in future research.
Naturally, pursuing this line of thought, we analyze the mean isoperimetric spectrum, both from analytic and graph theoretic points of view, and we prove a Federer-Fleming-type theorem (Section 5.1) as well as Cheeger-type inequalities connecting these parameters and the classical spectrum of eigenvalues in different levels (Section 5.2). Also, as a byproduct, it is shown that generalized Cheeger inequalities at the nth level seem to be strongly related to the concept of a *nodal domain* (e.g. see [33, 45] for the background).
Based on the fact that the isoperimetric problem is computationally a hard problem, in Section 5.3 we concentrate on some algorithmic considerations related to computation of the isoperimetric spectrum where we study the close relationships to the well-known k-means algorithm.

2 Preliminaries

In this section we go through some basic definitions and facts that will be used later. In what follows $\mathbb{R}$ and $\mathbb{R}^+$ are the sets of real and nonnegative real numbers, respectively, and for any real number $x \in \mathbb{R}$ we define

$$(x)^+ \stackrel{\text{def}}{=} \begin{cases} x & x > 0 \\ 0 & x \leq 0. \end{cases}$$

For an n-list of real numbers (repetition is allowed) as $(\zeta_1, \zeta_2, \ldots, \zeta_n)$, the mean n-list is denoted by $(\overline{\zeta}_1, \overline{\zeta}_2, \ldots, \overline{\zeta}_n)$, where

$$\overline{\zeta}_k \stackrel{\text{def}}{=} \frac{1}{k} \sum_{i=1}^{k} \zeta_i.$$

Hereafter, we adopt the notation $\mathcal{I}_n^k \stackrel{\text{def}}{=} \{k, k+1, \ldots, n\}$. Also, $\mathcal{I}_n \stackrel{\text{def}}{=} \mathcal{I}_n^1$.

2.1 Function spaces

If X is a set then $\mathcal{F}^d(X)$ stands for the set of all real functions $f : X \longrightarrow \mathbb{R}^d$, and also we define $\mathcal{F}(X) \stackrel{\text{def}}{=} \mathcal{F}^1(X)$. Similarly, $\mathcal{F}^+(X) \stackrel{\text{def}}{=} \{f \mid f : X \longrightarrow \mathbb{R}^+\}$. Also, for a positive and nowherezero weight function $\omega : X \longrightarrow \mathbb{R}^+ - \{0\}$ we define the inner product $\langle ., . \rangle_\omega$ and the norm $\|.\|_{p,\omega}$ on $\mathcal{F}(X)$ as

$$\langle f, g \rangle_\omega \stackrel{\text{def}}{=} \sum_{x \in X} f(x) g(x) \omega(x), \quad \|f\|_{p,\omega} \stackrel{\text{def}}{=} \left(\sum_{x \in X} |f(x)|^p \ \omega(x) \right)^{\frac{1}{p}},$$

respectively, where we usually use the subscript ω to refer to the product structure (e.g. $\mathcal{F}_\omega(X)$). Two functions $f, g \in \mathcal{F}_\omega(X)$ are said to be orthogonal with respect to ω, i.e. $f \perp_\omega g$, whenever $\langle f, g \rangle_\omega = 0$.
For any $f \in \mathcal{F}(X)$, $\text{supp}(f)$ stands for the set $\{v \in V(G) \mid f(v) \neq 0\}$. Also, for any subset $A \subseteq X$ the restriction of f to A is denoted by $f|_A$, i.e.,

$$f|_A(x) \stackrel{\text{def}}{=} \begin{cases} f(x) & x \in A \\ 0 & x \notin A. \end{cases}$$

The characteristic function of a subset $A \subseteq X$ is denoted by $\chi_A \stackrel{\text{def}}{=} 1|_A$ when X is clear from the context.
Moreover, for any real function f, the functions f^+ and f^- stand for the positive and negative parts of f, respectively; and consequently,

$$f = f^+ - f^- \quad \text{and} \quad |f| = f^+ + f^-.$$

For any two functions (or vectors) f, g, we write $f \leq g$ if

$$\forall\ v \in V(G) \quad f(v) \leq g(v).$$

Also, we write $f < g$ if $f \leq g$ and $f \neq g$.

2.2 Graphs and kernels

The main objective of this section is to introduce a common language of graphs and kernels that is accessible to both graph theorists and experts in functional analysis and also benefits from all aspects of the two points of view.
Throughout the paper, a *graph* $G = (V(G), E(G))$ is always assumed to be a finite directed graph (possibly with loops and without multiple edges), where $E(G) \subseteq V(G) \times V(G)$. Similarly, an *undirected graph* $\overline{G} = (V(\overline{G}), E(\overline{G}))$ is a finite set $V(\overline{G})$ along with a set of undirected edges $E(\overline{G})$, each element of which is a subset of $V(\overline{G})$ whose size is less than or equal to 2. When it is clear from the context, by abuse of notation, we use the same symbol uv both for the directed edge $(u, v) \in V(G) \times V(G)$ of a directed graph and also for a simple edge $\{u, v\}$ of an undirected graph.

For a given graph G, we use the natural notation, $\overleftrightarrow{G}$, for its symmetric directed base graph i.e. $V(\overleftrightarrow{G}) \stackrel{\text{def}}{=} V(G)$ and

$$(uv \in E(\overleftrightarrow{G}) \text{ and } vu \in E(\overleftrightarrow{G})) \Leftrightarrow (uv \in E(G) \text{ or } vu \in E(G)).$$

Moreover, for a given graph G, $\overline{G}$ stands for its symmetric undirected base graph i.e. $V(\overline{G}) \stackrel{\text{def}}{=} V(G)$ and

$$uv \in E(\overline{G}) \Leftrightarrow (uv \in E(G) \text{ or } vu \in E(G)).$$

Note that for an undirected graph $\overline{G} = (V(\overline{G}), E(\overline{G}))$ we may think of any simple edge uv as a subset $\{u, v\} \subseteq V(\overline{G})$. With this interpretation $\overleftrightarrow{G} = (V(\overleftrightarrow{G}), E(\overleftrightarrow{G}))$ is a directed graph obtained by replacing any simple edge $uv \in E(\overline{G})$ with two directed edges $uv \in E(\overleftrightarrow{G})$ and $vu \in E(\overleftrightarrow{G})$. Note that there is a one-to-one correspondence between undirected graphs and symmetric directed graphs, where the undirected presentation can be interpreted as a more compact version of expressing the same data.
Given any $n \times n$ matrix K whose rows and columns are indexed by the elements of an n-set V, in general, one can construct a graph $G_{_K} = (V, E)$ where

$$uv \in E \quad \Leftrightarrow \quad K(u, v) \neq 0.$$

Then, it is clear that from this point of view, the concept of a *weighted graph* contains the same data as the concept of a matrix, and moreover, symmetric graphs as well as undirected graphs correspond to the concept of symmetric matrices.

Notational assumption: Throughout the paper an *overlined* notation is usually adopted to refer to a symmetrization process or taking arithmetic means applied to the original concept.

For two given subsets X, Y of $V(G)$ we define

$$\overrightarrow{E}(X, Y) \stackrel{\text{def}}{=} \{uv \in E(G) \ \mid \ u \in X \ \& \ v \in Y\}.$$

Also, for a subset $Q \subset V(G)$ we define

$$\overrightarrow{E}(Q) \stackrel{\text{def}}{=} \overrightarrow{E}(Q, Q^c), \quad \overleftarrow{E}(Q) \stackrel{\text{def}}{=} \overrightarrow{E}(Q^c, Q),$$

and

$$\overleftrightarrow{E}(Q) \stackrel{\text{def}}{=} \overrightarrow{E}(Q) \cup \overleftarrow{E}(Q).$$

Hereafter, $\mathsf{K}_{_t}$ and $\mathsf{K}_{_{r,s}}$ stand for the (simple) complete graph on t vertices and the complete bipartite graph on two parts of sizes r and s, respectively.

2.3 Markov kernels and the energy space

Our major objective in this section is to present a standard symmetrization process as well as some basic facts about the theory of finite Markov chains with a graph theoretic emphasis (e.g. for more on this see [1, 18, 26, 42]). Particularly, we will show that the basic parameters used in this article as the weight functions i.e. the stationary distribution and the corresponding natural flow, are preserved in this setup, and consequently, one may talk about the connectivity parameters that are computable from the symmetric model of the corresponding undirected base graph. In this direction, we have tried to use the *overlined* notations for the parameters and concepts related to the undirected base graphs where we have used the *arrowed* notations for the general directed case. We will elaborate on the

details of this notational assumptions later in this section.
Hereafter, given a graph G, we assume that K is the kernel of a Markov chain on this graph and π is a nowherezero stationary distribution, i.e. $\pi K = \pi$ and $\pi(v) \neq 0$ for all $v \in V(G)$. In this setting, $\phi(u,v) \stackrel{\text{def}}{=} K(u,v)\pi(u)$ defines a nowherezero flow on G. Also, for any two disjoint sets $X, Y \subseteq V(G)$ we define

$$\pi(X) \stackrel{\text{def}}{=} \sum_{u \in X} \pi(u), \quad \overrightarrow{\partial}_{\phi}(X,Y) \stackrel{\text{def}}{=} \sum_{uv \in \overrightarrow{E}(X,Y)} \phi(u,v), \quad \overrightarrow{\partial}_{\phi}(X) \stackrel{\text{def}}{=} \overrightarrow{\partial}_{\phi}(X, X^c),$$

and $\overleftarrow{\partial}_{\phi}(X,Y)$ and $\overleftarrow{\partial}_{\phi}(X)$ analogously. Note that since ϕ is a flow, for every nonvoid subset $Q \subseteq V(G)$, we have

$$\overrightarrow{\partial}_{\phi}(Q) = \overleftarrow{\partial}_{\phi}(Q) = \overrightarrow{\partial}_{\phi}(Q^c).$$

By abuse of notation, we may write $\overrightarrow{\partial}(Q)$ for simplicity, if the flow is clear from the context. Within the same [4] setup, for the symmetric graph $\overline{G}$, we consider the kernel

$$\overline{K}(u,v) \stackrel{\text{def}}{=} \frac{1}{2}(K + K^*) = \frac{1}{2}\left(K(u,v) + \frac{K(v,u)\pi(v)}{\pi(u)}\right),$$

with the same stationary distribution π inducing the flow

$$\overline{\phi}(u,v) \stackrel{\text{def}}{=} \overline{K}(u,v)\pi(u) = \frac{1}{2}(\phi(u,v) + \phi(v,u))$$

on $\overline{G}$. We can also define $\overline{\partial}_{\overline{\phi}}(Q)$ similarly. Note that

$$\overline{\partial}_{\overline{\phi}}(Q) \stackrel{\text{def}}{=} \sum_{\substack{uv \in E(\overline{G}) \\ u \in Q, v \in Q^c}} \overline{\phi}(u,v) = \frac{1}{2}(\overrightarrow{\partial}_{\phi}(Q) + \overleftarrow{\partial}_{\phi}(Q)) = \overrightarrow{\partial}_{\phi}(Q). \tag{2}$$

This shows that for a given graph G, the outgoing flow from a subset $Q \subset V(G)$ is equal to the outgoing flow from $Q \subset V(\overline{G})$ in the symmetrized model, which justifies our transformation method from the directed case to the symmetric case, when dealing with connectivity parameters of graphs in terms of the corresponding flows. We will also prove a generalization of this fact in Lemma 2(a).
Now, we consider two linear Laplacian operators on $\mathcal{F}_{\pi}(G)$ as follows

$$\overrightarrow{\Delta} \stackrel{\text{def}}{=} id - K \quad \text{and} \quad \overline{\Delta} \stackrel{\text{def}}{=} id - \overline{K},$$

where id is the identity operator. It is clear that $\overline{K}$ and $\overline{\Delta}$ are self-adjoint operators on $\mathcal{F}_{\pi}(G)$ by definition, while K and $\overrightarrow{\Delta}$ may not be necessarily so, unless $K = K^*$ and $\overrightarrow{\Delta} = \overline{\Delta}$. Hence, when $|V(G)| = n$, one may order all real eigenvalues of $\overline{\Delta}$ as

$$0 = \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n. \tag{3}$$

(At times we may use superscripts as λ_2^G or λ_2^K to refer to the graph or the kernel when details are clear from the context.)
Also, it is a well-known fact (Perron-Frobenius theorem) that for a strongly connected graph G, the eigenspace corresponding to the eigenvalue $0 = \lambda_1^G$ is one-dimensional and is generated by the constant vector $\mathbf{1}$. Moreover, for any $n \times n$ self-adjoint matrix A, and for any $1 \leq k \leq n$, by Courant–Fischer variational principle (see [42]), one may write

$$\lambda_k^A = \min_{W \in \mathcal{W}_k} \max_{0 \neq f \in W} \left\{ \frac{\langle Af, f \rangle}{\|f\|^2} \right\} = \max_{W \in \mathcal{W}_{k-1}^{\perp}} \min_{0 \neq f \in W} \left\{ \frac{\langle Af, f \rangle}{\|f\|^2} \right\}, \tag{4}$$

[4] Note that for Riemannian manifolds $\partial(Q) = Vol(Boundary(Q))$ has the same property as a trivial flow with only a nonzero component to the complement.

in which

$$\mathcal{W}_{_k} \stackrel{\text{def}}{=} \{W \ \mid \ \dim(W) \geq k\}, \quad \mathcal{W}_{_k}^{\perp} \stackrel{\text{def}}{=} \{W \ \mid \ \dim(W^{\perp}) \leq k\},$$

and $\langle f, g\rangle$ is the inner product of the space on which A is defined and is self-adjoint.

2.4 Gradients, energy and their properties

Given a graph G, one may define the *directed*, *classical*, and *symmetric* gradients, respectively, as follows

- $\overrightarrow{\nabla} : \mathcal{F}_{_\pi}(G) \longrightarrow \mathcal{F}_{_\phi}(G)$ as $\overrightarrow{\nabla} f(uv) \stackrel{\text{def}}{=} (f(u) - f(v))^{+}$.
- $\nabla : \mathcal{F}_{_\pi}(G) \longrightarrow \mathcal{F}_{_\phi}(G)$ as $\nabla f(uv) \stackrel{\text{def}}{=} f(u) - f(v)$.
- $\overline{\nabla} : \mathcal{F}_{_\pi}(\overline{G}) \longrightarrow \mathcal{F}_{_{\overline{\phi}}}(\overline{G})$ as $\overline{\nabla} f(uv) \stackrel{\text{def}}{=} |f(u) - f(v)|$.

In the rest of this paper we will adopt the following framework.

Assumption: Following our previous notational assumption, hereafter, given any directed graph G (possibly with loops), we will be working with the measure spaces $(V(G), \pi)$ and $(E(G), \phi)$ as well as $(V(\overline{G}), \pi)$ and $(E(\overline{G}), \overline{\phi})$ for the corresponding undirected graph, (note that the last case also covers the case of simple graphs). In our notations, the subscript determines the function space under consideration (e.g. $\mathcal{F}_{_\phi}(G)$ stands for the set of all real functions defined on $E(G)$, the set of edges of a given graph G, equipped with an inner product weighted by ϕ). Thus we will be working within the frameworks $[G, (V(G), \pi), (E(G), \phi), \overrightarrow{\nabla}, \nabla, \overrightarrow{\Delta}]$ and $[\overline{G}, (V(\overline{G}), \pi), (E(\overline{G}), \overline{\phi}), \overline{\nabla}, \overline{\Delta}]$ for the (in general directed) graph G, and the corresponding undirected graph, respectively.

It ought to be noted that considering the inner-product space equipped with the weighted inner-product $\langle ., . \rangle_{_\pi}$ has the advantage of reflecting parts of the global structural properties of the base graph in the spectrum of the corresponding Laplacian operator (e.g. see [15, 16, 18, 26]), while this is not necessarily true when one uses the ordinary inner-product of $\mathbb{R}^n$ or symmetrization by the square root of the degree matrix (e.g. as in [9, 10, 11]). Let us start with the following well-known result.

Lemma 1. *For a given graph G, the classical gradient, ∇, is a linear operator and has an adjoint $\nabla^* : \mathcal{F}_{_\phi}(G) \longrightarrow \mathcal{F}_{_\pi}(G)$ defined as*

$$\nabla^* f(u) \stackrel{\text{def}}{=} \frac{1}{\pi(u)} \left(\sum_{uv \in E(G)} f(uv)\phi(u, v) - \sum_{vu \in E(G)} f(vu)\phi(v, u) \right).$$

Moreover, $2\overline{\Delta} = \nabla^* \nabla$.

Proof. Verification of the adjunction is straightforward. For the second equality, we have,

$$(\overline{\Delta} f)(u) = \frac{1}{\pi(u)} \sum_{v \in V(G)} (f(u) - f(v)) \ \overline{\phi}(u, v) = \frac{1}{\pi(u)} \sum_{v \in V(G)} \nabla f(uv) \ \overline{\phi}(u, v) = \frac{1}{2} \ \nabla^* \nabla f(u).$$

Also, note that,

$$\langle 2\overline{\Delta} f, g\rangle_{_\pi} = \langle \nabla^* \nabla f, g\rangle_{_\pi} = \langle \nabla f, \nabla g\rangle_{_\phi},$$

holds for all $f, g \in \mathcal{F}_{_\pi}(G)$. ■

The simple but important statement of Lemma 1 in a way presents the symmetrization process of constructing the undirected symmetric graph $\overline{G}$ from a given graph G, in an analytic sort of way. In other words, starting from a kernel K on a base graph G, and considering the operators ∇ and ∇^*, one may construct the symmetric Laplacian operator as $\overline{\Delta} = \frac{1}{2}\nabla^*\nabla$ that introduces a new kernel whose base graph is $\overline{G}$. Also, a classical and interesting fact is that if one starts from a graph G and considers the conservation of energy as Kirchhoff's node and loop laws, then one finds a Poisson's equation relating the current and voltage (i.e. potential) functions whose basic operator is the symmetric Laplacian $\overline{\Delta}$ on $\overline{G}$ (e.g. see [44]). Hence, in this sense, conservation of energy naturally is linked to connectivity through the symmetric model.
With this background, one of our main objectives can be described as finding methods that can reflect some of the *connectivity* properties of G in its related symmetric model $\overline{G}$, through the self-adjoint or symmetric operators defined on it. Therefore, it is natural to concentrate on well-behaved or induced operators on $\overline{G}$ (e.g. $\overline{\nabla} : \mathcal{F}_{\pi}(\overline{G}) \longrightarrow \mathcal{F}_{\overline{\phi}}(\overline{G})$) and consider their relationships to those of G. The following lemma summarizes some of the basic properties of these operators for further reference. Specially, note that Equation (2) is a consequence of part (a).

Lemma 2. *For any given graph G with a kernel K on it, and $f \in \mathcal{F}_{\pi}(G)$,*

a) $\|\overrightarrow{\nabla} f\|_{1,\phi} = \frac{1}{2}\ \|\nabla f\|_{1,\phi} = \|\overline{\nabla} f\|_{1,\overline{\phi}}$.

b) $\|\overrightarrow{\nabla} f\|_{1,\phi} = \|\overrightarrow{\nabla} f^{+}\|_{1,\phi} + \|\overrightarrow{\nabla} f^{-}\|_{1,\phi}$.

c) $\frac{1}{2}\ \|\nabla f\|^2_{2,\phi} = \|\overline{\nabla} f\|^2_{2,\overline{\phi}} = \langle \overline{\Delta} f, f\rangle_{\pi} = \langle \overrightarrow{\Delta} f, f\rangle_{\pi}$.

Proof. For (a) note that $2\overrightarrow{\nabla} f(uv) = \big(f(u) - f(v)\big) + |f(u) - f(v)|$. Since ϕ is a flow on $E(G)$, we have

$$\sum_{uv\in E(G)} \big(f(u) - f(v)\big)\ \phi(u,v) = \sum_{u\in V(G)} f(u)\ \big(\overrightarrow{\partial}(\{u\}) - \overleftarrow{\partial}(\{u\})\big) = 0$$

and consequently,

$$\begin{aligned} \|\overrightarrow{\nabla} f\|_{1,\phi} &= \sum_{uv\in E(G)} \overrightarrow{\nabla} f(uv)\ \phi(u,v) = \frac{1}{2}\sum_{uv\in E(G)} |f(u) - f(v)|\ \phi(u,v) \\ &= \frac{1}{2}\sum_{uv\in E(\overline{G})} \overline{\nabla} f(uv)\ \big(\phi(u,v) + \phi(v,u)\big) = \|\overline{\nabla} f\|_{1,\overline{\phi}}. \end{aligned}$$

Equality in (b) is clear. Also, (c) follows from Lemma 1 and the following equalities,

$$\begin{aligned} \langle (id - K)f, f\rangle_{\pi} &= \langle (id - \frac{1}{2}(K + K^*))f, f\rangle_{\pi} = \frac{1}{2}\|\nabla f\|^2_{2,\phi} \\ &= \frac{1}{2}\sum_{uv\in E(\overline{G})} |f(u) - f(v)|^2\ \big(\phi(u,v) + \phi(v,u)\big) = \|\overline{\nabla} f\|^2_{2,\overline{\phi}}. \end{aligned}$$

■

Clearly, in this approach, one needs some relations between the energy (Dirichlet) forms and different norms of the operators to construct the necessary connections needed. The following two lemmas demonstrate the most basic relationships.

Lemma 3. *For every $f \in \mathcal{F}_{\pi}(G)$ we have*

a) $\|\nabla f\|_{1,\phi} \leq \|\nabla f\|_{2,\phi}$.

b) $\|\overrightarrow{\nabla} f\|_{1,\phi} = \|\overline{\nabla} f\|_{1,\overline{\phi}} \leq \frac{\sqrt{2}}{2} \|\overline{\nabla} f\|_{2,\overline{\phi}}$.

Proof. Since ϕ is a flow we have $\sum_{uv \in E(G)} \phi(u,v) = 1$, and consequently, by Cauchy-Schwarz inequality,

$$\begin{aligned} \sum_{uv \in E(G)} |f(u) - f(v)|^2 \ \phi(u,v) &= \left(\sum_{uv \in E(G)} |f(u) - f(v)|^2 \ \phi(u,v) \right) \left(\sum_{uv \in E(G)} \phi(u,v) \right) \\ &\geq \left(\sum_{uv \in E(G)} |f(u) - f(v)| \ \phi(u,v) \right)^2 . \end{aligned}$$

Part (*b*) follows by a similar discussion. ■

Lemma 4. *For every* $0 \neq f \in \mathcal{F}_{\pi}(G)$ *we have*

a) $\frac{\|\nabla f^2\|_{1,\phi}}{\|f^2\|_{1,\pi}} \leq 2 \ \frac{\|\nabla f\|_{2,\phi}}{\|f\|_{2,\pi}}$.

b) $\frac{\|\overrightarrow{\nabla} f^2\|_{1,\phi}}{\|f^2\|_{1,\pi}} = \frac{\|\overline{\nabla} f^2\|_{1,\overline{\phi}}}{\|f^2\|_{1,\pi}} \leq \sqrt{2} \ \frac{\|\overline{\nabla} f\|_{2,\overline{\phi}}}{\|f\|_{2,\pi}}$.

Proof. The proof is clear by Lemma 2(c), Cauchy-Schwarz inequality (e.g. $(a+b)^2 \leq 2(a^2+b^2)$) and the following

$$\begin{aligned} \left(\frac{\sqrt{2} \ \|\overline{\nabla} f\|_{2,\overline{\phi}}}{\|f\|_{2,\pi}} \right)^2 &= \frac{\sum_{uv \in E(G)} |f(u) - f(v)|^2 \ \phi(u,v)}{\sum_{u \in V(G)} |f(u)|^2 \ \pi(u)} \times \frac{\sum_{uv \in E(G)} |f(u) + f(v)|^2 \ \phi(u,v)}{\sum_{uv \in E(G)} |f(u) + f(v)|^2 \ \phi(u,v)} \\ &\geq \frac{\left(\sum_{uv \in E(G)} |f(u)^2 - f(v)^2| \ \phi(u,v) \right)^2}{4 \left(\sum_{u \in V(G)} |f(u)|^2 \ \pi(u) \right)^2} = \left(\frac{\|\overrightarrow{\nabla} f^2\|_{1,\phi}}{\|f^2\|_{1,\pi}} \right)^2 . \end{aligned}$$

■

3 The isoperimetric spectrum

In this section we concentrate on the mean isoperimetric constant and its generalization. In this regard, our point of view is to consider a generalization that is, firstly, well-behaved computationally, and secondly, can present a good relation to the classical eigenvalues. Throughout the section, K is the kernel of a fixed Markov chain on the base graph G as before, and π is a nowherezero stationary distribution for this kernel.
It is a well-known fact from random-matrix theory and the recent literature that the behavior of the classical spectrum of the Laplacian operator is quite hard to predict and, as a matter of fact, is related to some deep problems in contemporary mathematics [23]. In our opinion,

one possible approach in this direction is to analyze a smooth function of the spectrum, that in a way contains a fair amount of data, rather than the eigenvalues themselves. Naturally, the most simple candidate for such a function can be considered to be the *arithmetic mean*, and consequently, there seems to be a fair chance that the behavior of the mean-spectrum, whose nth element is the mean of the first n eigenvalues, be more well-behaved than the spectrum itself. We should also mention the results of J. B. Hiriart-Urruty and D. Ye [31] that, in a sense, justifies this approach.
Therefore, based on the above-mentioned approach we will focus on the mean version of the isoperimetric constant and will generalize it as the most natural L^1 counterpart of the mean eigenvalue. It is interesting to note that this generalization leads to a definition for the nth isoperimetric number which is based on taking a minimum over all *n-disjoint* subsets of the ground-space, rather than its n-partitions, and also satisfies a Federer-Fleming-type theorem (Theorem 1). This difference, although disguised in the classical case $k = 2$ (see Proposition 1), seems to be quite nontrivial in general and will be our main motivation for the definition of a *supergeometric graph*.
It is not hard to check that there is a straightforward translation of almost all results of this section to the case of max-isoperimetric constants (see Section 5.2 for a precise definition) or the case of compact Riemannian manifolds (considering appropriate modifications).
In what follows we introduce the generalized isoperimetric number (in the mean case), and we investigate some of its basic properties. To begin, we set a couple of notations. The set $\mathcal{D}_{n}(G)$ is defined to be the set of all n-sets $\{Q_1, \ldots, Q_n\}$ with $\emptyset \neq Q_i \subseteq V(G)$ for all $1 \leq i \leq n$ such that for every pair $1 \leq i < j \leq n$ we have $Q_i \cap Q_j = \emptyset$. The set of *n-partitions* of a graph G, which is denoted by $\mathcal{P}_{n}(G)$, is the subset of $\mathcal{D}_{n}(G)$ that contains all n-sets $\{Q_1, \ldots, Q_n\}$ for which $\cup_{i=1}^{n} Q_i = V(G)$.
Now, we define the generalized mean isoperimetric constants as,

Definition 1. Given a graph G and a kernel K, the nth (mean) *isoperimetric constant* of G (with respect to K) is defined as follows

$$\iota_{n}(G, K) \stackrel{\text{def}}{=} \min_{\{Q_i\}_1^n \in \mathcal{D}_n(G)} \frac{1}{n} \left(\sum_{i=1}^{n} \frac{\vec{\partial}(Q_i)}{\pi(Q_i)} \right).$$

Also, considering the partitions, we define the following related constant,

$$\tilde{\iota}_{n}(G, K) \stackrel{\text{def}}{=} \min_{\{Q_i\}_1^n \in \mathcal{P}_n(G)} \frac{1}{n} \left(\sum_{i=1}^{n} \frac{\vec{\partial}(Q_i)}{\pi(Q_i)} \right).$$

We may exclude the kernel K from the notations, when it is fixed or is clear from the context. ♠

Some basic properties of the mean isoperimetric spectrum are stated in the following proposition.

Proposition 1. *For any graph G (and a given kernel K on it) and for all $1 \leq n \leq |V(G)|$ we have,*

a) $\iota_{n}(G) \leq \tilde{\iota}_{n}(G) \leq (1 - \frac{1}{n})\ \iota_{n}(G) + \frac{1}{n}$.

b) $\tilde{\iota}_{2}(G) = \iota_{2}(G)$.

c) $\tilde{\iota}_{n}(G) \leq (1 - \frac{1}{n^2})\ \tilde{\iota}_{n+1}(G) < \tilde{\iota}_{n+1}(G)$.

d) $\iota_{n}(G) \leq \iota_{n+1}(G)$.

Proof. The left-hand inequality of part (a) is clear by definitions. Assume that $\iota_{n}(G)$ is achieved by choosing $\{Q_{i}\}_{1}^{n} \in \mathcal{D}_{n}(G)$ and suppose that $\dfrac{\overrightarrow{\partial}(Q_{n})}{\pi(Q_{n})}$ is maximum of all $\dfrac{\overrightarrow{\partial}(Q_{i})}{\pi(Q_{i})}$, $i \in \mathcal{I}_{n}$. Then the partition $\{Q'_{i}\}_{1}^{n} \in \mathcal{P}_{n}(G)$ with $Q'_{i} \stackrel{\text{def}}{=} Q_{i}$ for all $i \in \mathcal{I}_{n-1}$ and $Q'_{n} \stackrel{\text{def}}{=} V(G) - (\cup_{i=1}^{n-1} Q_{i})$ will satisfy

$$\tilde{\iota}_{n}(G) \leq \frac{1}{n}\left(\frac{\overrightarrow{\partial}(Q'_{n})}{\pi(Q'_{n})} + \sum_{i=1}^{n-1}\frac{\overrightarrow{\partial}(Q_{i})}{\pi(Q_{i})}\right) \leq \frac{1}{n}(1 + (n-1)\ \iota_{n}(G)) = (1 - \frac{1}{n})\ \iota_{n}(G) + \frac{1}{n}.$$

For part (b), let $\{Q_{1}, Q_{2}\} \in \mathcal{D}_{2}(G)$ be such that $\iota_{2}(G)$ is achieved and let $Q^{*} \stackrel{\text{def}}{=} V(G) - (Q_{1} \cup Q_{2})$. Without loss of generality, assume that $\overrightarrow{\partial}(Q^{*}, Q_{1}) \leq \overrightarrow{\partial}(Q_{2}, Q^{*})$. Then for the partition $\{Q'_{1}, Q'_{2}\}$ with $Q'_{1} \stackrel{\text{def}}{=} Q_{1}$ and $Q'_{2} \stackrel{\text{def}}{=} Q_{2} \cup Q^{*}$ we have

$$2\ \tilde{\iota}_{2}(G) \leq \sum_{i=1}^{2}\frac{\overrightarrow{\partial}(Q'_{i})}{\pi(Q'_{i})} = \frac{\overrightarrow{\partial}(Q_{1})}{\pi(Q_{1})} + \frac{\overrightarrow{\partial}(Q_{2}, Q_{1}) + \overrightarrow{\partial}(Q^{*}, Q_{1})}{\pi(Q_{2}) + \pi(Q^{*})} \leq \sum_{i=1}^{2}\frac{\overrightarrow{\partial}(Q_{i})}{\pi(Q_{i})} = 2\ \iota_{2}(G).$$

The reverse inequality is clear from the definitions.
For part (c), let $\{Q_{i}\}_{1}^{n+1} \in \mathcal{P}_{n+1}(G)$ be a partition such that $\tilde{\iota}_{n+1}(G)$ is achieved. For every pair of indices $\{j,k\} \subseteq \mathcal{I}_{n+1}$ define

$$T_{j,k}^{n} \stackrel{\text{def}}{=} \frac{1}{n}\left(\frac{\overrightarrow{\partial}(Q_{j} \cup Q_{k})}{\pi(Q_{j} \cup Q_{k})} + \sum_{i \in \mathcal{I}_{n+1} - \{j,k\}}\frac{\overrightarrow{\partial}(Q_{i})}{\pi(Q_{i})}\right),$$

and let $w_{j,k} = \pi(Q_{j} \cup Q_{k})$. Note that $\sum_{1 \leq j < k \leq n+1} w_{j,k} = n$. Also

$$\begin{aligned}
n \sum_{1 \leq j < k \leq n+1} w_{j,k} T_{j,k}^{n} &= \sum_{1 \leq j < k \leq n+1} \overrightarrow{\partial}(Q_{j} \cup Q_{k}) \\
&\quad + \sum_{1 \leq j < k \leq n+1}\ \sum_{i \in \mathcal{I}_{n+1} - \{j,k\}} \pi(Q_{j} \cup Q_{k})\frac{\overrightarrow{\partial}(Q_{i})}{\pi(Q_{i})} \\
&= (n-1)\sum_{i=1}^{n+1}\overrightarrow{\partial}(Q_{i}) \\
&\quad + \sum_{i=1}^{n+1}(n-1)(1 - \pi(Q_{i}))\frac{\overrightarrow{\partial}(Q_{i})}{\pi(Q_{i})} \\
&= (n-1)\sum_{i=1}^{n+1}\frac{\overrightarrow{\partial}(Q_{i})}{\pi(Q_{i})}.
\end{aligned}$$

Thus,

$$\tilde{\iota}_{n}(G) \leq \min_{\{j,k\} \subseteq \mathcal{I}_{n+1}} T_{j,k}^{n} \leq \frac{1}{n}\sum_{1 \leq j < k \leq n+1} w_{j,k} T_{j,k}^{n} \leq \frac{n^{2}-1}{n^{2}}\ \tilde{\iota}_{n+1}(G).$$

For part (d), let $\{Q_{i}\}_{i \in \mathcal{I}_{n+1}} \in \mathcal{D}_{n+1}(G)$ be chosen such that $\iota_{n+1}(G)$ is achieved, and moreover, without loss of generality, assume that

$$\frac{\overrightarrow{\partial}(Q_{1})}{\pi(Q_{1})} \leq \cdots \leq \frac{\overrightarrow{\partial}(Q_{n+1})}{\pi(Q_{n+1})}.$$

Then clearly,

$$\iota_{n}(G) \leq \frac{1}{n}\sum_{i=1}^{n}\frac{\overrightarrow{\partial}(Q_{i})}{\pi(Q_{i})} \leq \frac{1}{n+1}\sum_{i=1}^{n+1}\frac{\overrightarrow{\partial}(Q_{i})}{\pi(Q_{i})} = \iota_{n+1}(G).$$

■

4 Some examples and special cases

As the first example, let us consider the case $n = 2$.

Example 1. Let G be a given directed graph. We have

$$\begin{aligned}
\tilde{\iota}_2(G) &= \min_{\{Q_i\}_1^2 \in \mathcal{P}_2(G)} \frac{1}{2}\left(\frac{\vec{\partial}(Q_1)}{\pi(Q_1)} + \frac{\vec{\partial}(Q_2)}{\pi(Q_2)}\right) \\
&= \min_{Q \subseteq V(G)} \frac{1}{2}\left(\frac{\vec{\partial}(Q)}{\pi(Q)} + \frac{\vec{\partial}(Q^c)}{\pi(Q^c)}\right) \\
&= \min_{Q \subseteq V(G)} \frac{1}{2}\left(\frac{\vec{\partial}(Q)}{\pi(Q)} + \frac{\vec{\partial}(Q)}{(1-\pi(Q))}\right) \\
&= \min_{Q \subseteq V(G)} \frac{\vec{\partial}(Q)}{2\pi(Q)(1-\pi(Q))},
\end{aligned}$$

which is the (mean version) of the classical Cheeger constant. Therefore, since we have $\tilde{\iota}_2(G) = \iota_2(G)$ by Proposition 1(b), our definition of the isoperimetric number for the classical case is justified. ♣

Given a strongly connected directed graph G, we define the natural random walk on G by

$$K(u,v) = \begin{cases} \frac{1}{d^+(u)} & uv \in E(G) \\ 0 & uv \notin E(G), \end{cases}$$

where $d^+(u)$ stands for the out-degree of vertex u. If the graph G is Eulerian, i.e. for every vertex $u \in V(G)$, we have $d^+(u) = d^-(u)$, then one can easily see that the distribution π, defined by $\pi(u) = \frac{d^+(u)}{|E(G)|}$ is the unique stationary distribution for the natural random walk on G which induces the flow ϕ on G, defined by $\phi(u,v) \stackrel{\text{def}}{=} \frac{1}{|E(G)|}$, whenever $uv \in E(G)$ and zero elsewhere. Hence, for every subset $Q \subseteq V(G)$, we have

$$\frac{\vec{\partial}(Q)}{\pi(Q)} = \frac{|\vec{E}(Q)|}{d^+(Q)}, \tag{5}$$

where $d^+(Q) \stackrel{\text{def}}{=} \sum_{u \in Q} d^+(u)$. Note that for any connected undirected graph G, the symmetric directed graph $\overleftrightarrow{G}$ is Eulerian, which shows that these arguments are valid in the case of undirected connected graphs as well.

4.1 Geometric graphs

By Proposition 1, for any given directed graph G with a kernel K and a nowherezero stationary distribution π on it, one can talk about the isoperimetric spectrum,

$$0 = \iota_1(G,K) \leq \iota_2(G,K) \leq \ldots \leq \iota_{|V(G)|}(G,K) \leq 1.$$

Also, note that if G has no loops then $\iota_{|V(G)|}(G,K) = 1$. On the other hand, by definitions, for any given graph G and for all $1 \leq n \leq |V(G)|$, we have $\iota_n(G,K) \leq \tilde{\iota}_n(G,K)$, that motivates the following definition (also see Theorem 1 and Section 5.3).

Definition 2. A graph G is said to be *n-geometric* with respect to a kernel K, if

$$\iota_n(G,K) = \tilde{\iota}_n(G,K).$$

A graph G is said to be *supergeometric* with respect to a kernel K, if it is n-geometric with respect to K, for every $2 \leq n \leq |V(G)|$. ♠

By definition and Proposition 1(b), any strongly connected graph is 2-geometric (with respect to any given kernel K). An easy observation is that for any graph without loops and with respect to any kernel,

$$|Q| = 1 \quad \Rightarrow \quad \frac{\overrightarrow{\partial}(Q)}{\pi(Q)} = 1.$$

This, for instance, shows that all simple graphs on a set of 6 vertices are supergeometric. In what follows we elaborate on going through the details of computing the mean isoperimetric constants of some well-known graphs, to provide examples of supergeometric graphs as well as cases for which the graph is far from being geometric.

Example 2. In this example we compute the isoperimetric spectra of complete graphs and complete bipartite graphs with respect to their natural random walks, and we show that they are supergeometric.
By Equation (5), for any $\{Q_i\}_1^n \in \mathcal{D}_n(V(\mathsf{K}_t))$, with $|Q_i| = t_i$, we have

$$\sum_{i=1}^{n} \frac{\overrightarrow{\partial}(Q_i)}{\pi(Q_i)} = \sum_{i=1}^{n} \frac{t_i(t-t_i)}{(t-1)t_i} = \frac{tn - \sum_i t_i}{(t-1)},$$

which is clearly minimized when $\{Q_i\}_1^n \in \mathcal{P}_n(\mathsf{K}_t)$. Therefore for all $n \in \mathcal{I}_t$ we have

$$\iota_n(\mathsf{K}_t) = \tilde{\iota}_n(\mathsf{K}_t) = \frac{t(n-1)}{n(t-1)},$$

and complete graphs are supergeometric.
Now, let X and Y be the two parts of the graph $\mathsf{K}_{r,s}$, with $|X| = r, |Y| = s$, and let $\{Q_i\}_1^n \in \mathcal{D}_n(V(\mathsf{K}_{r,s}))$, be such that $|Q_i \cap X| = x_i$ and $|Q_i \cap Y| = y_i$. By Equation (5), we have

$$\frac{1}{n}\sum_{i=1}^{n} \frac{\overrightarrow{\partial}(Q_i)}{\pi(Q_i)} = \frac{1}{n}\sum_{i=1}^{n} \frac{x_i(s-y_i) + y_i(r-x_i)}{sx_i + ry_i} = 1 - \frac{2}{n}\sum_{i=1}^{n} \frac{x_i y_i}{sx_i + ry_i}.$$

First, note that the function $\frac{x_i y_i}{sx_i + ry_i}$ is increasing with respect to both x_i and y_i, and consequently, one deduces that complete bipartite graphs are supergeometric.
Furthermore, as a special case, let s be a multiple of r, where we want to maximize the function $\frac{x_i y_i}{sx_i + ry_i}$ under constraints $\sum_{i=1}^n x_i = r$ and $\sum_{i=1}^n y_i = s$. Using Lagrange method we can see that the function is maximized when $sx_i = ry_i$, for every $i \in \mathcal{I}_n$. Thus, for every $n \in \mathcal{I}_r$, we have

$$\iota_n(\mathsf{K}_{r,s}) = \tilde{\iota}_n(\mathsf{K}_{r,s}) = 1 - \frac{2}{n}\sum_{i=1}^{n} \frac{sx_i}{r(s+s)} = 1 - \frac{1}{n}.$$

♣

Example 3. Let $G_t = (V, E)$ be the directed cycle with loops, where $V \stackrel{\text{def}}{=} \mathbb{Z}/t\mathbb{Z}$ and $E \stackrel{\text{def}}{=} \{(i,i), (i,i+1) |\ i \in V\}$. Considering the natural random walk on G_t, for every $Q \subset V$ we have

$$\frac{\overrightarrow{\partial}(Q)}{\pi(Q)} = \frac{s}{2|Q|},$$

where $s \stackrel{\text{def}}{=} |\{i \in Q |\ i+1 \notin Q\}|$. So when $Q \subsetneqq V$ is a nonvoid set of consecutive numbers, this quotient is minimized and is equal to $\frac{1}{2|Q|}$. Thus for every $2 \le n \le t$,

$$\iota_n(G_t) = \min_{\{Q_i\}_1^n \in \mathcal{D}_n(G_t)} \frac{1}{n}\sum_{i=1}^{n} \frac{\overrightarrow{\partial}(Q_i)}{\pi(Q_i)} = \min_{\{Q_i\}_1^n \in \mathcal{D}_n(G_t)} \frac{1}{2n}\sum_{i=1}^{n} \frac{1}{|Q_i|},$$

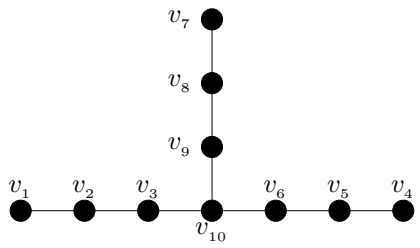

Figure 1: See Example 4.

which is clearly minimized when $\{Q_i\}_1^n \in \mathcal{P}_n(G_n)$. Consequently, the graph G_t is supergeometric and if $t = \lfloor \frac{t}{n} \rfloor n + r$, for some r, then for every $2 \leq n \leq t$,

$$\iota_n(G_t) = \tilde{\iota}_n(G_t) = \frac{1}{2n}\left(\frac{n-r}{\lfloor \frac{t}{n} \rfloor} + \frac{r}{\lfloor \frac{t}{n} \rfloor + 1}\right).$$

♣

In the following example we introduce a graph which is 2-geometric but not 3-geometric.

Example 4. Consider the simple graph G of Figure 1 along with its natural random walk, where we are going to compute $\iota_3(G)$ and $\tilde{\iota}_3(G)$. By considering disjoint sets

$$\{A_i \stackrel{\text{def}}{=} \{v_{3i-2}, v_{3i-1}, v_{3i}\} |\ i = 1, 2, 3\},$$

and the partition

$$\{B_1 \stackrel{\text{def}}{=} \{v_1, v_2, v_3\}, B_2 \stackrel{\text{def}}{=} \{v_4, v_5, v_6\}, B_3 \stackrel{\text{def}}{=} \{v_7, v_8, v_9, v_{10}\}\},$$

we have

$$\begin{aligned} \iota_3(G) &\leq \frac{1}{3}\sum_{i=1}^{3} \frac{\vec{\partial}(A_i)}{\pi(A_i)} = \frac{1}{3}(\frac{1}{5} + \frac{1}{5} + \frac{1}{5}) = \frac{1}{5}, \\ \tilde{\iota}_3(G) &\leq \frac{1}{3}\sum_{i=1}^{3} \frac{\vec{\partial}(B_i)}{\pi(B_i)} = \frac{1}{3}(\frac{1}{5} + \frac{1}{5} + \frac{2}{8}) = \frac{13}{60}. \end{aligned}$$

It is easy to verify the following claims (by a case study) for a subset $Q \subseteq V(G)$,

$$\begin{aligned} |Q| = 1 \quad &\Rightarrow \quad \frac{\vec{\partial}(Q)}{\pi(Q)} = 1, \\ |Q| = 2 \quad &\Rightarrow \quad \frac{\vec{\partial}(Q)}{\pi(Q)} \geq \frac{1}{3}, \\ |Q| \in \{3, 4, 5\} \quad &\Rightarrow \quad \frac{\vec{\partial}(Q)}{\pi(Q)} \geq \frac{1}{5}. \end{aligned}$$

To prove that $\iota_3(G) = \frac{1}{5}$ let $\{Q_1, Q_2, Q_3\}$ be a set of disjoint subsets for which the minimum is achieved with $|Q_1| \leq |Q_2| \leq |Q_3|$. Then by the previous claim it is clear that $|Q_1| \neq 1$ and hence we either have $|Q_1| = |Q_2| = 2$ or we must have $|Q_3| \leq 5$. Hence, again by the

previous claim in either case the mean flow is greater than or equal to $\frac{1}{5}$.
By a similar case study, one can characterize 3 different kinds of partitions as follows

$$\begin{aligned} & |Q_1| = 2, |Q_2| = 3, |Q_3| = 5, \\ \text{or} \quad & |Q_1| = 2, |Q_2| = 4, |Q_3| = 4, \\ \text{or} \quad & |Q_1| = 3, |Q_2| = 3, |Q_3| = 4, \end{aligned}$$

which shows that $\tilde{\iota}_3(G)$ is achieved for the partition $\{B_i |\ i = 1, 2, 3\}$. ♣

Example 5. In this example we show that, by modifying Example 4, we can construct a graph G for which $\tilde{\iota}_n(G) > \iota_{n+1}(G)$.
Let $G_n = (V_n, E_n)$ be a symmetric graph, where $V_n \overset{\text{def}}{=} \{u, x_i, y_i, z_i, w_i |\ 1 \leq i \leq n\}$. For every $i \in \mathcal{I}_n$, the induced graph on $\{x_i, y_i, z_i, w_i\}$ is a path of length 3 and the vertex u is adjacent to all vertices x_j, for all $j \in \mathcal{I}_n$. For $i \in \mathcal{I}_{n-1}$, let $A_i \overset{\text{def}}{=} \{x_i, y_i, z_i, w_i\}$ and also let $A_n \overset{\text{def}}{=} \{x_n, y_n\}$ and $A_{n+1} \overset{\text{def}}{=} \{z_n, w_n\}$. Then,

$$\iota_{n+1}(G_n) \leq \frac{1}{n+1} \sum_{i=1}^{n+1} \frac{\overrightarrow{\partial}(A_i)}{\pi(A_i)} = \frac{1}{n+1} \left(\frac{n-1}{7} + \frac{1}{3} + \frac{2}{4} \right).$$

Now, for $i \in \mathcal{I}_{n-1}$, let $B_i \overset{\text{def}}{=} \{x_i, y_i, z_i, w_i\}$ and also let $B_n \overset{\text{def}}{=} \{u, x_n, y_n, z_n, w_n\}$. Then, by a similar argument as in Example 4, one can prove that

$$\tilde{\iota}_n(G_n) = \frac{1}{n} \sum_{i=1}^{n} \frac{\overrightarrow{\partial}(B_i)}{\pi(B_i)} = \frac{1}{n} \left(\frac{n-1}{7} + \frac{n-1}{n+7} \right).$$

It is clear that if n is large enough, then $\iota_{n+1}(G_n) \leq (\frac{n}{n+1})\tilde{\iota}_n(G_n) < \tilde{\iota}_n(G_n)$. ♣

5 Computational aspects

5.1 A Federer-Fleming-type theorem

Our basic aim in this section is to find a functional definition through proving a Federer-Fleming-type theorem. This not only is quite important theoretically (e.g. see [40]) and along with Examples 4 and 5 justifies the correctness of our generalization, but also can be assumed as our first step to approximate isoperimetric constants using well-chosen test functions.
First, we define a couple of function spaces as follows.

Definition 3. We define the space of *unit positive functions* as,

$$\mathcal{U}_\pi^+(G) \overset{\text{def}}{=} \left\{ f \ \mid \ f \in \mathcal{F}_\pi^+(G) \text{ and } \|f\|_{1,\pi} = 1 \right\}.$$

Also, a class of functions $\{f_i\}_1^n$ is called *positive orthonormal*, if for all $1 \leq i \leq n$ we have $f_i \in \mathcal{U}_\pi^+(G)$ and moreover, for all pairs of indices $i \neq j$ we have $f_i \perp_\pi f_j$. In this regard we define

$$\mathcal{O}_n^+(G) \overset{\text{def}}{=} \left\{ \{f_i\}_1^n \ \mid \ \{f_i\}_1^n \text{ is positive orthonormal} \right\}.$$

$$\tilde{\mathcal{O}}_n^+(G) \overset{\text{def}}{=} \left\{ \{f_i\}_1^n \in \mathcal{O}_n^+(G) \ \mid \ \{\text{supp}(f_i)\}_1^n \in \mathcal{P}_n(G) \right\}.$$

♠

Now, given a kernel K and a nowherezero stationary distribution π, let us consider the following parameters which are naturally related to the constants $\iota_n(G)$ and $\tilde{\iota}_n(G)$,

$$\gamma_n(G,K) \stackrel{\text{def}}{=} \inf_{\{f_i\}_1^n \in \mathcal{O}_n^+(G)} \frac{1}{n}\left(\sum_{i=1}^n \|\vec{\nabla} f_i\|_{1,\phi}\right).$$

$$\tilde{\gamma}_n(G,K) \stackrel{\text{def}}{=} \inf_{\{f_i\}_1^n \in \tilde{\mathcal{O}}_n^+(G)} \frac{1}{n}\left(\sum_{i=1}^n \|\vec{\nabla} f_i\|_{1,\phi}\right).$$

As usual, we exclude the kernel when it is fixed or is clear from the context. First, we prove the following technical result.

Lemma 5. *For every function $f \in \mathcal{F}_\pi^+(G)$ with $\|f\|_{1,\pi} = 1$, there is a set $Q \subseteq \mathrm{supp}(f)$, such that $\dfrac{\vec{\partial}(Q)}{\pi(Q)} \leq \|\vec{\nabla} f\|_{1,\phi}$.*

Proof. We prove the claim by induction on the size of the range of f, $Range(f)$. If f takes only two values 0 and t_1, then $t_1 = \frac{1}{\pi(A)}$, where $A \stackrel{\text{def}}{=} f^{-1}(t_1)$ and $f = t_1\ \chi_A$. The proof is straightforward in this case.
Now, let $Range(f) = \{0, t_1, \ldots, t_n\}$ such that $0 < t_1 \leq \ldots \leq t_n$ and, moreover, for each $i \in \mathcal{I}_n$ let $A_i \stackrel{\text{def}}{=} f^{-1}(t_i)$ and $\pi_i \stackrel{\text{def}}{=} \pi(A_i)$. Then,

$$\begin{aligned}\|\vec{\nabla} f\|_{1,\phi} &= \sum_{uv \in E(G)} (f(u) - f(v))^+\ \phi(u,v)\\ &= c_1 t_1 + c_2 t_2 + \ldots + c_n t_n,\end{aligned}$$

for some real numbers c_i, where each c_i depends only on flows between the subsets A_i. Now, our objective is to find the minimum of the function

$$\psi(x_1, \ldots, x_n) \stackrel{\text{def}}{=} c_1 x_1 + \ldots + c_n x_n$$

subject to the constraints

$$\begin{cases} 0 \leq x_1 \leq \ldots \leq x_n, \\ g(x) \stackrel{\text{def}}{=} \sum_{i=1}^n \pi_i x_i - 1 = 0. \end{cases} \tag{6}$$

First, note that if $\frac{c_1}{\pi_1} = \ldots = \frac{c_n}{\pi_n} = \kappa$, then $\psi(x_1, \ldots, x_n) = \sum_i\ \kappa \pi_i x_i = \kappa$ everywhere. Therefore,

$$\|\vec{\nabla} f\|_{1,\phi} = \kappa = \frac{c_n}{\pi_n} = \frac{\vec{\partial}(A_n)}{\pi(A_n)}.$$

Now assume there exist $i \neq j$ such that $\frac{c_i}{\pi_i} \neq \frac{c_j}{\pi_j}$. By Lagrange method, the the minimum of ψ subject to the constraints (6) is equal to the minimum of the function $h(x,\lambda) = \psi(x) - \lambda g(x)$ under constraints

$$0 \leq x_1 \leq \ldots \leq x_n.$$

Since we have $\partial h / \partial x_i = c_i - \lambda \pi_i$, by assumption partial derivatives are not simultaneously zero, and consequently, g attains its minimum on a boundary point $(s_1, \ldots, s_n)$, i.e. there exists i_0 such that $s_{i_0} = s_{i_0+1}$. Now, define the function $\hat{f}$ to be equal to s_i on A_i for all i and zero elsewhere. Then, using (6), we have $\|\hat{f}\|_{1,\pi} = 1$ and

$$\|\vec{\nabla} \hat{f}\|_{1,\phi} = c_1 s_1 + \ldots + c_n s_n.$$

Therefore, by induction hypothesis we can find a subset $Q \subseteq \mathrm{supp}(\hat{f}) \subseteq \mathrm{supp}(f)$ such that

$$\frac{\overrightarrow{\partial}(Q)}{\pi(Q)} \leq \|\overrightarrow{\nabla}\hat{f}\|_{1,\phi} = \psi(s_1, \ldots, s_n) \leq \psi(t_1, \ldots, t_n) = \|\overrightarrow{\nabla} f\|_{1,\phi}.$$

■

The following theorem presents a functional definition for the mean isoperimetric spectrum.

Theorem 1. *For any graph G (and a given kernel K on it) and for all $1 \leq n \leq |V(G)|$ we have*

$$\iota_n(G) = \gamma_n(G) = \tilde{\gamma}_n(G).$$

Proof. By considering characteristic functions of sets we have $\gamma_n(G) \leq \iota_n(G)$. To prove equality, let $\{f_i\}_1^n \in \mathcal{O}_n^+(G)$ be chosen such that $\gamma_n(G)$ is achieved. By Lemma 5, for every $i \in \mathcal{I}_n$, there exists a set $Q_i \subseteq \mathrm{supp}(f_i)$, such that $\dfrac{\overrightarrow{\partial}(Q_i)}{\pi(Q_i)} \leq \|\overrightarrow{\nabla} f_i\|_{1,\phi}$. Since $\{f_i\}_1^n$ is positive orthonormal and $Q_i \subseteq \mathrm{supp}(f_i)$, we conclude that Q_i's are disjoint subsets, and consequently,

$$\iota_n(G) \leq \frac{1}{n}\sum_{i=1}^{n} \frac{\overrightarrow{\partial}(Q_i)}{\pi(Q_i)} \leq \frac{1}{n}\sum_{i=1}^{n} \|\overrightarrow{\nabla} f_i\|_{1,\phi} = \gamma_n(G).$$

For the second equality, by definition we have $\iota_n(G) = \gamma_n(G) \leq \tilde{\gamma}_n(G)$. Now, let $\{Q_i\}_1^n$ be a set of disjoint sets for which $\iota_n(G)$ is achieved. Also, let

$$Q' \stackrel{\text{def}}{=} \bigcup_{i=1}^{n-1} Q_i, \quad Q^* \stackrel{\text{def}}{=} V(G) - Q',$$

and $0 < \epsilon < \frac{1}{\pi(Q_n \cup Q^*)}$ be an arbitrary fixed number. For $i \in \mathcal{I}_{n-1}$, define functions $\{g_i\}_1^n \in \tilde{\mathcal{O}}_n^+(G)$ as $g_i \stackrel{\text{def}}{=} \frac{1}{\pi(Q_i)}\,\chi_{Q_i}$, and

$$g_n(u) \stackrel{\text{def}}{=} \begin{cases} \frac{1-\epsilon\ \pi(Q^*)}{\pi(Q_n)} & u \in Q_n \\ \epsilon & u \in Q^* \\ 0 & u \in Q'. \end{cases}$$

Therefore, we have

$$\begin{aligned} n\ \tilde{\gamma}_n(G) &\leq \sum_{i=1}^{n} \|\overrightarrow{\nabla} g_i\|_{1,\phi} \\ &= \sum_{i=1}^{n-1} \frac{\overrightarrow{\partial}(Q_i)}{\pi(Q_i)} + \frac{1-\epsilon\ \pi(Q^*)}{\pi(Q_n)}\ \overrightarrow{\partial}(Q_n) + \epsilon\left(\overrightarrow{\partial}(Q^*, Q') - \overrightarrow{\partial}(Q_n, Q^*)\right), \end{aligned}$$

and by tending ϵ to zero we get

$$\tilde{\gamma}_n(G) \leq \frac{1}{n}\left(\sum_{i=1}^{n} \frac{\overrightarrow{\partial}(Q_i)}{\pi(Q_i)}\right) = \iota_n(G).$$

■

This result along with Examples 4 and 5 show that the natural and correct definition of the mean isoperimetric constants is what is defined in terms of minimization over *disjoint* subsets of the domain and not *partitions*.

5.2 Spectral bounds and Cheeger-type inequalities

In this section we consider the problem of approximating the isoperimetric constants of a graph using its Laplacian spectrum and some more information from the eigenspaces. As a by product of this, we also prove generalized versions of Cheeger inequality for the isoperimetric spectrum. To begin, let us recall an interesting variational principle due to Ky Fan.

Theorem A. (e.g. see [2]) Ky Fan's minimum principle
Let $A \in \mathrm{End(V)}$ be a self-adjoint matrix operating on the ν-dimensional inner-product space V, and let

$$\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_\nu ,$$

be the set of eigenvalues of A ordered in an increasing order. Then for any $1 \leq n \leq \nu$ we have

$$\overline{\lambda}_n = \frac{1}{n}\left(\min_{UU^*=id_n} \mathrm{tr}(UAU^*) \right),$$

where $\overline{\lambda}_n$ is the average of the n smallest eigenvalues of A, U is an arbitrary $n \times \nu$ matrix, id_n is the $n \times n$ identity matrix, and (tr) *is the trace function.*

Note that another way of expressing Ky Fan's result is that, subject to the same conditions of Theorem A,

$$\overline{\lambda}_n = \frac{1}{n}\left(\min_{\substack{f_i \perp f_j \\ f_i \neq 0}} \sum_{i=1}^{n} \frac{\langle Af_i, f_i \rangle}{\|f_i\|_2^2} \right).$$

The second important fact is related to the concept of a *nodal domain* (e.g. see [5] and references therein). It is interesting to note that in the continuous case, the eigenfunctions of the ordinary Laplacian (say of a compact Riemannian manifold) is always a continuous function (essentially smooth) and by Rolle's theorem there is always a zero point between any two points with different signs. This fact, in a way, justifies the study of connected components of $f^{-1}(0)$ (as *nodal regions* [20, 27, 33]) for any eigenfunction f in the continuous case. However, when we are dealing with a discontinuous object as a graph, an eigenfunction can have opposite signs on the two endpoints of an edge, where this, on the one hand, makes the whole thing more complex, and on the other hand, it makes the space of eigenfunctions far richer.

Definition 4. If $f \in \mathcal{F}_\pi(G)$ and $Q \subseteq V(G)$, the pair (Q, Q^c) is called a *bipolar cut-set* for f if for any edge $uv \in \overleftrightarrow{E}(Q)$ we have $f(u)f(v) \leq 0$. Also, a subset Q is called a *nonnegative* (*nonpositive*) *bipolar part* of f if $f_1 \stackrel{\mathrm{def}}{=} f|_Q$ is a nonnegative (nonpositive) function on Q and (Q, Q^c) is a bipolar cut-set for f. A *signed* part of f is a subset Q that is either a nonnegative or a nonpositive bipolar part of f. Note that in this case $f = f_1 + f_2$ where $f_2 \stackrel{\mathrm{def}}{=} f|_{Q^c}$ and $f_1 \perp f_2$. Also, note that any *strong sign-graph* of f is clearly a signed part of f (e.g. see [5] for the definitions, other variations and background).
For a given real number $\zeta \in \mathbb{R}$, a real function $f \in \mathcal{F}(G)$ is said to be ζ-*excessive* (resp. ζ-*deficient*) for the kernel K if $Kf \leq \zeta f$ (resp. $Kf \geq \zeta f$). By abuse of language, a ζ-excessive (resp. ζ-deficient) function for $\overline{\Delta}$ is just referred to as a ζ-excessive (resp. ζ-deficient) function, if details are clear from the context. ♠

We will use the following lemma to prove a generalized Cheeger inequality later. It is instructive to mention that the lemma can also be deduced as a corollary of the well-known Duval-Reiner lemma (e.g. see [25] for the lemma and [5] for the history, erratum and a more detailed discussion).

Lemma 6. *Let G be graph, and $f \in \mathcal{F}(G)$ be a ζ-excessive (resp. ζ-deficient) function for $\overline{\Delta}$, such that a subset $Q \subseteq V(G)$ is a nonnegative (resp. nonpositive) bipolar part of f. Then, assuming $g \overset{\text{def}}{=} f|_{Q}$ we have*

$$\zeta \geq \frac{\|\overline{\nabla} g\|_{2,\overline{\phi}}^{2}}{\|g\|_{2,\pi}^{2}}.$$

Proof. Let Q be a nonnegative bipolar part of the ζ-excessive function f. If $u \in Q$ then $g(u) = f(u)$ and $g(v) \geq f(v)$ for all neighbors v of u, and so $\overline{\Delta} g(u) \leq \overline{\Delta} f(u) \leq \zeta f(u) = \zeta g(u)$. Also if $u \notin Q$ then $g(u) = 0$, and since $g \geq 0$, trivially $\overline{\Delta} g(u) \leq \zeta g(u)$. Hence by Lemma 2(c) we have

$$\|\overline{\nabla} g\|_{2,\overline{\phi}}^{2} = \langle \overline{\Delta} g, g \rangle_{\pi} \leq \zeta \langle g, g \rangle_{\pi} = \zeta \|g\|_{2,\pi}^{2}.$$

■

The following is the first half of the generalized Cheeger inequality.

Theorem 2. *For any given graph G we have $\overline{\lambda}_{n} \leq \iota_{n}(G)$.*

Proof. Let $\{Q_{i}\}_{1}^{n} \in \mathcal{D}_{n}(G)$ be chosen such that

$$\iota_{n}(G) = \frac{1}{n} \sum_{i=1}^{n} \frac{\overrightarrow{\partial}(Q_{i})}{\pi(Q_{i})}.$$

For every $i \in \mathcal{I}_{n}$ define

$$h_{i}(u) = \chi_{Q_{i}} \overset{\text{def}}{=} \begin{cases} 1 & u \in Q_{i} \\ 0 & u \notin Q_{i}. \end{cases}$$

Now, for each $i \in \mathcal{I}_{n}$ we have $\|h_{i}\|_{2,\pi}^{2} = \pi(Q_{i})$ and by Lemma 2,

$$\|\overline{\nabla} h_{i}\|_{2,\overline{\phi}}^{2} = \|\overline{\nabla} h_{i}\|_{1,\overline{\phi}} = \|\overrightarrow{\nabla} h_{i}\|_{1,\phi} = \overrightarrow{\partial}(Q_{i}).$$

Hence, by Ky Fan's minimum principle,

$$n\, \overline{\lambda}_{n} = \min_{f_{i} \perp_{\pi} f_{j}} \sum_{i=1}^{n} \frac{\langle \overline{\Delta} f_{i}, f_{i} \rangle_{\pi}}{\|f_{i}\|_{2,\pi}^{2}} \leq \sum_{i=1}^{n} \frac{\|\overline{\nabla} h_{i}\|_{2,\overline{\phi}}^{2}}{\|h_{i}\|_{2,\pi}^{2}} = n\, \iota_{n}(G).$$

■

Note that for the complete graph K_{t}, we have $\lambda_{i} = \frac{t}{t-1}$, for all $2 \leq i \leq t$. Also, for the complete bipartite graph $\mathsf{K}_{r,s}$, we have $\lambda_{i} = 1$, for all $2 \leq i \leq r+s-1$ and $\lambda_{r+s} = 2$. Thus, by Example 2, for the complete graph K_{t}, when $1 \leq n \leq t$ and also, for the complete bipartite graph $\mathsf{K}_{r,s}$, when s is a multiple of r and $1 \leq n \leq r$, equality holds in Theorem 2, which shows that the result is sharp.
For the second half of a generalized Cheeger inequality we need the following definition.

Definition 5. Let $\Gamma = (\zeta_{1}, \zeta_{2}, \ldots, \zeta_{n})$ be an n-list of real numbers. Then an n-list of real functions $F = (f_{1}, f_{2}, \ldots, f_{n})$ on a domain X along with n disjoint subsets $\mathcal{Q} = (Q_{1}, Q_{2}, \ldots, Q_{n})$ such that $Q_{i} \subseteq X$, is called a *compatible transverse set of functions* for $\overline{\Delta}$, if:

- $f_{i}|_{Q_{i}} \neq 0$.

- For each $1 \leq i \leq n$, the function $f_{_i}$ is a $\zeta_{_i}$-excessive (resp. ζ-deficient) function (with respect to $\overline{\Delta}$) on X.
- For each $1 \leq i \leq n$, the subset $Q_{_i}$ is a nonnegative (resp. nonpositive) bipolar part of $f_{_i}$.

♠

Theorem 3. *Consider a graph G and let $\Gamma = (\zeta_{_1}, \zeta_{_2}, \ldots, \zeta_{_n})$. If $F = (f_{_1}, f_{_2}, \ldots, f_{_n})$ along with $\mathcal{Q} = (Q_{_1}, Q_{_2}, \ldots, Q_{_n})$ is a compatible transverse set of functions for $\overline{\Delta}$, then*

$$2\,\overline{\zeta}_{_n} \;\geq\; \iota_{_n}(G)^2.$$

Proof. Let $0 \neq g_{_i} \overset{\text{def}}{=} f_{_i}|_{_{Q_{_i}}}$. Then,

$$\begin{aligned}\overline{\zeta}_{_n} \;&\geq \tfrac{1}{n} \sum_{i=1}^{n} \frac{\|\overline{\nabla} g_{_i}\|_{_{2,\overline{\phi}}}^{2}}{\|g_{_i}\|_{_{2,\pi}}^{2}} \geq \tfrac{1}{2n} \sum_{i=1}^{n} \frac{\|\overrightarrow{\nabla} g_{_i}^{2}\|_{_{1,\phi}}^{2}}{\|g_{_i}^{2}\|_{_{1,\pi}}^{2}} \\ &\geq \tfrac{1}{2} \left(\tfrac{1}{n} \sum_{i=1}^{n} \frac{\|\overrightarrow{\nabla} g_{_i}^{2}\|_{_{1,\phi}}}{\|g_{_i}^{2}\|_{_{1,\pi}}} \right)^{2} \geq \tfrac{1}{2}\, \iota_{_n}(G)^2,\end{aligned}$$

where the first and the second inequalities follow from Lemma 6 and 4, respectively, and the third one is a direct application of Cauchy-Schwarz inequality. ■

It ought to be noted that Theorems 2 and 3 together, can be considered as a *generalized* Cheeger inequality. In what follows we deduce a special case where one may get an explicit inequality for the mean spectrum.

Theorem 4. *Consider a kernel K on a base graph G. Let $F = (f_{_2}, f_{_3}, \ldots, f_{_{n+1}})$ be a list of eigenfunctions of $\overline{\Delta}$ for the list of eigenvalues $\Gamma = (\lambda_{_2}, \lambda_{_3}, \ldots, \lambda_{_{n+1}})$, respectively, such that along with $\mathcal{Q} = (Q_{_2}, Q_{_3}, \ldots, Q_{_{n+1}})$ form a compatible transverse set of functions for $\overline{\Delta}$. Then,*

$$\overline{\lambda}_{_n} \leq \iota_{_n}(G) \leq \sqrt{\frac{2(n+1)}{n}\; \overline{\lambda}_{_{n+1}}}. \tag{7}$$

Moreover, we would like to add that following the same scenario described for the mean version, one may define the nth max-isoperimetric constant as

$$\varsigma_{_n}(K, \pi) \overset{\text{def}}{=} \min_{\{Q_{_i}\}_1^n \in \mathcal{D}_n(G)} \left(\max_{1 \leq i \leq n} \frac{\overrightarrow{\partial}(Q_{_i})}{\pi(Q_{_i})} \right).$$

It is noteworthy that all of the previous mentioned results such as the Federer-Fleming theorem can also be verified for this version with appropriate modifications. For instance, we may state a more standard Cheeger inequality for the max-isoperimetric constant $\varsigma_{_n}$ using Theorems 2 and 3 and their counterparts, along with Courant-Fischer variational theorem as follows.

Theorem 5. *For a given graph G, let f be an eigenfunction of $\overline{\Delta}$ corresponding to the nth eigenvalue $\lambda_{_n}$. Also, let $(Q_{_1}, Q_{_2}, \ldots, Q_{_n})$ be a list of n disjoint nonempty subsets of $V(G)$ such that for every $1 \leq i \leq n$ we have $f|_{_{Q_{_i}}} \neq 0$ and each $Q_{_i}$ is a nonnegative or nonpositive bipolar part of f. Then,*

$$\frac{\lambda_{_n}}{2} \leq \varsigma_{_n}(G) \leq \sqrt{2\;\lambda_{_n}}, \quad \text{and} \quad \overline{\lambda}_{_n} \leq \iota_{_n}(G) \leq \sqrt{2\;\lambda_{_n}}. \tag{8}$$

Also, as a corollary of Theorem 5 by considering the fact that always the second eigenvalue has an eigenfunction with two nodal domains, we obtain the classical Cheeger inequality as,

$$\frac{\lambda_2}{2} \leq \iota_2(G) \leq \varsigma_2(G) \leq \sqrt{2\ \lambda_2}. \tag{9}$$

It also must be emphasized that a direct use of eigenvalues and eigenfunctions (not necessarily tuned with repetition) in Theorem 3 will definitely make a deviation from sharpness which can be easily verified by a comparison to the classical Cheeger inequality (Inequality (9)). Note that the classical Cheeger inequality is far from being sharp by a recent result of Montenegro and Tetali [39].
To provide some examples let us recall the following result.

Theorem B. [4, 5] *Let K be a kernel on a tree T and let f_n be an eigenfunction of $\overline{\Delta}$ with eigenvalue λ_n which does not vanish on any vertex. Then λ_n is simple and f_n has exactly n strong nodal domains.*

Therefore, a generalized Cheeger inequality is valid for any Markov chain on a tree T with a nowherezero eigenfunction f_n of an eigenvalue λ_n, i.e.

$$\max(\frac{\lambda_n}{2}, \overline{\lambda}_n) \leq \max(\frac{\lambda_n}{2}, \iota_n(T)) \leq \varsigma_n(T) \leq \sqrt{2\ \lambda_n}.$$

For more on the extensive literature of Markov chains on trees the interested reader is referred to [5, 37] and references therein.
On the other hand, it is quite interesting that even for the case of trees we do not know enough about the behavior of parameters discussed in this article, and as Example 4 shows one encounters nongeometric trees in very small cases. Hence, we believe that the following problem can be considered to be a nice starting point for the study of supergeometric graphs.

Problem 1. *Characterize the class of supergeometric trees.*

5.3 Algorithmic considerations

In this section we touch on some algorithmic aspects of the isoperimetry problem and we study its relationships to some well-known concepts as the k-means algorithm and the normalized cuts method. This section is mainly influenced by the seminal contribution of J. Malik and J. Shi [43] (also see [21]) that was brought to our attention after the presentation of the first two authors' article on the isoperimetric spectrum of graphs [19].
Following our notations in Section 3, for a set X, $\mathcal{D}_n(X)$ stands for the set of all n-sets $\{Q_i\}_1^n$, where Q_i's are nonempty disjoint subsets of X. Also $\mathcal{P}_n(X) \subseteq \mathcal{D}_n(X)$ consists of all n-partitions of X.

Definition 6. Given a function $f \in \mathcal{F}^d(X)$ and a weight function $\omega : X \to \mathbb{R}^+ - \{0\}$, for every $1 \leq n \leq |X|$, the cost function $\mathcal{C}_n^{f,\omega} : \mathcal{D}_n(X) \to \mathbb{R}^+$ is defined as follows

$$\mathcal{M}_n^{f,\omega}(\{Q_i\}_1^n) \stackrel{\text{def}}{=} \sum_{i=1}^{n} \sum_{u \in Q_i} \omega(u) \|f(u) - \mathbf{m}_i\|^2, \text{ where } \mathbf{m}_i \stackrel{\text{def}}{=} \frac{\sum_{u \in Q_i} \omega(u) f(u)}{\sum_{u \in Q_i} \omega(u)},$$

and

$$\mathcal{C}_n^{f,\omega}(\{Q_i\}_1^n) \stackrel{\text{def}}{=} \mathcal{M}_n^{f,\omega}(\{Q_i\}_1^n) + \sum_{u \in Q^*} \omega(u) \|f(u)\|^2,$$

where $\|.\|$ is the Euclidean L^2-norm of $\mathbb{R}^d$ and $Q^* = X - \cup_{i=1}^n Q_i$. Also, associated to the functions f and ω, we define the following parameters

$$\mu_n(f,\omega) \stackrel{\text{def}}{=} \min_{\mathcal{Q}\in\mathcal{D}_n(X)} \mathcal{C}_n^{f,\omega}(\mathcal{Q}), \quad \text{and} \quad \tilde{\mu}_n(f,\omega) \stackrel{\text{def}}{=} \min_{\mathcal{Q}\in\mathcal{P}_n(X)} \mathcal{C}_n^{f,\omega}(\mathcal{Q}).$$

♠

The well-known k-means algorithm seeks for the value of $\tilde{\mu}_n(f,\omega)$ and an n-partition on which the minimum is achieved. First, let's state the following simple lemma.

Lemma 7. *Given functions $f \in \mathcal{F}^d(X)$ and $\omega : X \to \mathbb{R}^+ - \{0\}$ on X, for all $1 \le n \le |X|$ and for every $\mathcal{Q} = \{Q_i\}_1^n \in \mathcal{D}_n(X)$, we have*

$$\mathcal{M}_n^{f,\omega}(\mathcal{Q}) = \sum_{i=1}^n \frac{1}{2\ \omega(Q_i)} \sum_{u,v\in Q_i} \omega(u)\omega(v)\|f(u)-f(v)\|^2.$$

Proof.

$$\begin{aligned}
\mathcal{M}_n^{f,\omega}(\mathcal{Q}) &= \sum_{i=1}^n \frac{1}{\omega(Q_i)^2} \sum_{u\in Q_i} \omega(u) \left\| \sum_{v\in Q_i} (f(u)-f(v))\ \omega(v) \right\|^2 \\
&= \sum_{i=1}^n \frac{1}{\omega(Q_i)^2} \sum_{u,v,w\in Q_i} \omega(u)\omega(v)\omega(w) \Big(\langle f(u),f(u)\rangle - \langle f(v),f(u)\rangle \\
&\quad -\langle f(w),f(u)\rangle + \langle f(v),f(w)\rangle \Big) = \sum_{i=1}^n \frac{1}{2\ \omega(Q_i)} \sum_{u,v\in Q_i} \omega(u)\omega(v)\|f(u)-f(v)\|^2.
\end{aligned}$$

■

Let G be a graph on ν vertices and K be a kernel on it, together with a stationary distribution π. Also, let D be the diagonal matrix defined as $D(u,u) \stackrel{\text{def}}{=} \pi(u)$. Define, the *normalized flow matrix* as,

$$\Phi \stackrel{\text{def}}{=} (id + \overline{K})D^{-1},$$

whose (u,v) entry can be described as

$$\Phi(u,v) = \begin{cases} \frac{\overline{\phi}(u,v)}{\pi(u)\pi(v)} & u \neq v, \\ \\ \frac{1}{\pi(u)} + \frac{\overline{\phi}(u,u)}{\pi(u)^2} & u = v, \end{cases}$$

that justifies the name. Now, if f is an eigenfunction for the eigenvalue λ of Φ, and we chose x in such a way that $\frac{f(x)}{\pi(x)} = \max_u \frac{|f(u)|}{\pi(u)}$, then

$$\lambda f(x) = (\Phi f)(x) = \frac{f(x)}{\pi(x)} + \sum_u \frac{\overline{K}(x,u)}{\pi(u)} f(u) \ge \frac{f(x)}{\pi(x)} \left(1 - \sum_u \overline{K}(x,u) \right) = 0,$$

which shows that Φ is a positive semidefinite matrix, and consequently, there exists a matrix P such that $\Phi = P^t P$. Let us define the function $p_K \in \mathcal{F}^\nu(G)$ such that $p_K(u)$ is uth column of P.

Proposition 2. *For every graph G on ν vertices and a kernel K on it with a nowherezero stationary distribution π, the following equations hold for all $1 \le n \le \nu$,*

$$\begin{aligned}
\mu_n(p_K,\pi) &= \nu - 2n + \mathrm{tr}(K) + n\ \iota_n(G), \qquad (10)\\
\tilde{\mu}_n(p_K,\pi) &= \nu - 2n + \mathrm{tr}(K) + n\ \tilde{\iota}_n(G).
\end{aligned}$$

Proof. Let $\mathcal{Q} = \{Q_i\}_1^n \in \mathcal{D}_n(G)$ be chosen arbitrary and let $Q^* = V(G) - \cup_{i=1}^n Q_i$. By Lemma 7,

$$\begin{aligned}
\mathcal{C}_n^{p_K,\pi}(\mathcal{Q}) &= \sum_{i=1}^n \frac{1}{2\ \pi(Q_i)} \sum_{u,v\in Q_i} \pi(u)\pi(v)\|p_K(u) - p_K(v)\|^2 + \sum_{u\in Q^*} \pi(u)\|p_K(u)\|^2 \\
&= \sum_{u\in V(G)} \pi(u)\langle p_K(u), p_K(u)\rangle - \sum_{i=1}^n \sum_{u,v\in Q_i} \frac{\pi(u)\pi(v)\langle p_K(u), p_K(v)\rangle}{\pi(Q_i)} \\
&= \sum_{u\in V(G)} (1 + K(u,u)) - \sum_{i=1}^n \sum_{u\in Q_i} \frac{\pi(u)}{\pi(Q_i)} - \sum_{i=1}^n \sum_{u,v\in Q_i} \frac{\pi(u)\overline{K}(u,v)}{\pi(Q_i)} \\
&= \nu + \sum_{u\in V(G)} K(u,u) - n - \sum_{i=1}^n \frac{\pi(Q_i) - \vec{\partial}(Q_i)}{\pi(Q_i)} \\
&= \nu - 2n + \mathrm{tr}(K) + \sum_{i=1}^n \frac{\vec{\partial}(Q_i)}{\pi(Q_i)}.
\end{aligned}$$

Now, the equations follow by taking minimum over $\mathcal{D}_n(G)$ and $\mathcal{P}_n(G)$. ■

This results along with Theorem 1 shows that the target of the standard k-means algorithm is not theoretically well-justified and must be redefined to be the set of *disjoint* subsets for which the minimum of $C_n^{f,\omega}$ is achieved. Besides, note that the left side of Equation (10) is always nonnegative, and consequently, one finds a lower bound for $\iota_n(G)$ as follows, which is good when n is large.

Corollary 1. *Let G be a graph on ν vertices and a kernel K on it with a nowherezero stationary distribution π. Then for every integer $1 \le n \le \nu$ we have*

$$\iota_n(G) \ge 2 - \frac{\nu + \mathrm{tr}(K)}{n}.$$

It should be noted that the set of functions $\{p_K(u) \mid u \in V(G)\}$ constitutes an orthogonal representation for G [35]. These relations along with relationships of the subject to the theory of weakly unitary invariant norms (e.g. see [2]), convex analysis on Hermitian matrices, and applications of semidefinite programming to the approximation problem are among areas that ought to be considered in forthcoming research.

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