

SHARP EDGE, VERTEX, AND MIXED CHEEGER INEQUALITIES FOR FINITE MARKOV KERNELS

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Abstract

We use the evolving set methodology of Morris and Peres to show Cheeger inequalities for bounding the spectral gap of a finite ergodic Markov kernel. This leads to sharp versions of several previous inequalities, including ones involving edge-expansion and/or vertex-expansion. A bound on the smallest eigenvalue also follows

1 Introduction

The Perron-Frobenius theorem guarantees that a finite, ergodic, reversible Markov kernel P has a real valued eigenbasis with eigenvalues $1 = \lambda_0(P) > \lambda_1(P) \geq \dots \geq \lambda_{n-1}(P) \geq -1$. The spectral gap $\lambda = 1 - \lambda_1(P)$ between the largest and second largest eigenvalues, or in the non-reversible case the gap $\lambda = 1 - \lambda_1\left(\frac{P+P^*}{2}\right)$ of the additive symmetrization, governs key properties of the Markov chain. Alon [1], Lawler and Sokal [7], and Jerrum and Sinclair [6] showed lower bounds on the spectral gap in terms of geometric quantities on the underlying state space, known as Cheeger inequalities [3]. Similarly, in the reversible case Diaconis and Stroock [4] used a Poincaré inequality to show a lower bound on $1 + \lambda_{n-1}$ which also has a geometric flavor.

Such inequalities have played an important role in the study of the mixing times of Markov chains. Conversely, in a draft of [8] the authors used their Evolving set bounds on mixing times to show a Cheeger inequality, but removed it from the final version as it was weaker than previously known bounds. We improve on their idea and find that our resulting Theorem 3.2 can be used to show sharp Cheeger-like lower bounds on λ , both in the edge-expansion sense of Jerrum and Sinclair, the vertex-expansion notion of Alon, and a mixture of both. These bounds typically improve on previous bounds by a factor of two, which is essentially all that can be hoped for as most of our bounds are sharp. Cheeger-like lower bounds on $1 + \lambda_{n-1}$

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follow as well, in terms of a notion of a fairly natural notion of edge-expansion which is yet entirely new.

The paper is organized as follows. In the preliminaries we review some mixing time and Evolving set results. This is followed in Section 3 by our main result, an Evolving set generalization of Cheeger’s inequality. In Section 4 this is used to show sharp versions of the edge expansion Cheeger Inequality and the vertex-expansion bounds of Alon and of Stoyanov. Similar bounds on λ_{n-1} , and more generally the second largest magnitude eigenvalue, are found in Section 5.

2 Preliminaries

All Markov chains in this paper will be finite and ergodic, and so in the remainder this will not be stated explicitly. Consider a Markov kernel P (i.e. transition probability matrix) on state space V with stationary distribution π . It is lazy if $P(x, x) \geq 1/2$ for every $x \in V$, and reversible if $P^* = P$ where the time-reversal $P^*(x, y) = \frac{\pi(y)P(y, x)}{\pi(x)}$. The ergodic flow from $A \subset V$ to $B \subset V$ is $Q(A, B) = \sum_{x \in A, y \in B} \pi(x)P(x, y)$. The total variation distance between distributions σ and π is $\|\sigma - \pi\|_{TV} = \frac{1}{2} \sum_{x \in V} |\sigma(x) - \pi(x)|$. Convergence of a reversible walk is related to spectral gap [6, 4] by

$$\frac{1}{2} (1 - \lambda)^n \leq \frac{1}{2} \lambda_{max}^n \leq \max_{x \in V} \|p_x^n - \pi\|_{TV} \leq \frac{1}{2} \frac{\lambda_{max}^n}{\min_{x \in V} \pi(x)} \tag{2.1}$$

where $p_x^n(y) = P^n(x, y)$ and $\lambda_{max} = \max\{\lambda_1(P), |\lambda_{n-1}(P)|\}$.

The results of this paper will be derived by using the Evolving set methodology of Morris and Peres [8]:

Definition 2.1. Given set $A \subset V$, a step of the *evolving set process* is given by choosing $u \in [0, 1]$ uniformly at random, and transitioning to the set

$$A_u = \{y \in V : Q(A, y) \geq u \pi(y)\} = \{y \in V : P^*(y, A) \geq u\}.$$

Denote an evolving set walk by $S_0, S_1, S_2, \dots, S_n$, the transition kernel by $K^n(A, S) = Prob(S_n = S | S_0 = A)$, and the expectation $E_n f(S_n) = \sum_{S_n \subset V} K^n(S_0, S_n) f(S_n)$.

The main result of [8] is a bound on the rate of convergence in terms of Evolving sets:

Lemma 2.2 (Equation (24) of [8]). *If $S_0 = \{x\}$ for some $x \in V$ then*

$$\|p_x^n - \pi\|_{TV} \leq \frac{1}{2 \pi(x)} E_n \sqrt{\min\{\pi(S_n), 1 - \pi(S_n)\}}.$$

A few easy identities will be required for our work. First, a Martingale type relation:

$$\int_0^1 \pi(A_u) du = \int_0^1 \sum_{x \in V} \pi(x) \delta_{Q(A, x) \geq u \pi(x)} du = \sum_{x \in V} \pi(x) \frac{Q(A, x)}{\pi(x)} = \pi(A) \tag{2.2}$$

Note that for a lazy walk $A \subset A_u$ if and only if $u \leq 1/2$, and otherwise $A_u \subset A$. The gaps between A and A_u are actually related to ergodic flow:

Lemma 2.3. *Given a lazy Markov kernel and $A \subset V$, then*

$$Q(A, A^c) = \int_{1/2}^1 (\pi(A) - \pi(A_u)) du = \int_0^{1/2} (\pi(A_u) - \pi(A)) du.$$

Proof. The second equality holds by (2.2). For the first, $A_u \subset A$ if $u > 1/2$ and so

$$\begin{aligned} \int_{1/2}^1 \pi(A_u) du &= \int_{1/2}^1 \sum_{x \in A} \pi(x) \delta_{Q(A,x) \geq u\pi(x)} du \\ &= \sum_{x \in A} \pi(x) \left(\frac{Q(A,x)}{\pi(x)} - \frac{1}{2} \right) = Q(A,A) - \frac{\pi(A)}{2} \end{aligned}$$

Finish by substituting in $Q(A,A) = Q(A,V) - Q(A,A^c) = \pi(A) - Q(A,A^c)$. □

In applying the Evolving set results we regularly use Jensen’s Inequality, that if f is a concave function and μ a probability measure then

$$\int f(g(u)) d\mu \leq f\left(\int g(u) d\mu\right). \tag{2.3}$$

3 A Generalized Cheeger Inequality

Recall that a Cheeger inequality is used to bound eigenvalues of the Markov kernel in terms of some geometric quantity. “The Cheeger Inequality” generally refers to the bound

$$\lambda \geq 1 - \sqrt{1 - h^2} \geq \frac{h^2}{2} \quad \text{where} \quad h = \min_{0 < \pi(A) \leq 1/2} \frac{Q(A,A^c)}{\pi(A)}. \tag{3.4}$$

The quantity h is known as the Cheeger constant, or Conductance, and measures how quickly the walk expands from a set into its complement. In the lazy case this can be interpreted as measuring how quickly the walk expands from a set A to a larger set in a single step. Our generalization of the Cheeger inequality will be expressed in terms of Evolving sets, with the Cheeger constant replaced by f -congestion:

Definition 3.1. A *weighting function* is a function $f : [0, 1] \rightarrow \mathbb{R}_{\geq 0}$ non-zero except possibly at $f(0)$ and $f(1)$. For weighting function f , the *f -congestion of a set $A \subset V$* is

$$\mathcal{C}_f(A) = \frac{\int_0^1 f(\pi(A_u)) du}{f(\pi(A))}$$

if $A \notin \{\emptyset, V\}$, otherwise $\mathcal{C}_f(A) = 1$. The *f -congestion* is $\mathcal{C}_f = \max_{0 < \pi(A) < 1} \mathcal{C}_f(A)$.

Small f -congestion usually indicates a rapid change in set sizes for the Evolving Set process. In [9] it is found that many measures of convergence rate (total variation, relative entropy, chi-square, etc.) can be bounded in terms of f -congestion, with different choices of f for each distance. The f -congestion is thus closely related to convergence of Markov chains, as is spectral gap, which in part explains why our main result holds:

Theorem 3.2. *If f is a weighting function, then for any reversible Markov kernel*

$$\lambda \geq 1 - \lambda_{max} \geq 1 - \mathcal{C}_f.$$

If $\forall a \in (0, 1/2) : f(a) \leq f(1 - a)$ then it suffices to let $\mathcal{C}_f = \max_{0 < \pi(A) \leq 1/2} \mathcal{C}_f(A)$.

Proof. Given $x \in V$, let $S_0 = \{x\}$, g be some weighting function, $A^\# = A$ if $\pi(A) \leq 1/2$ and $A^\# = A^c$ if $\pi(A) > 1/2$, and $M = \max_{\pi(A) \neq 0, 1} \frac{\sqrt{\pi(A^\#)}}{2g(\pi(A))}$. By Lemma 2.2,

$$\begin{aligned} \|\mathbf{p}_x^n - \pi\|_{TV} &\leq \frac{1}{2\pi(x)} \mathbf{E}_n \sqrt{\pi(S_n^\#)} \leq \frac{M}{\pi(x)} \mathbf{E}_n g(\pi(S_n)) \\ &= \frac{M}{\pi(x)} \mathbf{E}_{n-1} g(\pi(S_{n-1})) \mathcal{C}_g(S_{n-1}) \\ &\leq \frac{M}{\pi(x)} \mathcal{C}_g^n \mathbf{E}_0 g(\pi(S_0)) = \frac{Mg(\pi(x))}{\pi(x)} \mathcal{C}_g^n. \end{aligned}$$

The final inequality follows from $\mathcal{C}_g(S_{n-1}) \leq \mathcal{C}_g$, then induction. The first equality is

$$\mathbf{E}_n g(\pi(S_n)) = \mathbf{E}_{n-1} \mathbf{E}(g(\pi(S_n)) | S_{n-1}) = \mathbf{E}_{n-1} g(\pi(S_{n-1})) \mathcal{C}_g(S_{n-1}).$$

By equation (2.1),

$$\lambda_{max} \leq \sqrt[n]{2 \max_x \|\mathbf{p}_x^n - \pi\|_{TV}} \leq \sqrt[n]{2 \max_x \frac{Mg(\pi(x))}{\pi(x)} \mathcal{C}_g^n} \xrightarrow{n \rightarrow \infty} \mathcal{C}_g.$$

The first bound of the theorem (i.e. general case) follows by setting $g(a) = f(a)$. For the special case, let $g(a) = f(\min\{a, 1 - a\})$. Observe that $A_{1-u} \cup (A^c)_u = V$. Also, $x \in A_{1-u} \cap (A^c)_u$ exactly when $\mathbf{Q}(A, x) = (1 - u)\pi(x)$, which occurs for only a finite set of u 's since V is finite, so $A_{1-u} \cap (A^c)_u = \emptyset$ for a.e. u . Hence $\pi(A_{1-u}) = 1 - \pi((A^c)_u)$ almost everywhere, and so $\int_0^1 g(\pi(A_u)) du = \int_0^1 g(\pi((A^c)_u)) du$ and $\mathcal{C}_g(A) = \mathcal{C}_g(A^c) = \mathcal{C}_g(A^\#)$. Now, $g(\pi(A^\#)) = f(\pi(A^\#))$ and $g \leq f$, and so $\mathcal{C}_g(A) = \mathcal{C}_g(A^\#) \leq \mathcal{C}_f(A^\#)$. We conclude that $\lambda_{max} \leq \mathcal{C}_g = \max_A \mathcal{C}_g(A) = \max_{0 < \pi(A) \leq 1/2} \mathcal{C}_f(A)$, as desired. \square

Remark 3.3. For a non-reversible walk Theorem 3.2 holds with $1 - \lambda_{max}$ replaced by $1 - \lambda_*$, where $\lambda_* = \max_{i > 0} |\lambda_i|$ is the second largest magnitude (complex-valued) eigenvalue of \mathbf{P} . This follows from the related lower bound (see e.g. [9]):

$$\frac{1}{2} \lambda_*^n \leq \max_{x \in V} \|\mathbf{p}_x^n - \pi\|_{TV} \tag{3.5}$$

While intriguing, it is unclear if such a bound on $1 - \lambda_*$ has any practical application.

Remark 3.4. An anonymous reader notes that in order to prove our main result, Theorem 3.2, one can use weaker bounds than those of the form of (2.1) and (3.5). Instead, consider the well known-relation $\rho(A) = \lim_{k \rightarrow \infty} \|A^k\|^{1/k}$ (e.g. Corollary 5.6.14 of [5]), where spectral radius is defined by $\rho(A) = \max\{|\lambda| : \lambda \text{ is an eigenvalue of } A\}$, and $\|\cdot\| : M_n \rightarrow \mathbb{R}$ denotes any matrix norm. In the current setting let $\|A\|$ be the vector-norm $\|A\| = \sup_{v \in \mathbb{R}^n \setminus 0} \frac{\|Av\|_{1,\pi}}{\|v\|_{1,\pi}}$ where $\|v\|_{1,\pi} = \sum_{x \in V} \pi(x)|v(x)|$. Then, if E is the matrix with rows all equal to π ,

$$\begin{aligned} \lambda_*(\mathbf{P}) &= \lambda_*(\mathbf{P}^*) = \rho(\mathbf{P}^* - E) = \lim_{k \rightarrow \infty} \|(\mathbf{P}^* - E)^k\|^{1/k} \\ &= \lim_{k \rightarrow \infty} \|\mathbf{P}^{*k} - E\|^{1/k} = \lim_{k \rightarrow \infty} \max_{x \in V} (2\|\mathbf{p}_x^k - \pi\|_{TV})^{1/k} \end{aligned}$$

The first equality is because, for the reversal \mathbf{P}^* as defined in the first paragraph of the preliminaries, if $\vec{v}_i \mathbf{P} = \lambda_i \mathbf{P}$ for a row vector \vec{v}_i and eigenvalue λ_i , then $\mathbf{P}^* \left(\frac{\vec{v}_i}{\pi}\right)^t = \lambda_i \left(\frac{\vec{v}_i}{\pi}\right)^t$ where $\frac{\vec{v}_i}{\pi}(x) = \frac{\vec{v}_i(x)}{\pi(x)}$ is a row vector and \mathbf{P}^* acts by matrix multiplication.

4 Cheeger Inequalities

Special cases of Theorem 3.2 include bounds of the vertex type as in Alon [1], the edge type as in Jerrum and Sinclair [6], and mixtures of both.

4.1 Edge expansion

We first consider edge-expansion, i.e. ergodic flow, and in particular derive a bound in terms of the symmetrized Cheeger constant:

$$\tilde{h} = \min_{0 < \pi(A) < 1} \tilde{h}(A) \quad \text{where} \quad \tilde{h}(A) = \frac{Q(A, A^c)}{\pi(A)\pi(A^c)}.$$

This will be done by first showing a somewhat stronger bound, and then a few special cases will be considered including that of \tilde{h} .

Corollary 4.1. *If $f : [0, 1] \rightarrow \mathbb{R}_{\geq 0}$ not identically zero is such that f and f'' are concave, then the spectral gap of a Markov kernel satisfies*

$$\lambda \geq \min_{0 < \pi(A) < 1} \frac{Q(A, A^c)^2}{-f(\pi(A))/f''(\pi(A))}.$$

If $\forall a \in (0, 1/2) : f(a) \leq f(1 - a)$ then it suffices to minimize over $\pi(A) \in (0, 1/2]$.

Proof. First consider the reversible, lazy case. By Jensen’s Inequality (2.3) and Lemma 2.3,

$$\begin{aligned} \int_0^1 f(\pi(A_u)) du &= \frac{1}{2} \int_0^{1/2} f(\pi(A_u)) \frac{du}{1/2} + \frac{1}{2} \int_{1/2}^1 f(\pi(A_u)) \frac{du}{1/2} \\ &\leq \frac{1}{2} f \left(2 \int_0^{1/2} \pi(A_u) du \right) + \frac{1}{2} f \left(2 \int_{1/2}^1 \pi(A_u) du \right) \\ &= \frac{1}{2} f(\pi(A) + 2Q(A, A^c)) + \frac{1}{2} f(\pi(A) - 2Q(A, A^c)) \end{aligned}$$

Since f is concave then it is a weighting function (see definition 3.1), and so by Theorem 3.2,

$$\lambda \geq 1 - \mathcal{C}_f \geq \min_{0 < \pi(A) < 1} 1 - \frac{f(\pi(A) + 2Q(A, A^c)) + f(\pi(A) - 2Q(A, A^c))}{2f(\pi(A))} \tag{4.6}$$

More generally, consider the lazy reversible Markov kernel $P' = \frac{1}{2} \left(I + \frac{P+P^*}{2} \right)$. If $\{(\lambda_i, v_i)\}$ is an eigenbasis of $\frac{P+P^*}{2}$, then $\{(\frac{1+\lambda_i}{2}, v_i)\}$ is an eigenbasis for P' , and so $\lambda = 1 - \lambda_1 \left(\frac{P+P^*}{2} \right) = 2(1 - \lambda_1(P')) = 2\lambda_{P'}$. Also, $Q_{P'}(A, A^c) = \frac{1}{4} Q(A, A^c) + \frac{1}{4} Q_{P^*}(A, A^c)$, $Q_{P^*}(A, A^c) = Q(A^c, A)$, and $Q(A, A^c) = \pi(A) - Q(A, A) = \pi(A) - (\pi(A) - Q(A^c, A)) = Q(A^c, A)$, and so $Q_{P'}(A, A^c) = \frac{1}{2} Q(A, A^c)$. Hence, by equation (4.6),

$$\lambda = 2\lambda_{P'} \geq 2 \min_{0 < \pi(A) < 1} 1 - \frac{f(\pi(A) + Q(A, A^c)) + f(\pi(A) - Q(A, A^c))}{2f(\pi(A))} \tag{4.7}$$

$$\geq \min_{0 < \pi(A) < 1} \frac{Q(A, A^c)^2}{-f(\pi(A))/f''(\pi(A))}. \tag{4.8}$$

Equation (4.8) required that $f(x + \delta) + f(x - \delta) \leq 2f(x) + f''(x)\delta^2$. To show this let $F(x, \delta) = f''(x)\delta^2 + 2f(x) - f(x + \delta) - f(x - \delta)$. Observe that $\frac{\partial}{\partial \delta} F(x, \delta) = 2f''(x)\delta - f'(x + \delta) + f'(x - \delta) = 0$ at $\delta = 0$, and $\frac{\partial^2}{\partial \delta^2} F(x, \delta) = 2f''(x) - (f''(x + \delta) + f''(x - \delta)) \geq 0$ because f'' is concave. Hence $F(x, \delta)$ is convex in δ with minimum at $\delta = 0$, and therefore $F(x, \delta) \geq F(x, 0) = 0$. \square

We now show our first Cheeger inequality. If $A \subset V$ then $\mathbf{Q}(A, A^c) \geq \tilde{h}\pi(A)\pi(A^c)$, and so to maximize the lower bound of Corollary 4.1 in terms of \tilde{h} look for a concave f such that $c = \min_{x=\pi(A) \in (0,1)} \frac{x^2(1-x)^2}{-f(x)/f''(x)}$ is maximized, i.e. find a concave solution to $-f(x)/f''(x) \leq c^{-1}x^2(1-x)^2$ for some c . When $c = 1/4$ then $f(x) = \sqrt{x(1-x)}$ works, so $\lambda \geq c\tilde{h}^2 = \tilde{h}^2/4$. A more direct computation leads to a slightly stronger result:

Corollary 4.2. *The spectral gap of a Markov kernel satisfies*

$$\tilde{h} \geq \lambda \geq 2 \left(1 - \sqrt{1 - \tilde{h}^2/4} \right) \geq \frac{\tilde{h}^2}{4}.$$

Proof. The upper bound on λ is classical (e.g. [6]). The second lower bound follows from the first because $\sqrt{1-x} \leq 1-x/2$. For the first lower bound on λ , let $f(a) = \sqrt{a(1-a)}$, use \mathbf{Q}_A to denote $\mathbf{Q}(A, A^c)$, and apply (4.7) in the case that $\forall a \in (0, 1/2]: f(a) \leq f(1-a)$,

$$\begin{aligned} \lambda &\geq 2 \min_{0 < \pi(A) \leq 1/2} 1 - \frac{\sqrt{(\pi(A) + \mathbf{Q}_A)(\pi(A^c) - \mathbf{Q}_A)} + \sqrt{(\pi(A) - \mathbf{Q}_A)(\pi(A^c) + \mathbf{Q}_A)}}{2\sqrt{\pi(A)\pi(A^c)}} \\ &= 2 \min_{0 < \pi(A) \leq 1/2} 1 - \frac{\sqrt{1 + \tilde{h}(A)\pi(A^c)}\sqrt{1 - \tilde{h}(A)\pi(A)}}{2} - \frac{\sqrt{1 - \tilde{h}(A)\pi(A^c)}\sqrt{1 + \tilde{h}(A)\pi(A)}}{2} \end{aligned}$$

Simplify using Lemma 4.3 with $X = \frac{1}{2}(1 + \tilde{h}(A)\pi(A^c))$ and $Y = \frac{1}{2}(1 - \tilde{h}(A)\pi(A))$. \square

Lemma 4.3. *If $X, Y \in [0, 1]$ then*

$$\sqrt{XY} + \sqrt{(1-X)(1-Y)} \leq \sqrt{1 - (X - Y)^2}.$$

Proof. Let $g(X, Y) = \sqrt{XY} + \sqrt{(1-X)(1-Y)}$. Then

$$\begin{aligned} g(X, Y)^2 &= 1 - (X + Y) + 2XY \\ &\quad + \sqrt{[1 - (X + Y) + 2XY]^2 - [1 - 2(X + Y) + (X + Y)^2]}. \end{aligned}$$

Now, $\sqrt{a^2 - b} \leq a - b$ if $a^2 \geq b$, $a \leq \frac{1+b}{2}$ and $a \geq b$ (square both sides to show this). These conditions are easily verified when $a = 1 - (X + Y) + 2XY$ and $b = 1 - 2(X + Y) + (X + Y)^2$ for $X, Y \in [0, 1]$, and so

$$\begin{aligned} g(X, Y)^2 &\leq 2[1 - (X + Y) + 2XY] - [1 - 2(X + Y) + (X + Y)^2] \\ &= 1 + 2XY - X^2 - Y^2 = 1 - (X - Y)^2 \end{aligned}$$

\square

The Corollary is sharp on the two-point space $u - v$ with $P(u, v) = P(v, u) = 1$, because $\tilde{h} = 2$ and so the upper and lower bounds are equal. In contrast, “the Cheeger inequality” of (3.4) shows at best $\lambda \geq 1$, and so cannot be sharp for even this simple example.

Different choices of $f(a)$ work better if more is known about the dependence of $\tilde{h}(A)$ on set size:

Example 4.4. Consider the walk on the cycle $C_n = \mathbb{Z}/n\mathbb{Z}$ with $P(i, i \pm 1 \pmod n) = 1/2$. If $A \subset C_n$ then $Q(A, A^c) \geq 1/n$, and so the Cheeger Inequality shows only $\lambda \geq h^2/2 = 2/n^2$, whereas Corollary 4.2 improves this slightly to $\lambda \geq \tilde{h}^2/4 = 4/n^2$. To apply Corollary 4.1 directly, by the same argument as was done before Corollary 4.2, we solve the differential equation $-f/f'' \leq c^{-1}$, or $f'' + cf \geq 0$. The largest value of c with a concave solution is $c = \pi^2$ with $f(a) = \sin(\pi a)$. Although f'' is not concave, the function f can still be used in (4.7) to obtain

$$\begin{aligned} \lambda &\geq 2 \min_{x=\pi(A) \leq 1/2} 1 - \frac{\sin(\pi(x + Q(A, A^c))) + \sin(\pi(x - Q(A, A^c)))}{2 \sin(\pi x)} \\ &= 2 \min_{0 < \pi(A) \leq 1/2} 1 - \cos(\pi Q(A, A^c)) = 2(1 - \cos(\pi/n)) \approx \frac{\pi^2}{n^2}. \end{aligned}$$

A sharp bound can be obtained by evaluating $\mathcal{C}_{\sin(\pi a)}(A)$ exactly. As before, let $P' = \frac{1}{2} \left(I + \frac{P+P^*}{2} \right) = \frac{I+P}{2}$. If n is even then

$$\lambda = 2\lambda_{P'} \geq 2(1 - \mathcal{C}_{\sin(\pi a), P'}) = 1 - \cos(2\pi/n).$$

The final equality follows from computing $\mathcal{C}_{\sin(\pi a), P'} = \mathcal{C}_{\sin(\pi a), P'}(A)$, where A is any subset of $n/2$ consecutive vertices. A similar bound for the odd case is sharp as well.

4.2 Vertex-expansion

The Generalized Cheeger inequality can also be used to show Cheeger-like inequalities in terms of vertex-expansion (the number of boundary vertices), leading to sharp versions of bounds due to Alon [1], Bobkov, Houdré and Tetali [2] and Stoyanov [10].

Two notions of vertex-expansion are required:

Definition 4.5. If $A \subset V$ then the internal and external boundaries are $\partial_{in}(A) = \{x \in A : Q(x, A^c) > 0\}$ and $\partial_{out}(A) = \partial_{in}(A^c) = \{x \in A^c : Q(x, A) > 0\}$. The internal and external vertex expansion are

$$h_{in} = \min_{0 < \pi(A) \leq 1/2} h_{in}(A) \quad \text{and} \quad h_{out} = \min_{0 < \pi(A) \leq 1/2} h_{out}(A)$$

where

$$h_{in}(A) = \frac{\pi(\partial_{in}(A))}{\pi(A)} \quad \text{and} \quad h_{out}(A) = \frac{\pi(\partial_{out}(A))}{\pi(A)}.$$

Quantities \tilde{h}_{in} and $\tilde{h}_{in}(A)$ are defined similarly, but with $\pi(A)\pi(A^c)$ in the denominator. The minimum transition probability $P_0 = \min_{x \neq y \in V} \{P(x, y) : P(x, y) > 0\}$ will also be required.

Theorem 4.6. *The spectral gap of a reversible Markov kernel satisfies*

$$\begin{aligned} \lambda &\geq 1 - \sqrt{1 - h_{out}P_0} - P_0 \left(\sqrt{1 + h_{out}} - 1 \right) \geq \frac{P_0}{12} \min \{h_{out}^2, h_{out}\} \\ \lambda &\geq 1 - \sqrt{1 + h_{in}P_0} + P_0 \left(1 - \sqrt{1 - h_{in}} \right) \geq \frac{P_0}{8} h_{in}^2 \\ \lambda &\geq 1 - \sqrt{1 - \left(\frac{\tilde{h}_{in}P_0}{2} \right)^2} - P_0 \left(\sqrt{1 - \left(\frac{\tilde{h}_{in}}{2} \right)^2} - 1 \right) \geq \frac{P_0}{8} \tilde{h}_{in}^2. \end{aligned}$$

For the non-reversible case replace P_0 by $P_0/2$.

Proof. The proofs are not difficult and involve application of Jensen’s inequality (2.3) to upper bound $\int_0^1 f(\pi(A_u)) du$ with $f(a) = \sqrt{a}$ for inequalities 1 and 2, or $f(a) = \sqrt{a(1-a)}$ for inequality 3. Theorem 3.2 then induces a bound on λ . However, in order to avoid repeating nearly the same proof in both this and the following sub-section, we note that the first bound of Theorem 4.6 follows from the first bound of Theorem 4.8, with the substitution $h_{in}(A) \geq h(A)$, followed by the substitution $h(A) \geq P_0 h_{out}(A)$, and finishing with $h_{out}(A) \geq h_{out}$ (simple differentiation verifies that these substitutions can only decrease the bound of Theorem 4.8). Likewise, our second bound follows from the first bound of Theorem 4.8 and the substitution $h_{out}(A) \geq h(A)$ followed by $h(A) \geq P_0 h_{in}(A)$ and finally $h_{in}(A) \geq h_{in}$. The third bound of Theorem 4.6 follows from the second bound of Theorem 4.8 and the relations $\tilde{h}(A) \geq P_0 \tilde{h}_{in}(A)$ and $\tilde{h}_{in}(A) \geq \tilde{h}_{in}$.

For the simplified versions of the bounds use the approximations $\sqrt{1-x} \leq 1-x/2$ and $\sqrt{1+x} - 1 - x/2 \leq -\min\{x^2, x\}/12$ for the first bound, $\sqrt{1+x} \leq 1+x/2$ and $\sqrt{1-x} \leq 1-x/2 - x^2/8$ for the second, and $\sqrt{1-x} \leq 1-x/2$ for the third. \square

Stoyanov [10], improving on results of Alon [1] and Bobkov, Houdré and Tetali [2], showed that a reversible Markov kernel will satisfy

$$\begin{aligned} \lambda &\geq \max \left\{ \frac{P_0}{2} \left(1 - \sqrt{1 - h_{in}} \right)^2, \frac{P_0}{4} \left(\sqrt{1 + h_{out}} - 1 \right)^2 \right\} \\ &\geq \max \left\{ \frac{P_0}{8} h_{in}^2, \frac{P_0}{24} \min \{h_{out}^2, h_{out}\} \right\}. \end{aligned}$$

Theorem 4.6, and the approximations $\sqrt{1 - h_{out}P_0} \leq 1 - h_{out}P_0/2$ and $\sqrt{1 + h_{in}P_0} \leq 1 + h_{in}P_0/2$, leads to stronger bounds for reversible kernels:

$$\lambda \geq \frac{P_0}{2} \max \left\{ 1 - \sqrt{1 - h_{in}}, \sqrt{1 + h_{out}} - 1 \right\}^2 \tag{4.9}$$

$$\text{and } \lambda \geq \max \left\{ \frac{P_0}{8} \tilde{h}_{in}^2, \frac{P_0}{12} \min \{h_{out}^2, h_{out}\} \right\} \tag{4.10}$$

Remark 4.7. The h_{in} and h_{out} bounds in this section were not sharp, despite our having promised sharp bounds. These bounds were derived by use of the relation $\lambda \geq 1 - \mathcal{C}_{\sqrt{a}}$, but if $\mathcal{C}_{\sqrt{a(1-a)}}$ were used instead then we would obtain sharp, although quite complicated, bounds; these bounds simplify in the \tilde{h} and \tilde{h}_{in} cases, which is why we have used $\mathcal{C}_{\sqrt{a(1-a)}}$ for those two cases. Bounds based on $\mathcal{C}_{\sqrt{a(1-a)}}$ are sharp on the two-point space $u - v$ with $P(u, v) = P(v, u) = 1$.

4.3 Mixing edge and vertex expansion

We can easily combine edge and vertex-expansion quantities, and maximize at the set level rather than at a global level. For instance, in the reversible case

$$\lambda \geq \min_{0 < \pi(A) \leq 1/2} \max \left\{ \frac{1}{4} \tilde{h}(A)^2, \frac{P_0}{8} \tilde{h}_{in}(A)^2, \frac{P_0}{12} \min\{h_{out}(A)^2, h_{out}(A)\} \right\}.$$

Alternatively, we can apply Theorem 3.2 directly:

Theorem 4.8. *The spectral gap of a reversible Markov kernel satisfies*

$$\begin{aligned} \lambda &\geq \min_{\pi(A) \leq 1/2} 2 - P_0 \sqrt{1 - h_{in}(A)} - P_0 \sqrt{1 + h_{out}(A)} \\ &\quad - (1 - P_0) \sqrt{1 - \frac{h(A) - P_0 h_{in}(A)}{1 - P_0}} - (1 - P_0) \sqrt{1 + \frac{h(A) - P_0 h_{out}(A)}{1 - P_0}} \\ \lambda &\geq \min_{\pi(A) \leq 1/2} 2 - P_0 \sqrt{1 - \frac{\tilde{h}_{in}^2(A)}{4}} - \sqrt{1 - \frac{\tilde{h}^2(A)}{4}} - (1 - P_0) \sqrt{1 - \left(\frac{\tilde{h}(A) - P_0 \tilde{h}_{in}(A)}{2(1 - P_0)} \right)^2}. \end{aligned}$$

For the non-reversible case replace P_0 by $P_0/2$.

Proof. We begin by showing the first inequality.

Consider the lazy reversible case. Let $f(a) = \sqrt{a}$. It follows from Lemma 2.3 that $\int_0^{P_0} (\pi(A_u) - \pi(A)) du = P_0 \pi(\partial_{out}(A))$, that $\int_{P_0}^{1/2} (\pi(A_u) - \pi(A)) du = Q(A, A^c) - P_0 \pi(\partial_{out}(A))$, that $\int_{1-P_0}^1 (\pi(A) - \pi(A_u)) du = P_0 \pi(\partial_{in}(A))$, and that $\int_{1/2}^{1-P_0} (\pi(A) - \pi(A_u)) du = Q(A, A^c) - P_0 \pi(\partial_{in}(A))$. An application of Jensen’s Inequality leads to the bound

$$\begin{aligned} &\int_0^1 f(\pi(A_u)) du \\ &= P_0 \int_0^{P_0} f(\pi(A_u)) \frac{du}{P_0} + \left(\frac{1}{2} - P_0\right) \int_{P_0}^{1/2} f(\pi(A_u)) \frac{du}{1/2 - P_0} \\ &\quad + \left(\frac{1}{2} - P_0\right) \int_{1/2}^{1-P_0} f(\pi(A_u)) \frac{du}{1/2 - P_0} + P_0 \int_{1-P_0}^1 f(\pi(A_u)) \frac{du}{P_0} \\ &\leq P_0 \sqrt{\pi(A) + \pi(\partial_{out}(A))} + \left(\frac{1}{2} - P_0\right) \sqrt{\pi(A) + \frac{Q(A, A^c) - P_0 \pi(\partial_{out}(A))}{1/2 - P_0}} \\ &\quad + \left(\frac{1}{2} - P_0\right) \sqrt{\pi(A) - \frac{Q(A, A^c) - P_0 \pi(\partial_{in}(A))}{1/2 - P_0}} + P_0 \sqrt{\pi(A) - \pi(\partial_{in}(A))} \end{aligned}$$

Hence Theorem 3.2 leads to the bound

$$\begin{aligned} 1 - \lambda &\leq \max_{\pi(A) \leq 1/2} \mathcal{C}_f(A) = \frac{\int_0^1 f(\pi(A_u)) du}{f(\pi(A))} \\ &\leq \max_{\pi(A) \leq 1/2} P_0 \sqrt{1 + h_{out}(A)} + \left(\frac{1}{2} - P_0\right) \sqrt{1 + \frac{h(A) - P_0 h_{out}(A)}{1/2 - P_0}} \\ &\quad + \left(\frac{1}{2} - P_0\right) \sqrt{1 - \frac{h(A) - P_0 h_{in}(A)}{1/2 - P_0}} + P_0 \sqrt{1 - h_{in}(A)} \end{aligned}$$

To generalize to the non-lazy case consider the lazy walk $P' = \frac{I+P}{2}$ and use the relations $\lambda' = \frac{1}{2}\lambda$, $h'_{in}(A) = h_{in}(A)$, $h'_{out}(A) = h_{out}(A)$, $h'(A) = \frac{1}{2}h(A)$ and $P'_0 = P_0/2$. For the non-reversible case, use the result on reversible walks to bound the gap λ'' of the Markov kernel $P'' = \frac{P+P^*}{2}$, and then deduce a bound on λ via the relations $\lambda = \lambda''$, $h''_{in}(A) \geq h_{in}(A)$, $h''_{out}(A) \geq h_{out}(A)$, $h''(A) = h(A)$ and $P''_0 \geq P_0/2$.

Now for the second spectral bound. Given a lazy reversible walk, let $f(a) = \sqrt{a(1-a)}$. By Lemma 2.3, note that $\int_0^{1/2} (\pi(A_u) - \pi(A)) du = Q(A, A^c)$, that $\int_{1-P_0}^1 (\pi(A) - \pi(A_u)) du = P_0\pi(\partial_{in}(A))$ and $\int_{1/2}^{1-P_0} (\pi(A) - \pi(A_u)) du = Q(A, A^c) - P_0\pi(\partial_{in}(A))$. By Jensen's Inequality (2.3) and Theorem 3.2,

$$\begin{aligned}
 1 - \lambda &\leq \max_{\pi(A) \leq 1/2} \mathcal{C}_{\sqrt{a(1-a)}}(A) \\
 &\leq \max_{\pi(A) \leq 1/2} \frac{1}{2} \sqrt{\left(1 + 2\tilde{h}(A)\pi(A^c)\right)\left(1 - 2\tilde{h}(A)\pi(A)\right)} \\
 &\quad + \left(\frac{1}{2} - P_0\right) \sqrt{\left(1 - 2\frac{\tilde{h}(A) - P_0\tilde{h}_{in}(A)}{1 - 2P_0}\pi(A^c)\right)\left(1 + 2\frac{\tilde{h}(A) - P_0\tilde{h}_{in}(A)}{1 - 2P_0}\pi(A)\right)} \\
 &\quad + P_0 \sqrt{(1 - \tilde{h}_{in}(A)\pi(A^c))(1 + \tilde{h}_{in}(A)\pi(A))}
 \end{aligned} \tag{4.11}$$

If $\tilde{h}(A)$ and $\tilde{h}_{in}(A)$ are fixed then this is maximized when $\pi(A) = 1/2$ (see below), and so setting $\pi(A) = 1/2$ gives a bound for a lazy chain. In the general reversible case use the bound on the gap λ' of the lazy walk $P' = \frac{1}{2}(I + P)$ to deduce the result for λ via the relations $\lambda = 2\lambda'$, $\tilde{h}'_{in}(A) = \tilde{h}_{in}(A)$, $\tilde{h}'(A) = \tilde{h}(A)$ and $P'_0 = P_0/2$, as before. Use the same non-reversible reduction as before.

It remains only to show that (4.11) is maximized at $\pi(A) = 1/2$. Given $c \in [-1, 1]$ let $F_c(x) = \sqrt{(1 + c(1-x))(1 - cx)}$ where $x = \pi(A)$. Then (4.11) is just

$$\mathcal{C}_{\sqrt{a(1-a)}}(A) \leq P_0 F_{-\tilde{h}_{in}(A)}(x) + \frac{1 - 2P_0}{2} F_{-2\frac{\tilde{h}(A) - P_0\tilde{h}_{in}(A)}{1 - 2P_0}}(x) + \frac{1}{2} F_{2\tilde{h}(A)}(x).$$

To maximize this with respect to x , observe that $F'_c(x) = \frac{-c^4}{4[(1-cx)(1+c(1-x))]^{3/2}} \leq 0$ and so any sum $\sum \alpha_i F_{c_i}$ with $\alpha_i > 0$ is concave. It follows that if $(\sum \alpha_i F_{c_i})'(1/2) \geq 0$ then $\sum \alpha_i F_{c_i}(x)$ will be maximized in the interval $x \in [0, 1/2]$ at $x = 1/2$. In the case at hand, since $F'_c(1/2) = \frac{-c}{\sqrt{1-(c/2)^2}}$ the upper bound on $\mathcal{C}_{\sqrt{a(1-a)}}(A)$ differentiates as

$$\left. \frac{d}{dx} \right|_{x=1/2} = \frac{P_0\tilde{h}_{in}(A)}{\sqrt{1 - (\tilde{h}_{in}(A)/2)^2}} + \frac{\tilde{h}(A) - P_0\tilde{h}_{in}(A)}{\sqrt{1 - \left(\frac{\tilde{h}(A) - P_0\tilde{h}_{in}(A)}{1 - 2P_0}\right)^2}} - \frac{\tilde{h}(A)}{\sqrt{1 - \tilde{h}(A)^2}}, \tag{4.12}$$

which in turn differentiates as

$$\frac{\partial}{\partial \tilde{h}_{in}(A)} = \frac{P_0}{\left[1 - \left(\frac{\tilde{h}_{in}(A)}{2}\right)^2\right]^{3/2}} - \frac{P_0}{\left[1 - \left(\frac{\tilde{h}(A) - P_0\tilde{h}_{in}(A)}{1 - 2P_0}\right)^2\right]^{3/2}} \geq 0,$$

where the inequality is because $\tilde{h}(A) \leq \tilde{h}_{in}(A)/2$ (recall the chain is lazy). Then equation (4.12) is minimized when $\tilde{h}_{in}(A)$ is as small as possible, that is at $\tilde{h}_{in}(A) = 2\tilde{h}(A)$, at which point equation (4.12) is zero. Therefore equation (4.12) is non-negative, and from the comments above it follows that the upper bound on $\mathcal{C}_{\sqrt{a(1-a)}}(A)$ is maximized when $\pi(A) = 1/2$. \square

5 Bounding the smallest eigenvalue

The generalized Cheeger inequality can also be used to bound $1 - \lambda_{max}$ for a reversible walk, and more generally $1 - \lambda_*$ for a non-reversible walk, by examining \mathbb{P} directly instead of working with the lazy walk $\mathbb{P}' = \frac{1+\mathbb{P}}{2}$ as was done in the preceding proofs. Modified expansion quantities will be required, such as the following:

Definition 5.1. If $A \subset V$ then its *modified ergodic flow* is defined by

$$\Psi(A) = \frac{1}{2} \int_0^1 |\pi(A_u) - \pi(A)| du.$$

The *modified Cheeger constant* \tilde{h} is given by

$$\tilde{h} = \min_{0 < \pi(A) \leq 1/2} \tilde{h}(A) \quad \text{where} \quad \tilde{h}(A) = \frac{\Psi(A)}{\pi(A)\pi(A^c)}.$$

By Lemma 2.3, for a lazy chain $\Psi(A) = \mathbb{Q}(A, A^c)$ and hence also $\tilde{h}(A) = \tilde{h}(A)$. We can now show a lower bound on the eigenvalue gap:

Theorem 5.2. *Given a Markov kernel then*

$$1 - \lambda_* \geq 1 - \sqrt{1 - \tilde{h}^2} \geq \tilde{h}^2/2.$$

Proof. Let $f(a) = \sqrt{a(1-a)}$ and choose $\wp_A \in [0, 1]$ to be such that $\pi(A_u) \geq \pi(A)$ if $u < \wp_A$ and $\pi(A_u) \leq \pi(A)$ if $u > \wp_A$. Then $\Psi(A) = \int_0^{\wp_A} (\pi(A_u) - \pi(A)) du = \int_{\wp_A}^1 (\pi(A) - \pi(A_u)) du$ because $\int_0^1 \pi(A_u) du = \pi(A)$. By Jensen's Inequality,

$$\begin{aligned} \int_0^1 f(\pi(A_u)) du &= \wp_A \int_0^{\wp_A} f(\pi(A_u)) \frac{du}{\wp_A} + (1 - \wp_A) \int_{\wp_A}^1 f(\pi(A_u)) \frac{du}{1 - \wp_A} \\ &\leq \wp_A f\left(\pi(A) + \frac{\Psi(A)}{\wp_A}\right) + (1 - \wp_A) f\left(\pi(A) - \frac{\Psi(A)}{1 - \wp_A}\right) \end{aligned}$$

Hence, by the extension of Theorem 3.2 in Remark 3.3, we have

$$\begin{aligned} \lambda_* &\leq \max_{\pi(A) \leq 1/2} \mathcal{C}_{\sqrt{a(1-a)}}(A) = \max_{\pi(A) \leq 1/2} \frac{\int_0^1 \sqrt{\pi(A_u)(1 - \pi(A_u))} du}{\sqrt{\pi(A)\pi(A^c)}} \\ &\leq \frac{\sqrt{(\wp_A + \tilde{h}(A)\pi(A^c))(\wp_A - \tilde{h}(A)\pi(A))}}{\sqrt{(1 - \wp_A - \tilde{h}(A)\pi(A^c))(1 - \wp_A + \tilde{h}(A)\pi(A))}} \end{aligned}$$

To finish let $X = \wp_A + \tilde{h}(A)\pi(A^c)$ and $Y = \wp_A - \tilde{h}(A)\pi(A)$ in Lemma 4.3. \square

For an isoperimetric interpretation of this, note that in Lemma 4.17 of [9] it was shown that

$$\Psi(A) = \min_{\substack{B \subset V, v \in V, \\ \pi(B) \leq \pi(A^c) < \pi(B \cup v)}} \mathbf{Q}(A, B) + \frac{\pi(A^c) - \pi(B)}{\pi(v)} \mathbf{Q}(A, v).$$

To understand this, observe that B contains those vertices where $\frac{\mathbf{Q}(A, x)}{\pi(x)}$ is minimized, i.e. with a minimum fraction of their stationary distribution due to ergodic flow from A , and v is the vertex with the next smallest $\frac{\mathbf{Q}(A, v)}{\pi(v)}$. So, given some set A , then $\Psi(A)$ is the worst-case ergodic flow from A into a set of size $\pi(A^c)$.

Hence, in our results, to bound λ consider the (worst-case) ergodic flow from a set A to its complement A^c (i.e. $\mathbf{Q}(A, A^c)$), whereas to bound λ_* use the worst-case ergodic flow from a set A to a set the same size as its complement A^c (i.e. $\Psi(A)$).

Just as in the examples of Section 4, a careful choice of f can give better results than the general bound.

Example 5.3. Consider the cycle walk of Example 4.4. Given $x = \frac{k}{n} \leq \frac{1}{2}$, define sets $\mathcal{A}_x = \{0, 2, 4, \dots, 2k - 2\}$ and $\mathcal{B}_x = \mathcal{A}_x \cup \{-1, -2, -3, \dots, -n + 2k\}$. Then $\min_{\pi(A)=x} \Psi(A) = \mathbf{Q}(\mathcal{A}_x, \mathcal{B}_x)$. It follows that $\hbar = 4\mathbf{Q}(\mathcal{A}_{1/2}, \mathcal{B}_{1/2}) = 0$ if n is even and so $1 + \lambda_{n-1} \geq 0$, while $\hbar = \frac{2n}{n^2-1} > \frac{2}{n}$ if n is odd and so $1 + \lambda_n \geq \hbar^2/2 \geq 2/n^2$.

The bound for n even was optimal. To improve on the case of n odd, note that a bound similar to the lower bound of Corollary 4.1 holds for $\Psi(A)$ as well. Since $\Psi(A) \geq 1/2n$ for all $A \subset V$, this again suggests taking $f(a) = \sin(\pi a)$, and so if n is odd then

$$1 - \lambda_{max} \geq 1 - \mathcal{C}_{\sin(\pi a)} = 1 - \cos(2\pi\Psi(\mathcal{A}_{\frac{n-1}{2n}})) = 1 - \cos\left(\frac{\pi}{n}\right)$$

This is again an equality.

Vertex-expansion lower bounds for $1 - \lambda_*$ (and hence also $1 - \lambda_{max}$) hold as well. For instance, if $\hat{P}_0 = \min_{x, y \in V} \{P(x, y) : P(x, y) > 0\}$ (note that $x = y$ is permitted) then

$$\hat{h}_{out} = \min_{0 < \pi(A) \leq 1/2} \min_{\pi(B) = \pi(A^c)} \frac{\pi(\{x \in B : \mathbf{Q}(A, x) > 0\})}{\pi(A)}$$

if π is uniform. Working through a vertex-expansion argument shows the relation $1 - \lambda_* \geq \frac{\hat{P}_0}{12} \min\{\hat{h}_{out}^2, \hat{h}_{out}\}$.

Example 5.4. A vertex-expander is a lazy walk where $h_{out} \geq \epsilon > 0$. Analogously, we might define a non-lazy vertex-expander to be a walk where $\hat{h}_{out} \geq \epsilon > 0$. If the expander is regular of degree d then

$$1 - \lambda_{max} \geq \frac{\min\{\hat{h}_{out}^2, \hat{h}_{out}\}}{12d} \geq \frac{\epsilon^2}{12d},$$

which (up to a small factor) generalizes the relation $1 - \lambda_{max} \geq \frac{\epsilon^2}{4d}$ for the lazy walk.

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