A NOTE ON THE POINCARÉ AND CHEEGER INEQUALITIES FOR SIMPLE RANDOM WALK ON A CONNECTED GRAPH

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ABSTRACT. In 1991, Persi Diaconis and Daniel Stroock obtained two canonical path bounds on the second largest eigenvalue for simple random walk on a connected graph, the Poincaré and Cheeger bounds, and they raised the question as to whether the Poincaré bound is always superior. In this paper, we present some background on these issues, provide an example where Cheeger beats Poincaré, establish some sufficient conditions on the canonical paths for the Poincaré bound to triumph, and show that there is always a choice of paths for which this happens.

1. BACKGROUND AND NOTATION

Let G = G(X, E) be any simple, connected, undirected, and unweighted graph with edge set E and finite vertex set X. For each $(x, y) \in X \times X$ with $x \neq y$, choose a unique oriented path $\gamma_{x,y}$ from x to y. Let Γ denote this collection of canonical paths (also known as a routing) and define

$$n = |X|, \ d = \max_{x \in X} \deg(x), \ \gamma_* = \max_{\gamma \in \Gamma} |\gamma|, \ \text{and} \ b = \max_{\overrightarrow{e} \in \overrightarrow{E}} |\{\gamma \in \Gamma : \gamma \ni \overrightarrow{e}\}|.$$

Note that in the definition of b, the *bottleneck number* of (G, Γ) , the maximum is taken over directed edges and so is to be distinguished from the related concept of the *edge-forwarding index* of (G, Γ) (see [7]). We distinguish directed and undirected edges by adorning the former with an arrow, and if e is an undirected edge connecting vertices x and y, we write $e = \{x, y\}$. Throughout this paper, the term *path* refers to a sequence of vertices where successive terms are connected by an edge. Repeated vertices are allowed, but no edge may appear more than once. (Some authors refer to such a path as a *trail.*) If \overrightarrow{e} is an edge from x to y, we write $\gamma \ni e, \gamma \ni \overrightarrow{e}$ if the vertex sequence defining γ contains x and y as consecutive terms, x preceding yin the latter case. The length of a path is defined as the number of edges it contains: $|\gamma| = |\{e \in E : \gamma \ni e\}|$.

A simple random walk on G begins at some vertex x_0 and then proceeds by moving to a neighboring vertex chosen uniformly at random. This defines a Markov process $\{X_k\}$ with state space X, transition probabilities

$$K(x,y) = \begin{cases} \frac{1}{\deg(x)}, & \{x,y\} \in E\\ 0, & \text{otherwise} \end{cases}$$

and stationary distribution

$$\pi(x) = \frac{\deg(x)}{2|E|}.$$

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This Markov chain is irreducible and reversible, thus the operator K defined by

$$[K\phi](x) = \sum_{y \in X} K(x, y)\phi(y)$$

is a self-adjoint contraction on $L^2(\pi)$ with real eigenvalues

$$1 = \beta_0 > \beta_1 \ge \ldots \ge \beta_{n-1} \ge -1$$

whose corresponding eigenfunctions are orthogonal with respect to the inner product

$$\langle \phi, \psi \rangle_{\pi} = \sum_{x \in X} \phi(x) \psi(x) \pi(x).$$

It is of interest to estimate $\beta_* = \max \{\beta_1, |\beta_{n-1}|\}$ as this quantity can be used to bound the *r*-step distance to stationarity. For example, when K is reversible with respect to π , letting K_x^r denote the distribution of X_r given that $X_0 = x$, we have the classical bound on the total variation distance to stationarity [2]

$$\|K_x^r - \pi\|_{TV} \le \frac{1}{2}\beta_*^r \sqrt{\frac{1 - \pi(x)}{\pi(x)}}$$

More generally, consideration of the Jordan normal form of the transition matrix shows that the exponential rate of convergence of any ergodic Markov chain is governed by the second largest eigenvalue (in magnitude). Because one can often ensure that $\beta_1 \ge |\beta_{n-1}|$ - by adding holding probabilities, for example - much of the research has focused on bounding β_1 .

In the above setting, Diaconis and Stroock [2] give the Poincaré inequality

$$\beta_1 \le 1 - \frac{2\left|E\right|}{d^2 \gamma_* b}$$

and the Cheeger inequality

$$\beta_1 \le 1 - \frac{|E|^2}{2d^4b^2}.$$

These inequalities are corollaries of results that hold for all irreducible, reversible Markov chains and are based on geometric techniques (derived by their namesakes) for bounding the spectral gap of the Laplacian on a Riemannian manifold. Both ultimately rely on the variational characterization of the eigenvalues of the discrete Laplacian L = I - K:

$$1 - \beta_1 = \inf_{\phi \text{ nonconstant}} \frac{\mathcal{E}(\phi, \phi)}{\operatorname{Var}_{\pi}(\phi)}$$

where $\mathcal{E}(\phi, \phi)$ is the Dirichlet form

$$\mathcal{E}(\phi,\phi) = \langle \phi, L\phi \rangle_{\pi} = \frac{1}{2} \sum_{x,y \in X} [\phi(x) - \phi(y)]^2 \pi(x) K(x,y)$$

and

$$\operatorname{Var}_{\pi}(\phi) = \langle \phi - E_{\pi}[\phi], \phi - E_{\pi}[\phi] \rangle_{\pi} = \frac{1}{2} \sum_{x,y \in X} [\phi(x) - \phi(y)]^2 \pi(x) \pi(y)$$

is the variance of ϕ with respect to π , $E_{\pi}[\phi] = \langle \phi, 1 \rangle_{\pi}$ being the corresponding expectation. This characterization follows easily from the Courant-Fischer theorem [4] and the properties of K.

The use of canonical paths in this framework originated in the work of Jerrum and Sinclair on approximating the permanent of a 0-1 matrix [5]. For the purposes of this exposition, we will only be considering the aforementioned inequalities for random walks on graphs, but it should be noted that they are both overestimates of the more general Poincaré and Cheeger bounds. Also, observe that the variational characterization immediately gives lower bounds on β_1 by evaluating the Rayleigh quotient at any nonconstant ϕ . The interested reader is encouraged to consult [2] for the general bounds, their proofs, and the derivation of these particular cases for random walk on a graph.

Though both inequalities are valid for any choice of Γ , their utility hinges upon a clever selection of canonical paths. In particular, one seeks to minimize $\gamma_* b$ for Poincaré and b for Cheeger. It was noted in [2] that the Poincaré bound is often superior, regardless of the choice of Γ , but it was left as an open question whether this is always the case. A little algebra shows that this is equivalent to asking whether $4d^2b \geq \gamma_* |E|$ for all choices of Γ . In addition to better understanding eigenvalue estimates for simple random walk on connected graphs, knowledge of the conditions under which the preceding inequality holds is of interest in its own right. For example, bounds relating standard graph theoretic quantities with measures of bottlenecking may be useful in applications involving network management or optimal distribution.

Jason Fulman and Elizabeth Wilmer [3] have shown that Poincaré beats Cheeger for simple random walk on trees, for which there is only one choice of canonical paths. They also show that for any vertex transitive graph, such as the Cayley graph of a group with a symmetric generating set, and any collection of paths Γ , one has the inequality $bd^2 \geq D |E|$ where D = diam(G). Thus Poincaré beats Cheeger for random walk on vertex transitive graphs whenever $\gamma_* \leq 4D$. In particular, this implies that the Poincaré bound is superior in these graphs when the paths are taken to be geodesics.

For more background and examples, the reader is referred to [2] and [3]. Other useful references include [5, 6, 1]. By way of a counterexample, we answer the question posed by Diaconis and Stroock in the negative. Moreover, we extend the work of Fulman and Wilmer by providing more general criteria for the Poincaré bound to prevail.

2. A Counterexample

Consider the case when G is a complete graph on n vertices. Then d = n - 1 and $|E| = \binom{n}{2}$. Now let γ be a Hamiltonian path with initial vertex x_0 and terminal vertex y_0 , and define a routing Γ by letting $\gamma_{x,y}$ be the unique (length 1) oriented geodesic from x to y for each $(x, y) \in X \times X \setminus \{(x_0, y_0)\}$ and letting $\gamma_{x_0,y_0} = \gamma$. Then $\gamma_* = |\gamma| = n - 1$ and b = 2. The conjectured inequality is thus

$$8(n-1)^2 = 4d^2b \ge \gamma_* |E| = (n-1)\left(\frac{n^2 - n}{2}\right)$$

Because this fails when $n \ge 17$, there are infinitely many graphs where Cheeger beats Poincaré for some choice of canonical paths, hence the Poincaré bound is not uniformly superior to the Cheeger bound. Observe that since the left hand side is $\Omega(n^2)$ and the right hand side is $\Omega(n^3)$, the inequality cannot be salvaged by adjusting constants. Also, this particular choice of paths is kind of an overkill in that the argument actually shows that if one path in Γ has length greater than $16\frac{n-1}{n}$ and the rest are geodesics, then we still get a counterexample. At the other extreme, observe that when n is odd, we can take the long path, γ , to be an Eulerian cycle with an edge deleted, and when n is even, we can take γ to be an Eulerian cycle on a subgraph on n-1 vertices with an edge deleted. These constructions show that counterexamples appear in all complete graphs on $n \ge 7$ vertices. Let us now examine the case of a complete graph on $n \ge 3$ vertices a little closer. The transition probabilities are given by

$$K(x,y) = \frac{1}{n-1} \left(1 - \delta_x(y)\right),$$

so it is easy to see that G has 1 as a simple eigenvalue and its only other eigenvalue is $-\frac{1}{n-1}$ with multiplicity n-1. The preceding analysis shows that if we take Γ as above, then the Poincaré bound is

$$\beta_1 \le 1 - \frac{n}{2(n-1)^2}$$

and the Cheeger bound is

$$\beta_1 \le 1 - \frac{n^2}{32(n-1)^2}$$

Neither bound is remotely sharp, but Cheeger certainly comes out on top for n sufficiently large. If we take Γ to be the unique set of geodesics, in which case $\gamma_* = b = 1$, then we obtain a Poincaré bound of

$$1 - \frac{2\,|E|}{d^2\gamma_* b} = -\frac{1}{n-1}.$$

The corresponding Cheeger bound is

$$1 - \frac{|E|^2}{2d^4b^2} = 1 - \frac{1}{8}\left(\frac{n}{n-1}\right)^2.$$

Because γ_* and b are small as they can be in this case, these are the best possible bounds.

Thus even though we have an example where Cheeger beats Poincaré (on a vertex transitive graph), it involves a choice of paths that yields terrible bounds while the best possible choice of paths gives an ideal Poincaré bound that is much better than the optimal Cheeger bound. Perhaps then the relevant question is whether the best possible Poincaré bound is always better than the best possible Cheeger bound. If the Poincaré v. Cheeger conjecture is stated in terms of optimal bounds, then one can stipulate that the paths do not have repeated vertices as allowing them to contain cycles can only increase the bottleneck number and the longest path length. However, the counterexample shows that this restriction alone does not guarantee that the Poincaré bound is uniformly better than the Cheeger bound. Moreover, for an arbitrary graph, there is no reason to suspect that the optimal Poincaré bound is realized by a choice of paths which gives the optimal Cheeger bound since a choice of paths which minimizes $\gamma_* b$ need not minimize b (and vice versa), so this question is more involved than asking when $4d^2b \geq \gamma_* |E|$. Indeed, it seems that a resolution of this issue would require some characterization of the collections of canonical paths that yield the best bounds, which is probably both the most important and the most difficult problem associated with these path-based eigenvalue inequalities.

At this point, we observe that the construction of the counterexample involved a choice of canonical paths with one exceptionally long path and many shorter paths. This is no coincidence. For any choice of paths, Γ , there are $M = \sum_{\gamma \in \Gamma} |\gamma|$ oriented edges counting multiplicity. Since there are a total of 2 |E| oriented edges in the graph, the pigeonhole principle implies $b \geq \frac{M}{2|E|}$. In terms of the average path length, $\bar{\gamma} = \frac{1}{n^2} \sum_{\gamma \in \Gamma} |\gamma|$, we get the inequality $b \geq \frac{n^2 \bar{\gamma}}{2|E|}$. (Note that we are including the *n* empty paths in this average.)

This shows that a sufficient condition for Poincaré to beat Cheeger is that $2d^2n^2\bar{\gamma} \ge \gamma_* |E|^2$. Because $2|E| = \sum_{x \in X} \deg(x) \le dn$, it follows that Poincaré beats Cheeger whenever $8\bar{\gamma} \ge \gamma_*$. This idea was used implicitly in [3], but the author feels that it is significant enough to be stated directly as

Theorem 1. For any simple connected graph G, if Γ is a set of canonical paths that satisfies $8\bar{\gamma} \ge \gamma_*$, then $4d^2b \ge \gamma_* |E|$, hence the Poincaré bound is superior to the Cheeger bound for this choice of paths.

Thus in order for the Cheeger inequality to prevail, the longest path length must exceed the average path length considerably. When attention is restricted to geodesic paths, this shows that Poincaré beats Cheeger whenever the mean distance is at least one eighth of the diameter. In addition to providing a nice general criterion, this observation shows that Poincaré beats Cheeger along geodesics for a larger class of graphs than just those which are vertex transitive.

Recalling the inequality $b \ge \frac{M}{2|E|}$ where $M = \sum_{\gamma \in \Gamma} |\gamma|$, one sees that M is minimized when Γ is taken to be a collection of geodesics. This choice also minimizes γ_* , though there could be other choices of canonical paths not consisting entirely of geodesics for which $\gamma_* = \text{Diam}(G)$. This suggests that geodesic paths are often a good starting point for finding optimal bounds. Of course $\frac{M}{2|E|}$ is only a lower bound for b and there are often many choices for Γ such that all paths are geodesics, so this is in no way a sufficient criterion for optimization. Indeed, one can sometimes reduce b without increasing γ_* by taking a slight detour in traveling between certain vertices. A little thought will show that this is the case in the following graph.



Still, for the reasons indicated above and the fact that geodesics are often among the more obvious choices for canonical paths, it would be interesting to know more about when Poincaré beats Cheeger along geodesics and when geodesic routings yield optimal bounds (as in the case of complete graphs). All of the examples in [2] and [3] used geodesic paths, but the above graph shows that this is not always the best choice.

3. Spanning Trees

In this section, we show that if Γ is taken to be the set of canonical paths along any spanning tree of any simple connected graph, then the Poincaré bound is strictly better than the Cheeger bound. Specifically, we have $d^2b \geq \gamma_* |E|$ for such Γ . Moreover, the inequality is strict whenever the graph has more than two vertices, or equivalently, when $d \geq 2$. Since every connected graph has at least one spanning tree, this will show that there is always a choice of paths for which Poincaré beats Cheeger.

To begin, let G = G(X, E) be a simple connected graph on |X| = n vertices and let T be any spanning tree for G. Then we can define $\Gamma = \Gamma(T)$ to be the (unique) set of paths along T. We will show that Poincaré beats Cheeger for such routings by first dealing with the case where γ_* is large and then using the results of [3] to handle the remaining case. We note at the outset that as there is only one connected graph with d = 1and it is easily verified that $d^2b = 1 = \gamma_* |E|$ in this case, we can assume throughout that $d \ge 2$. Now let us say that that a routing is subordinate with respect to a path $\gamma_{x,y} = v_0, v_1, ..., v_m$ if for all $0 \le i < j \le m$ with $v_i \ne v_j, \gamma_{v_i,v_j} = v_i, v_{i+1}, ..., v_j$. With this terminology, we can dispense with the large γ_* case using the following lemma.

Lemma 1. If Γ is subordinate with respect to a longest path γ which is cycle-free and satisfies $\gamma_* = |\gamma| > \frac{4|E|}{d^2} - 2$, then $d^2b > \gamma_* |E|$.

Proof.

$$b \ge \left\lfloor \frac{\gamma_* + 1}{2} \right\rfloor \left((\gamma_* + 1) - \left\lfloor \frac{\gamma_* + 1}{2} \right\rfloor \right) \ge \frac{\gamma_*(\gamma_* + 2)}{4}$$

because if $\gamma = v_0, v_1, ..., v_{\gamma_*}$, then for all $0 \le i < j \le \gamma_*, \gamma_{v_i, v_j} = v_i, v_{i+1}, ..., v_j$, so there are $\lfloor \frac{\gamma_* + 1}{2} \rfloor$ initial vertices and $(\gamma_* + 1) - \lfloor \frac{\gamma_* + 1}{2} \rfloor$ terminal vertices of paths through a central edge of γ . Consequently, if $\gamma_* > \frac{4|E|}{d^2} - 2$ (thus $d^2\gamma_* + 2d^2 > 4 |E|$), then

$$d^{2}b \geq d^{2}\frac{\gamma_{*}(\gamma_{*}+2)}{4} = \gamma_{*}\frac{d^{2}\gamma_{*}+2d^{2}}{4} > \gamma_{*}\left|E\right|.$$

Since a spanning tree routing is subordinate with respect to each of its paths, Lemma 1 shows that if $\Gamma = \Gamma(T)$ is the set of canonical paths along a spanning tree T of G, then the Poincaré bound is strictly better than the Cheeger bound whenever $\gamma_* > \frac{4|E|}{d^2} - 2$.

We now note that for any connected graph G on n vertices, we must have $|E| \ge n-1$. When |E| = n-1, G is a tree and there is only one choice of canonical paths. In this case, every path is subordinate with respect to the longest path, which has length $\gamma_* = |E| = n-1$, so the first line in the proof of Lemma 1 shows that

$$b \ge \frac{\gamma_*(\gamma_*+2)}{4} > \frac{1}{4}\gamma_* |E|.$$

Since $d \ge 2$ whenever n > 2, we see that if G is a graph on n > 2 vertices with |E| = n - 1, then $d^2b > \gamma_* |E|$. Consequently, we can assume henceforth that $|E| \ge n$.

For the remaining case, we appeal to Theorem 4 in [3], the proof of which is included for completeness.

Lemma 2. Let T be a tree with n vertices having maximal degree $d_T \ge 2$ and bottleneck number b_T . Then

$$b_T \ge \frac{(n-1)^2}{d_T^2}.$$

Proof. Since T is a tree with n vertices, T has n-1 edges, and for any oriented edge e, the number of pairs of vertices (x, y) with $e \in \gamma_{x,y}$ is of the form k(n-k), $1 \le k \le \frac{n}{2}$ where deletion of edge e cuts T into two components of size k and n-k, respectively. Because k(n-k) is increasing in k for $1 \le k \le \frac{n}{2}$, it is enough to show there exists an edge e^* whose removal divides T into two components, the smaller of which has size at least $\frac{n-1}{dr}$. Given such an edge, we have

$$b_T \ge \left(\frac{n-1}{d_T}\right) \left(n - \frac{n-1}{d_T}\right) \ge \left(\frac{(d_T - 1)(n-1)^2}{d_T^2}\right) \ge \frac{(n-1)^2}{d_T^2}.$$

Thus we need only to demonstrate the existence of e^* . To this end, note that if there is an edge which cuts T into two pieces of equal size, then we may take this edge to be e^* . Otherwise, the deletion of any edge divides T into two pieces of size k and n - k, respectively, where k < n - k. In this case, we can orient the edges by directing each edge from its endpoint in the component of size k to its endpoint in the component of size n - k. Because there are n vertices and n - 1 edges, there must exist a vertex v^* with indegree 0. Since $\deg(v^*) \leq d_T$, there must be some edge leaving v^* whose deletion cuts T into two components, the smaller of which has size at least $\frac{n-1}{d_T}$. Calling this edge e^* establishes the result.

Now by Lemma 1, we can assume that $\gamma_* \leq \frac{4|E|}{d^2} - 2$. Also, since $d \geq 2$ implies there are at least 3 vertices in G (and thus in T), the maximal degree of the vertices in T is $d_T \geq 2$. Because $d \geq d_T$, Lemma 2 shows that

$$b = b_T \ge \frac{(n-1)^2}{d_T^2} \ge \frac{(n-1)^2}{d^2}$$

Therefore, since $2|E| = \sum_{x \in X} \deg(x) \le nd$, and we may assume also that $|E| \ge n$, we have

$$\gamma_* |E| \le \left(\frac{4|E|}{d^2} - 2\right) |E| = \frac{(2|E|)^2}{d^2} - 2|E| \le n^2 - 2n < d^2 \frac{(n-1)^2}{d^2} \le d^2 b$$

We record the above result as

Theorem 2. For any simple connected graph G, if Γ is taken to be the set of paths along any spanning tree of G, then $d^2b \geq \gamma_* |E|$ for this choice of Γ . If G has at least 3 vertices, then the inequality is strict.

Since every connected graph has at least one spanning tree, we have the immediate corollary

Corollary 1. For every simple connected graph, there is a choice of canonical paths such that the Poincaré bound is strictly better than the Cheeger bound.

4. Concluding Remarks

We have established that Poincaré is not uniformly superior to Cheeger for all simple connected graphs and Cheeger is not uniformly superior to Poincaré for any simple connected graph. Strictly speaking, this resolves the question put forth by Diaconis and Stroock, but it would be nice to know whether the best possible Poincaré bounds are always better than the best possible Cheeger bounds. A more complete characterization of the choice of canonical paths for which Poincaré beats Cheeger would likely prove helpful in settling this question. Lemma 1 and Theorems 1 and 2 offer partial results in this direction and subsume all previous findings, but the matter is still far from being resolved. Perhaps examining the case of geodesic routings more closely would shed some light on these issues. Also, since every connected graph can be obtained by adding edges to a spanning tree or deleting edges from a complete graph, it may be possible to obtain related results using surgery methods in conjunction with the above analyses of these extreme cases. Lastly, and probably of greatest practical importance, one would like to know more about how to find routings which yield the best bounds.

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