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Modulus of continuity eigenvalue bounds for homogeneous graphs and convex subgraphs with applications to quantum Hamiltonians

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A B S T R A C T

We adapt modulus of continuity estimates to the study of spectra of combinatorial graph Laplacians, as well as the Dirichlet spectra of certain weighted Laplacians. The latter case is equivalent to stoquastic Hamiltonians and is of current interest in both condensed matter physics and quantum computing. In particular, we introduce a new technique which bounds the spectral gap of such Laplacians (Hamiltonians) by studying the limiting behavior of the oscillations of their solutions when introduced into the heat equation. Our approach is based on recent advances in the PDE literature, which include a proof of the fundamental gap theorem by Andrews and Clutterbuck.

1. Introduction

In this paper, we investigate the spectral structure of combinatorial graph Laplacians by adapting recent advances in the spectral theory of Schrödinger operators on $\mathbb{R}^n$. A combinatorial Laplacian L corresponding to a connected graph G of N vertices has eigenvalues $0 < \lambda_1(L) \leq \lambda_2(L) \leq \cdots \leq \lambda_{N-1}(L)$ and corresponding eigenvectors $u_0, u_1, u_2, \ldots, u_{N-1}$. In part of what follows, we focus on the spectral gap of L, or the difference in its two lowest eigenvalues. In this case, because L always has lowest eigenvalue 0, the spectral gap is simply $\lambda_1(L)$.

To proceed, we introduce a technique based largely on the work of Ben Andrews, Julie Clutterbuck, and collaborators [1–6]. Additionally, we attempt an approach similar to [5] to bounding the spectral gap $\gamma(H)$ of the physically-motivated case of a Hermitian matrix $H = L + W$, where W is some diagonal matrix.

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Recently, these matrices have been called "stoquastic Hamiltonians" in the physics literature [9].[1] That the lowest eigenvalue of H is no longer 0 and the corresponding eigenvector is nonuniform makes determining the spectral gap of H a more challenging problem than that of L alone. In this paper, we reduce such a bound to an estimate involving the log-concavity of the lowest eigenvector u_0 of H.

Because this is the first attempt at applying these techniques to graph spectra, we simplify our problem by considering only *homogeneous* graphs and their strongly convex subgraphs. A homogeneous graph G has an associated group $\mathcal{H}$ and the edges associated with any vertex of G may be identified with the elements of a particular generating set $\mathcal{K}$ for $\mathcal{H}$. (For a formal definition, see Section 2.1.) We consider only the case such that $g^{-1} \in \mathcal{K}$ if and only if $g \in \mathcal{K}$ and therefore the graph is undirected. Also, we assume that the graph is *invariant*, or that the generating set $\mathcal{K}$ is invariant under conjugation by elements $g \in \mathcal{K}$. A subgraph $S \subseteq G$ with vertex set $V(S)$ is *strongly convex* if for each pair of vertices $x, y \in V(S)$, all of the shortest paths in G from x to y are also contained in S [13].

Our approach follows [5], where the authors proved the Fundamental Gap Conjecture. In particular, we study the behavior of oscillations in functions defined on the graph $V(S)$. In [5], the authors studied the time-extended behavior of these oscillation terms when introduced into the heat equation, since such terms cannot decay any slower than $Ce^{-\lambda_1(L)t}$ for some constant C. These oscillation terms are characterized by a modulus of continuity, a construct which typically tracks how uniformly continuous a function is, but we can think of as quantifying the size of oscillations separated by a particular distance. More specifically, for a function $f : V(S) \longrightarrow \mathbb{R}$ we say that it has modulus of continuity η if

$$|f(y) - f(x)| \leq \eta(d(y, x)) \text{ for all } y, x \in V(S)$$

where $d(y, x)$ is the shortest path length between vertices $y, x \in V(S)$. We will further formalize this modulus in Section 3.1.

By sacrificing some tightness, one can apply modulus of continuity estimates without utilizing the heat equation at all. Instead one can derive bounds in terms of the ℓ^2-norm of the modulus. Nonetheless, our intuition stems from the heat equation and we expect that the heat equation will prove useful in subsequent work, so we derive our results from this perspective.

In Section 3.1, we prove the primary result of this paper:

Theorem 1. *Let L be the combinatorial Laplacian for a strongly convex subgraph $S \subseteq G$ of an invariant homogeneous graph G. Then,*

$$\lambda_1(L) \geq 2\left(1 - \cos\left(\frac{\pi}{D+1}\right)\right)$$

where D is the diameter of S.

This theorem gives a nice lower bound to the spectral gap of combinatorial Laplacians in terms of the diameter of the corresponding graph. Although there is a long history of results comparing eigenvalues to diameters, this particular bound relates $\lambda_1(L)$ to the first eigenvalue of the path graph of $D + 1$ vertices. This bound is also tight, since it is always achieved for $S \subset G$ such that S is the path graph with D edges. As a corollary to Theorem 1, this bounds the eigenvalues of the normalized Laplacian $\mathcal{L}$ of S. Thus, this

[1] The term "stoquastic" comes from the resemblance to stochastic matrices. Up to normalization, stoquastic matrices are equivalent to sub-stochastic matrices (*cf.* [14,15]). The spectral properties of sub-stochastic matrices have been previously studied in [18]. In graph theory, the current setting, these Hamiltonians correspond to Laplacians of subgraphs of weighted graphs with Dirichlet boundary, as discussed in Section 4 and elaborated on in [13].

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