Graph Theoretic Uncertainty Principles

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***Abstract*—We develop a graph theoretic set of uncertainty principles with tight bounds for difference estimators acting simultaneously in the graph domain and the frequency domain. We show that the eigenfunctions of a modified graph Laplacian operator dictate the upper and lower bounds for the inequalities.**

I. Introduction

Analysis on graphs is a key component to many techniques in data analysis, dimension reduction, and analysis on fractals. The Fourier transform on a graph has been defined using the spectrum of the graph Laplacian, see, e.g., [7], [2], [13], [12], [11], [10], [9], [5], [3], and [1]. In [1], the authors define the notion of spread in the spectral and graph domains using the analytic properties of the graph Fourier transform. The eigenvalues and eigenvectors of the graph Laplacian play a central role in determining what values of spread are feasible. Motivated by this result, we extend the notion of discrete uncertainty principles such as those introduced in [6], [14], and [4]. We show that for the graph setting, the cyclic structure of the discrete Fourier transform is no longer present for the graph Fourier transform. As a result, the support theorems (such as in [4]) are no longer guaranteed. Finally, we extend the frame uncertainty principle introduced by Lammers and Maeser in [8].

The structure of the paper is as follows. In Section II, we provide a short overview of elementary graph theory, and we establish notation. Section III motivates the choice of the graph Fourier transform by analogy to the L^1 Fourier transform, and examines a special case of the cyclic graph, where columns of the discrete Fourier transform matrix are eigenfunctions of the graph Laplacian. An additive graph uncertainty principle is established in Section IV. In Section V, we extend a result from [8] to the graph setting. In Section VI, we provide uncertainty analysis on a complete graph. Theorems 4.1 and 5.2 are the main results of the paper. Finally, we discuss future directions concerning graph theoretical uncertainty.

II. Weighted Graphs

A graph $G = \{V, \mathbf{E} \subseteq V \times V, w\}$ consists of a set V of vertices, a set $\mathbf{E}$ of edges consisting of pairs of elements of V, and a weight function $w : V \times V \to \mathbb{R}^+$. For $u, v \in V$, $w(u,v) > 0$ if $(u,v) \in \mathbf{E}$ and is zero otherwise. If $w(u,v) = 1$ for all $(u,v) \in \mathbf{E}$, then we say G is "unit weighted." There is no restriction on the size of the set V, but we shall restrict our attention to $|V| = N < \infty$. We also assume that the set $\{v_j\}_{j=0}^{N-1} = V$ has an arbitrary, but fixed ordering.

For all graphs, we define the *adjacency* matrix A component-wise as $A_{m,n} = w(v_m, v_n)$. If A is symmetric, that is, if $w(v_n, v_m) = A_{n,m} = A_{m,n} = w(v_m, v_n)$, then we say G is undirected. If a graph has loops, that is $w(v_j, v_j) > 0$ for some $v_j \in V$, then A has nonzero diagonal entries. Unless otherwise specified, we shall assume that our graphs are undirected and have no loops.

The *degree* d of a vertex v_j is defined by $deg(v_j) = \sum_{n=0}^{N-1} w(v_j, v_n) = \sum_{n=0}^{N-1} A_{j,n}$. We can then define a diagonal *degree matrix* $D = \text{diag}\,(deg(v_0), deg(v_1), ..., deg(v_{N-1}))$. There are two common choices for the graph Laplacian:

$$\begin{aligned} L &= D - A \\ \mathcal{L} &= I - D^{-1/2} A D^{-1/2}, \end{aligned}$$

where I is the $N \times N$ identity. L is defined as the *unnormalized graph Laplacian*, while $\mathcal{L}$ is defined as the *normalized graph Laplacian*. We shall restrict our results to the unnormalized graph Laplacian and refer to it as the Laplacian. Define the $|\mathbf{E}| \times |V|$ *unnormalized* *incidence matrix* M with element $M_{k,j}$ for edge e_k and vertex v_j by:

$$M_{k,j} = \begin{cases} 1, & \text{if } e_k = (v_j, v_l) \text{ and } j < l \\ -1, & \text{if } e_k = (v_j, v_l) \text{ and } j > l \\ 0, & \text{otherwise.} \end{cases}$$

Define the diagonal $|\mathbf{E}| \times |\mathbf{E}|$ *weight matrix* $W = diag(w(e_0), w(e_1), ..., w(e_{|\mathbf{E}|-1}))$.

Noting that $L = M^*WM = \left(W^{\frac{1}{2}}M\right)^* \left(W^{\frac{1}{2}}M\right)$, where $\cdot^*$ denotes the conjugate transpose of an operator $\cdot$, we conclude that L is real, symmetric, and positive semidefinite. By the spectral theorem, L must have an orthonormal basis $\{\chi_l\}$ of eigenvectors with associated eigenvalues $\{\lambda_l\}$ ordered as $0 = \lambda_0 < \lambda_1 \leq \lambda_2 \leq ... \leq \lambda_{N-1}$. Let χ be the matrix whose l^{th} column is given by χ_l. Let Δ be the diagonalization of L, that is, $\chi^* L \chi = \Delta = diag(\lambda_0, ..., \lambda_{N-1})$. We shall use this set of eigenfunctions to define the graph Fourier transform.

III. The Graph Fourier Transform

Functions f defined on a graph G will be written notationally as a vector $f \in \mathbb{R}^N$ where $f[j]$ for $j = 0, ..., N-1$ is the value of the function f evaluated at the vertex v_j. We say $f \in l^2(G)$, and use the standard l^2 norm: $\|f\| = \left(\sum_{j=0}^{N-1} |f[j]|^2\right)^{1/2}$.

Given this space $l^2(G)$ of real-valued functions on the set V of vertices of the graph G, it is natural to define a Fourier transform based on the structure of G. To motivate this definition, we examine the *Fourier transform* on $L^1(\mathbb{R})$, viz.,

$$\widehat{f}(\gamma) = \int_{\mathbb{R}} f(t) e^{-2\pi i t \gamma} d\gamma,$$

and the formal *inverse Fourier transform*,

$$f(t) = \int_{\widehat{\mathbb{R}}} \widehat{f}(\gamma) e^{2\pi i t \gamma}\, d\gamma,$$

where $\widehat{\mathbb{R}} = \mathbb{R}$ is considered the frequency domain. The functions $e^{2\pi i t\gamma}$, $\gamma \in \widehat{\mathbb{R}}$, are the eigenfunctions of the Laplacian operator $\frac{d^2}{dt^2}$ since we have $\frac{d^2}{dt^2} e^{2\pi i t \gamma} = -4\pi^2\gamma^2 e^{2\pi i t\gamma}$. If $\widehat{f} \in L^1(\widehat{\mathbb{R}})$, then the inverse Fourier transform is an expansion of the function f in terms of the eigenfunctions with coefficients $\widehat{f}(\gamma)$. With this in mind, we use the eigenvectors of the graph Laplacian to define the *graph Fourier transform* $\widehat{f}$ of $f \in l^2(G)$ as follows:

$$\forall l = 0, 1, ..., N-1, \quad \widehat{f}[l] = \langle \chi_l, f \rangle,$$

or, equivalently, $\widehat{f} = \chi^* f$. It is clear from the orthonormality of the basis, $\{\chi_l\}$, that $\chi^* = \chi^{-1}$. Thus, the *inverse graph Fourier transform* is given by $\chi\widehat{f} = \chi\chi^* f = If = f$, or, equivalently, $f[j] = \sum_{l=0}^{N-1} \langle \chi_l, f \rangle \chi_l[j]$.

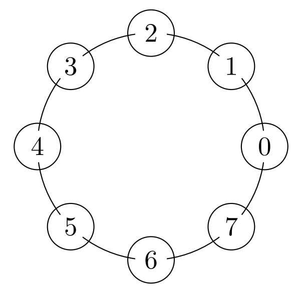

Fig. 1. **A unit weighted circulant graph with 8 vertices.** The graph Laplacian associated with this graph is the classical discrete Laplacian.

Example 3.1: An interesting special case of the graph Fourier transform occurs when the graph is a unit weighted circulant graph as in Figure 1. If T is the $N \times N$ matrix defined by

$$T_{i,j} = \begin{cases} 1 & i = j-1 \\ 1 & i = N-1, j = 0 \\ 0 & \text{otherwise,} \end{cases}$$

then the Laplacian is given by $L = 2T^0 - T - T^{N-1}$, where $T^0 = I$ is the $N \times N$ identity.

If $0 \leq j \leq N-1$, then an orthonormal eigenbasis for T^j is given by

$$\chi_l = \left(1/\sqrt{N}\right) [W^{0l}, W^{1l}, ..., W^{(N-1)l}]^*,$$

for $W = e^{-2\pi i/N}$ and $l = 0, 1, ..., N-1$. Indeed, we have $T^j \chi_l = W^{-jl}\chi_l$, and so χ_l is an eigenvector with the associated eigenvalue W^{-jl}. Therefore, L has the set $\{\chi_l\}$ of orthonormal eigenvectors, with eigenvalues $\lambda_l = -2\cos(2\pi l/N) + 2 = 4\sin^2(\pi l/N)$ for $l = 0, ..., N-1$.

The *unitary* $N \times N$ *discrete Fourier transform (DFT) matrix* is

$$DFT = \frac{1}{\sqrt{N}} \left(W^{mn}\right).$$

Therefore $\Lambda = (DFT)^* PM$ is the matrix whose columns are formed by the set $\{\chi_l\}$ reordered such that the columns are arranged in ascending order of their eigenvalues, and where PM is the permutation matrix that achieves this reordering. Hence, the graph Fourier transform $\Lambda^* = PM^*(DFT)$ generated by a circulant graph may be viewed as a permutation of the discrete Fourier transform.

Graphs, similar to those in Example 3.1, provide an additional motivation for defining the graph Fourier transform by way of eigenvectors of the graph Laplacian.

In fact, the DFT is essentially a special case of the graph Fourier transform. Motivated by this example, we shall examine general uncertainty principles that arise from the graph setting.

IV. A Graph Uncertainty Principle

In the classical $L^2(\mathbb{R})$ setting, we have the additive Heisenberg uncertainty principle:

$$\|f(t)\|^2 \leq 2\pi \left(\|tf(t)\|^2 + \left\|\gamma \widehat{f}(\gamma)\right\|^2 \right). \qquad (1)$$

For a function $f \in \mathcal{S}(\mathbb{R})$, the space of Schwartz functions on $\mathbb{R}$, inequality (1) is equivalent to:

$$\|f(t)\|^2 \leq \left(\left\|\widehat{f'}(\gamma)\right\|^2 + \|f'(t)\|^2 \right). \qquad (2)$$

To achieve a graph analog of inequality (2), we must define the notion of a derivative or difference operator in the graph setting. To do this, we examine the following product:

$$W^{1/2}Mf = D_r f$$

where $D_r = W^{1/2}M$. We refer to D_r as the difference operator for the graph G because it generates the weighted difference of f across each edge of G:

$$(D_r f)[k] = (f[j] - f[i])\,(w(e_k))^{1/2},$$

where $e_k = (v_j, v_i)$ and $j < i$. Because of this property, it is common to refer to $D_r f$ as the derivative of f (see [1]). In the case of the unit weighted circulant graph, D_r is the difference operator in [8]. With this in mind, we establish a graph Fourier transform inequality of the form of (2).

Theorem 4.1: Let G be a weighted, connected, and undirected graph. Then, for any non-zero function $f \in l^2(V)$, the following inequalities hold:

$$0 < \|f\|^2\, \tilde{\lambda}_0 \leq \|D_r f\|^2 + \left\|D_r \widehat{f}\right\|^2 \leq \|f\|^2\, \tilde{\lambda}_{N-1}, \quad (3)$$

where $0 < \tilde{\lambda}_0 \leq \tilde{\lambda}_1 \leq ... \leq \tilde{\lambda}_{N-1}$ are the ordered real eigenvalues of $L+\Delta$. Furthermore, the bounds are sharp.

Proof: Noting that

$$\begin{aligned}\|D_r f\|^2 &= \langle D_r f, D_r f\rangle \\ &= \langle f, \chi\Delta\chi^* f\rangle \\ &= \left\langle \widehat{f}, \Delta\widehat{f}\right\rangle\end{aligned}$$

and, similarly, that $\left\|D_r \widehat{f}\right\|^2 = \left\langle \widehat{f}, L\widehat{f}\right\rangle$, we have

$$\|D_r f\|^2 + \left\|D_r \widehat{f}\right\|^2 = \left\langle \widehat{f}, (L+\Delta)\widehat{f}\right\rangle.$$

Assuming $\tilde{\lambda}_0 > 0$, Inequality (3) follows directly from $L+\Delta$ being symmetric and positive semidefinite, and by applying the properties of the Rayleigh quotient to $L+\Delta$. To prove positivity of $\tilde{\lambda}_0$, note that for $\left\langle \widehat{f}, (L+\Delta)\widehat{f}\right\rangle = 0$ we must have $\langle h, \Delta h\rangle = 0 = \langle h, Lh\rangle$ for some $h \neq 0$. This is impossible as we have, for non-zero h, $\langle h, \Delta h\rangle = 0$ if and only if $h = c[1, 0, ..., 0]^*$ for some $c \neq 0$. This implies $\langle h, Lh\rangle = deg(v_0) > 0$ due to the connectivity of the graph. ■

A direct consequence of Theorem 4.1 is that for a constant function $f = c\chi_0$ ($c \neq 0$) we have $\|D_r c\widehat{\chi_0}\| > 0$. Hence, $D_r f = 0$ in the graph domain implies a non-constant function in the graph Fourier domain.

V. A Graph Frame Uncertainty Principle

As a generalization of the work by Lammers and Maeser in [8], we show that the modified Laplacian operator $L + \Delta$ will dictate an additive uncertainty principle for frames. Let

$$E = \begin{bmatrix} e_0 & e_1 & ... & e_{N-1} \end{bmatrix}$$

be a $d \times N$ matrix whose columns form a Parseval frame for $\mathbb{C}^d$, i.e. $EE^* = I_{d\times d}$. If we let $\mathcal{D} = T^0 - T$, then $\mathcal{D}^* = T^0 - T^{N-1}$, and the classical Laplacian in the discrete setting is given by $L_c = \mathcal{D}^*\mathcal{D} = 2T^0 - T - T^{N-1}$. Let $\|\cdot\|_{fr}$ denote the Frobenius norm. The following result holds.

Theorem 5.1: (Lammers and Maeser [8]) For fixed dimension d and $N \geq d \geq 2$, the following inequalities hold for all $d \times N$ Parseval frames:

$$\begin{aligned} 0 < G(N,d) &\leq \|\mathcal{D}DFTE^*\|_{fr}^2 + \|\mathcal{D}E^*\|_{fr}^2 \\ &\leq H(N,d) \\ &\leq 8d. \end{aligned} \qquad (4)$$

Furthermore, the minimum (maximum) occurs when columns of E^* the d orthonormal eigenvectors corresponding to the d smallest (largest) eigenvalues of $L_c + \Delta_c$ where L_c is the classical Laplacian and Δ_c is its diagonalization. The constant $G(N,d)$ is the sum of those d smallest eigenvalues, and $H(N,d)$ is the sum of those d largest eigenvalues.

To extend the inequalities in Theorem 5.1 to the graph Fourier transform setting, we apply D_r to the frame's conjugate transpose E^* and to the graph Fourier transform $\chi^* E^*$, and then find bounds for the Frobenius norms.

Theorem 5.2: For any graph G as in Theorem 4.1, the following inequalities hold for all $d \times N$ Parseval frames E:

$$\sum_{j=0}^{d-1} \tilde{\lambda}_j \leq \|D_r \chi^* E^*\|_{fr}^2 + \|D_r E^*\|_{fr}^2 \leq \sum_{j=N-d}^{N-1} \tilde{\lambda}_j, \quad (5)$$

where $\left\{\tilde{\lambda_j}\right\}$ is the ordered set of real, non-negative eigenvalues of $L + \Delta$. Furthermore, these bounds are sharp.

Proof: Writing out the Frobenius norms as trace operators yield:

$$\|D_r \chi^* E^*\|_{fr}^2 + \|D_r E^*\|_{fr}^2 = tr(E\chi D_r^* D_r \chi^* E^*) + tr(D_r E^* E D_r^*). \quad (6)$$

Using the invariance of the trace when reordering products, we have $\|D_r \chi^* E^*\|_{fr}^2 + \|D_r E^*\|_{fr}^2$

$$\begin{aligned} &= tr(L\chi^* E^* E\chi) + tr(LE^* E) \\ &= tr(L\chi^* E^* E\chi) + tr(\chi\Delta\chi^* E^* E) \\ &= tr((L + \Delta)\chi^* E^* E\chi). \end{aligned}$$

The operator $\Delta + L$ is real, symmetric, and positive semidefinite. By the spectral theorem, it has an orthonormal eigenbasis P that, upon conjugation, diagonalizes $\Delta + L$:

$$P^*(\Delta + L)P = \tilde{\Delta} = \text{diag}(\tilde{\lambda_0}, \tilde{\lambda}_1, ..., \tilde{\lambda}_{N-1}).$$

Hence, we have

$$\begin{aligned} \|D_r \chi E^*\|_{fr}^2 + \|D_r E^*\|_{fr}^2 &= tr((\Delta + L)\chi^* E^* E\chi) \\ &= tr(P\tilde{\Delta}P^*\chi^* E^* E\chi) \\ &= tr(\tilde{\Delta}P^*\chi^* E^* E\chi P) \\ &= \sum_{j=0}^{N-1} (K^*K)_{j,j} \tilde{\lambda}_j, \end{aligned}$$

where $K = E\chi P$. The matrix K is a Parseval frame because unitary transformations of Parseval frames are Parseval frames . Therefore, $tr(K^*K) = tr(KK^*) = d$. K^*K is also the product of matrices with operator norm ≤ 1. Therefore, each of the entries, $(K^*K)_{j,j}$, satisfies $0 \leq (K^*K)_{j,j} \leq 1$. Hence, minimizing (maximizing) $\sum_{j=0}^{N-1} (K^*K)_{j,j} \tilde{\lambda}_j$ is achieved if

$$(K^*K)_{j,j} = \begin{cases} 1 & j < d \ (j \geq N-d) \\ 0 & j \geq d \ (j < N-d). \end{cases}$$

Choosing E to be the first (last) d rows of $(\chi P)^*$ accomplishes this. The positivity of the bounds follows from the proof of Theorem 4.1 ∎

VI. THE COMPLETE GRAPH

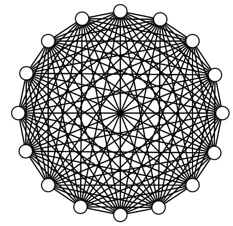

Fig. 2. **A unit weighted complete graph with 16 vertices.**

Unit weighted graphs for which every vertex is connected directly to every other vertex, as in Figure 2, are referred to as *complete graphs*. A complete graph with N vertices has graph Laplacian $L = NI - O$ where O is an $N \times N$ matrix each of whose elements is 1. The minimal polynomial $m(x)$ for L is given by $m(x) = x(x - N)$, and the characteristic polynomial is $c(x) = x(x - N)^{N-1}$. As is the case with all connected graphs, the eigenspace associated with the null eigenvalue is the constant vector $\chi_0 = \left(1/\sqrt{N}\right)[1, ..., 1]^*$. Let $\chi_1 = \left(1/\sqrt{2}\right)[1, -1, 0, ..., 0]$. Then $\langle \chi_0, \chi_1 \rangle = 0$ and $L\chi_1 = N\chi_1$. Upon solving for the $N - 2$ remaining orthonormal eigenvectors χ_l for $l = 2, ..., N - 1$, we define the complete graph Fourier transform $\chi_c^* = [\chi_0, \chi_1, \chi_2, ..., \chi_{N-1}]^*$. We then have $\widehat{\chi_1} = [0, 1, 0, ..., 0]^*$, and

$$|supp(\chi_1)|\,|supp(\widehat{\chi_1})| = 2 < N$$

for $N \geq 3$; and we see that the support theorems in [4] do not hold for graphs. Alternatively, applying Theorem 4.1, we have, for $N > 2$, that

$$\|f\|^2 (N - \sqrt{N}) \leq \|D_r f\|^2 + \left\|D_r \widehat{f}\right\|^2 \leq \|f\|^2 2N.$$

Similarly, applying Theorem 5.2, we have, for $2 \leq d \leq N$ and any $d \times N$ Parseval frame E, that

$$2N(d - 1) \leq \|D_r \chi^* E^*\|_{fr}^2 + \|D_r E^*\|_{fr}^2 .$$

VII. DISCUSSION

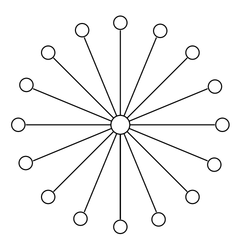

Fig. 3. **A unit weighted star graph with 17 vertices.**

The complete graph, as in Figure 2 provides a structure to illuminate the results of our work. However, the graph Laplacian associated with the complete graph is invariant when the labeling of elements of V are permuted. This property is not true in general, as most graph Laplacians only have invariant eigenvalues when these permutations occur. For example, the star graph (see Figure 3) Laplacian L is highly dependent on what labeling the center vertex receives, but the diagonalization Δ of L is invariant under permutations of labels in V. As a result, the actual lower bounds in Theorems 4.1 and 5.2, while still always positive, change values depending on the labeling of vertices. We leave analysis of the effects of permuting labels to future discussion.

VIII. Acknowledgements

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