Fourier Analysis on Graphs

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Primary Sources


Secondary Sources

Why study graphs?

- Graph theory has developed into a useful tool in applied mathematics.
- Vertices correspond to different sensors, observations, or data points. Edges represent connections, similarities, or correlations among those points.
Outline

1. Graphs and the Graph Laplacian
2. Graph Fourier Transform and other Time-Frequency Operations
3. Windowed Graph Fourier Frames
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1. Graphs and the Graph Laplacian
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Denote a graph by $G = G(V, E)$.
Vertex set $V = \{x_i\}_{i=1}^N$. $|V| = N < \infty$.
Edge set, $E$:

$$E = \{(x, y) : x, y \in V \text{ and } x \sim y\}.$$

We only consider *undirected graphs* in which the edge set, $E$, is symmetric, that is $x \sim y \implies y \sim x$.

We consider a function on a graph $G(V, E)$ to be defined on the vertex set, $V$. That is, we consider functions $f : V \to \mathbb{C}$.
The **degree of** $x$, denoted $d_x$, to be the number of edges connected to point $x$.

A graph is **connected** if for any $x, y \in V$ there exists a sequence $\{x_j\}_{j=1}^K \subseteq V$ such that $x = x_0$ and $y = x_K$ and $(x_j, x_{j+1}) \in E$ for $j = 0, ..., K - 1$. 
Laplace’s operator

In \( \mathbb{R} \), Laplace’s operator is simply the second derivative: We can express this with the second difference formula

\[
f''(x) = \lim_{h \to 0} \frac{f(x + h) - 2f(x) + f(x - h)}{h^2}.
\]

Suppose we discretize the real line by its dyadic points, i.e., \( x = k/2^n \) for \( k \in \mathbb{Z}, n \in \mathbb{N} \). Each vertex has an edge connecting it to its two closest neighbors.

\[
f''(x) = \lim_{n \to \infty} \frac{f(x + \frac{1}{2^n}) - 2f(x) + f(x - \frac{1}{2^n})}{(\frac{1}{2^n})^2}.
\]

This is the sum of all the differences of \( f(x) \) with \( f \) evaluated at all its neighbors (and then properly renormalized).
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Graph Laplacian

**Definition**

The pointwise formulation for the Laplacian acting on a function $f : V \to \mathbb{R}$ is

$$\Delta f(x) = \sum_{y \sim x} f(x) - f(y).$$

- For a finite graph, the Laplacian can be represented as a matrix.
  Let $D$ denote the $N \times N$ degree matrix, $D = \text{diag}(d_x)$.
  Let $A$ denote the $N \times N$ adjacency matrix,

  $$A(i, j) = \begin{cases} 1, & \text{if } x_i \sim x_j \\ 0, & \text{otherwise}. \end{cases}$$

  Then the unweighted graph Laplacian can be written as

  $$L = D - A.$$

  Equivalently,

  $$L(i, j) = \begin{cases} d_{x_i}, & \text{if } i = j \\ -1, & \text{if } x_i \sim x_j \\ 0, & \text{otherwise}. \end{cases}$$
Graph Laplacian

$L = D - A$

- Matrix $L$ is called the unweighted Laplacian to distinguish it from the renormalized Laplacian, $\mathcal{L} = D^{-1/2}LD^{1/2}$, used in some of the literature on graphs.
- $L$ is a symmetric matrix since both $D$ and $A$ are symmetric.
Spectrum of the Laplacian

- $L$ is a real symmetric matrix and therefore has nonnegative eigenvalues $\{\lambda_k\}_{k=0}^{N-1}$ with associated orthonormal eigenvectors $\{\varphi_k\}_{k=0}^{N-1}$.

- If $G$ is finite and connected, then we have
  \[ 0 = \lambda_0 < \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_{N-1}. \]

- The spectrum of the Laplacian, $\sigma(L)$, is fixed but one’s choice of eigenvectors $\{\varphi_k\}_{k=0}^{N-1}$ can vary. Throughout the paper, we assume that the choice of eigenvectors are fixed.

- Since $L$ is Hermetian ($L = L^*$), then we can choose the eigenbasis $\{\varphi_k\}_{k=0}^{N-1}$ to be entirely real-valued.

- Let $\Phi$ denote the $N \times N$ matrix where the $k$th column is precisely the vector $\varphi_k$.

- Easy to show that $\varphi_0 \equiv 1/\sqrt{N}$. 
Figure: Eigenfunctions corresponding to the first six nonzero eigenvalues. Minnesota road graph (2642 vertices)
Figure: Eigenfunctions corresponding to the first six nonzero eigenvalues. Level-8 graph approximation to Sierpinski gasket (9843 vertices)
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Motivation

In the classical setting, the Fourier transform on $\mathbb{R}$ is given by

$$\hat{f}(\xi) = \int_{\mathbb{R}} f(t) e^{-2\pi i \xi t} \, dt = \langle f, e^{2\pi i \xi t} \rangle.$$ 

This is precisely the expansion of $f$ in terms of the eigenvalues of the eigenfunctions of the Laplace operator.

Analogously, we define the graph Fourier transform of a function, $f : V \to \mathbb{R}$, as the expansion of $f$ in terms of the eigenfunctions of the graph Laplacian.
The **graph Fourier transform** is defined as

\[ \hat{f}(\lambda_l) = \langle f, \varphi_l \rangle = \sum_{n=1}^{N} f(n) \varphi_l^*(n). \]

Notice that the graph Fourier transform is only defined on values of \( \sigma(L) \).

The **inverse Fourier transform** is then given by

\[ f(n) = \sum_{l=0}^{N-1} \hat{f}(\lambda_l) \varphi_l(n). \]

If we think of \( f \) and \( \hat{f} \) as \( N \times 1 \) vectors, we then these definitions become

\[ \hat{f} = \Phi^* f, \quad f = \Phi \hat{f}. \]
Parseval’s Identity

With this definition one can show that Parseval’s identity holds. That is for any \( f, g : V \rightarrow \mathbb{R} \) we have

\[
\langle f, g \rangle = \langle \hat{f}, \hat{g} \rangle.
\]

Proof.
This can be seen easily using the matrix notation since \( \Phi \) is an orthonormal matrix. That is,

\[
\langle \hat{f}, \hat{g} \rangle = \hat{f}^* \hat{g} = (\Phi^* f)^* \Phi^* g = f^* \Phi \Phi^* g = f^* g = \langle f, g \rangle.
\]

This immediately gives us Plancherel’s identity:

\[
\| f \|_{\ell^2}^2 = \sum_{n=1}^{N} |f(n)|^2 = \sum_{l=0}^{N-1} |\hat{f}(\lambda_l)|^2 = \| \hat{f} \|_{\ell^2}^2.
\]
In Euclidean setting, modulation is multiplication of a Laplacian eigenfunction.

**Definition**

For any \( k = 0, 1, \ldots, N - 1 \) the graph modulation operator \( M_k \), is defined as

\[
(M_k f)(n) = \sqrt{N} f(n) \varphi_k(n).
\]

Notice that since \( \varphi_0 \equiv \frac{1}{\sqrt{N}} \) then \( M_0 \) is the identity operator.

On \( \mathbb{R} \), modulation in the time domain = translation in the frequency domain,

\[
\hat{M}_\xi \hat{f}(\omega) = \hat{f}(\omega - \xi).
\]

The graph modulation does *not* exhibit this property due to the discrete nature of the spectral domain.
$G = \text{SG}_6$
\[ \hat{f}(\lambda_l) = \delta_2(l) \implies f = \varphi_2. \]
$G = \text{Minnesota}$

$\hat{f}(\lambda_1) = \delta_2(l) \quad \implies \quad f = \varphi_2.$
Classically, for signals $f, g \in L^2(\mathbb{R})$ we define the convolution as

$$f \ast g(t) = \int_{\mathbb{R}} f(u)g(t - u) \, du.$$ 

However, there is no clear analogue of translation in the graph setting. So we exploit the property

$$(\hat{f} \ast \hat{g})(\xi) = \hat{f}(\xi)\hat{g}(\xi),$$

and then take inverse Fourier transform.

**Definition**

For $f, g : V \to \mathbb{R}$, we define the *graph convolution* of $f$ and $g$ as

$$f \ast g(n) = \sum_{l=0}^{N-1} \hat{f}(\lambda_l)\hat{g}(\lambda_l)\varphi_l(n).$$
Properties of graph convolution

\[ f \ast g(n) = \sum_{l=0}^{N-1} \hat{f}(\lambda_l) \hat{g}(\lambda_l) \varphi_l(n). \]

**Proposition**

For \( \alpha \in \mathbb{R} \), and \( f, g, h : V \rightarrow \mathbb{R} \) then the graph convolution defined above satisfies the following properties:

1. \( \hat{f} \ast \hat{g} = \hat{f} \hat{g} \).
2. \( \alpha(f \ast g) = (\alpha f) \ast g = f \ast (\alpha g) \).
3. **Commutativity**: \( f \ast g = g \ast f \).
4. **Distributivity**: \( f \ast (g + h) = f \ast g + f \ast h \).
5. **Associativity**: \( (f \ast g) \ast h = f \ast (g \ast h) \).
Example

Consider the function \( g_0 : V \rightarrow \mathbb{R} \) by setting \( \hat{g}_0(\lambda_l) = 1 \) for all \( l = 0, \ldots, N - 1 \). Then,

\[
g_0(n) = \sum_{l=0}^{N-1} \varphi_l(n).
\]

Then for any signal \( f : V \rightarrow \mathbb{R} \)

\[
f(n) = \sum_{l=0}^{N-1} \hat{f}(\lambda_l) \varphi_l(n) = \sum_{l=0}^{N-1} \hat{f}(\lambda_l) \hat{g}_0(\lambda_l) \varphi_l(n) = f \ast g_0(n).
\]
Graph Translation

- For signal $f \in L^2(\mathbb{R})$, the translation operator, $T_u$, can be thought of as a convolution with $\delta_u$.

- On $\mathbb{R}$ we can calculate
  \[
  \hat{\delta}_u(k) = \int_{\mathbb{R}} \delta_u(x)e^{-2\pi ikx} \, dx = e^{2\pi iku} (= \varphi_k(u)).
  \]

- Then by taking the convolution on $\mathbb{R}$ we have
  \[
  (T_u f)(t) = (f * \delta_u)(t) = \int_{\mathbb{R}} \hat{f}(k)\hat{\delta}_u(k)\varphi_k(t) \, dk = \int_{\mathbb{R}} \hat{f}(k)\varphi^*_k(u)\varphi_k(t) \, dk.
  \]

**Definition**

For any $f : V \to \mathbb{R}$ the *graph translation operator*, $T_i$, is defined to be

\[
(T_if)(n) = \sqrt{N}(f * \delta_i)(n) = \sqrt{N} \sum_{l=0}^{N-1} \hat{f}(\lambda_l)\varphi^*_i(i)\varphi_i(n).
\]
Example - Movie

\( G = \text{Minnesota} \)

\( f = \mathbb{1}_1 \)
\[ G = \text{Minnesota} \]
\[ \hat{f} (\lambda_i) = e^{-5\lambda_i} \]
Example - Movie

\[ G = S G_6 \]
\[ \hat{f}(\lambda_i) = e^{-5\lambda_i} \]
Example - Movie

$G = \text{Minnesota}$

$\hat{f} \equiv 1$
The generalized graph translation possesses many of the nice properties of our usual notion of translation in Euclidean space.

**Proposition**

For any \( f, g : V \to \mathbb{R} \) and \( i, j \in \{1, 2, \ldots, N\} \) then

1. \( T_i(f \ast g) = (T_i f) \ast g = f \ast (T_i g) \).
2. \( T_i T_j f = T_j T_i f \).
Corollary

Given a graph, $G$, with real valued eigenvectors. For any $i, n \in \{1, ..., N\}$ and for any function $f : V \rightarrow \mathbb{R}$ we have

$$T_i f(n) = T_n f(i).$$

Corollary

Given a graph, $G$, with real valued eigenvectors. Let $\alpha$ be a multiindex, i.e. $\alpha = (\alpha_1, \alpha_2, ..., \alpha_K)$ where $\alpha_j \in \{1, ..., N\}$ for $1 \leq j \leq K$ and let $\alpha_0 \in \{1, ..., N\}$. We let $T_\alpha$ denote the composition $T_{\alpha_1} \circ T_{\alpha_2} \circ \cdots \circ T_{\alpha_K}$. Then for any $f : V \rightarrow \mathbb{R}$, we have

$$T_\alpha f(\alpha_0) = T_\beta f(\beta_0),$$

where $\beta = (\beta_1, ..., \beta_K)$ and $(\beta_0, \beta_1, \beta_2, ..., \beta_K)$ is any permutation of $(\alpha_0, \alpha_1, ..., \alpha_K)$. 
Not-so-nice Properties of Translation operator

- In general, the set of translation operators \( \{ T_i \}_{i=1}^N \) do not form a group like in the classical Euclidean setting.
- \( T_i T_j \neq T_{i+j} \).
- If \( \Phi \) is the DFT matrix, then \( T_i T_j = T_{i+j} \pmod{N} \).
- In general, Can we even hope for \( T_i T_j = T_{i \circ j} \) for some semigroup operation, \( \circ : \{1,\ldots,N\} \times \{1,\ldots,N\} \rightarrow \{1,\ldots,N\} \)?
Not-so-nice Properties of Translation operator

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- If \( \Phi \) is the DFT matrix, then \( T_i T_j = T_{i+j} \mod N \).

- In general, Can we even hope for \( T_i T_j = T_i \cdot j \) for some semigroup operation, \( \cdot : \{1, \ldots, N\} \times \{1, \ldots, N\} \rightarrow \{1, \ldots, N\} \)?
When is graph translation a semigroup operation?

Theorem (B. & O.)

Given a graph, $G$, with eigenvector matrix $\Phi = [\varphi_0 | \cdots | \varphi_{N-1}]$. Graph translation on $G$ is a semigroup, i.e. $T_i T_j = T_{i \cdot j}$ for some semigroup operator $\cdot : \{1, \ldots, N\} \times \{1, \ldots, N\} \rightarrow \{1, \ldots, N\}$, only if $\Phi = (1/\sqrt{N}) H$, where $H$ is a Hadamard matrix.

- $H$ is a Hadamard matrix only if $N = 1, 2, \text{ or } 4k$. Sufficiency is an open conjecture.

Theorem (Barik, Fallat, Kirkland)

If $G$ has a normalized Hadamard eigenvector matrix, $\Phi = (1/\sqrt{N}) H$, then $G$ must be $k$-regular and all eigenvalues must be even integers.
The translation operator is not isometric.

\[ \| T_i f \|_{\ell^2} \neq \| f \| \]

We do have the following estimates on the operator \( T_i \):

\[ |\hat{f}(0)| \leq \| T_i f \|_{\ell^2} \leq \sqrt{N} \max_{l \in \{0,1,\ldots,N-1\}} \| \varphi_l \|_{\infty} \| f \|_{\ell^2} \]

Additionally, \( T_i \) is need not be injective, and therefore not invertible.
1. Graphs and the Graph Laplacian

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3. Windowed Graph Fourier Frames
Given a window function \( g : V \rightarrow \mathbb{R} \), we define a \textit{windowed graph Fourier atom} by

\[
g_{i,k}(n) := (M_k T_i g)(n) = N \varphi_k(n) \sum_{l=0}^{N-1} \hat{g}(\lambda_l) \varphi^*_l(i) \varphi_l(n).
\]

The \textit{windowed graph Fourier transform} of function \( f : V \rightarrow \mathbb{R} \) is defined by

\[
Sf(i, k) := \langle f, g_{i,k} \rangle.
\]
Theorem

If \( \hat{g}(0) \neq 0 \), then \( \{g_{i,k}\}_{i=1,2,...,N; k=0,1,...,N-1} \) is a frame. That is for all \( f : V \to \mathbb{R} \),

\[
A \|f\|_{\ell^2}^2 \leq \sum_{i=1}^{N} \sum_{k=0}^{N-1} |\langle f, g_{i,k} \rangle|^2 \leq B \|f\|_{\ell^2}^2
\]

where

\[
A := \min_{n=1,2,...,N} \{N \|T_n g\|_{\ell^2}^2\}, \quad B := \max_{n=1,2,...,N} \{N \|T_n g\|_{\ell^2}^2\}
\]

And we have the estimate:

\[
0 < N|\hat{g}(0)|^2 \leq A \leq B \leq N^2 \max_{l=0,1,...,N-2} \|\varphi_l\|_{\infty}^2 \|g\|_{\ell^2}^2.
\]
Theorem

Provided the window, \( g \), has non-zero mean, i.e. \( \hat{g}(0) \neq 0 \), then for any \( f : V \to \mathbb{R} \),

\[
f(n) = \frac{1}{N \| T_n g \|_{\ell^2}^2} \sum_{i=1}^{N} \sum_{k=0}^{N-1} Sf(i, k)g_{i,k}(n).
\]

Proof requires basic algebraic manipulations and results given on the graph translation operators.
Further questions/topics

Other ways to represent/approximate functions

- Polynomials on graphs
  - Polynomial is defined to be a function, $f$, for which $\Delta^n f = 0$ for finite $n$.
  - Trivial for finite graphs. Not trivial for some infinite graphs.

- Sampling
  - Also trivial for finite graphs

- Band limiting functions
What is the boundary of a graph?

- If a graph boundary, $\partial V \subseteq V$, is defined, this allows us to compute Dirichlet eigenvalues.
  - The Laplacian as we’ve defined it here corresponds to functions on graphs with Neumann boundary conditions.
- One good definition of boundary vertices are those vertices that user has special control over
  - Connections with Schrödinger Eigenmaps
- Other ways to “extract” a boundary
  - Largest radius via shortest path metric or effective resistance metric.
  - Some techniques work well on certain graphs, poorly on others.
Thank you!

