Fourier Analysis on Graphs

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for Harmonic Analysis and Applications

Sources

Primary Sources

[2] David I Shuman, Benjamin Ricaud, and Pierre Vandergheynst, *Vertex-frequency analysis on graphs*, preprint, (2013).

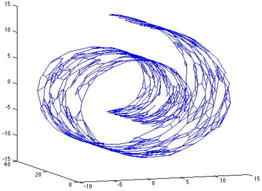
[3] David K Hammond, Pierre Vandergheynst, and Rémi Gribonval *Wavelets on graphs via spectral graph theory*, Applied and Computational Harmonic Analysis **30** (2011) no. 2, 129-150.

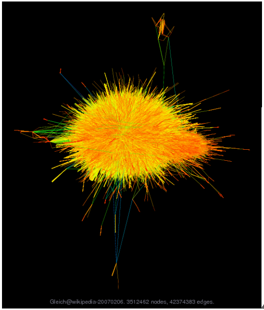
Secondary Sources

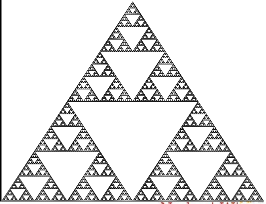
[1] Fan RK Chung, *Spectral Graph Theory*, vol. 92, American Mathematical Soc., 1997.

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

Outline

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Graph Preliminaries

- 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 $f : V \to \mathbb{C}$

Graph Preliminaries, cont.

- 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 it's 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 it's 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,

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

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Graph Laplacian

$$L = D - A$$

- Matrix L is called the unweighted Laplacian to distinguish it from the renormalized Laplacian, $\mathcal{L} = D^{-1/2} L D^{1/2}$, 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 Φ denote the $N \times N$ matrix where the kth column is precisely the vector φ_k.
- Easy to show that $\varphi_0 \equiv 1/\sqrt{N}$.

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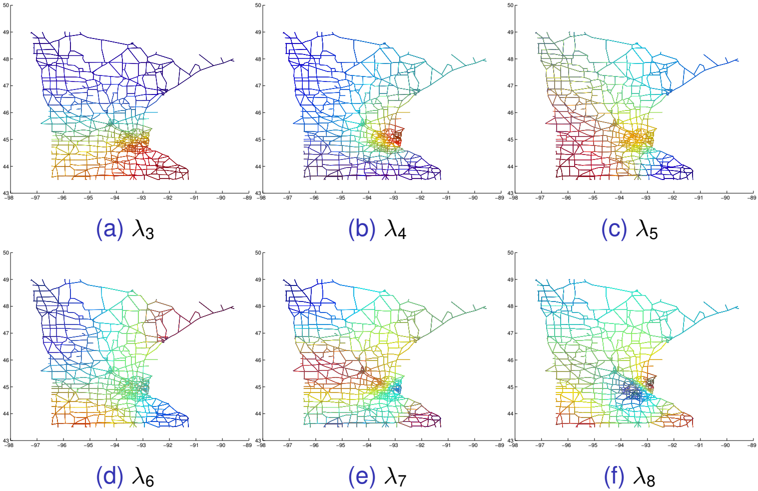
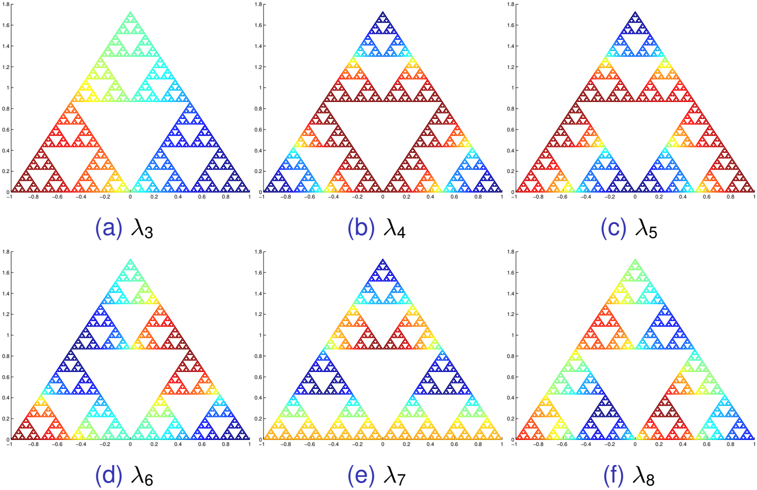


(a) λ_3 (b) λ_4 (c) λ_5

(d) λ_6 (e) λ_7 (f) λ_8

Figure : Eigenfunctions corresponding to the first six nonzero eigenvalues. Minnesota road graph (2642 vertices)

Data Sets - Sierpinski gasket graph approximation

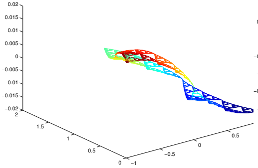


(a) λ_3 (b) λ_4 (c) λ_5

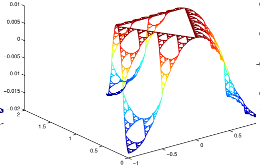
(d) λ_6 (e) λ_7 (f) λ_8

Figure : Eigenfunctions corresponding to the first six nonzero eigenvalues. Level-8 graph approximation to Sierpinski gasket (9843 vertices)

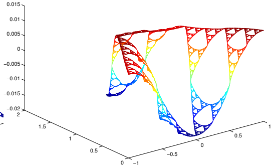
Data Sets - Sierpinski gasket graph approximation



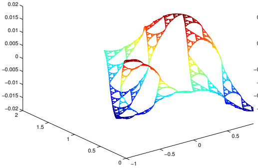
(a) λ_3



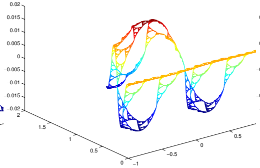
(b) λ_4



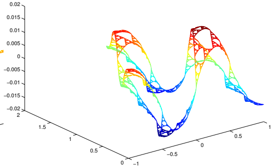
(c) λ_5



(d) λ_6



(e) λ_7



(f) λ_8

Figure : Eigenfunctions corresponding to the first six nonzero eigenvalues. Level-8 graph approximation to Sierpinski gasket (9843 vertices)

Outline

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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.

Graph Fourier Transform

Definition

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 $f, g : V \to \mathbb{R}$ we have

$$\langle f, g \rangle = \langle \hat{f}, \hat{g} \rangle.$$

Proof.

This can be seen easily using the matrix notation since Φ 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:

$$\|f\|_{\ell^2}^2 = \sum_{n=1}^{N} |f(n)|^2 = \sum_{l=0}^{N-1} |\hat{f}(\lambda_l)|^2 = \left\|\hat{f}\right\|_{\ell^2}^2.$$

Graph Modulation

- In Euclidean setting, modulation is multiplication of a Laplacian eigenfunction.

Definition

For any $k = 0, 1, ..., N-1$ 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,

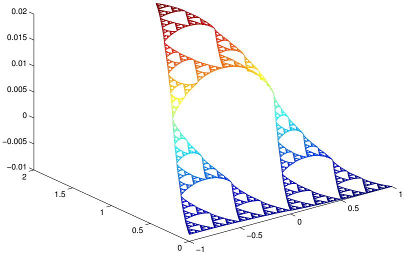
$$\widehat{M_\xi f}(\omega) = \hat{f}(\omega - \xi).$$

The graph modulation does *not* exhibit this property due to the discrete nature of the spectral domain.

Example - Movie

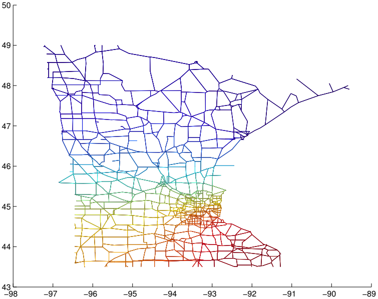
$G = \mathrm{SG}_6$

$\hat{f}(\lambda_l) = \delta_2(l) \implies f = \varphi_2.$



Example - Movie

G =Minnesota
$\hat{f}(\lambda_l) = \delta_2(l) \implies f = \varphi_2$.



Graph Convolution - Motivation and Definition

- Classically, for signals $f, g \in L^2(\mathbb{R})$ we define the convolution as

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

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

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

and then take inverse Fourier transform.

Definition

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

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

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Properties of graph convolution

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

Proposition

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

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

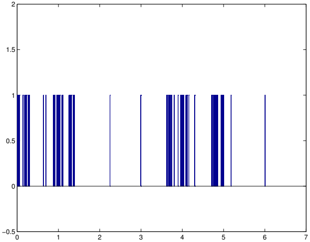
Example

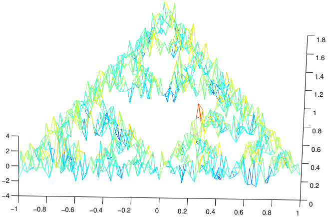
Consider the function $g_0 : V \to \mathbb{R}$ by setting $\hat{g}_0(\lambda_l) = 1$ for all $l = 0, ..., N-1$. Then,

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

Then for any signal $f : V \to \mathbb{R}$

$$\begin{aligned} f(n) &= \sum_{l=0}^{N-1} \hat{f}(\lambda_l)\varphi_l(n) = \sum_{l=0}^{N-1} \hat{f}(\lambda_l)\hat{g}_0(\lambda_l)\varphi_l(n) \\ &= f * g_0(n). \end{aligned}$$





Graph Translation

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

$$(T_u f)(t) = (f * \delta_u)(t) = \int_{\mathbb{R}} \hat{f}(k)\hat{\delta}_u(k)\varphi_k(t)\, dk = \int_{\mathbb{R}} \hat{f}(k)\varphi_k^*(u)\varphi_k(t)\, dk$$

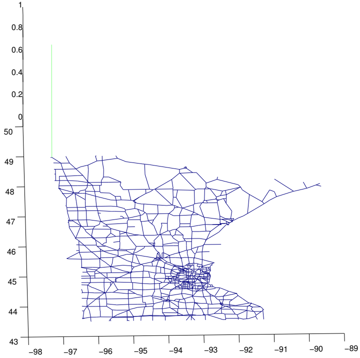
Definition

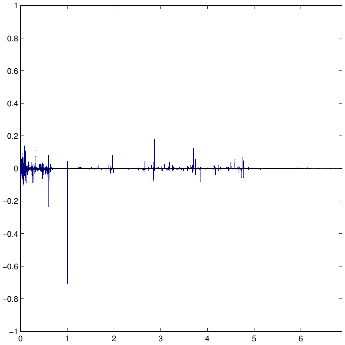
For any $f : V \to \mathbb{R}$ the *graph translation operator*, T_i, is defined to be

$$(T_i f)(n) = \sqrt{N}(f * \delta_i)(n) = \sqrt{N} \sum_{l=0}^{N-1} \hat{f}(\lambda_l)\varphi_l^*(i)\varphi_l(n).$$

Example - Movie

$G =$Minnesota
$f = \mathbb{1}_1$





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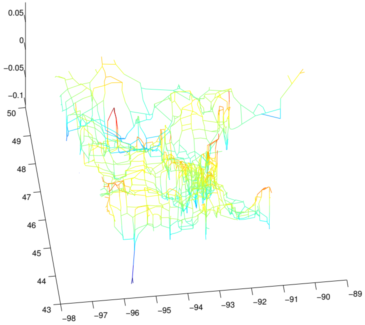
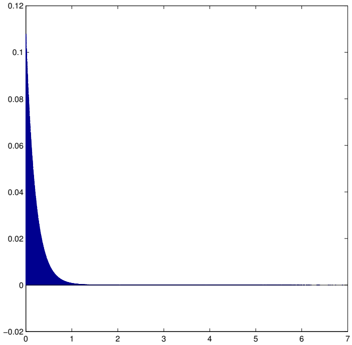
Example - Movie

$G =$Minnesota
$\hat{f}(\lambda_l) = e^{-5\lambda_l}$





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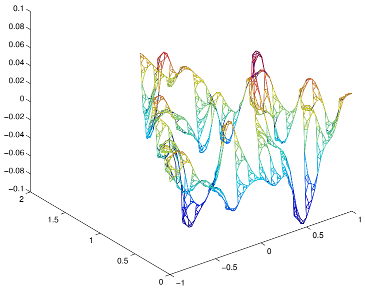
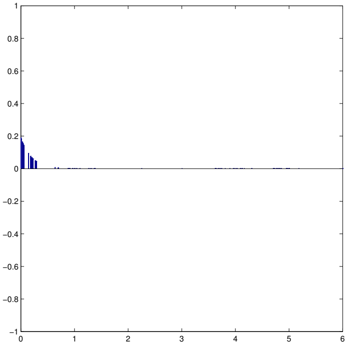
Example - Movie

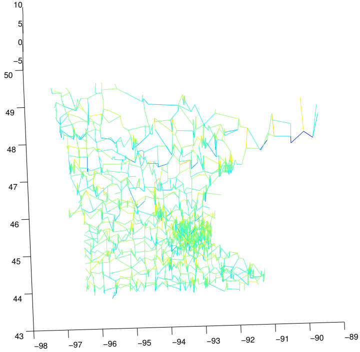
$G = \mathrm{SG}_6$
$\hat{f}(\lambda_l) = e^{-5\lambda_l}$

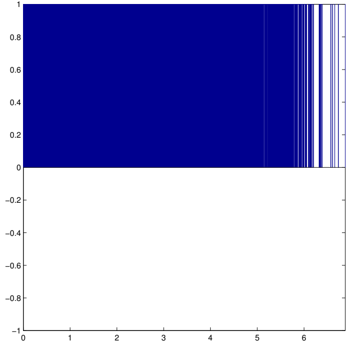




Example - Movie

$G =$Minnesota
$\hat{f} \equiv 1$





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Properties of Translation operator

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* $i, j \in \{1, 2, ..., N\}$ *then*

1. $T_i(f * g) = (T_i f) * g = f * (T_i g)$.
2. $T_i T_j f = T_j T_i f$.

Properties of Translation operator

Corollary

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

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

Corollary

Given a graph, G, with real valued eigenvectors. Let α 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_α denote the composition $T_{\alpha_1} \circ T_{\alpha_2} \circ \cdots \circ T_{\alpha_K}$. Then for any $f : V \to \mathbb{R}$, 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 Φ is the DFT matrix, then $T_i T_j = T_{i+j \pmod N}$.
- In general, Can we even hope for $T_i T_j = T_{i \bullet j}$ for some semigroup operation, $\bullet : \{1, ..., N\} \times \{1, ..., N\} \to \{1, ..., N\}$?

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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. $T_i T_j = T_{i\bullet j}$ for some semigroup operator $\bullet : \{1,...,N\} \times \{1,...,N\} \to \{1,...,N\}$, only if $\Phi = (1/\sqrt{N})H$, where H is a Hadamard matrix.

- H is a Hadamard matrix only if $N = 1, 2$, or $4k$. Sufficiency is 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.

Not-so-nice Properties of Translation operator

- 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.

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Outline

Windowed Graph Fourier Transform

- Given a window function $g : V \to \mathbb{R}$, we define a *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 *windowed graph Fourier transform* of function $f : V \to \mathbb{R}$ is defined by

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

Windowed Graph Fourier Frames

Theorem

If $\hat{g}(0) \neq 0$*, then* $\{g_{i,k}\}_{i=1,2,\ldots,N;k=0,1,\ldots,N-1}$ *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

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

And we have the estimate:

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

Reconstruction Formula

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

Further questions/topics

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!

- Fan RK Chung, *Spectral Graph Theory*, vol. 92, American Mathematical Soc., 1997.
- Pierre Vandergheynst David I Shuman, Benjamin Ricaud, *Vertex-frequency analysis on graphs*, preprint (2013).
- David K Hammond, Pierre Vandergheynst, and Rémi Gribonval, *Wavelets on graphs via spectral graph theory*, Applied and Computational Harmonic Analysis **30** (2011), no. 2, 129–150.

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