Dictionary Design for Graph Signal Processing

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Signal Processing on Graphs



Some Typical Graph Signal Processing Problems

Compression / Visualization





Denoising

Earth data source: Frederik Simons





Orthonormal Dictionaries



Orthonormal Dictionaries (cont.)



$$f = \alpha$$

$$f = \sum_{\ell} \alpha_{\ell} u_{\ell} = \sum_{\ell} \langle f, u_{\ell} \rangle u_{\ell}$$

Overcomplete Dictionaries and Sparsity



- Given an overcomplete Φ , there are infinitely many choices of α that lead to the same signal f
- Useful to *sparsely* represent signals \longrightarrow few non-zero coefficients in α

Motivating Example: Denosing

• Tikhonov regularization for denoising: $\operatorname{argmin}_{f} \left\{ ||f - y||_{2}^{2} + \gamma f^{T} \mathcal{L} f \right\}$



• Wavelet denoising: $\operatorname{argmin}_{a} \left\{ ||f - W^*a||_2^2 + \gamma ||a||_{1,\mu} \right\}$



Motiving Example: Compression

Piecewise-Smooth Signal with Discontinuities



Diffusion Wavelet Coefficients, Sorted by Magnitude





Motivating Example: Any Structure?



Dictionary Design for Signals on Graphs





Desirable Characteristics

- Ability to sparsely represent signals few non-zero coefficients in α
- Ability to capture the relevant characteristics of signals to extract information
- Computationally efficient to apply Φ and Φ^{T}

Frames

- Overcomplete dictionary of matoms in \mathbb{R}^n forms a frame if $A||f||_2^2 \leq \sum_{i=1}^m |\langle f, \phi_i \rangle|^2 \leq B||f||_2^2,$ $\forall f \in \mathbb{R}^n$
- Desirable to have a *tight* frame (A=B), because then the frame operator ΦΦ* is a multiple of the identity operator; equivalently,

$$f = \frac{1}{A} \sum_{i=1}^{m} \langle f, \phi_i \rangle \phi_i, \ \forall f \in \mathbb{R}^n$$

Christensen, Frames and bases, 2008



Kovačević and Chebira, Life beyond bases: The advent of frames, SPM, 2007

Why Do We Need New Dictionaries?



To identify and exploit structure in the data, we need to account for the intrinsic geometric structure of the underlying graph data domain

The Essence of the Problem



- Weighted graphs are irregular structures that lack a shift-invariant notion of translation
- Many simple yet fundamental concepts that underlie classical signal processing techniques become significantly more challenging in the graph setting

Approach: Leverage Intuition from Euclidean Settings to Develop New Mathematical Tools for the Graph Setting



Survey of Approaches to Graph Signal Dictionary Design



Analytic Versus Trained Dictionaries

- Rubinstein et al., Dictionaries for sparse representation modeling, Proc. IEEE, 2010
- Analytic dictionaries: adapted to graph structure, but not Analytic dictionaries: adapted to graph structure, but not Analytic dictionaries: adapted to graph structure, but not
- Dictionary learning: adapt dictionary to training data
 - Aharon et al., The K-SVD, TSP, 2003
 - Engan et al., Method of optimal directions for frame design, ICASSP, 1999
 - These general methods do not explicitly account for graph structure
 - <u>Parametric training</u>: force some structure upon the dictionary (e.g., to incorporate graph topology, ensure an efficient computational implementation), but use training signals to learn parameters

Survey of Approaches to Graph Signal Dictionary Design

- Graph Fourier transform
- Vertex domain designs
- Diffusion-based designs
- Windowed graph Fourier transform
- Spectral domain designs
- Generalized filter banks

Combinatorial Graph Laplacian

- Connected, undirected, weighted graph $\mathcal{G} = \{\mathcal{V}, \mathcal{E}, W\}$
- Degree matrix D: zeros except diagonals, which are sums of weights of edges incident to corresponding node

Non-normalized graph Laplacian: $\mathcal{L} := D - W$

 Complete set of orthonormal eigenvectors and associated real, non-negative eigenvalues:

$$\mathcal{L}u_{\ell} = \lambda_{\ell}u_{\ell},$$

ordered w.l.o.g. s.t.

$$0 = \lambda_0 < \lambda_1 \leq \lambda_2 ... \leq \lambda_{N-1} := \lambda_{\max}$$

• Discrete difference operator: $(\mathcal{L}f)(i) = \sum_{j \in \mathcal{N}_i} W_{i,j}[f(i) - f(j)]$



$$W = \begin{bmatrix} 0 & .3 & .1 & 0 \\ .3 & 0 & .2 & .5 \\ .1 & .2 & 0 & .7 \\ 0 & .5 & .7 & 0 \end{bmatrix}$$

$$D = \left[\begin{array}{rrrr} .4 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1.2 \end{array} \right]$$

Graph Fourier Transform

- Graph Laplacian eigenvectors are the analog of complex exponentials: Values of the eigenvectors associated with low eigenvalues change less rapidly across connected vertices
- Different choices of graph Fourier basis include combinatorial/normalized/random walk Laplacian eigenbasis or generalized eigenbasis of adjacency matrix



The GFT Incorporates the Graph Structure



The GFT Incorporates the Graph Structure



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Vertex Domain Designs

Spatial Wavelets



Crovella and Kolaczyk, Graph wavelets for spatial traffic analysis, INFOCOM, 2003

Wang and Ramchandran, Random multi resolution representations for arbitrary sensor network graphs, ICASSP, 2006



$\begin{bmatrix} \mathbf{f} \\ \mathbf{f} \end{bmatrix} = \begin{bmatrix} \mathbf{a} \\ \mathbf{c} \end{bmatrix}$



- Narang and Ortega, Lifting based wavelet transforms on graphs, APSIPA, 2009
 - Jansen et al., R. Stat. Soc. Ser. B, 2009
- Shen and Ortega, TSP, 2010
 - Rustamov, Wavelets on graphs via deep learning, NIPS, 2013

Gavish et al., Multiscale wavelets on trees, graphs and high dimensional data, ICML, 2010

- Murtagh, J. Classification, 2007
- Lee et al., Ann. Appl. Stats., 2008

Ram et al., TSP, 2011

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Diffusion-Based Designs

• Start with a unit of energy at a single vertex and let it diffuse:



• How much it diffuses over a fixed time depends on the graph structure:



Coifman and Lafon, Diffusion maps, ACHA, 2006

Multiresolution Scaling Function Spaces (Approximation Spaces)



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Diffusion Wavelet Atoms



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Classical Windowed Fourier Transform

- Localized Fourier analysis joint descriptions of signals' temporal and spectral behavior
 - Localized oscillations appear frequently in audio processing, vibration analysis, radar detection, etc.
 - e.g., identify musical notes and melody at different times
- Windowed (short-time) Fourier transform of $f \in L^2(\mathbb{R})$:

$$Sf(s,\xi) := \langle f, g_{s,\xi} \rangle = \int_{-\infty}^{\infty} f(t) \overline{g(t-s)} e^{-2\pi i \xi t} dt$$





• The atoms $g_{s,\xi}$ are localized in time and frequency:





Generalized Translation/Localization

- Define a generalized convolution by imposing that convolution in the vertex domain is multiplication in the graph spectral domain
- Define generalized translation via generalized convolution with a delta

Functions on the Real Line

For $f \in L^2(\mathbb{R})$, in the weak sense $(T_s f)(t) := f(t - s)$ $= (f * \delta_s)(t)$ $= \int_{\mathbb{R}} \hat{f}(\xi) e^{-2\pi i \xi s} e^{2\pi i \xi t} d\xi$

Functions on the Vertices of a Graph

For $f \in \mathbb{R}^N$, we define $(T_i f)(n) := \sqrt{N}(f * \delta_i)(n)$ $= \sqrt{N} \sum_{\ell=0}^{N-1} \hat{f}(\lambda_\ell) u_\ell^*(i) u_\ell(n)$



Properties of Generalized Translation/ Localization

Warning 1: Do not have the group structure of classical translation:

 $T_i T_j \neq T_{i+j}$

- Warning 2: Unlike the classical case, generalized translation operators are not unitary, so ||T_ig||₂ ≠ ||g||₂ in general
- However, the mean is preserved: $\sum_{n} (T_i g)(n) = \sum_{n} g(n)$

Theorem (Smoothness of \hat{g} leads to localization of $T_i g$ around vertex i)

Let $\hat{g} : [0, \lambda_{\max}] \to \mathbb{R}$ be a kernel and define $d_{in} := d_{\mathcal{G}}(i, n)$. Then

$$|(T_ig)(n)| \leq \sqrt{N}B_{\hat{g}}(d_{in}-1),$$

where $B_{\hat{g}}(K)$ is the minimax polynomial approximation error over all polynomials of degree K:

$$B_{\hat{g}}(K) := \inf_{\widehat{p_{K}}} \left\{ \sup_{\lambda \in [0, \lambda_{\max}]} |\hat{g}(\lambda) - \widehat{p_{K}}(\lambda)| \right\}.$$

Windowed Graph Fourier Transform

1 Translate a window g to each vertex of the graph



2 Multiply each component of the graph signal f of interest by the corresponding component of the translated window T_ig

Take the graph Fourier transform of $f \cdot * T_i g$ (recall analysis)

Shuman et al., Vertex-frequency analysis on graphs, ACHA, 2016

Windowed Graph Fourier Transform (cont.)

• Windowed graph Fourier atoms: $g_{i,k} := M_k T_i g$



Spectrogram Examples





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Spectrogram Examples

• Spectrogram = frequency-lapse video







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Example 2 (Tikhonov regularization): We observe a noisy graph signal $\mathbf{y} = \mathbf{f}$ Gaussian noise, and wish to recover \mathbf{f}_0 . To enforce a priori information that the the underlying graph, we include a regularization term of the form $\mathbf{f}^{\mathsf{T}} \mathcal{L} \mathbf{f}$, and,

Spectral Graph Wavelets^{the under}

 $\arg\min_{\mathbf{f}} \left\{ \|\mathbf{f} - \mathbf{y}\|_2^2 + \gamma \mathbf{f}^{\mathrm{T}} \boldsymbol{\ell} \mathbf{f} \right\}.$

Hammond et al., Wavelets on graphs vithe proposition 1]) the optimal reconstruction is given by

• Generalized dilation:



• Spectral graph wavelet $a_{k} (scale t_{k}) = \left[s \atop 1 + \gamma \lambda_{\ell} \right] \hat{y}(\lambda_{\ell}) u_{\ell}(i),$ centered at vertex n: or, equivalently, $\mathbf{f} = \hat{h}(\mathcal{L})\mathbf{y}$, where $\hat{h}(\lambda) := \frac{1}{1+\gamma\lambda}$ can be viewed as a low-pass As an example, in the figure below, we take the 512 x 512 cameraman in $\mathcal{N} = 1$ Gaussian noise with mean zero and standard deviation 0.1 to get a noisy signa $\psi_{s,n}($ in tho<u>ds</u> to Tenois the signal. In the first method we apply a symmetric two size 72 x 72 with two different standard deviations: 1.5 and 3.5. In the second the pixels by connecting each pixel to *its* (horizontal, vertical, and diagonal hei (??) between two neighboring pixels according to the similarity of the nois y in edges of the semi-local graph are independent of the noisy image, but the dis bereni-theores hering pixel values in the noisy image. For the Gaussian wei We then perform the low-pass graph filtering (??) to reconstruct the image. The anisptropic diffusion image smoothing method of [?]. In all image displays, we threshold the values to the [0,1] interval. The zoomed version of the top row of images. Comparing the results of the two smooth sufficiently in smoother areas of the image, the classical Gaussian filt The graph spectral filtering method does not smooth as much across the image image is encoded in the graph Laplacian via the noisy image. Gaussian-Filtered Ga Original Image (S)(Std. Dev. = 1.5)37

Spectral Graph Wavelet Localization



Translated Kernel Variants



Leonardi and Van De Ville, Tight wavelet frames on multislice graphs, TSP, 2013
 Shuman et al., Spectrum-adapted tight graph wavelet and vertex-frequency frames, TSP, 2015

Translated Kernel Variants (cont.)

• Restrict kernels to be polynomials of a given degree, and learn the polynomial coefficients from a training data set



Zhang et al., Learning of structured graph dictionaries, ICASSP, 2012
Thanou et al., Learning parametric dictionaries for signals on graphs, TSP, 2014

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1D Wavelets Via Filter Banks

Classical 2-Channel Critically Sampled Filter Bank



- To extend to the graph setting, we need appropriate notions of downsampling, upsampling, filtering, graph reduction
- Some issues that arise:
 - Difficulty generalizing conditions on filters ensuring properties such as perfect reconstruction, orthogonality
 - Preserving a meaningful correspondence between filtering at different resolution levels

Iterating Low Pass Branch Yields Wavelets



Generalized Operators Downsampling and Graph Reduction

Downsampling



- Downsampling + graph reduction = a multiresolution of graphs
- Methods used here:
 - Graph downsampling by polarity of Laplacian eigenvector associated with largest eigenvalue
 - Kron reduction with spectral sparsification
- Alternative: coarse graining



Generalized Operators Graph Spectral Filtering

- Filtering: represent an input signal as a combination of other signals, and amplify or attenuate the contributions of some of the component signals
- In classical signal processing, the most common choice of basis the complex exponentials, which results in frequency filtering

$$f(t) \longrightarrow FT \longrightarrow \hat{f}(\xi) \longrightarrow \hat{g} \longrightarrow \hat{g}(\xi)\hat{f}(\xi) \longrightarrow IFT \longrightarrow \Phi f(t)$$

$$f(t)=20\cos(2\pi(1)t) + 2\cos(2\pi(11)t) \qquad \hat{f}(\xi) \qquad \hat{f}(\xi) \qquad \hat{f}(\xi) \qquad \hat{f}(\xi) \hat{g}(\xi) \qquad \Phi f(t)$$

$$\stackrel{20}{\xrightarrow{10}} \stackrel{10}{\xrightarrow{0}} \stackrel{10}{\xrightarrow{$$

Example: Image Denoising by Low-Pass Graph Filtering

$$f(n) \longrightarrow GFT \longrightarrow \hat{f}(\lambda_{\ell}) \longrightarrow \hat{g} \longrightarrow \hat{g}(\lambda_{\ell}) \hat{f}(\lambda_{\ell}) \longrightarrow IGFT \longrightarrow \Phi f(n)$$



Shuman et al., The emerging field of signal processing on graphs, SPM, 2013

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Architecture Example 1: A Multiscale Pyramid Transform for Graph Signal



- Generalization of classical Laplacian pyramid of Burt and Adelson
- Overcomplete transform
- Replace classical prediction step (upsample then low pass filter) with a graph interpolation operator
- fterate on $x^{(j+1)}$: Yields a multi-resolution of the underlying graph and a multi-resolution approximation of the the graph signal



Shuman et al., A multiscale pyramid transform for graph signals, TSP, 2016

A Multiscale Pyramid Transform for Graph Signals Multiresolution Examples



A Multiscale Pyramid Transform for Graph Signals Multiresolution Examples





A Multiscale Pyramid Transform for Graph Signals Compression Example



Figure: Compression example. (a) The original piecewise-smooth signal with a discontinuity on the Stanford bunny. (b) The sorted magnitudes of the 15346 pyramid transform coefficients. (c) The reconstruction from the 2724 coefficients with the largest magnitudes, using the least squares synthesis.

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A Multiscale Pyramid Transform for Graph Signals Denoising Example



Figure: Denoising example. (a) Piecewise constant signal on the Minnesota graph. (b) Noisy observation with $\sigma = \frac{1}{2}$. (c) Denoised signal reconstructed after hard thresholding the prediction errors of a two-level pyramid transform.



Shuman et al., A multiscale pyramid transform for graph signals, TSP, 2016

Architecture Example 2: M-Channel Critically Sampled Graph Filter Bank

Architecture



Jin and Shuman., An M-channel critically sampled filter bank for graph signals, ICASSP, 2017

Sampling and Interpolation

- How to sample a graph signal and interpolate from the samples?
- Subset V_s of vertices is a <u>uniqueness set</u> for a subspace P iff: If two signals in the subspace P have the same values on the vertices in the uniqueness set, then they are the same signal
- Partition into uniqueness sets for ideal filter bank subspaces:

Jin and Shuman., An M-channel critically sampled filter bank for graph signals, ICASSP, 2017

How to Evaluate Dictionaries / Open Research Questions

Dictionaries Galore

Approach

• Which multiscale transforms for signals on graphs are well-suited for which signal processing tasks, which classes of signals, and which types of graphs?

1. Signal Models and Sparsity

- For signals on Euclidean data domains, we have results characterizing classes of signals that are well-approximated by different transforms
 - e.g., piecewise-smooth 1D signals by wavelets, 2D cartoons with curvilinear discontinuities by curvelets/shearlets
- Connections between properties of graph signals, the graph structure, and the decay of transform coefficients?
- Empirically, many of the proposed transforms sparsely represent smooth and piecewise smooth graph signals, but there is little in the way of theoretical guarantees to date

Mathematical Models for Graph Signals

- Bandlimited or concentrated on specific parts of the spectrum
 - with noise
 - approximately bandlimited with some extra components (model mismatch)
- Globally smooth/low pass
- Piecewise-smooth/locally regular
- Linear combination (possibly sparse) of some dictionary atoms
 - variational splines (Green's functions)
 - Pesenson, Sampling in Paley-Wiener spaces
 - on combinatorial graphs, T. AMS, 2008
 - overlapping local patterns

Thanou et al., Learning parametric

dictionaries for signals on graphs, TSP, 2014

Piecewise-smooth

Notions of Global Regularity

Notions of Local Regularity

Local Variation

$$|\nabla_m \mathbf{f}||_2 = \left[\sum_{n \in \mathcal{N}_m} w(m, n) \left[f(n) - f(m)\right]^2\right]^{\frac{1}{2}}$$

Hölder Regularity A graph signal f is (C, α, r) -Hölder regular with respect to the graph \mathcal{G} at vertex $n \in \mathcal{V}$ if

$$|f(n) - f(m)| \le C[d_{\mathcal{G}}(m, n)]^{\alpha}, \ \forall m \in \mathcal{N}(n, r)$$

Gavish et al., ICML, 2010

Laplacian as Derivative

- $(\mathcal{L}^k f)(n)$ as a measure of local regularity of f in a neighborhood of radius k around vertex n
 - If f is constant on a neighborhood of radial k around vertex n, this quantity is equal to 0

Ricaud et al., SPIE, 2013

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2. Application-Driven Developments

- Which mathematical models actually match graph signals found in applications?
- Can we collectively build a set of applications/problems to empirically explore and compare the behavior of different dictionaries to better understand what works well when?
- How can specific signal processing tasks arising in certain applications inform dictionary design?
- Recent applications include brain signals, road traffic, video compression, epidemic outbreaks, climate data, and social networks

3. Cumulative Coherence of Atoms

- Ideally, atoms should not be too correlated with each other
- An extreme example:

• Cumulative coherence for a given sparsity level k

$$\mu_1(k) := \max_{|\Theta|=k} \max_{\psi \in \mathcal{D}_{\{1,2,\dots,N \cdot M\} \setminus \Theta}} \sum_{\theta \in \Theta} \frac{|\langle \psi, \mathcal{D}_{\theta} \rangle|}{||\psi||_2 ||\mathcal{D}_{\theta}||_2}$$

 $|/_{a}, \mathcal{T} \rangle|$

4. Vertex-Frequency Tiling

• To sparsely represent large classes of signals, it can be desirable for dictionary atoms to be jointly localized in vertex (time) and graph spectral (frequency) domains

Signals on the Real Line

WGFT

Graph Signals on the Path Graph

SGWT

• For signals on the real line, the Heisenberg uncertainty principle characterizes the tradeoff in resolution between the two domains

4. Vertex-Frequency Tiling (cont.)

• Unlike the complex exponentials, the graph Laplacian eigenvectors can be localized (highly concentrated on a small region of the graph)

Saito and Woei, RIMS Kokyuoku, 2011

• As a result, some graph signals may be simultaneously localized in both the vertex and graph spectral domains

4. Vertex-Frequency Tiling: Open Questions

- How are structural properties of weighted graphs theoretically related to the (non-)localization of the graph Laplacian eigenvectors?
- Different ways to measure spreads in the two domains?
- New uncertainty principles?

- Uncertainty principles can be used to show unexpected things are *possible*
- Example: partial, noisy observation of a bandlimited signal recoverable because a bandlimited signal cannot be concentrated on missing values (provided few enough values are missing and/or bandlimit is low enough)

Donoho and Stark, Uncertainty principles and signal recovery, 1989

Theoretical results characterizing fundamental limits of graph signals such as uncertainty principles inform dictionary design

Agaskar and A spectral graph uncertainty principle, T. Info. Theory, 2013 Pasdeloup et A. Toward an uncertainty principle for weighted graphs, 2015 Tsitsvero et al., Signals on graphs: Uncertainty principle and sampling, 2015 Perraudin et al., Global and local uncertainty principles, 2016

5. Scalable/Distributed Implementations

- Routines that avoid full eigendecompositions
 - e.g., polynomial approximations for graph spectral filtering
 - fast graph Fourier transforms?

- Reduce storage and communication requirements in distributed settings
- Leverage numerical linear algebra literature / form collaborations with researchers from that area
- Connections with solving symmetric, diagonallydominant systems of equations

Spielman, http://www.cs.yale.edu/homes/spielman/precon/precon.html
 Saad, Iterative methods for sparse linear systems, 2003
 Livne and Brandt, Lean algebraic multigrid: Fast graph Laplacian linear solver, 2012
 Vishnoi, Lx=b Laplacian solvers and their algorithmic applications, 2013

6. Graph Construction and Choice of Graph Fourier Basis

- Different choices of graph construction (choosing edges and weights, directed/undirected)
- Different notions of distance (geodesic/shortest path, resistance, diffusion, algebraic)
- Different choices of graph Fourier basis
- Recent flurry of work on graph topology identification/learning

Explore

- <u>https://lts2.epfl.ch/gsp/</u>
- <u>https://www.macalester.edu/~dshuman1/publications.html</u>

Summary

- Weighted graphs are a flexible tool to represent a wide variety of topologically-complicated data domains
- To identify and exploit structure in the data, we need to design dictionaries that incorporate the intrinsic geometric structure of the underlying data domain
- Try to leverage intuition from computational harmonic analysis of signals on Euclidean domains
 - Some ideas generalize relatively straightforwardly (e.g., notion of frequency)
 - However, signals and transforms on graphs can have surprising properties due to the irregularity of the data domains (e.g., uncertainty principle)
- Field is *emerging*
 - Requires more connections/iterations between dictionary design, theory, algorithms, and applications
 - Application of these techniques to real science and engineering problems is in its infancy