Learning Sparse Representations for Graph Signals

Pascal Frossard, EPFL

HIM Workshop on Harmonic Analysis, Graphs and Learning March 16th, 2016





Structured data



Brain signals





Mobility patterns





Structured, but irregular data ...

• Traditional signal processing in Euclidean space





• Irregular (graph) structures: new challenges for signal processing?







Acknowledgements



Dorina Thanou



Xiaowen Dong



David Shuman



Pierre Vandergheynst



Phil Chou



Antonio Ortega



Sunil Narang





Agenda

- Graph Signal Processing Basics
 - Main definitions and operators
- Adaptive Graph Signal Representations
 - Graph Spectral Dictionaries
 - Dictionary Learning Algorithm
 - Applications of Graph Spectral Dictionaries
- Inferring Graphs from Observations
 - Factor Analysis Model
 - Graph Learning Algorithm
 - Illustrative Applications



Signals on Graphs

- Connected, undirected, weighted graph $\mathcal{G} = (V, E, W)$ where $W_{i,j}$ is the weight of the edge e = (i, j)
- Graph signal: a function $f: \mathcal{V} \to \mathbb{R}$ that assigns real values to each vertex of the graph
- Graph description:
 - Degree matrix D : diagonal matrix with sum of weights of incident edges
 - Laplacian matrix ${\cal L}$: difference operator defined based on ${\bf W}$









(Unormalized) Laplacian

• Laplacian is a difference operator $\mathcal{L} := \mathbf{D} - \mathbf{W}$

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

- It is a real symmetric matrix
- It has a complete set of eigenvectors $\{\mathbf{u}_{\ell}\}_{\ell=0,1,\dots,N-1}$
- The eigenvectors are associated with real, nonnegative eigenvalues $\{\lambda_{\ell}\}_{\ell=0,1,...,N-1}$

$$\mathcal{L}\mathbf{u}_{\ell} = \lambda_{\ell}\mathbf{u}_{\ell}, \ \forall \ell = 0, 1, \dots, N-1$$

• Its spectrum is defined as $\sigma(\mathcal{L}) := \{\lambda_0, \lambda_1, \dots, \lambda_{N-1}\}$ $0 = \lambda_0 < \lambda_1 \le \lambda_2 \dots \le \lambda_{N-1} := \lambda_{\max}$





Laplacian example



$$G = \{V, E\}$$
$$D = diag(degree(v_1) \dots degree(v_n))$$
$$\mathcal{L} := \mathbf{D} - \mathbf{W}$$



- Symmetric
- Off-diagonal entries non-positive
- Rows sum up to zero
- Has a complete set of orthonormal eigenvectors: $L = \chi \Lambda \chi^T$

 $0 = \lambda_0 < \lambda_1 \le \ldots \le \lambda_{n-1}$







Normalized Laplacian

- The normalized Laplacian is another popular graph matrix
- Each weight $W_{i,j}$ is normalised by $\frac{1}{\sqrt{d_i d_j}}$

$$\tilde{\mathcal{L}} := \mathbf{D}^{-\frac{1}{2}} \mathcal{L} \mathbf{D}^{-\frac{1}{2}}$$
$$(\tilde{\mathcal{L}}f)(i) = \frac{1}{\sqrt{d_i}} \sum_{j \in \mathcal{N}_i} W_{i,j} \left[\frac{f(i)}{\sqrt{d_i}} - \frac{f(j)}{\sqrt{d_j}} \right]$$

- The set of eigenvalues is $0 = \tilde{\lambda}_0 < \tilde{\lambda}_1 \leq \ldots \leq \tilde{\lambda}_{\max} \leq 2$
- The normalized Laplacian has often stability benefits





Graph Fourier Transform

 The eigenvectors of the graph Laplacian are used for defining the Graph Fourier Transform

$$\begin{array}{ll} \text{GFT} & \text{IGFT} \\ \hat{f}(\lambda_{\ell}) := \langle \mathbf{f}, \mathbf{u}_{\ell} \rangle = \sum_{i=1}^{N} f(i) u_{\ell}^{*}(i) & f(i) = \sum_{\ell=0}^{N-1} \hat{f}(\lambda_{\ell}) u_{\ell}(i) \end{array}$$

 This is analogous to the classical Fourier Transform built on eigenfunctions of the 1-D Laplace operator

$$\hat{f}(\xi) := \langle f, e^{2\pi i\xi t} \rangle = \int f(t)e^{-2\pi i\xi t}dt$$
$$-\Delta(e^{2\pi i\xi t}) = -\frac{\partial^2}{\partial t^2}e^{2\pi i\xi t} = (2\pi\xi)^2 e^{2\pi i\xi t}$$





Notion of 'frequency'

 The graph Laplacian eigenvalues and eigenvectors carry a notion of frequency







Dual representations

 Graph signals represented in either the vertex or the spectral domains (kernels, or graph Fourier multipliers)







Frequency filtering

 Analogously to classical filtering, one can perform graph spectral filtering with transfer function $\hat{h}(\lambda_{\ell})$

$$\hat{f}_{out}(\lambda_{\ell}) = \hat{f}_{in}(\lambda_{\ell})\hat{h}(\lambda_{\ell})$$
$$f_{out}(i) = \sum_{\ell=0}^{N-1} \hat{f}_{in}(\lambda_{\ell})\hat{h}(\lambda_{\ell})u_{\ell}(i)$$

- Equivalently
- $f = \hat{h}(\mathbf{C})f$ In matrix notation:

$$\hat{h}(\mathcal{L}) := \mathbf{U} \begin{bmatrix} \hat{h}(\lambda_0) & \mathbf{0} \\ & \hat{h}(\lambda_0) \end{bmatrix} \mathbf{U}^{\mathrm{T}}$$
$$\begin{pmatrix} \hat{h}(\lambda_{N-1}) \end{bmatrix} \mathbf{U}^{\mathrm{T}}$$





Filtering in the vertex domain

• Linear combination of values at neighbour vertices

$$f_{out}(i) = b_{i,i} f_{in}(i) + \sum_{j \in \mathcal{N}(i,K)} b_{i,j} f_{in}(j)$$

K

- localized linear transform

• Example: polynomial filter as $\hat{h}(\lambda_{\ell}) = \sum_{k=0}^{N} a_k \lambda_{\ell}^k$ $f_{out}(i) = \sum_{\ell=0}^{N-1} \hat{f}_{in}(\lambda_{\ell}) \hat{h}(\lambda_{\ell}) u_{\ell}(i)$ $= \sum_{j=1}^{N} f_{in}(j) \sum_{k=0}^{K} a_k \left(\mathcal{L}^k\right)_{i,j} \longrightarrow b_{i,j} := \sum_{k=d_{\mathcal{G}}(i,j)}^{K} a_k \left(\mathcal{L}^k\right)_{i,j}$





Translation on graphs

- The classical translation $(T_u f)(t) := f(t u)$ does not generalise to non-regular graphs
- A generalized translation operator on graphs can still be defined as

 $T_n:\mathbb{R}^N\to\mathbb{R}^N$

$$(T_n g)(i) := \sqrt{N}(g * \delta_n)(i) = \sqrt{N} \sum_{\ell=0}^{N-1} \hat{g}(\lambda_\ell) u_\ell^*(n) u_\ell(i)$$
$$\delta_n(i) = \begin{cases} 1 & \text{if } i = n\\ 0 & \text{otherwise} \end{cases} \quad (f * h)(i) := \sum_{\ell=0}^{N-1} \hat{f}(\lambda_\ell) \hat{h}(\lambda_\ell) u_\ell(i)$$





Translation example



Translation of the heat kernel to different locations of the Minnesota graph







Transforms on graphs

- Localized transforms are ideal to analyse graph signals
 - analysis properties and scalable implementations
 - GFT is unfortunately not a local transform
- Wavelet transforms are particularly interesting
 - localization in both the vertex and spectral domains
 - different designs in the vertex or the spectral domain [Shuman:2013]
 - example: Spectral Graph Wavelets [Hammond:2011]

 $\boldsymbol{\Psi}^{SGWT}: \mathbb{R}^N \to \mathbb{R}^{N(K+1)} \qquad \boldsymbol{\Psi}^{SGWT} = [\boldsymbol{\Psi}^{SGWT}_{scal}; \boldsymbol{\Psi}^{SGWT}_{t_1}; \dots; \boldsymbol{\Psi}^{SGWT}_{t_K}]$

- Dilations and translations of a band-pass kernel $\psi_{t_k,i}^{SGWT} := T_i \mathcal{D}_{t_k} \mathbf{g} = \widehat{\mathcal{D}_{t_k}g}(\mathcal{L}) \boldsymbol{\delta}_i$
- Translation of a low-pass kernel $\psi_{scal,i}^{SGWT} := T_i \mathbf{h} = \hat{h}(\mathcal{L}) \boldsymbol{\delta}_i$

• Such transforms do not explicitly adapt to the data :(





SGWT illustration



[Shuman:2013]





Data-adaptive representations

• Sparse graph signal representation



- We want to have an efficient structured representation Φ that is adapted to data: graph spectral dictionaries





Dictionary for Graph Signals

- Our objective: meaningful graph signal representations that
 - ✓ reveal relevant structural properties of the graph signals/extract important features on graphs
 - ✓ sparsely represent different classes of signals on graphs



How can we define atoms on graphs?





Sparse signal model

- Graph signals can be approximated by a small number of localized components
 - e.g., multiple processes started at different vertices







Parametric graph atoms

- A set of generating kernels $\{\widehat{g_s}(\cdot)\}_{s=1,2,...,S}$ represent the spectral characteristics of the signals
- The kernels are chosen to be smooth polynomial of degree K in order to form localized graph features

$$\hat{g}(\lambda_{\ell}) = \sum_{k=0}^{n} \alpha_k \lambda_{\ell}^k, \quad \ell = 0, ..., N - 1$$

• A graph atom is the translation of the kernel to vertex *n*

$$T_n g = \sqrt{N} (g * \delta_n) = \sqrt{N} \sum_{\ell=0}^{N-1} \sum_{k=0}^K \alpha_k \lambda_\ell^k \chi_\ell^*(n) \chi_\ell = \sqrt{N} \sum_{k=0}^K \alpha_k (\mathcal{L}^k)_n$$

 \mathcal{L} : normalized Laplacian, χ_{ℓ} : eigen







Dictionary Structure

- A parametric graph dictionary $\mathcal{D} = [\mathcal{D}_1, \mathcal{D}_2, ..., \mathcal{D}_S]$ is a concatenation of *S* subdictionaries
- Each subdictionary is built on a specific kernel

$$\mathcal{D}_s = \widehat{g_s}(\mathcal{L}) = \chi \left(\sum_{k=0}^K \alpha_{sk} \Lambda^k \right) \chi^T = \sum_{k=0}^K \alpha_{sk} \mathcal{L}^k$$

- Each atom (column of \mathcal{D}_s) corresponds to a K-hop localized pattern centered on a node of the graph, i.e.,

 $T_n g_s$





Dictionary Learning Problem

- Learning consists in computing $\{\alpha_{sk}\}_{s=1,2,\ldots,S;\ k=1,2,\ldots,K}$
- Given a set of training signals $Y = [y_1, y_2, ..., y_M] \in \mathbb{R}^{N \times M}$ on the graph \mathcal{G} , solve







Alternating optimisation

Algorithm 1 Parametric Dictionary Learning on Graphs

- 1: Input: Signal set Y, initial dictionary $\mathcal{D}^{(0)}$, target signal sparsity T_0 , polynomial degree K, number of subdictionaries S, number of iterations *iter*
- 2: Output: Sparse signal representations X, polynomial coefficients α
- 3: Initialization: $\mathcal{D} = \mathcal{D}^{(0)}$
- 4: for i = 1, 2, ..., iter do:
- 5: Sparse Approximation Step:
- 6: (a) Scale each atom in \mathcal{D} to a unit norm
- 7: (b) Update X using Sparse Coding
- 8: (c) Rescale X, \mathcal{D} to recover the polynomial structure
- 9: Dictionary Update Step:
- 10: Compute the polynomial coefficients α and update the dictionary

11: **end for**





Properties of the dictionary

- By construction, the dictionary is a frame
- The coherence depends on the graph

$$\phi \le \max_{n \ne n', s, s'} \frac{\nu (\sum_{\ell=0}^{N-1} |\widehat{g_s}(\ell) \widehat{g_{s'}}(\ell)|^2)^{1/2} \|deg\|^2}{|\widehat{g_s}(\lambda_0)| |\widehat{g'_s}(\lambda_0)| \sqrt{deg_n} \sqrt{deg_{n'}}}$$

- Parametric structure: easy dictionary description
 - it has only (K+1)S parameters
- Polynomial form: efficient implementation, esp. when the graph is sparse
 - Both forward and adjoint operators can be efficiently applied

$$\mathcal{D}^T y = \sum_{s=1}^S \sum_{k=0}^K \alpha_{sk} \mathcal{L}^k y \qquad \qquad \mathcal{D}\mathcal{D}^T y = \sum_{s=1}^S \widehat{g_s}^2(\mathcal{L}) y$$





Recovery on synthetic data







Approximation on synthetic data







Real World Datasets

	Flickr		Traffic		Brain
V	Nodes: 245 vertices in the Trafalgar Square (London), each representing a geographical area	~	Nodes: 439 detector stations in Alameda County, CA	v	Nodes: 88 brain regions of contiguous voxels
V	Edges : Assign edge when distance < 30m	V	Edges : Assign edge when distance < 13km	V	Edges : Assign edge if anatomical distance < 40 mm
V	Graph signals: Daily number of distinct users that took photos between Jan. 2010 and June 2012	V	Graph signals: Daily number of bottlenecks (in minutes) between Jan. 2007 to May. 2013	v	Graph signals: fMRI signals acquired on five subjects, in different states, 1290 signals per subject
	Provide and		400 Filerito Walnut Creek Walnut Creek W		





Approximation performance



- As the sparsity level increases, the localisation property becomes beneficial
- The polynomial dictionary is able to learn local patterns in areas of the graph that do not show up in the training signals





Examples of Learned Atoms

• Most common atoms in OMP expansions







Applications of graph dictionaries

- Graph dictionaries apply to many sparse problems
 - sparsity prior on graphs
 - helpful when smooth priors are insufficient
- Graph dictionaries also define features on graphs
 - learning or clustering applications
- By construction, spectral graph dictionaries lead to effective implementations
 - distributed processing applications in networks









3D Point Cloud Sequences



- No explicit spatio-temporal geometry structure
 - Frames have different number of points
 - No association between points over time
- Graph localised features can be used to match frames





Graph-based Motion Estimation



Graph SP representation used for motion estimation and compensation, and eventually predictive coding







Motion Compensation - Example



(a) reference + target frame

(b) sparse correspondences between frames

(c) motion compensated reference frame + target frame

 The sparse set of matching vertices are accurate and welldistributed in space





3D Color Compression Results



Compression of 10 frames in each sequence using predictive coding [Zhang:2014]





Distributed processing

- Graph signal: function on a network
 - e.g., measurement in a wireless sensor network
- Signal processing tasks
 - denoising, reconstruction, inference
- Communication constraints
 - centralised processing is not possible
 - no node fully knows the signal
 - only local communication









Processing on graphs: denoising

Denoising (LASSO) problem

$$x^* = \min_{x} \|y - \mathcal{D}x\|_2^2 + \kappa \|x\|_1$$

Iterative soft thresholding solution

$$\mathcal{S}_{\kappa\tau} = \begin{cases} 0 & \text{if } |z| \le \mu\tau\\ z - \operatorname{sgn}(z)\kappa\tau & \text{otherwise} \end{cases}$$

$$x^{t} = S_{\kappa\tau} \left(x^{(t-1)} + 2\tau \mathcal{D}^{T} \left(y - \mathcal{D} x^{(t-1)} \right) \right), \ t = 1, 2, \dots$$

 Distributed solution feasible as the dictionarybased operators can be distributed!





Illustration: adjoint operator



Distributed computation of $\mathcal{D}^{\mathcal{T}} y$

Similar operations for the computation of $\mathcal{D}x$ and $\mathcal{D}\mathcal{D}^{\mathcal{T}}y$







Denoising experiments







The graph learning problem



Challenge:

- How to define models of relationships between signals and graph?
- How to learn graphs that enforce desirable properties of graph signals?





Factor analysis framework

 Graph signal observations could be represented explained by unobserved latent variables



representation matrix (Eigenvector matrix of graph Laplacian)





Statistical model

$$x = \chi h + u_x + \epsilon$$

- Gaussian prior on latent variable $h \sim \mathcal{N}(0, \Lambda^{\dagger})$ with Λ^{\dagger} the pseudo-inverse of the eigenvalue matrix Λ of the graph Laplacian L
- Probabilities given as

$$\begin{split} p(x|h) &\sim \mathcal{N}(\chi h + u_x, \sigma_{\epsilon}^2 I_n), \\ p(x) &\sim \mathcal{N}(u_x, L^{\dagger} + \sigma_{\epsilon}^2 I_n) \quad \text{with} \quad L^{\dagger} = \chi \Lambda^{\dagger} \chi^T \end{split}$$

• χ : eigenvector of covariance of x

$$L^{\dagger} + \sigma_{\epsilon}^2 I_n = \chi (\Lambda^{\dagger} + \sigma_{\epsilon}^2 I_n) \chi^T$$





'Classical' regularisation problem

If
$$u_x = 0$$

 $h_{MAP}(x) := \arg \max_h p(h|x) = \arg \max_h p(x|h)p(h)$
 $h_{MAP}(x) = \arg \min_h (-\log p_E(x - \chi h) - \log p_H(h))$
 $h_{MAP}(x) = \arg \min_h \left(-\log e^{-(x - \chi h)^T (x - \chi h)} - \alpha \log e^{-h^T \Lambda h} \right)$
 $h_{MAP}(x) = \arg \min_h ||x - \chi h||_2^2 + \alpha h^T \Lambda h$
smoothness term
 $h^T \Lambda h = (\chi^T x)^T \Lambda \chi^T x = x^T \chi \Lambda \chi^T x = x^T L x$





Graph learning problem

• When the graph is unknown,

$$\begin{split} \min_{\chi,\Lambda,h} ||x - \chi h||_2^2 + \alpha \ h^T \Lambda h \\ \min_{L,y} ||x - y||_2^2 + \alpha \ y^T Ly. \end{split}$$

$$\min_{L \in \mathbb{R}^{n \times n}, Y \in \mathbb{R}^{n \times p}} ||X - Y||_F^2 + \alpha \operatorname{tr}(Y^T L Y) + \beta ||L||_F^2,$$

s.t. $\operatorname{tr}(L) = n,$
 $L_{ij} = L_{ji} \leq 0, \ i \neq j,$
 $L \cdot \mathbf{1} = \mathbf{0},$





Graph learning algorithm

Alternating optimisation

Step 1: $\arg\min_{L} \alpha tr(Y^{T}LY) + \beta ||L||_{F}^{2}$ s.t. $tr(L) = n, \quad L = L^{T}, \quad off(L) \le 0, \quad L\mathbf{1} = \mathbf{0}$

Step 2: $\arg\min_{Y} ||X - Y||_F^2 + \alpha tr(Y^T L Y)$

Both steps are convex optimization problems :)

Algorithm 6 Graph Learning for Smooth Signal Representation (GL-SigRep)

- 1: Input: Input signal X, number of iterations *iter*, α , β
- 2: Output: Output signal Y, graph Laplacian L
- 3: Initialization: Y = X
- 4: for t = 1, 2, ..., iter do:
- 5: Step to update Graph Laplacian L:
- 6: Solve the optimization problem of Eq. (6.24) to update L.
- 7: Step to update Y:
- 8: Solve the optimization problem of Eq. (6.25) to update Y.
- 9: end for

10: $L = L^{iter}, Y = Y^{iter}$.





Results: Synthetic data







Analysis of meteorological data

• The learned graph can be used for partitioning entities into several clusters, e.g., [Ng, NIPS'01]











Learning brain networks







Summary

- Graph Signal Processing: joint consideration of the signal and the structure
- Structured adaptive representations lead to computationally effective operators
- In general, the graph is not known!

Many open challenges :)







References

- D. I Shuman, S. K. Narang, P. Frossard, A. Ortega, and P. Vandergheynst, "The emerging field of signal processing on graphs: Extending high dimensional data analysis to networks and other irregular domains," IEEE Signal Process. Mag., vol. 30, no. 3, pp. 83–98, May 2013
- D. Thanou, D. I Shuman, and P. Frossard, "Learning Parametric Dictionaries for Signals on Graphs", IEEE Trans. Signal Process., vol. 62, no. 15, Aug. 2014
- D. Thanou, and P. Frossard, "Multi-graph learning of spectral graph dictionaries", IEEE ICASSP 2015 (best student paper award).
- X. Zhang, X. Dong, and P. Frossard, "Learning of structured graph dictionaries," in Proc. IEEE Int. Conf. Acc., Speech, and Signal Process., Kyoto, Japan, Mar. 2012, pp. 3373 3376.
- D. Thanou, P. A. Chou, and P. Frossard, "Graph-based compression of dynamic 3D point cloud sequences," IEEE Transactions on Image Processing, April 2016
- X. Dong, D. Thanou, P. Frossard, P. Vandergheynst, "Learning Laplacian Matrix in Smooth Graph Signal Representations," submitted to IEEE Transactions on Signal Processing, 2015
- D. Thanou and P. Frossard, "Distributed Signal Processing with Graph Spectral Dictionaries", Proceedings of the 53rd Annual Allerton Conference on Communication, Control, and Computing, UIUC, IL, USA, October 2015.



