Spectral Graph Dictionaries

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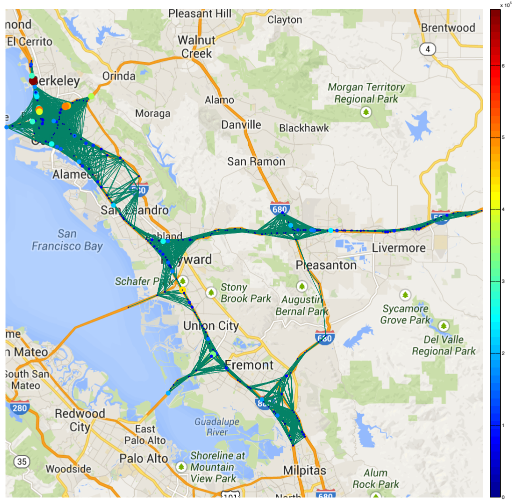
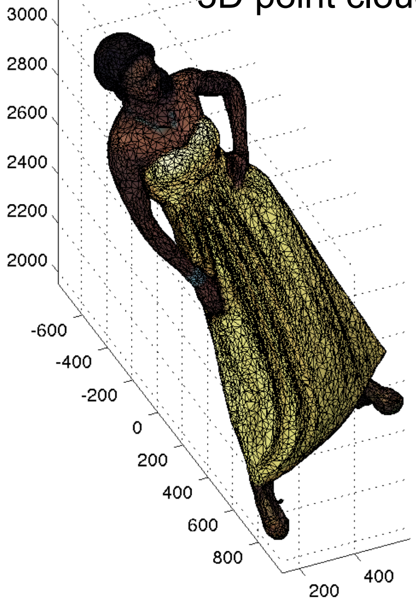
(Joint work with Dorina Thanou and David Shuman)

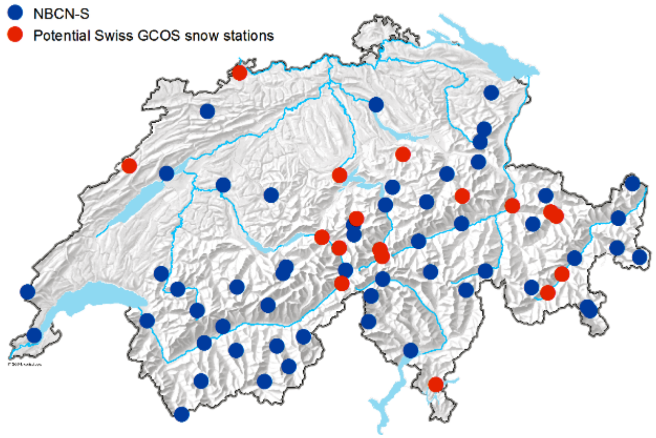
Structured data



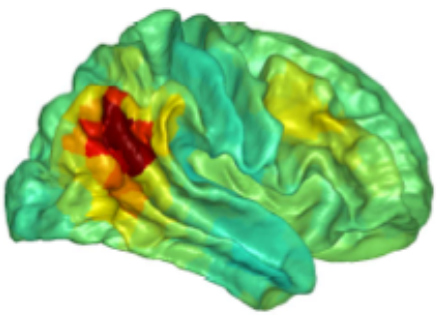
Traffic bottlenecks

3D point clouds

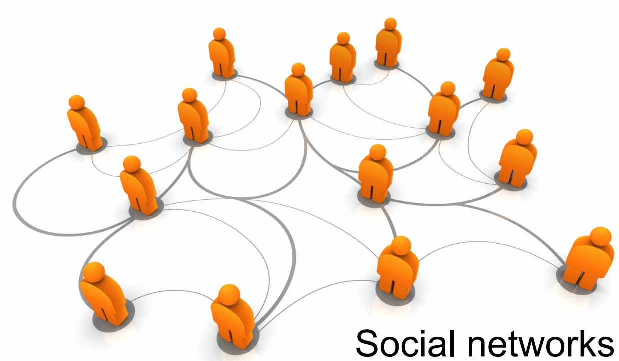




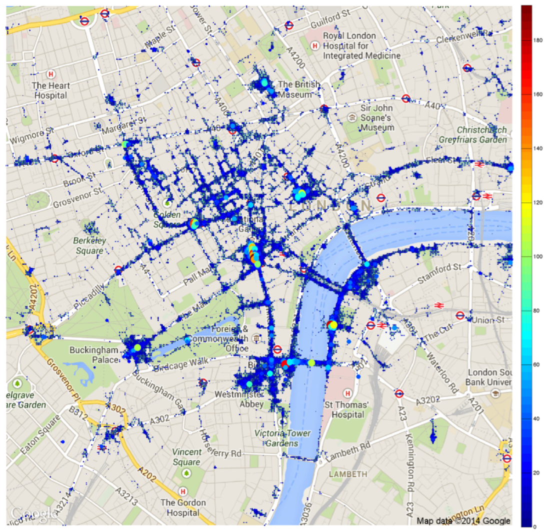
Sensor networks



Brain signals



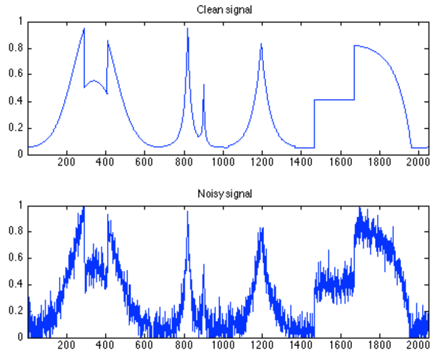
Social networks



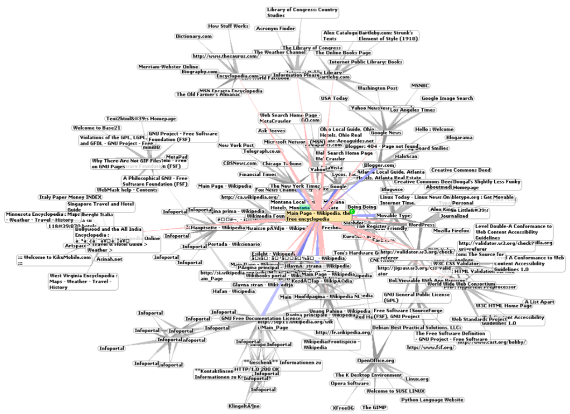
Mobility patterns

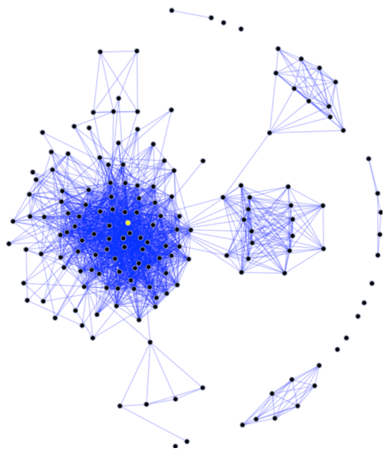
Structured, but irregular data …

- Traditional signal processing in Euclidean space



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





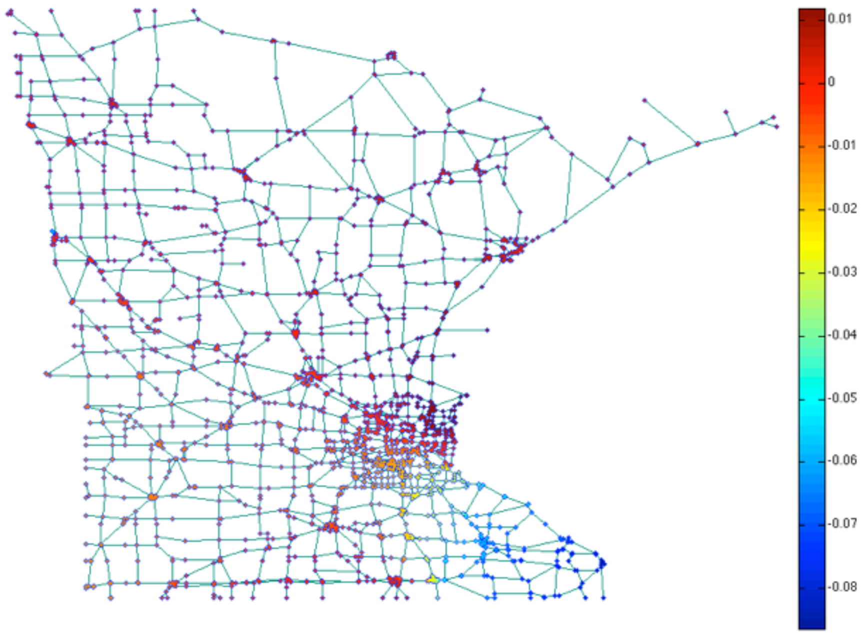
Challenges on graphs

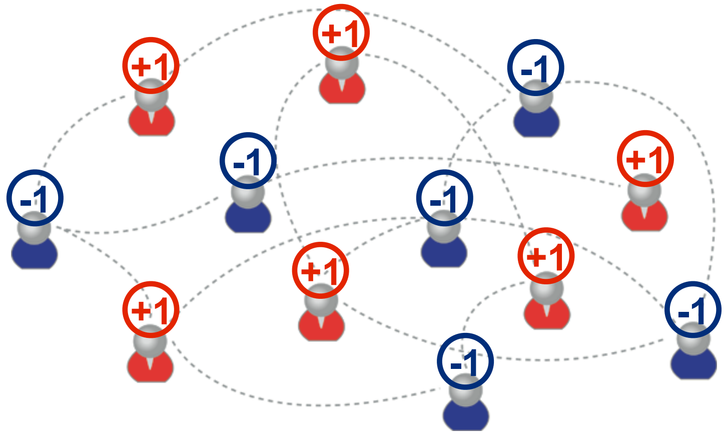
- Data processing on irregular domains raises important questions:
  - how to incorporate the graph structure into *localised* transforms?
  - how to leverage invaluable intuitions from Euclidian framework?
  - how to design computationally effective methods?

- Sparsity is very helpful in classical settings - and for graphs?
  - could we define sparse representations on graphs?
  - could we build efficient dictionaries adapted to graphs?

Signal Processing on Graphs

- Objective: to process, analyse, reconstruct signals that live on networks or irregular structures



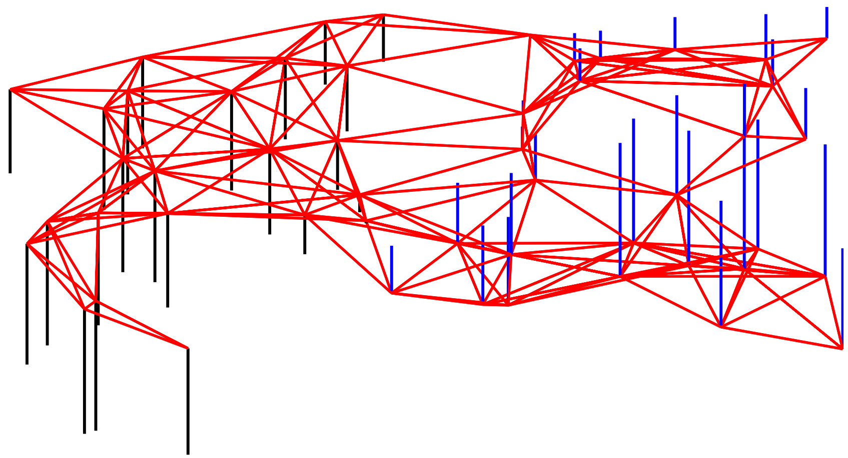


- Framework: emerging field of graph signal processing
  - algebraic and spectral graph theoretic concepts
  - harmonic analysis

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 $\mathbf{D}$: diagonal matrix with sum of weights of incident edges
  - Laplacian matrix $\mathcal{L}$: difference operator defined based on $\mathbf{W}$

(Unormalized) Laplacian

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

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

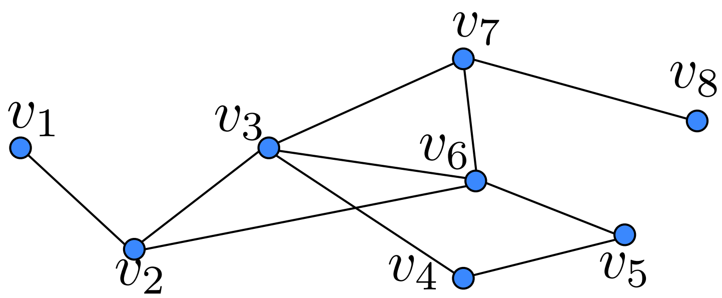
- It is a real symmetric matrix
- It has a complete set of eigenvectors $\{\mathbf{u}_\ell\}_{\ell=0,1,\ldots,N-1}$
- The eigenvectors are associated with real, nonnegative eigenvalues $\{\lambda_\ell\}_{\ell=0,1,\ldots,N-1}$

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

- Its spectrum is defined as $\sigma(\mathcal{L}) := \{\lambda_0, \lambda_1, \ldots, \lambda_{N-1}\}$

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

Laplacian example



$$G = \{V, E\}$$

$$D = diag(degree(v_1) \quad \ldots \quad degree(v_n))$$

$$\mathcal{L} := \mathbf{D} - \mathbf{W}$$

$$\begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix} \Rightarrow \begin{pmatrix} 1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 3 & -1 & 0 & 0 & -1 & 0 & 0 \\ 0 & -1 & 4 & -1 & 0 & -1 & -1 & 0 \\ 0 & 0 & -1 & 2 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & -1 & 0 & -1 & 4 & -1 & 0 \\ 0 & 0 & -1 & 0 & 0 & -1 & 3 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 \end{pmatrix}$$

$\mathbf{W}$ $\qquad$ $\mathcal{L}$

- Symmetric
- Off-diagonal entries non-positive
- Rows sum up to zero
- Has a complete set of orthonormal eigenvectors: $L = \chi \Lambda \chi^T$
  $0 = \lambda_0 < \lambda_1 \leq \ldots \leq \lambda_{n-1}$

Normalized Laplacian

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

$$\tilde{\mathcal{L}} := \mathbf{D}^{-\frac{1}{2}} \mathcal{L} \mathbf{D}^{-\frac{1}{2}}$$

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

- 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

GFT

$$\hat{f}(\lambda_\ell) := \langle \mathbf{f}, \mathbf{u}_\ell \rangle = \sum_{i=1}^{N} f(i) u_\ell^*(i)$$

IGFT

$$f(i) = \sum_{\ell=0}^{N-1} \hat{f}(\lambda_\ell) u_\ell(i)$$

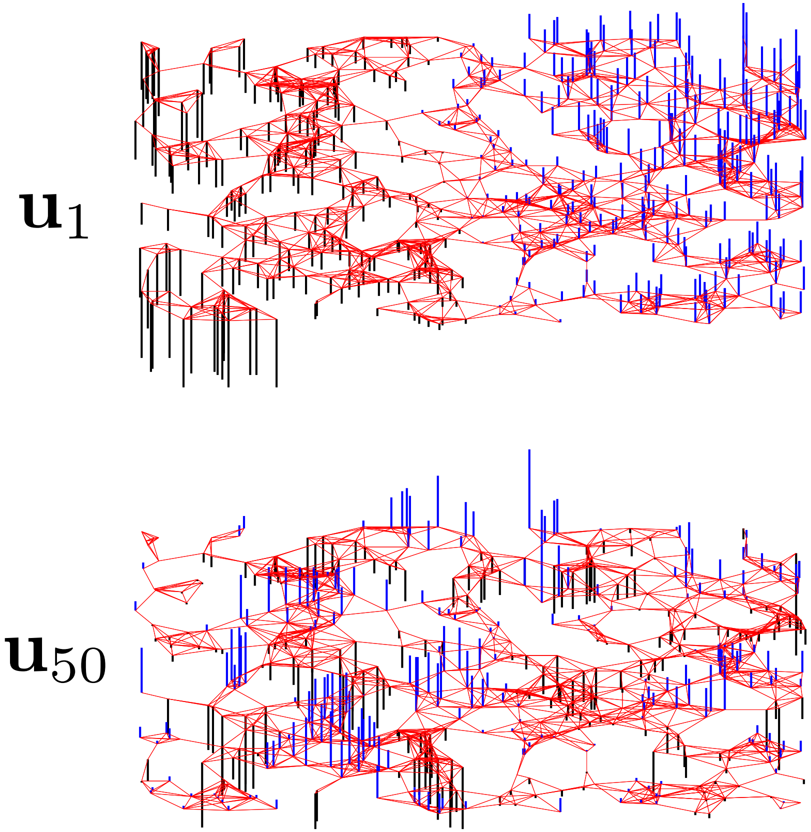
- This is analogous to the classical Fourier Transform built on eigenfunctions of the 1-D Laplace operator

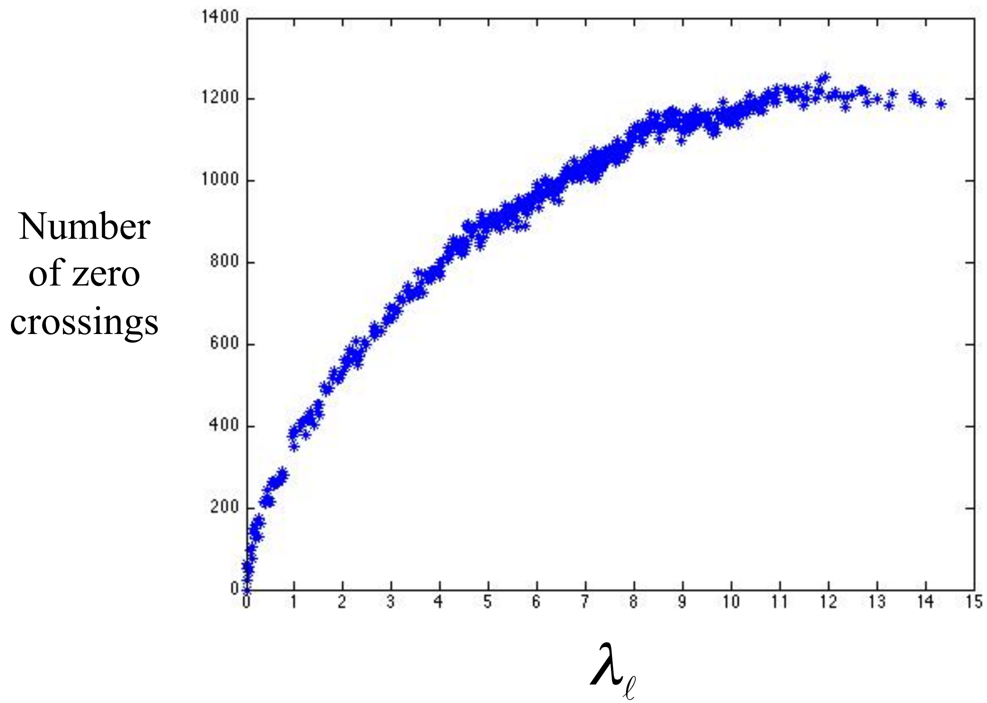
$$\hat{f}(\xi) := \langle f, e^{2\pi i \xi t} \rangle = \int_{\mathbb{R}} f(t) e^{-2\pi i \xi t} dt$$

$$-\Delta(e^{2\pi i \xi t}) = -\frac{\partial^2}{\partial t^2} e^{2\pi i \xi t} = (2\pi\xi)^2 e^{2\pi i \xi t}$$

Notion of 'frequency'

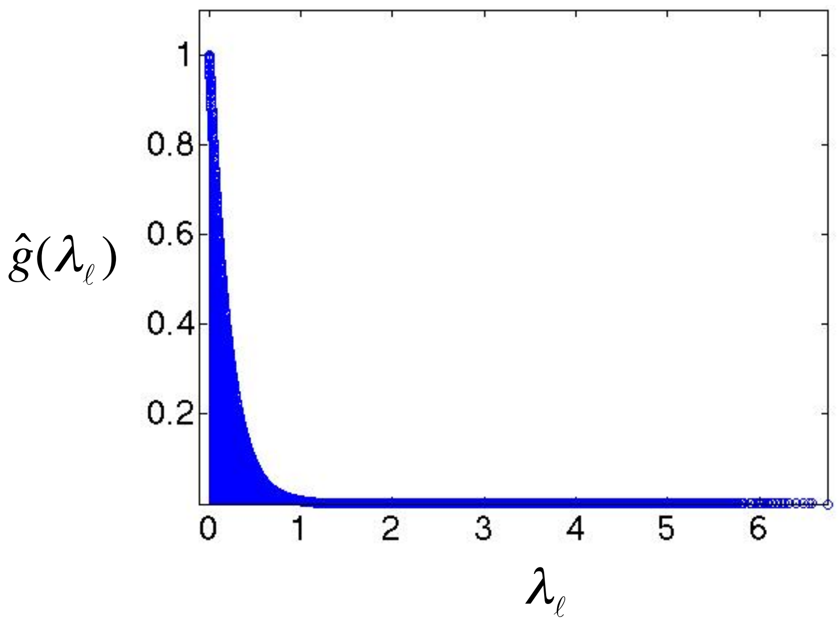
- The graph Laplacian eigenvalues and eigenvectors carry a notion of frequency



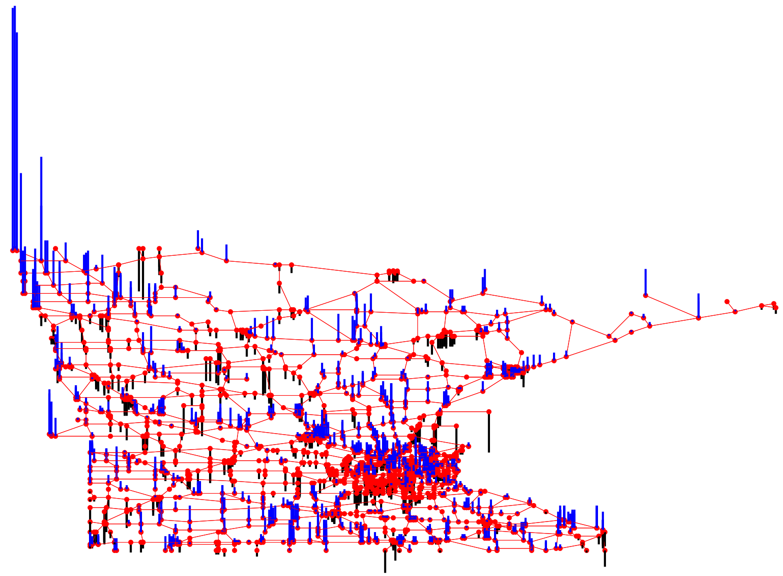


Dual representations

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



$$\hat{g}(\lambda_\ell) = e^{-5\lambda_\ell}$$



$$g(n) \xleftarrow{IGFT} \hat{g}(\lambda_\ell)$$

Local Smoothness

- **Assumption**: strong interplay between signal and graph
  - Signal analysis driven by data structure
- Local smoothness at vertex i

$$\|\nabla_i \mathbf{f}\|_2 := \left[\sum_{j \in \mathcal{N}_i} W_{i,j} \left[f(j) - f(i) \right]^2 \right]^{\frac{1}{2}}$$

  - with the gradient $\nabla_i \mathbf{f} := \left[\left\{ \sqrt{W_{i,j}} \left[f(j) - f(i) \right] \right\}_{\text{for } j \in \mathcal{V} \text{ s.t. } e=(i,j) \in \mathcal{E}} \right]$

Global Smoothness

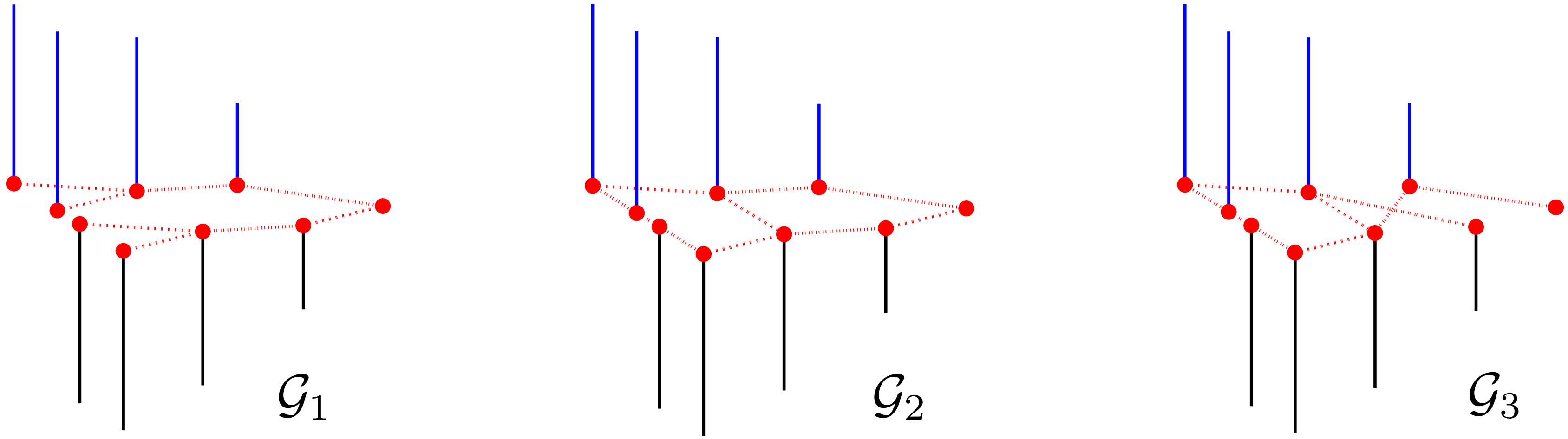
- **Assumption**: strong interplay between signal and graph
  - Signal analysis driven by data structure
- Global smoothness

$$S_p(\mathbf{f}) := \frac{1}{p} \sum_{i \in V} \|\nabla_i \mathbf{f}\|_2^p = \frac{1}{p} \sum_{i \in V} \left[\sum_{j \in \mathcal{N}_i} W_{i,j} \left[f(j) - f(i) \right]^2 \right]^{\frac{p}{2}}$$

  - with $p = 1$: total variation of the signal wrt the graph
  - with $p = 2$: graph Laplacian quadratic form

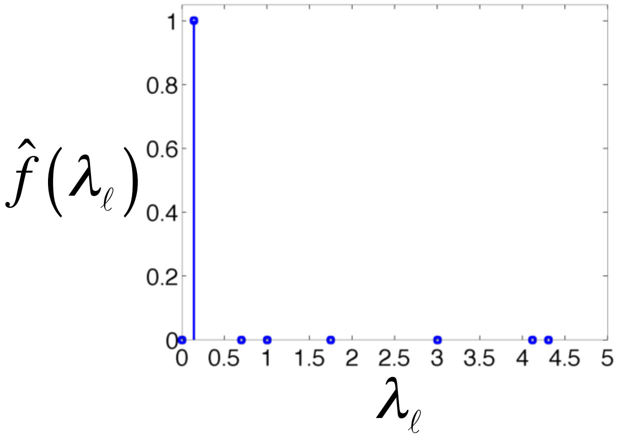
$$S_2(\mathbf{f}) = \frac{1}{2} \sum_{i \in V} \sum_{j \in \mathcal{N}_i} W_{i,j} \left[f(j) - f(i) \right]^2 = \sum_{(i,j) \in \mathcal{E}} W_{i,j} \left[f(j) - f(i) \right]^2 = \mathbf{f}^{\mathrm{T}} \mathcal{L} \mathbf{f}$$

Importance of the graph

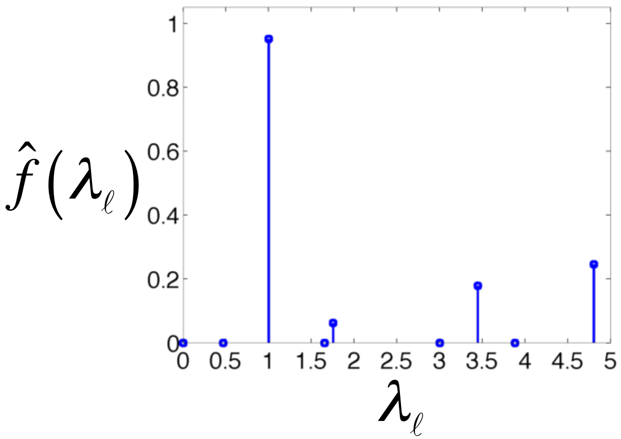


The same signal has different smoothness wrt different graphs

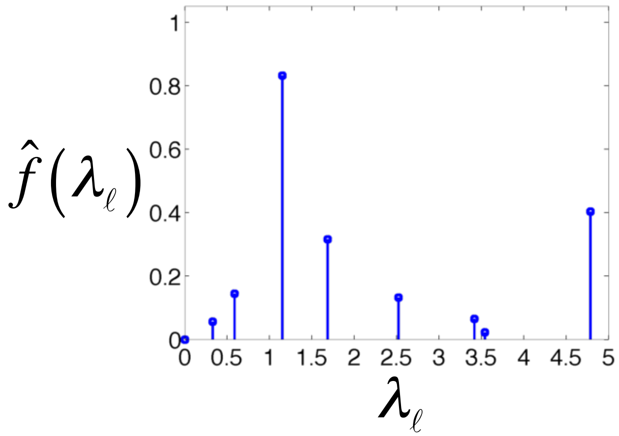
$\mathbf{f}^{\mathrm{T}}\mathcal{L}_1\mathbf{f} = 0.14$



$\mathbf{f}^{\mathrm{T}}\mathcal{L}_2\mathbf{f} = 1.31$



$\mathbf{f}^{\mathrm{T}}\mathcal{L}_3\mathbf{f} = 1.81$



Frequency filtering

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

$$\hat{f}_{out}(\lambda_\ell) = \hat{f}_{in}(\lambda_\ell)\hat{h}(\lambda_\ell)$$

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

- In matrix notation: $$\mathbf{f}_{out} = \hat{h}(\mathcal{L})\mathbf{f}_{in}$$

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

Example: Tikhonov regularization

- Consider a classical denoising problem
  - noisy signal $\mathbf{y} = \mathbf{f}_0 + \boldsymbol{\eta}$
  - smooth regularization prior $\mathbf{f}^{\mathrm{T}} \mathcal{L} \mathbf{f}$
  - optimization problem: $\underset{\mathbf{f}}{\operatorname{argmin}} \left\{ \|\mathbf{f} - \mathbf{y}\|_2^2 + \gamma \mathbf{f}^{\mathrm{T}} \mathcal{L} \mathbf{f} \right\}$
  - optimal solution

$$f_*(i) = \sum_{\ell=0}^{N-1} \left[\frac{1}{1 + \gamma \lambda_\ell} \right] \hat{y}(\lambda_\ell) u_\ell(i) \quad \text{or} \quad \mathbf{f} = \hat{h}(\mathcal{L}) \mathbf{y} \text{ with } \hat{h}(\lambda) := \frac{1}{1 + \gamma \lambda}$$

Original Noisy Gaussian filtering Graph filtering

Filtering in the vertex domain

- Linear combination of values at neighbour vertices

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

  - localized linear transform

- Example: polynomial filter as $\hat{h}(\lambda_\ell) = \sum_{k=0}^{K} a_k \lambda_\ell^k$

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

$$= \sum_{j=1}^{N} f_{in}(j) \sum_{k=0}^{K} a_k \left(\mathcal{L}^k\right)_{i,j} \rightarrow b_{i,j} := \sum_{k=d_{\mathcal{G}}(i,j)}^{K} a_k \left(\mathcal{L}^k\right)_{i,j}$$

Localization of polynomials

- **Lemma** [Hammond:2011]**:** for any two vertices *i* and *j*, if the minimal hop distance $d_{\mathcal{G}}(i,j) > s$ then $\left(\mathcal{L}^s\right)_{i,j} = 0$

  - *Proof:* $\mathcal{L}_{i,j} = 0$ if *i* and *j* are not connected

    $\left(\mathcal{L}^s\right)_{i,j} = \sum \mathcal{L}_{i,k_1}\mathcal{L}_{k_1,k_2}\dots\mathcal{L}_{k_{s-1},j}$ over s-1 length sequences

    By contra. $\left(\mathcal{L}^s\right)_{i,j} \neq 0$ $\Longrightarrow$ at least one non-zero term in the sum

    $\Longrightarrow \exists$ a path of length $d_{\mathcal{G}}(i,j) \leq s$

- Kernels defined by smooth polynomial functions of the Laplacian are localised in the vertex domain

$$\hat{h}(\lambda_\ell) = \sum_{k=0}^{K} a_k \lambda_\ell^k \quad \text{and} \quad f_{in}(j) = \begin{cases} 1 & \text{if } j = n \\ 0 & \text{otherwise} \end{cases} \quad \Longrightarrow \quad f_{out}(i) = \sum_{k=0}^{K} a_k \left(\mathcal{L}^k\right)_{i,n}$$

localized within K hops of *n* !

Convolution

- The classical convolution does not generalise to the graph settings
  - $h(t-\tau)$ does not have any equivalent on graphs

$$f_{out}(t) = \int_{\mathbb{R}} f_{in}(\tau)h(t-\tau)d\tau =: (f_{in} * h)(t)$$

- Instead, it can be defined by multiplication in the graph spectral domain

$$(f * h)(i) := \sum_{\ell=0}^{N-1} \hat{f}(\lambda_\ell)\hat{h}(\lambda_\ell)u_\ell(i)$$

Translation on graphs

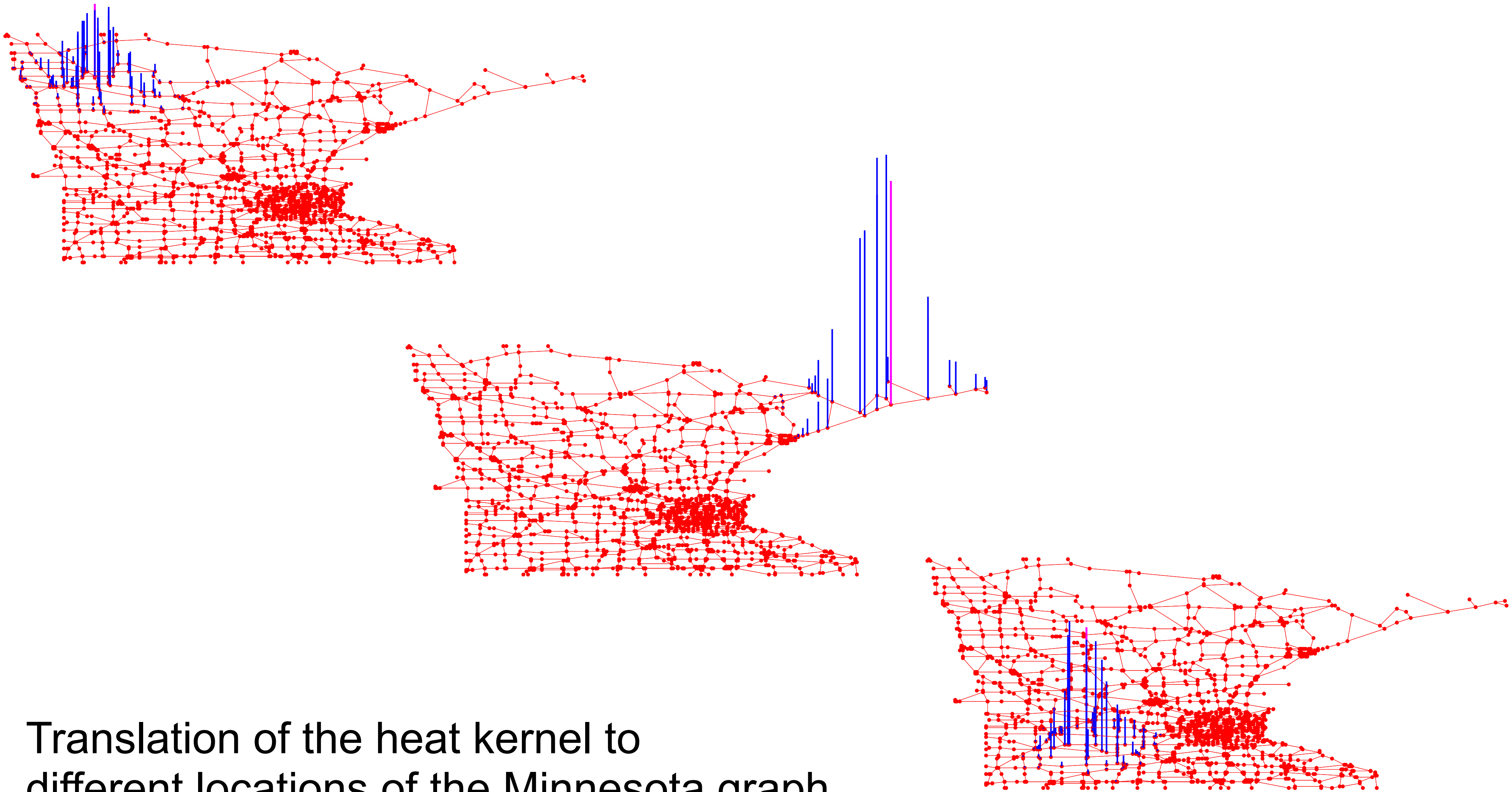
- The classical translation $(T_u f)(t) := f(t-u)$ does not generalise to non-regular graphs
- A generalized translation operator on graphs can still be defined as

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

$$(T_n g)(i) := \sqrt{N}(g * \delta_n)(i) = \sqrt{N} \sum_{\ell=0}^{N-1} \hat{g}(\lambda_\ell) u_\ell^*(n) u_\ell(i)$$

$$\delta_n(i) = \begin{cases} 1 & \text{if } i = n \\ 0 & \text{otherwise} \end{cases}$$

Translation example



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

Transforms on graphs

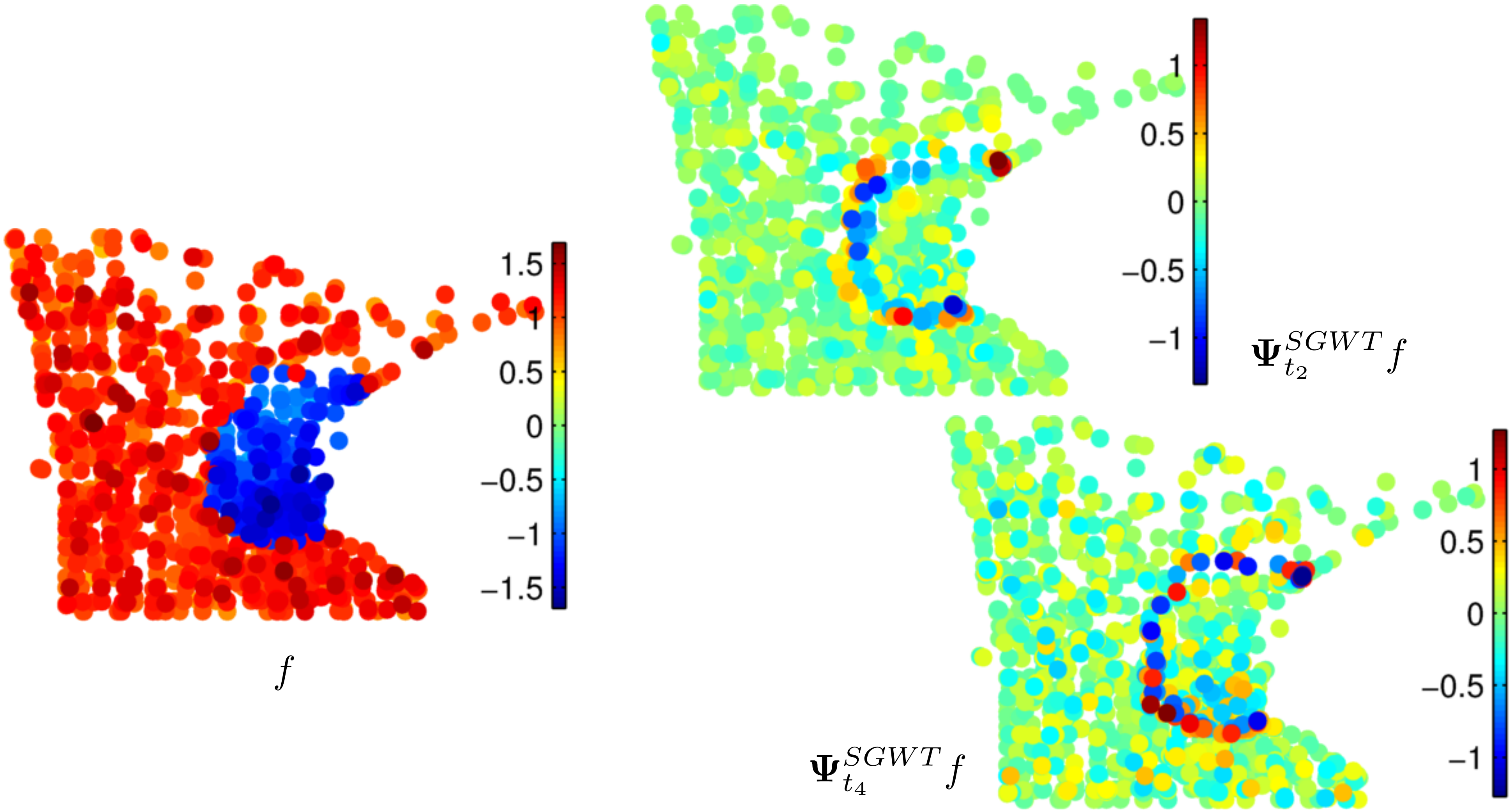
- Localized transforms are ideal to analyse graph signals
  - analysis properties and scalable implementations
- Wavelet transforms are particularly interesting
  - localization in both the vertex and spectral domains
  - different designs in the vertex or the spectral domain [Shuman:2013]
  - *Example*: Spectral Graph Wavelets [Hammond:2011]

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

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

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

SGWT illustration



[Shuman:2013]

Another SGWT illustration

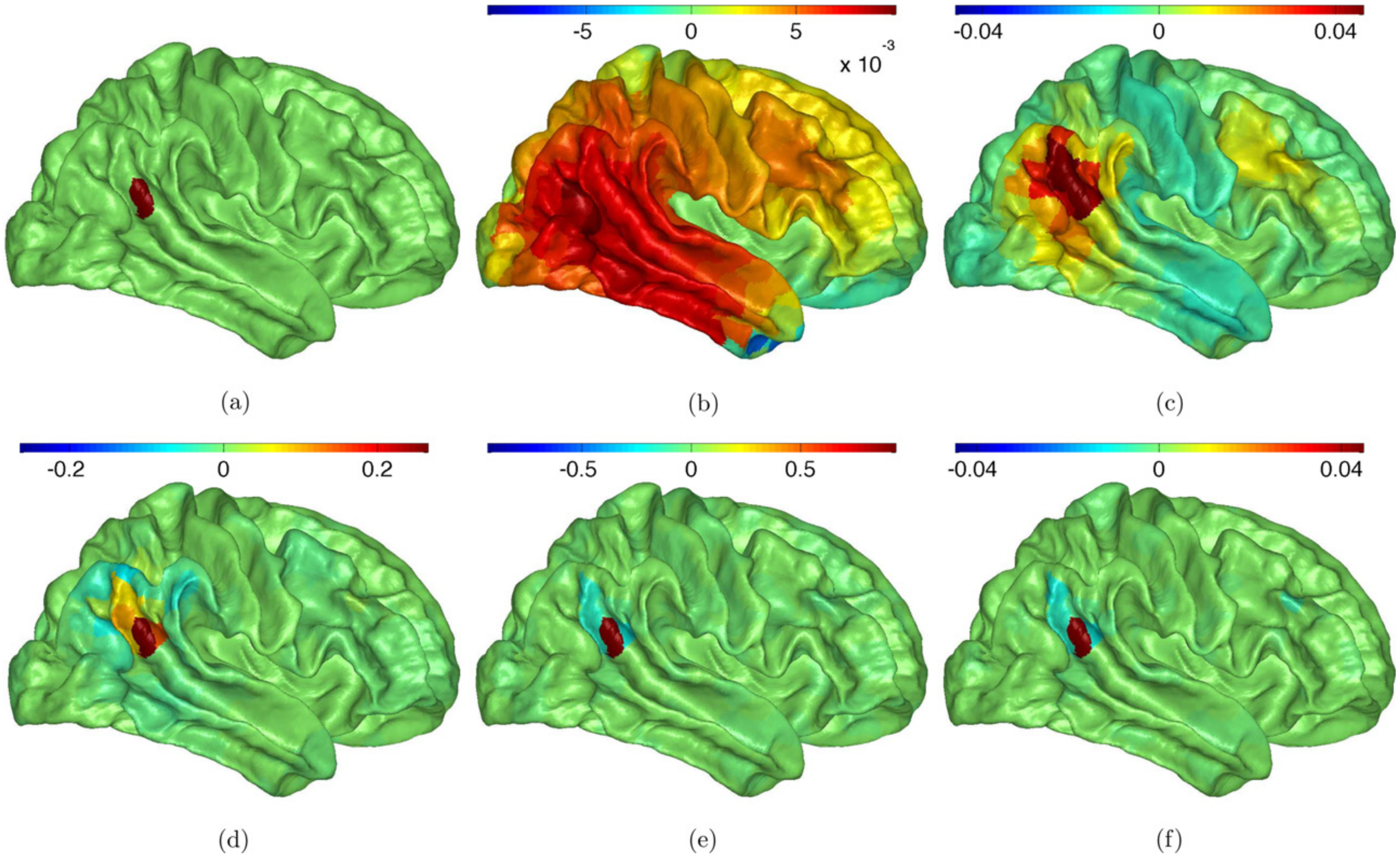
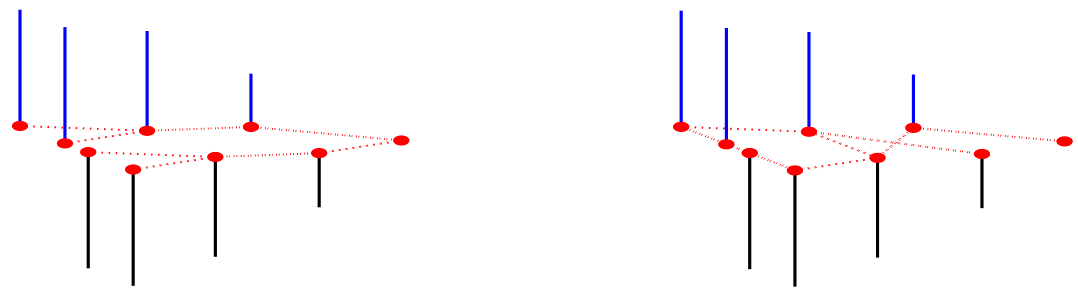


Fig. 5. Spectral graph wavelets on cerebral cortex, with $K = 50$, $J = 4$ scales. (a) ROI at which wavelets are centered, (b) scaling function, (c)–(f) wavelets, scales 1–4.

[Hammond:2011]

Better adaptation to data?

- The representation can be adapted to the data by numerical optimisation
- Dictionary Learning could be performed naively on graph signals represented as vectors
  - K-SVD, Method of Optimal Directions (MOD), etc
  - Agnostic to the graph structure :(
    - Permutation of indexes changes the dictionary
    - Different graph signals with the same representation



- Costly, highly non-structured representations :(

Bridging the gap…

- Sparse graph signal representation

$$\mathbf{y} = \mathbf{\Phi x} \quad \text{s.t.} \quad \|\mathbf{x}\|_0 \leq T_0$$

structure-based methods

$\mathbf{\Phi}$ defined
via mathematical structures
(*transforms*):
Fourier, wavelets...

not data-specific!

numerical methods

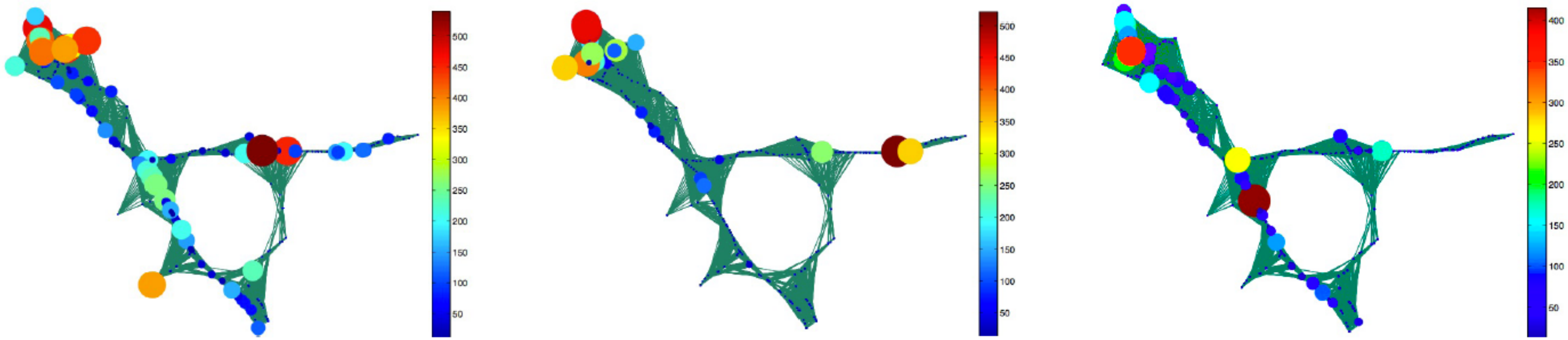
$\mathbf{\Phi}$ learned
via training samples
(*dictionary learning*):
sparse coding, MOD, K-SVD...

not graph-specific!

- We want to have an efficient structured representation $\mathbf{\Phi}$ 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



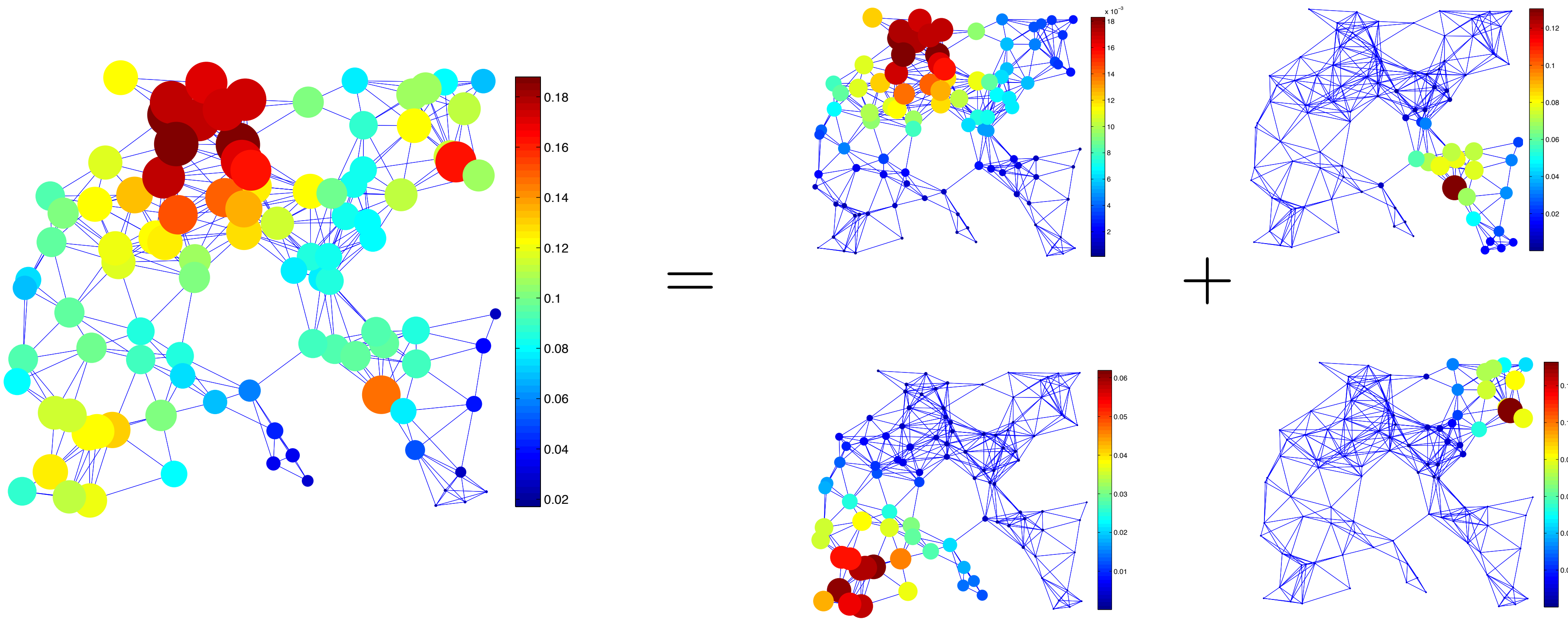
(a) Day 1 (b) Day 2 (c) Day 3

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

$e^{-\tau_1 \mathcal{L}} \delta_i, \tau_1 = 15$ $\quad$ $e^{-\tau_2 \mathcal{L}} \delta_i, \tau_2 = 3$



Parametric graph atoms

- A set of generating kernels $\{\widehat{g_s}(\cdot)\}_{s=1,2,\ldots,S}$ 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

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

- 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 : eigenvector

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.,

$$\frac{1}{\sqrt{N}} T_n g_s$$

Dictionary design constraints

- The kernels have to be nonnegative and bounded

$$0 \leq \widehat{g}_s(\lambda) \leq c, \ \forall \lambda \in [0, \lambda_{\max}]$$

$$0 \preceq \mathcal{D}_s \preceq cI, \quad \forall s \in \{1, 2, ..., S\},$$

  - Each subdictionary is positive semi-definite with max eigenvalue bounded by *c*

- The kernels should cover the full spectrum

$$c - \epsilon_1 \leq \sum_{s=1}^{S} \widehat{g}_s(\lambda) \leq c + \epsilon_2, \ \text{for all } \lambda \in [0, \lambda_{\max}]$$

$$(c - \epsilon_1)I \preceq \sum_{s=1}^{S} \mathcal{D}_s \preceq (c + \epsilon_2)I$$

Frame bounds

- With

$$\begin{cases} \mathcal{D}_s = \sum_{k=0}^{K} \alpha_{sk} \mathcal{L}^k \\ 0 \leq \widehat{g_s}(\lambda) \leq c, \ \forall \lambda \in [0, \lambda_{\max}] \\ c - \epsilon_1 \leq \sum_{s=1}^{S} \widehat{g_s}(\lambda) \leq c + \epsilon_2, \ \text{for all } \lambda \in [0, \lambda_{\max}] \end{cases}$$

the set of atoms $\{d_{s,n}\}_{s=1,2,\ldots,S,n=1,2,\ldots,N}$ form a frame

$$\frac{(c-\epsilon_1)^2}{S} \|y\|_2^2 \leq \sum_{n=1}^{N} \sum_{s=1}^{S} |\langle y, d_{s,n} \rangle|^2 \leq (c+\epsilon_2)^2 \|y\|_2^2 \qquad \forall y \in \mathbb{R}^N$$

Proof

By generalisation of the Theorem 5.6 in [Hammond:2011]

$$\sum_{n=1}^{N}\sum_{s=1}^{S}|\langle y, d_{s,n}\rangle|^2 = \sum_{\ell=0}^{N-1}|\hat{y}(\lambda_\ell)|^2\sum_{s=1}^{S}|\widehat{g_s}(\lambda_\ell)|^2, \quad \forall\lambda\in\sigma(\mathcal{L}). \tag{1}$$

From the constraints on the spectrum of kernels $\{\widehat{g_s}(\cdot)\}_{s=1,2,\dots,S}$ we have

$$\sum_{s=1}^{S}|\widehat{g_s}(\lambda_\ell)|^2 \le \left(\sum_{s=1}^{S}\widehat{g_s}(\lambda_\ell)\right)^2 \le (c+\epsilon_2)^2, \quad \forall\lambda\in\sigma(\mathcal{L}). \tag{2}$$

Moreover, from the left side of the second design constraint and the Cauchy-Schwarz inequality, we have

$$\frac{(c-\epsilon_1)^2}{S} \le \frac{\left(\sum_{s=1}^{S}\widehat{g_s}(\lambda_\ell)\right)^2}{S} \le \sum_{s=1}^{S}|\widehat{g_s}(\lambda_\ell)|^2, \quad \forall\lambda\in\sigma(\mathcal{L}). \tag{3}$$

Combining (1), (2) and (3) yields the desired result.

Dictionary Learning Problem

- Learning consists in computing $\{\alpha_{sk}\}_{s=1,2,...,S;\ k=1,2,...,K}$
- 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

$$\begin{aligned} \underset{\alpha \in \mathbb{R}^{(K+1)S},\ X \in \mathbb{R}^{SN \times M}}{\operatorname{argmin}} \quad & \{ ||Y - \mathcal{D}X||_F^2 + \mu \|\alpha\|_2^2 \} \\ \text{subject to} \quad & \|x_m\|_0 \leq T_0, \quad \forall m \in \{1, ..., M\}, \\ & \mathcal{D}_s = \sum_{k=0}^{K} \alpha_{sk} \mathcal{L}^k, \quad \forall s \in \{1, 2, ..., S\} \\ & 0 \preceq \mathcal{D}_s \preceq c, \quad \forall s \in \{1, 2, ..., S\} \\ & (c - \epsilon_1) I \preceq \sum_{s=1}^{S} \mathcal{D}_s \preceq (c + \epsilon_2) I, \end{aligned}$$

The spectral constraints guarantee that:
1. The learned kernels cover the whole spectrum
2. The dictionary is a frame

Alternating optimisation

Algorithm 1 Parametric Dictionary Learning on Graphs

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

Sparse Coding Step

- The dictionary (α) is fixed
- The sparse coding coefficients are computed with

$$\underset{X}{\operatorname{argmin}} ||Y - \mathcal{D}X||_F^2 \text{ subject to } \|x_m\|_0 \leq T_0$$

$$\forall m \in \{1, ..., M\}$$

- this can be solved by greedy algorithmms, like OMP
- it can also be solved by convex relaxation using iterative soft thresholding, for example

Dictionary Update Step

- The coefficients *X* are fixed, the dictionary is updated with

$$\underset{\alpha \in \mathbb{R}^{(K+1)S}}{\operatorname{argmin}} \left\{ ||Y - \mathcal{D}X||_F^2 + \mu \|\alpha\|_2^2 \right\}$$

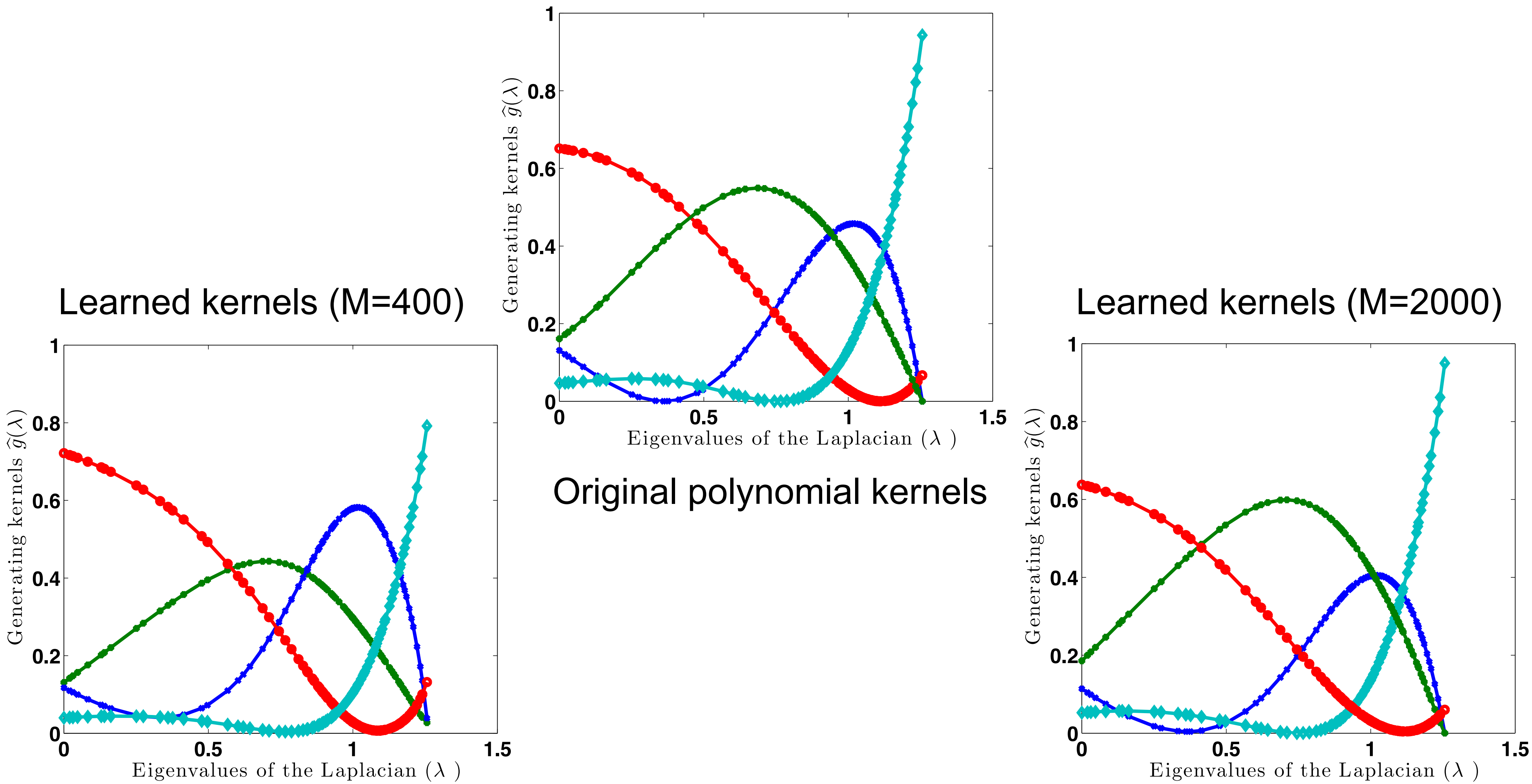
$$\text{subject to} \quad \mathcal{D}_s = \sum_{k=0}^{K} \alpha_{sk} \mathcal{L}^k, \quad \forall s \in \{1, 2, ..., S\}$$

$$0 \preceq \mathcal{D}_s \preceq cI, \quad \forall s \in \{1, 2, ..., S\}$$

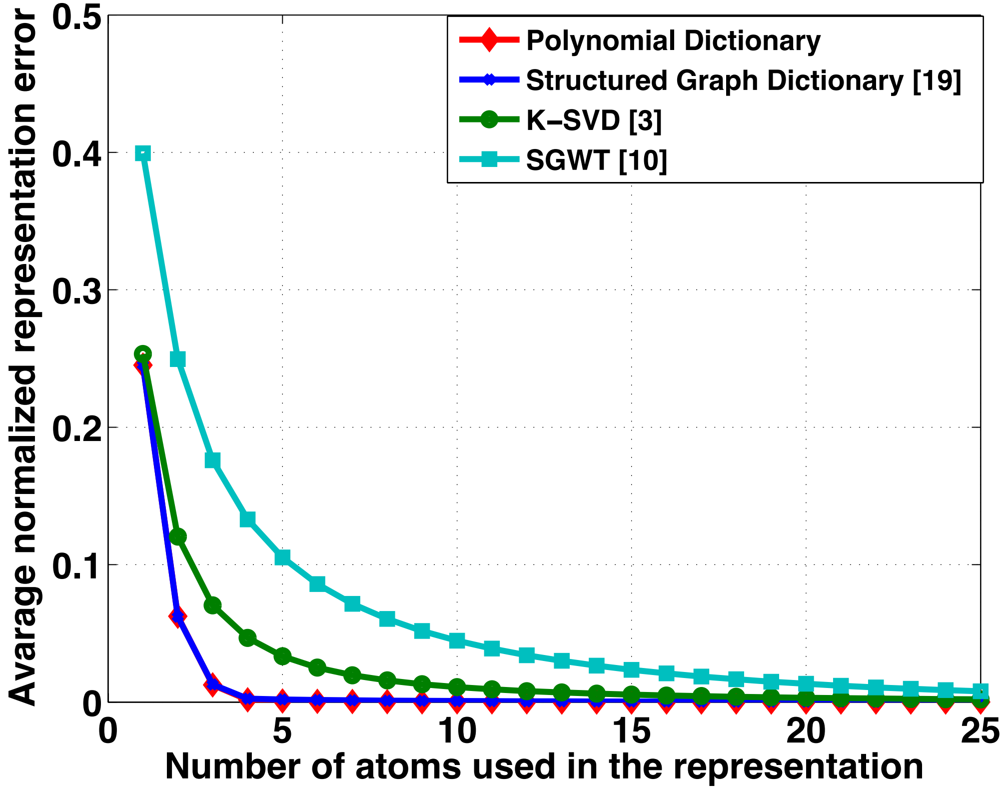
$$(c - \epsilon_1) I \preceq \sum_{s=1}^{S} \mathcal{D}_s \preceq (c + \epsilon_2) I.$$

- quadratic function with affine constraints, solved by interior point methods or ADMM

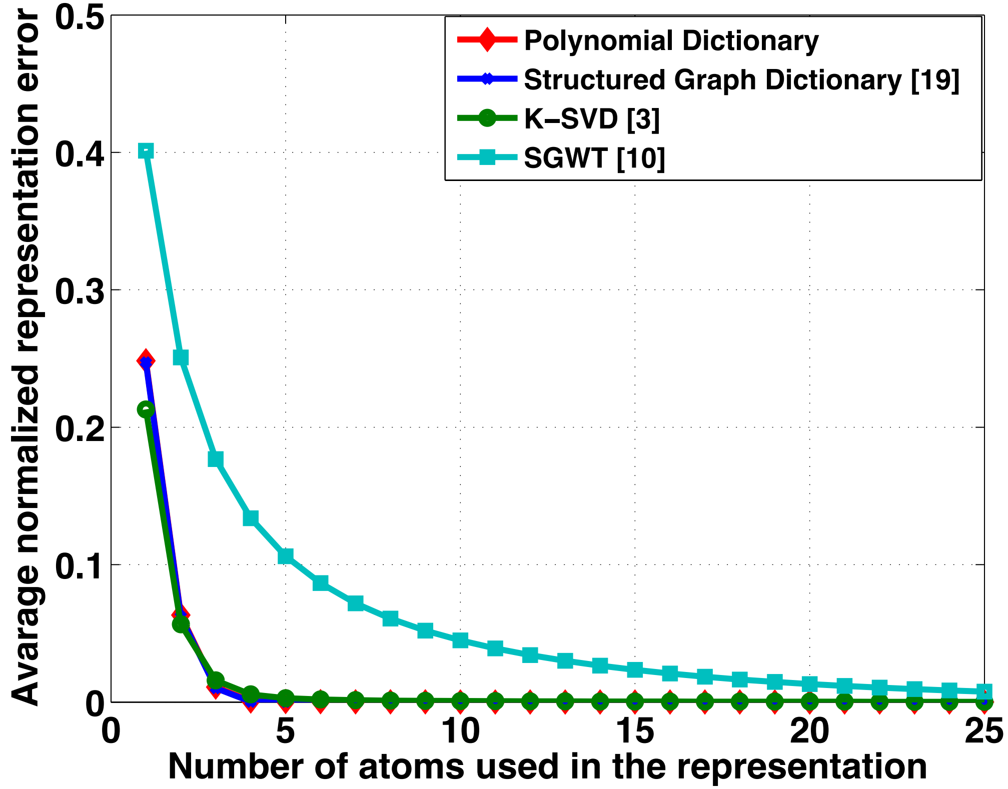
Recovery on synthetic data



Approximation on synthetic data

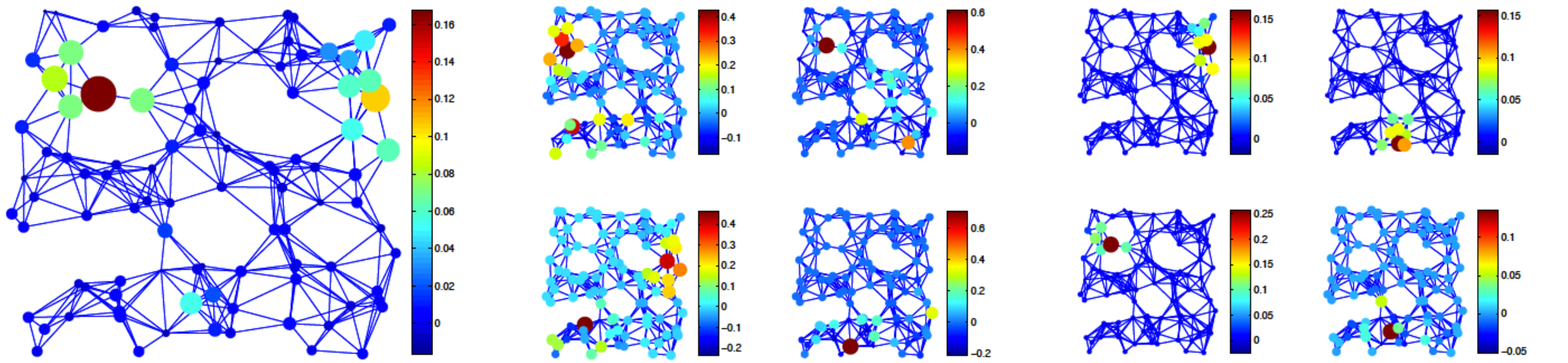


M=400



M=2000

Examples of atoms



(a) Graph Signal

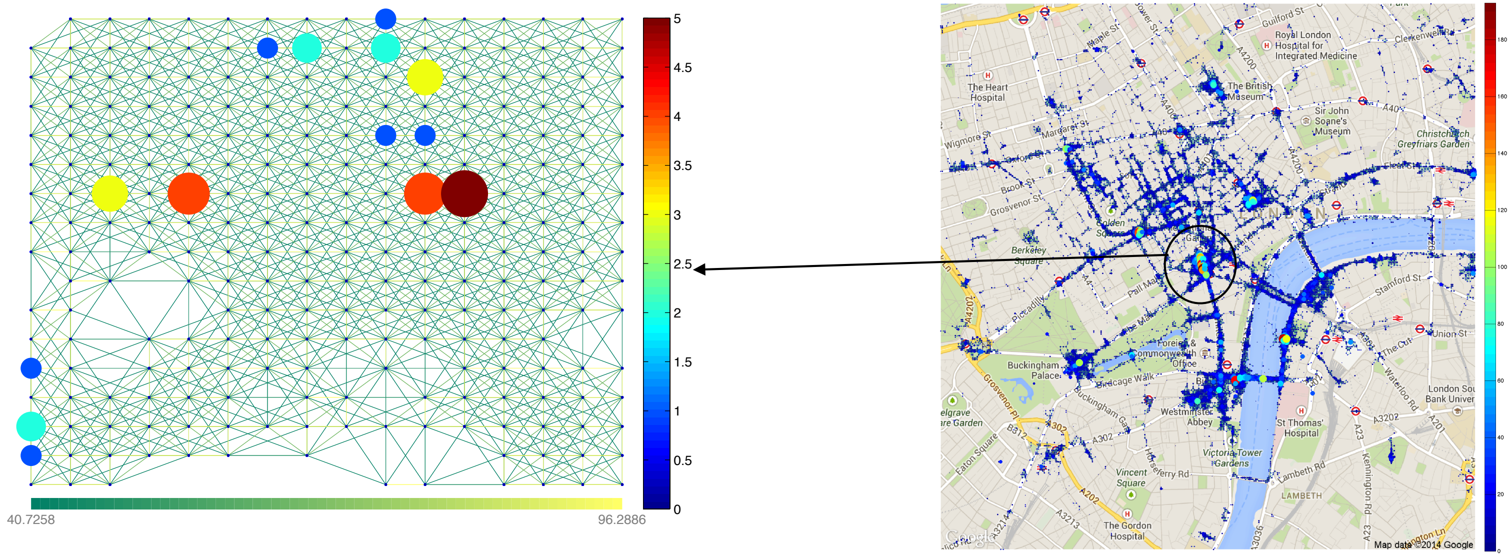
(b) Atomic decomposition with OMP in the K-SVD dictionary

(c) Atomic decomposition with OMP in the Polynomial dictionary

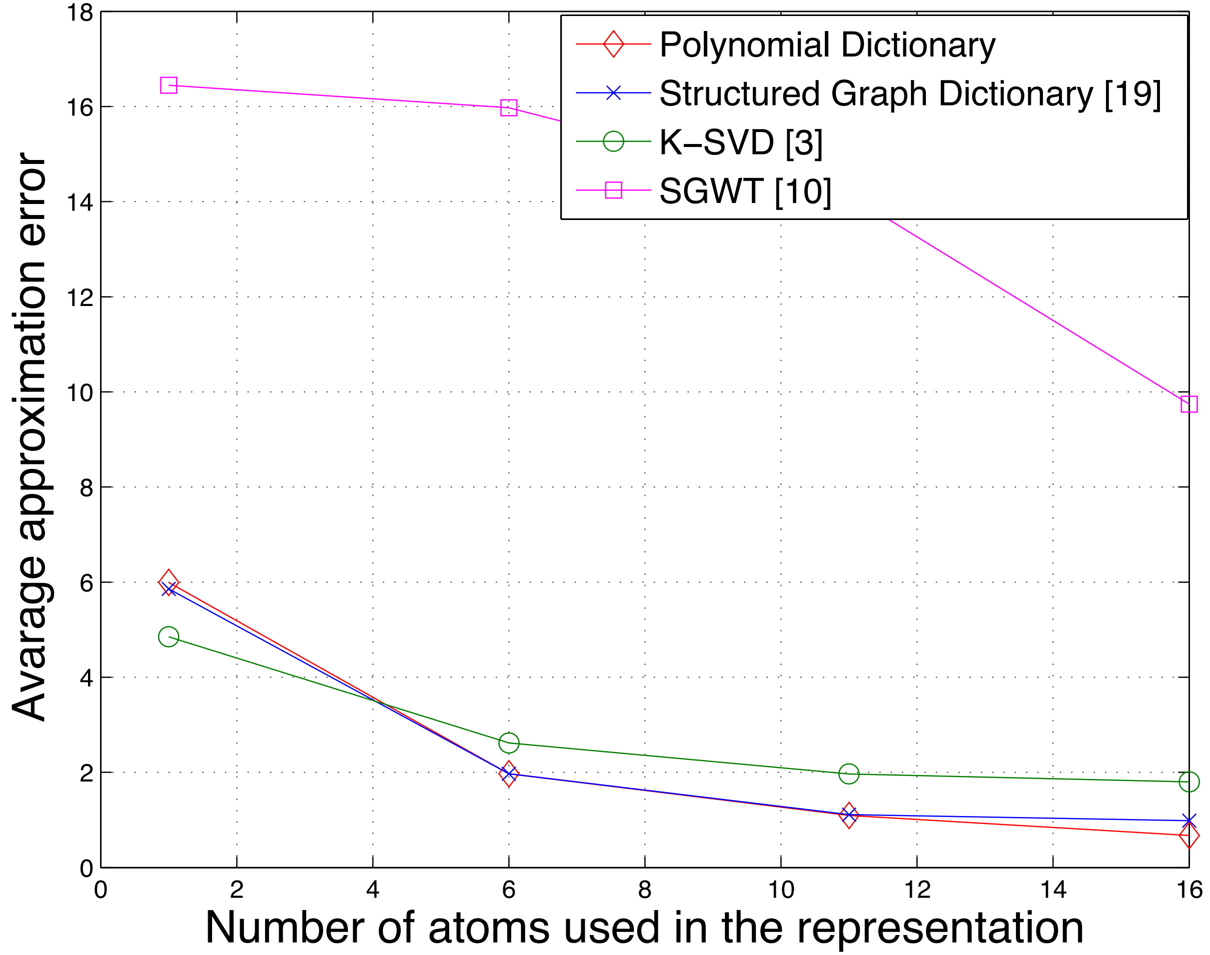
The K-SVD atoms have global support while the polynomial dictionary atoms are well localized on the graph

Flickr dataset

- Nodes: 245 vertices around Trafalgar Square (London), each representing a geographical area 10x10m^2
- Assign edges when distance < 30m
- Graph Signals: Daily number of distinct users that took photos between Jan. 2010 and June 2012

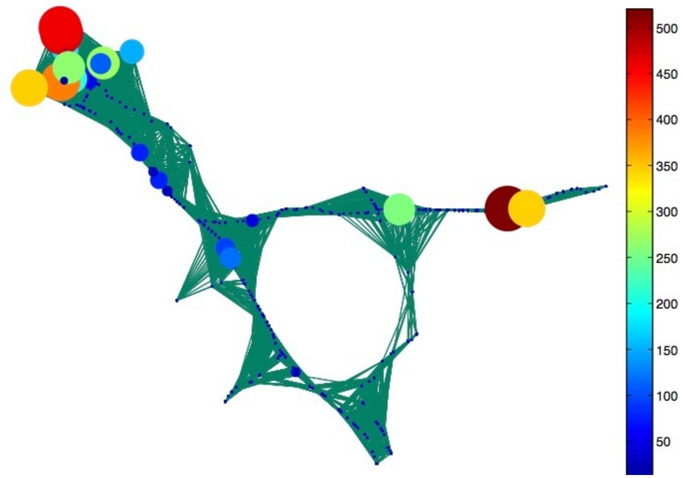


Flickr signal approximation

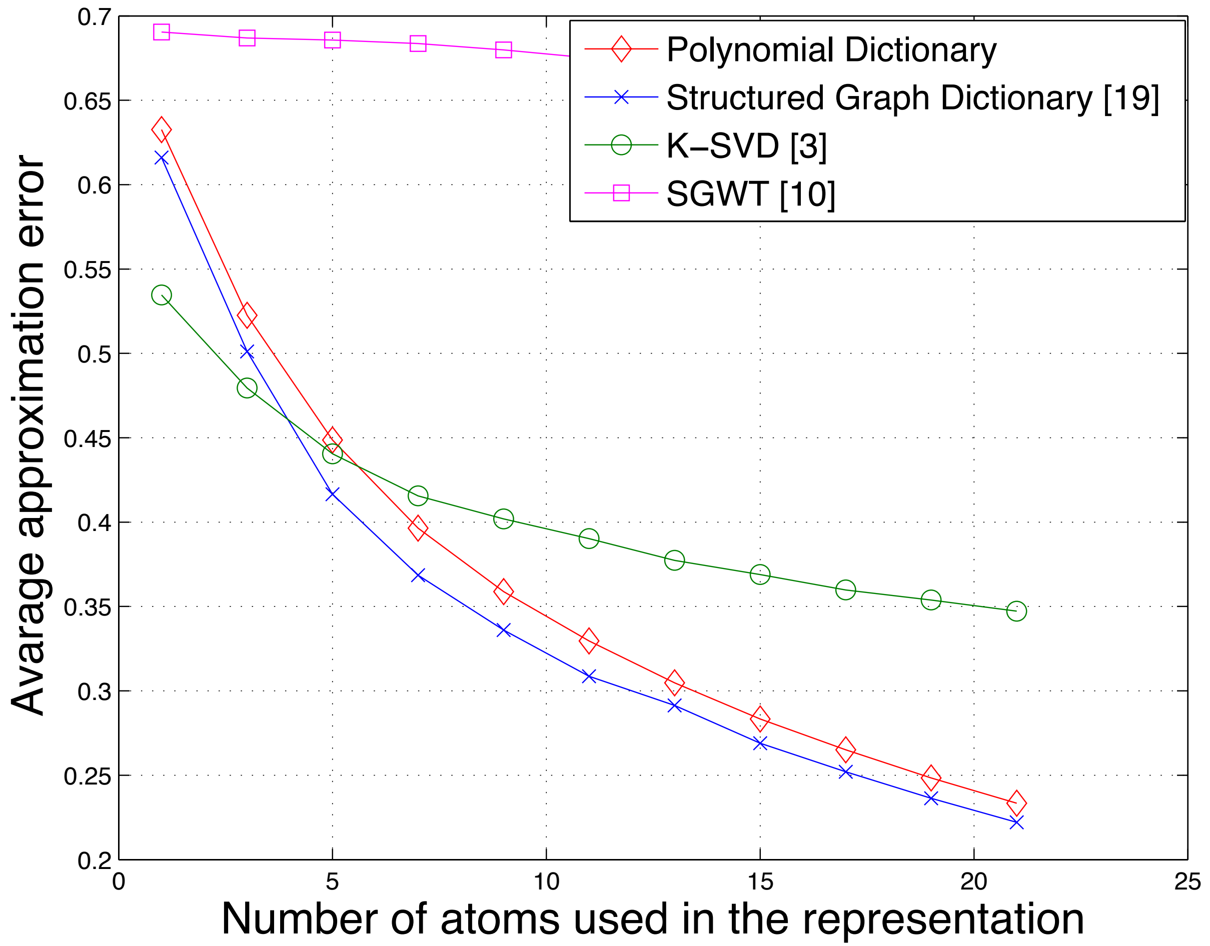


Traffic dataset

- Nodes: 439 detector stations in Alameda County, CA
- Assign edge when distance < 13km
- Graph Signals: Daily number of bottlenecks (in minutes) between Jan. 2007 to May. 2013

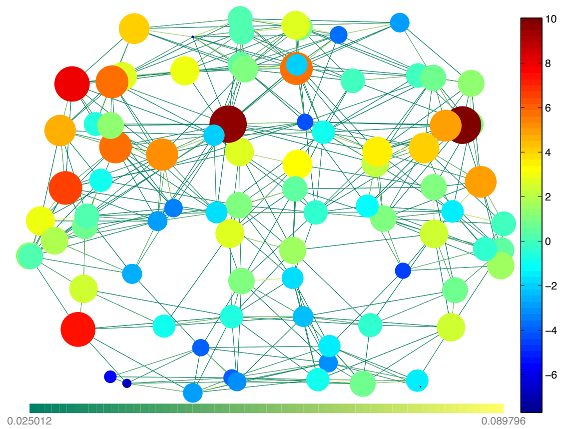


Traffic signal approximation

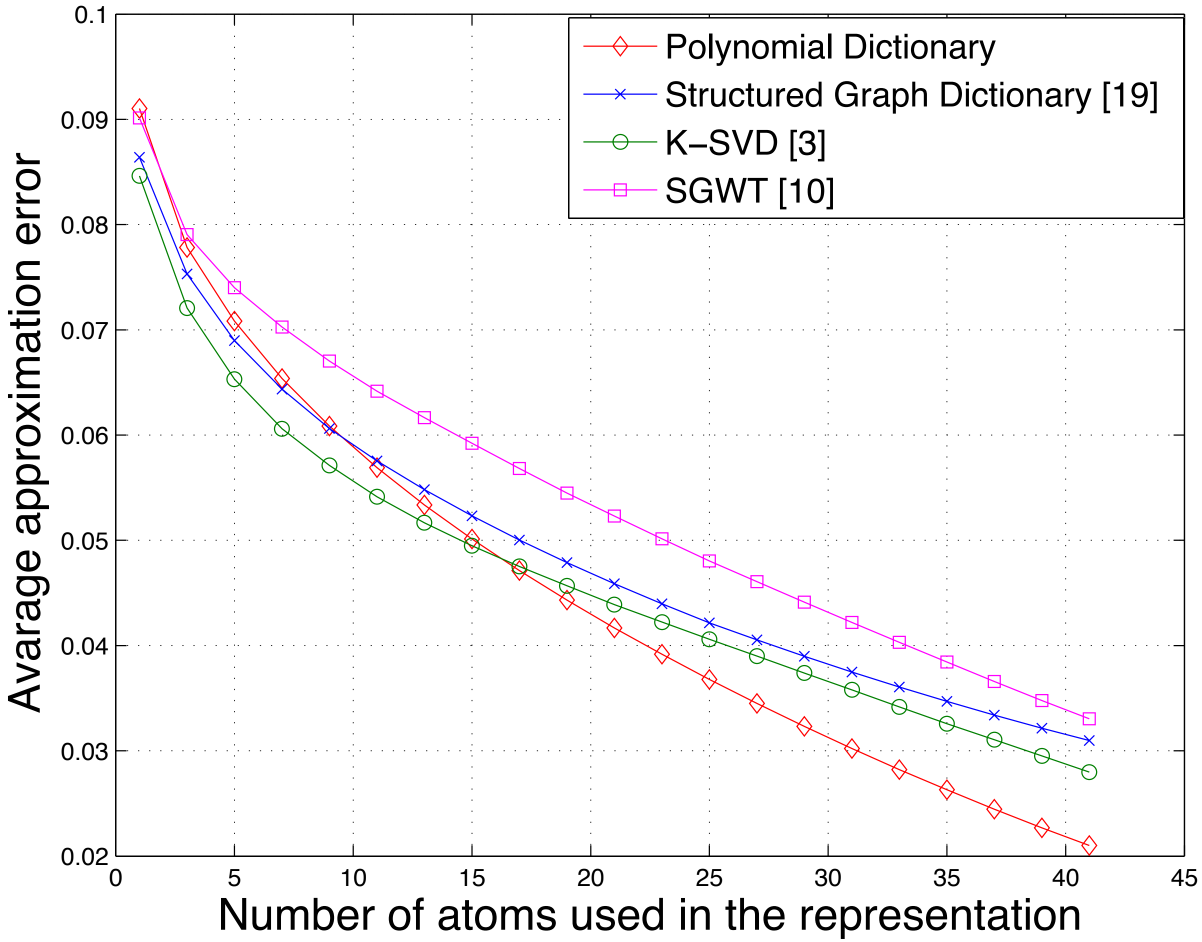


Brain dataset

- Nodes: 90 brain regions of contiguous voxels
- Edges assigned if anatomical distance < 40 mm
- Graph Signals: fMRI signals acquired on five subjects, in different states - 1290 signals per subject

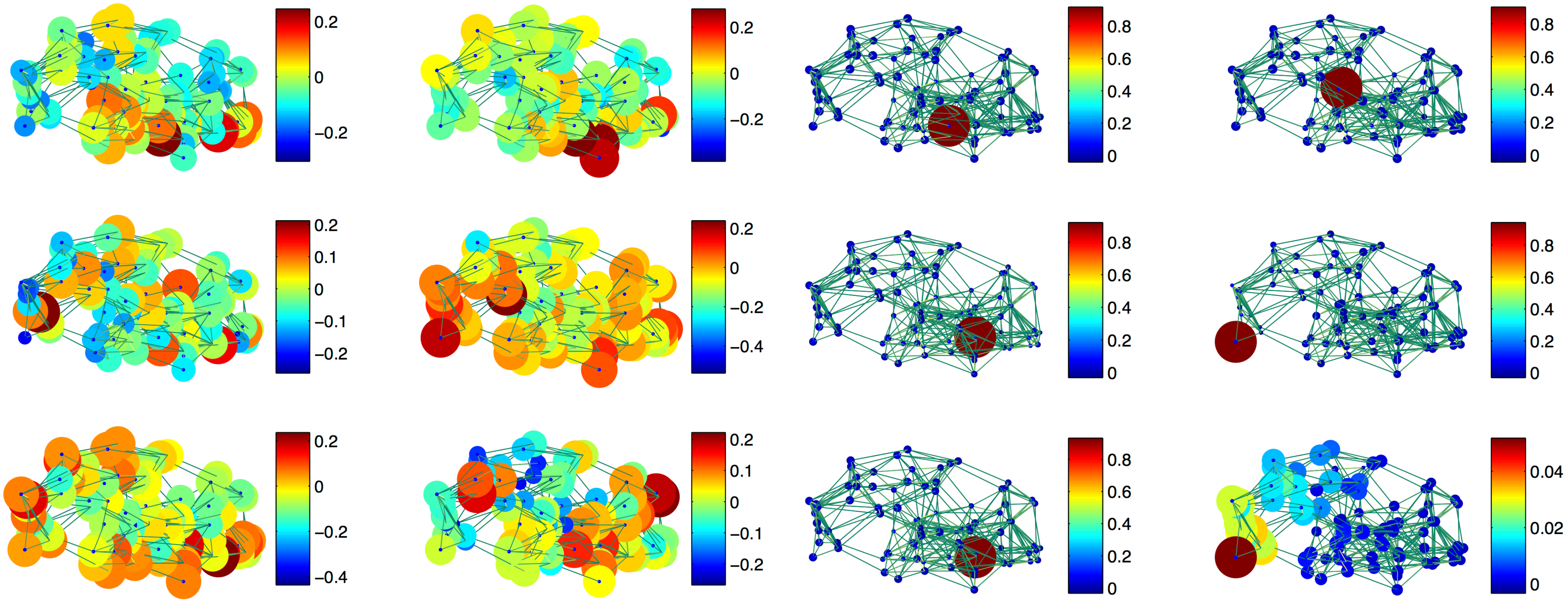


Brain signal approximation



Examples of Learned Atoms

- Most common atoms in OMP expansions



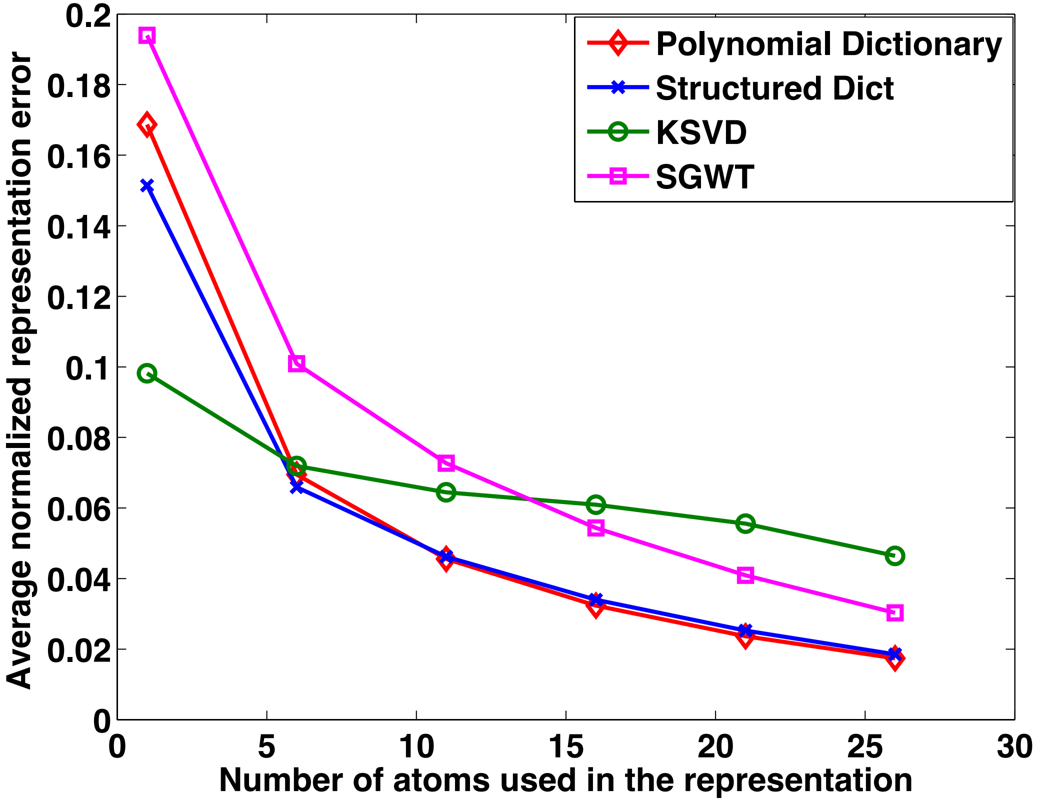
K-SVD Dictionary

Polynomial Graph Dictionary

Twitter dataset

- Graph: a social network of 63 Twitter users

- Training & Testing signals: 4032 & 4032 signals with number of tweets that each user has posted during several time intervals



Benefits of the structure

- The dictionary is easy to describe (e.g., store, or transmit)
  - it has only $(K+1)S$ parameters

- Efficient implementation, esp. when the graph is sparse
  - Both forward and adjoint operators can be efficiently applied
  - Both operators are the main components of many sparsity-based applications

$\mathcal{D}^T y = \sum_{s=1}^{S} \sum_{k=0}^{K} \alpha_{sk} \mathcal{L}^k y$ is $O(K|\mathcal{E}| + NSK)$ since $\{\mathcal{L}^k y\}_{k=0,2,\ldots,K}$ is $O(K|\mathcal{E}|)$

$\mathcal{D}\mathcal{D}^T y = \sum_{s=1}^{S} \widehat{g_s}^2(\mathcal{L}) y$ similar, with a polynomial of degree $K' = 2K$

Example: Iterative soft thresholding

- Lasso regularisation problem

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

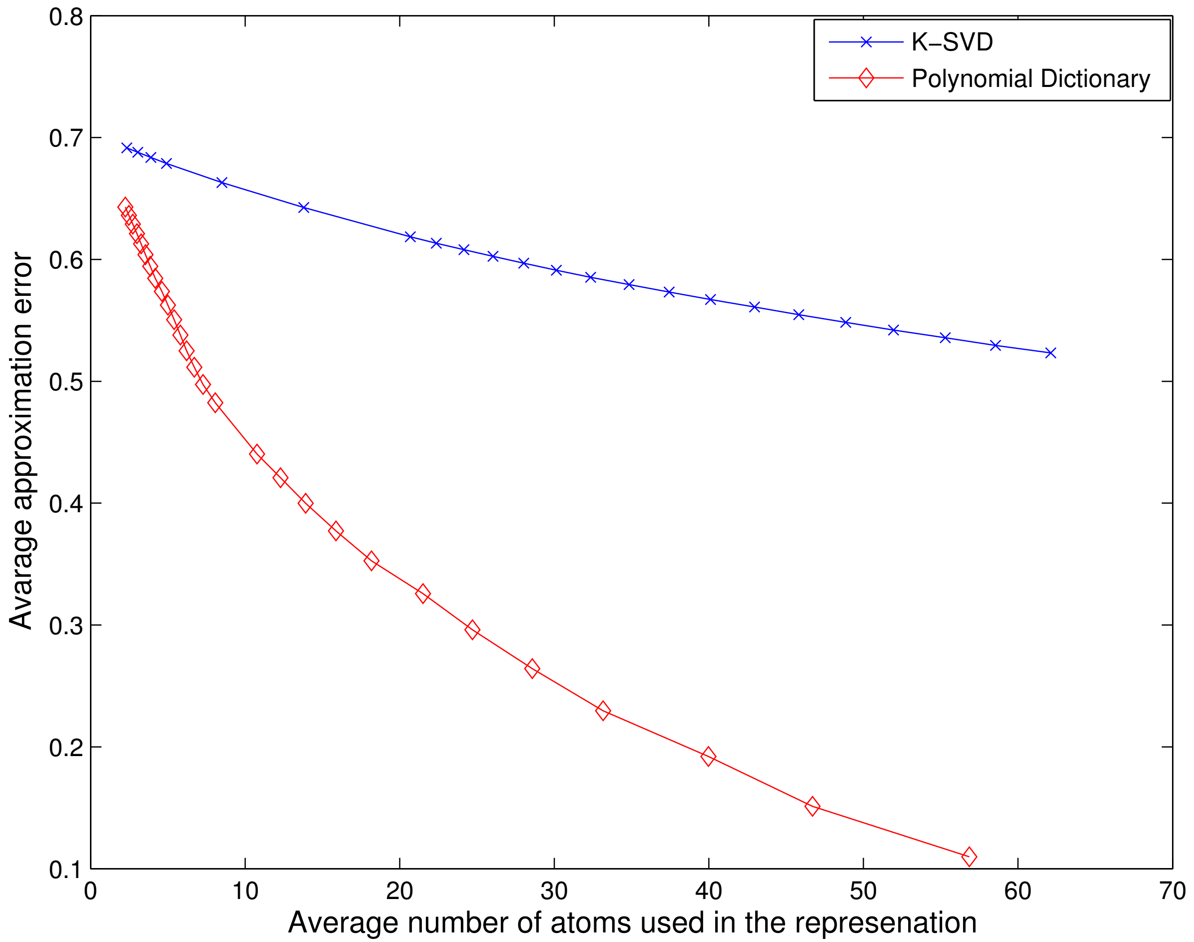
- It can be solved by iterative soft thresholding with

$$x^t = \mathcal{S}_{\kappa\tau}\left(x^{(t-1)} + 2\tau\mathcal{D}^T \; (y - \mathcal{D}x^{(t-1)})\right), \; t = 1, 2, \ldots$$

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

  - both dictionary-based operators are ‘easy’ to compute

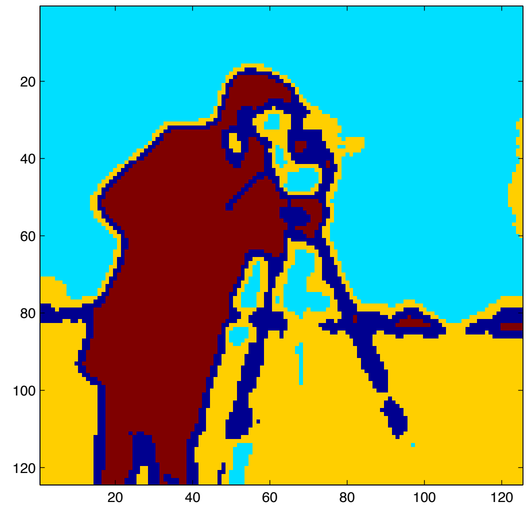
Illustrative Lasso performance



Iterative soft thresholding on traffic bottleneck signals

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



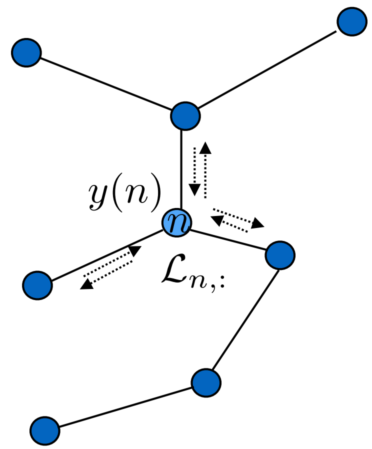


Image Segmentation Example

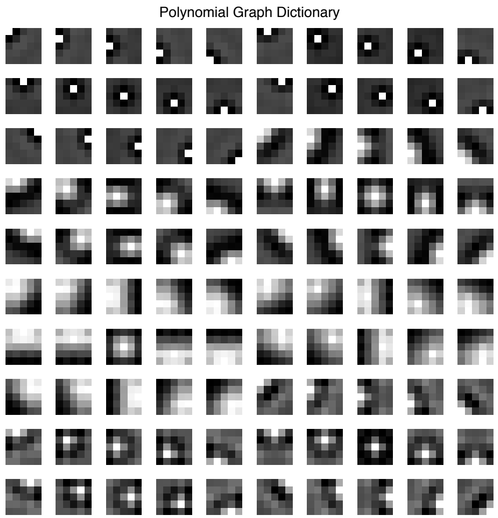
- Dictionary construction
  - For each pixel (node), build a 5x5 patch
    - each pixel connected to its horizontal and vertical neighbors
    - graphs signal is the pixel luminance value
  - Learn a dictionary from patch signals with $S = 4, K = 15$

- Segmentation
  - Process each signal with the learned filters i.e.,

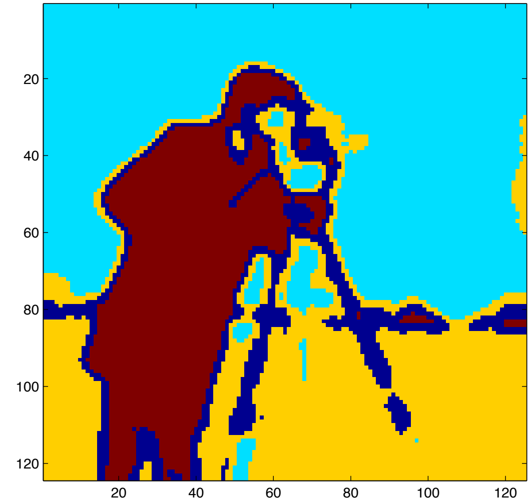
$$\mathcal{D}_s^T y_j = \sum_{\ell=0}^{N-1} \widehat{y_j}(\lambda_\ell)\widehat{g_s}(\lambda_\ell)\chi_\ell$$

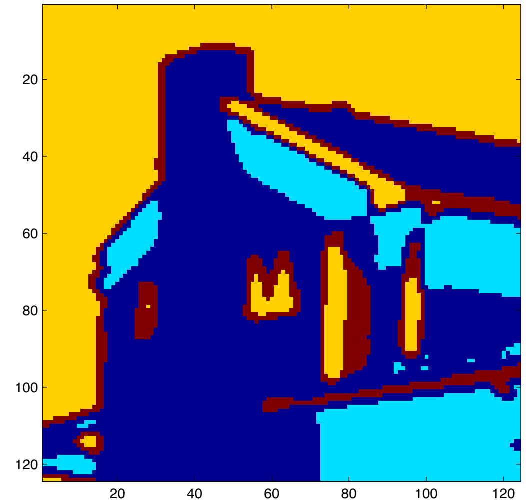
  - Node feature: mean and variance of the filtered signals
  - Clustering: K-means on the feature vectors

Clustering results



Atoms learned on patches

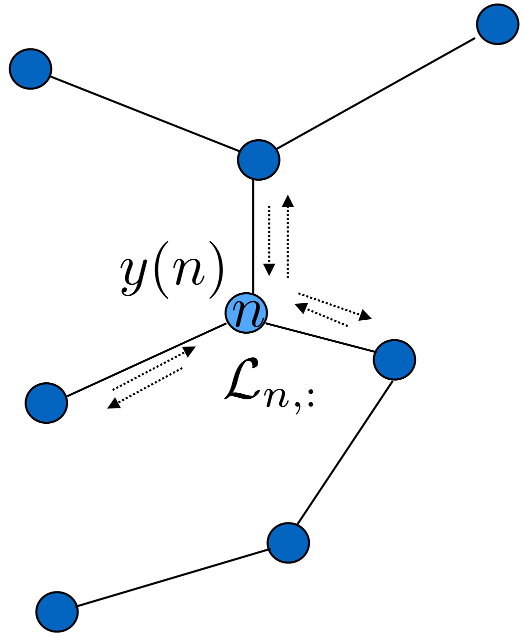




Clustering results

Distributed processing

- Centralised processing may be impossible
  - network with communication constraints
  - no node knows fully the signal



- Settings for distributed processing
  - Each node *n* knows
    - its own reading of *y*
    - the *n*th row of the Laplacian
    - the coefficients used in the dictionary
  - Signal is processed distributively

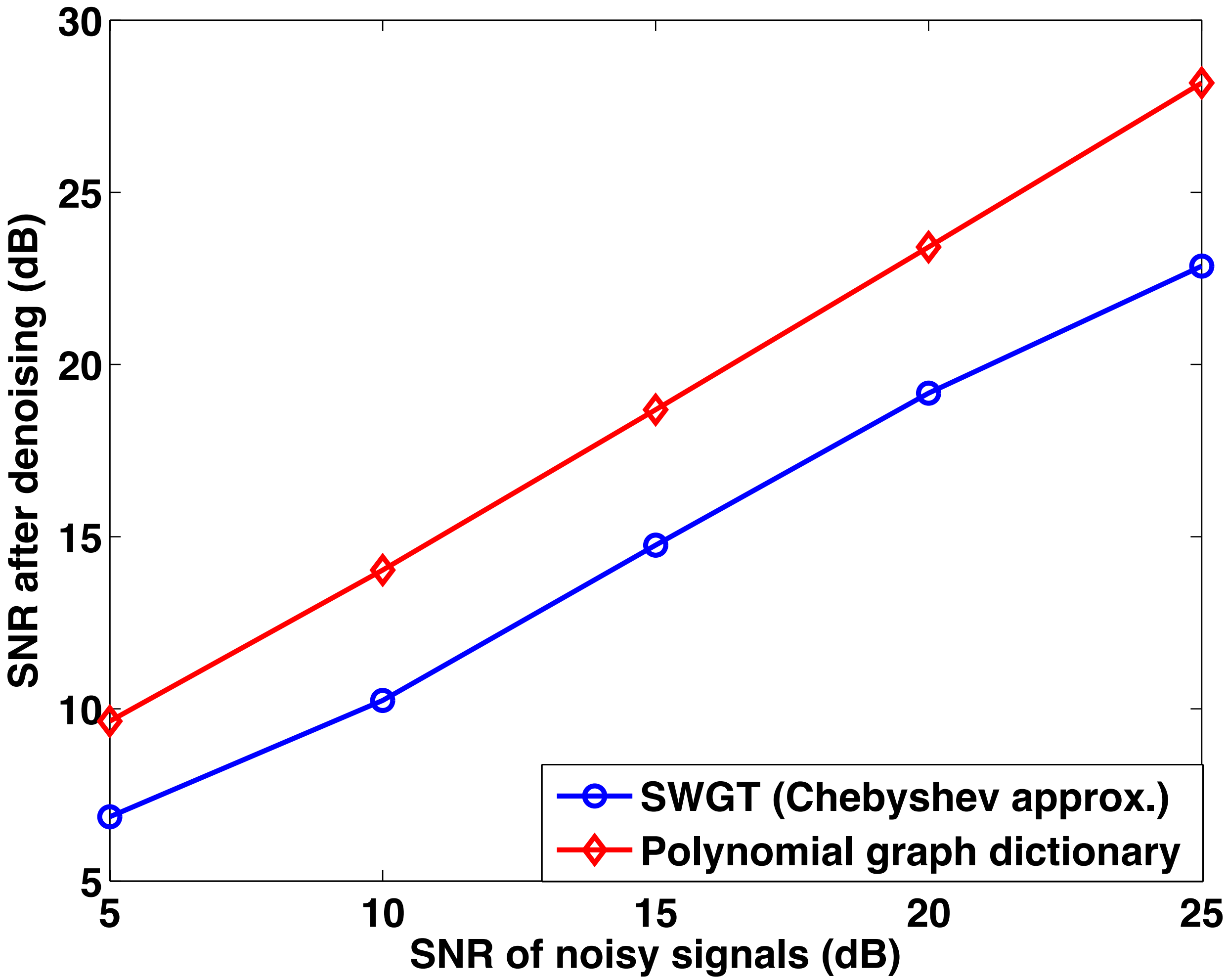
Good news: the spectral dictionary can be distributed!

Distributed processing of adjoint

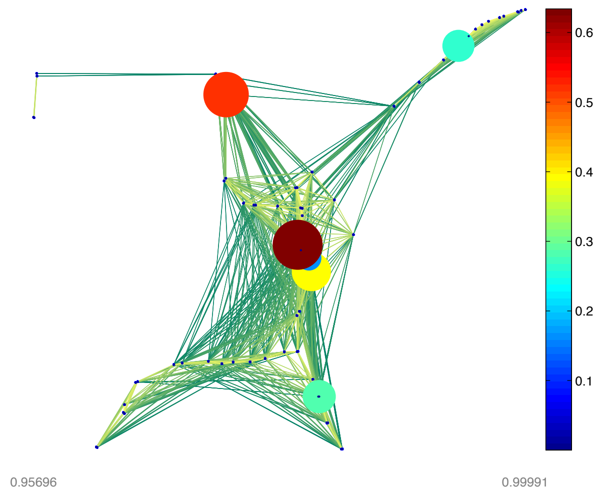
Algorithm 1 Distributed computation of $\mathcal{D}^T y$

Inputs at node n**:** $y(n), \mathcal{L}_{n,:}, \alpha = [\alpha_1; ...; \alpha_S]$
Output at node n**:** $\{(\mathcal{D}^T y)_{(s-1)N+n}\}_{s=1,..,S}$
Transmit $y(n)$ to all neighbors $\mathcal{N}_n$
Receive $y(m)$ from neighbors $\mathcal{N}_n$
Compute and store $c_n^1 = (\mathcal{L}^T y)_n$.
for $k = 2, ..., K$ **do:**
    Transmit $c_n^{k-1} = (\mathcal{L}^T c^{k-2})_n$ to all the neighbors
    Receive c_m^{k-1} from all the neighbors $m \in \mathcal{N}_n$.
end for
for $s = 1, .., S$ **do**
    Compute $(\mathcal{D}^T y)_{(s-1)N+n} = \alpha_{0s} y(n) + \sum_{k=1}^{K} \alpha_{ks} c_n^k$
end for

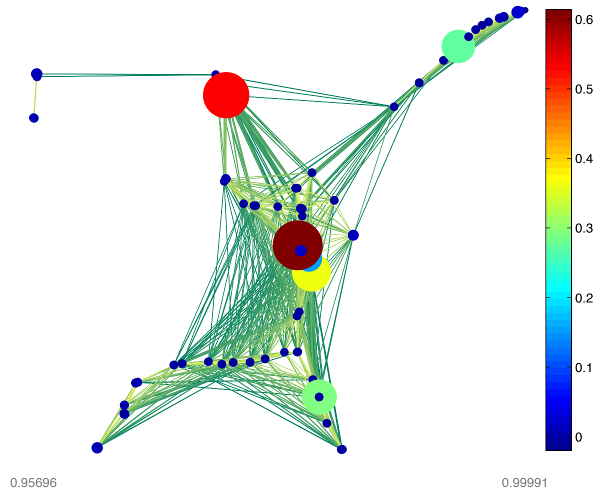
Denoising experiments



Distributed denoising with 100 ISTA iterations



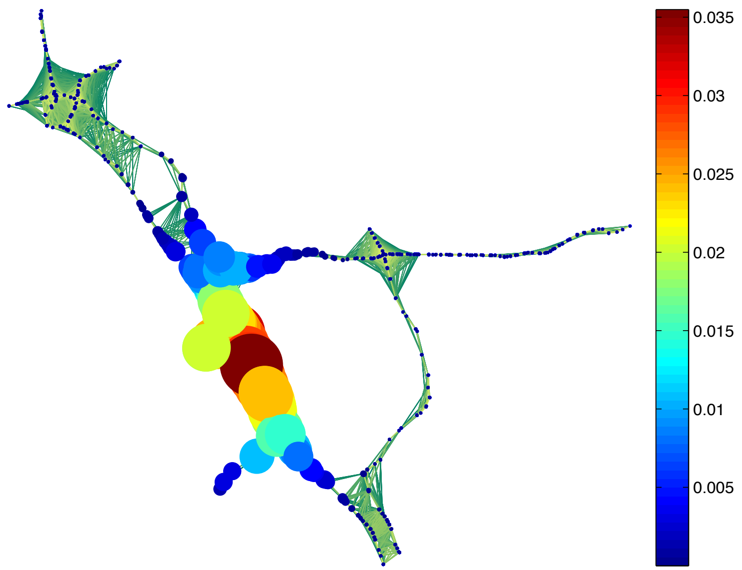
Clean traffic bottleneck signal

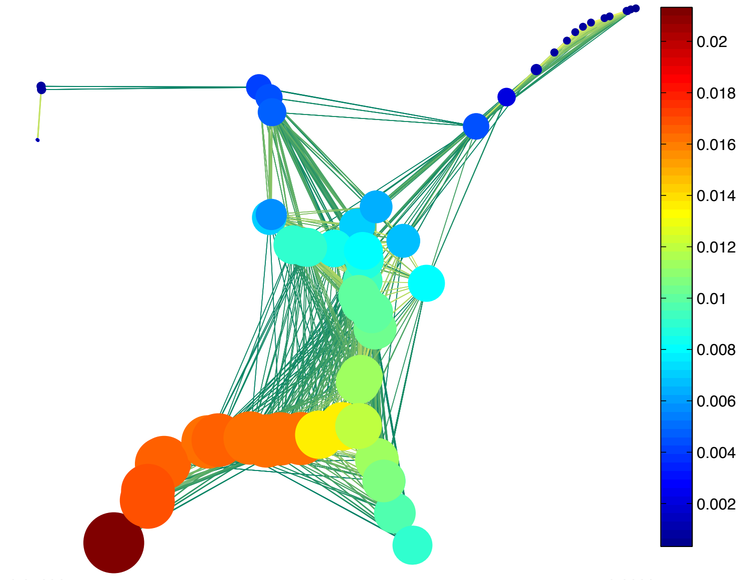


Denoised traffic bottleneck signal [24 dB]

Next? Signals on Multiple Graphs

- A process could be observed on different graphs (e.g., traffic bottlenecks in different cities)





- The evolution of the process depends on the graph: the observations may be visually different

Graph Signal Model

- We consider graph signals that are linear combinations of a few overlapping local processes at different nodes (localized patterns)

- Given a set of processes $\mathcal{P} = \{g_s(\mathcal{G})\}_{s=1}^{S}$, a signal y on a graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ can be decomposed as:

$$y = \sum_{g \in \widetilde{\mathcal{P}}, n \in \widetilde{\mathcal{V}}} y_{g,n}, \quad \text{where } \widetilde{\mathcal{P}} \subseteq \mathcal{P}, \widetilde{\mathcal{V}} \subseteq \mathcal{V}$$

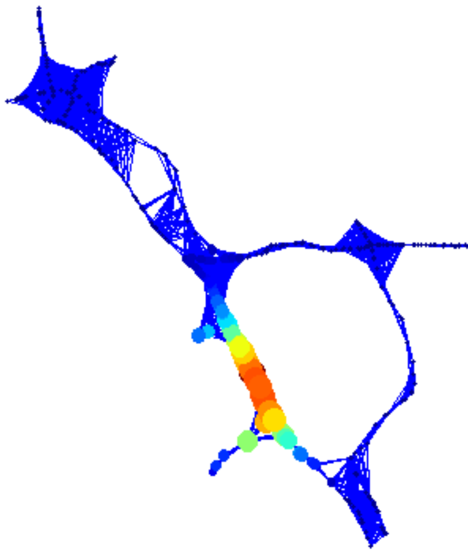
sparse set of components

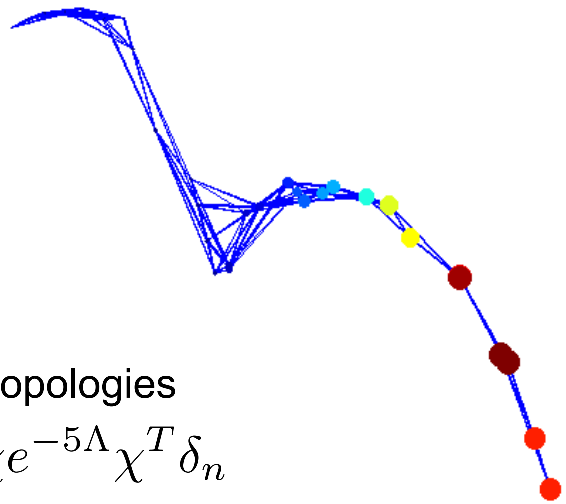
- The same processes may evolve across different topologies

Multi-graph dictionary learning

- **Problem:** Learn atoms for effective representation of signals, that are collected on different graph topologies

- **Main assumption:** Signals on different topologies may share similar spectral characteristics





- same process evolving in two different topologies
- signal observation: $y = e^{-5\mathcal{L}}\delta_n = \chi e^{-5\Lambda}\chi^T\delta_n$

Multi-Graph Dictionary Learning Problem

- Given a set of training signals $Y_t = [y_{t1}, y_{t2}, ..., y_{tM_t}]$, living on the weighted graphs $\mathcal{G}_t, t = \{1, 2, ..., T\}$, solve:

$$\underset{\alpha \in \mathbb{R}^{(K+1)S},\ X_t \in \mathbb{R}^{SN \times M_t}}{\text{argmin}} \left\{ \sum_{t=1}^{T} \frac{1}{M_t} ||Y_t - \mathcal{D}_t X_t||_F^2 + \mu ||\alpha||_2^2 \right\}$$

$$\text{subject to} \quad \|X_t^m\|_0 \leq \gamma, \quad \forall m \in \{1, ..., M_t\},$$

$$\mathcal{D}_t^s = \sum_{k=0}^{K} \alpha_{sk} \mathcal{L}_t^k, \forall s \in \{1, 2, ..., S\},$$

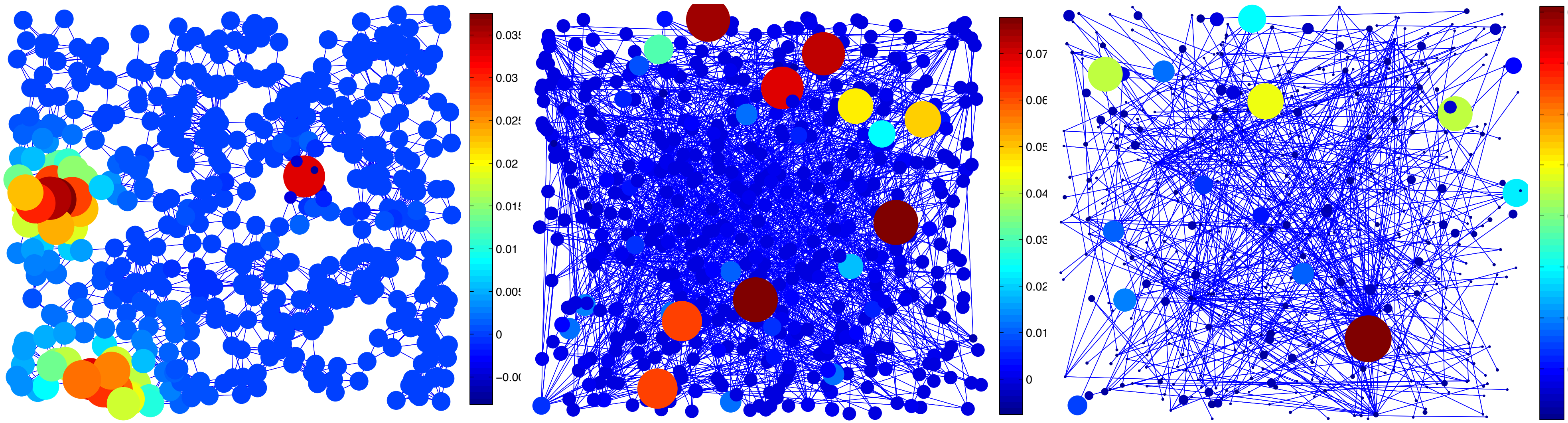
$$0 \preceq \mathcal{D}_t^s \preceq c, \forall s \in \{1, 2, ..., S\},$$

Each subdictionary captures the same process evolving in different topologies

Same polynomial coefficients for all topologies

Synthetic Experiments

- Generate 3 graphs $\mathcal{G}_1, \mathcal{G}_2, \mathcal{G}_3$ of 500 nodes



(a) RBF model $\mathcal{G}_1$

(b) Forest Fire model $\mathcal{G}_2$

(c) Barabasi-Albert model $\mathcal{G}_3$

Synthetic Graph Processes

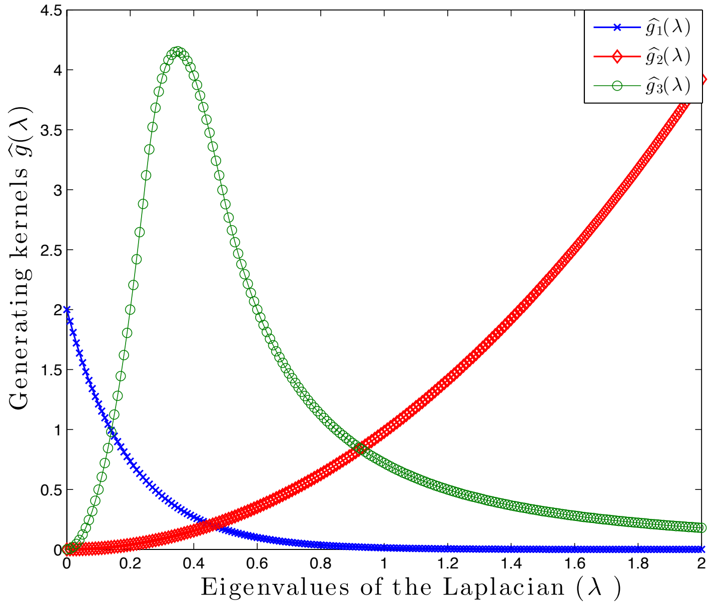
- Consider 3 subdictionaries generated from the following processes:
  1) Heat diffusion kernel $\widehat{g}_1(\lambda) = e^{-5\lambda}$ → $\mathcal{D}^1 = \chi \widehat{g}_1(\Lambda) \chi^T$
  2) Wave kernel $\widehat{g}_2(\lambda) = e^{-(0.01-\log\lambda)^2}$ → $\mathcal{D}^2 = \chi \widehat{g}_2(\Lambda) \chi^T$
  3) Spectral graph wavelet kernel (bandpass filter)
     $\widehat{g}_3(\lambda) = \widehat{g}(4.1\lambda)$ → $\mathcal{D}^3 = \chi \widehat{g}_3(\Lambda) \chi^T$

- Training signals: linear combination of a few atoms of the above subdictionaries on one graph

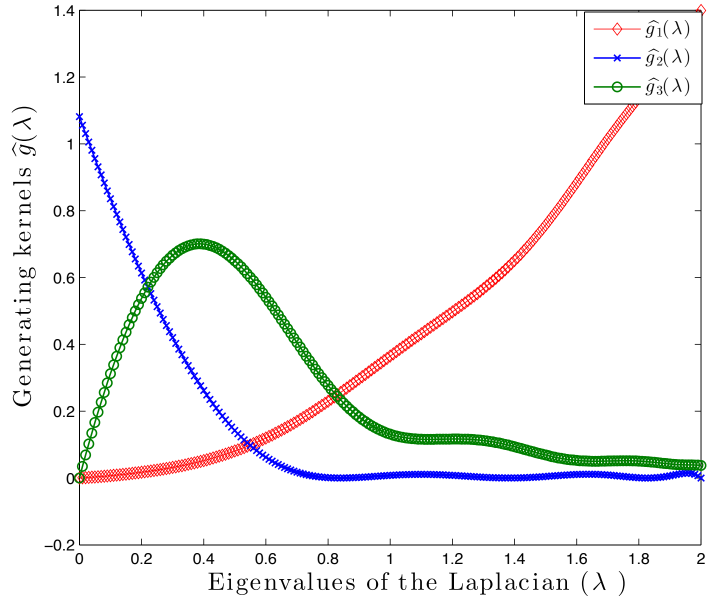
$$y_t = [\mathcal{D}_t^1 \ \mathcal{D}_t^2 \ \mathcal{D}_t^3]x, \quad \text{where} \quad \|x\|_0 \leq 4$$

Recovery of Graph Processes

- Processes are learned jointly from 1200 training signals on the three graphs $(M = M_1 = M_2 = M_3 = 400)$



Original kernels

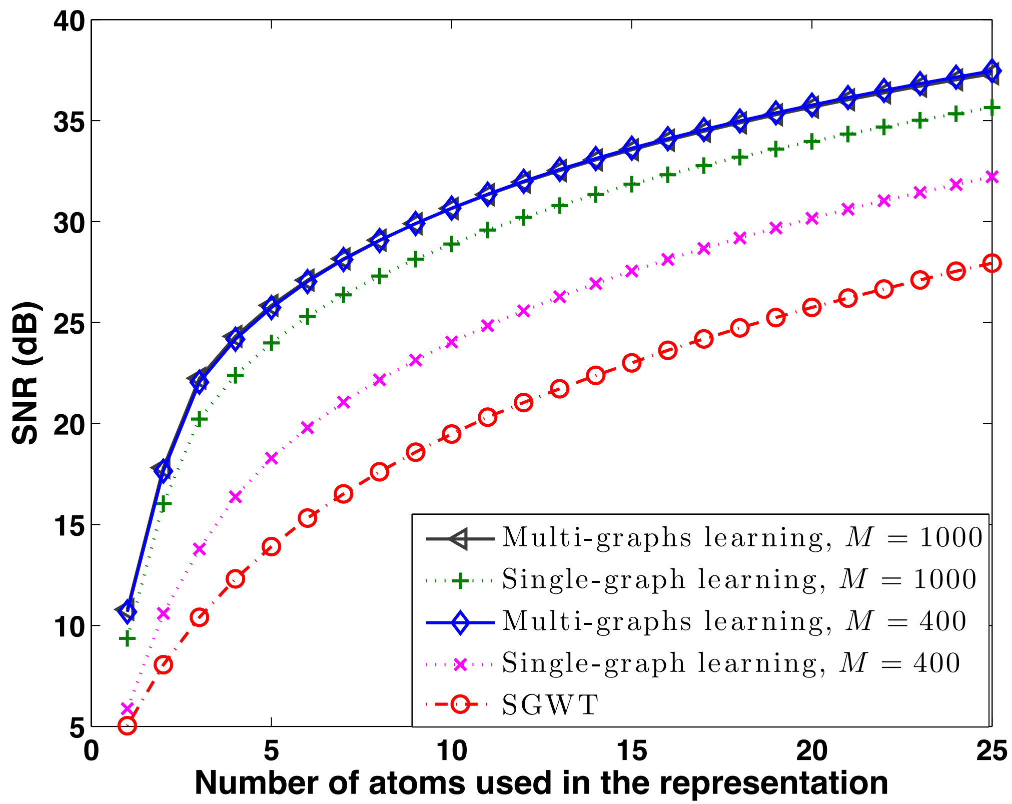


Learned kernels

- The proposed algorithm is able to recover the continuous processes

Representation of Synthetic Signals

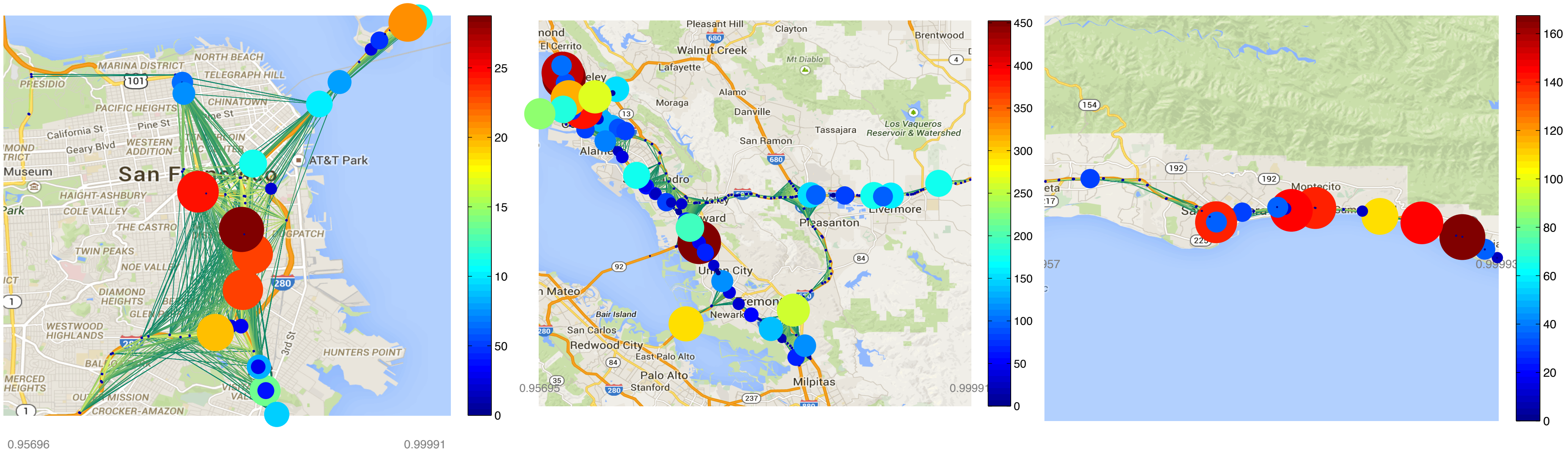
- Learn a dictionary for different sizes of the training set



- Joint learning compensates for the lack of training signals in each graph separately

Representation of Traffic Signals

- Consider bottleneck signals[1] from Jan. 2007-Aug.2014 on three different graphs:

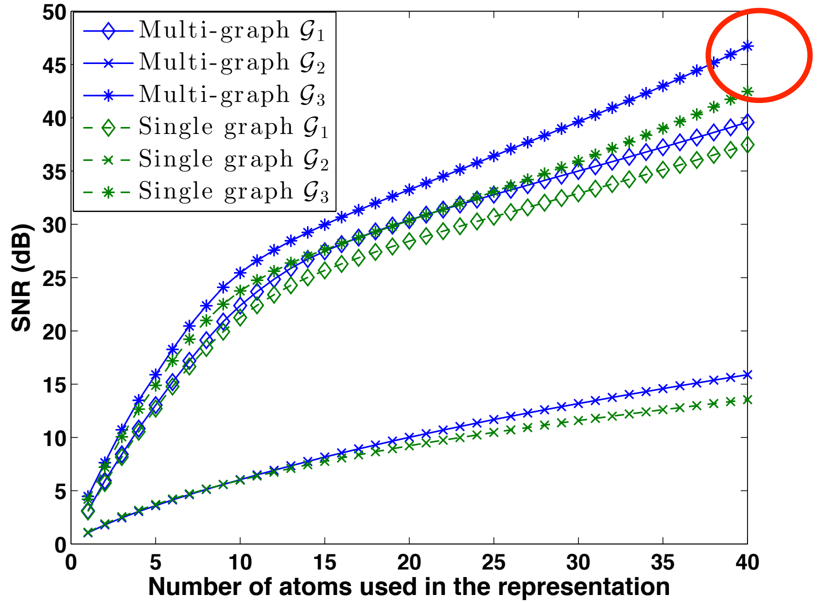


(a) San Francisco ($\mathcal{G}_1$) **(b) Alameda** ($\mathcal{G}_2$) **(c) Santa Barbara** ($\mathcal{G}_3$)

[1]The data are publicly available at http://pems.dot.ca.gov.

Representation of Traffic Signals

- Learn a dictionary from training signals on different graphs: 1383 signals in San Francisco, 1386 in Alameda, 447 in Santa Barbara
- Approximate with the learned kernels testing signals on specific graph



- Joint learning outperforms independent learning on each graph

Summary

- Take-home messages:
  - Graph signal processing is a very generic and promising framework
  - Polynomial matrix functions of the graph Laplacian seems to be a flexible structure for sparsely representing graph signals
  - Polynomial kernels lead to effective implementations

- Still many open questions:
  - Development of applications where the kernel information could be beneficial, such as classification, learning, etc
  - Limits of multi-graph dictionary learning
  - Definition of the optimal graph topology

Acknowledgments

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- many others…

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