

## Signal Processinc SpaRTaN-Mace, itering Strikechool <br> Pierre Vandergheynst LON F Federal Institute of Technology

April is Autism Awareness Month: https://www.autismspeaks.org/wordpress-tags/autism-awareness-month

## Signal Processing on Graphs




## Some Typical Processing Problems

Compression / Visualization


Many interesting new contributions with a SP perspective
[Coifman, Maggioni, Kolaczyk, Ortega, Ramchandran, Moura, Lu, Borgnat] or IP perspective [EIMoataz, Lezoray]
See review in 2013 IEEE SP Mag


## Outline

- Introduction:
- Graphs and elements of spectral graph theory, with emphasis on functional calculs
- Kernel Convolution:
- Localization, filtering, smoothing and applications
- An application to spectral clustering that unifies some of the themes you've heard of during the workshop: machine learning, compressive sensing, optimisation algorithms, graphs


# Elements of Spectral Graph Theory 

Reference: F. Chung, Spectral Graph Theory

## Definitions

A graph $G$ is given by a set of vertices and «relationships» between them encoded in edges $\mathrm{G}=(V, E)$

A set $V$ of vertices of cardinality $|V|=N$
A set $E$ of edges: $e \in E, \quad e=(u, v)$ with $u, v \in V$
Directed edge: $e=(u, v), \quad e^{\prime}=(v, u)$ and $e \neq e^{\prime}$
Undirected edge: $e=(u, v), \quad e^{\prime}=(v, u)$ and $e=e^{\prime}$
A graph is undirected if it contains only undirected edges
A weighted graph has an associated non-negative weight function:

$$
w: V \times V \rightarrow \mathbb{R}^{+} \quad(u, v) \notin E \Rightarrow w(u, v)=0
$$

## Matrix Formulation

Connectivity captured via the (weighted) adjacency matrix

$$
\begin{array}{ll}
W(u, v)=w(u, v) & \text { with obvious restriction for unveighted graphs } \\
W(u, u)=0 & \text { no lops }
\end{array}
$$

Let $d(u)$ be the degree of $u$ and $\mathbf{D}=\operatorname{diag}(\mathrm{d})$ the degree matrix
Graph Laplacians, Signals on Graphs

$$
\mathcal{L}=\mathbf{D}-\mathbf{W} \quad \mathcal{L}_{\text {norm }}=\mathbf{D}^{-1 / 2} \mathcal{L} \mathbf{D}^{-1 / 2}
$$

Graph signal: $f: V \rightarrow \mathbb{R}$
Laplacian as an operator on space of graph signals

$$
\mathcal{L} f(u)=\sum_{v \sim u} w(u, v)(f(u)-f(v))
$$

## Some differential operators

The Laplacian can be factorized as $\mathcal{L}=\mathbf{S S}^{*}$
Explicit form of the incidence matrix (unweighted in this example):

$$
e=(u, v)
$$


$\mathbf{S}^{*} f(u, v)=f(v)-f(u)$ is a gradient

$$
\mathbf{S} g(u)=\sum_{(u, v) \in E} g(u, v)-\sum_{\left(v^{\prime}, u\right) \in E} g\left(v^{\prime}, u\right) \text { is a negative divergence }
$$

## Properties of the Laplacian

Laplacian is symmetric and has real eigenvalues
Moreover: $\langle f, \mathcal{L} f\rangle=\sum_{u \sim v} w(u, v)(f(u)-f(v))^{2} \geq 0 \quad$ Dirichlet form
positive semi-definite, non-negative eigenvalues
Spectrum: $0=\lambda_{0} \leq \lambda_{1} \leq \ldots \lambda_{\max }$
$G$ connected: $\lambda_{1}>0$
$\lambda_{i}=0$ and $\lambda_{i+1}>0 \quad G$ has $i+1$ connected components
Notation: $\langle f, \mathcal{L} g\rangle=f^{t} \mathcal{L} g$

## Measuring Smoothness

$\langle f, \mathcal{L} f\rangle=\sum_{u \sim v}(f(u)-f(v))^{2} \geq 0$
is a measure of «how smooth » $f$ is on $G$
Using our definition of gradient: $\nabla_{u} f=\left\{S^{*} f(u, v), \forall v \sim u\right\}$
Local variation $\left\|\nabla_{u} f\right\|_{2}=\sqrt{\sum_{v \sim u}\left|S^{*} f(u, v)\right|^{2}}$
Total variation $|f|_{T V}=\sum_{u \in V}\left\|\nabla_{u} f\right\|_{2}=\sum_{u \in V} \sqrt{\sum_{v \sim u}\left|S^{*} f(u, v)\right|^{2}}$

## Notions of Global Regularity for Graph

B Discrete Calculus, Grady and Polimeni, 2010
$\left.\begin{gathered}\text { Ddge } \\ \text { Derivative }\end{gathered} \frac{\partial \mathbf{f}}{\partial e}\right|_{m}:=\sqrt{w(m, n)}[f(n)-f(m)]$

Graph
Gradient

$$
\nabla_{m} \mathbf{f}:=\left[\left\{\left.\frac{\partial \mathbf{f}}{\partial e}\right|_{m}\right\}_{e \in \mathcal{E} \text { s.t. } e=(m, n)}\right]
$$

Local
Variation

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

Quadratic
Form

$$
\frac{1}{2} \sum_{m \in V}\left\|\nabla_{m} \mathbf{f}\right\|_{2}^{2}=\sum_{(m, n) \in \mathcal{E}} w(m, n)[f(n)-f(m)]^{2}=\mathbf{f}^{\mathrm{T}} \mathcal{L} \mathbf{f}
$$

## Smoothness of Graph Signals


$\mathbf{f}^{\mathrm{T}} \mathcal{L}_{1} \mathbf{f}=0.14$
$\mathcal{G}_{2}$

$\mathbf{f}^{\mathrm{T}} \mathcal{L}_{2} \mathbf{f}=1.31$
$\mathcal{G}_{3}$

$\mathbf{f}^{\mathrm{T}} \mathcal{L}_{3} \mathbf{f}=1.81$

## Remark on Discrete Calculus

Discrete operators on graphs form the basis of an interesting field aiming at bringing a PDE-like framework for computational analysis on graphs:

- Leo Grady: Discrete Calculus
- Olivier Lezoray, Abderrahim Elmoataz and co-workers: PDEs on graphs:
- many methods from PDEs in image processing can be transposed on arbitrary graphs
- applications in vision (point clouds) but also machine learning (inference with graph total variation)


## Laplacian eigenvectors

Spectral Theorem: Laplacian is PSD with eigen decomposition

$$
\begin{gathered}
\mathcal{L}=\mathbf{D}-\mathbf{W} \quad\left\{\left(\lambda_{\ell}, \mathbf{u}_{\ell}\right)\right\}_{\ell=0,1, \ldots, N-1} \\
\mathcal{L}=\mathbf{U} \boldsymbol{\Lambda} \mathbf{U}^{t}
\end{gathered}
$$

That particular basis will play the role of the Fourier basis:

## Graph Fourier Transform, Coherence

$$
\begin{array}{r}
\hat{f}\left(\lambda_{\ell}\right):=\left\langle\mathbf{f}, \mathbf{u}_{\ell}\right\rangle=\sum_{i=1}^{N} f(i) u_{\ell}^{*}(i) \\
\mu:=\max _{\ell, i}\left|\left\langle\mathbf{u}_{\ell}, \delta_{i}\right\rangle\right| \in\left[\frac{1}{\sqrt{N}}, 1[ \right.
\end{array}
$$

Graph Coherence

## Important remark on eigenvectors

$$
\mu:=\max _{\ell, i}\left|\left\langle\mathbf{u}_{\ell}, \delta_{i}\right\rangle\right| \in\left[\frac{1}{\sqrt{y}},\right.
$$

Optimal - Fourier case
What does that mean ??


Eigenvectors of modified path graph

## Examples: Cut and Clustering

$C(A, B):=\sum_{i \in A, j \in B} W[i, j] \operatorname{RatioCut}(A, \bar{A}):=\frac{1}{2} \frac{C(A, \bar{A})}{|A|}+\frac{1}{2} \frac{C(A, \bar{A})}{|\bar{A}|}$ $\min _{A \subset V} \operatorname{RatioCut}(A, \bar{A}) \quad f[i]=\left\{\begin{array}{cl}\sqrt{|\bar{A}| /|A|} & \text { if } i \in A \\ -\sqrt{|A| /|\bar{A}|} & \text { if } i \in \bar{A}\end{array}\right.$

$$
\|f\|=\sqrt{|V|} \text { and }\langle f, 1\rangle=0
$$

$$
f^{t} \mathcal{L} f=|V| \cdot \operatorname{RatioCut}(A, \bar{A})
$$


Relaxed problem Looking for a smooth partition function


## Examples: Cut and Clustering

## Spectral Clustering

$$
\arg \min _{f \in \mathbb{R}^{|V|}} f^{t} \mathcal{L} f \text { subject to }\|f\|=\sqrt{|V|} \text { and }\langle f, 1\rangle=0
$$

By Rayleigh-Ritz, solution is second eigenvector $\mathbf{u}_{1}$
Remarks: Natural extension to more than 2 sets Solution is real-valued and needs to be quantized. In general, k-MEANS is used.
First $k$ eigenvectors of sparse Laplacians via Lanczos, complexity driven by eigengap $\left|\lambda_{k}-\lambda_{k+1}\right|$

Spectral clustering $:=$ embedding +k -MEANS

$$
\forall i \in V: i \mapsto\left(u_{0}(i), \ldots, u_{k-1}(i)\right)
$$

## Graph Embedding/Laplacian Eigenmaps

Goal: embed vertices in low dimensional space, discovering geometry

$$
\begin{aligned}
& \left(x_{1}, \ldots x_{N}\right) \mapsto\left(y_{1}, \ldots y_{N}\right) \\
& x_{i} \in \mathbb{R}^{d} \quad y_{i} \in \mathbb{R}^{k} \quad k<d
\end{aligned}
$$

Good embedding: nearby points mapped nearby, so smooth map


## Graph Embedding/Laplacian Eigenmaps

Goal: embed vertices in low dimensional space, discovering geometry

$$
\begin{aligned}
& \left(x_{1}, \ldots x_{N}\right) \mapsto\left(y_{1}, \ldots y_{N}\right) \\
& x_{i} \in \mathbb{R}^{d} \quad y_{i} \in \mathbb{R}^{k} \quad k<d
\end{aligned}
$$

Good embedding: nearby points mapped nearby, so smooth map minimize variations/ maximize smoothness of embedding

$$
\sum_{i, j} W[i, j]\left(y_{i}-y_{j}\right)^{2}
$$

## Laplacian Eigenmaps

$$
\mathcal{L} \mathbf{y}=\lambda \mathbf{D} \mathbf{y}
$$



## Laplacian Eigenmaps


[Belkin, Niyogi, 2003]

## Remark on Smoothness

## Linear / Sobolev case

Smoothness, loosely defined, has been used to motivate various methods and algorithms. But in the discrete, finite dimensional case, asymptotic decay does not mean much

$$
\|\nabla f\|_{2}^{2} \leq M \Leftrightarrow f^{t} \mathcal{L} f \leq M \Leftrightarrow \sum_{\ell} \lambda_{\ell}|\hat{f}(\ell)|^{2} \leq M, \begin{array}{rr} 
\\
E_{K}(f)=\left\|f-P_{K}(f)\right\|_{2} & E_{K}(f) \leq \frac{\|\nabla f\|_{2}}{\sqrt{\lambda_{K+1}}}
\end{array}
$$

$$
|\hat{f}(\ell)| \leq \frac{\sqrt{M}}{\sqrt{\lambda_{\ell}}}
$$

## Smoothness of Graph Signals Revisited

$$
\begin{aligned}
& \mathcal{G}_{1} \\
& \mathcal{G}_{2} \\
& \mathbf{f}^{\mathrm{T}} \mathcal{L}_{1} \mathbf{f}=0.14 \\
& \mathbf{f}^{\mathrm{T}} \mathcal{L}_{2} \mathbf{f}=1.31 \\
& \mathbf{f}^{\mathrm{T}} \mathcal{L}_{3} \mathbf{f}=1.81
\end{aligned}
$$

## Functional calculus

It will be useful to manipulate functions of the Laplacian

$$
\mathcal{L}^{k} \mathbf{u}_{\ell}=\lambda_{\ell}^{k} \mathbf{u}_{\ell} \xrightarrow{f(\mathcal{L}), f: \mathbb{R} \mapsto \mathbb{R}} \text { polynomials }
$$

Symmetric matrices admit a (Borel) functional calculus

## Borel functional calculus for symmetric matrices

$$
f(\mathcal{L})=\sum_{\ell \in \mathcal{S}(\mathcal{L})} f\left(\lambda_{\ell}\right) \mathbf{u}_{\ell} \mathbf{u}_{\ell}^{t}
$$

Use spectral theorem on powers, get to polynomials
From polynomial to continuous functions by Stone-Weierstrass
Then Riesz-Markov (non-trivial !)

## Example: Diffusion on Graphs

Consider the following « heat »diffusion model

$$
\frac{\partial f}{\partial t}=-\mathcal{L} f \quad \frac{\partial}{\partial t} \hat{f}(\ell, t)=-\lambda_{\ell} \hat{f}(\ell, t) \quad \hat{f}(\ell, 0):=\hat{f}_{0}(\ell)
$$

$$
\hat{f}(\ell, t)=e^{-t \lambda_{\ell}} \hat{f}_{0}(\ell) \quad f=e^{-t \mathcal{L}} f_{0} \quad \text { by functional calculus }
$$

Explicitly:

$$
f(i)=\sum_{j \in V} \sum_{\ell} e^{-t \lambda_{\ell}} u_{\ell}(i) u_{\ell}(j) f_{0}(j)
$$

$$
e^{-t \mathcal{L}}=\sum_{\ell} e^{-t \lambda_{\ell}} \mathbf{u}_{\ell} \mathbf{u}_{\ell}^{t} \quad=\sum_{\ell} e^{-t \lambda_{\ell}} u_{\ell}(i) \sum_{j \in V} u_{\ell}(j) f_{0}(j)
$$

$$
e^{-t \mathcal{L}}[i, j]=\sum_{\ell} e^{-t \lambda_{\ell}} u_{\ell}(i) u_{\ell}(j)=\sum_{\ell} e^{-t \lambda_{\ell} \hat{f}_{0}(\ell)} u_{\ell}(i)
$$

## Example: Diffusion on Graphs

examples of heat kernel on graph



$$
\begin{aligned}
& f_{0}(j)=\delta_{k}(j) \\
& f(i)=\sum_{\ell} e^{-t \lambda_{\ell}} \hat{f}_{0}(\ell) u_{\ell}(i) \\
&=\sum_{\ell} e^{-t \lambda_{\ell}} u_{\ell}(k) u_{\ell}(i)
\end{aligned}
$$



## Simple De-Noising Example

Suppose a smooth signal $f$ on a graph


$$
\begin{gathered}
\|\nabla f\|_{2}^{2} \leq M \Leftrightarrow f^{t} \mathcal{L} f \leq M \\
|\hat{f}(\ell)| \leq \frac{\sqrt{M}}{\sqrt{\lambda_{\ell}}}
\end{gathered}
$$

But you observe only a noisy version $y$

$$
y(i)=f(i)+n(i)
$$

Noisy
Original


## Simple De-Noising Example

## De-Noising by Regularization

$$
\underset{f}{\operatorname{argmin}}\|f-y\|_{2}^{2} \text { s.t. } f^{t} \mathcal{L} f \leq M
$$

$\underset{f}{\operatorname{argmin}} \frac{\tau}{2}\|f-y\|_{2}^{2}+f^{\mathrm{T}} \mathcal{L}^{r} f \quad \square \mathcal{L}^{r} f_{*}+\frac{\tau}{2}\left(f_{*}-y\right)=0$

Graph Fourier


$$
\begin{aligned}
\widehat{\mathcal{L}^{r} f_{*}}(\ell)+\frac{\tau}{2}\left(\widehat{f_{*}}(\ell)-\hat{y}(\ell)\right)=0, & \\
& \forall \ell \in\{0,1, \ldots, N-1\}
\end{aligned}
$$



$$
\widehat{f}_{*}(\ell)=\frac{\tau}{\tau+2 \lambda_{\ell}^{r}} \hat{y}(\ell) \quad \text { "Low pass" filtering! }
$$

Convolution with a kernel: $\hat{f}(\ell) \hat{g}\left(\lambda_{\ell} ; \tau, r\right) \Rightarrow g(\mathcal{L} ; \tau, r)$

## Simple De-Noising Example

## $\operatorname{argmin}_{f}\left\{\|f-y\|_{2}^{2}+\gamma f^{T} \mathcal{L} f\right\}$



Original


Noisy

$\square \mathcal{L}^{r} f_{*}+\frac{\tau}{2}\left(f_{*}-y\right)=0$


$$
\widehat{f}_{*}(\ell)=\frac{\tau}{\tau+2 \lambda_{\ell}^{r}} \hat{y}(\ell) \text { "Low pass" filtering ! }
$$

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

# Convolution with a kernel and localization 

## "Convolutions" and "Translations"

$$
(f * g)(n)=\sum_{\ell} \hat{f}(\ell) \hat{g}(\ell) u_{\ell}(n)
$$

Inherits a lot of properties of the usual convolution associativity, distributivity, diagonalized by GFT

$$
\begin{aligned}
g_{0}(n):= & \sum_{\ell} u_{\ell}(n) \\
& \mathcal{L}(f * g)=(\mathcal{L} f) * g=f *(\mathcal{L} g)
\end{aligned}
$$

Use convolution to induce translations

$$
\left(T_{i} f\right)(n):=\sqrt{N}\left(f * \delta_{i}\right)(n)=\sqrt{N} \sum_{\ell} \hat{f}(\ell) u_{\ell}^{*}(i) u_{\ell}(n)
$$

## Localising a Kernel

Hammond et al., Wavelets on graphs via spectral graph theory, ACHA, 2011

- Action of the localisation operator on a spectral kernel

$$
\left(T_{i} f\right)(n):=\sqrt{N}\left(f * \delta_{i}\right)(n)=\sqrt{N} \sum_{\ell} \hat{f}(\ell) u_{\ell}^{*}(i) u_{\ell}(n)
$$



## The Agonizing Limits of Intuition

The Graph Fourier and Kronecker bases are not necessarily mutually unbiased

$$
\mu:=\max _{\ell, i}\left|\left\langle\mathbf{u}_{\ell}, \delta_{i}\right\rangle\right| \in\left[\frac{1}{\sqrt{N}}, 1[\right.
$$

Laplacian eigenvectors (Fourier modes!) can be well localized

- phenomenon not yet fully understood, under intense study
- can be observed in lots of experimental data graphs
- not universal: known classes of random and regular graphs have delocalized eigenvectors

$$
1 \leqslant\left\|T_{i}\right\|_{2} \leqslant \sqrt{N} \mu
$$

- the limit towards low coherence seems well-behaved (all regular properties emerge)
- HOWEVER in average:

$$
\frac{1}{N} \sum_{i=1}^{N}\left\|T_{i}\right\|_{2}^{2}=1
$$


(a)

(d)

(b)

(e)

(c)

(f)

## Kernel Localization

The operator $T$ should be understood as kernel localization:
From a kernel $\hat{g}(s)$ generate localized instances:
Kernel Localization

$$
\hat{g}: \mathbb{R}^{+} \mapsto \mathbb{R}
$$

$$
T_{j} g(i)=\sum_{\ell} \hat{g}\left(\lambda_{\ell}\right) u_{\ell}(i) u_{\ell}(j)
$$

By functional calculus, the linear operator

$$
f \mapsto g(\mathcal{L}) f
$$

is the kernelized convolution.

## Polynomial Localization

Given a spectral kernel $g$, construct the family of features:

$$
\phi_{n}(m)=\left(T_{n} g\right)(m) \quad \phi_{n}(m)=\sqrt{N} \sum_{\ell=0}^{N-1} \hat{g}\left(\lambda_{\ell}\right) u_{\ell}(m) u_{\ell}^{*}(n)
$$

Are these features localized?
Polynomial Kernels are $K$-Localized

$$
\widehat{p_{K}}\left(\lambda_{\ell}\right)=\sum_{k=0}^{K} a_{k} \lambda_{\ell}^{k} \quad \text { if } d(i, n)>K, \text { then }\left(T_{i} p_{K}\right)(n)=0
$$

## Polynomial Localization

Given a spectral kernel $g$, construct the family of features:

$$
\phi_{n}(m)=\left(T_{n} g\right)(m) \quad \phi_{n}(m)=\sqrt{N} \sum_{\ell=0}^{N-1} \hat{g}\left(\lambda_{\ell}\right) u_{\ell}(m) u_{\ell}^{*}(n)
$$

Are these features localized?

Suppose the GFT of the kernel is smooth enough (K+1 different.)
Construct an order $K$ polynomial approximation:

$$
\phi_{n}^{\prime}(m)=\left\langle\delta_{m}, P_{K}(\mathcal{L}) \delta_{n}\right\rangle \quad \text { Exactly localized in a } K \text {-ball around } n
$$

$\phi_{n}(m)=\left\langle\delta_{m}, g(\mathcal{L}) \delta_{n}\right\rangle \leadsto$ Should be well localized within $K$-ball around n !

## Polynomial Localization - Extended

$f$ is $(K+1)$-times differentiable:

$$
\inf _{q_{K}}\left\{\left\|f-q_{K}\right\|_{\infty}\right\} \leq \frac{\left[\frac{b-a}{2}\right]^{K+1}}{(K+1)!2^{K}}\left\|f^{(K+1)}\right\|_{\infty}
$$

Let $K_{i n}:=d(i, n)-1$

$$
\left|\left(T_{i} g\right)(n)\right| \leq \sqrt{N} \inf _{\overline{p_{K_{i n}}}}\left\{\sup _{\lambda \in\left[0, \lambda_{\max }\right]}\left|\hat{g}(\lambda)-\widehat{p_{K_{i n}}}(\lambda)\right|\right\}=\sqrt{N} \underset{\operatorname{pinf}_{K_{i n}}}{ }\left\{\left\|\hat{g}-\widehat{p_{K_{i n}}}\right\|_{\infty}\right\}
$$

## Regular Kernels are Localized

If the kernel is $d(i, n)$-times differentiable:

$$
\left|\left(T_{i} g\right)(n)\right| \leq\left[\frac{2 \sqrt{N}}{d_{i n}!}\left(\frac{\lambda_{\max }}{4}\right)^{d_{i n}} \sup _{\lambda \in\left[0, \lambda_{\max }\right]}\left|\hat{g}^{\left(d_{i n}\right)}(\lambda)\right|\right]
$$

## Polynomial Localization - Extended

Example: for the heat kernel $\hat{g}(\lambda)=e^{-\tau \lambda}$

$$
\frac{\left|\left(T_{i} g\right)(n)\right|}{\left\|T_{i} g\right\|_{2}} \leq \frac{2 \sqrt{N}}{d_{i n}!}\left(\frac{\tau \lambda_{\max }}{4}\right)^{d_{i n}} \leq \sqrt{\frac{2 N}{d_{i n} \pi}} e^{-\frac{1}{12 d_{i n}+1}}\left(\frac{\tau \lambda_{\max } e}{4 d_{i n}}\right)^{d_{i n}}
$$

We can estimate an explicit measure of spread in terms of the degrees:

$$
\begin{aligned}
& \Delta_{i}^{2}(f)=\frac{1}{\|f\|_{2}^{2}} \sum_{n=1}^{N} d_{i n}^{2}[f(n)]^{2} \\
& \Delta_{i}^{2}\left(T_{i} g\right) \leq \frac{\tau N \lambda_{\max } D_{i}}{(2 \pi)^{\frac{3}{2}}} e^{\frac{\tau \lambda_{\max e^{2}\left(D_{\max }-1\right)}^{4}}{2}} \\
& \tau \rightarrow 0 \Rightarrow T_{i} g \rightarrow \delta_{i}, \Delta_{i}^{2}\left(T_{i} g\right) \rightarrow 0 \\
& \tau \rightarrow+\infty \Rightarrow T_{i} g \rightarrow \frac{1}{\sqrt{N}}, \Delta_{i}^{2}\left(T_{i} g\right) \rightarrow \frac{1}{N} \sum_{n=1}^{N} d(i, n)^{2}
\end{aligned}
$$

## Remark on Implementation

Not necessary to compute spectral decomposition


Then wavelet operator expressed with powers of Laplacian:

$$
g(t \mathcal{L}) \simeq \sum_{k=0}^{K-1} a_{k}(t) \mathcal{L}^{k}
$$

And use sparsity of Laplacian in an iterative way

## Remark on Implementation

$$
\tilde{W}_{f}(t, j)=\left(p(\mathcal{L}) f^{\#}\right)_{j} \quad\left|W_{f}(t, j)-\tilde{W}_{f}(t, j)\right| \leq B\|f\|
$$

sup norm control (minimax or Chebyshev)

$$
\tilde{W}_{f}\left(t_{n}, j\right)=\left(\frac{1}{2} c_{n, 0} f^{\#}+\sum_{k=1}^{M_{n}} c_{n, k} \bar{T}_{k}(\mathcal{L}) f^{\#}\right)_{j}
$$

$\bar{T}_{k}(\mathcal{L}) f=\frac{2}{a_{1}}\left(\mathcal{L}-a_{2} I\right)\left(\bar{T}_{k-1}(\mathcal{L}) f\right)-\bar{T}_{k-2}(\mathcal{L}) f$

## Shifted Chebyshev polynomial

Computational cost dominated by matrix-vector multiply with (sparse) Laplacian matrix
Complexity: $O\left(\sum_{n=1}^{J} M_{n}|E|\right) \quad$ Note: "same" algorithm for adjoint !


## Non-local Wavelet Frame

- Non-local Wavelets are ...

... Graph Wavelets on Non-Local Graph

increasing scale
Interest: good adaptive sparsity basis


## Localization / Uncertainty

Competition between smoothness and localization in the spectral representation of kernels

$$
\text { Remark: } \quad \sigma_{t}^{2} \sigma_{\omega}^{2}=C \int_{\mathbb{R}} d t|t f(t)|^{2} \int_{\mathbb{R}} d t\left|f^{\prime}(t)\right|^{2}
$$

Smooth kernels can be used to construct controlled localized features
Example: Spectral Graph Wavelets

Localization/Smoothness generate sparsity (but more on that later)

## Summary so far

- We now have a simple black box theory to design and apply linear filters on graph data
- results on localisation, uncertainty
- fast, scalable algorithm
- all sorts of filter banks studied and used in litterature
- We can use filter banks to construct graph equivalent of linear transforms (wavelets, Gabor,..)
- We can extend stationary signal models
- (sub)-sampling theory


## Goal

Given partially observed information at the nodes of a graph


Can we robustly and efficiently infer missing information?
What signal model ?
How many observations ?
Influence of the structure of the graph?

## Notations

## L is real, symmetric PSD

orthonormal eigenvectors $\mathrm{U} \in \mathbb{R}^{n \times n}$ Graph Fourier Matrix non-negative eigenvalues $\boldsymbol{\lambda}_{1} \leqslant \boldsymbol{\lambda}_{2} \leqslant \ldots, \boldsymbol{\lambda}_{n}$

$$
\mathrm{L}=\mathrm{U} \wedge \mathrm{U}^{\top}
$$

$k$-bandlimited signals $\quad \boldsymbol{x} \in \mathbb{R}^{n}$
Fourier coefficients $\quad \hat{\boldsymbol{x}}=\mathrm{U}^{\top} \boldsymbol{x}$

$$
\boldsymbol{x}=\mathrm{U}_{k} \hat{\boldsymbol{x}}^{k} \quad \hat{\boldsymbol{x}}^{k} \in \mathbb{R}^{k}
$$

$$
\mathrm{U}_{k}:=\left(\boldsymbol{u}_{1}, \ldots, \boldsymbol{u}_{k}\right) \in \mathbb{R}^{n \times k}
$$

## Sampling Model

$$
\begin{gathered}
\boldsymbol{p} \in \mathbb{R}^{n} \quad \boldsymbol{p}_{i}>0 \quad\|\boldsymbol{p}\|_{1}=\sum_{i=1}^{n} \boldsymbol{p}_{i}=1 \\
\mathrm{P}:=\operatorname{diag}(\boldsymbol{p}) \in \mathbb{R}^{n \times n}
\end{gathered}
$$

Draw independently $m$ samples (random sampling)

$$
\mathbb{P}\left(\omega_{j}=i\right)=\boldsymbol{p}_{i}, \quad \forall j \in\{1, \ldots, m\} \text { and } \forall i \in\{1, \ldots, n\}
$$

$$
\begin{gathered}
\boldsymbol{y}_{j}:=\boldsymbol{x}_{\omega_{j}}, \quad \forall j \in\{1, \ldots, m\} \\
\boldsymbol{y}=\mathrm{M} \boldsymbol{x}
\end{gathered}
$$

## Sampling Model

$$
\frac{\left\|\mathrm{U}_{k}^{\top} \boldsymbol{\delta}_{i}\right\|_{2}}{\left\|\mathrm{U}^{\top} \boldsymbol{\delta}_{i}\right\|_{2}}=\frac{\left\|\mathrm{U}_{k}^{\top} \boldsymbol{\delta}_{i}\right\|_{2}}{\left\|\boldsymbol{\delta}_{i}\right\|_{2}}=\left\|\mathrm{U}_{k}^{\top} \boldsymbol{\delta}_{i}\right\|_{2}
$$

How much a perfect impulse can be concentrated on first $k$ eigenvectors
Carries interesting information about the graph
Ideally: $\quad \boldsymbol{p}_{i}$ large wherever $\left\|\mathrm{U}_{k}^{\top} \boldsymbol{\delta}_{i}\right\|_{2}$ is large

## Graph Coherence

$$
\begin{aligned}
& \nu_{\boldsymbol{p}}^{k}:=\max _{1 \leqslant i \leqslant n}\left\{\boldsymbol{p}_{i}^{-1 / 2}\left\|\mathrm{U}_{k}^{\top} \boldsymbol{\delta}_{i}\right\|_{2}\right\} \\
& \text { Rem: } \quad \nu_{\boldsymbol{p}}^{k} \geqslant \sqrt{k}
\end{aligned}
$$

## Stable Embedding

Theorem 1 (Restricted isometry property). Let M be a random subsampling matrix with the sampling distribution $\boldsymbol{p}$. For any $\delta, \epsilon \in(0,1)$, with probability at least $1-\epsilon$,

$$
\begin{equation*}
(1-\delta)\|\boldsymbol{x}\|_{2}^{2} \leqslant \frac{1}{m}\left\|\mathrm{MP}^{-1 / 2} \boldsymbol{x}\right\|_{2}^{2} \leqslant(1+\delta)\|\boldsymbol{x}\|_{2}^{2} \tag{1}
\end{equation*}
$$

for all $\boldsymbol{x} \in \operatorname{span}\left(\mathrm{U}_{k}\right)$ provided that

$$
\begin{equation*}
m \geqslant \frac{3}{\delta^{2}}\left(\nu_{\boldsymbol{p}}^{k}\right)^{2} \log \left(\frac{2 k}{\epsilon}\right) \tag{2}
\end{equation*}
$$

$\mathrm{MP}^{-1 / 2} \boldsymbol{x}=\mathrm{P}_{\Omega}^{-1 / 2} \mathrm{M} \boldsymbol{x} \quad$ Only need M , re-weighting offline

$$
\left(\nu_{\boldsymbol{p}}^{k}\right)^{2} \geqslant k
$$

Need to sample at least $k$ nodes

Proof similar to CS in bounded ONB but simpler since model is a subspace (not a union)

## Stable Embedding

$$
\left(\nu_{\boldsymbol{p}}^{k}\right)^{2} \geqslant k \quad \text { Need to sample at least } k \text { nodes }
$$

## Can we reduce to optimal amount ?

$$
\text { Variable Density Sampling } \quad \boldsymbol{p}_{i}^{*}:=\frac{\left\|\mathrm{U}_{k}^{\top} \boldsymbol{\delta}_{i}\right\|_{2}^{2}}{k}, \quad i=1, \ldots, n
$$

is such that: $\quad\left(\nu_{\boldsymbol{p}}^{k}\right)^{2}=k \quad$ and depends on structure of graph

Corollary 1. Let M be a random subsampling matrix constructed with the sampling distribution $\boldsymbol{p}^{*}$. For any $\delta, \epsilon \in(0,1)$, with probability at least $1-\epsilon$,

$$
(1-\delta)\|\boldsymbol{x}\|_{2}^{2} \leqslant \frac{1}{m}\left\|\mathrm{MP}^{-1 / 2} \boldsymbol{x}\right\|_{2}^{2} \leqslant(1+\delta)\|\boldsymbol{x}\|_{2}^{2}
$$

for all $\boldsymbol{x} \in \operatorname{span}\left(\mathrm{U}_{k}\right)$ provided that

$$
m \geqslant \frac{3}{\delta^{2}} k \log \left(\frac{2 k}{\epsilon}\right)
$$

## Recovery Procedures

$$
\begin{array}{ll}
\boldsymbol{y}=\mathrm{M} \boldsymbol{x}+\boldsymbol{n} & \boldsymbol{y} \in \mathbb{R}^{m} \\
& \boldsymbol{x} \in \operatorname{span}\left(\mathrm{U}_{k}\right) \quad \text { stable embedding }
\end{array}
$$

Standard Decoder

$$
\min _{\boldsymbol{z} \in \operatorname{span}\left(U_{k}\right)}\left\|\mathrm{P}_{\Omega}^{-1 / 2}(\mathrm{M} \boldsymbol{z}-\boldsymbol{y})\right\|_{2}
$$

re-weighting for RIP
need projector

## Recovery Procedures

$$
\begin{array}{ll}
\boldsymbol{y}=\mathrm{M} \boldsymbol{x}+\boldsymbol{n} & \boldsymbol{y} \in \mathbb{R}^{m} \\
& \boldsymbol{x} \in \operatorname{span}\left(\mathrm{U}_{k}\right) \quad \text { stable embedding }
\end{array}
$$

Efficient Decoder:

$$
\min _{\boldsymbol{z} \in \mathbb{R}^{n}}\left\|\mathrm{P}_{\Omega}^{-1 / 2}(\mathrm{M} \boldsymbol{z}-\boldsymbol{y})\right\|_{2}^{2}+\gamma\left(\boldsymbol{z}^{\top} g(\mathrm{~L}) \boldsymbol{z}\right.
$$

soft constrain on frequencies efficient implementation

## Analysis of Standard Decoder

## Standard Decoder:

$$
\min _{\boldsymbol{z} \in \operatorname{span}\left(\mathrm{U}_{k}\right)}\left\|\mathrm{P}_{\Omega}^{-1 / 2}(\mathrm{M} \boldsymbol{z}-\boldsymbol{y})\right\|_{2}
$$

Theorem 1. Let $\Omega$ be a set of $m$ indices selected independently from $\{1, \ldots, n\}$ with sampling distribution $\boldsymbol{p} \in \mathbb{R}^{n}$, and M the associated sampling matrix. Let $\epsilon, \delta \in(0,1)$ and $m \geqslant \frac{3}{\delta^{2}}\left(\nu_{\boldsymbol{p}}^{k}\right)^{2} \log \left(\frac{2 k}{\epsilon}\right)$. With probability at least $1-\epsilon$, the following holds for all $\boldsymbol{x} \in \operatorname{span}\left(\mathrm{U}_{k}\right)$ and all $\boldsymbol{n} \in \mathbb{R}^{m}$.
i) Let $\boldsymbol{x}^{*}$ be the solution of Standard Decoder with $\boldsymbol{y}=\mathrm{M} \boldsymbol{x}+\boldsymbol{n}$. Then,

$$
\begin{equation*}
\left\|\boldsymbol{x}^{*}-\boldsymbol{x}\right\|_{2} \leqslant \frac{2}{\sqrt{m(1-\delta)}}\left\|\mathrm{P}_{\Omega}^{-1 / 2} \boldsymbol{n}\right\|_{2} \tag{1}
\end{equation*}
$$

Exact recovery when noiseless

## Analysis of Efficient Decoder

Efficient Decoder:

$$
\min _{\boldsymbol{z} \in \mathbb{R}^{n}}\left\|\mathrm{P}_{\Omega}^{-1 / 2}(\mathrm{M} \boldsymbol{z}-\boldsymbol{y})\right\|_{2}^{2}+\boldsymbol{z}^{\top} g(\mathrm{~L}) \boldsymbol{z}
$$

Filter reshapes Fourier coefficients

$$
\begin{array}{cc}
h: \mathbb{R} \rightarrow \mathbb{R} \quad \boldsymbol{x}_{h}:=\mathrm{U} \operatorname{diag}(\hat{\boldsymbol{h}}) \mathrm{U}^{\top} \boldsymbol{x} \in \mathbb{R}^{n} \\
\hat{\boldsymbol{h}}=\left(h\left(\boldsymbol{\lambda}_{1}\right), \ldots, h\left(\boldsymbol{\lambda}_{n}\right)\right)^{\top} \in \mathbb{R}^{n} \\
p(t)=\sum_{i=0}^{d} \alpha_{i} t^{i} \quad \boldsymbol{x}_{p}=\mathrm{U} \operatorname{diag}(\hat{\boldsymbol{p}}) \mathrm{U}^{\top} \boldsymbol{x}=\sum_{i=0}^{d} \alpha_{i} \mathrm{~L}^{i} \boldsymbol{x}
\end{array}
$$

Pick special polynomials and use e.g. recurrence relations for fast filterin (with sparse matrix-vector multiply only)

## Analysis of Efficient Decoder

Efficient Decoder:

$$
\begin{aligned}
& \min _{\boldsymbol{z} \in \mathbb{R}^{n}} \| \mathrm{P}_{\Omega}^{-1 / 2}(\mathrm{M} \boldsymbol{z}-\boldsymbol{y}) \|_{2}^{2}+\boldsymbol{z}^{\top} g(\mathrm{~L}) \boldsymbol{z} \\
& \text { non-negative }
\end{aligned}
$$

Favours reconstruction of approximately band-limited signals

Ideal filter yields Standard Decoder

$$
i_{\lambda_{k}}(t):= \begin{cases}0 & \text { if } t \in\left[0, \lambda_{k}\right] \\ +\infty & \text { otherwise }\end{cases}
$$

## Analysis of Efficient Decoder

Theorem 1. Let $\Omega, \mathrm{M}, \mathrm{P}, m$ as before and $M_{\max }>0$ be a constant such that $\left\|\mathrm{MP}^{-1 / 2}\right\|_{2} \leqslant M_{\max }$. Let $\epsilon, \delta \in(0,1)$. With probability at least $1-\epsilon$, the following holds for all $\boldsymbol{x} \in \operatorname{span}\left(\mathrm{U}_{k}\right)$, all $\boldsymbol{n} \in \mathbb{R}^{n}$, all $\gamma>0$, and all nonnegative and nondecreasing polynomial functions $g$ such that $g\left(\boldsymbol{\lambda}_{k+1}\right)>0$.

Let $\boldsymbol{x}^{*}$ be the solution of Efficient Decoder with $\boldsymbol{y}=\mathrm{M} \boldsymbol{x}+\boldsymbol{n}$. Then,

$$
\begin{align*}
\left\|\boldsymbol{\alpha}^{*}-\boldsymbol{x}\right\|_{2} \leqslant \frac{1}{\sqrt{m(1-\delta)}}\left[\left(2+\frac{M_{\max }}{\sqrt{\gamma g\left(\boldsymbol{\lambda}_{k+1}\right)}}\right) \|\right. & \mathrm{P}_{\Omega}^{-1 / 2} \boldsymbol{n} \|_{2} \\
& \left.+\left(M_{\max } \sqrt{\frac{g\left(\boldsymbol{\lambda}_{k}\right)}{g\left(\boldsymbol{\lambda}_{k+1}\right)}}+\sqrt{\gamma g\left(\boldsymbol{\lambda}_{k}\right)}\right)\|\boldsymbol{x}\|_{2}\right] \tag{1}
\end{align*}
$$

and

$$
\begin{equation*}
\left\|\boldsymbol{\beta}^{*}\right\|_{2} \leqslant \frac{1}{\sqrt{\gamma g\left(\boldsymbol{\lambda}_{k+1}\right)}}\left\|\mathrm{P}_{\Omega}^{-1 / 2} \boldsymbol{n}\right\|_{2}+\sqrt{\frac{g\left(\boldsymbol{\lambda}_{k}\right)}{g\left(\boldsymbol{\lambda}_{k+1}\right)}}\|\boldsymbol{x}\|_{2} \tag{2}
\end{equation*}
$$

where $\boldsymbol{\alpha}^{*}:=\mathrm{U}_{k} \mathrm{U}_{k}^{\top} \boldsymbol{x}^{*}$ and $\boldsymbol{\beta}^{*}:=\left(\mathrm{I}-\mathrm{U}_{k} \mathrm{U}_{k}^{\top}\right) \boldsymbol{x}^{*}$.

## Analysis of Efficient Decoder

Noiseless case:
$\left\|\boldsymbol{x}^{*}-\boldsymbol{x}\right\|_{2} \leqslant \frac{1}{\sqrt{m(1-\delta)}}\left(M_{\max } \sqrt{\frac{g\left(\boldsymbol{\lambda}_{k}\right)}{g\left(\boldsymbol{\lambda}_{k+1}\right)}}+\sqrt{\gamma g\left(\boldsymbol{\lambda}_{k}\right)}\right)\|\boldsymbol{x}\|_{2}+\sqrt{\frac{g\left(\boldsymbol{\lambda}_{k}\right)}{g\left(\boldsymbol{\lambda}_{k+1}\right)}}\|\boldsymbol{x}\|_{2}$
$g\left(\boldsymbol{\lambda}_{k}\right)=0+$ non-decreasing implies perfect reconstruction

## Otherwise:

choose $\gamma$ as close as possible to 0 and seek to minimise the ratio $g\left(\boldsymbol{\lambda}_{k}\right) / g\left(\boldsymbol{\lambda}_{k+1}\right)$
Choose filter to increase spectral gap?
Clusters are of course good
Noise:

$$
\left\|\mathrm{P}_{\Omega}^{-1 / 2} \boldsymbol{n}\right\|_{2} /\|\boldsymbol{x}\|_{2}
$$

## Estimating the Optimal Distribution

$$
\text { Need to estimate }\left\|\mathrm{U}_{k}^{\top} \boldsymbol{\delta}_{i}\right\|_{2}^{2}
$$

Filter random signals with ideal low-pass filter:

$$
\begin{aligned}
& \boldsymbol{r}_{{\lambda_{\boldsymbol{\lambda}}}}=\mathrm{U} \operatorname{diag}\left(\boldsymbol{\lambda}_{1}, \ldots, \boldsymbol{\lambda}_{k}, 0, \ldots, 0\right) \mathrm{U}^{\top} \boldsymbol{r}=\mathrm{U}_{k} \mathrm{U}_{k}^{\top} \boldsymbol{r} \\
& \mathbb{E}\left(\boldsymbol{r}_{b_{\boldsymbol{\lambda}_{k}}}\right)_{i}^{2}=\boldsymbol{\delta}_{i}^{\top} \mathrm{U}_{k} \mathrm{U}_{k}^{\top} \mathbb{E}\left(\boldsymbol{r} \boldsymbol{r}^{\top}\right) \mathrm{U}_{k} \mathrm{U}_{k}^{\top} \boldsymbol{\delta}_{i}=\left\|\mathrm{U}_{k}^{\top} \boldsymbol{\delta}_{i}\right\|_{2}^{2}
\end{aligned}
$$

In practice, one may use a polynomial approximation of the ideal filter and:

$$
\begin{gathered}
\tilde{\boldsymbol{p}}_{i}:=\frac{\sum_{l=1}^{L}\left(\boldsymbol{r}_{c_{\lambda_{k}}}^{l}\right)_{i}^{2}}{\sum_{i=1}^{n} \sum_{l=1}^{L}\left(\boldsymbol{r}_{c_{\lambda_{k}}}^{l}\right)_{i}^{2}} \\
L \geqslant \frac{C}{\delta^{2}} \log \left(\frac{2 n}{\epsilon}\right)
\end{gathered}
$$

## Estimating the Eigengap

Again, low-pass filtering random signals:
$(1-\delta) \sum_{i=1}^{n}\left\|\mathrm{U}_{j^{*}}^{\top} \boldsymbol{\delta}_{i}\right\|_{2}^{2} \leqslant \sum_{i=1}^{n} \sum_{l=1}^{L}\left(\boldsymbol{r}_{b_{\lambda}}^{l}\right)_{i}^{2} \leqslant(1+\delta) \sum_{i=1}^{n}\left\|\mathrm{U}_{j^{*}}^{\top} \boldsymbol{\delta}_{i}\right\|_{2}^{2}$
Since: $\quad \sum_{i=1}^{n}\left\|\mathrm{U}_{j^{*}}^{\top} \boldsymbol{\delta}_{i}\right\|_{2}^{2}=\left\|\mathrm{U}_{j^{*}}\right\|_{\text {Frob }}^{2}=j^{*}$

We have: $(1-\delta) j^{*} \leqslant \sum_{i=1}^{n} \sum_{l=1}^{L}\left(\boldsymbol{r}_{b_{\lambda}}^{l}\right)_{i}^{2} \leqslant(1+\delta) j^{*}$

Dichotomy using the filter bandwidth

## Experiments

## Community graph



## Experiments







## Experiments



## Experiments


(a)


## Compressive Spectral Clustering

Clustering equivalent to recovery of cluster assignment functions

Well-defined clusters $->$ band-limited assignment functions!

Generate features by filtering random signals


## Compressive Spectral Clustering

Clustering equivalent to recovery of cluster assignment functions

Well-defined clusters -> band-limited assignment functions!

Generate features by filtering random signals

$$
\text { by Johnson-Lindenstrauss } \quad \eta=\frac{4+2 \beta}{\epsilon^{2} / 2-\epsilon^{3} / 3} \log n
$$

Each feature map is smooth, therefore keep

$$
m \geqslant \frac{6}{\delta^{2}} \nu_{k}^{2} \log \left(\frac{k}{\epsilon^{\prime}}\right)
$$

Use k-means on compressed data and feed into Efficient Decoder ${ }^{68}$

## Compressive Spectral Clustering



## Outlook



- Application of graph signal processing techniques to real science and engineering problems is in its infancy
- Connections with "traditional" signal processing, machine learning, ...


## Thank you!

