Analyse de données en grande dimension sur graphes et réseaux

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Mathématiques et Grandes Dimensions
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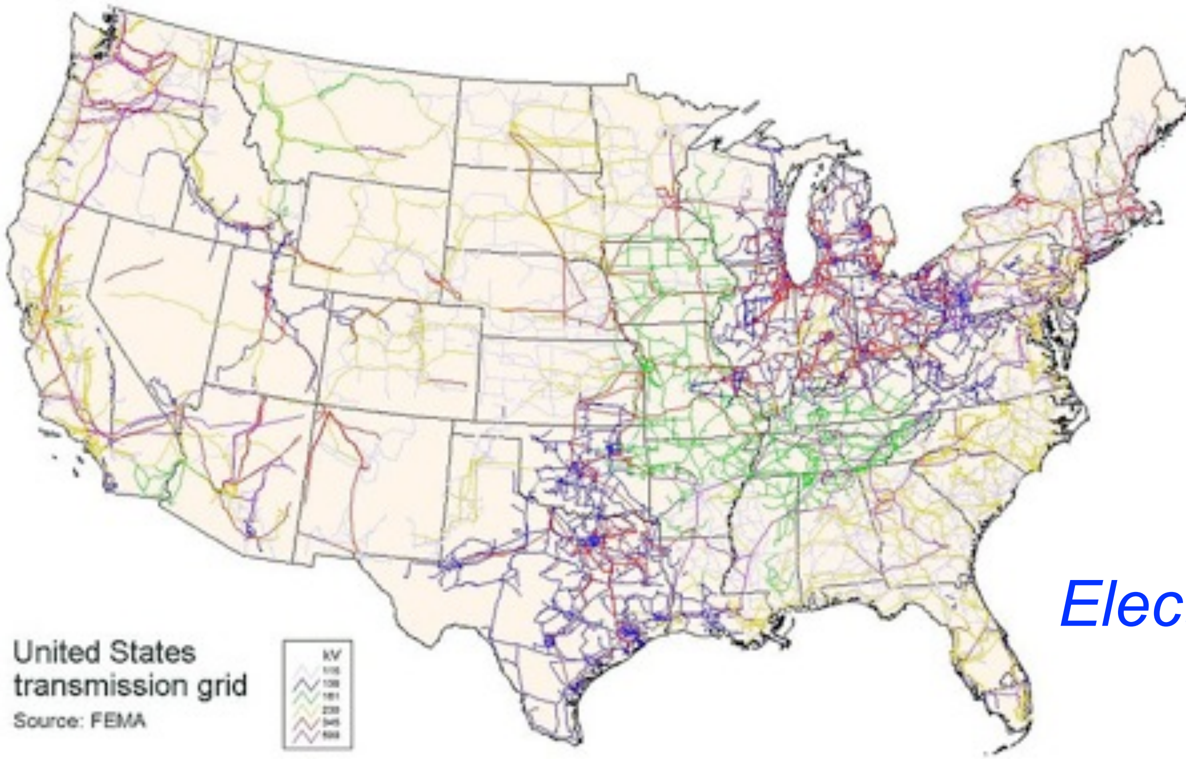
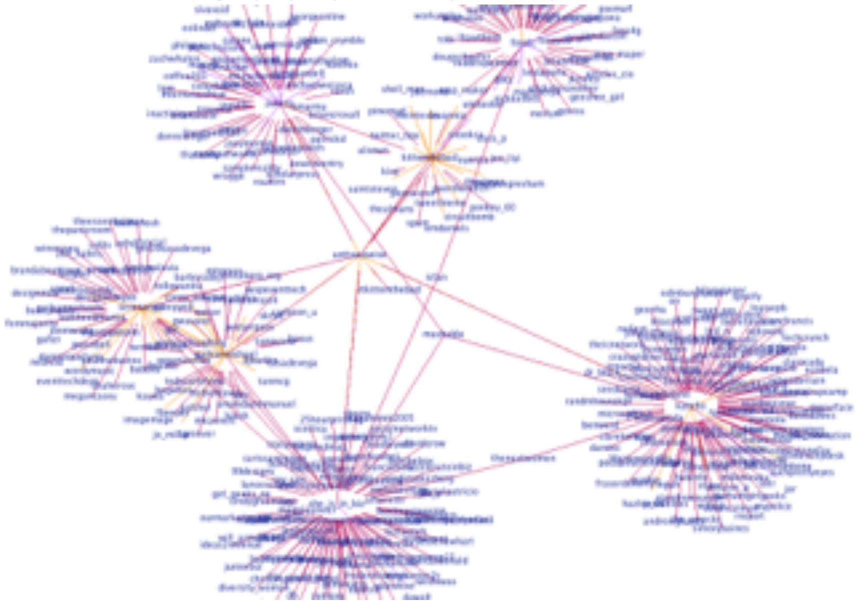
Graphs for Data Modeling



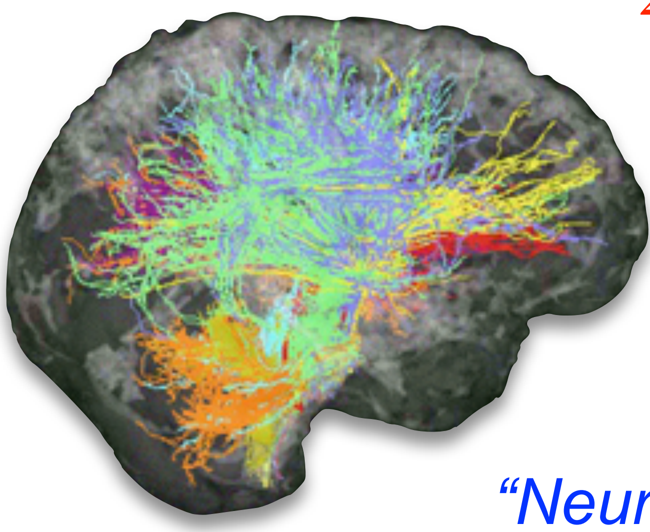
Electrical Network

Social Network



2010: 980 exabytes of new digital information

Big Data



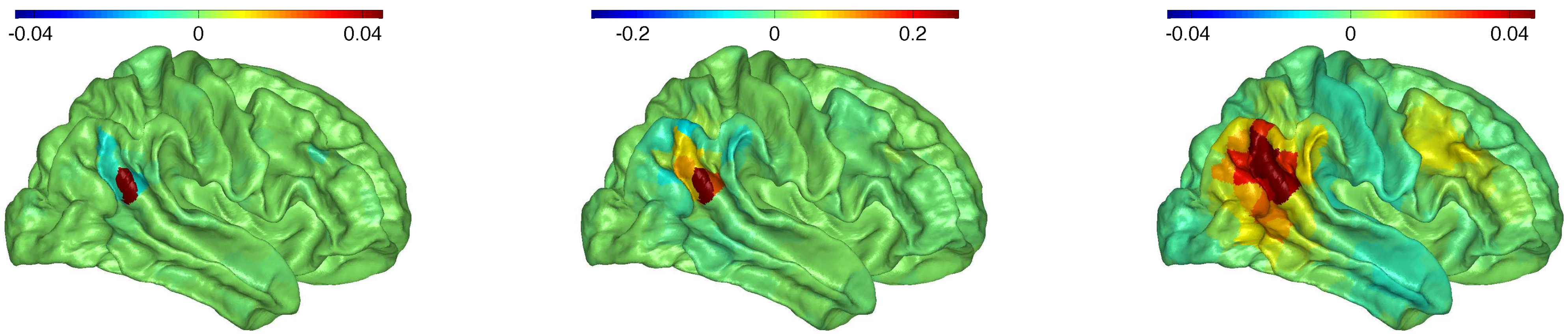
"Neuronal" Network

Ubiquitous sensing

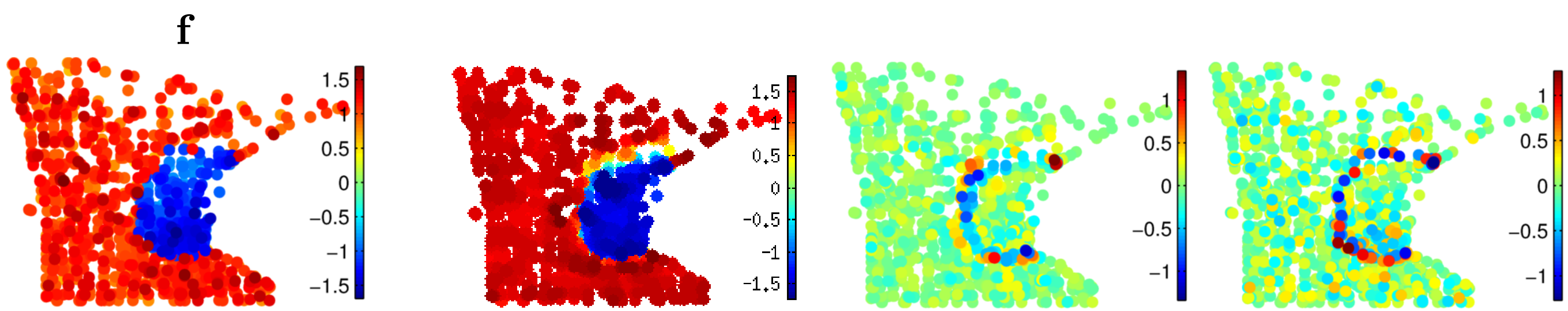
Graphs for Data Modeling

To process or analyze one typically extracts “features” or apply transforms

Local multi-scale averages or multi-scale differentials (wavelets)



The localization/scale properties often induces interesting effects such as sparsity:



Outline

- Wavelets on (undirected) graps
  - Definitions, implementation
  - Localization
- Schematic application to (transductive) learning

Graphs, Laplacian and Spectral Theory

$G = (V, E, w)$ weighted, undirected graph

Non-normalized Laplacian: $\mathcal{L} = D - A$ Real, symmetric

$$(\mathcal{L}f)(i) = \sum_{i \sim j} w_{i,j}(f(i) - f(j))$$

Why Laplacian ? $\mathbb{Z}^2$ with usual stencil

$$(\mathcal{L}f)_{i,j} = 4f_{i,j} - f_{i+1,j} - f_{i-1,j} - f_{i,j+1} - f_{i,j-1}$$

In general, graph laplacian from nicely sampled manifold converges to Laplace-Beltrami operator

Remark:

$$\mathcal{L}^{norm} = D^{-1/2}\mathcal{L}D^{-1/2} = I - D^{-1/2}AD^{-1/2}$$

Graphs, Laplacian and Spectral Theory

eigen decomposition of Laplacian $\Rightarrow$ Spectral Graph Theory

$$\{\chi_l\}_{l=0,1,\ldots,N-1} \qquad 0 = \lambda_0 < \lambda_1 \leq \lambda_2 \ldots \leq \lambda_{N-1} := \lambda_{\max}$$

The Graph Laplacian induces a convenient Fourier-like transform

$$\hat{f}(\ell) := \langle f, \chi_l \rangle = \sum_{n=1}^{N} \chi_\ell^*(n) f(n)$$

$$\boxed{\mu := \max_{\substack{\ell \in \{0,1,\ldots,N-1\} \\ i \in \{1,2,\ldots,N\}}} |\langle \chi_\ell, \delta_i \rangle| \in \left[\frac{1}{\sqrt{N}}, 1\right]}$$

Smoothness via Laplacian

Example (Belkin, Niyogi)

Affinity between data points represented by edge weights (affinity matrix W)

measure of smoothness:
$$\Delta f = \sum_{i,j \in X} \mathbf{W}_{ij}(f(x_i) - f(x_j))^2$$
$$= \mathbf{f}^t L \mathbf{f} \quad L = W - D$$

Revisit ridge regression:
$$\|\mathbf{X}_S^t \beta - \mathbf{y}\|_2^2 + \alpha\|\beta\|_2^2 + \gamma\beta^t \mathbf{X} L \mathbf{X}^t \beta$$

Solution is smooth in graph "geometry"

$$\|f\|_{G,2s}^2 = \sum_l \lambda_l^{2s} |\hat{f}(\lambda_l)|^2$$ discrete Sobolev semi-norm on G

Smoothness via Laplacian

$$\operatorname*{argmin}_f \frac{\tau}{2}\|f - y\|_2^2 + f^{\mathrm{T}}\mathcal{L}^r f \quad \Rightarrow \quad \mathcal{L}^r f_* + \frac{\tau}{2}(f_* - y) = 0$$

Graph Fourier

$$\Rightarrow \quad \widehat{\mathcal{L}^r f_*}(\ell) + \tfrac{\tau}{2}\left(\widehat{f_*}(\ell) - \hat{y}(\ell)\right) = 0, \quad \forall \ell \in \{0, 1, \ldots, N-1\}$$

$$\Rightarrow \quad \widehat{f_*}(\ell) = \frac{\tau}{\tau + 2\lambda_\ell^r}\hat{y}(\ell)$$

"Low pass" filtering !

Simple linear features: $\hat{f}(\ell)\hat{g}(\lambda_\ell; p) \Rightarrow g(\mathcal{L}; p)$

"Convolutions" and "Translations"

$$(f * g)(n) := \sum_{\ell=0}^{N-1} \hat{f}(\ell)\hat{g}(\ell)\chi_\ell(n)$$

Inherits a lot of properties of the usual convolution

associativity, distributivity, diagonalized by GFT

$$g_0(n) \ := \ \textstyle\sum_{\ell=0}^{N-1} \chi_\ell(n) \quad \Longrightarrow \quad f * g_0 = f$$

$$\mathcal{L}(f * g) = (\mathcal{L}f) * g = f * (\mathcal{L}g)$$

Use convolution to induce translations

$$(T_i f)\,(n) := \sqrt{N}(f * \delta_i)(n) = \sqrt{N}\sum_{\ell=0}^{N-1} \hat{f}(\ell)\chi_\ell^*(i)\chi_\ell(n)$$

Spectral Graph Wavelets

$G=(E,V)$ a weighted undirected graph, with Laplacian $\mathcal{L} = D - A$

Dilation operates through operator: $T_g^t = g(t\mathcal{L})$

Translation (localization):

Define $\psi_{t,j} = T_g^t \delta_j$ response to a delta at vertex j

$$\psi_{t,j}(i) = \sum_{\ell=0}^{N-1} g(t\lambda_\ell)\chi_\ell^*(j)\chi_\ell(i) \qquad \mathcal{L}\chi_\ell(j) = \lambda_\ell \chi_\ell(j)$$

$$\psi_{t,a}(u) = \int_{\mathbb{R}} d\omega\, \hat{\psi}(t\omega) e^{-j\omega a} e^{j\omega u}$$

And so formally define the graph wavelet coefficients of f:

$$W_f(t,j) = \langle \psi_{t,j}, f \rangle \qquad W_f(t,j) = T_g^t f(j) = \sum_{\ell=0}^{N-1} g(t\lambda_\ell)\hat{f}(\ell)\chi_\ell(j)$$

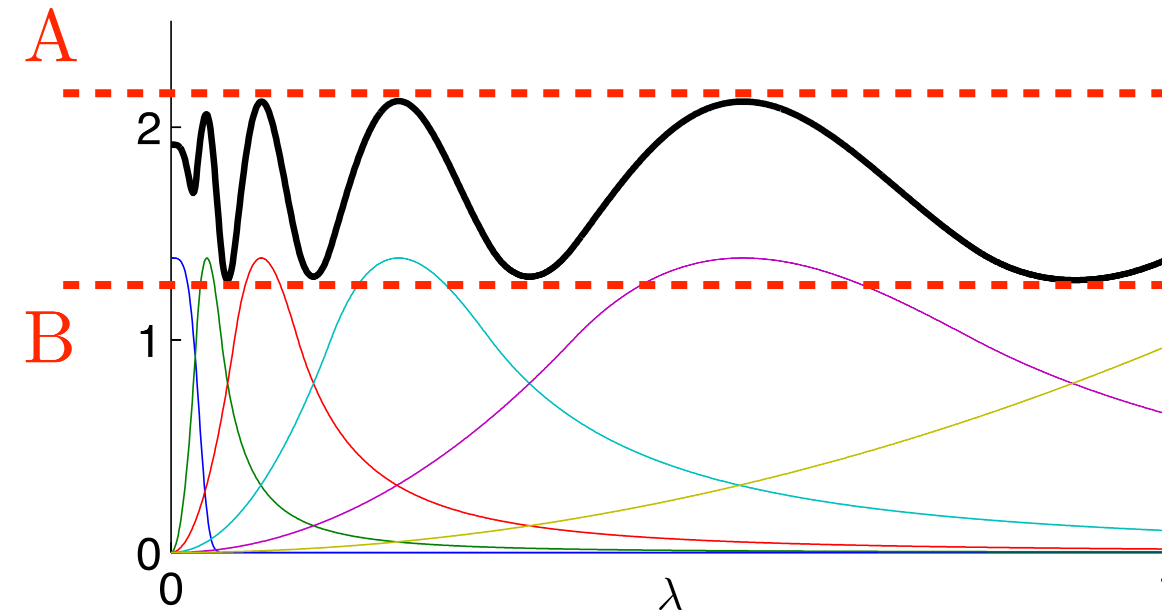
Frames

$\exists\, A, B > O,\ \exists h : \mathbb{R}_+ \to \mathbb{R}_+$ (i.e. scaling function)

$$0 < A \leqslant h^2(u) + \sum_s g(t_s u)^2 \leqslant B < \infty$$

scaling function *wavelets*

$\phi_n = T_h \delta_n = h(\mathcal{L})\delta_n$

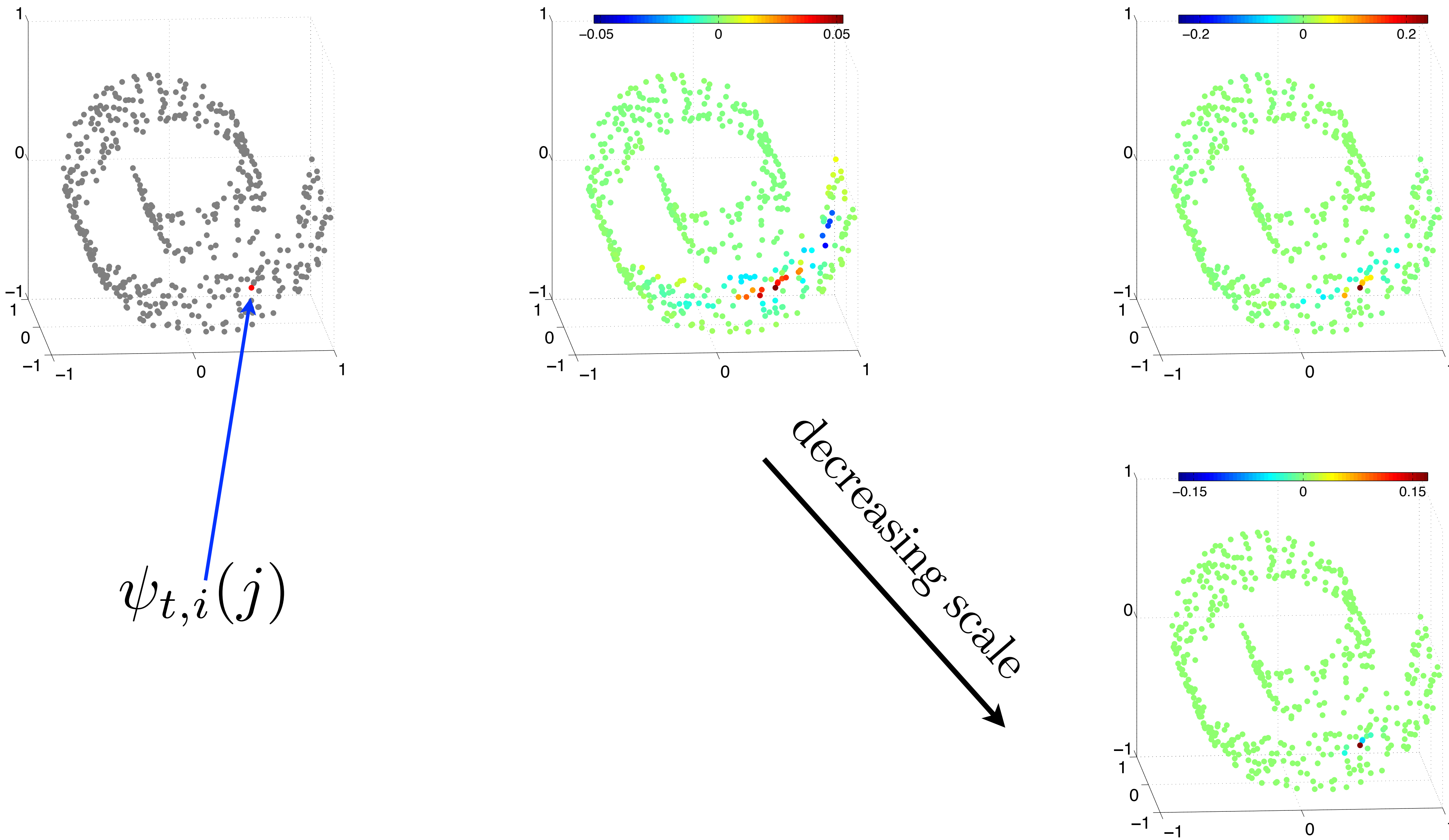


A simple way to get a tight frame:

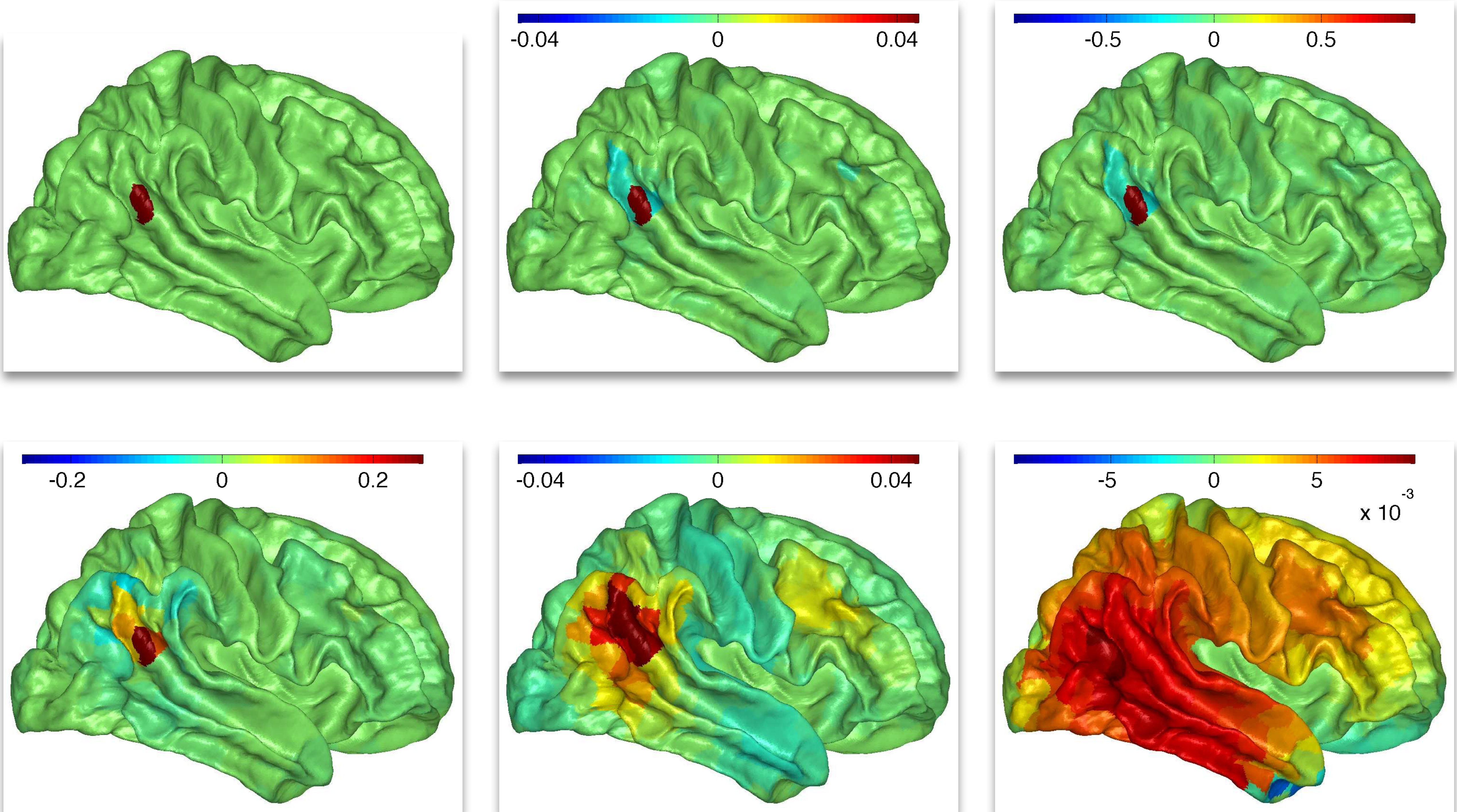
$$\gamma(\lambda_\ell) = \int_{1/2}^{1} \frac{dt}{t}\, g^2(t\lambda_\ell) \implies \tilde{g}(\lambda_\ell) = \sqrt{\gamma(\lambda_\ell) - \gamma(2\lambda_\ell)}$$

for any admissible kernel g

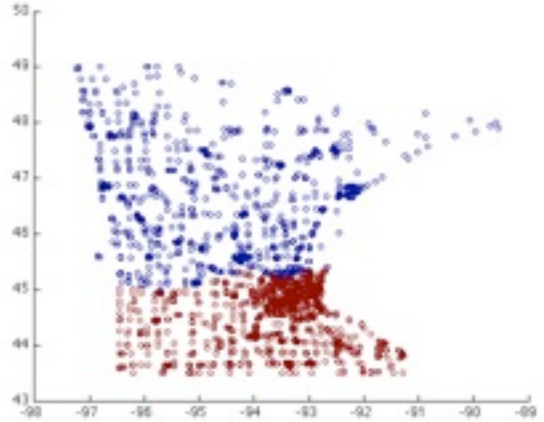
Scaling & Localization



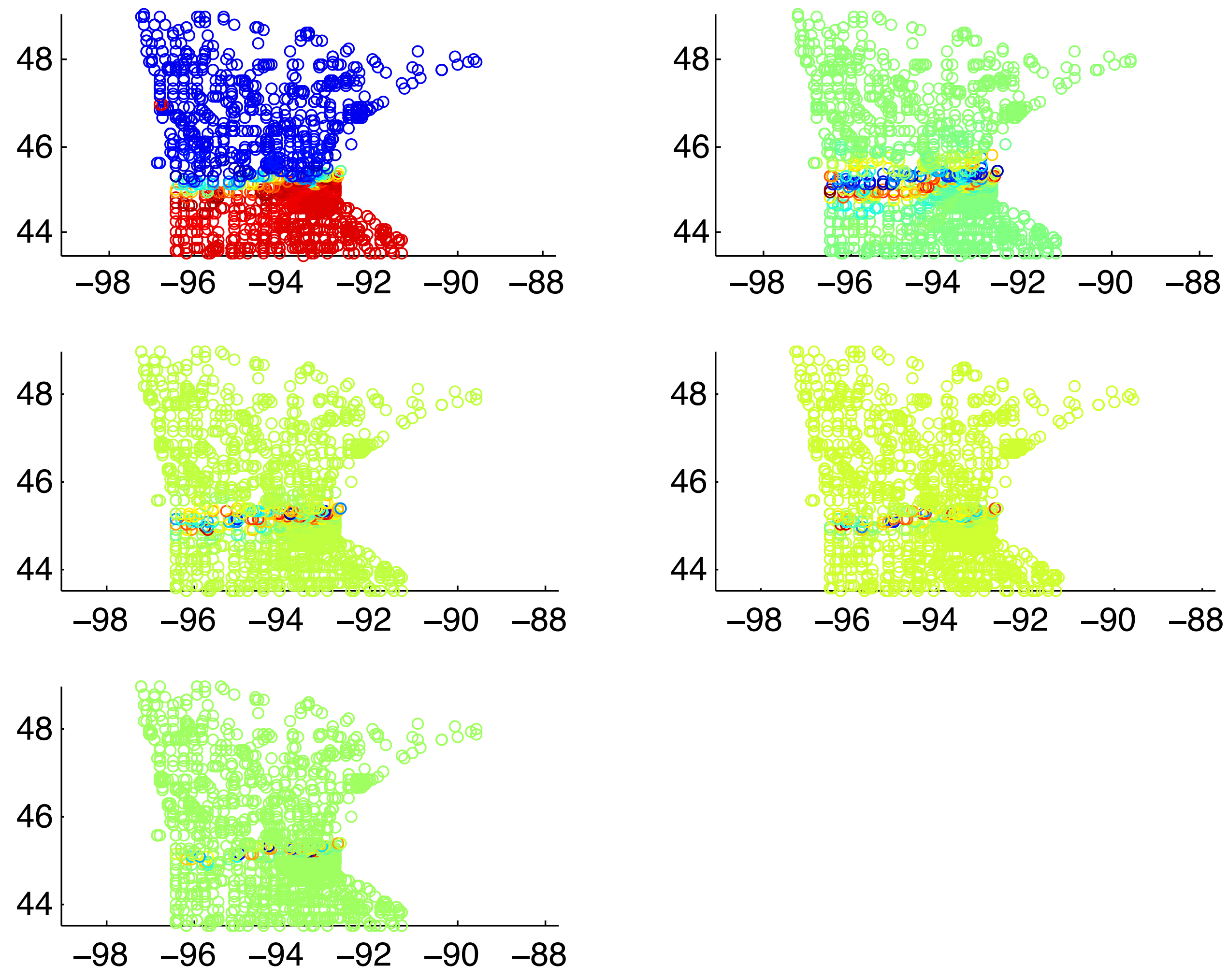
Example



Sparsity and Smoothness on Graphs



scaling functions coeffs



Polynomial Localization

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

$$\phi_n(m) = \big(T_n g\big)(m) \qquad \phi_n(m) = \sqrt{N} \sum_{\ell=0}^{N-1} \hat{g}(\lambda_\ell)\chi_\ell^*(m)\chi_\ell^*(n)$$

Are these features localized ?

Suppose the GFT of the kernel is smooth enough (K+1 different.):

$$B = \sup_x |\hat{g}^{(K+1)}(x)|$$

Construct an order K polynomial approximation:

$$\sup_\ell |\hat{g}(x) - P_K(x)| \leq \frac{B}{2^K (K+1)!}$$

Polynomial Localization

$$\sup_{\ell} |\hat{g}(x) - P_K(x)| \leq \frac{B}{2^K (K+1)!}$$

Now consider:

$$\phi_n(m) = \langle \delta_m, g(\mathcal{L}) \delta_n \rangle$$

$$\phi'_n(m) = \langle \delta_m, P_K(\mathcal{L}) \delta_n \rangle$$

Exactly localized in a K-ball around n

The original feature is well-localized in a K-ball around n:

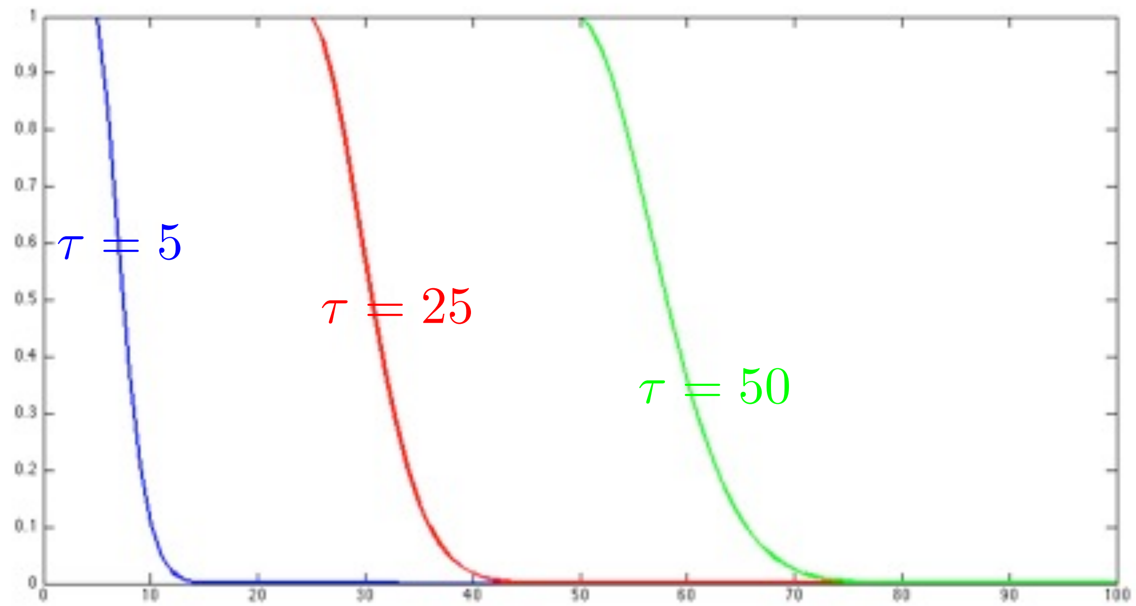
$$B_{\hat{g}}(K) = \inf_{\widehat{p_k}} \left\{ \sup_{\lambda \in [0, \lambda_{\max}]} |\hat{g}(\lambda) - \widehat{p_k}(\lambda)| \right\}$$

$$d_{in} > K \quad |(T_i g)(n)| \leq \sqrt{N} B_{\hat{g}}(d_{in} - 1)$$

Bounds on Localization

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

$$\frac{|(T_i g)(n)|}{\|T_i g\|_2} \leq \frac{2\sqrt{N}}{d_{in}!} \left(\frac{\tau\lambda_{\max}}{4} \right)^{d_{in}} \leq \sqrt{\frac{2N}{d_{in}\pi}} e^{-\frac{1}{12d_{in}+1}} \left(\frac{\tau\lambda_{\max} e}{4d_{in}} \right)^{d_{in}}$$



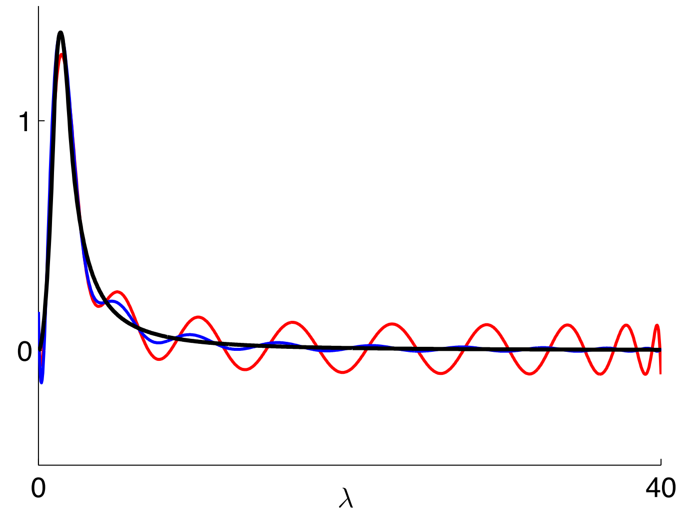
Remark on Implementation

Not necessary to compute spectral decomposition for filtering

Polynomial approximation :

$$g(t\omega) \simeq \sum_{k=0}^{K-1} a_k(t) p_k(\omega)$$

ex: Chebyshev, minimax



Then wavelet operator expressed with powers of Laplacian:

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

And use sparsity of Laplacian in an iterative way

Remark on Implementation

$$\tilde{W}_f(t,j) = \left(p(\mathcal{L})f^{\#}\right)_j \qquad |W_f(t,j) - \tilde{W}_f(t,j)| \leq B\|f\|$$

sup norm control (minimax or Chebyshef)

$$\tilde{W}_f(t_n,j) = \left(\frac{1}{2}c_{n,0}f^{\#} + \sum_{k=1}^{M_n} c_{n,k}\overline{T}_k(\mathcal{L})f^{\#}\right)_j$$

$$\overline{T}_k(\mathcal{L})f = \frac{2}{a_1}(\mathcal{L} - a_2 I)\left(\overline{T}_{k-1}(\mathcal{L})f\right) - \overline{T}_{k-2}(\mathcal{L})f$$

Computational cost dominated by matrix-vector multiply with (sparse) Laplacian matrix.

In particular $O(\sum_{n=1}^{J} M_n|E|)$

http://wiki.epfl.ch/sgwt

Note: “same” algorithm for adjoint !

LTS EPFL LTS2

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Transductive Learning

Let X be an array of data points $x_1, x_2, ..., x_n \in \mathbb{R}^d$

Each point has a desired class label $y_k \in Y$ (suppose binary)

At training you have the labels of a subset S of X $\quad |S| = l < n$

Getting data is easy but labeled data is a scarce resource

GOAL: predict remaining labels

Rationale: minimize empirical risk on your training data such that

- your model is predictive
- your model is simple, does not overfit
- your model is "stable" (depends continuously on your training set)
- ...

Transductive Learning

Ex: Linear regression $y_k = \beta \cdot x_k + b$

Empirical Risk: $\|\mathbf{X}^t\beta - \mathbf{y}\|_2^2 \Longrightarrow \beta = (\mathbf{X}\mathbf{X}^t)^{-1}X\mathbf{y}$

if not enough observations, regularize (Tikhonov):

$$\|\mathbf{X}^t\beta - \mathbf{y}\|_2^2 + \alpha\|\beta\|_2^2 \Longrightarrow \beta = (\mathbf{X}\mathbf{X}^t + \alpha\mathbf{I})^{-1}X\mathbf{y}$$

Ridge Regression

Questions:

How can unlabeled data be used ?

More general linear model with a dictionary of features ?

$$\|\mathbf{\Phi}_X\beta - \mathbf{y}\|_{2,S}^2 + \alpha\mathcal{S}(\beta)$$

dictionary depends on data points

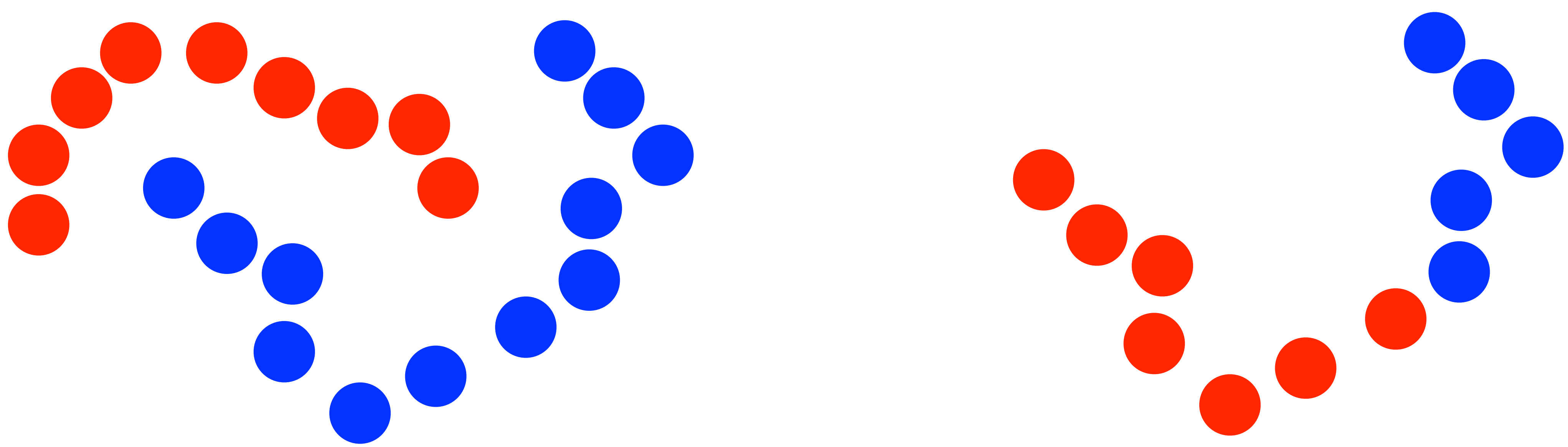
simplifies/stabilizes selected model

Learning on/with Graphs

How can unlabeled data be used ?

Assumption:

target function is not globally smooth but it is locally smooth over regions of data space that have some geometrical structure



Use graph to model this structure

Transduction & Representation

More general linear model with a dictionary of features ?

$\boldsymbol{\Phi}_X$ dictionary of features on the complete data set (data dependent)

$\boldsymbol{M}$ restricts to labeled data points (mask)

$$\arg\min_{\beta} \|\mathbf{y} - \mathbf{M}\boldsymbol{\Phi}_X \beta\|_2^2 + \alpha \mathcal{S}(\beta)$$

Empirical Risk

Model Selection penalty, sparsity ?
Smoothness on graph ?

Important Note: our dictionary will be data dependent but its construction is not part of the above optimization

Sparsity and Transduction

$$\arg\min_{\beta} \|\mathbf{y} - \mathbf{M}\mathbf{\Phi}_X \beta\|_2^2 + \alpha \boxed{\mathcal{S}(\beta)}$$

Since sparsity = smoothness on graph, why not simple LASSO ?

$$\arg\min_{\beta} \|\mathbf{y} - \mathbf{M}\mathbf{\Phi}_X \beta\|_2^2 + \alpha \|\beta\|_1$$

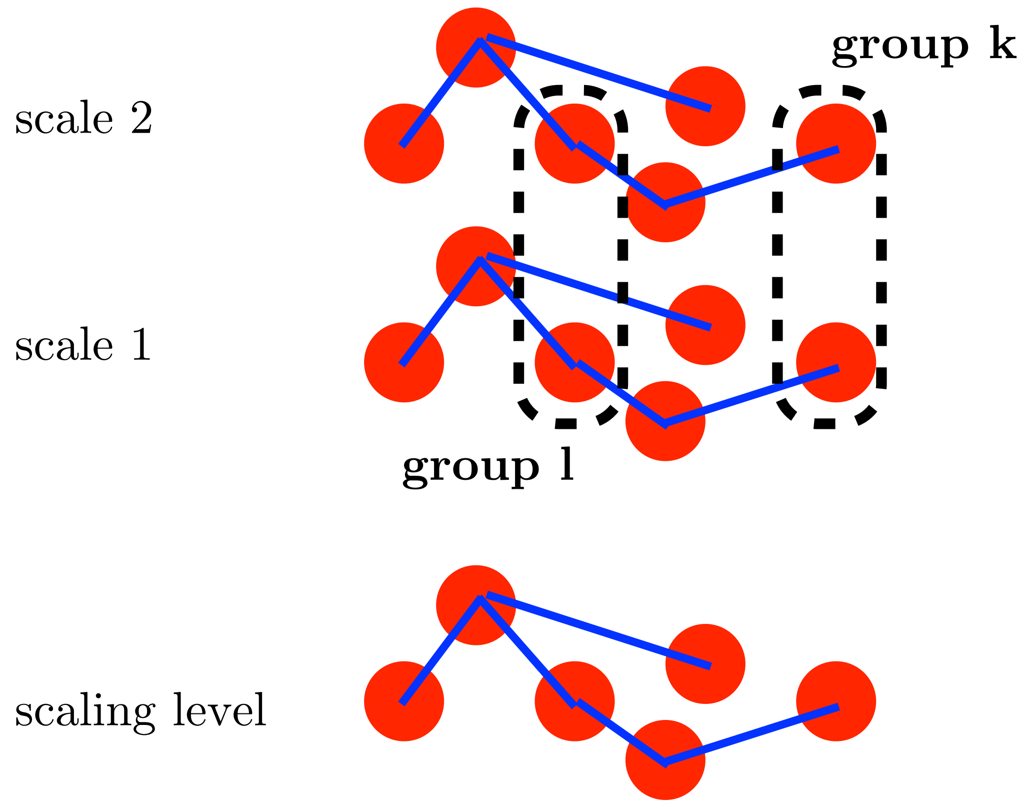
Bad Idea:

We *know* there are strongly correlated coefficients (LASSO will kill some of them)

Group Sparsity

Scaling functions not sparse are optimized separately

Group potentially correlated variables (scales)



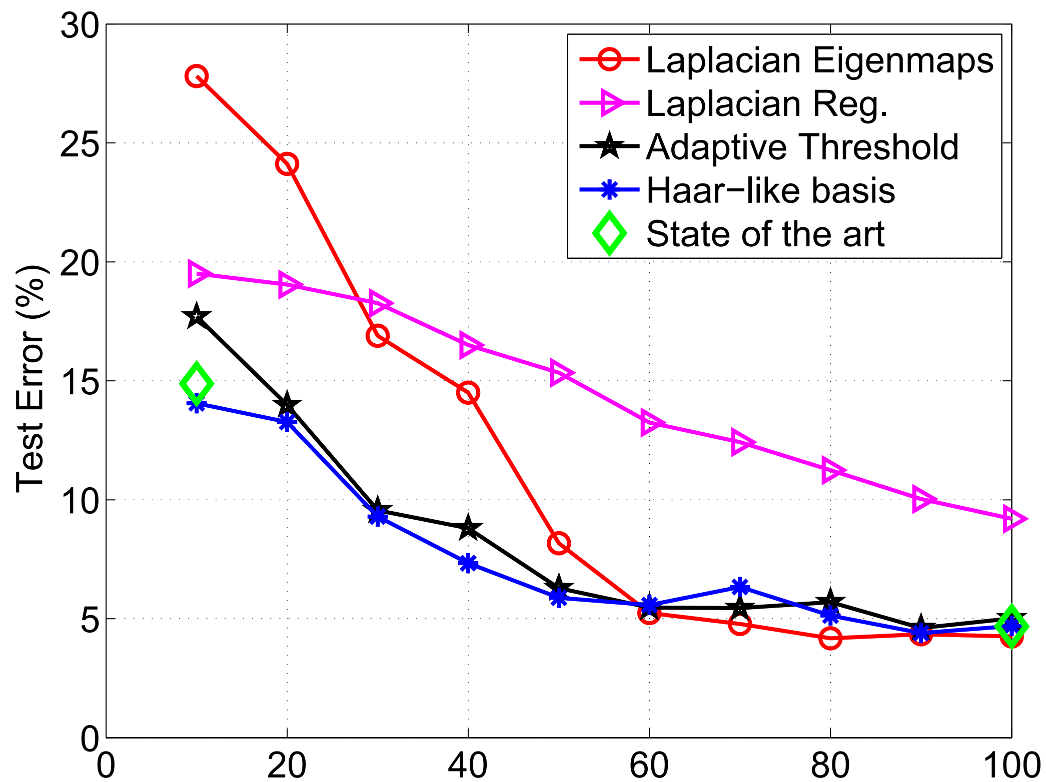
Few groups should be active = local smoothness

Inside group, all coefficients can be active

Formulate with mixed-norms $\|\beta\|_{p,q}$

Simple model, no overlap, optimized like LASSO

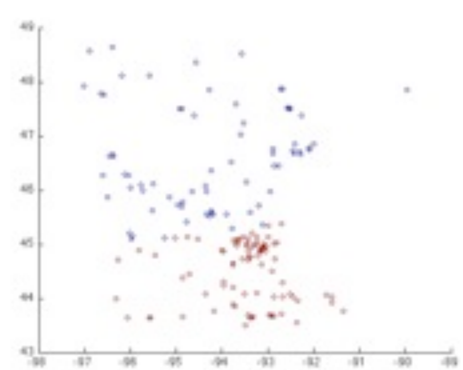
Preliminary Results



2-class USPS

Simulation results from Gavish et al, ICML 2010

5% labeled



recovered

Conclusions

- Processing data on graphs is still an emerging field.
- Interesting connections with other areas
- How to scale computations ?
- Diverse applications:
  - fMRI [Leonardi, Van de Ville, 2012], cortical smoothing
  - Network Analysis [Tremblay, Borgnat, 2012]
  - Learning, Distributed regularization [Shuman et al, 2012]