Harmonic Analysis on Graphs
Global vs. Multiscale Approaches

Boaz Nadler

Weizmann Institute of Science, Rehovot, Israel

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Joint work with
Matan Gavish (WIS/Stanford), Ronald Coifman (Yale), ICML 10’
Challenge: Organization / Understanding of Data

In many fields massive amounts of data collected or generated,

EXAMPLES:

financial data, multi-sensor data, simulations, documents, web-pages, images, video streams, medical data, astrophysical data, etc.
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Need to organize / understand their structure
Inference / Learning from data
Classical vs. Modern Data Analysis Setup and Tasks

**Classical Setup:**

- Data typically in a (low-dimensional) Euclidean Space.
- Small to medium sample sizes ($n < 1000$)
- Either all data unlabeled (unsupervised) or all labeled (supervised).
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- Huge datasets, with \( n = 10^6 \) samples or more. Few labeled data.
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Question: Harmonic Analysis in such settings
Harmonic Analysis and Learning

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geometry of space $X \Rightarrow$ bases for $\{ f : X \rightarrow \mathbb{R} \}$
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Simplest Example: $X = [0, 1]$

Construct (multiscale) basis $\{\Psi_i\}$, that allows control of $|\langle f, \Psi_i \rangle|$ for some (smooth) class of functions $f$.

Theorem: $\psi$ smooth wavelet, $\psi_{\ell,k}$ - wavelet basis, $f : [0, 1] \to \mathbb{R}$, then

$$|f(x) - f(y)| < C|x - y|^\alpha \iff |\langle f, \psi_{\ell,k} \rangle| \leq C'2^{-\ell(\alpha + 1/2)}$$
Harmonic analysis wisdom for $f : \mathbb{R}^d \to \mathbb{R}$
Setting

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- Expand $f$ in orthonormal basis $\{\psi_i\}$ (e.g. wavelet)

$$f = \sum_i \langle f, \psi_i \rangle \psi_i$$
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- Useful when $f$ well approximated by a few terms
  (“fast coefficient decay” / sparsity)
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Can this work on general datasets?

Need data-adaptive basis $\{\psi_i\}$ for space of functions $f : X \to \mathbb{R}$
Harmonic Analysis on Graphs

Setup: We are given dataset $X = \{x_1, \ldots, x_N\}$ with similarity / affinity matrix $W_{i,j}$

Goal: Statistical inference of smooth $f : X \rightarrow \mathbb{R}$

- Denoise $f$
- SSL / Regression / classification: extend $f$ from $\tilde{X} \subset X$ to $X$
Semi-Supervised Learning

In many applications - easy to collect lots of unlabeled data, BUT labeling the data is expensive.

Question: Given (small) labeled set $\tilde{X} \subset X = \{x_i, y_i\} (y = f(x))$, construct $\hat{f}$ to label rest of $X$. 
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Key Assumption:

function \( f(x) \) has some smoothness w.r.t graph affinities \( W_{i,j} \).

otherwise - unlabeled data is useless or may even harm prediction.
The Graph Laplacian

In most previous approaches, key object is

**GRAPH LAPLACIAN:**

\[ L = D - W \]

where \( D_{ii} = \sum_j W_{ij} \),
Global Graph Laplacian Based SSL Methods

Zhu, Ghahramani, Lafferty, SSL using Gaussian fields and harmonic functions [ICML, 2003], Azran [ICML 2007]

\[ f(x) = \arg \min_{f(x_i)=y_i} \frac{1}{n^2} \sum_{i,j=1}^{n} W_{i,j}(f_i - f_j)^2 = \arg \min \frac{1}{n^2} f^T L f \]

Y. Bengio, O. Delalleau, N. Le Roux, [2006]
D. Zhou, O. Bousquet, T. Navin Lal, J. Weston, B. Scholkopf
[NIPS 2004]

\[ f(x) = \arg \min \left[ \frac{1}{n^2} \sum_{i,j=1}^{n} W_{i,j}(f_i - f_j)^2 + \lambda \sum_{i=1}^{\ell} (f_i - y_i)^2 \right] \]
Global Graph-Laplacian Based SSL

Belkin & Niyogi (2003): Given similarity matrix $W$ find first few eigenvectors of Graph Laplacian, $Le_j = (D - W)e_j = \lambda_j e_j$. Expand

$$
\hat{f} = \sum_{j=1}^{p} a_j e_j
$$

Estimate coefficients $a_j$ from labeled data.
Statistical Analysis of Laplacian Regularization

[N., Srebro, Zhou, NIPS 09’]

**Theorem:** In the limit of large unlabeled data from Euclidean space, with \( W_{i,j} = K(\|x_i - x_j\|) \), Graph Laplacian Regularization Methods

\[
f(x) = \arg \min \left[ \frac{1}{n^2} \sum_{i,j=1}^{n} W_{i,j}(f_i - f_j)^2 + \lambda \sum_{i=1}^{\ell} (f_i - y_i)^2 \right]
\]

are well posed for underlying data in 1-d, but *are not well posed* for data in dimension \( d \geq 2 \).

In particular, in limit of infinite unlabeled data, \( f(x) \rightarrow \text{const} \) at all unlabeled \( x \).
Eigenvector-Fourier Methods

Belkin, Niyogi [2003], suggested a different approach based on the Graph Laplacian $L = W - D$:

Given similarity $W$, find first few eigenvectors $(W - D)e_j = \lambda_j e_j$, Expand

$$\hat{y}(x) = \sum_{j=1}^{p} a_j e_j$$

Find coefficients $a_j$ by least squares,

$$(\hat{a}_1, \ldots, \hat{a}_p) = \arg \min \sum_{j=1}^{l} (y_j - \hat{y}(x_j))^2.$$
Toy example

Example: USPS benchmark
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- $X$ is USPS (ML benchmark) as 1500 vectors in $\mathbb{R}^{16 \times 16} = \mathbb{R}^{256}$
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- Affinity $W_{i,j} = \exp \left( - \| x_i - x_j \|^2 \right)$
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**Example: USPS benchmark**

- $X$ is USPS (ML benchmark) as 1500 vectors in $\mathbb{R}^{16 \times 16} = \mathbb{R}^{256}$
- Affinity $W_{i,j} = \exp \left( -\|x_i - x_j\|^2 \right)$
- $f : X \to \{1, -1\}$ is the class label.
Toy example: visualization by kernel PCA
Toy example: Prior art?
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Generalizing Fourier: The Graph Laplacian eigenbasis
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- Typical coefficient decay rate in Fourier basis: \text{polynomial}
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In Euclidean setting

- Typical coefficient decay rate in Fourier basis: \textbf{polynomial}
- \textbf{But} in wavelet bases: \textbf{exponential}
Toy example: Graph Laplacian Eigenbasis

Coefficient decay rate of labels function

$| < \psi_i, f > |$

Coefficient # i
Toy example: Graph Laplacian Eigenbasis

Coefficient decay rate of labels function

log_{10} | \langle \psi_i, f \rangle |
Toy example: Graph Laplacian Eigenbasis
Challenge: build multiscale "wavelet-like" bases on $X$
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1. Construct adaptive multiscale basis on general dataset
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Previous Works
- Diffusion Wavelets [Coifman and Maggioni]
- Multiscale Methods for Data on Graphs [Jansen, Nason, Silverman]
- Wavelets on Graphs via Spectral Graph Theory [Hammond et al.]
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Our Work
- (Relatively) Simple Construction
- Accompanying Theory.
Toy example: intriguing experiment

Coefficient decay rate of labels function

\[ \langle \psi_i, f \rangle \]

Coefficient \# \(i\)

Laplacian eigenbasis
Toy example: intriguing experiment

Coefficient decay rate of labels function

- **Laplacian eigenbasis**
- **Haar-like basis**

\[ |\langle \psi_i, f \rangle| \]

Coefficient \# i
Toy example: intriguing experiment
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Cumulative energy

\[ \sqrt{\sum_{k<i} \langle \psi_i, f \rangle^2} \]

Coefficient # i

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Cumulative energy

- Blue: Laplacian eigenbasis
- Red: Haar-like basis

Coefficient # i

\[ \sqrt{\sum_{k<i} | \psi_k(f) |^2} \]
Challenge and Result
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Key Results

1. Partition tree on $X$ induces “wavelet” Haar-like bases
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1. Partition tree on $X$ induces “wavelet” Haar-like bases
2. Assuming “Balanced” tree

\[ f \text{ smooth } \Leftrightarrow \text{ fast coefficient decay} \]
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The Haar Basis on $[0, 1]$
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Hierarchical partition of $X$
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Partition Tree (Dendrogram)
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Partition Tree ⇒ Haar-like basis

[Lee, N., Wasserman, AOAS 08’]

Simple Observation:

Hierarchical Tree → Multi-Resolution Analysis of Space of Functions
⇒ Haar-like multiscale basis
Partition Tree $\Rightarrow$ Haar-like basis

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Hierarchical Tree $\rightarrow$ Mutli-Resolution Analysis of Space of Functions
$\rightarrow$ Haar-like multiscale basis

$$V = \{ f \mid f : X \rightarrow \mathbb{R} \}$$

$$V^\ell = \{ f \mid f \text{ constant at partitions at level } \ell \}$$
Partition Tree $\Rightarrow$ Haar-like basis

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$$V = \{f \mid f : X \to \mathbb{R}\}$$

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$$V^1 \subset V^2 \subset \ldots V^L = V$$

[Lee, N., Wasserman, AOAS 08']
Partition Tree $\Rightarrow$ Haar-like basis
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\[
\ell = 1 \\
\ell = 2 \\
\ell = 3 \\
\psi_{2,2}
\]
Partition Tree ⇒ Haar-like basis

\[ \psi_{3,1} \]
Partition Tree $\Rightarrow$ Haar-like basis

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Toy example: Haar-like basis function
Smoothness $\iff$ Coefficient decay

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Particular example of Space of Homogeneous Type [Coifman & Weiss]
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- Measure smoothness of $f : X \rightarrow \mathbb{R}$ in tree metric

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**Theorem:**
Let $f : X \rightarrow \mathbb{R}$. Then

$$|f(x_i) - f(x_j)| \leq C d(x_i, x_j)^{\alpha} \iff |\langle f, \psi_{\ell,i} \rangle| \leq C' q^{-\ell(\alpha + 1/2)}.$$

where
- $q$ measures the tree balance
- $\alpha$ measures function smoothness w.r.t. tree

Particular example of Space of Homogeneous Type [Coifman & Weiss]
Application: SSL

Given dataset $X$ with weighted graph $G$, similarity matrix $W$, labeled points $\{x_i, y_i\}$,

1. Construct a balanced hierarchical tree of graph
2. Construct corresponding Haar-like basis
3. Estimate coefficients from labeled points
Toy Example: Benchmarks
Toy Example: MNIST 8 vs. $\{3,4,5,7\}$
Summary
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5. *Computational experiments* motivate *theory and vice-versa*
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The End

www.wisdom.weizmann.ac.il/∼nadler