New directions in graph-based learning: Active learning, Hamilton-Jacobi equations on graphs, and elliptic regularity

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School of Mathematics
University of Minnesota

IPAM Hamilton-Jacobi Opening Day
March 9, 2020
Outline

1. Introduction and background

2. New directions
   - Hamilton-Jacobi equations on graphs
   - Active Learning
   - Elliptic regularity
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2. New directions
   - Hamilton-Jacobi equations on graphs
   - Active Learning
   - Elliptic regularity
Quick intro to learning

**Fully supervised:** Given training data \((x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)\) with \(x_i \in \mathcal{X}\) and \(y_i \in \mathcal{Y}\), learn a function

\[
(1) \quad u : \mathcal{X} \to \mathcal{Y} \quad \text{for which } u(x_i) \approx y_i \text{ for } i = 1, \ldots, n.
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**Semi-supervised learning:** Given additional unlabeled data \(x_{n+1}, \ldots, x_{n+m}\) for \(m \geq 1\), use both the labeled and unlabeled data to learn \(f\).
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**Unsupervised learning:** Algorithms that use only the unlabeled data \(x_1, \ldots, x_n\), such as clustering.
Example: Automated image captioning
Example: Automated image captioning

A woman is throwing a **frisbee** in a park.

A **dog** is standing on a hardwood floor.

A **stop** sign is on a road with a mountain in the background.

A little **girl** sitting on a bed with a teddy bear.

A **group of people** sitting on a boat in the water.

A **giraffe** standing in a forest with **trees** in the background.

Example: Automated image captioning fail

(-11.269838) a woman holding a baby giraffe in a zoo

[Andrej Karpathy’s NeuralTalk]
Graph-based learning

In semi-supervised and unsupervised learning, we often build a graph \((\mathcal{X}, \mathcal{W})\):
- \(\mathcal{X} \subset \mathbb{R}^d\) are the vertices and
- \(\mathcal{W} = (w_{xy})_{x,y \in \mathcal{X}}\) are the nonnegative edge weights.
- \(w_{xy} \approx 1\) if \(x, y\) similar, and \(w_{xy} \approx 0\) when dissimilar.

The graph Laplacian:
\[
L_u(x) = \sum_{y \in \mathcal{X}} w_{xy} (u(y) - u(x)) = 0.
\]

Laplacian regularized semi-supervised learning [Zhu et al., (2003)]

Propagate labels on a graph by harmonic extension.

Spectral clustering [Shi and Malik (2000)] [Ng, Jordan, and Weiss (2002)]

Embed a graph into \(\mathbb{R}^k\) by projecting onto eigenspaces of \(L\).

Laplacian eigenmaps [Belkin and Niyogi (2003)], Diffusion maps [Coifman and Lafon (2006)]
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**MNIST (70,000 28 × 28 pixel images of digits 0-9)**

<table>
<thead>
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Laplace learning on MNIST

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<th>1000</th>
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<td>Laplace</td>
<td>93.2 (2.3)</td>
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Average accuracy over 10 trials with standard deviation in brackets.

Weight matrix constructed with the Scattering Transform [Bruna and Mallat, 2013].
Spectral embedding: MNIST

Digits 1 and 2 from MNIST visualized with spectral projection
Spectral embedding: MNIST

Digits 1 (blue) and 2 (red) from MNIST visualized with spectral projection
Random geometric graph ($\varepsilon$-ball graph)

Assume the vertices of the graph are

$$\mathcal{X}_n = \{x_1, \ldots, x_n\}$$

where $x_1, \ldots, x_n$ are a sequence of i.i.d. random variables on $\Omega \subset \mathbb{R}^d$ with positive density $\rho$, and the weights are given by

$$w_{xy} = \eta\left(\frac{|x - y|}{\varepsilon}\right),$$

where $\eta : [0, \infty) \rightarrow [0, 1]$ is smooth with compact support.
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where \(x_1, \ldots, x_n\) are a sequence of i.i.d. random variables on \(\Omega \subset \mathbb{R}^d\) with positive density \(\rho\), and the weights are given by

\[ w_{xy} = \eta \left( \frac{|x - y|}{\varepsilon} \right), \]

where \(\eta : [0, \infty) \rightarrow [0, 1]\) is smooth with compact support. In particular, we assume

\[
\begin{cases} 
\eta(t) \geq 1, & \text{if } 0 \leq t \leq \frac{1}{2} \\
\eta(t) = 0, & \text{if } t > 1 \\
\eta(t) \geq 0, & \text{for all } t \geq 0.
\end{cases}
\]

**Manifold assumption:** Also common to assume \(x_1, \ldots, x_n\) are supported on a smooth manifold \(\mathcal{M}\) embedded in \(\mathbb{R}^d\). 

Calder (UofM)

Graph-based learning

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Let

\[ \varepsilon_k(x) = \text{Distance from } x \text{ to } k^{\text{th}} \text{ nearest neighbor.} \]

- Non-symmetric (or directed) \( k \)-nn graph

\[ w_{xy} = \eta \left( \frac{|x - y|}{\varepsilon_k(x)} \right). \]
k-nearest neighbor graph

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$$w_{xy} = \eta \left( \frac{|x - y|}{\varepsilon_k(x)} \right).$$

- Various ways to symmetrize:

$$w_{xy} = \eta \left( \frac{|x - y|}{\varepsilon_k(x)} \right) + \eta \left( \frac{|x - y|}{\varepsilon_k(y)} \right)$$

$$w_{xy} = \eta \left( \frac{|x - y|}{\min\{\varepsilon_k(x), \varepsilon_k(x)\}} \right)$$

$$w_{xy} = \eta \left( \frac{|x - y|}{\max\{\varepsilon_k(x), \varepsilon_k(x)\}} \right)$$
Synthetic Gaussian Data
$k$-nn graph

$k = 5$, Sparsity $\leq 1\%$
Random geometric graph

$\epsilon = 0.25$, Sparsity $\sim 1.7\%$, Disconnected graph
Continuum limits in graph-based learning

The limit is taken jointly as $n \to \infty$ and $\varepsilon \to 0$.

- Early work [Hein et al., 2007] established pointwise consistency for smooth functions, with high probability

$$\mathcal{L}u = \rho^{-1} \text{div} (\rho^2 \nabla u) + O(\varepsilon).$$
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- $\Gamma$-convergence framework developed in [Trillos & Slepčev 2016] for variational convergence.
  - Continuum limit for total variation on graphs [Trillos & Slepčev 2016].
  - Spectral convergence rates [Trillos et al., 2018], [Calder & Trillos 2019].
  - Many other applications.
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- Maximum principle and viscosity solution approach [Calder, 2018].
Convergence rates

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<tr>
<th>Eigenmode</th>
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</tbody>
</table>

**Table:** Rates of convergence of the form $O(\varepsilon^b)$ (value of $b$ is shown) for eigenvalues and eigenvectors of the graph Laplacian on the 2-sphere. Errors are averaged over 100 trials with $n$ ranging from $n = 500$ to $n = 10^5$.

Rates of convergence for

$$\varepsilon = \left( \frac{\log n}{n} \right)^{1/(d+2)}.$$

Sharpest known convergence rates are $O(\varepsilon)$ [Calder & Trillos 2019].
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   - Elliptic regularity
Some new directions

Previous/current work has focused on continuum limits: $F_{n,\varepsilon} \to F$, which gives

- Well-posedness/stability results
- New understandings of algorithms

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3. Elliptic regularity for graph Laplacians
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- Establish performance guarantees for algorithms
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Hamilton-Jacobi equations on graphs

The graph eikonal equation gives a “nearest neighbor” classifier:

\[
\begin{cases}
\min_{y \sim x} \{ \nabla u(x, y) + w_{xy} \} = 0, & \text{if } x \in \mathcal{X} \setminus \Gamma \\
u(x) = 0, & \text{if } x \in \Gamma.
\end{cases}
\]

(3)

Here, \( \nabla u(x, y) = u(y) - u(x) \) and \( w_{xy} = |x - y| \).
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Performance on MNIST

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<td>82.3 (1.0)</td>
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Hamilton-Jacobi equations on graphs

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Question: How can we incorporate information about the data distribution \(\rho\) into Hamilton-Jacobi equations on graphs for classification?
Hamilton-Jacobi equations on graphs

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<td>96.9 (0.1)</td>
<td>97.1 (0.1)</td>
<td>97.6 (0.1)</td>
<td>97.7 (0.0)</td>
</tr>
<tr>
<td>eikonal (0.3 sec.)</td>
<td>82.3 (1.0)</td>
<td>89.0 (0.5)</td>
<td>90.6 (0.4)</td>
<td>93.4 (0.1)</td>
<td>93.7 (0.1)</td>
</tr>
</tbody>
</table>

**Question:** How can we incorporate information about the data distribution \( \rho \) into Hamilton-Jacobi equations on graphs for classification?

**Question:** Are more general HJ-equations \( H(x, \nabla u) = 0 \) useful?
Outline

1. Introduction and background

2. New directions
   - Hamilton-Jacobi equations on graphs
   - Active Learning
   - Elliptic regularity
Active learning

**Main question:** Which data points should be queried for labels?
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Using PageRank to choose labeled points

<table>
<thead>
<tr>
<th># Labels/class</th>
<th>10</th>
<th>50</th>
<th>100</th>
<th>500</th>
<th>1000</th>
</tr>
</thead>
<tbody>
<tr>
<td>Laplace</td>
<td>93.2 (2.3)</td>
<td>96.9 (0.1)</td>
<td>97.1 (0.1)</td>
<td>97.6 (0.1)</td>
<td>97.7 (0.0)</td>
</tr>
<tr>
<td>PR Laplace</td>
<td>95.4 (0.0)</td>
<td>97.2 (0.0)</td>
<td>97.3 (0.0)</td>
<td>97.4 (0.0)</td>
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</tr>
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<td>93.7 (0.1)</td>
</tr>
<tr>
<td>PR eikonal</td>
<td>85.6 (0.0)</td>
<td>92.4 (0.0)</td>
<td>93.6 (0.0)</td>
<td>95.1 (0.0)</td>
<td>95.0 (0.0)</td>
</tr>
</tbody>
</table>
Inverse problem?

To formulate the active learning problem, consider Laplace learning with $\Gamma \subset \mathcal{X}$ labels

\begin{equation}
\begin{cases}
\mathcal{L} u(x) = 0, & \text{if } x \in \mathcal{X} \setminus \Gamma \\
u(x) = g(x), & \text{if } x \in \Gamma,
\end{cases}
\end{equation}

and add another label at $z \in \mathcal{X}$:

\begin{equation}
\begin{cases}
\mathcal{L} u_z(x) = 0, & \text{if } x \in \mathcal{X} \setminus \Gamma \\
u_z(x) = g(x), & \text{if } x \in \Gamma \cup \{z\}.
\end{cases}
\end{equation}

We should choose $z$ to minimize $\|u_z - g\|$?

Can we do this efficiently, and under what models for $g$?

Can the connection to continuum PDEs or Hamilton-Jacobi equations be utilized?
Elliptic regularity on graphs

Some of the most useful tools in PDE theory are regularity results.
Elliptic regularity on graphs

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For the \( p \)-Laplacian on a random geometric graph we have the following:

**Theorem (Calder, 2018)**

If \( \mathcal{L}_p u = 0 \) and \( p > d \), then for every \( 0 < \alpha < \frac{p-d}{p-1} \) there exists \( C, \delta > 0 \) such that

\[
|u(x) - u(y)| \leq C(|x - y|^\alpha + \varepsilon^\alpha)
\]

holds for all \( x, y \in \mathcal{X}_n \) with probability at least

\[
1 - \exp \left( -\delta n \varepsilon^q + C \log(n) \right),
\]

where \( q = \max\{d + 4, 3d/2\} \).
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$$1 - \exp \left( -\delta n\varepsilon^q + C \log(n) \right),$$

where $q = \max\{d + 4, 3d/2\}$.

A similar result is implicit in [Slepčev & Thrope, 2019].

Outline

1 Introduction and background

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Elliptic regularity on graphs

**Question:** Given a random geometric graph model, how regular are solutions of graph Poisson equations

\[ \mathcal{L}u(x) = f(x) \quad \text{for } x \in \mathcal{X} \]

Regularity can be Hölder, Lipschitz, \( C^{k,\alpha} \) or Sobolev spaces.

A very preliminary result in the manifold setting:

**Theorem (Calder, Lewicka, Trillos 2020)**

With probability greater than \( 1 - n^{-\exp(-cn\varepsilon d + 4)} \), solutions of (7) satisfy

\[ |u(x) - u(y)| \leq C(\|f\|_{\infty} + \|u\|_{\infty})(|x - y| + \varepsilon) \]

for all \( x, y \in \mathcal{X} \cap M \).

The proof of the theorem uses stochastic coupling of random walks. A direct application is \( L_{\infty} \) spectral convergence rates.
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**Theorem (Calder, Lewicka, Trillos 2020)**

*With probability greater than $1 - n^k \exp(-cn\varepsilon^{d+4})$ solutions of (7) satisfy*

\[ |u(x) - u(y)| \leq C(\|f\|_\infty + \|u\|_\infty)(|x - y| + \varepsilon) \]

*for all $x, y \in \mathcal{X} \cap M$. *

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Question: Given a random geometric graph model, how regular are solutions of graph Poisson equations

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\]

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My chalkboard tutorial talk is based off Chapter 5 in the Calculus of Variations lecture notes available on my personal website: