Graph-Based Learning: Theory and Applications

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Mathematics of Machine Learning Course
Brigham Young University
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Outline

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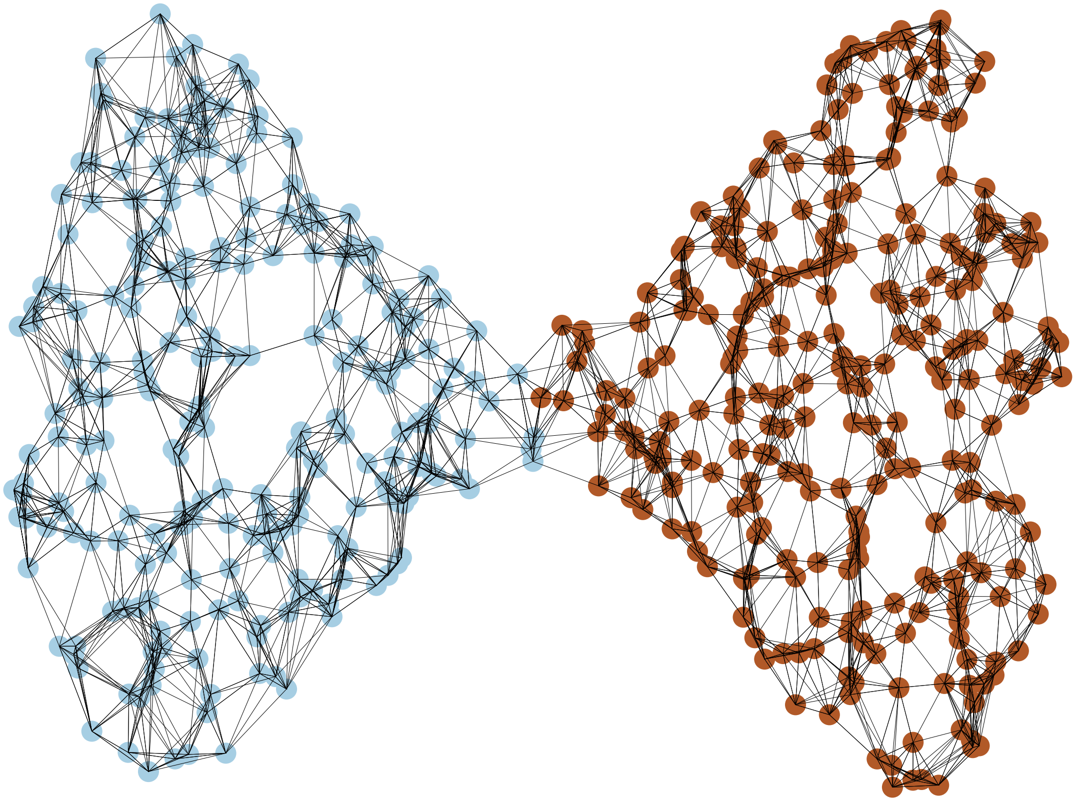
Graph-based learning

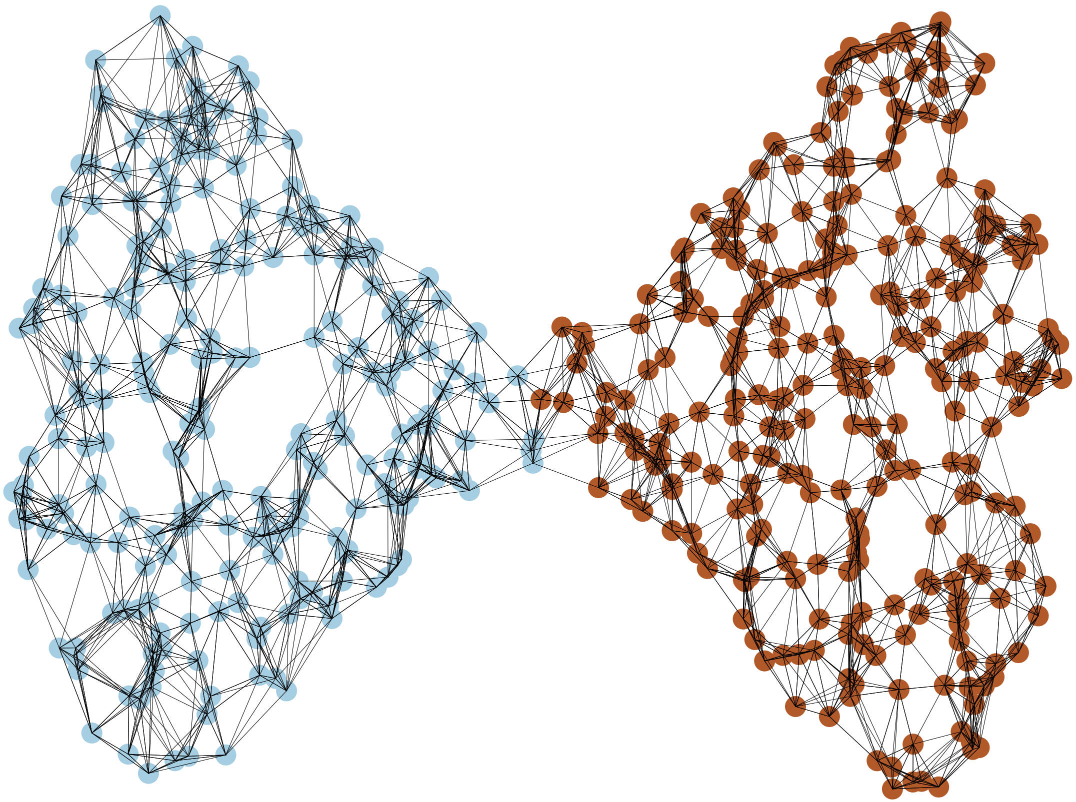
Let $(\mathcal{X}, \mathcal{W})$ be a graph.

- $\mathcal{X} \subset \mathbb{R}^d$ are the vertices.
- $\mathcal{W} = (w_{xy})_{x,y\in\mathcal{X}}$ are nonnegative edge weights.
- w_{xy} is large when x and y are similar, and small or $w_{xy} = 0$ otherwise.

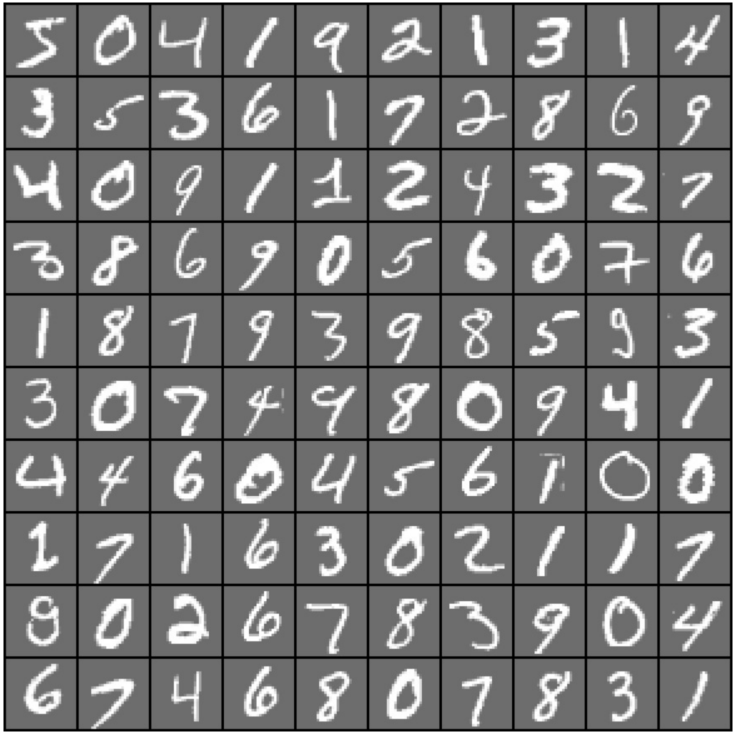


Some common graph-based learning tasks

1. Clustering (grouping similar datapoints)
2. Semi-supervised learning (propagating labels)
3. Dimension reduction (spectral embeddings)



MNIST (70,000 28×28 pixel images of digits 0-9)



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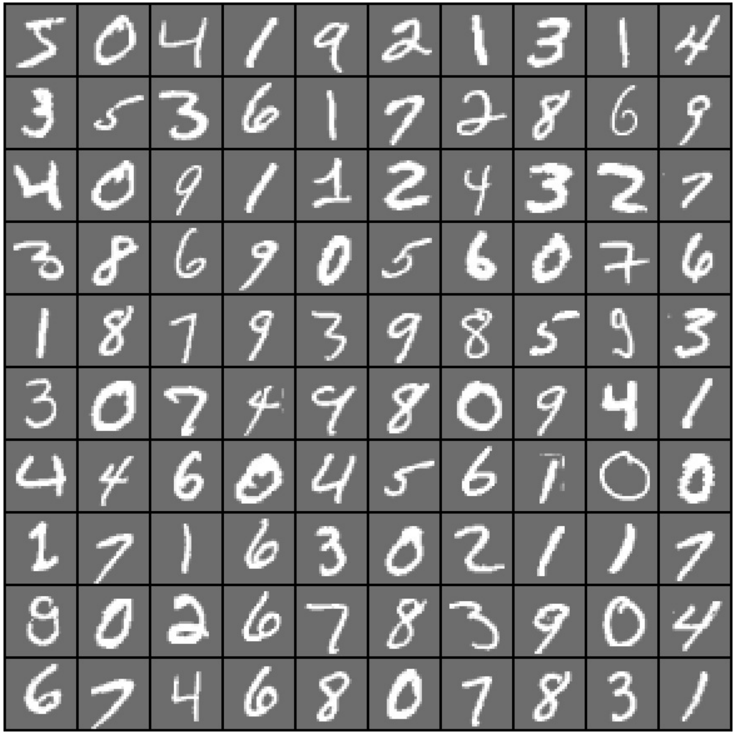

- Each image is a datapoint

$$x \in \mathbb{R}^{28\times 28} = \mathbb{R}^{784}.$$

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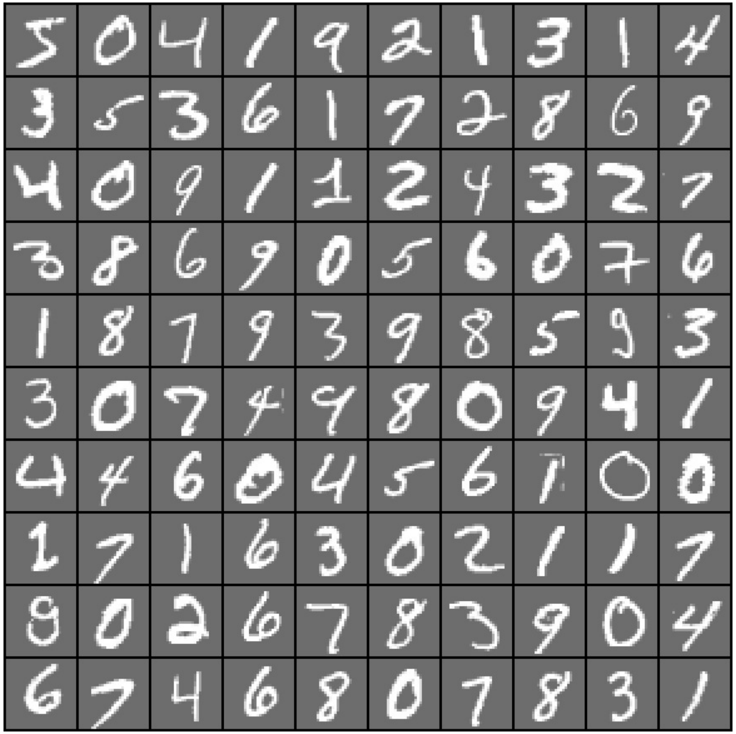

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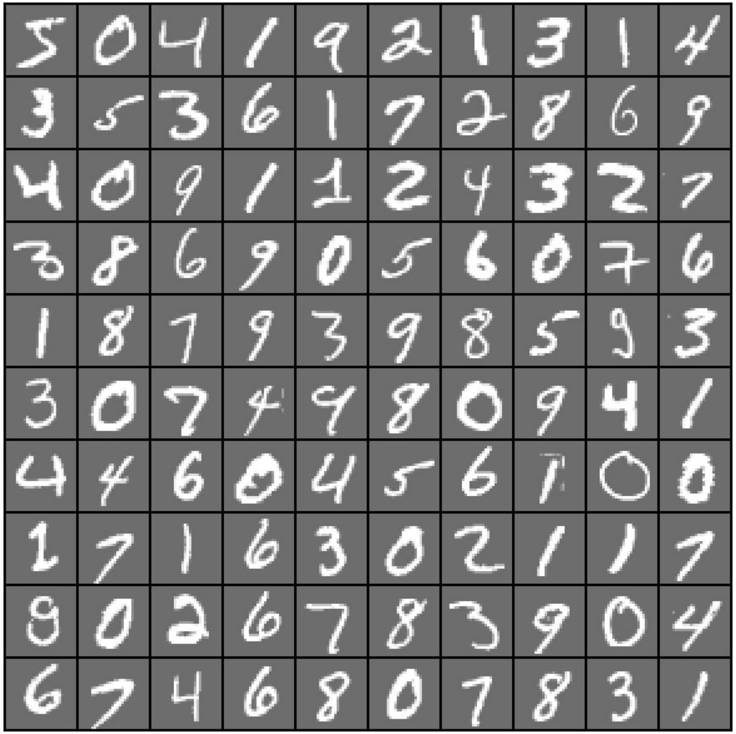

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- Geometric weights:

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

- k-nearest neighbor graph:

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

Clustering MNIST

https://divamgupta.com

Graph cuts

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Consider binary clustering (two classes). We can try to minimize a graph cut energy

$$\text{(Min-Cut)} \qquad \min_{A \subset \mathcal{X}} \mathrm{Cut}(A) := \sum_{\substack{x,y \in \mathcal{X} \\ x \in A, y \notin A}} w_{xy}.$$

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Tends to produce unbalanced classes (e.g., $A = \{x\}$).

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$$\text{(Balanced-Cut)} \qquad \min_{A \subset \mathcal{X}} \frac{\mathrm{Cut}(A)}{\mathrm{Vol}(A)\mathrm{Vol}(\mathcal{X} \setminus A)},$$

where

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Gives good clusterings but very computationally hard (NP-hard).

Spectral clustering

For $A \subset \mathcal{X}$ set

$$u(x) = \begin{cases} 1, & \text{if } x \in A \\ 0, & \text{otherwise.} \end{cases}$$

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This allow us to write the balanced cut problem as

$$\min_{u:\mathcal{X} \to \{0,1\}} \frac{\displaystyle\sum_{x,y \in \mathcal{X}} w_{xy}(u(x) - u(y))^2}{\displaystyle\sum_{x,y,x',y' \in \mathcal{X}} u(x) w_{xy} (1 - u(y')) w_{x'y'}}.$$

Spectral clustering

Consider solving the similar, relaxed, problem

$$\min_{\substack{u:\mathcal{X}\to\mathbb{R} \\ \sum_{x\in\mathcal{X}} u(x)\neq 0}} \frac{\displaystyle\sum_{x,y\in\mathcal{X}} w_{xy}(u(x)-u(y))^2}{\displaystyle\sum_{x\in\mathcal{X}} u(x)^2}.$$

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The solution is the smallest non-trivial eigenvector (Fiedler vector) of the graph Laplacian

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Binary spectral clustering:

1. Compute Fiedler vector $u : \mathcal{X} \to \mathbb{R}$.
2. Set $A = \{x \in \mathcal{X} \ : \ u(x) > 0\}$.

Spectral clustering

Spectral clustering: To cluster into k groups:

1. Compute first k eigenvectors of the graph Laplacian $\mathcal{L}$:

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$$\Psi(x) = (u_1(x), u_2(x), \dots, u_k(x)).$$
3. Cluster the point cloud $\mathcal{Y} = \Psi(\mathcal{X})$ with your favorite clustering algorithm (often k-means).

Spectral methods in data science

Spectral methods are widely used for dimension reduction and clustering in data science and machine learning.

- Spectral clustering [Shi and Malik (2000)] [Ng, Jordan, and Weiss (2002)]
- Laplacian eigenmaps [Belkin and Niyogi (2003)]
- Diffusion maps [Coifman and Lafon (2006)]

Outline

Graph-based semi-supervised learning

Given:

- Graph $(\mathcal{X}, \mathcal{W})$
- Labeled nodes $\Gamma \subset \mathcal{X}$ and labels $g : \Gamma \to \mathbb{R}^k$,
- The i^{th} class has label vector $g(x) = e_i = (0, , \dots, 0, 1, 0, \dots, 0)$.

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Applications of semi-supervised learning

1. Speech recognition
2. Classification (images, video, website, etc.)
3. Inferring protein structure from sequencing

Why semi-supervised?

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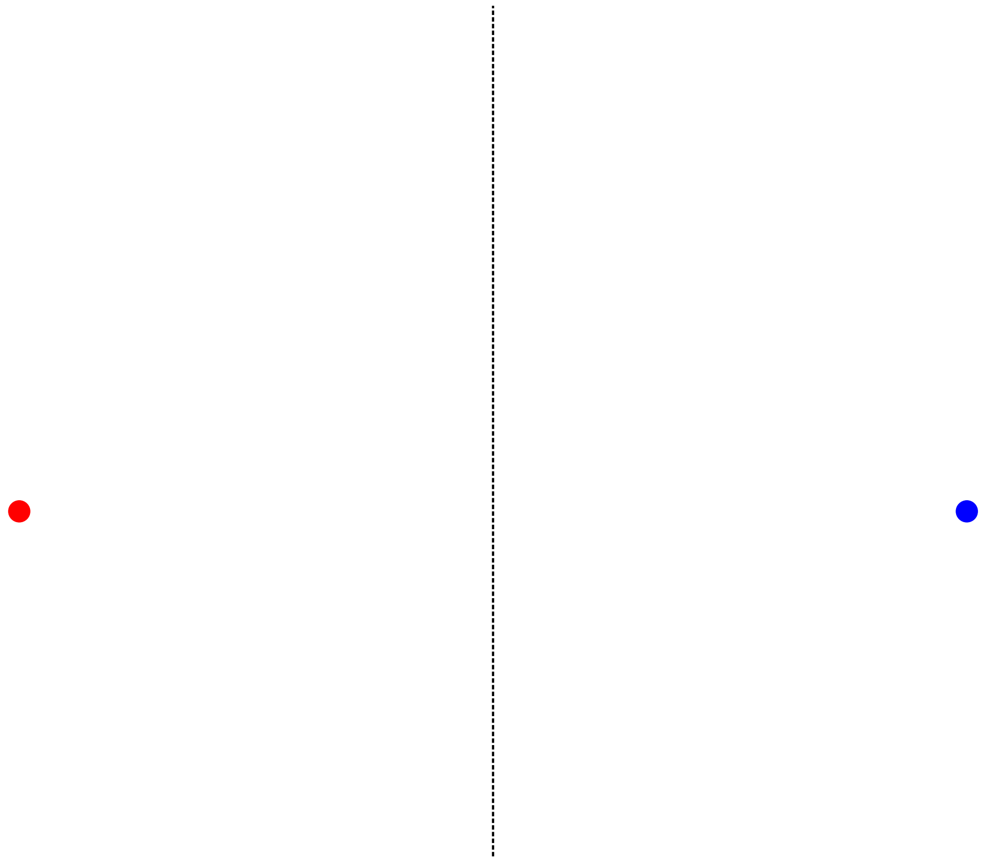

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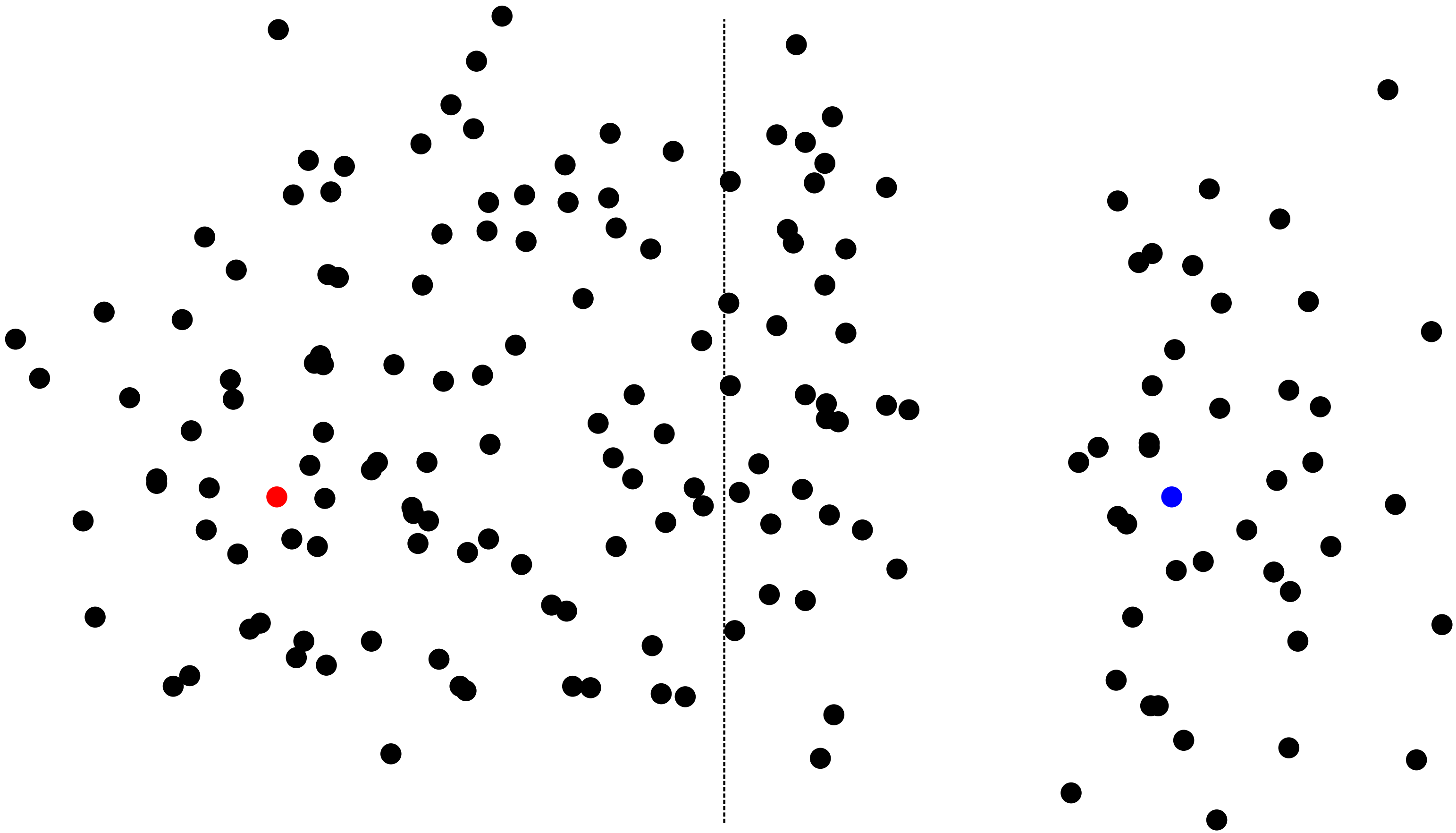

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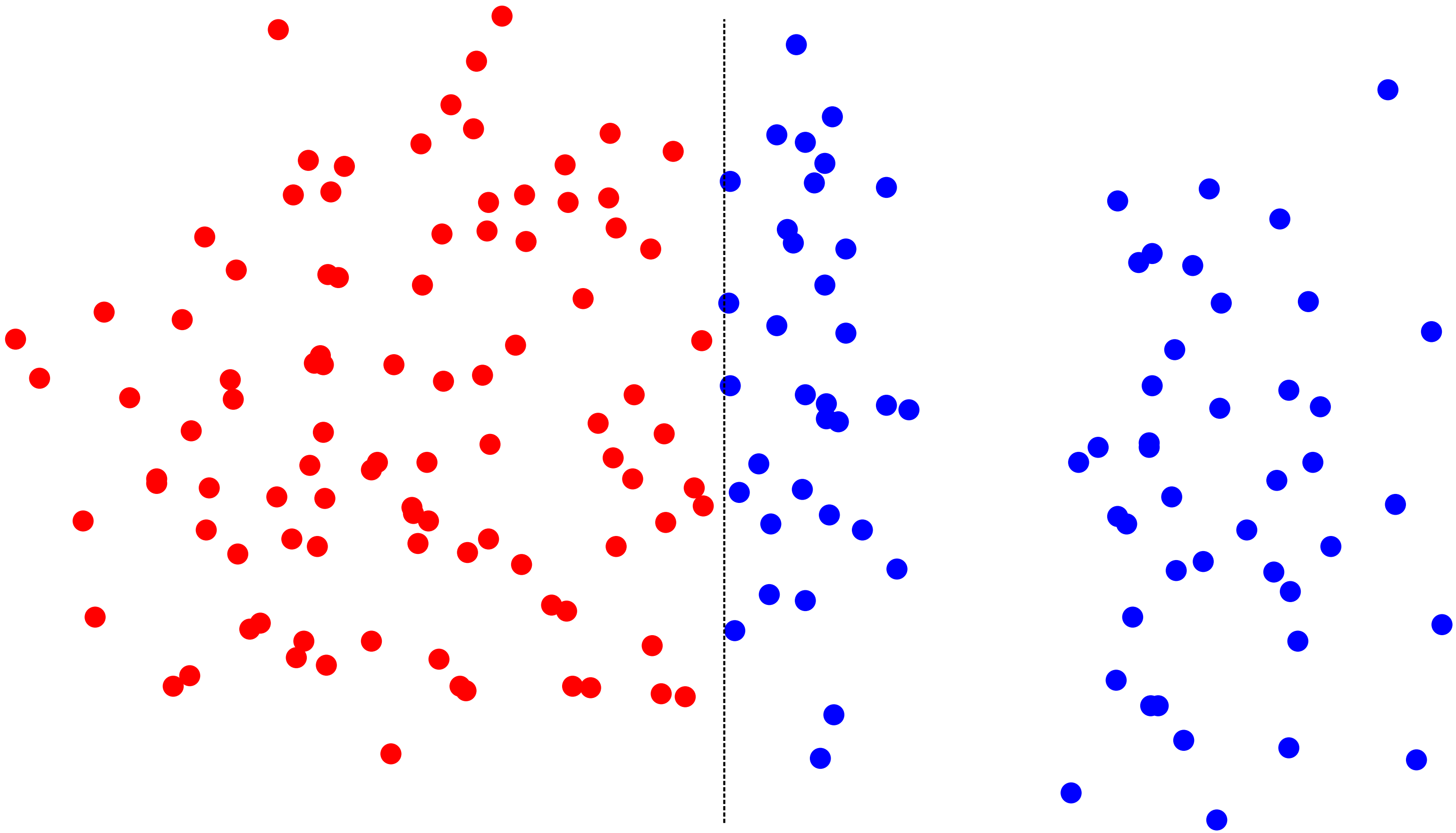

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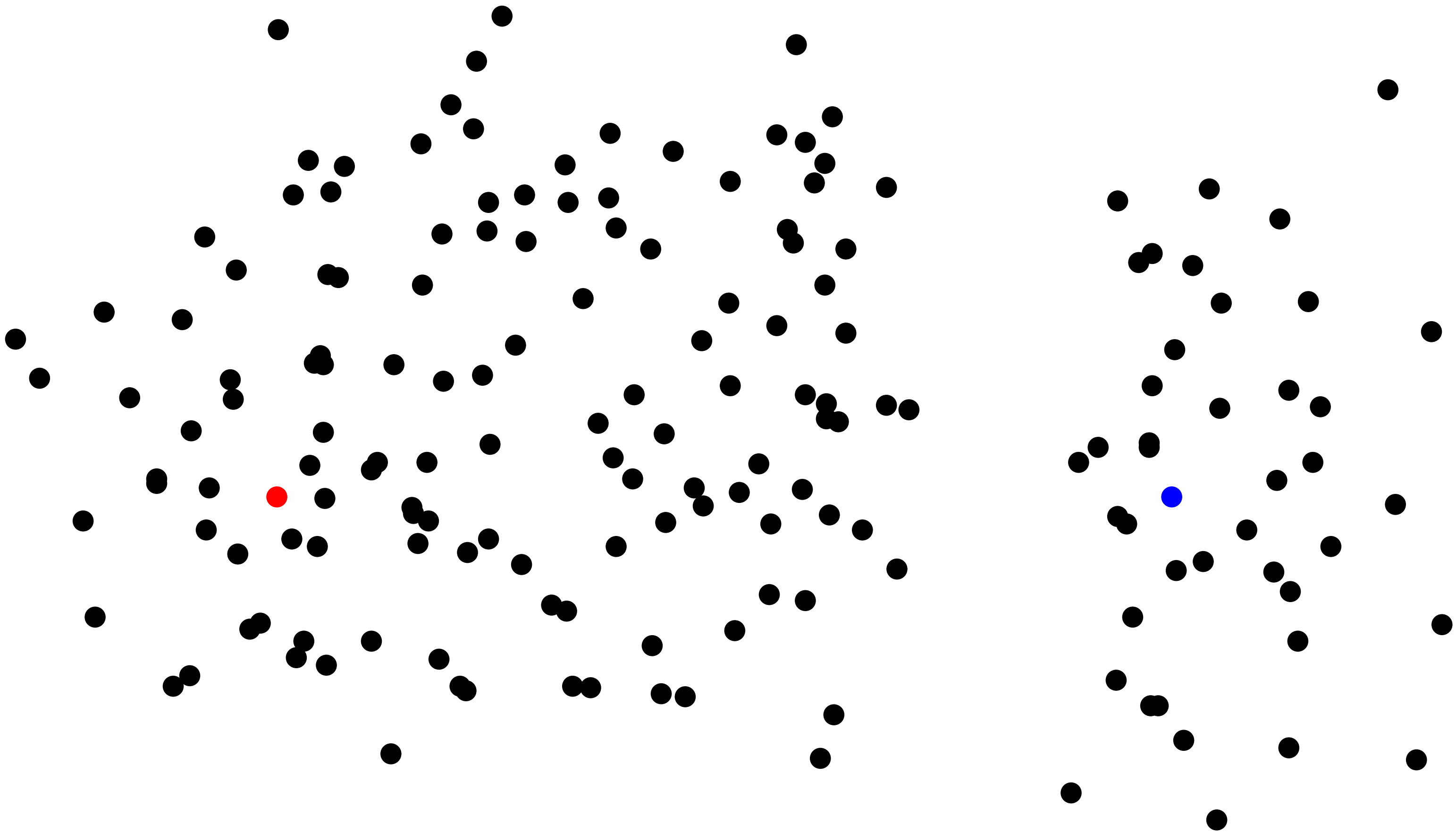

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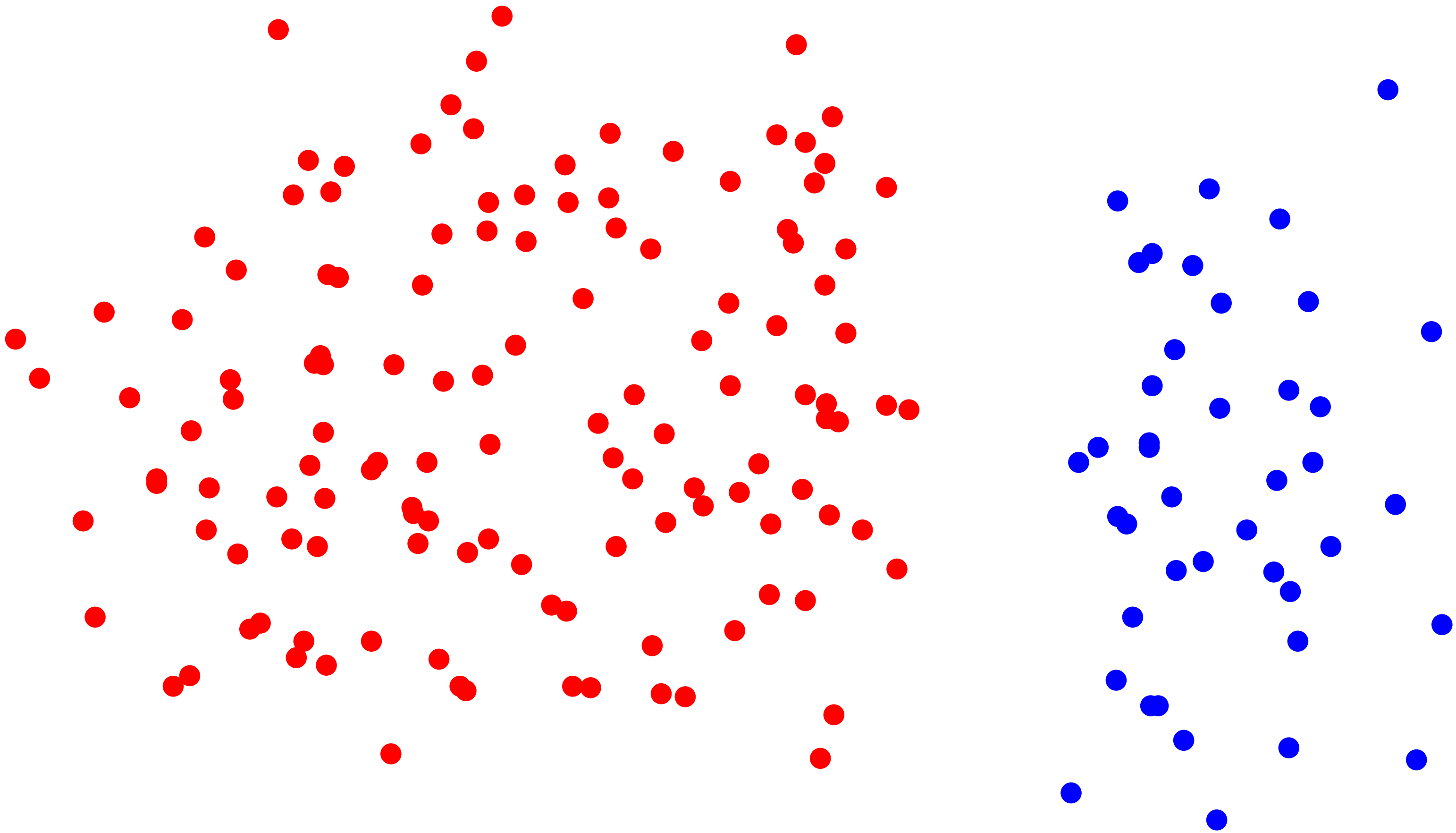

Laplacian regularization

Laplacian regularized semi-supervised learning solves the Laplace equation

$$\begin{cases} \mathcal{L}u = 0 & \text{in } \mathcal{X} \setminus \Gamma, \\ u = g & \text{on } \Gamma, \end{cases}$$

where $u : \mathcal{X} \to \mathbb{R}^k$, and $\mathcal{L}$ is the graph Laplacian

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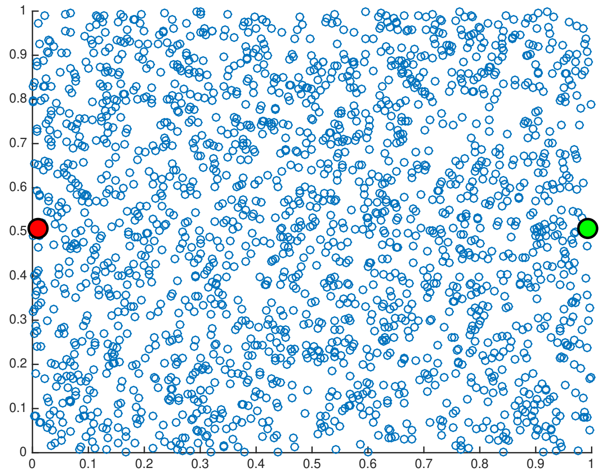
The label decision for vertex $x \in \mathcal{X}$ is determined by the largest component of $u(x)$

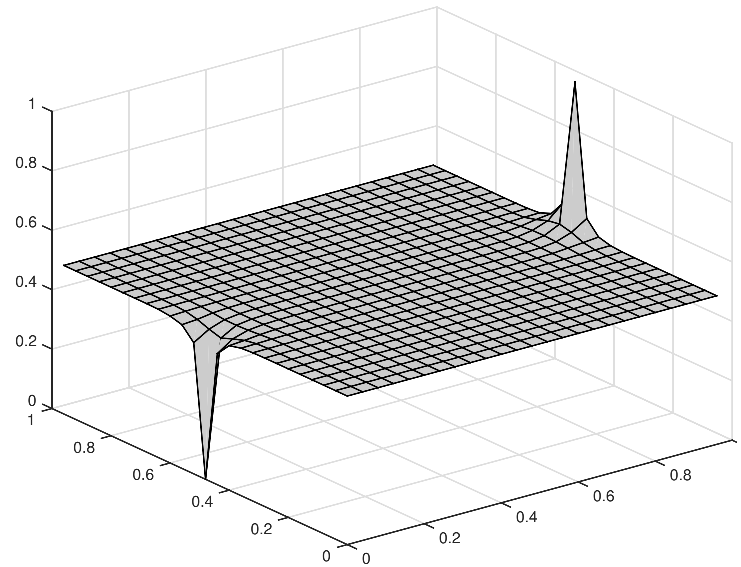
$$\ell(x) = \operatorname*{argmax}_{j \in \{1,\dots,k\}} \{u_j(x)\}.$$

References:

- Original work [Zhu et al., 2003]
- Learning [Zhou et al., 2005, Ando and Zhang, 2007]
- Manifold ranking [He et al., 2006, Zhou et al., 2011, Xu et al., 2011]

Ill-posed with small amount of labeled data





- Graph is $n = 10^5$ i.i.d. random variables uniformly drawn from $[0,1]^2$.
- $w_{xy} = 1$ if $|x - y| < 0.01$ and $w_{xy} = 0$ otherwise.
- Two labels: $g(x) = 0$ at the Red point and $g(x) = 1$ at the Green point.

[Nadler et al., 2009]

Recent work

The low-label rate problem was originally identified in [Nadler 2009].

A lot of recent work has attempted to address this issue with new graph-based classification algorithms at low label rates.

- Higher-order regularization: [Zhou and Belkin, 2011], [Dunlop et al., 2019]
- p-Laplace regularization: [Alaoui et al., 2016], [Calder 2018,2019], [Slepcev & Thorpe 2019]
- Re-weighted Laplacians: [Shi et al., 2017], [Calder & Slepcev, 2019]
- Centered kernel method: [Mai & Couillet, 2018]
- Poisson Learning: [Calder, Cook, Thorpe, Slepcev, ICML 2020]

Poisson learning

At low label rates one should replace Laplace learning

$$\begin{cases} \mathcal{L}u = 0, & \text{in } \mathcal{X}, \\ u = g, & \text{on } \Gamma, \end{cases}$$

with Poisson learning

$$\mathcal{L}u(x) = \sum_{y \in \Gamma} (g(y) - \overline{g})\delta_{xy},$$

subject to $\sum_{x \in \mathcal{X}} d(x)u(x) = 0$, where $\overline{g} = \frac{1}{|\Gamma|} \sum_{y \in \Gamma} g(y)$.

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In both cases, the label decision is the same:

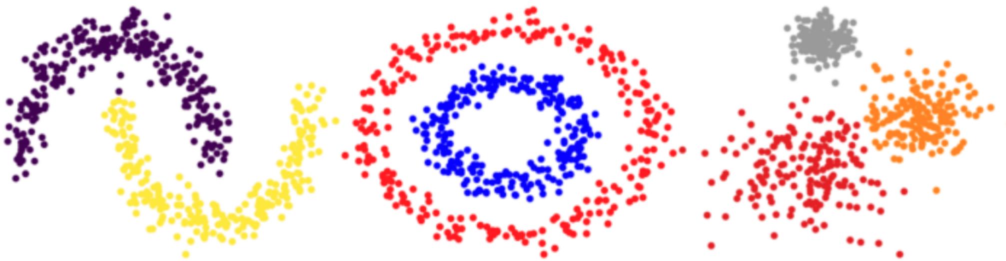
$$\ell(x) = \operatorname*{argmax}_{j \in \{1,\ldots,k\}} \{u_j(x)\}.$$

J. Calder, B. Cook, M. Thorpe, and D. Slepčev. **Poisson Learning: Graph based semi-supervised learning at very low label rates.** *International Conference on Machine Learning (ICML), PMLR 119:1306–1316*, 2020.

Outline

GraphLearning Python Package (Click Here)

Graph-based Clustering and Semi-Supervised Learning



This python package is devoted to efficient implementations of modern graph-based learning algorithms for both semi-supervised learning and clustering. The package implements many popular datasets (currently MNIST, FashionMNIST, cifar-10, and WEBKB) in a way that makes it simple for users to test out new algorithms and rapidly compare against existing methods.

This package reproduces experiments from the paper

Calder, Cook, Thorpe, Slepcev. Poisson Learning: Graph Based Semi-Supervised Learning at Very Low Label Rates., Proceedings of the 37th International Conference on Machine Learning, PMLR 119:1306-1316, 2020.

Installation

Install with

```
pip install graphlearning
```

https://github.com/jwcalder/GraphLearning

Outline

Pointwise consistency on random geometric graphs

Let $X_1, X_2, \ldots, X_n$ be a sequence of i.i.d random variables on $\Omega \subset \mathbb{R}^d$ with density $\rho \in C^2(\Omega)$, where Ω is open and bounded with a smooth boundary, and $\rho \geq \rho_{min} > 0$.

The random geometric graph Laplacian applied to $u : \Omega \to \mathbb{R}$ is

$$\mathcal{L}u(x) = \sum_{i=1}^{n} \eta\left(\frac{|X_i - x|}{\varepsilon}\right)(u(X_i) - u(x)),$$

where $\varepsilon > 0$ is the connectivity length scale (bandwidth) and $\eta : \mathbb{R} \to \mathbb{R}$ is smooth, nonnegative and has compact support in $[0, 1]$.

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where $\varepsilon > 0$ is the connectivity length scale (bandwidth) and $\eta : \mathbb{R} \to \mathbb{R}$ is smooth, nonnegative and has compact support in $[0, 1]$.

Today we'll prove that when u is C^3 we have

$$\frac{2}{\sigma_\eta n \varepsilon^{d+2}} \mathcal{L}u(x) = \rho^{-1} \mathrm{div}\left(\rho^2 \nabla u\right) + \underbrace{O\left(n^{-1/2}\varepsilon^{-1-d/2}\right)}_{\text{Variance}} + \underbrace{O(\varepsilon)}_{\text{Bias}}.$$

with high probability, provided $B(x, \varepsilon) \subset \Omega$.

Discrete to continuum convergence

Manifold assumption: Let $x_1, \ldots, x_n$ be a sequence of i.i.d. random variables with density ρ supported on a d-dimensional compact, closed, and connected Riemannian manifold $\mathcal{M}$ embedded in $\mathbb{R}^D$, where $d \ll D$. Fix a finite set of points $\Gamma \subset \mathcal{M}$ and set

$$\mathcal{X}_n := \underbrace{\{x_1, \ldots, x_n\}}_{\text{Unlabeled}} \cup \underbrace{\Gamma}_{\text{Labeled}}.$$

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Conjecture

Let $n \to \infty$ and $\varepsilon = \varepsilon_n \to 0$ so that $\lim_{n\to\infty} \frac{n\varepsilon_n^{d+2}}{\log n} = \infty$. Let u_n be the solution of the Poisson learning problem

$$\left(\frac{2}{\sigma_\eta n \varepsilon_n^{d+2}}\right) \mathcal{L} u_n(x) = \sum_{y\in\Gamma} (g(y) - \overline{g})(n\delta_{xy}) \quad \textit{for } x \in \mathcal{X}_n.$$

Then with probability one $u_n \to u$ locally uniformly on $\mathcal{M} \setminus \Gamma$ as $n \to \infty$, where $u \in C^\infty(\mathcal{M} \setminus \Gamma)$ is the solution of the Poisson equation

$$-\mathit{div}_{\mathcal{M}} \left(\rho^2 \nabla_{\mathcal{M}} u\right) = \sum_{y\in\Gamma} (g(y) - \overline{g})\delta_y \quad \textit{on } \mathcal{M}.$$

Concentration of measure

Theorem (Bernstein's inequality)

Let $Y_1, \dots, Y_n$ be i.i.d. with mean $\mu = \mathbb{E}[Y_i]$ and variance $\sigma^2 = \mathbb{E}[(Y_i - \mathbb{E}[Y_i])^2]$, and assume $|Y_i| \le M$ almost surely for all i. Then for any $t > 0$

$$\mathbb{P}\left(\left|\frac{1}{n}\sum_{i=1}^n Y_i - \mu\right| > t\right) \le 2\exp\left(-\frac{nt^2}{2\sigma^2 + 4Mt/3}\right). \tag{1}$$

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Let $\delta > 0$ and choose $t > 0$ so that $\delta = 2\exp\left(-\frac{nt^2}{2\sigma^2+4Mt/3}\right)$. Then we get

$$\left|\frac{1}{n}\sum_{i=1}^n Y_i - \mu\right| \leq \sqrt{\frac{2\sigma^2|\log\frac{\delta}{2}|}{n}} + \frac{4M|\log\frac{\delta}{2}|}{3n}$$

with probability at least $1 - \delta$.

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$$\left|\frac{1}{n}\sum_{i=1}^n Y_i - \mu\right| \leq \sqrt{\frac{2\sigma^2|\log\frac{\delta}{2}|}{n}} + \frac{4M|\log\frac{\delta}{2}|}{3n}$$

with probability at least $1-\delta$. Provided $M \leq C\sqrt{n}\sigma$ we can write

$$\frac{1}{n}\sum_{i=1}^n Y_i = \mu + O\left(\sqrt{\frac{\sigma^2}{n}}\right) \quad \text{w.h.p.}$$

Proof of Pointwise consistency

$$\mathcal{L}u(x) = \sum_{i=1}^{n} \underbrace{\eta\left(\frac{|x_i - x|}{\varepsilon}\right)\left(u(x_i) - u(x)\right)}_{Y_i}$$

$$|Y_i| \leq C\varepsilon = M.$$

$$\sigma^2 = \mathrm{Var}(Y_i) \sim \int_{B(x,\varepsilon)} \eta\left(\frac{|y-x|}{\varepsilon}\right)^2 \overbrace{\left(u(y) - u(x)\right)^2}^{O(\varepsilon^2)} \rho(x)^2 \, dx$$

$$\sim \varepsilon^{d+2}$$

Bernstein:

$$\frac{1}{n}\mathcal{L}u(x) = \overbrace{\int_{B(x,\varepsilon)} \eta\left(\frac{|x-y|}{\varepsilon}\right)(u(y)-u(x))\,\rho(y)\,dy}^{Au(x)} + \underbrace{O\left(\sqrt{\frac{\varepsilon^{d+2}}{n}}\right)}_{\text{variance}}.$$

Taylor expansions in $Au(x)$ after $z = \frac{x-y}{\varepsilon}$

$$Au(x) = \varepsilon^d \int_{B(0,1)} \eta(|z|)(u(x+\varepsilon z)-u(x))\,\rho(x+\varepsilon z)\,dz$$

$$\rho(x+\varepsilon z) = \rho(x) + \varepsilon \nabla\rho(x)\cdot z + O(\varepsilon^2)$$

$$u(x+\varepsilon z) - u(x) = \varepsilon \nabla u(x)\cdot z + \frac{\varepsilon^2}{2} z^T \nabla^2 u(x) z + O(\varepsilon^3)$$

① $\cancel{\varepsilon \nabla u(x)\cdot z \, \rho(x)}$ odd function over $B(0,1) \Longrightarrow 0$

② $\varepsilon^2 (\nabla\rho(x)\cdot z)(\nabla u(x)\cdot z)$

③ $\rho(x)\frac{\varepsilon^2}{2} z^T \nabla^2 u(x) z$

$$② \int_{B(0,1)} \eta(|z|)\,(\nabla \rho(x)\cdot z)\,(\nabla u(x)\cdot z)\,dz$$

$$= \sum_{i,j=1}^{n} \rho_{x_i}(x)\, u_{x_j}(x) \underbrace{\int_{B(0,1)} \eta(|z|)\, z_i z_j \, dz}_{\substack{= 0 \text{ if } i \neq j \\ =: \sigma_\eta \text{ if } i = j}}$$

$$= \sigma_\eta \nabla \rho(x) \cdot \nabla u(x)$$

(3)

$$\frac{1}{2}\rho(x)\int_{B(0,1)} \eta(|z|)\, z^T \nabla^2 u(x)\, z \, dz$$

$$= \frac{1}{2}\rho(x)\sum_{i,j=1}^{n} u_{x_i x_j}(x) \int_{B(0,1)} \eta(|z|)\, z_i z_j \, dz$$

$$= \frac{1}{2}\rho(x)\sum_{i=1}^{n} u_{x_i x_i}\sigma_\eta$$

$$= \frac{\sigma_\eta}{2}\rho(x)\,\Delta u(x).$$

Hence

$$Au(x) = \varepsilon^{d+2}\sigma_\eta\left(\frac{1}{2}\rho\Delta u + \nabla u\cdot\nabla\rho\right) + O(\varepsilon^{d+3})$$

$$= \frac{\sigma_\eta}{2}\varepsilon^{d+2}\rho^{-1}\left(\rho^2\Delta u + 2\rho\nabla\rho\cdot\nabla u\right) + O(\varepsilon^{d+3})$$

$$= \frac{\sigma_\eta}{2}\varepsilon^{d+2}\rho^{-1}\,\mathrm{div}(\rho^2\nabla u) + O(\varepsilon^{d+3})$$

Therefore

$$\frac{1}{n}\mathcal{L}u(x) = \frac{\sigma_\eta}{2}\varepsilon^{d+2}\rho^{-1}\operatorname{div}(\rho^2\nabla u) + O(\varepsilon^{d+3})$$

$$+ O\left(\sqrt{\frac{\varepsilon^{d+2}}{n}}\right)$$

and so

Bias

$$\frac{2}{\sigma_\eta n\varepsilon^{d+2}}\mathcal{L}u(x) = \rho^{-1}\operatorname{div}(\rho^2\nabla u) + O(\varepsilon)$$

$$+ O\left(\sqrt{\frac{1}{n\varepsilon^{d+2}}}\right)$$

Variance.