

# Higher Order Poisson Regularization for Graph-Based Semi-Supervised Learning

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UMN Honors Thesis

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# Outline

- 1 Introduction
- 2 Graph-Based Semi-Supervised Learning
  - Laplacian Learning
  - Higher Order Poisson Learning
- 3 Algorithm Development
  - Spectral Numerical Approximation
- 4 Simulation Results
- 5 Current and Future Works
- 6 References

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- ▶ Classification (More on this later)
- ▶ Regression (Draw Inferences for Demographic Information from limited Census Data)

# Mathematical Framework to Learning

**Fully supervised:** In fully supervised learning, we are given training data  $(x_i, y_i)$  for  $i = 1, \dots, n$ , where  $x_i \in \mathcal{X}$  are the data points and  $y_i \in \mathcal{Y}$  are the known labels.

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❷ **Transductive learning:** Learn a function

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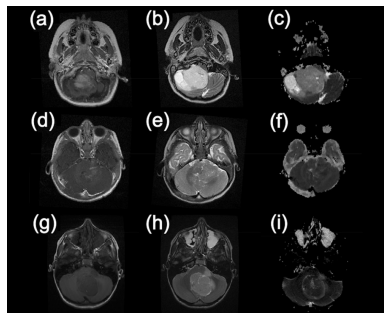
**Why** do we want to use semi-supervised learning?

It is oftentimes **expensive and labor intensive** to obtain labeled data, and we normally have an **abundance** of unlabeled data.

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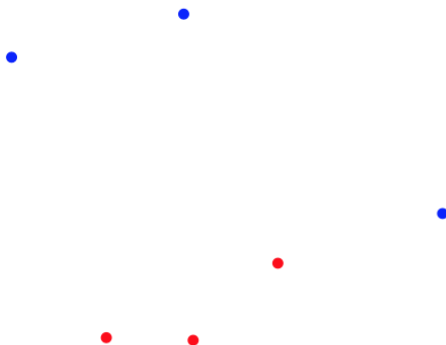


Figure: Three labels per class is given.

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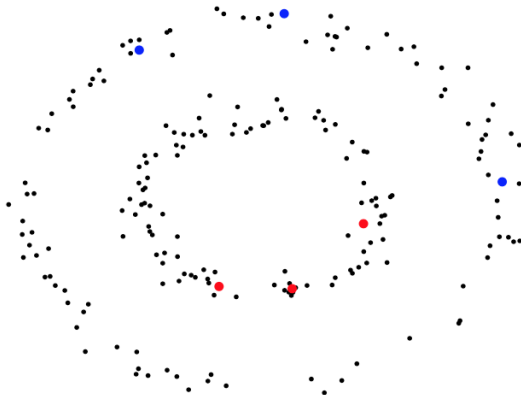


Figure: When both labeled and unlabeled data is given.

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- ➌ We are given a labelling function  $g : \Gamma \rightarrow \mathbf{R}^k$  such that the  $i^{\text{th}}$  class has label vector  $g(x) = e_i = (0, \dots, 0, 1, 0, \dots, 0)$ .

**Task:** Extend the labels from  $\Gamma$  to the entire graph  $\mathcal{X}$ .

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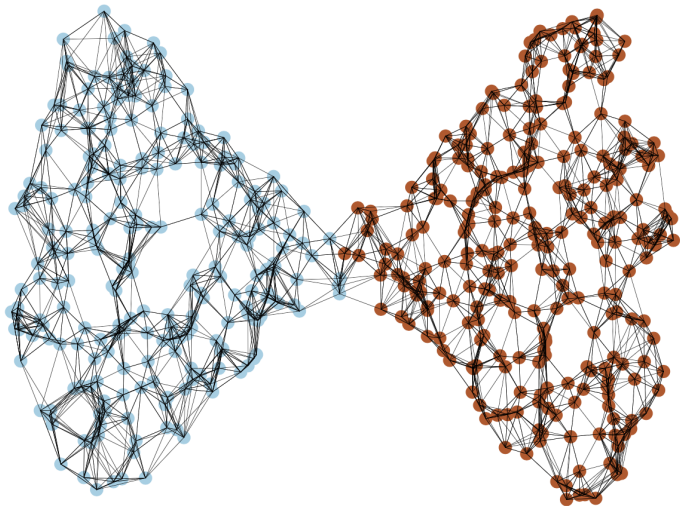
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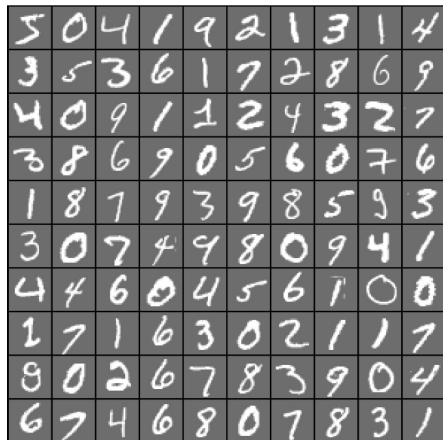
## Semi-supervised smoothness assumption

**Similar** points  $x, y \in \mathcal{X}$  in **high density** regions of the graph should have similar labels.

# Example graph

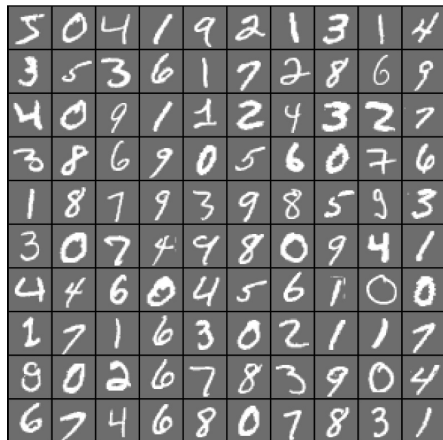


# MNIST (70,000 $28 \times 28$ pixel images of digits 0-9)





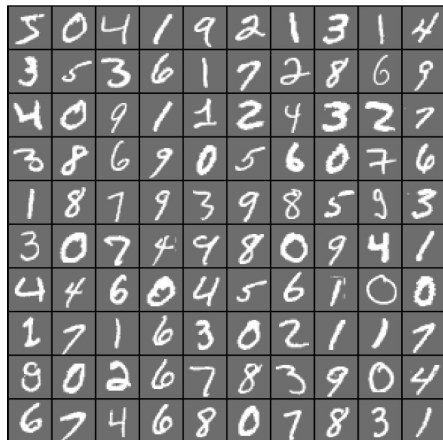
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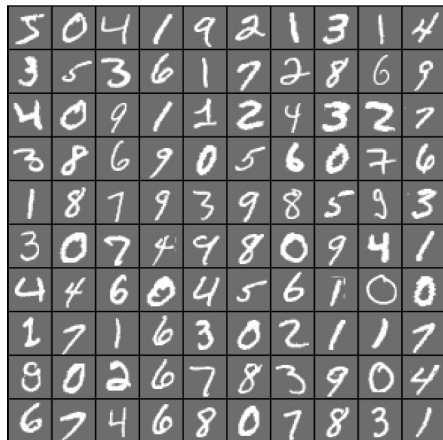
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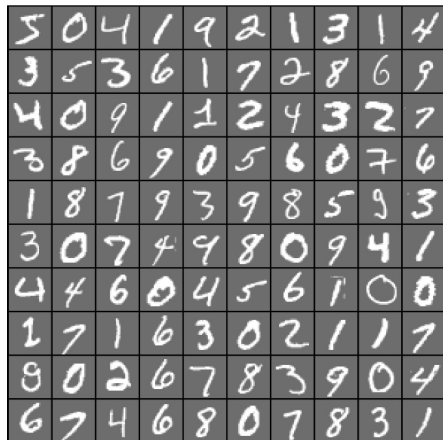
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- $k$ -nearest neighbor graph:

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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  $u : \mathcal{X} \rightarrow \mathbb{R}^k$ , 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]

# Variational interpretation

Laplace learning is equivalent to the variational problem

$$\min_{u:\mathcal{X}\rightarrow\mathbb{R}^k} \left\{ \sum_{x,y\in\mathcal{X}} w_{xy} |u(x) - u(y)|^2 : u(x) = g(x) \text{ for all } x \in \Gamma \right\}.$$



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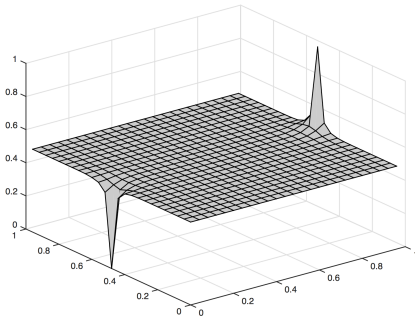
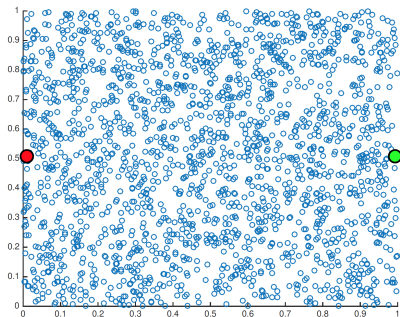
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Many soft-constrained versions have been proposed

$$\min_{u:\mathcal{X}\rightarrow\mathbb{R}^k} \left\{ \sum_{x,y\in\mathcal{X}} w_{xy} |u(x) - u(y)|^2 + \lambda \sum_{x\in\Gamma} \ell(u(x), g(x)) \right\}.$$

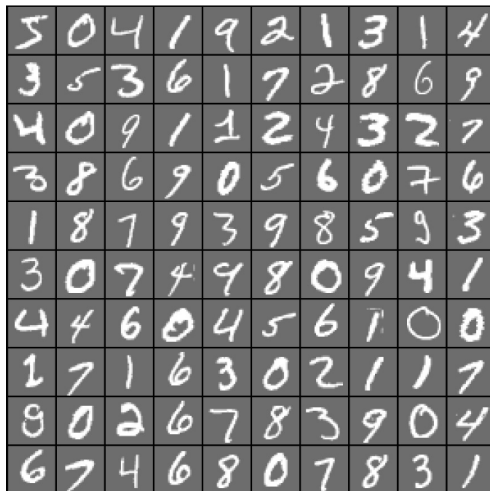
# Ill-posed with small amount of labeled data



- 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]

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[Y. LeCun, L. Bottou, Y. Bengio, and P. Haffner. "Gradient-based learning applied to document recognition." Proceedings of the IEEE, 86(11):2278-2324, November 1998.]

# Laplace learning on MNIST at low label rates

# Labels per class	1	2	3	4	160
Laplace Learning	16.1 (6.2)	28.2 (10.3)	42.0 (12.4)	57.8 (12.3)	97.0 (0.1)
Nearest Neighbor	65.4 (5.2)	74.2 (3.3)	77.8 (2.6)	80.7 (2.0)	92.4 (0.2)

- Average accuracy over 100 trials with standard deviation in brackets.
- Nearest neighbor is geodesic graph-nearest neighbor.

# 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, 2020]

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# Higher Order Poisson Learning

We propose the higher order Poisson (HOP) learning

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

subject to  $\sum_{x \in \mathcal{X}} u(x) = 0$ , where  $\bar{g} = \frac{1}{|\Gamma|} \sum_{y \in \Gamma} g(y)$  and  $m \in \mathbf{Z}^+$ .

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The label decision is the same as before:

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The higher order Poisson learning problem is equivalent to the variational problem

$$(2) \quad \min_{u \in \ell_0^2(\mathcal{X})} \left\{ \frac{1}{2} (u, \mathcal{L}^m u) - \sum_{x \in \Gamma} (g(x) - \bar{g}) \cdot u(x) \right\}.$$

where  $\bar{g} = \frac{1}{|\Gamma|} \sum_{x \in \Gamma} g(x)$  is the average label vector.

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## Theorem 1 (Existence and Uniqueness of Solution for HOP Learning)

*Assume that  $\mathcal{G}$  is connected. Then there exists a unique minimizer  $u \in \ell_0^2(\mathcal{X})$  of (2) and furthermore it satisfies the Euler-Lagrange equation for higher order Poisson learning*

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*Suppose that the graph Laplacian operator  $\mathcal{L}$  is defined on a connected graph  $\mathcal{G}$ . The kernel of the graph Laplacian operator is the set of constant function on  $\mathcal{X}$ . In other words, we have*

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## Lemma 3

*The range of the graph Laplacian operator is the set of unweighted mean-zero functions on  $\mathcal{X}$ . In other words, we have*

$$\text{range}(\mathcal{L}) = \mathcal{L}(\mathcal{X}) = \{v \in \ell^2(\mathcal{X}) : \sum_{i=1}^n v(x_i) = 0\},$$

*where  $\mathcal{L}$  is the graph Laplacian operator and  $\mathcal{X}$  is explicitly written out as  $\mathcal{X} := \{x_1, \dots, x_n\}$  with  $n \in \mathbf{Z}^+$ .*

# Preliminary Results

## Lemma 4

*Let  $\mathcal{L}$  be the graph Laplacian operator,  $\mathcal{X}$  be explicitly written as  $\mathcal{X} := \{x_1, \dots, x_n\}$  with  $n \in \mathbb{Z}^+$ , and  $m \in \mathbb{Z}^+$  be given. Then we have*

$$\ker(\mathcal{L}^m) = \ker(\mathcal{L}) = \{v \in \ell^2(\mathcal{X}) : v(x) = v(y) \text{ for all } x, y \in \mathcal{X}\},$$

*and*

$$\text{range}(\mathcal{L}^m) = \text{range}(\mathcal{L}) = \{v \in \ell^2(\mathcal{X}) : \sum_{i=1}^n v(x_i) = 0\}.$$

*In other words, the kernel and range of the higher order Laplacian is the same as the kernel and range of the graph Laplacian.*

# Sketch of the Proof for the Theorem

“Proof:” Consider the Euler Lagrange equation for HOP learning problem

$$\mathcal{L}^m u(x) = \sum_{y \in \Gamma} (g(y) - \bar{g}) \delta_{xy} = \begin{cases} g(x) - \bar{g}, & \text{when } x \in \Gamma, \\ 0, & \text{when } x \notin \Gamma. \end{cases}$$

Thus the existence of solution as range of  $\mathcal{L}^m$  is the set of mean zero functions.

The solution is unique up to a constant function as the kernel of  $\mathcal{L}^m$  is a set of constant functions.

The variational interpretation then comes naturally by taking the variations of the energy term

$$E(u) = \frac{1}{2}(u, \mathcal{L}^m u) - \sum_{x \in \Gamma} (g(x) - \bar{g}) \cdot u(x). \quad \square$$



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# Algorithm Development

To solve the Euler-Lagrange equation for higher order Poisson learning

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

we need to construct the inverse matrix  $(\mathcal{L}^m)^{-1}$ . This can be done through spectral numerical approximation.

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# Algorithm Development

## Theorem 5 (Spectral Numerical Approximation)

*The solution of the Euler-Lagrange equation for higher order Poisson learning*

$$\mathcal{L}^m u(x) = \sum_{y \in \Gamma} (g(y) - \bar{g}) \delta_{xy}$$

*can be approximated by*

$$u(x) \approx (\mathcal{L}_N^m)^{-1} \sum_{y \in \Gamma} (g(y) - \bar{g}) \delta_{xy}$$

*where*

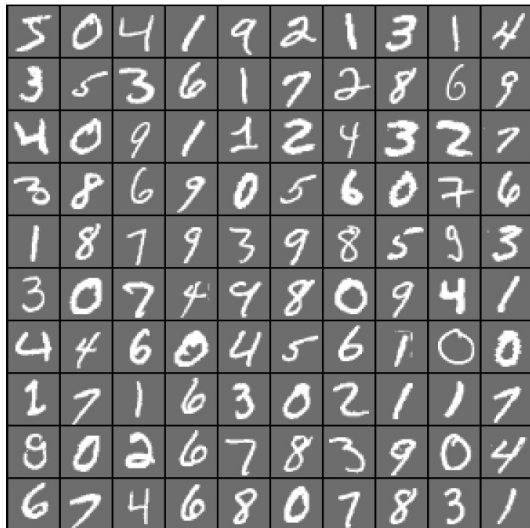
$$(\mathcal{L}_N^m)^{-1} = V_N \Lambda_{N,m} V_N^T$$

*with  $V_N$  being the matrix of first  $N$  (in terms of the ascending order of eigenvalues) eigenvectors as its columns and  $\Lambda_{N,m} = \text{diag}((\lambda_i^{-m})_{i=1, \dots, N})$  being the diagonal matrix with diagonal entries equal to the inverse of the first  $N$  eigenvalues.*

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# MNIST

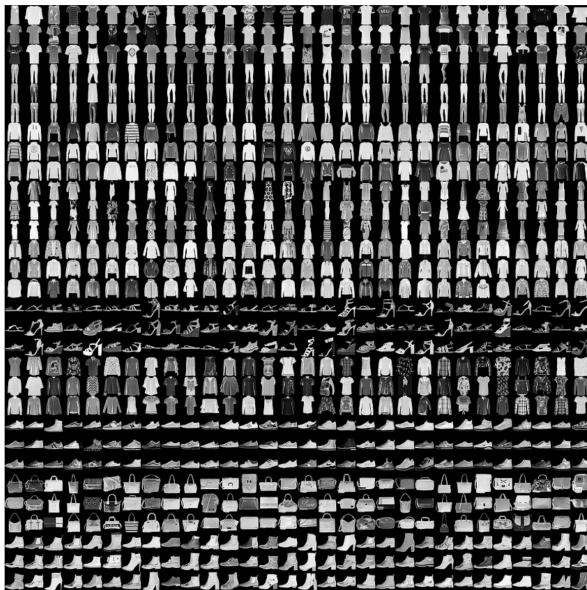


# Simulation Results (MNIST)

Figure: Mean(Standard Deviation) Classification Accuracy over 100 Trials

# LABELS PER CLASS	1	2	3	4	5
HOP WITH $N = 20$ & $m = 1.0$	<b><u>91.6 (3.9)</u></b>	<b><u>94.3 (1.6)</u></b>	<b><u>95.0 (0.8)</u></b>	95.1 (0.6)	95.3 (0.5)
HOP WITH $N = 30$ & $m = 1.0$	90.9 (3.8)	94.3 (1.5)	94.9 (1.1)	<b><u>95.3 (0.9)</u></b>	<b><u>95.6 (0.8)</u></b>
POISSON	90.2 (4.0)	93.6 (1.6)	94.5 (1.1)	94.9 (0.8)	95.3 (0.7)

# Fashion-MNIST





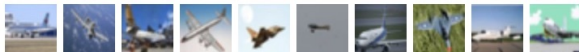
# Simulation Results (Fashion-MNIST)

Figure: Mean(Standard Deviation) Classification Accuracy over 100 Trials

# LABELS PER CLASS	1	2	3	4	5
HOP WITH $N = 10$ & $m = 0.4$	<u><b>61.7 (5.2)</b></u>	65.6 (4.1)	68.5 (2.6)	69.5 (2.2)	69.7 (2.1)
HOP WITH $N = 20$ & $m = 0.7$	60.7 (4.8)	<u><b>65.8 (4.4)</b></u>	69.4 (2.8)	70.6 (2.6)	71.4 (2.3)
HOP WITH $N = 30$ & $m = 0.8$	59.9 (4.7)	65.6 (4.2)	<u><b>69.5 (2.7)</b></u>	70.8 (2.5)	72.0 (2.3)
HOP WITH $N = 30$ & $m = 0.7$	59.6 (4.7)	65.5 (4.2)	69.4 (2.7)	<u><b>70.9 (2.5)</b></u>	<u><b>72.1 (2.2)</b></u>
POISSON	60.8 (4.6)	<u><b>66.1 (3.9)</b></u>	<u><b>69.6 (2.6)</b></u>	<u><b>71.2 (2.2)</b></u>	<u><b>72.4 (2.3)</b></u>

# Cifar-10

**airplane**



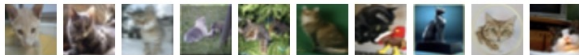
**automobile**



**bird**



**cat**



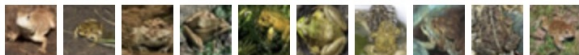
**deer**



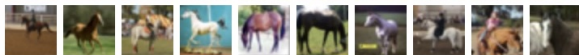
**dog**



**frog**



**horse**



**ship**



**truck**

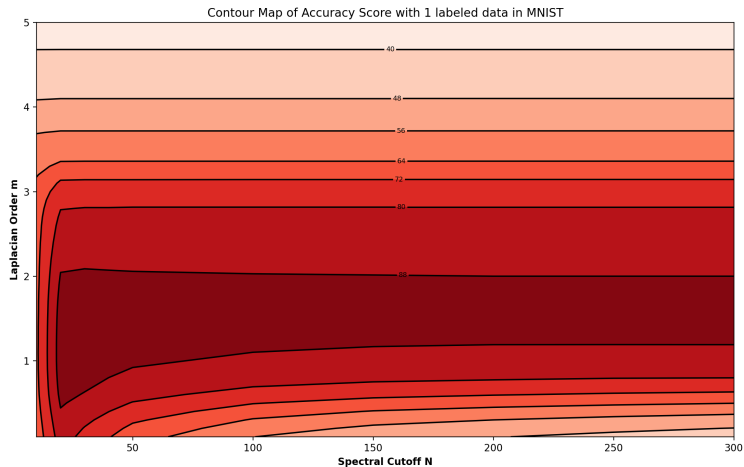


# Simulation Results (Cifar-10)

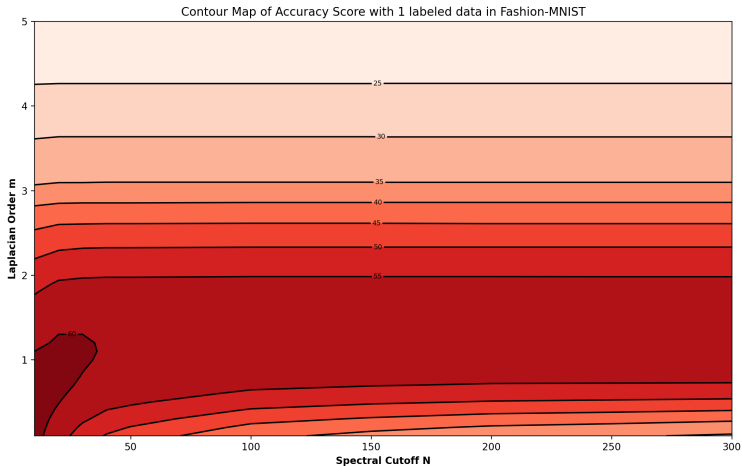
Figure: Mean(Standard Deviation) Classification Accuracy over 100 Trials

# LABELS PER CLASS	1	2	3	4	5
HOP WITH $N = 20$ & $m = 0.3$	<b><u>41.8 (5.5)</u></b>	47.7 (5.3)	51.0 (3.9)	53.1 (3.1)	54.4 (2.7)
HOP WITH $N = 20$ & $m = 0.1$	41.7 (5.5)	<b><u>47.8 (5.3)</u></b>	<b><u>51.0 (3.8)</u></b>	<b><u>53.2 (3.1)</u></b>	<b><u>54.5 (2.7)</u></b>
POISSON	40.7 (5.5)	46.5 (5.1)	49.9 (3.4)	52.3 (3.1)	53.8 (2.6)

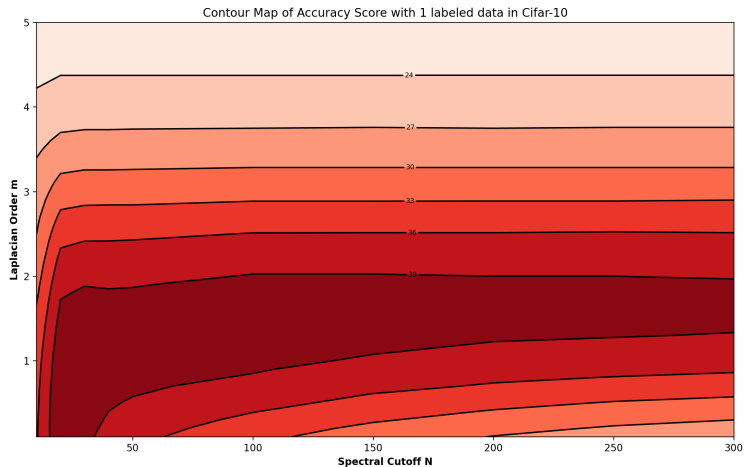
# Contour Graphs for Simulation Results (MNIST)



# Contour Graphs for Simulation Results (Fashion-MNIST)



# Contour Graphs for Simulation Results (Cifar-10)



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# Current and Future Works



# Current and Future Works

We observe that:

# Current and Future Works

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- The lower the spectral cutoff  $N$  is, the better result we have in terms of classification accuracy in general (Spectral Embedding and Clustering).
- The combination of the spectral cutoff  $N$  and the Laplacian operator order  $m$  plays a great role in the classification accuracy score.

# Current and Future Works

We observe that:

- The lower the spectral cutoff  $N$  is, the better result we have in terms of classification accuracy in general (Spectral Embedding and Clustering).
- The combination of the spectral cutoff  $N$  and the Laplacian operator order  $m$  plays a great role in the classification accuracy score.

Future works may want to investigate for a criterion to find the best combination between the spectral cutoff  $N$  and the Laplacian operator order  $m$ .

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**Code:** <https://github.com/DingjunB/Honors-Thesis.git>

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