DARTMOUTH

Randomization & Approximation in Machine Learning and Neural Network Pruning

Math 76 Final Project

Warren Shepard Sri Korandla Tushar Aggarwal

August 2024

Dr. Alice Schwarze

Table of contents

Basic Randomization & Approximation in ML

Randomization & Approximation as we know it

The randomization techniques from class mostly involve **splitting** or **modifying data** randomly:

- splitting data into training and testing subsets

```
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.3, random_state=42)
```

- bagging/bootstrapping procedures
- random parameter/weight initialization in neural networks

Approximation is of course the goal of machine learning, but we often use *exact* algorithms in ML models instead of approximation algorithms

What else can Randomization & Approximation be used for

- Optimization:
  - trade "accuracy" for speed
  - oftentimes algorithms have $\geq 90\%$ accuracy
- In neural networks
  - "Prune" connections (somewhat) at random to get a smaller model with higher accuracy
- Sometimes, allowing some error is more "realistic" leading to a higher accuracy
  - higher accuracy's could also be because of a reduction in over fitting

Example: k Approximate Nearest Neighbors

Naive Solution

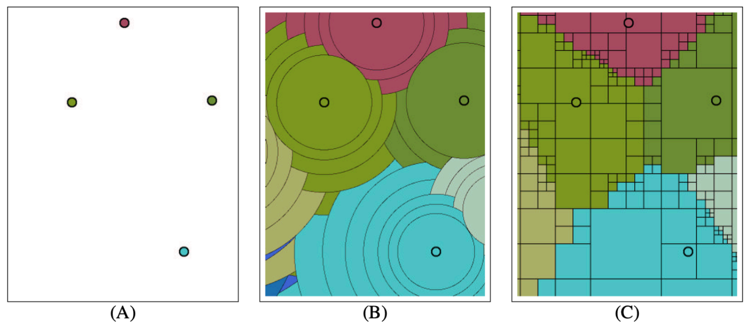
Problem: Given a set of vectors S in a data space and a similarity measure DIST (for example euclidean distance) find the k nearest ("most similar") neighbors to some input x.

Brute force solution: compare to every other point

```
procedure BRUTE-KNN(x, S, DIST, k = 1)
    Compute DIST(x, s) ∀ s ∈ S
    return k points (s ∈ S) with smallest DIST values
```

Issue: expensive and **redundant** (especially in higher dimensions and when there is lots of training data); $O(n)$ lookup

k Approximate Nearest Neighbors (kANN)



A) data points; B) & C) approximate nearest neighbor [3]

Locality Sensitive Hashing (LSH)

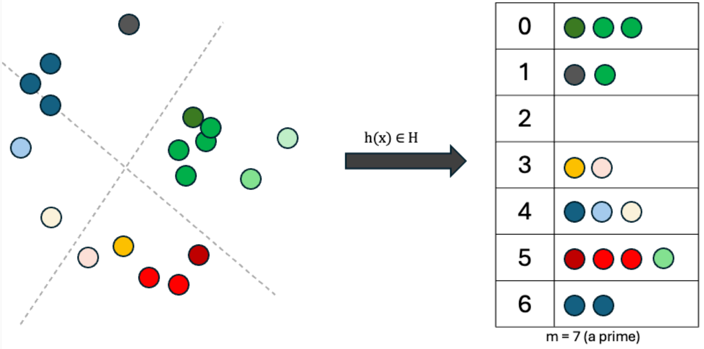
Hashing:

- hash function: $f : U \to [n]$ where $|U| >> n$ and n is (usually) prime
- typically, two inputs have a very low probability of ”colliding” (their output is the same)
  - inputs will have different ”hashes” even if they are very similar

Locality Sensitive Hashing (LSH)

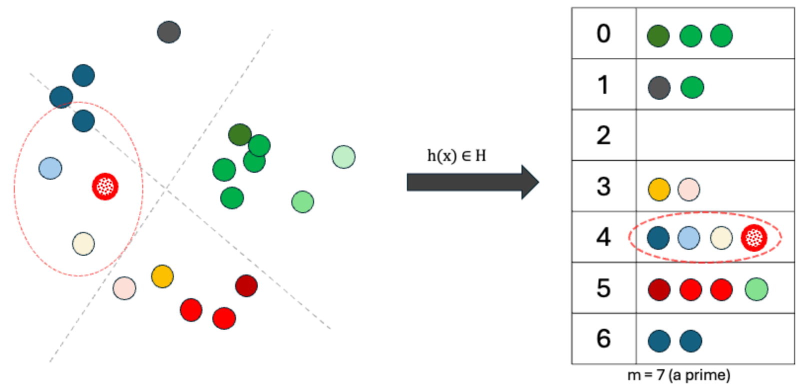
- two inputs which are similar have a high probability of colliding [3]
- can be used to solve kANN with high accuracy and in less time

LSH Preprocessing



Pre processing for LSH; completed in $O(n)$ time

LSH Query



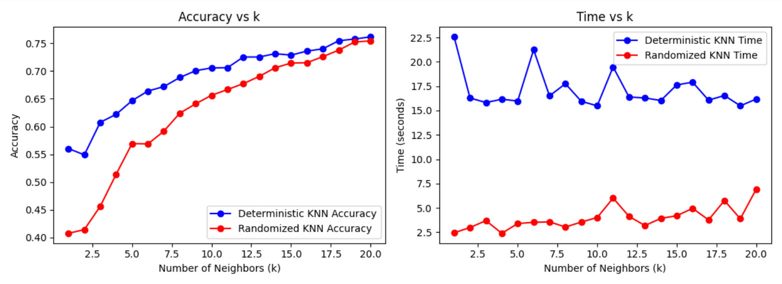
Querying for LSH; completed in $O(1)$ time per query

Approximate-KNN Experiment

- using PyNNdescent package for kANN implementation [5]
  - uses modern kANN algorithm [1], written in python
  - accuracy converges to 90%
- Naive brute force implementation hand written in python
  - did not use an implementation from scikitlearn because compiled in C
  - best to have implementation we are comparing all in the same language

Results

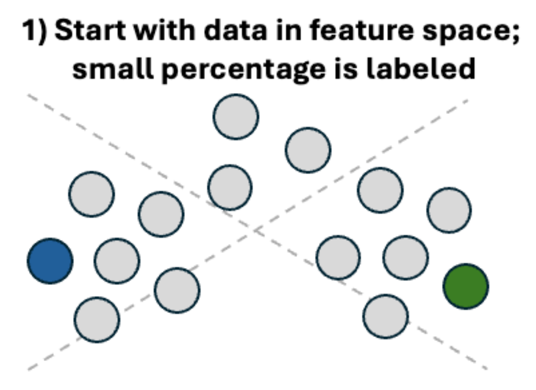
```
# Generate a synthetic dataset with 10,000 samples and 1,000 features
X, y = make_classification(n_samples=10000, n_features=200, n_informative=50, n_classes=3,
        random_state=42)
```



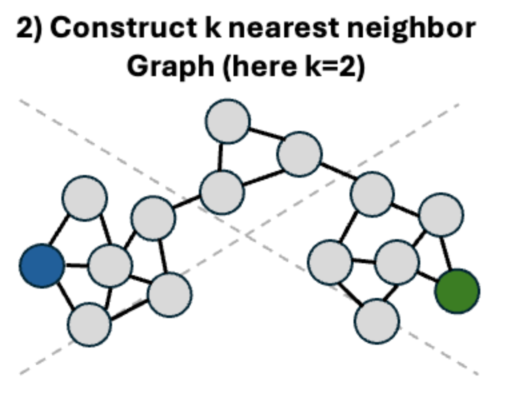
kNN vs kANN **raw** accuracy and time comparison

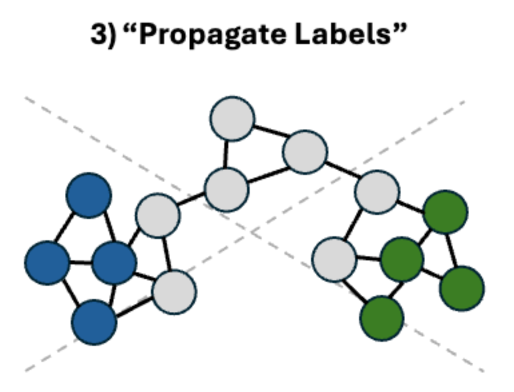
Graph-Based Semi-Supervised Learning

Graph-Based Semi-Supervised Learning

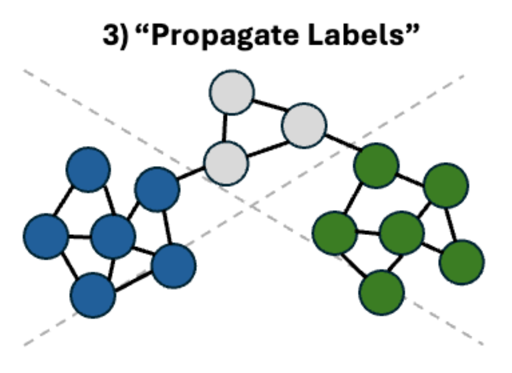


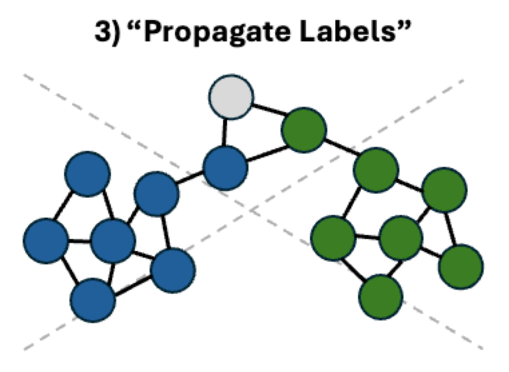
Graph-Based Semi-Supervised Learning



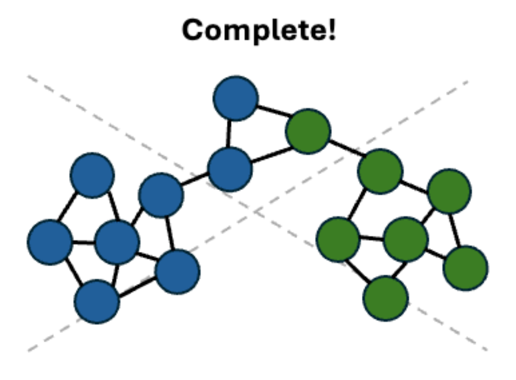

3) “Propagate Labels”

Graph-Based Semi-Supervised Learning

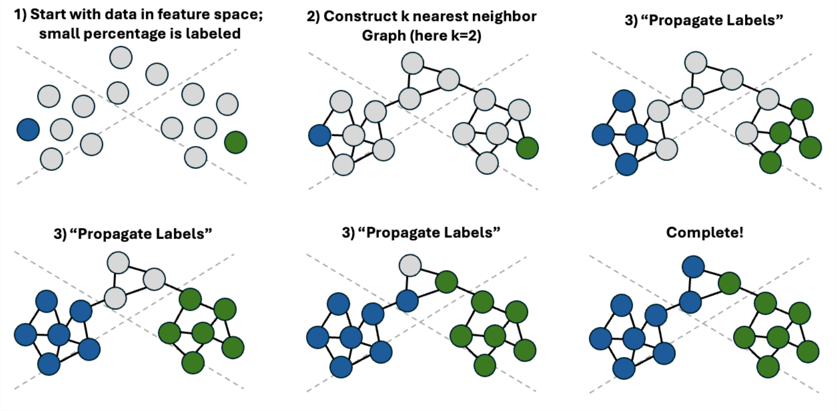



3) “Propagate Labels”

Graph-Based Semi-Supervised Learning



Graph-Based Semi-Supervised Learning



Graph-Based Semi-Supervised Learning

- Constructing the k Nearest Neighbor Graph dominates runtime
- Most Label Propagation Algorithms (LPA) are **simple** and **near linear** in time

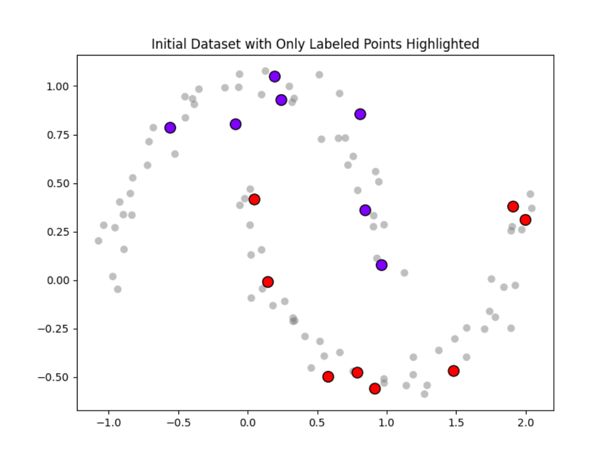
Parameters:

- $y :=$ initial labels; $y_i :=$ label of node i; -1 if unlabeled
- $W :=$ adjacency matrix of nearest neighbors graph
- $\alpha \in [0, 1] :=$ "clamping factor" indicating influence of initial labels **per iteration**

Update Rules:

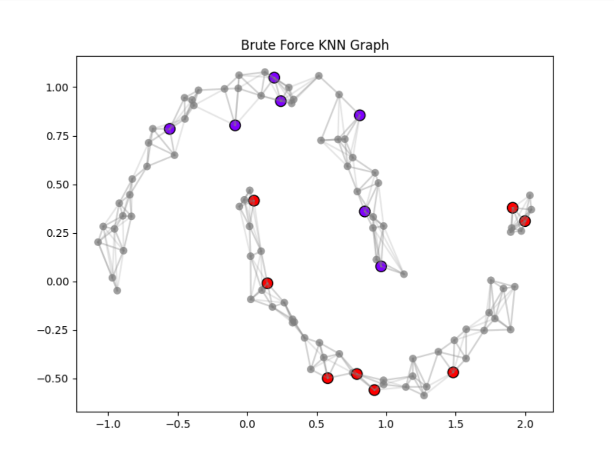
- $F_{ic}^{(0)} \leftarrow \begin{cases} 1 & \text{if } y_i = c \\ 0 & \text{otherwise} \end{cases}$ F_{ic} is the **confidence** of node i having label c
- $F_{ic}^{(t+1)} \leftarrow \underbrace{\alpha W F^{(t)}}_{\text{propagate from neighbors}} + \underbrace{(1-\alpha) F^{(0)}}_{\text{account for initial labels}}$
- $y_i^* \leftarrow \mathbf{arg\,max}_c\, F_{ic}^{(t_{\max})}$ y_i^* is the vector of **final labels**

Results I



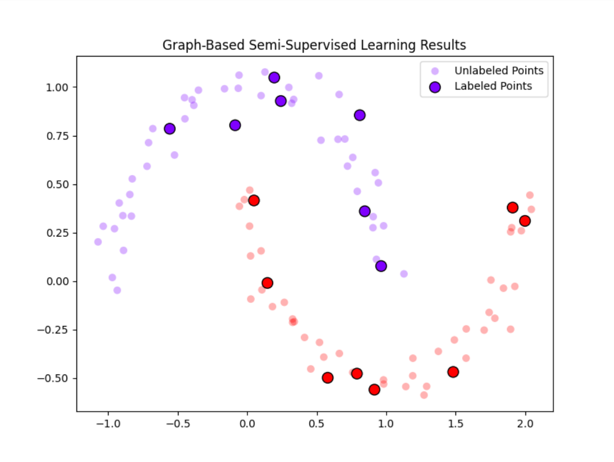
Initial Dataset with Only Labeled Points Highlighted
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0

Results I



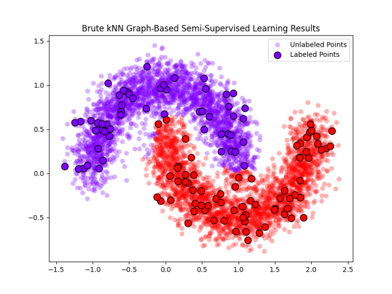
Nearest Neighbor graph with $k = 5$

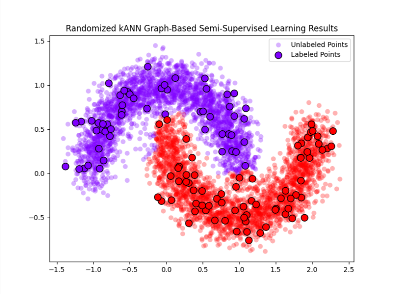
Results I



Final labels using $\alpha = .99$

Results II

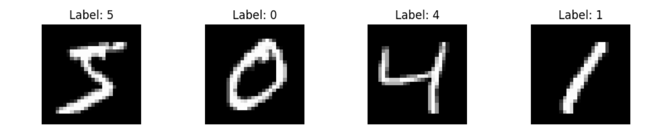




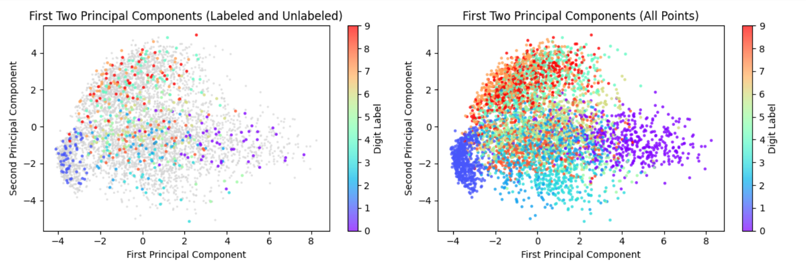
- Time: 4.20 seconds
- Accuracy: 0.976

- Time: 2.89 seconds
- Accuracy: 0.977

MNIST Dataset Preprocessing



- Normalized signal to take value $\in [0, 1]$
- PCA to extract top 50 principle components
- masked 90% of labels to simulate semi-supervised learning; kept full label set for accuracy testing



MNIST Dataset Results

* Ran with A100 GPU runtime on Google Colab
* Parameters:

Using Brute Force kNN:

- Accuracy: 0.933
- Total Time: 18.81 minutes
- Time to construct kNN-graph: 17.14 minutes

Using k Approximate NN:

- Accuracy: 0.955
- Time: 1.79 minutes
- Time to construct kANN-graph: [redacted]

MNIST Dataset Results

* Ran with A100 GPU runtime on Google Colab
* Parameters:

Using Brute Force kNN:

- Accuracy: 0.933
- Total Time: 18.81 minutes
- Time to construct kNN-graph: 17.14 minutes

Using k Approximate NN:

- Accuracy: 0.955
- Time: 1.79 minutes
- Time to construct kANN-graph: **< 6.2 seconds**

MNIST Dataset Results

* Ran with A100 GPU runtime on Google Colab
* Parameters:

Using Brute Force kNN:

- Accuracy: 0.933
- Total Time: 18.81 minutes
- Time to construct kNN-graph: 17.14 minutes

Using k Approximate NN:

- Accuracy: 0.955
- Time: 1.79 minutes
- Time to construct kANN-graph: **< 6.2 seconds**

Approximate NN-graph construction is over 165 times faster than the naive

The Problem With (our) Label Propagation (implementation)

- In theory, LPA can be parallelized
    - instead of executing **sequentially**, tasks are executed **simultaneously** on multiple units (i.e. CPU/GPU)
- No early stopping
    - the number of iterations is a parameter
    - stop early if there is no/little change between two consecutive iterations
- ~~Not leveraging sparse matrices~~
    - MNIST PCA is not sparse!

LPA Implementation Improvements & Results

Improvements:

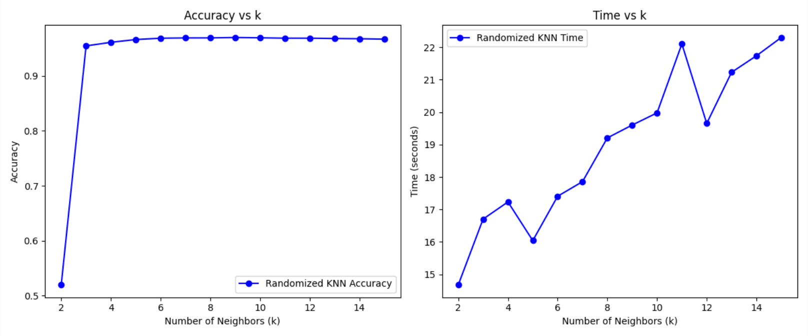
- Parallelization did not help
- Early stopping helped significantly and easy to implement

New results using k Approximate NN:

- Accuracy: 0.966
- Time: 16 seconds
- Time to construct kANN-graph: $\approx$ 6 seconds
- LPA time: **10 seconds**; **over 10 times faster**

Note: accuracy is 1% higher, which indicates initial model may have been slightly overfit

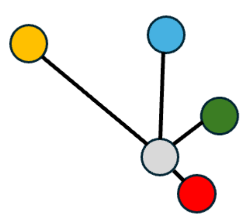
Hyper-Parameter (k) tuning



Accuracy (left) and time (right) comparison for $k \in [2 : 15]$

Note: Increase in time is a result of NN-graph construction, not LPA

The Inefficiency with LPA (in this context)



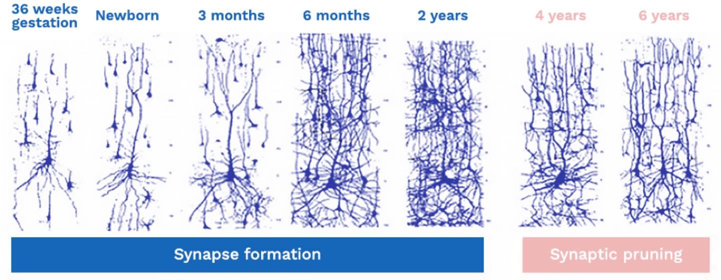
- we do not consider distances to nearest neighbors
- however, we already calculated these distances in kNN
- in kANN we did not, but it would take negligible time to compute distances
- Idea: if we consider distances to nearest neighbors in LPA, it could potentially be more accurate

Randomized Pruning in Neural Networks

Why Prune?

- ”It is widely acknowledged that large and sparse models have higher accuracy than small and dense models” [4]
- pruning a model prevents over-fitting
- pruned models also require a fraction of the space a unpruned model would need in memory

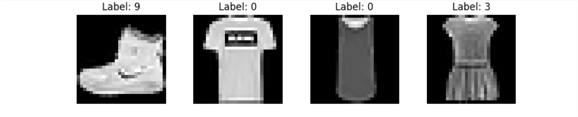
Neurology Inspiration



Synaptic pruning in the brain [2]

Dataset and Neural Network Architecture

- We use a simple architecture recommended by tensorflow
- We prune connections on one layer (more detail on next slide)
- pruning is done by setting pruned weights (outgoing to next layer) to zero
- Inspiration for randomized pruning: ”Breaking through Deterministic Barriers: Randomized Pruning Mask Generation and Selection” [4]



MNIST Fashion Dataset

RESULTS

Network	Pruning Strategy	Accuracy
No Pruning	No pruning is applied. All connections are retained.	87.68%
Threshold Fraction Pruning	Prune a specified fraction of connections with the smallest weights.	86.63%
Random Pruning	Prune a random subset of connections, regardless of their weights or importance.	64.56%
Importance-Weighted Random Pruning	Prune connections probabilistically based on their importance, where more important connections are less likely to be pruned.	78.06%
Fractional Random Threshold Pruning	First, select a fraction of connections with the smallest weights. Then, randomly prune a smaller fraction of these selected connections.	87.47%

Summary of Pruning Strategies for Five Neural Networks

Questions???

References i

W. Dong, M. Charikar, and K. Li.
Efficient k-nearest neighbor graph construction for generic similarity measures.
In Proceedings of the 20th international conference on World wide web, pages 577–586. ACM, 2011.

J. Embrace.
Synaptic growth, synesthesia, and savant abilities.
Embrace Autism, 2024.
Accessed: 2024-08-12.

S. Har-Peled, P. Indyk, and R. Motwani.
Approximate nearest neighbor: Towards removing the curse of dimensionality.
Theory of Computing, 8:321–350, 2012.
Special issue in honor of Rajeev Motwani.

J. Li, W. Gao, Q. Lei, and D. Xu.
Breaking through deterministic barriers: Randomized pruning mask generation and selection.
arXiv preprint arXiv:2310.13183, 2023.
Accessed: 2024-08-14.

PyNNDescent Developers.
PyNNDescent Documentation, 2024.
Accessed: 2024-08-14.