ENTERPRISE-SCALE TOPOLOGICAL DATA ANALYSIS USING SPARK

Anshuman Mishra, Lawrence Spracklen
Alpine Data

Spark summit
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DATA SCIENCE AND ENGINEERING AT SCALE
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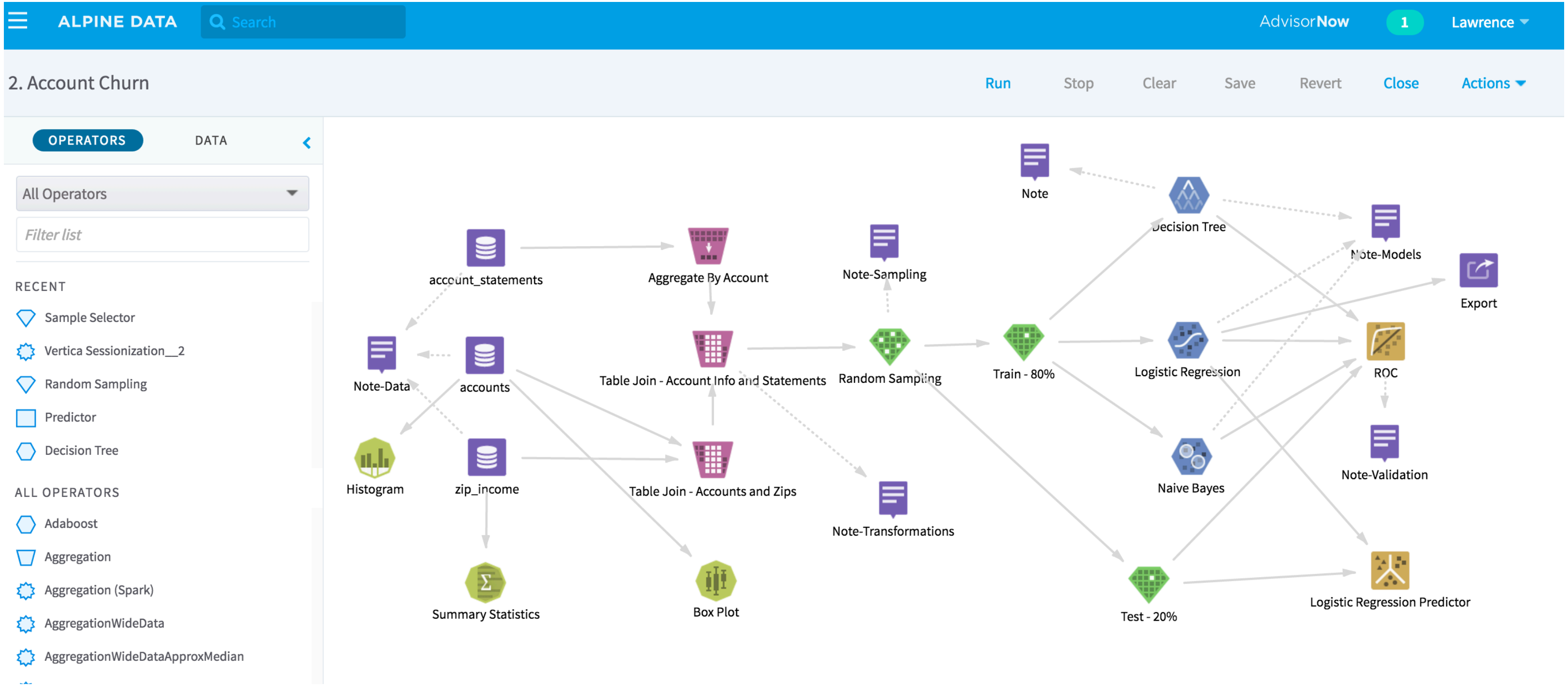
Alpine Data



ALPINE DATA
Search
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2. Account Churn
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OPERATORS
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Filter list
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Random Sampling
Predictor
Decision Tree
ALL OPERATORS
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Aggregation
Aggregation (Spark)
AggregationWideData
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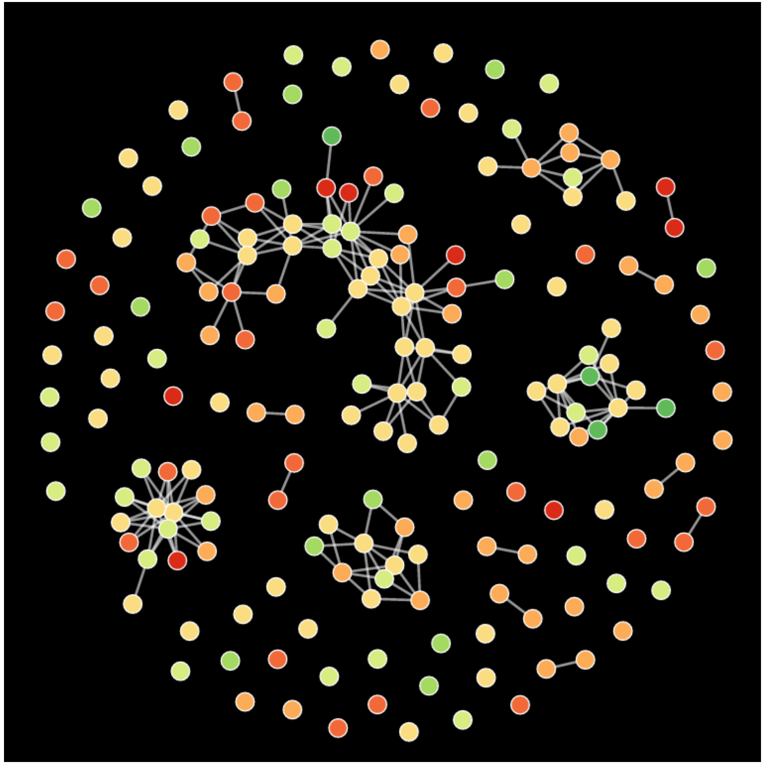
account_statements
Aggregate By Account
Note-Sampling
Note
Decision Tree
Note-Models
Export
Note-Data
accounts
Table Join - Account Info and Statements
Random Sampling
Train - 80%
Logistic Regression
ROC
Histogram
zip_income
Table Join - Accounts and Zips
Naive Bayes
Note-Validation
Note-Transformations
Summary Statistics
Box Plot
Test - 20%
Logistic Regression Predictor

What we'll talk about

- What's TDA and why should you care
- Deep dive into Mapper and bottlenecks
- **Betti Mapper** - scaling Mapper to the enterprise

Can anyone recognize this?



We built the first open-source scalable implementation of TDA Mapper

- Our implementation of Mapper beats a naïve version on Spark by **8x-11x*** for moderate to large datasets
  - 8x: avg. 305 s for Betti vs. non-completion in 2400 s for Naïve (100,000 x 784 dataset)
  - 11x: avg. 45 s for Betti vs. 511 s for Naïve (10,000 x 784 dataset)
- We used a novel combination of locality-sensitive hashing on Spark to increase performance

TDA AND MAPPER: WHY SHOULD WE CARE?

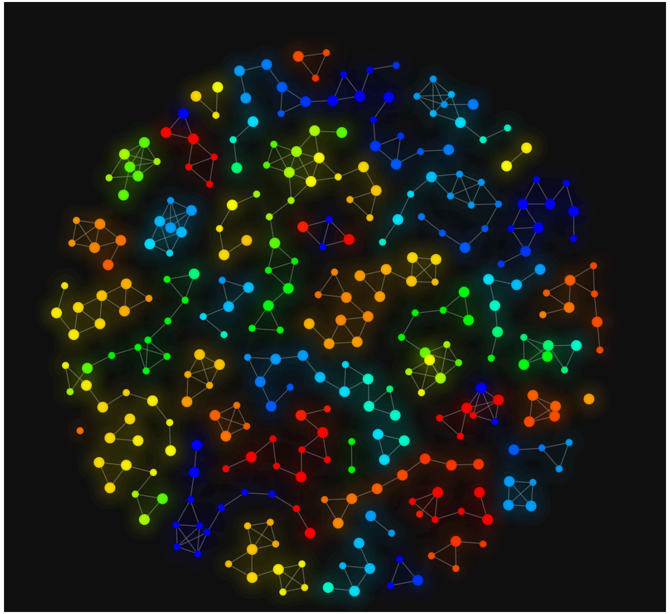
Conventional ML carries the "curse of dimensionality"

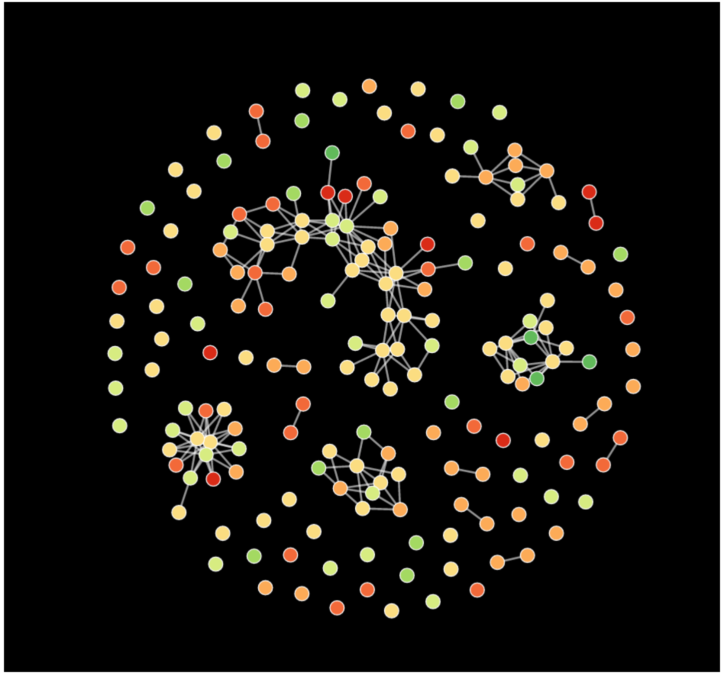
- As d $\rightarrow \infty$, all data points are packed away into corners of a corresponding d-dimensional hypercube, with little to separate them
- Instance learners start to choke
- Detecting anomalies becomes tougher

How does TDA (Mapper) help?

- ***"Topological Methods for the Analysis of High Dimensional Data Sets and 3D Object Recognition"***, G. Singh, F. Memoli, G. Carlsson, Eurographics Symposium on Point-Based Graphics (2007)
- Algorithm consumes a dataset and generates a topological summary of the whole dataset
- Summary can help identify localized structures in high-dimensional data

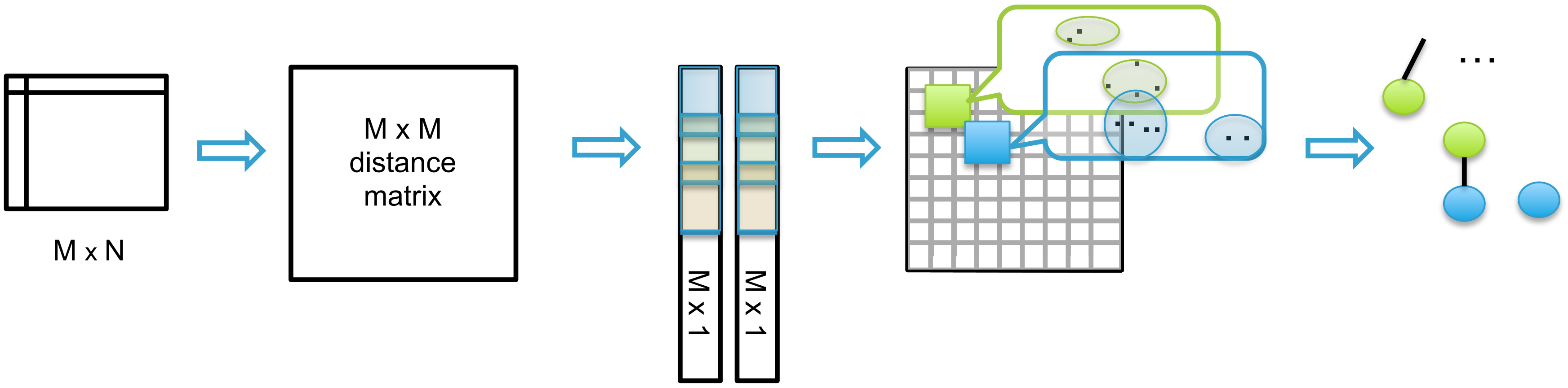
Some examples of Mapper outputs



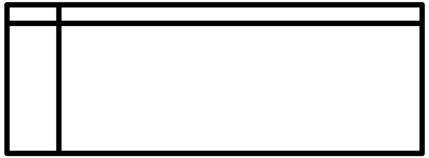


DEEP DIVE INTO MAPPER

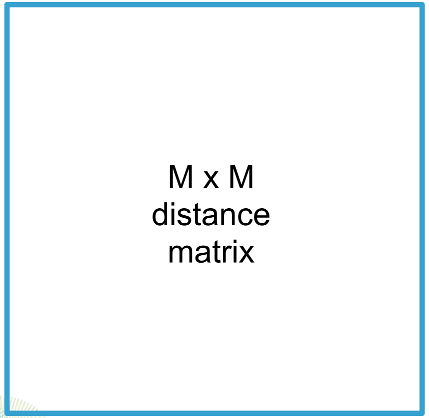
Mapper: The 30,000 ft. view



Mapper: 1. Choose a Distance Metric



M x N

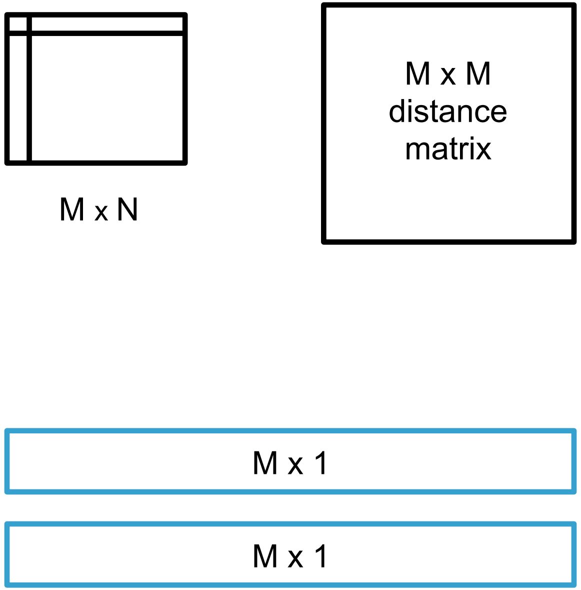


The **1st step** is to **choose a distance metric** for the dataset, in order to **compute a distance matrix**.

This will be used to capture similarity between data points.

Some examples of distance metrics are Euclidean, Hamming, cosine, etc.

Mapper: 2. Compute filter functions



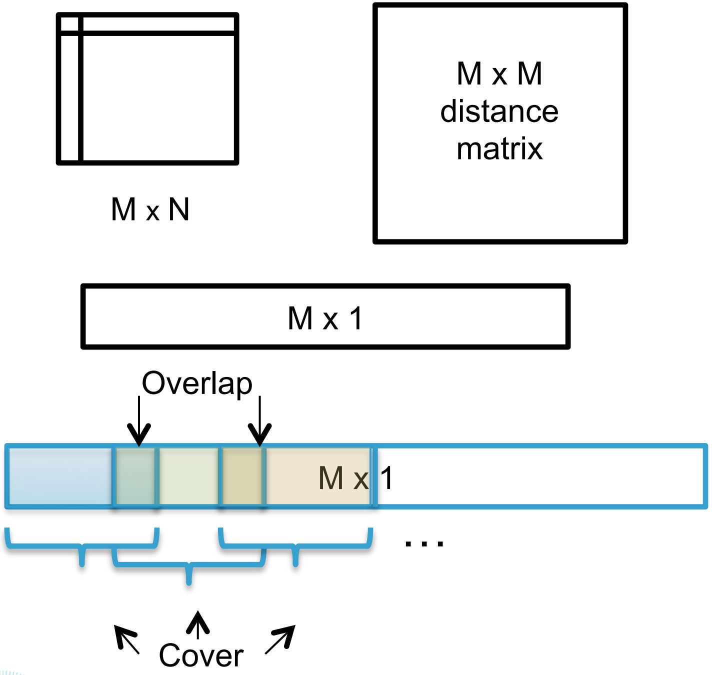
Next, **filter functions** (aka **lenses**) are chosen to map data points to a single value on the real line.

These filter functions can be based on:

- Raw features
- Statistics – mean, median, variance, etc.
- Geometry – distance to closest data point, furthest data point, etc.
- ML algorithm outputs

Usually two such functions are computed on the dataset.

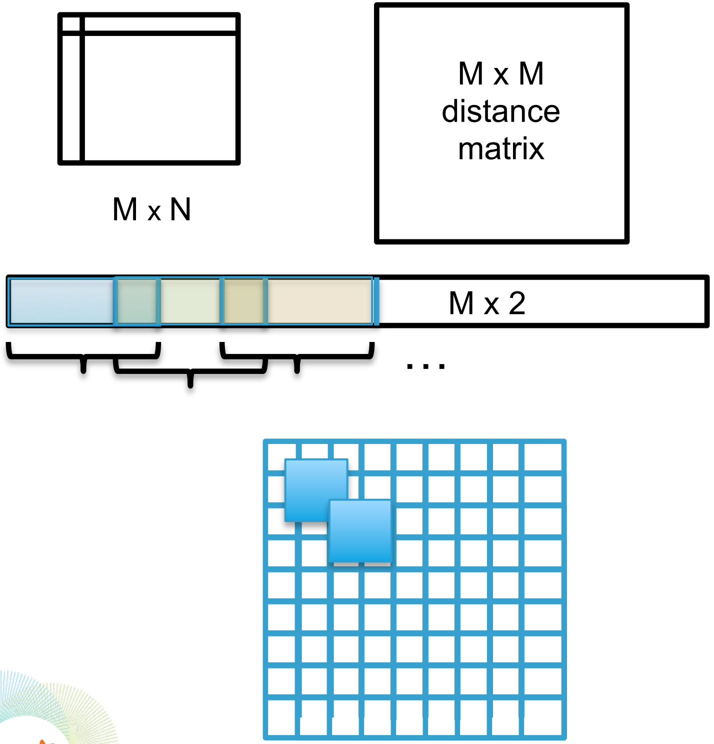
Mapper: 3. Apply cover & overlap



Next, the ranges of each filter application are “chopped up” into overlapping segments or intervals using two parameters: **cover** and **overlap**

- Cover (aka **resolution**) controls how many intervals each filter range will be chopped into, e.g. 40,100
- Overlap controls the degree of overlap between intervals (e.g. 20%)

Mapper: 4. Compute Cartesians

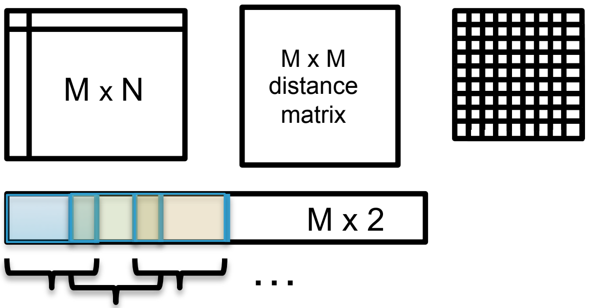


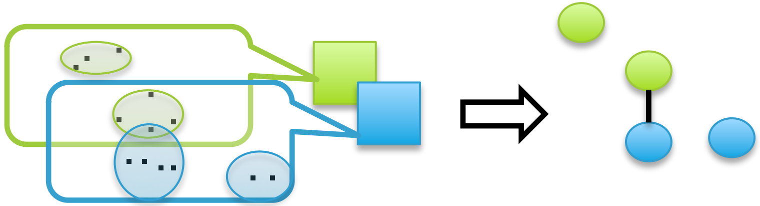
The next step is to compute the Cartesian products of the range intervals (from the previous step) and assign the original data points to the resulting two-dimensional regions based on their filter values.

Note that **these two-dimensional regions will overlap** due to the parameters set in the previous step.

In other words, there will be points in common between these regions.

Mapper: 5. Perform clustering



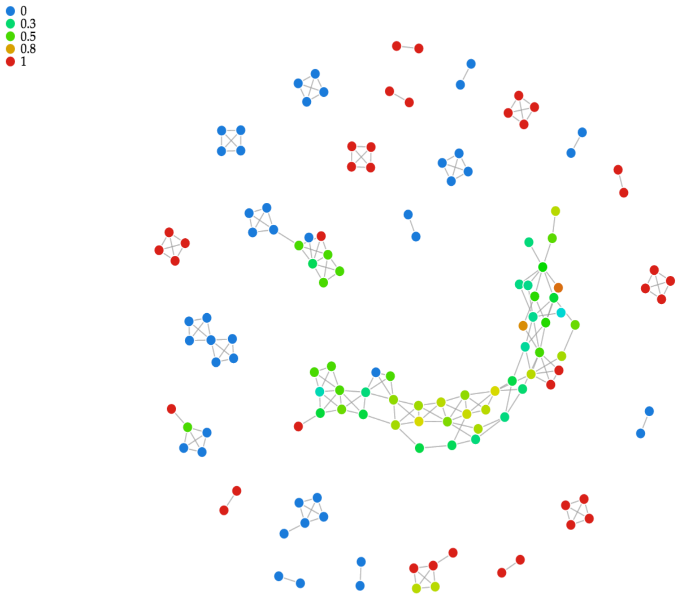


The penultimate stage in the Mapper algorithm is to **perform clustering in the original high-dimensional space** for each (overlapping) region.

Each cluster will be represented by a node; since regions overlap, some clusters will have points in common. **Their corresponding nodes will be connected via an unweighted edge**.

The kind of clustering performed is immaterial. Our implementation uses DBSCAN.

Mapper: 6. Build TDA network



Finally, by joining nodes in topological space (re: clusters in feature space) that have points in common, one can derive a topological network in the form of a graph.

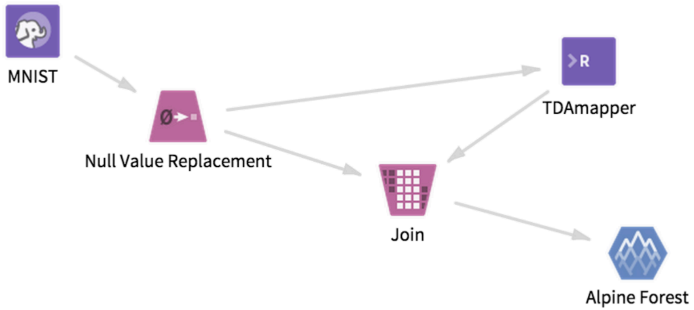
Graph coloring can be performed to capture localized behavior in the dataset and derive hidden insights from the data.

Open source Mapper implementations

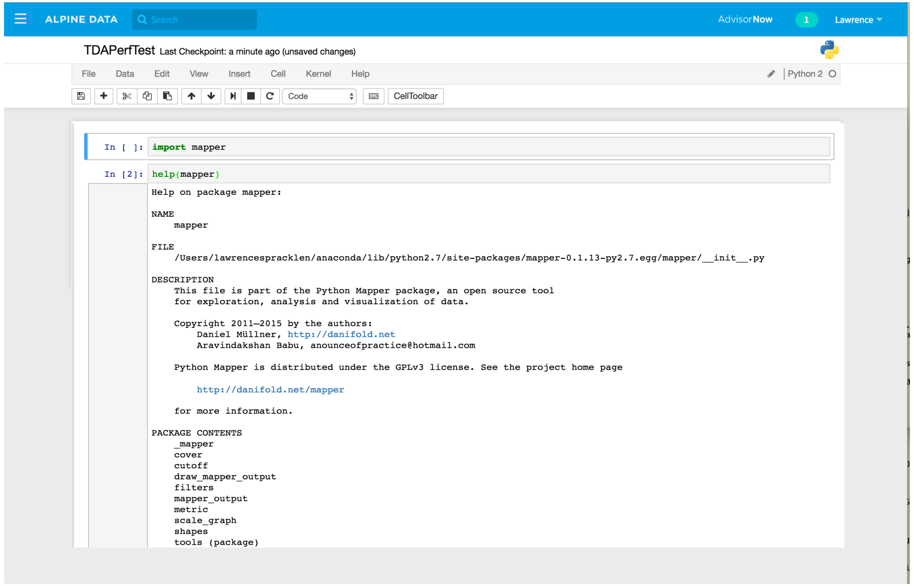
- Python:
  - Python Mapper, Mullner and Babu: http://danifold.net/mapper/
  - Proof-of-concept Mapper in a Kaggle notebook, @mlwave: https://www.kaggle.com/triskelion/digit-recognizer/mapping-digits-with-a-t-sne-lens/notebook
- R:
  - TDAmapper package
- Matlab:
  - Original mapper implementation

Alpine TDA

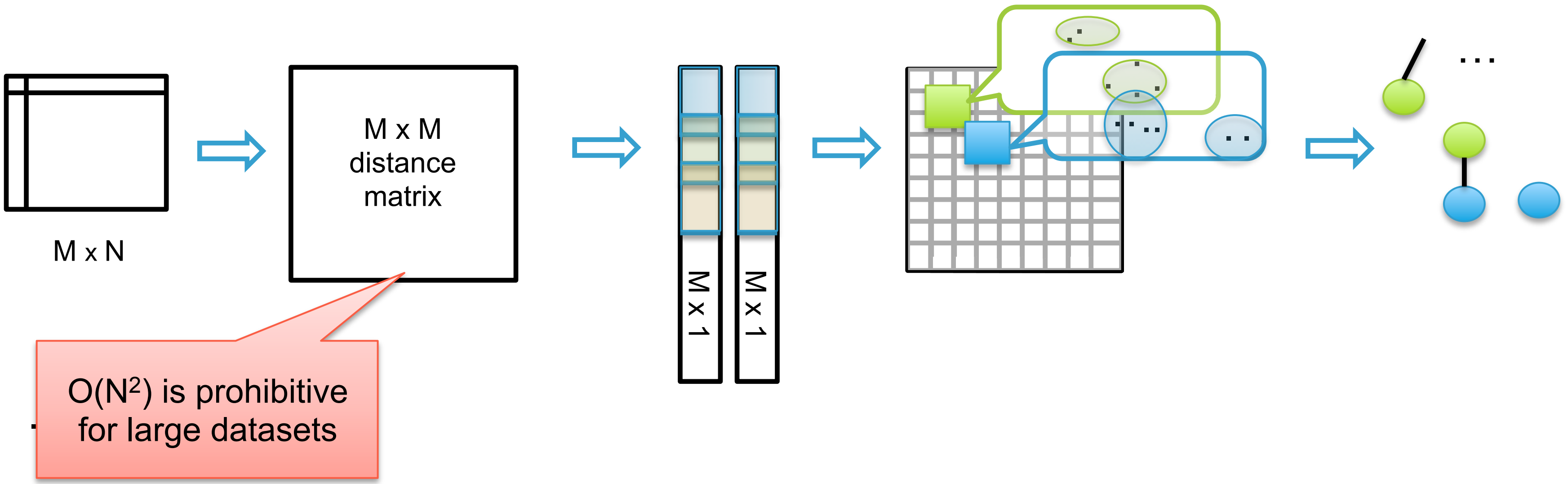
R



Python



Mapper: Computationally expensive!



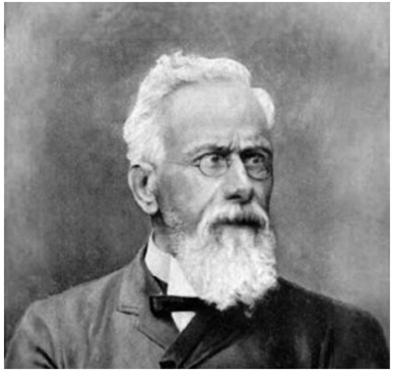
Single-node open source Mappers choke on large datasets (generously defined as > 10k data points with >100 columns)

Rolling our own Mapper..

- Our Mapper implementation
  - Built on PySpark 1.6.1
  - Called **Betti Mapper**
  - Named after Enrico Betti, a famous topologist

X

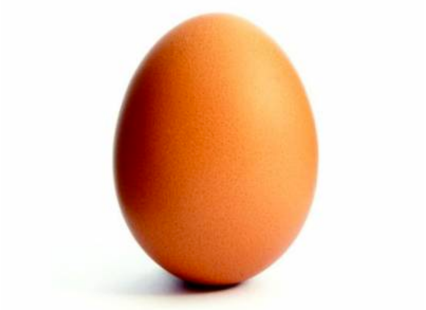
✔



Multiple ways to scale Mapper

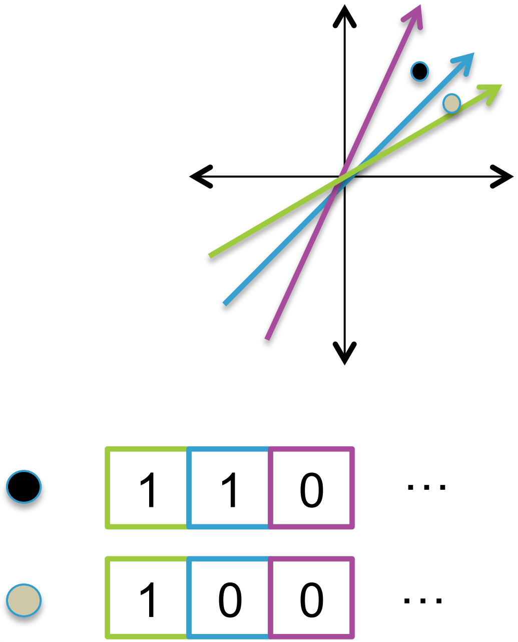
1. **Naïve Spark implementation**
   - ✓ Write the Mapper algorithm using (Py)Spark RDDs
   - – Distance matrix computation still performed over entire dataset on driver node
2. **Down-sampling / landmarking (+ Naïve Spark)**
   - ✓ Obtain manageable number of samples from dataset
   - – Unreasonable to assume global distribution profiles are captured by samples
3. **LSH Prototyping!!!!?!**

What came first?



- We use Mapper to detect structure in high-dimensional data using the concept of similarity.
- BUT we need to measure similarity so we can sample efficiently.
- We could use stratified sampling, but then what about
  - Unlabeled data?
  - Anomalies and outliers?
- LSH is a lower-cost first pass capturing similarity for cheap and helping to scale Mapper

Locality sensitive hashing by random projection



- We draw random vectors with same dimensions as dataset and compute dot products with each data point
- If dot product > 0, mark as 1, else 0
- Random vectors serve to slice feature space into bins
- Series of projection bits can be converted into a single hash number

- We have found good results by setting # of random vectors to: *floor*(log_2 *|M|*)

Scaling with LSH Prototyping on Spark

✓ Fastest scalable implementation

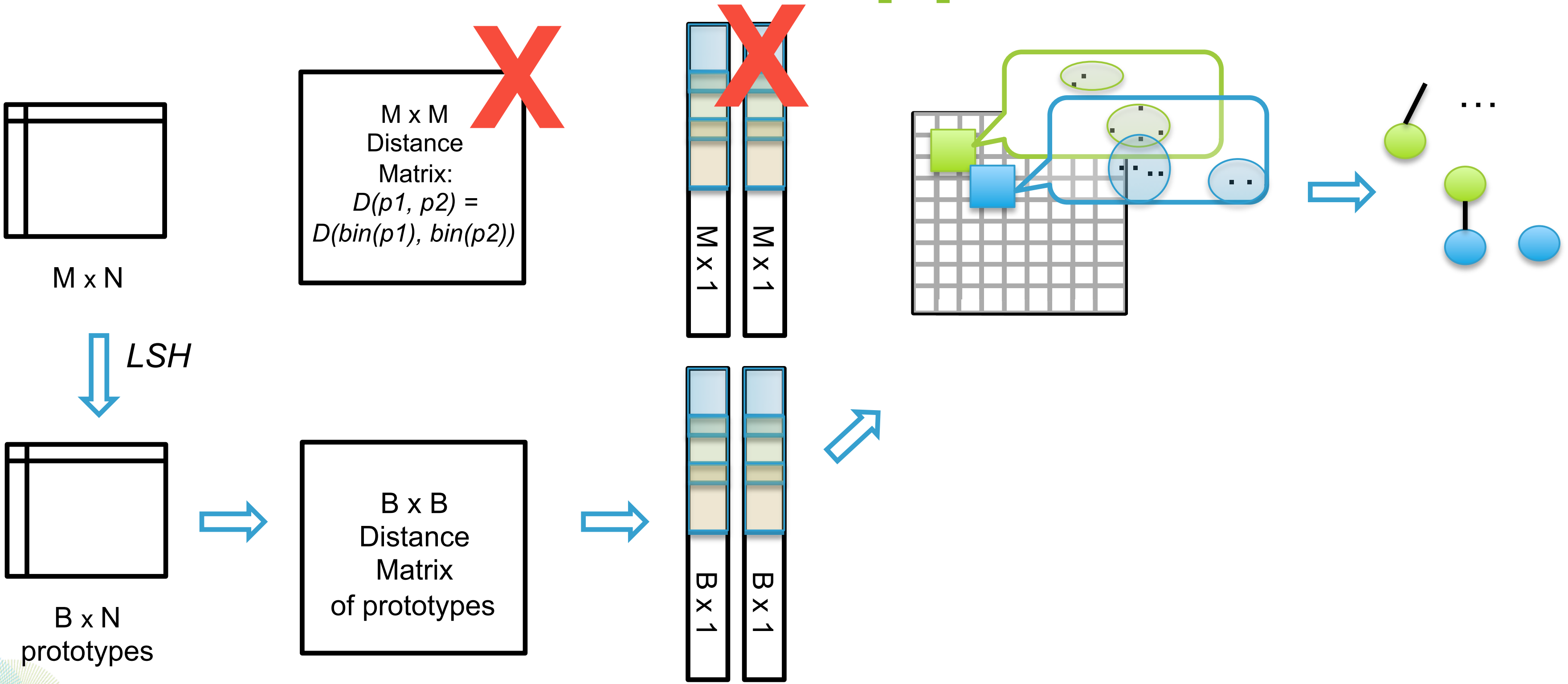
✓ # of random vectors controls # of bins and therefore fidelity of topological representation

✓ LSH binning tends to select similar points (inter-bin distance > intra-bin distance)

1. Use Locality Sensitive Hashing (SimHash / Random Projection) to drop data points into bins
2. Compute "**prototype**" points for each bin corresponding to bin centroid
   – can also use median to make prototyping more robust
3. Use binning information to compute topological network:

   $dist_{MxM}$ => $dist_{BxB}$, where B is no. of prototype points (1 per bin)

Betti Mapper

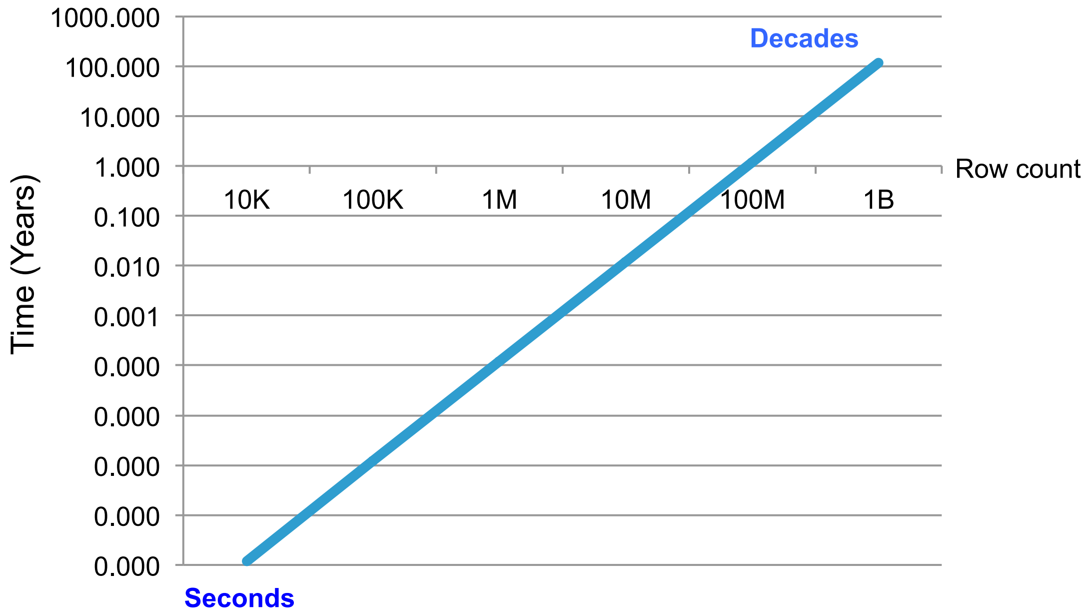


IMPLEMENTATION PERFORMANCE

Using pyspark

- Simple to “sparkify” an existing python mapper implementation
- Leverage the rich python ML support to greatest extent
  - Modify only the computational bottlenecks
- Numpy/Scipy is essential
- Turnkey Anaconda deployment on CDH

Naïve performance



- 4TFLOP/s GPGPU (100% util)
- 5K Columns
- Euclidean distance

Our Approach

Build and test three implementations of Mapper

1. Naïve Mapper on Spark
2. Mapper on Spark with sampling (5%, 10%, 25%)
3. Betti Mapper: LSH + Mapper (8v, 12v, 16v)

Test Hardware

Macbook Pro, mid 2014

- 2.5 GHz Intel® Core i7
- 16 GB 1600 MHz DDR3
- 512 GB SSD

Spark Cluster on Amazon EC2

- Instance type: *r3.large*
- Node: 2 vCPU, 15 GB RAM, 32 GB SSD
- 4 workers, 1 driver
- 250 GB SSD EBS as persistent HDFS
- Amazon Linux, Anaconda 64-bit 4.0.0, PySpark 1.6.1

Spark Configuration

Spark 1.6.1 Spark Master at spark://ec2-54-144-84-194.compute-1.amazonaws.com:7077

URL: spark://ec2-54-144-84-194.compute-1.amazonaws.com:7077
REST URL: spark://ec2-54-144-84-194.compute-1.amazonaws.com:6066 *(cluster mode)*
Alive Workers: 4
Cores in use: 8 Total, 8 Used
Memory in use: 54.8 GB Total, 48.0 GB Used
Applications: 1 Running, 13 Completed
Drivers: 0 Running, 0 Completed
Status: ALIVE

Workers

Worker Id	Address	State	Cores	Memory
worker-20160607230300-10.181.116.235-48249	10.181.116.235:48249	ALIVE	2 (2 Used)	13.7 GB (12.0 GB Used)
worker-20160607230300-10.234.189.40-49750	10.234.189.40:49750	ALIVE	2 (2 Used)	13.7 GB (12.0 GB Used)
worker-20160607230300-10.79.189.26-47663	10.79.189.26:47663	ALIVE	2 (2 Used)	13.7 GB (12.0 GB Used)
worker-20160607230302-10.136.69.111-36008	10.136.69.111:36008	ALIVE	2 (2 Used)	13.7 GB (12.0 GB Used)

- --driver-memory 8g
- --executor-memory 12g (each)
- --executor-cores 2
- No. of executors: 4

Dataset Configuration

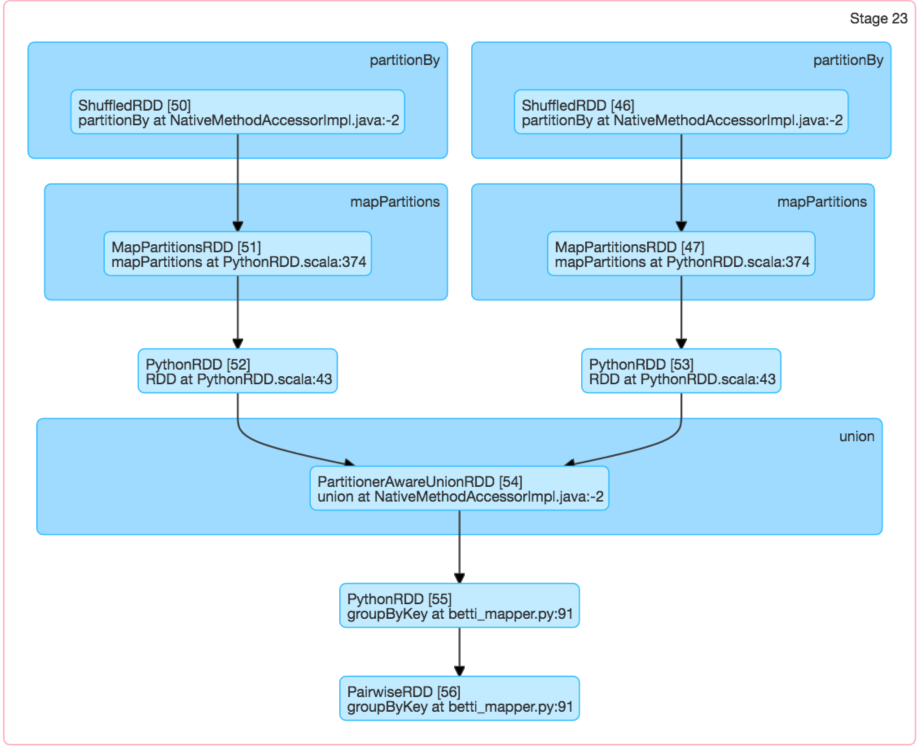
Filename	Size (MxN)	Size (bytes)
MNIST_1k.csv	1000 rows x 784 cols	1.83 MB
MNIST_10k.csv	10,000 rows x 784 cols	18.3 MB
MNIST_100k.csv	100,000 rows x 784 cols	183 MB
MNIST_1000k.csv	1,000,000 rows x 784 cols	1830 MB

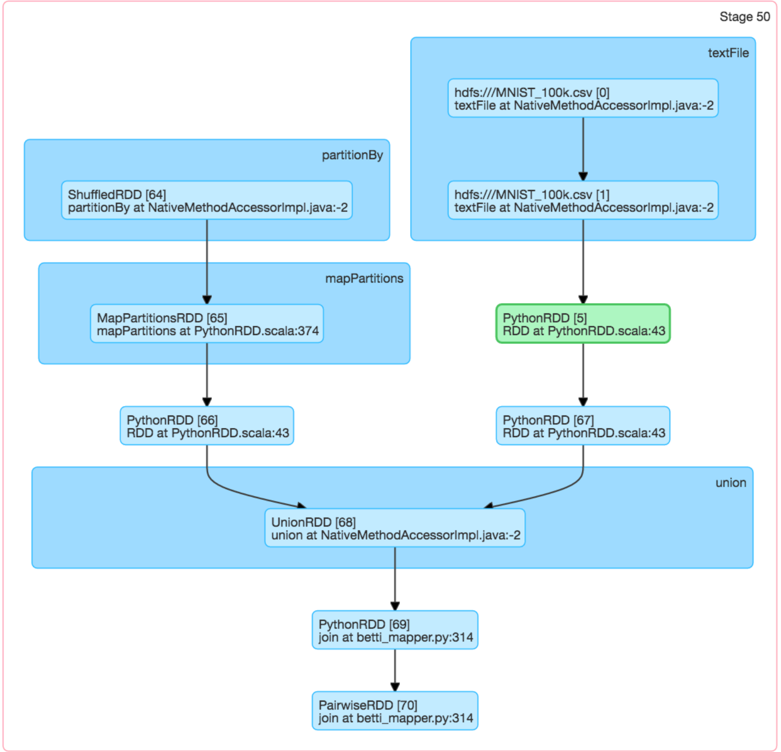
The datasets are sampled with replacement from the original MNIST dataset available for download using Python's *scikit-learn* library *(mldata* module*)*

Test Harness

- Runs test cases on cluster
- Test case:
  - <mapper type, dataset size, no. of vectors>
- Terminates when runtime exceeds 40 minutes

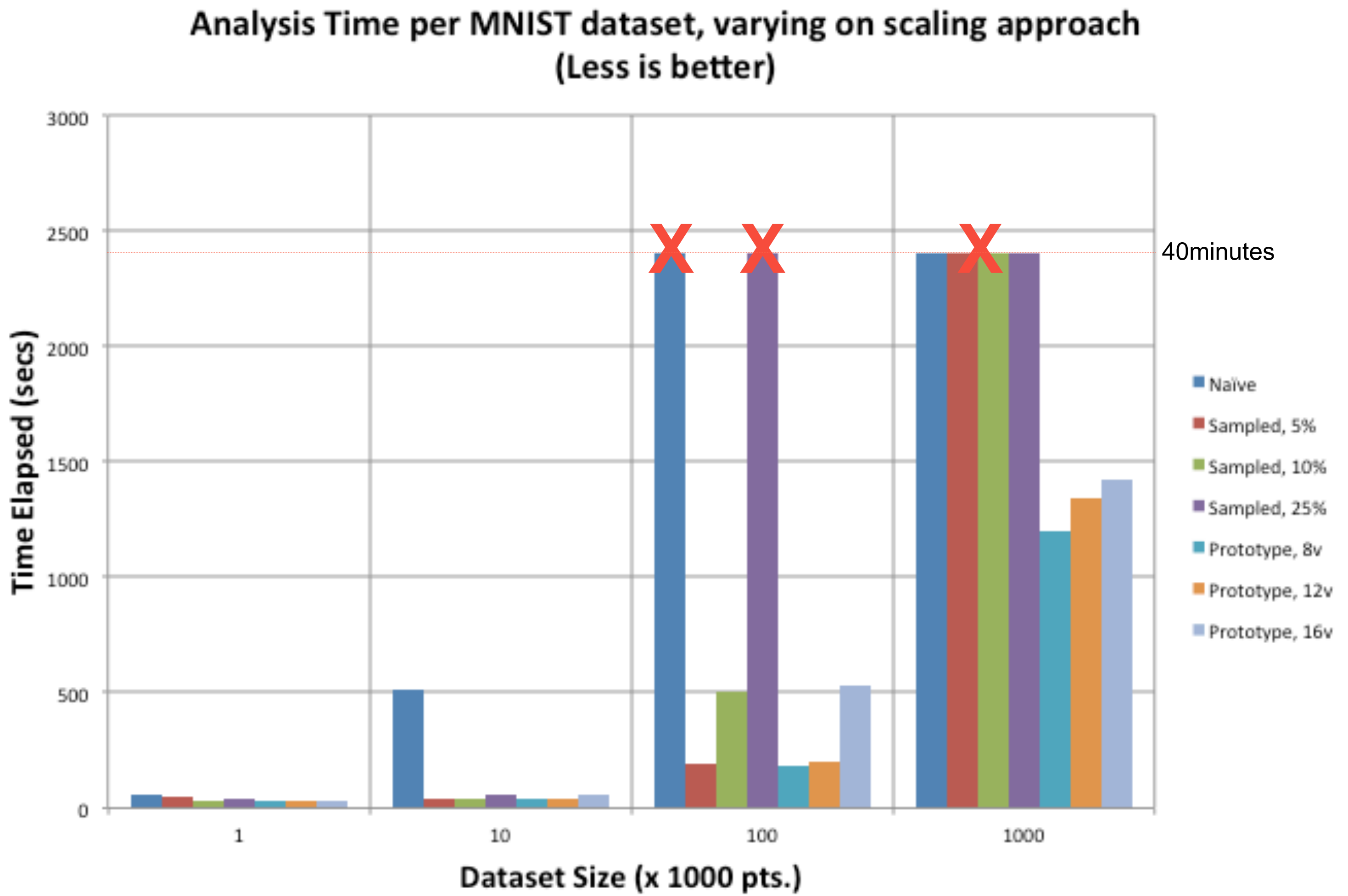
Some DAG Snapshots

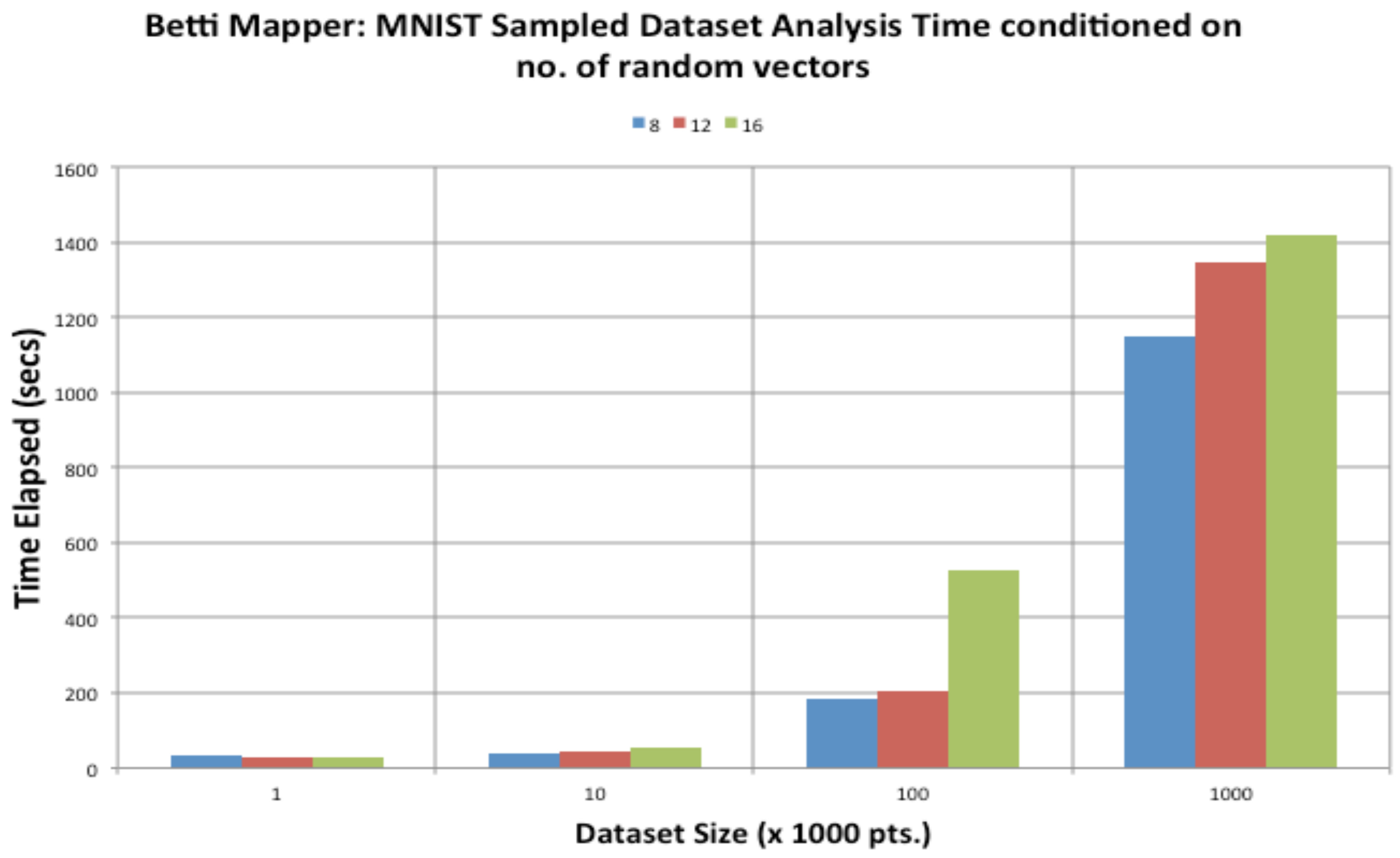




Clustering and node assignment

Graph coloring by median digit


Analysis Time per MNIST dataset, varying on scaling approach
(Less is better)
Time Elapsed (secs)
3000
2500
2000
1500
1000
500
0
1
10
100
1000
Dataset Size (x 1000 pts.)
40minutes
X
X
X
Naïve
Sampled, 5%
Sampled, 10%
Sampled, 25%
Prototype, 8v
Prototype, 12v
Prototype, 16v



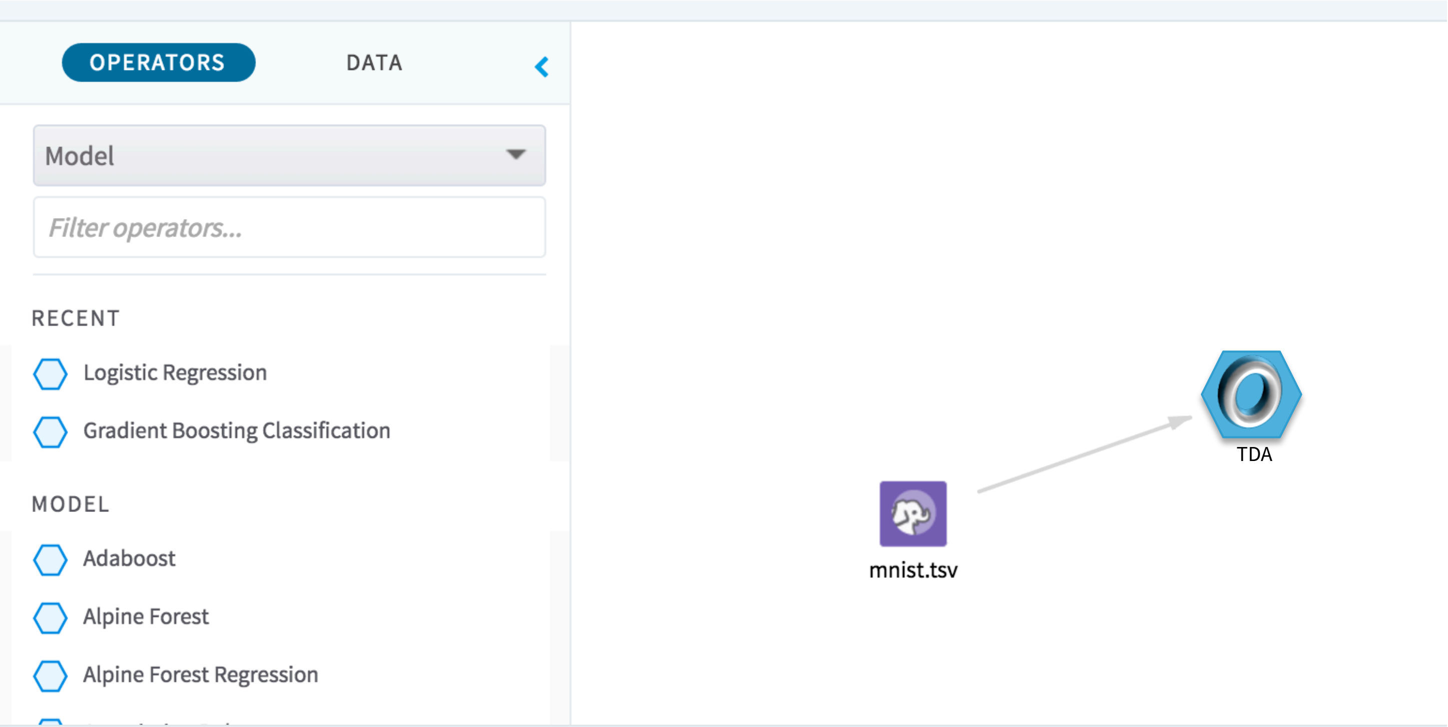
Betti Mapper: MNIST Sampled Dataset Analysis Time conditioned on no. of random vectors
8
12
16
1600
1400
1200
1000
800
600
400
200
0
Time Elapsed (secs)
1
10
100
1000
Dataset Size (x 1000 pts.)

Future Work

- Test other LSH schemes
- Optimize Spark code and leverage existing codebases for distributed linear algebra routines
- Incorporate as a machine learning model on the Alpine Data platform

ALPINE DATA™

Alpine Spark TDA



Key Takeaways

- Scaling Mapper algorithm is non-trivial but possible
- Gaining control over fidelity of representation is key to gaining insights from data
- Open source implementation of Betti Mapper will be made available after code cleanup! ☺

References

- “**Topological Methods for the Analysis of High Dimensional Data Sets and 3D Object Recognition**”*,* G. Singh, F. Memoli, G. Carlsson, *Eurographics Symposium on Point-Based Graphics (2007)*
- “**Extracting insights from the shape of complex data using topology**”, P. Y. Lum, G. Singh, A. Lehman, T. Ishkanov, M. Vejdemo-Johansson, M. Alagappan, J. Carlsson, G. Carlsson, *Nature Scientific Reports (2013)*
- “**Online generation of locality sensitive hash signatures**”, B. V. Durme, A. Lall, *Proceedings of the Association of Computational Linguistics 2010 Conference Short Papers (2010)*
- PySpark documentation: http://spark.apache.org/docs/latest/api/python/

Acknowledgements

- Rachel Warren
- Anya Bida

Alpine is Hiring

- Platform engineers
- UX engineers
- Build engineers
- Ping me : lawrence@alpinenow.com

Q & (HOPEFULLY) A

THANK YOU.

anshuman@alpinenow.com
lawrence@alpinenow.com