A Massively Scalable Architecture for Learning Representations from Heterogeneous Graphs

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TODAY'S TALK

How to handle heterogeneity in training large graph embedding models

1. Overview & Background
2. Our Approach
3. Results

Who we are

Bayan Bruss

Anish Khazane

SECTION ONE: OVERVIEW

A quick background on graph embeddings & some of the issues related to scaling them

People are can be disproportionately attracted to content that is sensational or provocative.

Machine learning systems that learn how to serve content are prone to optimizing towards these types of content.

Capital One

Some common problems and solutions

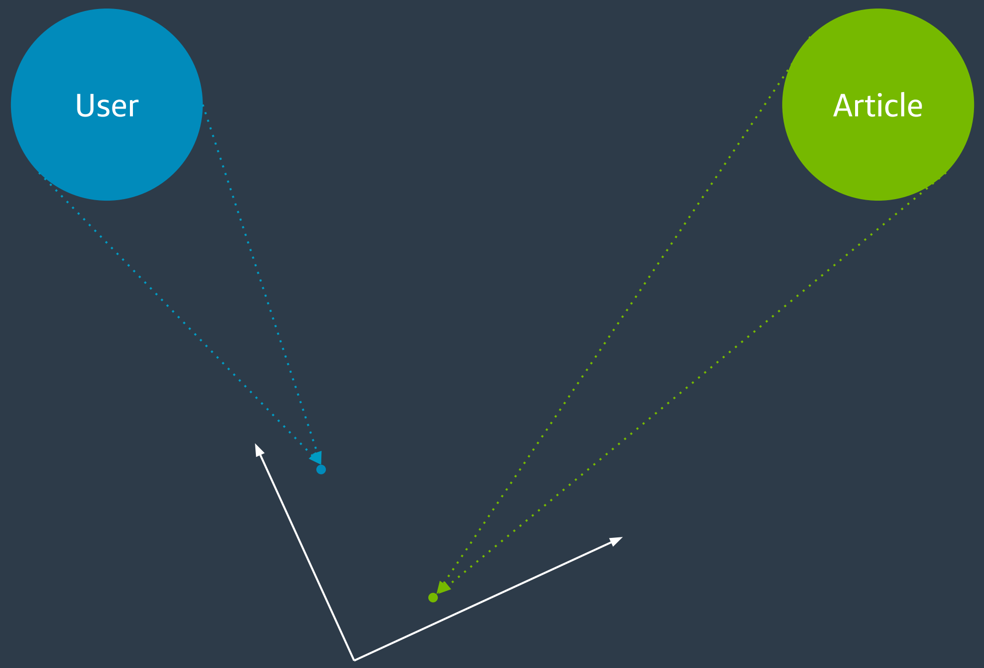
1. If this is a problem with content (spam, violent, racist, homophobic, etc.) -> Flag & demote content that is deemed objectionable

2. If this is a problem with users (fake accounts, malicious actors) -> Eliminate fraudulent accounts

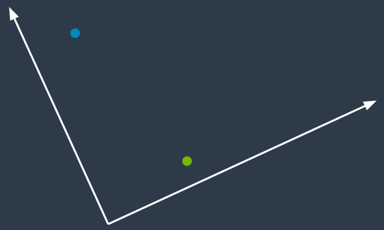
What’s missing?

Basic mechanics of a neural network recommender

Basic mechanics of a neural network recommender



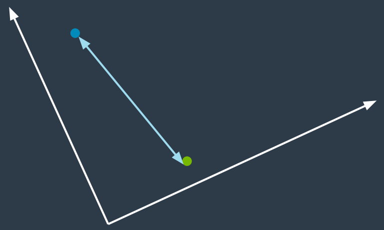
Basic mechanics of a neural network recommender



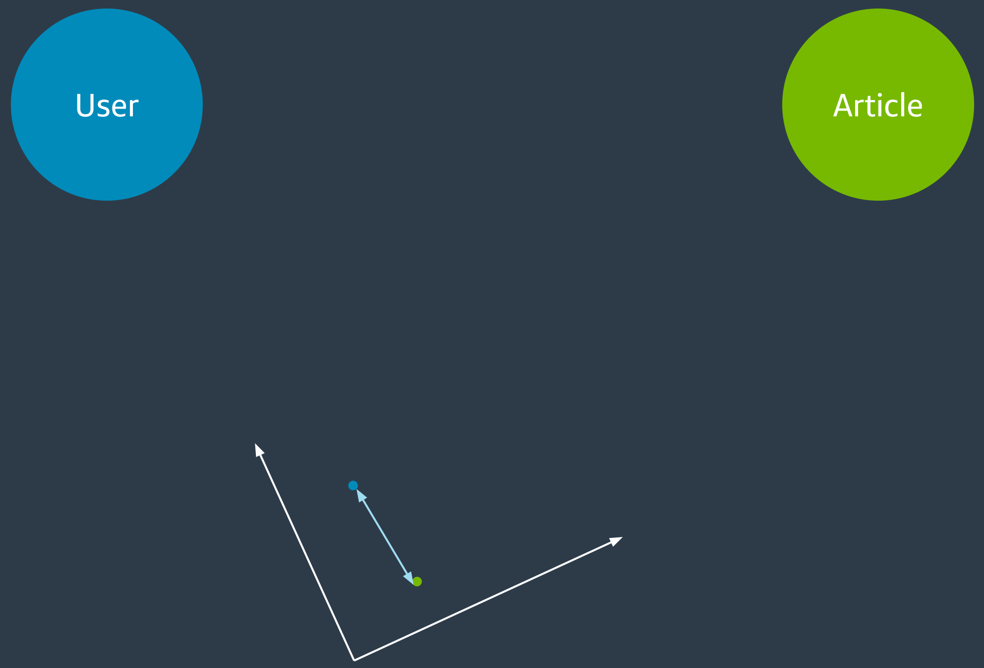
Basic mechanics of a neural network recommender

User

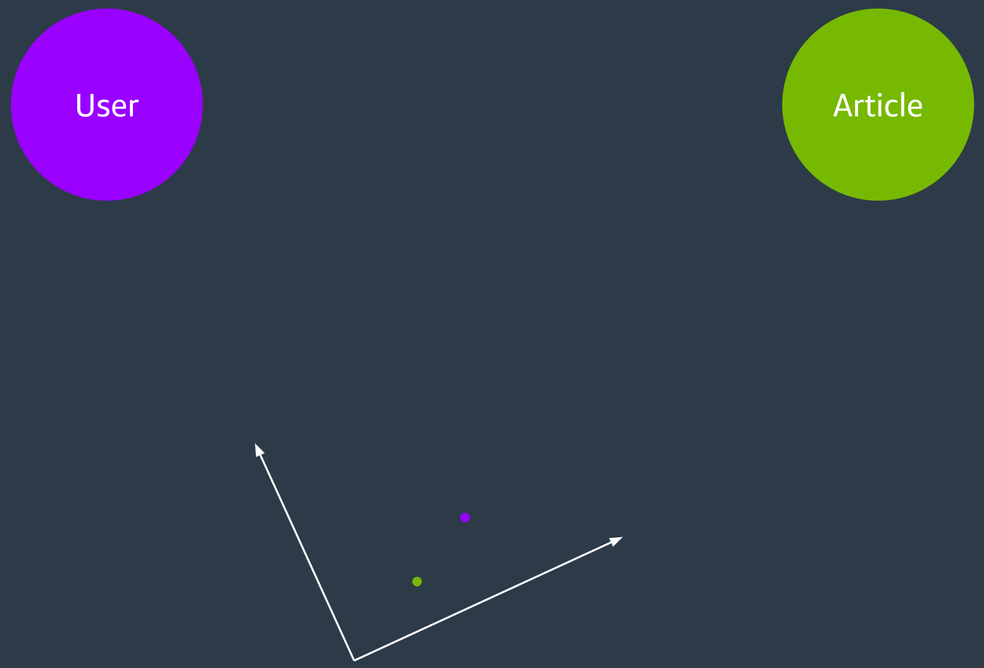
Article



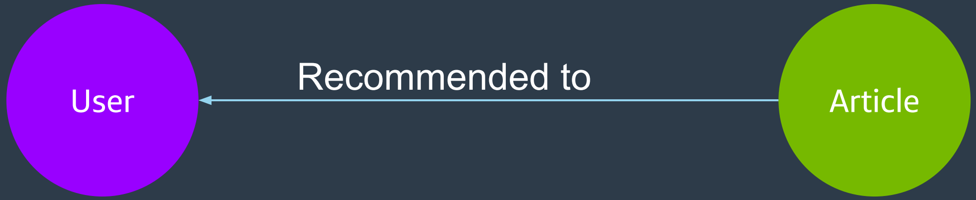
Basic mechanics of a neural network recommender

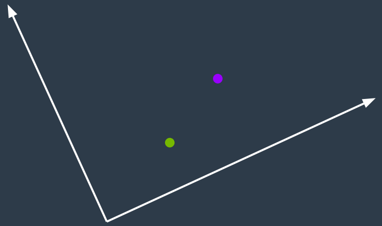


Basic mechanics of a neural network recommender



Basic mechanics of a neural network recommender





How can we add more fidelity to these models?

1. Treat heterogeneous graphs as containing distinct element types

2. Model interactions depending what type of entity is involved

A brief history of graph embeddings

Most Common Objective:

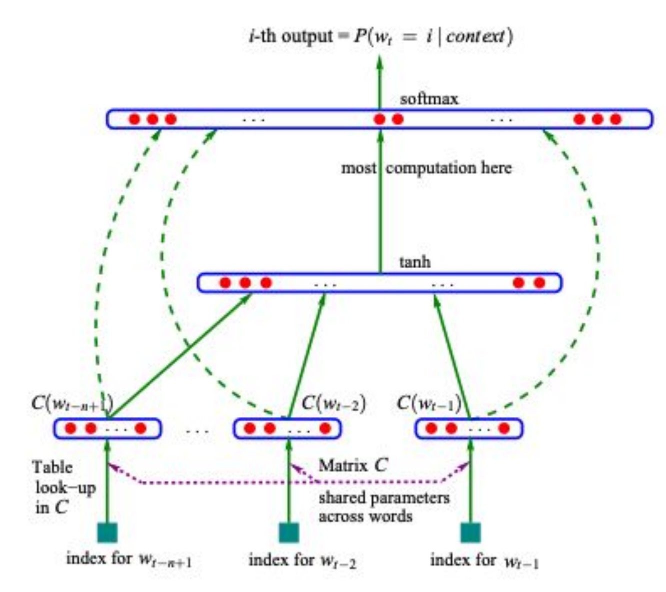
- Learn a continuous vector for each node in a graph that preserves some local or global topological features about the neighborhood of that node

Early Efforts Focused on Explicit Matrix Factorization

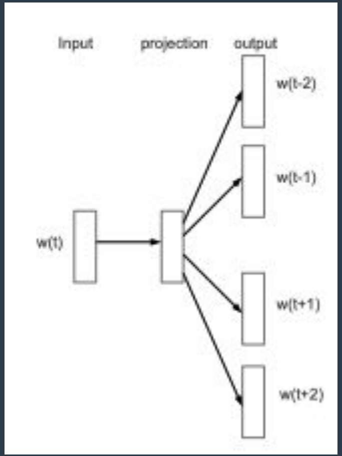
- Not very scalable
- Highly tuned to specific topological attributes

Meanwhile over in the language modeling world

Word2Vec world blows things open



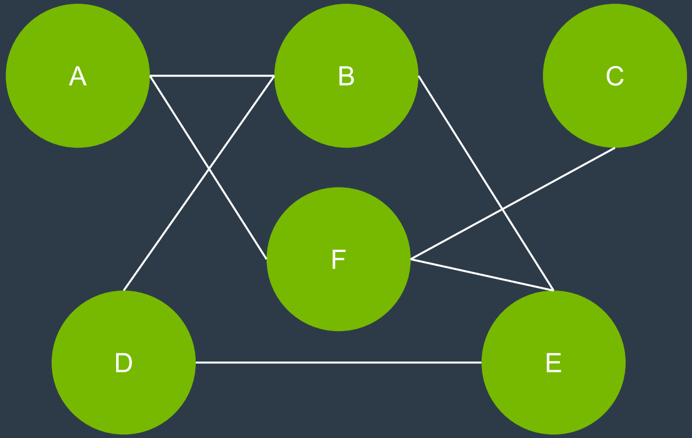
Y Bengio, R Ducharme, P Vincent, C Jauvin. A neural probabilistic language model. Journal of machine learning research, 2003



Mikolov, Tomas, et al. "Distributed representations of words and phrases and their compositionality." *Advances in neural information processing systems*. 2013.

Quickly ported to graph embeddings

Walks on a graph can be likened to sentences in a document



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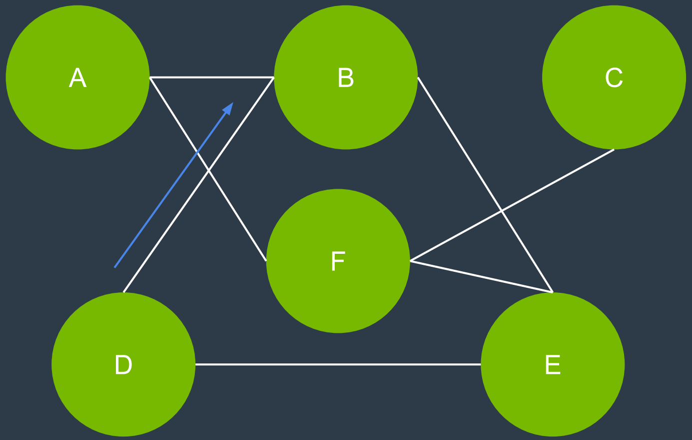

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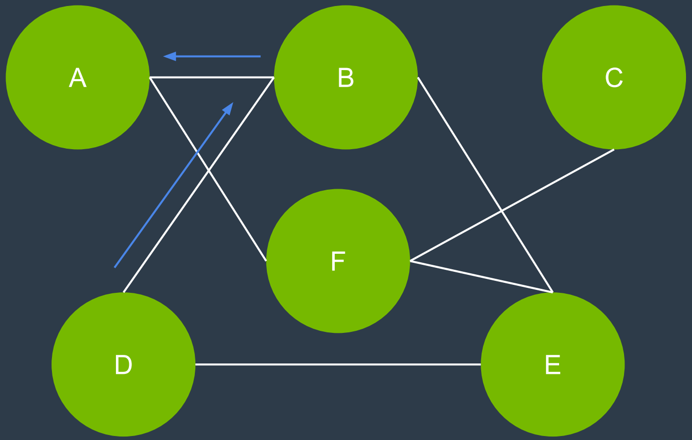

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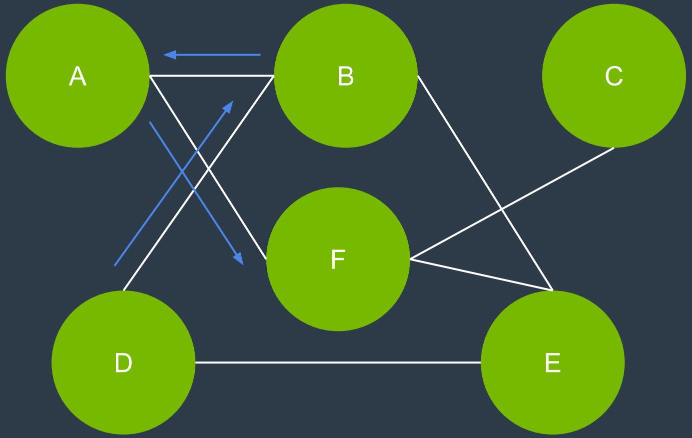

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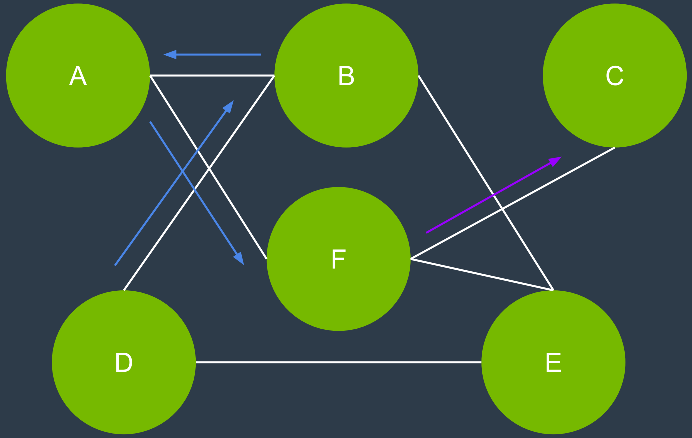

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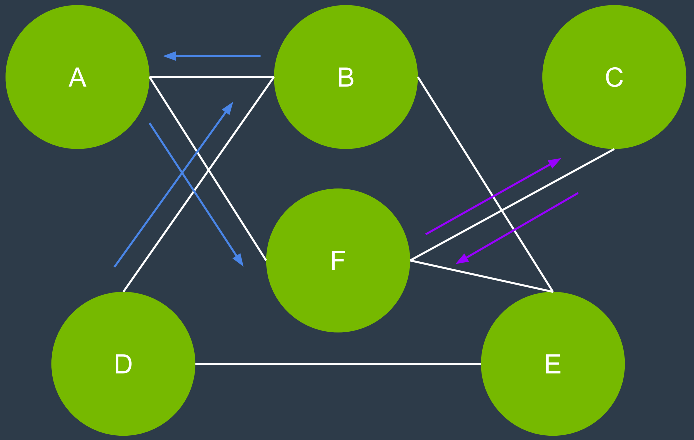

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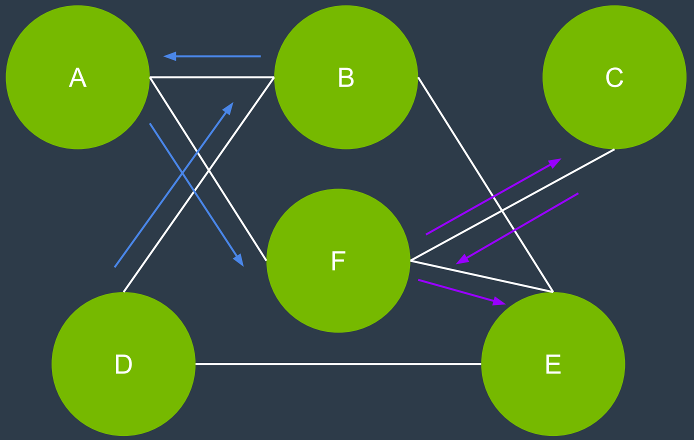
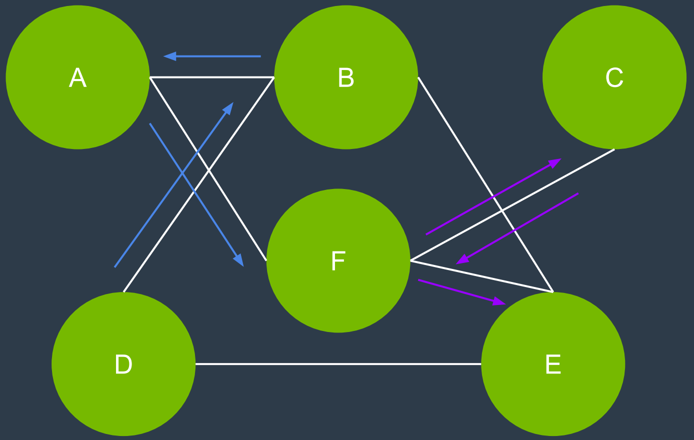


Quickly ported to graph embeddings

Walks on a graph can be likened to sentences in a document



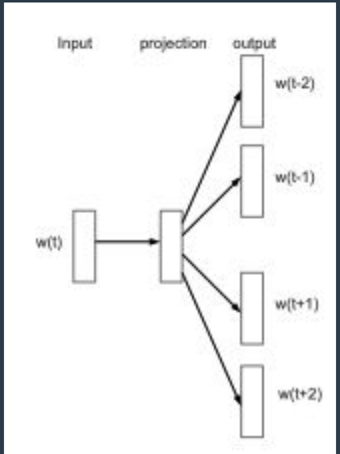
["D", "B", "A", "F"]

["F", "C", "F", "E"]

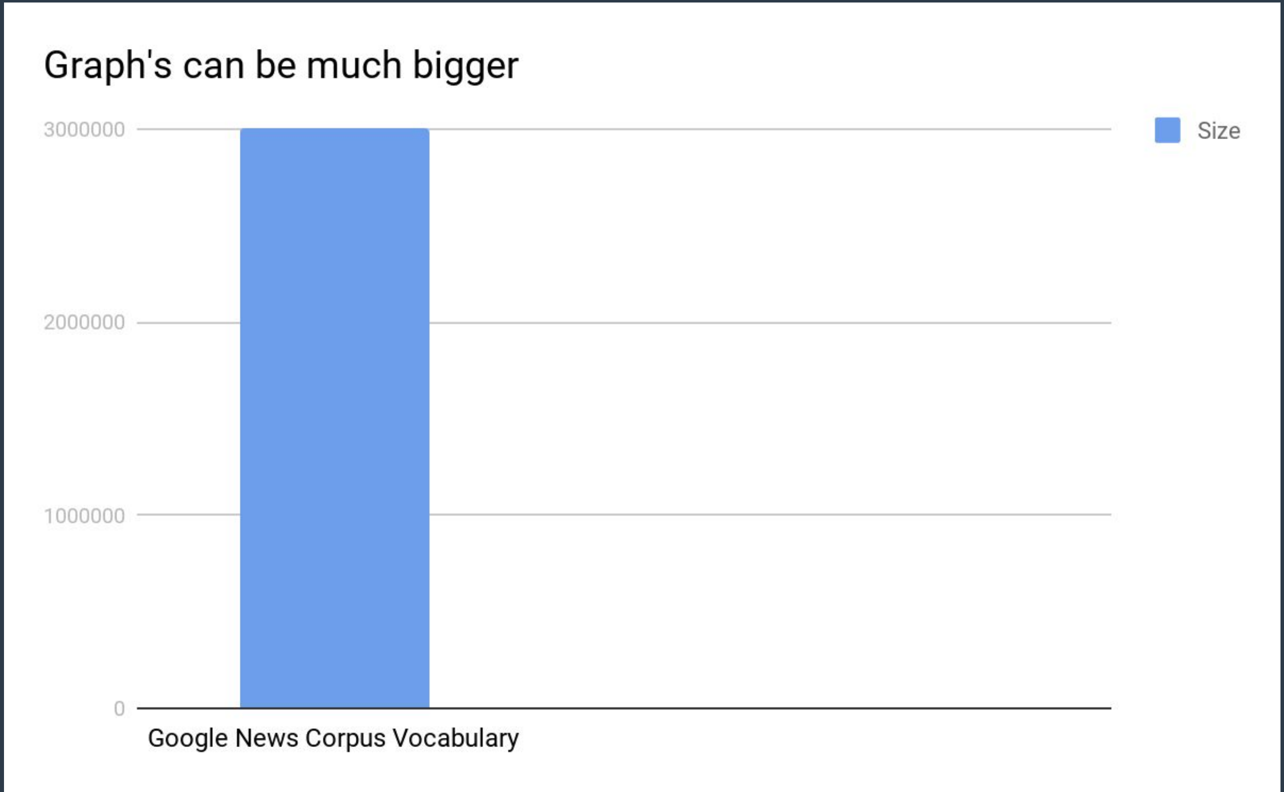
Walks on graphs can be treated as sentences

["D", "B", "A", "F"]

["F", "C", "F", "E"]



Graphs are different from language



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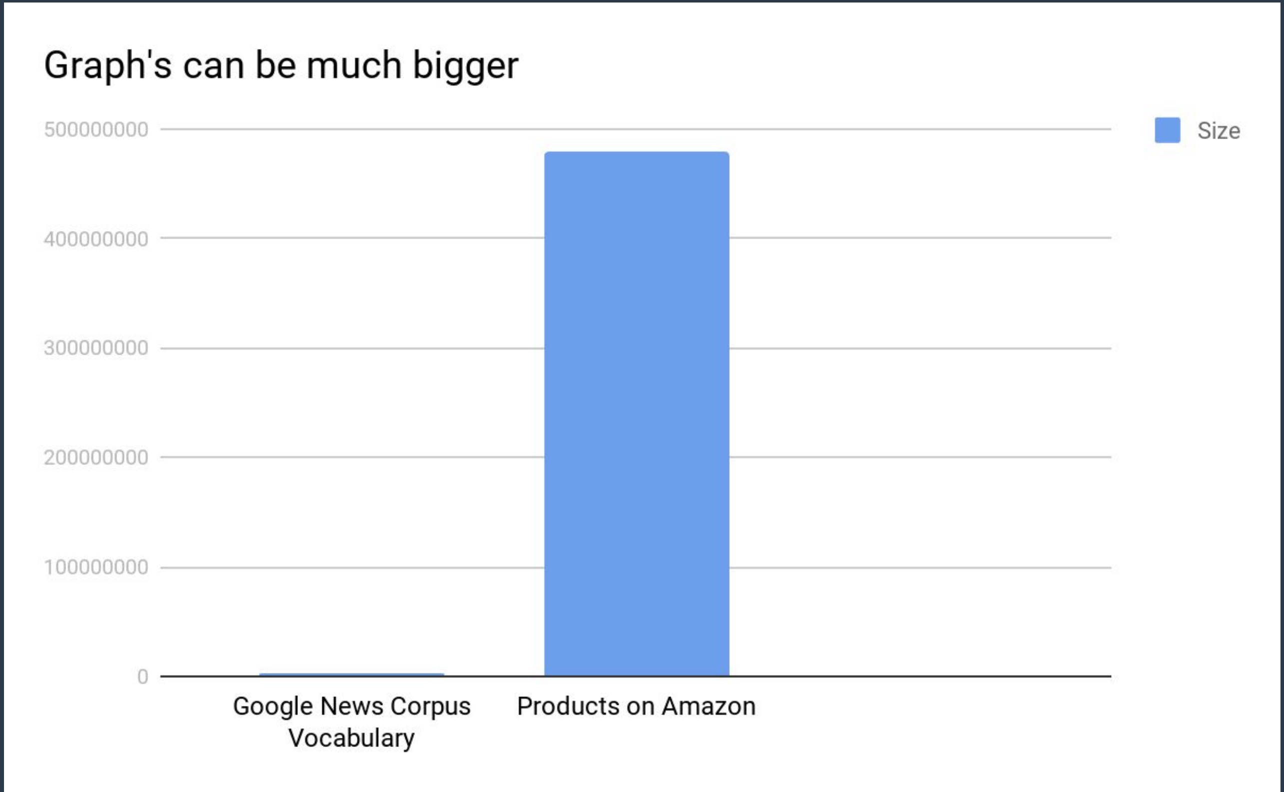

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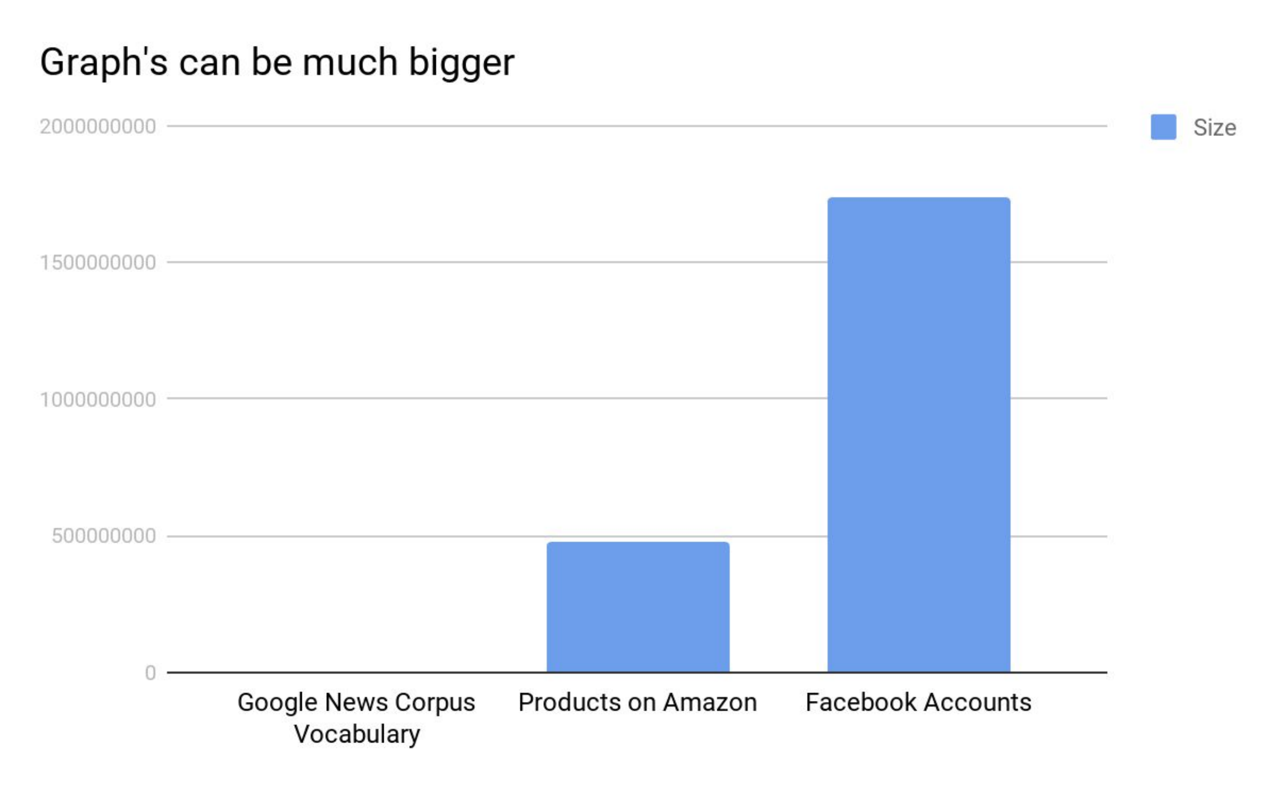
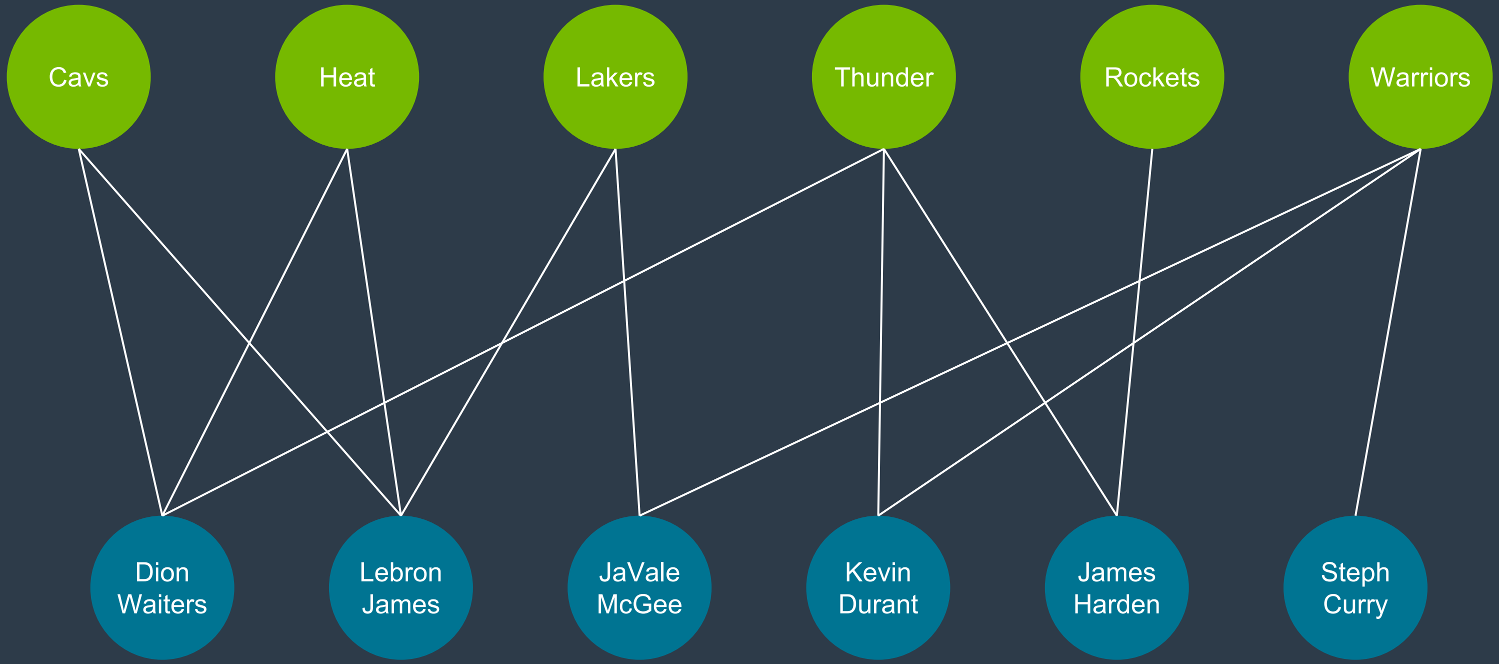


Graphs can be heterogeneous



All this makes scale an even bigger challenge

Homogeneous graphs are difficult

<u>Dimensionality</u>: Millions or even billions of nodes

<u>Sparsity</u>: Each node only interacts with a small subset of other nodes

Quickly hit limits on all resources

1) An embedding space is a N X D dimensional matrix where each row corresponds to a row.
2) D is typically 100 - 200 (an arbitrary hyperparameter)
3) A 500M node graph would be 200 - 400 GB
4) Cannot hold in GPU memory
5) Quickly exceeds limits of a single worker
6) Lots of little vector multiplication ideal for GPUs
7) Sharding because of connectedness - sharding the matrix is challenging

Heterogeneous graphs are even harder

Have to keep K possible embedding spaces with N nodes for each

Have to have an architecture that routes to the right embedding space

It’s also hard from an algorithmic perspective

We’re working on this too but not the focus of today’s talk

See interesting articles

- Metapath2Vec: Scalable Representation Learning for Heterogeneous Networks
- CARL: Content-Aware representation Learning for Heterogeneous Graphs

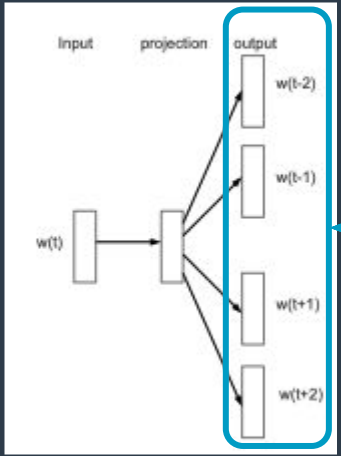
SECTION TWO: OUR APPROACH

Applied Research: An architecture for handling heterogeneity at scale

Capital One

Quick Primer on Negative Sampling

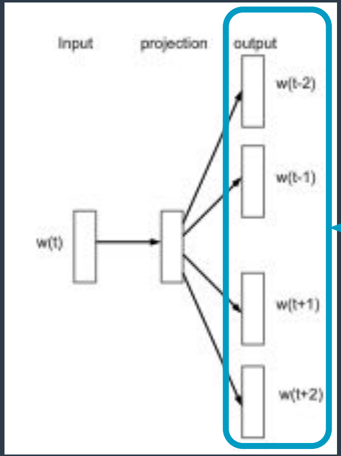
Original SkipGram Model



Need to compute softmax over entire vocabulary for each input

Quick Primer on Negative Sampling

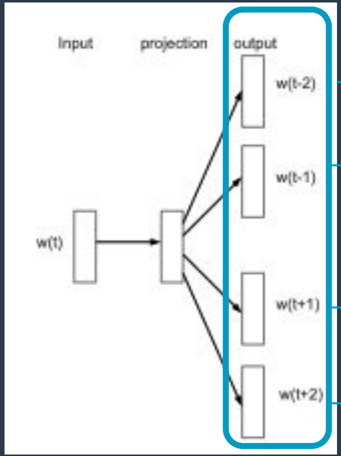
Original SkipGram Model



VERY EXPENSIVE!

Softmax can be approximated by binary classification task

Original SkipGram Model



Binary Discriminator

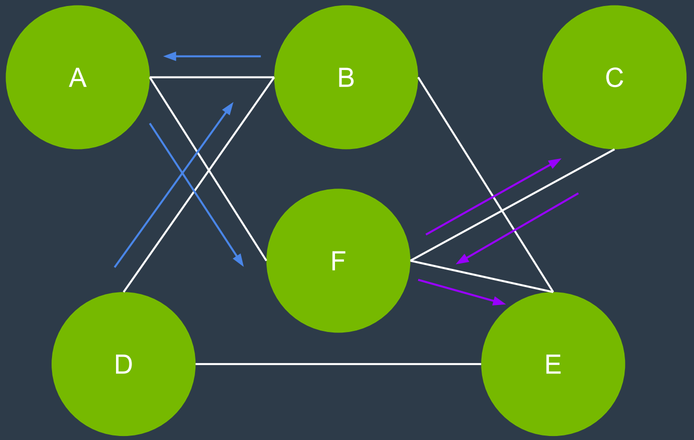
w(t-2) vs negative samples

w(t-1) vs negative samples

w(t+1) vs negative samples

w(t+2) vs negative samples

Use non-edges to generate negative samples



Negatives for B

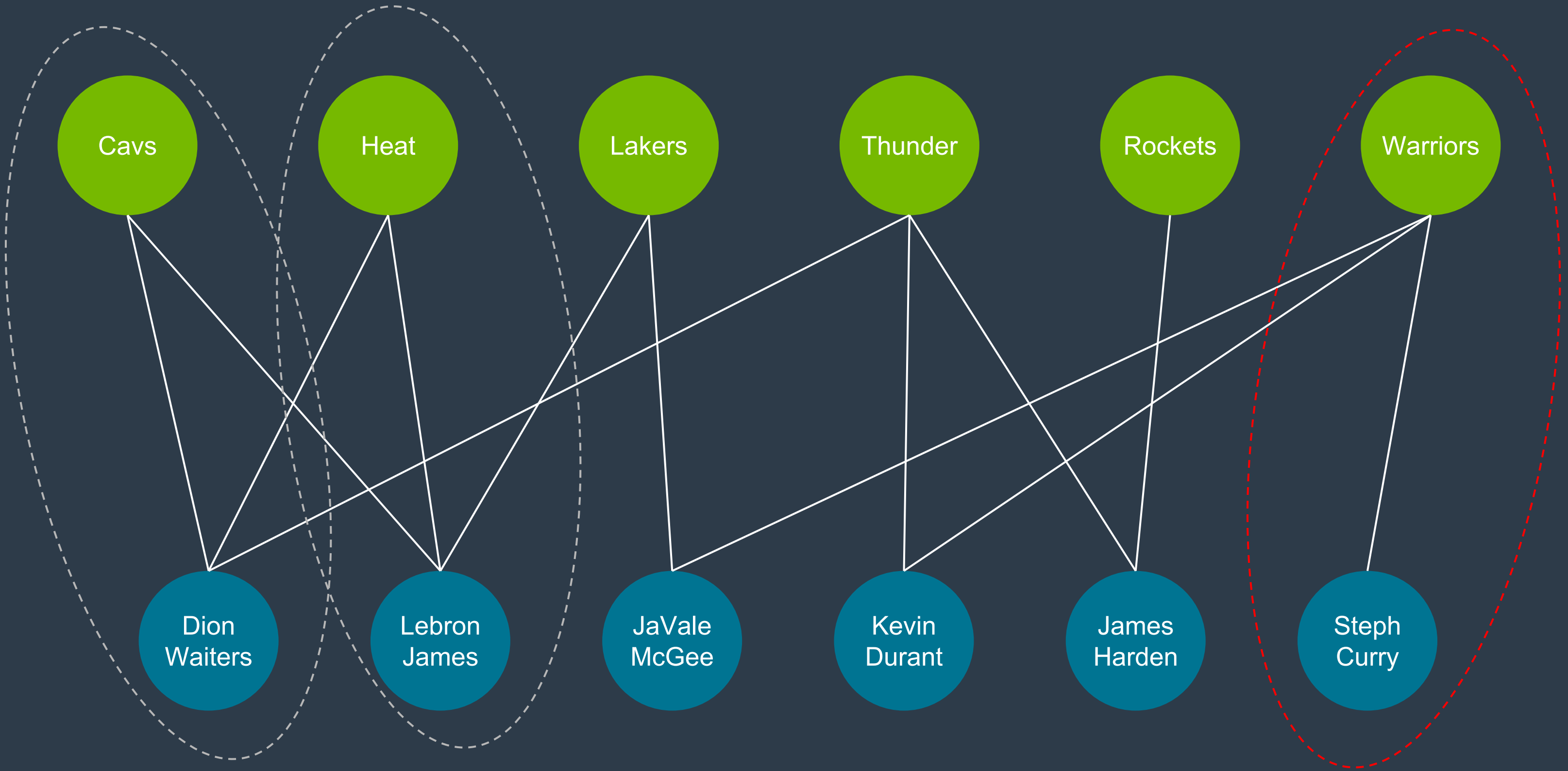
["F", "C", "F"]

["D", "B", "A", "F"]

Context for B

["F", "C", "F", "E"]

Walking on heterogeneous graph



How to distribute (parallelize) training

1. Split the training set across a number of workers that execute in parallel asynchronously and unaware of the existence of each other.

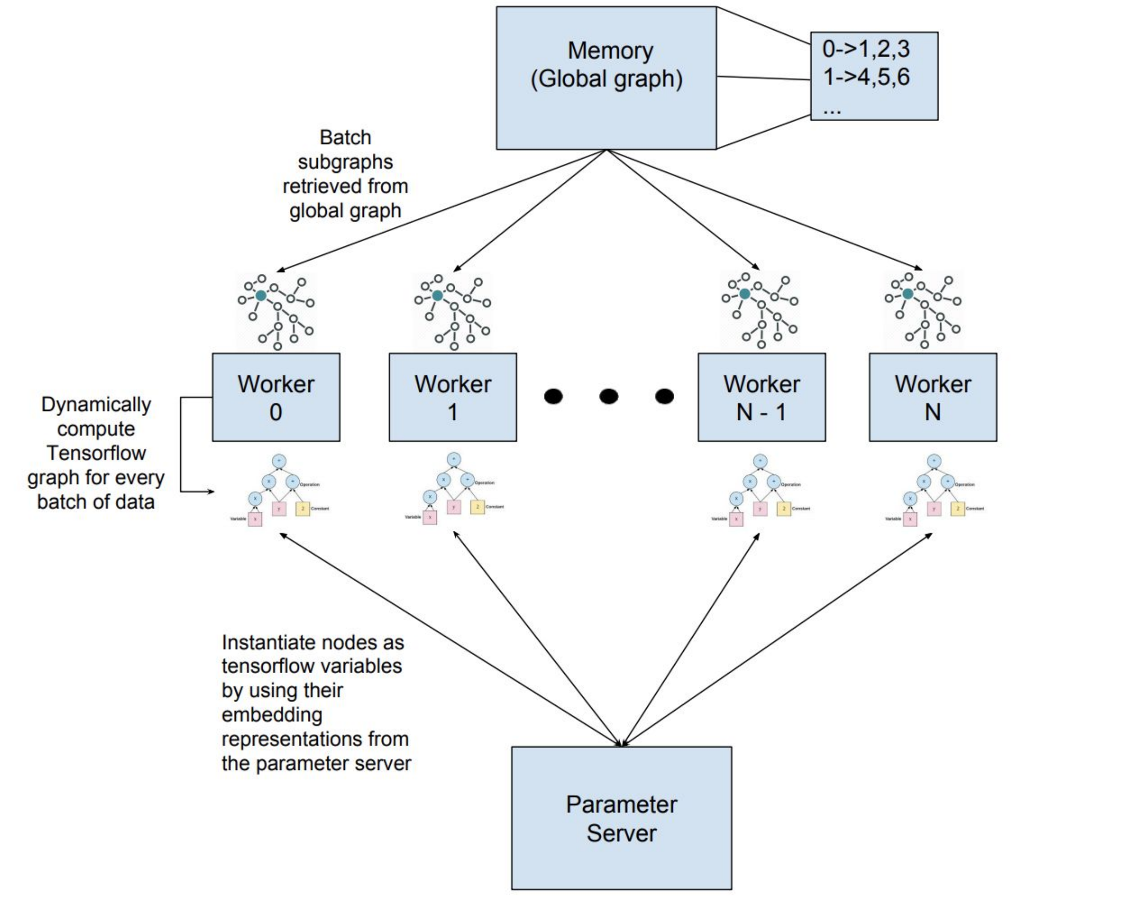
2. Create some form of centralized parameter repository that allows learning to be shared across all the workers.

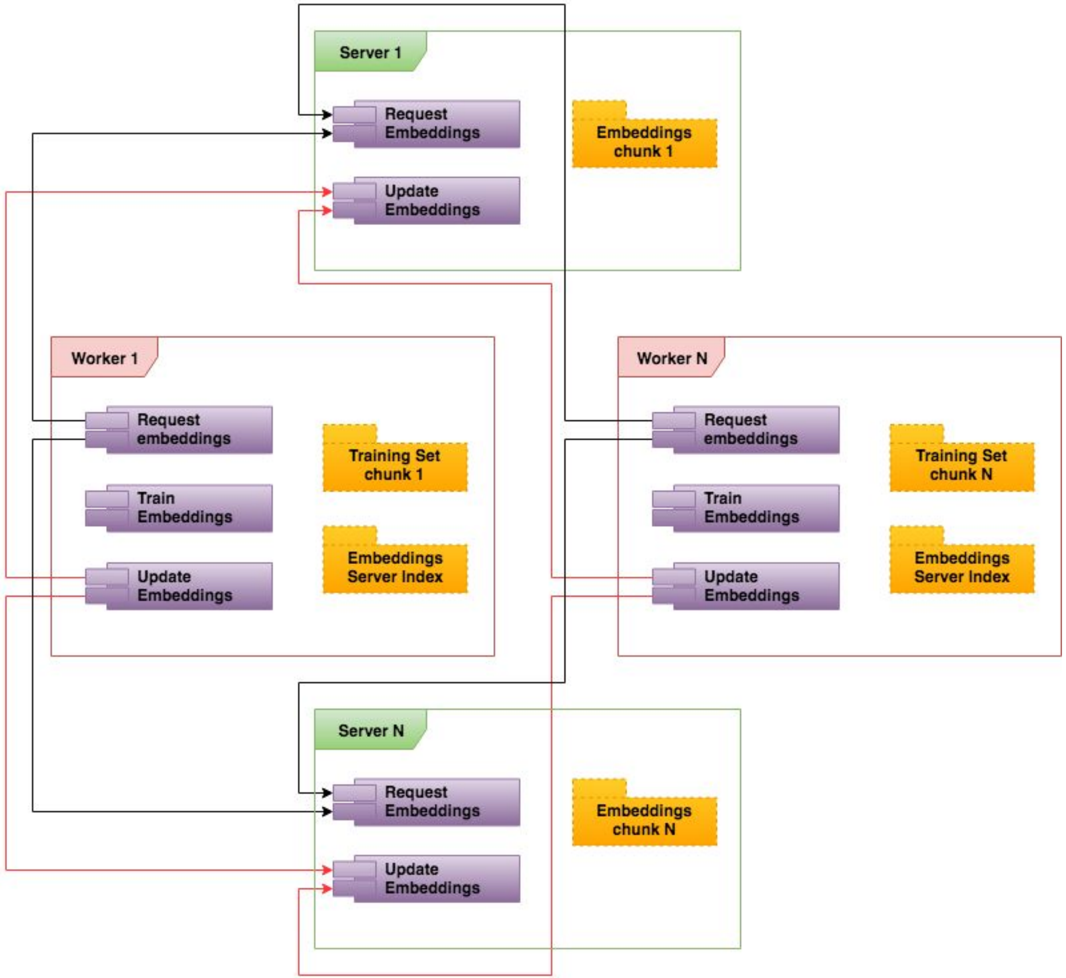
Parameter server partitioning

- A parameter server can hold the embeddings table which contains the vectors corresponding to each node in the graph.

- The embeddings table is a N x M table, where N is the number of nodes in the graph and M is a hyperparameter that denotes the number of embedding dimensions.

Variable Tensorflow Computational Graphs



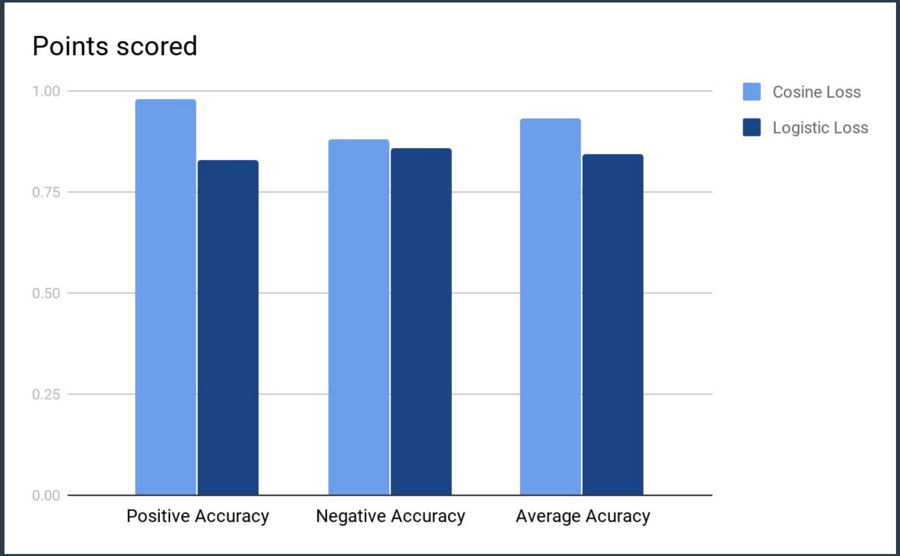


Server 1
Request Embeddings
Update Embeddings
Embeddings chunk 1
Worker 1
Request embeddings
Train Embeddings
Update Embeddings
Training Set chunk 1
Embeddings Server Index
Worker N
Request embeddings
Train Embeddings
Update Embeddings
Training Set chunk N
Embeddings Server Index
Server N
Request Embeddings
Update Embeddings
Embeddings chunk N

SECTION THREE: RESULTS

Capital One Heterogeneous Data

Node Type A:	18, 856, 021
Node Type B:	32, 107, 404
Total Nodes:	50, 963, 425
Edges:	280, 422, 628



Train Time: 3 Days on 28 workers

Friendster Graph

Publicly available dataset

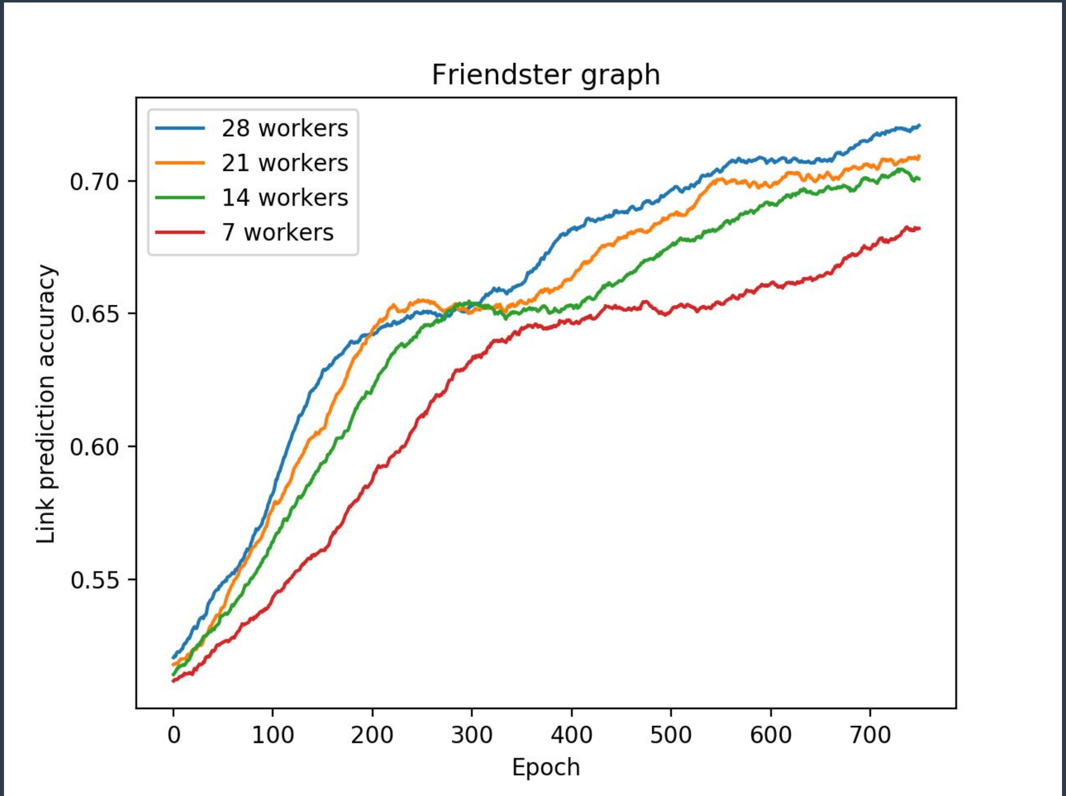
68,349,466 vertices (users)

2,586,147,869 edges (friendships)

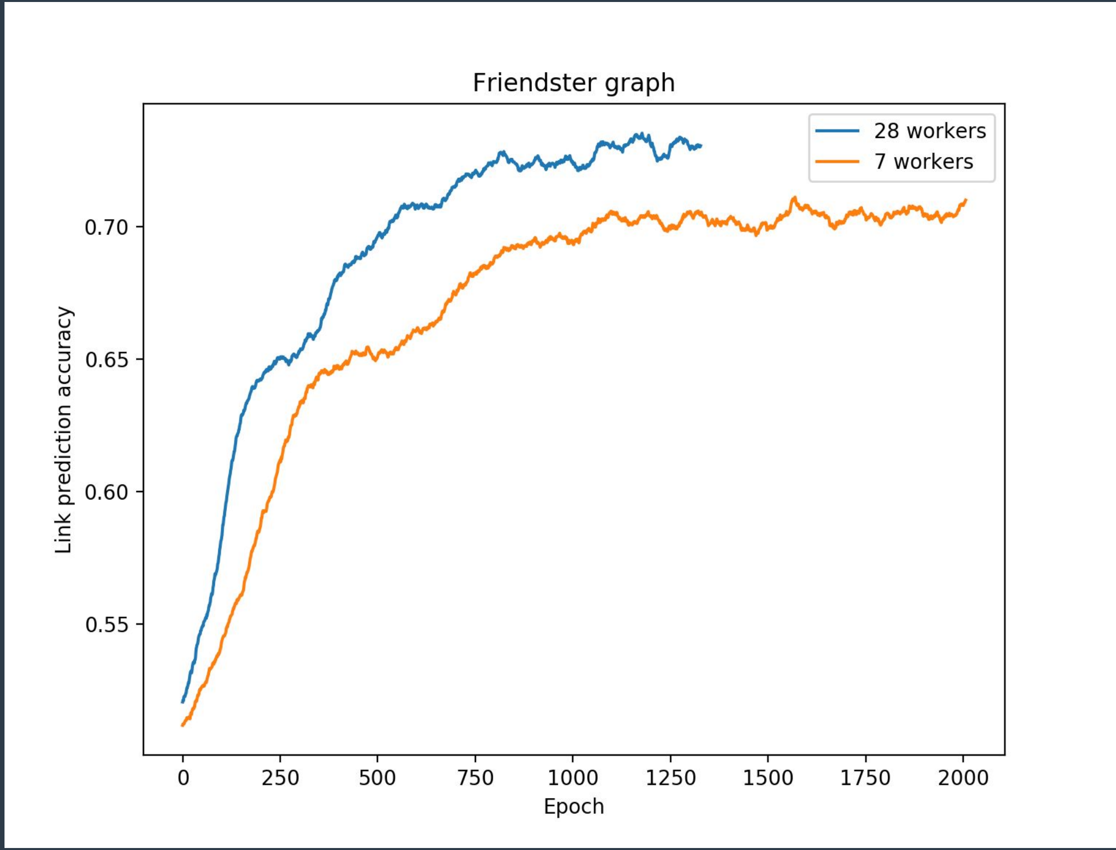
Sampled 80 positive and 5 * 80 negative edges per node as training data.

The data was shuffled, split into chunks and distributed across workers

Friendster Graph



Friendster Graph



Implications

Scalability:

- More nodes per entity type
- More entity types

Convergence:

- Faster as number of workers increases

Limitations and Future Directions

Limitations

- Python performance
- Not partitioning the embedding space
- Recomputing the computational graph for each batch could be optimized

Future Directions

- Evaluate c++ variant of architecture
- Intelligent partitioning of graph so that each worker gets a component of the graph and only has to go to the server for small subset of nodes in other components

THANK YOU