The Examples of How to Design Distributed GML systems

Driven by Industrial-purpose Application

Ethan Zhu

Department of Computer Science and Technology
Nanjing University

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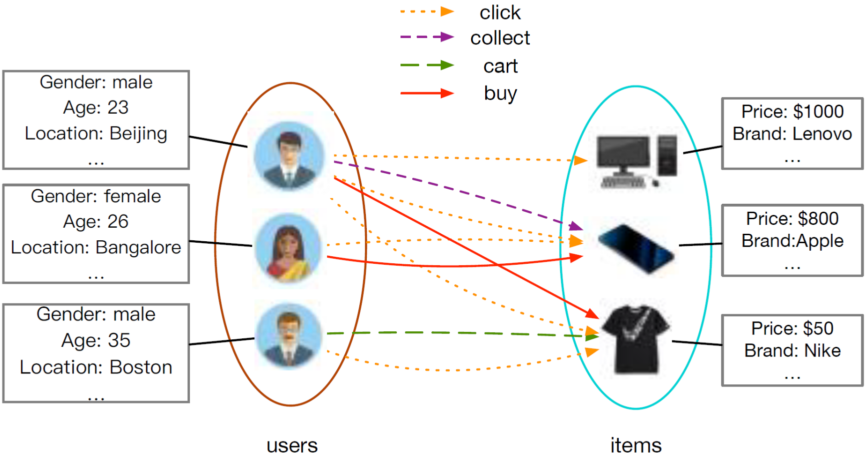
Attributed Heterogeneous Graph



We are faced with

- Large scale graph datasets
  - ✓ Billion of vertices and billion of edges
  - ✓ Multiple types of vertices and edges
  - ✓ Nodes and edges has high demension features
- Converting the graph data into a low dimensional space
  - ✓ Keeping both the structural and property information to the maximum due to data dependency
- Scale-up and Scale-out
  - ✓ Limited stand-alone resources → (scale-up e.g. Amazon X-large)
  - ✓ Communication overhead is high in distributed environment → (scale-out)
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Designing and implementation GML systems···

Problem Definition

- Given an input graph G, which is a simple graph or an AHG, and a predefined number d on the dimension of embedding where $d \ll |V|$, the embedding problem is to convert the graph G into the d-dimensional space such that the graph property is preserved as much as possible.
- GNN is a special kind of graph embedding method, which learns the embedding results by applying graph neural networks.
- We concentrate on the vertex-level embedding.
- The output of the GNN is an embedding vector and will be fed into the downstream machine learning tasks, such as classification, link prediction and etc.

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We need to solve that

- How to elegantly integrate the heterogeneous information to be an unified embedding result
  - ✓ How to keep both the structural and property information to the maximum
- How to ensure scalability and fault tolerance
- How to improve the time and space efficiencies of GNN on large-scale graphs
- How to design efficient incremental GNN methods on dynamic graphs
- ...

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Overview of Papers

AliGraph: A Comprehensive Graph Neural Network Platform

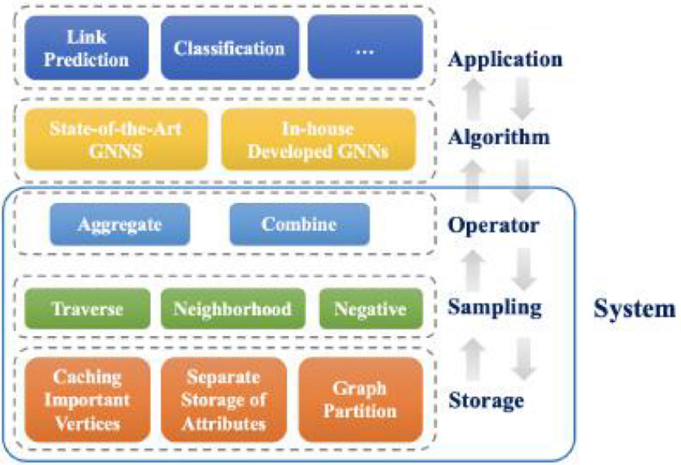
Rong Zhu, Kun Zhao, Hongxia Yang*, Wei Lin, Chang Zhou, Baole Ai, Yong Li, Jingren Zhou
Alibaba Group
{red.zr, kun.zhao, yang.yhx, weilin.lw, ericzhou.zc, jiufeng.ly, jingren.zhou}@alibaba-inc.com

AGL: A Scalable System for Industrial-purpose Graph Machine Learning

Dalong Zhang, Xin Huang, Ziqi Liu, Jun Zhou, Zhiyang Hu, Xianzheng Song, Zhibang Ge, Lin Wang, Zhiqiang Zhang, Yuan Qi

Ant Financial Services Group, Hangzhou, China
{dalong.zdl, huangxi.hx, ziqiliu, jun.zhoujun, zhiyang.hzhy, xianzheng.sxz, zhibang.zg, fred.wl,,lingyao.zzq, yuan.qi}@antfin.com

Solution 1: Aligraph [1]



[1] AliGraph: A Comprehensive Graph Neural Network Platform https://dl.acm.org/doi/pdf/10.14778/3352063.3352127

The property of different methods

Category	Method	Heterogeneous Node	Heterogeneous Edge	Attributed	Dynamic	Large-Scale
Classic Graph Embedding	DeepWalk	✗	✗	✗	✗	✗
	Node2Vec	✗	✗	✗	✗	✗
	LINE	✗	✗	✗	✗	✗
	NetMF	✗	✗	✗	✗	✗
	TADW	✗	✗	✓	✗	✗
	LANE	✗	✗	✓	✗	✗
	ASNE	✗	✗	✓	✗	✗
	DANE	✗	✗	✓	✗	✗
	ANRL	✗	✗	✓	✗	✗
	PTE	✗	✓	✗	✗	✗
	Methpath2Vec	✗	✓	✗	✗	✗
	HERec	✗	✓	✗	✗	✗
	HNE	✗	✗	✗	✗	✗
	PMNE	✗	✓	✓	✗	✗
	MVE	✗	✓	✓	✗	✗
	MNE	✗	✓	✓	✗	✗
	Mvn2Vec	✗	✓	✓	✗	✗
GNN	Structural2Vec	✗	✗	✓	✗	✗
	GCN	✗	✗	✓	✗	✗
	FastGCN	✗	✗	✓	✗	✗
	AS-GCN	✗	✗	✓	✗	✗
	GraphSAGE	✗	✗	✓	✗	✗
	HEP	✓	✓	✓	✗	✗
	AHEP	✓	✓	✓	✗	✓
	GATNE	✓	✓	✓	✗	✓
	Mixture GNN	✓	✓	✓	✗	✗
	Hierarchical GNN	✓	✓	✓	✗	✗
	Bayesian GNN	✗	✓	✓	✗	✗
	Evolving GNN	✗	✓	✓	✓	✗

GNN framework

Algorithm 1: GNN Framework

Input: network $\mathcal{G}$, embedding dimension $d \in \mathbb{N}$, a vertex feature $\mathbf{x}_v$ for each vertex $v \in \mathcal{V}$ and the maximum hops of neighbors $k_{max} \in \mathbb{N}$.

Output: embedding result $\mathbf{h}_v$ of each vertex $v \in \mathcal{V}$

```
h_v^(0) ← x_v
for k ← 1 to k_max do
    for each vertex v ∈ V do
        S_v ← SAMPLE(Nb(v))
        h'_v ← AGGREGATE(h_u^(k-1), ∀u ∈ S)
        h_v^(k) ← COMBINE(h_v^(k-1), h'_v)
    normalize all embedding vectors h_v^(k) for all v ∈ V
h_v ← h_v^(k_max) for all v ∈ V return h_v as the embedding result for all v ∈ V
```

$\mathbf{h}_v^{(0)} \leftarrow \mathbf{x}_v$

for $k \leftarrow 1$ *to* k_{max} **do**

- **for** *each vertex* $v \in \mathcal{V}$ **do**
  - $S_v \leftarrow \textsc{Sample}(Nb(v))$
  - $\mathbf{h}'_v \leftarrow \textsc{Aggregate}(\mathbf{h}_u^{(k-1)}, \forall u \in S)$
  - $\mathbf{h}_v^{(k)} \leftarrow \textsc{Combine}(\mathbf{h}_v^{(k-1)}, \mathbf{h}'_v)$
- normalize all embedding vectors $\mathbf{h}_v^{(k)}$ for all $v \in \mathcal{V}$

$\mathbf{h}_v \leftarrow \mathbf{h}_v^{(k_{max})}$ for all $v \in \mathcal{V}$ return $\mathbf{h}_v$ as the embedding result for all $v \in \mathcal{V}$

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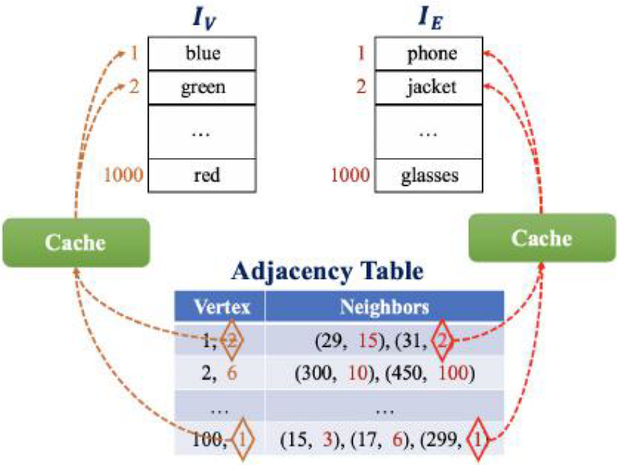
- Using the k-hop neighbors to keep structure and properties information

System optimization technique: Storage

- AliGraph platform is build on a distributed environment
  - ✓ Graph partition to minimize the number of crossing edges whose endpoints are in different workers.
    - The whole graph is divided and separately stored in different workers.
    - The goal of graph partition is to minimize the number of crossing edges whose endpoints are in different workers.
    - Aligraph includes four built-in state-of-the-art graph partition algorithms.
    - Users can choose the best partition strategy based on their own needs.
  - ✓ Separate storage of attributes
    - It is similar to normal form.
    - It increases the access time for retrieving the attributes.
  - ✓ Caching Neighbors of Important Vertices to reduce the communication cost
    - The trade-off exists between time and space.
    - It exists a user-specified threshold.

Separate storage of attributes



Partition and Caching

Algorithm 2: Partition and Caching

Input: graph $\mathcal{G}$, partition number p, cache depth h, threshold $\tau_1, \tau_2, \ldots, \tau_h$
Output: p subgraphs

Initialize p graph servers
for *each edge* $e = (u, v) \in \mathcal{E}$ **do**
  $j = \textsc{Assign}(u)$
  Send edge e to the j-th partition
for *each vertex* $v \in V$ **do**
  for $k \leftarrow 1$ *to* h **do**
    Compute $D_i^{(k)}(v)$ and $D_o^{(k)}(v)$
    if $\boxed{\frac{D_i^{(k)}(v)}{D_o^{(k)}(v)} \geq \tau_k}$ **then**
      Cache the 1 to k-hop out-neighbors of v on each partition where v exists

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    Send edge e to the j-th partition
for each vertex v ∈ V do
    for k ← 1 to h do
        Compute D_i^(k)(v) and D_o^(k)(v)
        if D_i^(k)(v) / D_o^(k)(v) ≥ τ_k then
            Cache the 1 to k-hop out-neighbors of v on each partition where
              v exists
```

Sampling

- TRAVERSE: is used to sampling a batch of vertices or edges from the whole partitioned subgraphs.
- NEIGHBORHOOD: will generate the context for a vertex. The context of this vertex may be one or multi hop neighbors, which are used to encode this vertex.
- NEGATIVE: is used to generate negative samples to accelerate the convergence of the training process.

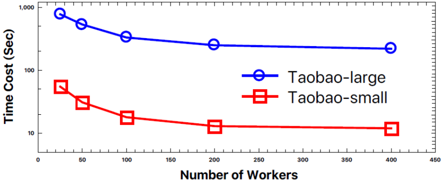
Operator

- Aggregate
  - ✓ Convolution operation
  - ✓ Elementwise mean, max-pooling neural network and long short-term memory (LSTMs)
- Combine
  - ✓ Concat ...

System Evaluation

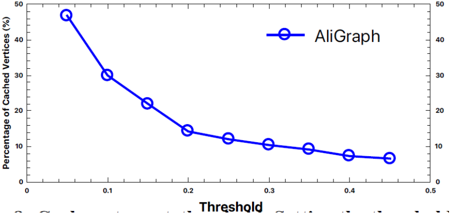
Dataset	# user vertices	# item vertices	# user-item edges	# item-item edges	# attributes of user	# attributes of item
Taobao-small	147,970,118	9,017,903	442,068,516	224,129,155	27	32
Taobao-large	483,214,916	9,683,310	6,587,662,098	231,085,487	27	32

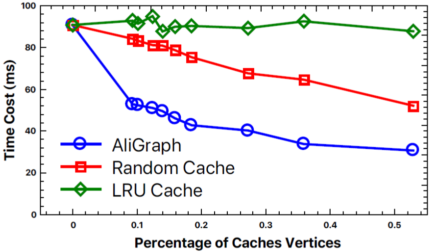
- Graph Build
  - ✓ The graph building time explicitly decreases w.r.t. the number of workers
  - ✓ AliGraph can build large-scale graphs in minutes, e.g. 5 minutes for Taobao-large.



System Evaluation

- Effects of Caching Neighbors





System Evaluation

- Effects of Sampling

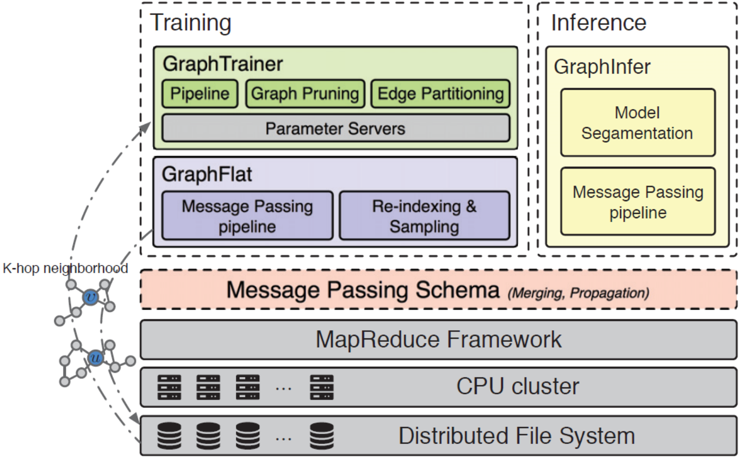
Dataset	Setting		Time (ms)		
	# of workers	Cache Rate	TRAVERSE	NEIGHBORHOOD	NEGATIVE
Taobao-small	25	18.46%	2.59	45.31	6.22
Taobao-large	100	17.68%	2.62	52.53	7.52

- Sampling methods are very efficient which finish between a few milliseconds to no more than 60ms.
- Sampling methods are efficient and scalable.

Conclusions

- In-memory processing systems using rpc comunication with the different workers.
- Using k-hop neighbors to keep structure and properties information.
- Design a series of optimization strategy.

Solution 2: AGL [2]



[2] AGL: A Scalable System for Industrial-purpose Graph Machine Learning http://www.vldb.org/pvldb/vol13/p3125-zhang.pdf

How to keep structure and properties information

- K-hop Neighborhood: The K-hop neighborhood w.r.t. a target node v, denoted as G_v^K , is defined as the induced attributed subgraph of G whose node set is $V_v^K = \{v\} \cup \{u : d(v,u) \leq k\}$, where $d(v,u)$ denotes the length of the shortest path from u to v.

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- This is different from an Aligraph.

Theorem 1. Let $\mathcal{G}_v^K$ be the K-hop neighborhood w.r.t. the target node v, then $\mathcal{G}_v^K$ contains the **sufficient and necessary information** for a K layers GNN model, which follows the paradigm of Equation 1, to generate the embedding of node v.

First, the 0^{th} layer embedding is directly assigned by the raw feature, i.e., $\mathbf{h}_v^{(0)} = \mathbf{x}_v$, which is also the 0-hop neighborhood. And then, from Equation 1, it's easy to find that the output embedding of v in each subsequent layer is generated only based on the embedding of the 1-hop in-edge neighbors w.r.t. v from the previous layer. Therefore, by applying mathematical induction, it's easy to prove Theorem 1. Moreover, we can extend the theorem to a batch of nodes. That is, the intersection of the K-hop neighborhoods w.r.t. a batch of nodes provides the sufficient and necessary information for a K layers GNN model to generate all the node embeddings in the batch. This simple theorem implies that in a K layers GNN model the target node's embedding at the K^{th} layer only depends on its K-hop neighborhood, rather than the entire graph.

GraphFlat

- GraphFlat is to generate independent K-hop neighborhoods.
- It is based on message passing.
- Those tiny K-hop neighborhoods are flattened to a protobuf strings and stored on a distributed file system.
- The k-hop neighborhood is self-contained, so we can load one or a batch of them rather than the entire graph into memory, and do the training similar to any other traditional learning methods

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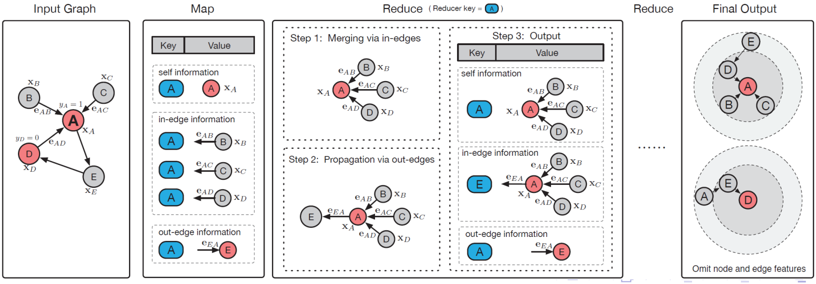


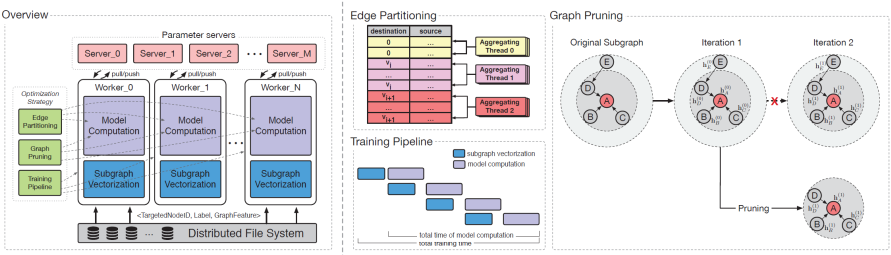
Hub node

- In network science, a hub is a node with a number of links that greatly exceeds the average.
- In the Reduce phase of GraphFlat, reducers that process such "hub" nodes could be much slower than others thus damage the load balances of GraphFlat.
- The huge K-hop neighborhoods w.r.t. those "hub" nodes may cause the Out Of Memory (OOM) problem.

System optimization technique: Sampling and Indexing

- Re-indexing: update shuffle keys using suffixes when exceeds a pre-defined threshold.
- Sampling framework: reduce the scale of the K-hop neighborhoods, especially for those "hub" nodes.
- Inverted indexing: replace the reindexed shuffle key with the original shuffle key.

GraphTrainer



- Training workers of GraphTrainer is independent of each other.
- Training workflow
  - ✓ subgraph vectorization
    - ∗ Adjacency matrix, A_α
    - ∗ Node feature matrix, X_α
    - ∗ Edge feature matrix, E_α
  - ✓ model computation
    - ∗ forward and backward

Datasets

Indices	Cora	PPI	Ogbn	UUG
#Nodes	2,708	56,944	2,449,029	6.23×10^9
#Edges	5,429	818,716	61,859,140	3.38×10^{11}
#feature	1,433	50	100	656
#Classes	7	121	47	2
#Train	140	44,906	196,615	1.2×10^8
#Valid	500	6,514	39,323	5×10^6
#Test	1,000	5,524	2,213,091	1.5×10^7
#Layers	2	3	3	2
Embedding	16	64	256	8
#Epochs	200	200	20	10

System Evaluation

- Effectiveness

Datasets	Methods	Base	PyG	DGL	AliGraph	AGL
Cora (Accuracy)	GCN	0.813	0.818	0.811	0.802	0.811
	GAT	0.830	0.831	0.828	0.823	0.830
PPI (micro-F1)	GraphSage	0.598	0.632	0.636	–	0.635
	GAT	0.973	0.983	0.976	–	0.977
Ogbn (Accuracy)	GCN	0.757	–	–	0.723	0.744
	GraphSage	0.780	–	–	0.745	0.775
UUG (AUC)	GCN	–	–	–	–	0.681
	GraphSage	–	–	–	–	0.708
	GAT	–	–	–	–	0.867

System Evaluation

- Efficiency

	GCN			GraphSAGE			GAT		
	1-layer	2-layer	3-layer	1-layer	2-layer	3-layer	1-layer	2-layer	3-layer
PyG	3.49	6.43	9.62	4.47	6.98	10.15	44.29	65.32	85.21
DGL	1.09	1.35	1.62	1.14	1.39	1.64	16.14	21.47	26.03
AGL_{base}	0.48	2.75	4.10	0.46	2.47	3.94	4.75	25.72	36.86
$\text{AGL}_{+\text{pruning}}$	0.48	1.93	3.23	0.46	1.67	2.99	4.75	13.88	20.01
$\text{AGL}_{+\text{partition}}$	0.42	1.22	1.60	0.34	0.97	1.39	4.63	22.65	33.45
$\text{AGL}_{+\text{pruning\&partition}}$	**0.42**	**1.13**	**1.52**	**0.34**	**0.88**	**1.35**	**4.63**	**13.73**	**18.63**

图: Time cost(s) per epoch on PPI in Standalone mode

Conclusions

- Construction of K-hop neighborhood, an information-complete subgraph for each node
- AGL provides the scalability, fault tolerance using mature infrastructures such as MapReduce.

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Key Insight

How to keep the structure and properties information···

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Future Work

- The k-hop neighberhoods design is very enlightening. I see if I can further think about it here, or use this solution idea in reverse to optimize the system.

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References I

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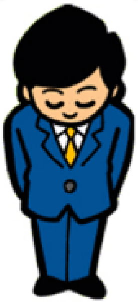
Thank you!
Welcome for any questions!



Jun-peng Zhu
Department of Computer Science and Technology
Nanjing University