Efficient Graph Computation for Node2Vec

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ABSTRACT

Node2Vec is a state-of-the-art general-purpose feature learning method for network analysis. However, current solutions cannot run Node2Vec on large-scale graphs with billions of vertices and edges, which are common in real-world applications. The existing distributed Node2Vec on Spark incurs significant space and time overhead. It runs out of memory even for mid-sized graphs with millions of vertices. Moreover, it considers at most 30 edges for every vertex in generating random walks, causing poor result quality.

In this paper, we propose Fast-Node2Vec, a family of efficient Node2Vec random walk algorithms on a Pregel-like graph computation framework. Fast-Node2Vec computes transition probabilities during random walks to reduce memory space consumption and computation overhead for large-scale graphs. The Pregel-like scheme avoids space and time overhead of Spark’s read-only RDD structures and shuffle operations. Moreover, we propose a number of optimization techniques to further reduce the computation overhead for popular vertices with large degrees. Empirical evaluation show that Fast-Node2Vec is capable of computing Node2Vec on graphs with billions of vertices and edges on a mid-sized machine cluster. Compared to Spark-Node2Vec, Fast-Node2Vec achieves 7.7–122× speedups.

1. INTRODUCTION

Graph is an important big data model, widely used to represent real-world entities and relationships in applications ranging from the World Wide Web [1], social networks [6], publication networks [18], to protein-protein interaction networks in bioinformatics [13]. One promising approach to network (graph) analysis is to construct feature vectors to represent vertices or edges in a graph such that classical machine learning algorithms can be applied to the resulting vectors or edges for network analysis tasks, such as node classification [16] and link prediction [6]. Node2Vec [5] is a state-of-the-art general-purpose feature learning method for network analysis. It has been shown that Node2Vec achieves better accuracy than other competitive feature learning solutions, including Spectral Clustering [15], DeepWalk [12], and LINE [14], as well as a number of popular heuristic solutions [5].

Node2Vec extends the Skip-gram model [8] to the network analysis scenario. The Skip-gram model is originally studied in the text analysis scenario [8][9]. The goal is to automatically learn a feature vector for every word. The first step is to sample the neighbor words for every word. Based on the samples, it then formulates and solves an optimization problem using Stochastic Gradient Descent (SGD) to obtain the vector representations of words. In the text scenario, the neighbor words of a word can be easily defined as the t words prior to and t words following the target word in sentences, where t is a parameter (e.g., 5). Therefore, one of the main challenges to employ this idea to graphs is to compute the neighbors of a vertex in a graph.

The main distinctive characteristic of Node2Vec is that it proposes a biased 2nd-order random walk model to sample neighbors of every vertex in a graph, upon which the optimization problem similar to that in the original text analysis scenario [9] is solved to obtain the vertex feature vectors. This random walk model combines BFS and DFS in a flexible manner so that local and global structures of the vertex neighborhood can both be captured. In this way, it is capable of supporting different varieties of graphs and analysis tasks well. The Node2Vec paper reports the run times for graphs with up to 1 million vertices and 10 million edges. In this paper, we are interested in efficiently supporting Node2Vec on large-scale graphs with billions of vertices and edges, which are common in real-world applications.

Problems of Existing Node2Vec Implementations.

There are two reference implementations (i.e. Python and C++) on the Node2Vec project page[3]. Both of them run on a single machine and perform well on small graphs. However, the data structures for large-scale graphs with billion of vertices cannot fit into the main memory of a single machine, demanding distributed graph computation solutions.

Spark[21] [21] is a popular distributed computation framework for big data processing. Compared to the previous MapReduce framework [3], Spark takes advantage of in-memory processing and caching to significantly improve computation efficiency. There is a Node2Vec implementation on

http://snap.stanford.edu/node2vec/
https://spark.apache.org/
While it leverages Spark to compute Node2Vec on larger graphs using a cluster of machines, there are two main problems of Spark-Node2Vec.

First, Spark-Node2Vec is not an exact Node2Vec implementation. For every vertex, it considers at most 30 edges with the highest weights for computing the biased random walks in order to save memory space for storing the transition probabilities. However, a popular vertex in a real-world graph (e.g., a social network) can have thousands or even millions of edges. As a result, Spark-Node2Vec samples only a very small fraction of neighbors of a popular vertex (e.g., 3% of 1K neighbors, 0.003% of 1M neighbors). This significantly degrades the quality of the resulting vectors, as will be shown in our experimental study in Section 4.

Second, Spark-Node2Vec runs out of memory and incurs significant overhead for even mid-sized graphs. Spark’s core data structure is RDD, which is a distributed data set that allows parallel computation across multiple worker machine nodes. To simplify data consistency and fault tolerance, Spark’s RDD is designed to be read-only. That is, any modification to an RDD will result in a new RDD. However, every random walk step needs to update the sampled walks. A typical configuration runs 10 rounds of random walks, each with 80 steps. Therefore, Spark-Node2Vec incurs frequent creations of new RDDs, which consume the main memory space quickly. Moreover, the solution employs an RDD Join operation in selecting the transition probabilities at every step of the random walks. The Join operation performs data re-distribution, a.k.a. shuffle, which spills intermediate data to disks, incurring significant I/O overhead.

Our Solution: Fast-Node2Vec on a Pregel-Like Graph Computation Framework. We propose a Fast-Node2Vec algorithm on a Pregel-like graph computation framework \(^7\) to address the problems of the existing solutions. Node2Vec consists of a biased random walk stage and a Skip-Gram computation stage. As the former constitutes 98.8% of the total execution time of Spark-Node2Vec, we mainly focus on improving the Node2Vec random walk stage in this paper.

First, we employ GraphLite\(^4\), an open-source C/C++ implementation of Pregel \(^7\) in order to avoid the overhead in Spark. Pregel is a distributed in-memory graph computation framework. Graph computation is implemented as programs running on individual vertices. In contrast to Spark, vertex states are updated in place and vertices communicate through messages in main memory and across network. Therefore, the Pregel framework does not incur the RDD creation and the shuffle overhead as in Spark.

Second, Fast-Node2Vec computes the transition probabilities on demand during random walks. It does not precompute and store all the transition probabilities before random walks. As Node2Vec performs a 2nd-order random walk, the transition probability depends on a pair of vertices in the last two steps in a random walk. Therefore, for a vertex \(V_i\) with \(d_i\) neighbors in an undirected graph, there are \(d_i^2\) transition probabilities. The total number of transition probabilities for all vertices is much larger than the number of vertices and the number of edges added up together. This is especially the case in power-law graphs, where a small number of popular vertices have high degrees. We find that the total amount of memory space required to store all transition probabilities of large-scale graphs can be magnitudes larger than the total memory size of the machine cluster used in our evaluation. Therefore, Fast-Node2Vec performs on-demand computation of transition probabilities in order to reduce the memory space and support large-scale graphs.

Third, we further analyze the computation overhead in Fast-Node2Vec. We find that the communication of vertex neighbors is a significant source of overhead, especially for popular vertices with a large number of neighbors. To reduce this overhead, we propose and study a family of Fast-Node2Vec algorithms: (i) For vertices in the same graph partition, we can directly read the neighbor information without sending messages (FN-Local); (ii) To find the common neighbors of a popular vertex \(B\) and a low-degree vertex \(S\), we may always send \(S\)’s neighbors to \(B\) (FN-Switch); (iii) After receiving the neighbor information of a popular vertex \(B\) from a remote graph partition, we can cache it locally and reuse it (FN-Cache). The above Fast-Node2Vec algorithms are all exact implementation of Node2Vec random walks. In addition, we propose a variant of Fast-Node2Vec (FN-Approx) that approximately computes next moves at popular vertices with low overhead and bounded errors.

Finally, we perform extensive experiments to empirically evaluate all the proposed algorithms using both real-world and synthetic data sets. Our experimental results on a mid-sized cluster of 12 machines show that our proposed Fast-Node2Vec solutions are capable of computing Node2Vec for large-scale graphs with billions of vertices in a reasonable amount of time. Compared to Spark-Node2Vec, our proposed Fast-Node2Vec solutions achieve 7.7–122x speedups.

Contributions of the Paper:

1. We propose Fast-Node2Vec, a family of efficient Node2Vec random walk algorithms on a Pregel-like graph computation framework. Fast-Node2Vec computes transition probabilities during random walks to reduce memory space consumption and computation overhead for large-scale graphs.

2. We analyze the behavior of the Node2Vec random walks and show that popular vertices with a large number of edges incur significant overhead in message sizes and computations. Then we propose and study a number of optimization techniques (including FN-Cache and FN-Approx) to reduce the overhead.

3. We perform extensive experiments to empirically evaluate our proposed solutions. In our experiments, we see that (i) Spark-Node2Vec has both poor result quality and poor efficiency. (ii) Fast-Node2Vec is capable of supporting graphs with billions vertices and edges using a mid-sized machine cluster. Similar computing resources are often available to academic researchers. (iii) Compared to Spark-Node2Vec, Fast-Node2Vec solutions achieve 7.7–122x speedups speedups. (iv) As the vertex distribution of a graph becomes more and more skewed, our optimization techniques to reduce the overhead of popular vertices become more effective.

The rest of the paper is organized as follows. Section 2 briefly overviews existing Node2Vec solutions. Section 3 presents the technical details for improving the efficiency of Node2Vec using Fast-Node2Vec on a Pregel-Like graph computation framework. Section 4 compares Fast-Node2Vec with Spark-Node2Vec, and studies the proposed optimiza-
Upon the first-generation framework, MapReduce [3], by putting the results of intermediate computation steps in memory, thereby reducing I/O overhead to access the underlying distributed file system (e.g. HDFS) in MapReduce. The core data structure in Spark is RDD (Resilient Distributed Data sets). An RDD is an immutable, distributed data set. Operations (a.k.a. transformations) on an RDD can be performed in parallel across all the partitions of the RDD. GraphX is a graph computation framework built on top of Spark. It represents vertices, edges, and intermediate states as RDDs, and implements graph computations using RDD transformations, such as joins.

Spark-Node2Vec implements random walks in two phases:

(i) **Preprocessing phase**: Spark-Node2Vec pre-computes all transition probabilities and allocates RDDs for storing the transition probabilities to facilitate random walks. Every edge stores three arrays of equal length. One array records the neighbors of the destination vertex. The other two arrays are initialized using the transition probabilities for Alias Sampling [17]. Every vertex contains an array of (neighbor, edge weight) pairs. To reduce the allocated memory space and computation overhead, Spark-Node2Vec trims the graph by removing edges. It preserves only 30 edges with the top most edge weights for every vertex.

(ii) **Random walk phase**: Spark-Node2Vec simulates random walks starting from all vertices based on the pre-computed transition probabilities. It computes one step of all walks in every loop iteration. This is achieved by joining the last two walk steps, the pre-computed transition probabilities for edges, and the recorded edge weights for vertices. The computed random walks are recorded in an RDD, where the walk length grows one step per iteration for every vertex.

Spark-Node2Vec incurs both poor quality and poor efficiency:

- **Poor quality**: The trim idea over-simplifies the random walk process. For a vertex $v$ with $d >> 30$ outgoing edges, Spark-Node2Vec would explore only 30 neighbors of $v$. For $d = 1000$, this is 3% of all neighbors. For $d = 1$ million, merely 0.003% of the neighbors are preserved. This significantly deviates from the Node2Vec random walk model. As will be shown in Section 4, node classification accuracy suffers drastically because of the problematic trim idea.

- **Poor efficiency**: Even with the much simplified graph after trimming, the efficiency of Spark-Node2Vec is still poor. There are two main causes. First, Spark RDDs are read-only; Recording random walk steps in every iteration will result in a copy-on-write and the creation of a new RDD. Second, the computation performs frequent join transformations. However, a join often involves a shuffle operation, which prepares data by sorting or hash partitioning. Unfortunately, shuffle often needs to spill the intermediate data to disks, incurring significant disk I/O overhead. As a result, Spark-Node2Vec has a difficult time processing even mid-sized graphs, as will be shown in Section 4.

### 3. FAST-NODE2VEC

We present Fast-Node2Vec in this section. We begin by describing our choice of graph computation framework in Section 3.1. Then, we describe the main components of the
Fast-Node2Vec algorithm in Section 3.2. After that, we analyze the computation to understand its efficiency bottleneck in Section 3.3 and propose a number of techniques to improve Fast-Node2Vec in Section 3.4.

3.1 GraphLite: a Pregel-Like Distributed Graph Computation Framework

Pregel [7] is a distributed in-memory graph computation framework. GraphLite [9] is a lightweight open-source C/C++ implementation of Pregel. We choose GraphLite to run Node2Vec in order to avoid the costs of RDDs and shuffles in Spark, as discussed in Section 2.2.

In the Pregel model, a graph algorithm is implemented as a vertex-centric compute function. The system consists of a master machine node and a number of worker nodes connected through a data center network, as depicted in Figure 3. The graph is partitioned across the workers at the beginning of the computation. The system runs the graph computation in a series of supersteps. At the beginning of a superstep, the master broadcasts a start message to all workers. Upon receiving this message, each worker iterates through all the vertices and invokes the compute function for every vertex in its graph partition. Then workers send done messages to the master. The master starts the next superstep only after all the workers are done with the current superstep. In this way, the computation follows the Bulk Synchronous Parallel model: The master enforces a global barrier between two supersteps: Within each superstep, compute is run in parallel across workers.

The compute function on a vertex is typically implemented with three main parts: (i) receiving incoming messages from the previous superstep; (ii) computing and updating the state of the vertex in light of the incoming messages; (iii) sending messages to other vertices that will be delivered in the next superstep.

Figure 3 illustrates the internal data structures of a worker. There are an array of vertex states, an array of vertex out-edges, and structures for managing messages. In a superstep, incoming messages to the vertices in the local partition are appended to the global received message list. At the start of the next superstep, the messages are then delivered into the per-vertex in-message lists, which are processed in the compute function invoked later in the superstep.

Compared to Spark, the Pregel model has the following advantages. First, vertex states are updated in place, while Spark incurs RDD copy-on-write cost and consumes much more memory space. Second, vertices communicate through messages that are managed in main memory, while Spark’s shuffle operation may incur significant file I/O overhead.

GAS model and Node2Vec. Apart from the Pregel model, another popular graph computation model is GAS proposed in PowerGraph [4]. The GAS model divides the compute function into three functions: Gather, Apply, and Scatter. While GAS can efficiently support many graph computation tasks, such as PageRank, we find that GAS may not be suitable for Node2Vec because the incoming messages in Node2Vec cannot be aggregated and there are no broadcasting outgoing messages. Consequently, the GAS approach does not introduce additional benefits for Node2Vec.

3.2 Fast-Node2Vec on GraphLite

We aim to run Node2Vec efficiently on graphs with billions of vertices and edges using a mid-sized cluster of machines. Such computing resources are often available to researchers in academia. In our experiments, we use a cluster of 12 machines, each with 128GB of memory and 40 cores. Since Pregel performs distributed computation in memory, we aim to restrict the total memory consumption in Node2Vec to the aggregate memory size in the cluster (i.e., 1.5TB).

In the original Node2Vec [5], all transition probabilities are pre-computed before simulating the random walks. This approach is followed by both the single-machine reference implementations and Spark-Node2Vec. However, this approach consumes a large amount of memory. Let us consider an undirected graph for simplicity. Directed graphs can be analyzed similarly. Let the degree of a vertex $V_i$ be $d_i$. As shown in Figure 2 there is an $\alpha_{pq}(u, V, x)$ for each pair of $u$ and $x$, which are $V_i$’s neighbors. Thus, the number of $\alpha$’s at $V_i$ is equal to $d_i^2$. Alias sampling [17] requires 8-byte space per probability. Therefore, the space for all the transition probabilities can be computed as follows:

$$\text{Memory}_{\text{TransProb}} = 8 \sum d_i^2 \geq 8 \left( \sum d_i \right)^2 = 8 nd^2$$  \hspace{1cm} (1)

where $n$ is the number of vertices and $d$ is the average vertex degree. Here, we estimate the total amount of space required to store all the transition probabilities of a social network. Real-world social networks (e.g., Twitter, Facebook, WeChat) often have over a billion vertices. The number of friends of an average user is on the order of 100 to 1000. Therefore, if $n = 1G$ and $d = 100$, it requires a space of 80 TB. If $n = 1G$ and $d = 1000$, it takes 8 PB to store all transition probabilities. The space required is clearly much larger than the aggregate memory space available in a mid-sized cluster.

Given this observation, we propose to compute the transition probability on demand during the biased random walk. Algorithm 1 lists the pseudo-code for Fast-Node2Vec on GraphLite. There are several interesting design choices in this algorithm. First, the algorithm simulates $n$ random walks, one per starting vertex, where $n$ is the number of vertices in the graph. At superstep $s$, it computes step $s$ for all $n$ random walks. Second, there are two types of messages: STEP and NEIG. The STEP message reports a sampled step in a random walk. The NEIG message sends the neighbors of the current vertex to the next-step vertex $x$ in the random walk. All messages are labelled with the associated starting vertex ID (Line 9). Third, the sampled walk steps are stored in the value of the starting vertex (Line 5 and 11). This is achieved by sending the STEP message with the sampled step as the value field to the starting vertex (Line 20). Fourth, if a random walk moves from $v$ to $x$, then the compute at $v$ will send $v$’s neighbor vertex IDs to $x$ (Line 22). In this way, $x$ can easily figure out the shared neighbors between $x$ and $v$ for the transition probability...
computation (Line 17). Finally, we note that multiple random walks may arrive at the same vertex in some step. The algorithm deals with this complexity by grouping messages based on the starting vertex IDs (Line 13 and 16).

We now explain how to compute transition probabilities. A vertex can access its outgoing edges in the out-edge array based on the starting vertex IDs (Line 13 and 16). Therefore, in superstep \(s\), we need to figure out the distance \(dist(u, x)\) between \(u\) and every neighbor \(x\) of \(v\). In Algorithm 1, in superstep \(s - 1\), compute at \(u\) has already sent \(u\)’s neighbors to \(v\) (Line 22). Therefore, in superstep \(s\), compute at \(v\) will receive \(u\)’s neighbors in incoming messages (Line 12-14). The three cases of distances in Figure 2 means that \(x\) is \(u\), \(x\) is a common neighbor of \(u\) and \(v\), and all other cases. It is easy to find out if \(x\) is a common neighbor of \(u\) and \(v\) by using a hash set. In this way, we obtain the unnormalized transition probabilities, then use them to perform the biased sample at \(v\) (Line 18).

### 3.3 Analysis of Fast-Node2Vec Computation

Figure 4 shows the change in the memory space consumed during the Fast-Node2Vec computation on com-Friendster, the largest real-world graph in our evaluation (c.f. Section 3.1). We see that the amount of memory consumed quickly increases, and then flattens after about 10 supersteps. To understand this behavior, we consider the memory consumed during graph computation. There are mainly three parts that consume significant amount of memory: (i) the graph topology, including vertices and edges; (ii) the vertex values and edge weights; (iii) the \(STEP\) and \(NEIG\) messages. In the Node2Vec computation, the graph topology is unchanged and the memory space allocated for the vertex values and the edge weights keeps the same. Therefore, part (i) and part (ii), shown as base usage in Figure 4, do not contribute to the increase in the observed memory consumption. On the other hand, the memory consumed by messages grow significantly, as shown in Figure 4. The number of \(STEP\) messages is equal to \(n\), the number of vertices, in Fast-Node2Vec. The size of a \(STEP\) message is always the same. Therefore, the memory consumed by all \(STEP\) messages is the same in the entire computation. In contrast, the \(NEIG\) message sizes change significantly.

We analyze the relationship of the vertex degrees and the frequency of vertices to appear in the resulting random walks, as shown in Figure 5. The X-axis shows equi-width buckets of degrees. For example, the bucket 600 contains all vertices with degrees between 400 and 600. The height of the bar represents the average times for a vertex in this bucket to be sampled in the Node2Vec random walks. From Figure 5, we see that the higher the vertex degree, the more frequently that the vertex is sampled in the random walks.

We can explain this phenomenon as follows. For a vertex \(v\), if a random walk arrives at one of \(v\)’s neighbors, there is a chance for the random walk to move to \(v\). The higher the degree of \(v\), the more neighbors that \(v\) has, the more likely...
that the previous vertex in the random walk is a neighbor of \( v \). This effect means that random walks will tend to visit large-degree vertices. We know that the higher the degree of \( v \), the larger size \( v \)'s NEIG messages take. At the beginning, there is a walk at every vertex. Gradually, more and more large-degree vertices appear in the walk. Therefore, the memory consumed by NEIG messages increases. When this behavior becomes stable, the memory consumed becomes flat.

While Figure 4 and Figure 5 show the results for one set of Node2Vec \((p, q)\) parameters, we see similar behaviors across different parameter settings.

### 3.4 Optimization Techniques

We have seen that the neighbor messages can consume a large amount of memory. This is especially the case for power-law graphs where a small number of vertices have very large degrees. We call such vertices popular vertices. The memory consumption effectively determines the graph sizes that can be supported in a mid-sized cluster. In this subsection, we propose a number of techniques to reduce the message sizes for saving memory and improve the efficiency of Fast-Node2Vec.

**FN-Local: Exploiting local graph partition.** Consider an NEIG message sent from \( u \) to \( v \). The purpose of this message is to notify \( v \) of \( u \)'s neighbors. This is only necessary if \( u \) and \( v \) are in separate workers. If both \( u \) and \( v \) are in the same worker, \( v \) is able to directly read \( u \)'s neighbors from the out-edge array. We call an NEIG message between vertices in the same worker a local NEIG message. We extend the GraphLite framework with an API that allows a vertex to visit another vertex’s information in the same worker. Then FN-Local uses this API to reduce all the local NEIG messages.

**FN-Switch: Switching the destination of NEIG messages from popular vertices to unpopular vertices.** The NEIG message size is proportional to the number of neighbors of a vertex. Consider an NEIG message from \( u \) to \( v \), where \( u \) is a popular vertex and \( v \) is an unpopular vertex. The purpose of this message is to facilitate the computation of common neighbors between \( u \) and \( v \). However, since a popular vertex has a large number of neighbors, the message size from \( u \) to \( v \) is very large.

An interesting observation is that the common neighbors between \( u \) and \( v \) can also be computed at \( u \) if \( v \) sends all its neighbors to \( u \). In addition, after \( u \) knows all \( v \)'s neighbors, it can perform the full computation of transition probabilities and random walk simulation on behalf of \( v \). In other words, it is possible to switch the destination of the NEIG message, asking \( v \) to send its neighbors to \( u \). Since \( v \) has much fewer neighbors than \( u \), this idea may significantly reduce the message size.

While this destination switching idea seems promising at first sight, back-of-envelope computation shows that it could significantly increase the overall run time. There is a significant problem to implement this idea. There are two messages for computing the random walk step: \( u \) must notify \( v \) that it wants \( v \) to send back an NEIG message; Then \( v \) sends the NEIG message to \( u \). This means that the random walk step needs two supersteps. This breaks Fast-Node2Vec’s behavior that it computes the same step of all random walks in every superstep. Consider a random walk that consists of alternating popular and unpopular vertices. Half of the moves are from a popular vertex to an unpopular vertex. Every such move takes one extra superstep. Thus, the entire random walk will take 50% more supersteps to complete, incurring significant time overhead.

**FN-Cache: Caching neighbors of remote popular vertices.** If a popular vertex \( u \) sends its neighbors to a vertex \( v \) in a remote worker \( W \), \( v \) can cache \( u \)'s neighbors in a global data structure at worker \( W \) so that later computation at any vertices in worker \( W \) can directly access this information without \( u \) re-sending costly NEIG messages.

To implement this idea, we extend GraphLite to expose an API for looking up the worker ID of a vertex. A popular vertex \( u \) will remember in an WorkerSent set to which remote workers it has sent NEIG messages. Before sending an NEIG message, \( u \) checks to see if the destination vertex \( v \)'s worker is in the WorkerSent set. If no, \( u \) sends a normal NEIG message and records \( v \)'s worker ID in the WorkerSent set. If yes, \( u \) sends a special NEIG message with a special (otherwise unused) value to notify \( v \) to look up \( u \)'s neighbors locally. In this way, this technique can significantly improve the efficiency of Fast-Node2Vec as will be shown in Section 4.

**FN-Multi: Simulating random walks using multiple rounds.** After the above optimizations, it is possible that the memory space required by Fast-Node2Vec is still too large to fit into the aggregate memory size in the machine cluster. We would like to gracefully handle such situations. We observe that the random walks starting from different vertices are independent of each other. Therefore, it is not necessary to run all \( n \) random walks at the same time. Instead, we can simulate the random walks in \( k \) rounds. In each round, we simulate \( n/k \) random walks. This technique will reduce the memory space for managing messages and for recording random walks by about a factor of \( k \) times. Note that we cannot remove any vertex or edge from the graph to reduce memory space for vertices and edges. This is because every vertex and every edge may still be visited in the subset of random walks.

**FN-Approx: Approximately computing the random walk steps at popular vertices.** The cost of computing the transition probabilities and simulating a random walk step at vertex \( v \) is \( O(d_v) \), where \( d_v \) is \( v \)'s degree. Therefore, popular vertices take much longer time for this computation. We would like to reduce the computation cost at popular vertices.

Consider an NEIG message from an unpopular vertex \( u \) to a popular vertex \( v \). We can derive the upper and lower bounds for an individual transition probability at \( v \). Suppose \( 1 \leq \frac{d_v}{d_u} \leq 1 \). Let \( d_u \) be \( u \)'s degree. Then the bounds for the transition probability from \( v \) to a neighbor \( x \) that is not \( u \) are as follows:

\[
\text{Lower Bound} = \frac{\text{Weight}_{\text{min}}}{\left(\frac{1}{p} + \frac{d_v - d_u}{q}\right)\text{Weight}_{\text{max}}} \quad (2)
\]

\[
\text{Upper Bound} = \frac{\text{Weight}_{\text{max}}}{\left(\frac{1}{p} + d_u + \frac{d_v - d_u}{q}\right)\text{Weight}_{\text{min}}} \quad (3)
\]

The numerator is the unnormalized transition probability. Its minimal value is \( \text{Weight}_{\text{min}} \), which is the product of the
minimal \( \alpha = 1 \) (when \( x \) is not \( u \)) and the minimal edge weight. Its maximal value is \( \text{Weight}_{\text{max}} \), which is the product of the maximal \( \alpha \) and the maximal edge weight. For the denominator, the minimal value is achieved when all of \( u \)'s \( d_u \) neighbors are also \( v \)'s neighbors. The maximal value is achieved when \( u \) and \( v \) do not have common neighbors. Similarly, we can obtain the upper and lower bounds for other value combinations of \( p \) and \( q \).

Note that \( d_u < d_v \). In many real-world scenarios, the difference between \( \text{Weight}_{\text{min}} \) and \( \text{Weight}_{\text{max}} \) is small. (For example, in a great many cases, edge weights are 1 for all edges). Therefore, the above lower bound is close to \( q/d_v \), and the above upper bound is close to \( 1/d_u \). As \( d_u \) is very large, the difference between the lower and the upper bounds can be very small.

Based on this observation, we propose FN-Approx, an approximate Fast-Node2Vec algorithm. At a popular vertex \( v \), if the last step \( u \) is an unpopular vertex, FN-Approx computes the difference between the upper and the lower bounds. If the difference is below a pre-defined threshold (e.g., 1e-3), FN-Approx will simply sample the step based on the static edge weights without considering the 2nd order effect. In this way, FN-Approx can significantly reduce the time overhead for computing transition probabilities at popular vertices. We study the impact of this approximation on the efficiency and the accuracy of the solution in Section 4.

4. EVALUATION

In this section, we empirically evaluate the efficiency of our proposed Fast-Node2Vec algorithms. We apply the algorithms to a number of large-scale real-world and synthetic graphs.

4.1 Experimental Setup

Machine Configuration. We run all experiments on a cluster of 12 machines, each of which is equipped with two Intel(R) Xeon(R) E5-2650 v3 CPU @ 2.30GHz (10 cores, 2 threads/core) and 128GB DRAM. The machine runs stock Ubuntu 16.04 with Linux Kernel version 4.4.0-112-generic. The machine nodes are connected through 10 Gbps Ethernet. The measured network bandwidth is between 9.4 and 9.6 Gbps. We compile C-Node2Vec, GraphLITE, and the Fast-Node2Vec algorithms using g++ version 5.4.0 with optimization level -O3. For Spark-Node2Vec, we run Spark version 2.2.0 using Java version 1.8 and Scala version 2.11. We deploy a cluster of 11 Spark workers and 1 Spark master and set the driver memory and executor memory size as 100 GB for Spark-Node2Vec evaluation to utilize almost all memory available on the machine nodes.

Data Sets. Table 1 summarizes the real-world and synthetic data sets used in the evaluation. The real-world graphs are described in the following:

- **BlogCatalog** [20]: This is a social network between authors on the BlogCatalog site. Vertices are labelled with topic categories provided by authors. This is the same data set used in the Node2Vec paper [5]. We use this data set to evaluate not only the efficiency the algorithms, but also the accuracy of the resulting vector representations for the node classification task.

- **com-LiveJournal** [19]: This is the friendship social network of the LiveJournal blogging website. There are 4 million vertices and 34.7 million edges in the graph.

- **com-Orkut** [19]: This is a social network of the Orkut site. Compared to com-LiveJournal, this graph contains slightly smaller number of vertices (3.1 million) but much larger number of edges (117.2 million). The average vertex degree of com-Orkut is 4.3 times as large as that of com-LiveJournal.

- **com-Friendster** [19]: This is a network of social relationships of the users on the Friendster site. Containing 1.8 billion edges, com-Friendster is the largest real-world data set in the evaluation.

In addition to the real-world graphs, we generate synthetic graphs that follow the RMAT [2] model. In the RMAT model, a graph with \( 2^K \) vertices is generated using four parameters \((a, b, c, d)\), where \( a+b+c+d = 1 \). The \( 2^K \times 2^K \) adjacency matrix is conceptually divided into four \( 2^{K-1} \times 2^{K-1} \) sub-matrices. An edge is randomly generated in the top-left, top-right, bottom-left, and bottom-right sub-matrices with probability \( a, b, c, \) and \( d \), respectively. This process is recursively applied to every sub-matrix. That is, a \( 2^i \) matrix is conceptually divided into four \( 2^{i-1} \times 2^{i-1} \) matrices, where \( i = K, K - 1, \ldots, 2 \). Given that an edge is to be generated in a \( 2^i \times 2^i \) matrix, the probability that this edge belongs to one of its four \( 2^{i-1} \times 2^{i-1} \) sub-matrices follows the \((a, b, c, d)\) distribution. We use a graph generation tool called TrillionC [11] to generate large-scale RMAT graphs. We vary \((a, b, c, d)\) to generate three sets of graphs with different characteristics:

- **ER-K graphs**: We set \((a, b, c, d)\) to \((0.25, 0.25, 0.25, 0.25)\) to generate Erdos-Renyi (ER) graphs with \( 2^K \) vertices and an average degree of 10. Note that the edges in this graph are uniformly distributed. There is no skew in the vertex degree distribution. We use this graph because the Node2Vec paper [5] reports run times for ER graphs with up to 1 million vertices and 10 million edges. We would like to compare our solution with the original Node2Vec, and show that our solution can scale up to 1 billion vertices and 10 billion edges. Therefore, we vary \( K \) from 20 to 30 to generate graphs with 1 million to 1.1 billion vertices.

Table 1: Graphs used in the evaluation.

| Graph                  | \(|V|\)  | \(|E|\)  | Max Degree |
|------------------------|--------|--------|-----------|
| BlogCatalog            | 10.3K  | 334.9K | 3.584     |
| com-LiveJournal        | 4.0M   | 34.7M  | 14.815    |
| com-Orkut              | 3.1M   | 117.2M | 58.999    |
| com-Friendster         | 65.6M  | 1.8G   | 8.447     |
| ER-20                  | 1.0M \((2^{20})\) | 10.5M  | 29        |
| ER-22                  | 4.2M \((2^{22})\) | 41.9M  | 31        |
| ER-24                  | 16.8M \((2^{24})\) | 167.8M | 31        |
| ER-26                  | 67.1M \((2^{26})\) | 671.1M | 32        |
| ER-28                  | 268.4M \((2^{28})\) | 2.7G   | 33        |
| ER-30                  | 1.1G \((2^{30})\) | 10.7G  | 35        |
| WeC-20                 | 1.0M \((2^{20})\) | 104.8M | 1.053     |
| WeC-22                 | 4.2M \((2^{22})\) | 419.4M | 1.745     |
| WeC-24                 | 16.8M \((2^{24})\) | 167.8M | 2.316     |
| WeC-26                 | 67.1M \((2^{26})\) | 6.7G   | 2.771     |
| Skew-1                 | 4.2M \((2^{22})\) | 419.4M | 2.098     |
| Skew-2                 | 4.2M \((2^{22})\) | 419.4M | 8.420     |
| Skew-3                 | 4.2M \((2^{22})\) | 419.4M | 23.594    |
| Skew-4                 | 4.2M \((2^{22})\) | 419.2M | 36.914    |

https://github.com/chan150/TrillionC
WeC-K graphs: We model a WeChat-like social network, where the upper bound of the number of friends per user is 5,000 and the average number of friends is about 100. We generate a set of WeC-K graphs with $2^K$ vertices and $100 \times 2^K$ edges. Without loss of generality, suppose $c + d \geq a + b$. Then the vertex with the largest degree is the last vertex with high probability. We can compute the parameters to ensure the expected degree of the last vertex is 5000. While the resulting parameters vary slightly for different $K$, we choose (0.18, 0.25, 0.25, 0.32) as the representative parameters to generate all WeC-K graphs so that the graphs are comparable to the Skew-S graphs.

Skew-S graphs: We generate a set of graphs with $2^{22}$ vertices and an average degree of 100, while varying the skewness of the data. We set the parameters $(a, b, c, d)$ so that the number of edges in the bottom-right part of the matrix is about $S$ times as many as that in the top-left part of the matrix, i.e. $d = S a$. In addition, we set $b = c = 0.25$. When $S = 1$, there is no skew. In general, when $S \geq 5000$, RMAT generates graphs with power-law characteristics. The higher the $S$, the more skew the vertex degrees are. We vary $S$ from 1 to 5. Note that WeC-22 is Skew-1.78 (0.32/0.18 = 1.78).

Algorithms to Compare. We evaluate the following solutions in the experiments:

- C-Node2Vec: This is the single-machine C++ reference implementation from the Node2Vec project web page. We use this implementation for two purposes: (i) comparing accuracy of applying the various solutions to the node classification task; and (ii) evaluating the scalability using the ER-K graphs.

- Spark-Node2Vec: This is the Node2Vec implementation on Spark. It preserves up to 30 edges per vertex, and computes the transition probabilities before running the biased random walk.

- FN-Base: This is Algorithm 1, the baseline Fast-Node2Vec algorithm, which computes transition probabilities on demand and runs on GraphLite, a Pregel-Like Graph Computation Framework (cf. Section 3.2).

- FN-Local: FN-Local improves FN-Base by allowing vertices to visit edge information of other vertices in the local graph partitions (cf. Section 3.4). In this way, it reduces the $NEIG$ messages for local vertices.

- FN-Switch: FN-Switch switches the destination of $NEIG$ messages from popular to unpopular vertices (cf. Section 3.4). However, this may incur more rounds of messages and thus more supersteps.

- FN-Cache: FN-Cache improves FN-Local by caching neighbors of the most popular vertices in order to reduce the amount of messages for popular vertices (cf. Section 3.4). As the other FN algorithms all give exact results, we use FN-Exact to represent them for the purpose of comparing accuracy of applying the solutions to the node classification task.

Measurements. We compare both the result quality and the efficiency of the above solutions in our experiments. In the efficiency comparison, we will focus only on the run time of performing the Node2Vec random walks. For each combination of solutions, graphs, and Node2Vec parameters, we compute 80-step biased random walks for all vertices in the graph.

4.2 Accuracy of Node Classification

The first question that we would like to answer is what is the impact of the quality of the generated random walks on the accuracy of the node classification task. We use the BlogCatalog data set, in which vertex labels are available, for this purpose. Figure 6 compares the accuracy of the node classification task using the vector representations generated by C-Node2Vec, Spark-Node2Vec, FN-Exact, and FN-approx. From left to right, the figure shows the micro-F1 and macro-F1 scores with two sets of Node2Vec parameters. The higher the scores, the better the solution. From Figure 6 we see that:

1. The accuracy of Spark-Node2Vec is dramatically worse than the other solutions. This is because Spark-Node2Vec preserves only up to 30 edges for every vertex in order to save memory space, significantly restricting the random walk destinations and thus altering the behavior of Node2Vec random walks.

2. FN-exact achieves similar accuracy as C-Node2Vec. FN-exact (i.e., FN-Base, FN-Local, FN-Switch, FN-Cache)
implements the 2nd-order biased random walk exactly as defined in Node2Vec [5]. Therefore, it has similar quality as the reference implementation, C-Node2Vec.

(3) Interestingly, FN-approx, our proposed approximate solution, achieves similar accuracy compared to FN-exact and C-Node2Vec. This shows that the quality degradation caused by the approximate computation on peripheral vertices is negligible. This approximation technique works in practice.

### 4.3 Efficiency on Real-World Graphs

Figures 7(a)-(c) compare the execution time of all seven solutions: C-Node2Vec, Spark-Node2Vec, FN-Base, FN-Local, FN-Cache, FN-Approx, and FN-Switch. For each graph, we run experiments with two sets of Node2Vec \((p, q)\) parameters. From the figures, we can see the following trends:

1. **C-Node2Vec**, a single-machine solution, cannot support very large graphs, such as com-Orkut. When the space required by the graph and the Node2Vec algorithm is too large to fit into the memory of a single machine, it is desirable to run distributed Node2Vec solutions.

2. **Spark-Node2Vec** is by far the slowest solution. Spark-Node2Vec tries to reduce memory space by restricting the number of edges per vertex to 30. As shown in Section 4.2, this trick drastically degrades the quality of the solution. However, even with this trick, Spark-Node2Vec still runs out of memory for com-Orkut on our 12-node cluster. Moreover, it suffers from the inefficiency of read-only RDDs and the I/O intensive shuffle operations.

3. **FN-Base achieves 7.7-22x speedups over Spark-Node2Vec for the cases that Spark-Node2Vec can support.** The improvements of FN-Base are twofold. First, FN-Base employs a Pregel-like graph computation platform that avoids the overhead of RDDs and disk I/Os in Spark. Second, FN-Base computes the transition probabilities on the fly, thereby significantly reducing the memory required to store the transition probabilities. Suppose each probability requires 8-byte space. Then, the total amount of memory saved for storing the transition probabilities is 3.0GB, 68.6GB, 731.9GB for BlogCatalog, com-LiveJournal, and com-Orkut, respectively.

4. **FN-Local’s execution time is quite similar to that of FN-Base.** While FN-Local reduces the NEIG messages between vertices in the same graph partition, we find that the direct memory visits at a vertex \(u\) to retrieve the edge information of another vertex \(v\) may incur expensive CPU cache misses, which is especially the case when \(v\)’s degree is small. As a result, the overall benefit is not as large as we expected.

5. **FN-Cache and FN-Approx achieve 1.5–1.9x and 1.8–5.6x speedups over FN-Base, respectively.** FN-Cache employs...
caching for the edge information of popular vertices. In this way, it significantly reduces the cost of NEIG messages. FN-Approx performs approximate computation (random sampling) on popular vertices when the estimation errors are low. This further reduces the computation overhead. Overall, compared to Spark-Node2Vec, FN-Cache and FN-Approx achieve 11.9–40.8x and 13.8–122x speedups, respectively.

(6) **FN-Switch has the longest run time among the Fast-Node2Vec solutions.** The switch of an NEIG message requires an additional message to be sent, thereby increasing the total number of supersteps in the graph computation. This effect significantly offsets the potential benefit of switching the NEIG messages, resulting in poor efficiency.

From Figure [6] and Figure [7], we can conclude that Spark-Node2Vec has both poor result quality and poor efficiency. Moreover, among the Fast-Node2Vec solutions, FN-Switch has poor efficiency and FN-Local achieves similar execution time as FN-Base. Therefore, we will not consider Spark-Node2Vec, FN-Local, and FN-Switch any more in the rest of the evaluation.

**The com-Friendster Graph.** Figure [8] compares the execution time of FN-Base, FN-Cache, and FN-Approx for the com-Friendster Graph. com-Friendster is the largest real-world graph with 1.8 billion edges. The total amount of space required to store all the transition probabilities is 11.6TB, much larger than the total memory size (∼1.5TB) of our 12-node cluster. Therefore, the pre-computation approach is not possible. Computing the transition probabilities on the fly is a must for larger graphs. Taking this approach, FN-Base computes the full Node2Vec random walks in about 3.3 hours. This shows that FN-Base is capable of processing large-scale real-world graphs in a reasonable amount of time using a mid-sized cluster of machines.

However, FN-Base has already consumed the majority of memory for com-Friendster. Hence, FN-Cache has only limited amount of memory available for caching edge information for popular vertices, which does not show significant benefit.

### 4.4 Scalability on ER-K Graphs

Figure [9] shows the scalability of FN-Base and C-Node2Vec on the ER-K graphs varying the number of vertices from $2^{20}$ (about 1 million) to $2^{30}$ (about 1 billion). The two figures show the results for two sets of Node2Vec $(p, q)$ parameters.

Both the X-axis and the Y-axis are in the log-scale. From Figure [9], we see that as the graph size increases, C-Node2Vec scales linearly. However, it runs out of memory for ER-K graphs, where $K \geq 26$. In comparison, our Fast-Node2Vec solution scales linearly while the number of vertices increases from 1 million to 1 billion. FN-Base computes Node2Vec random walks on the largest ER-K graph, i.e. ER-30, in about 2.3 hours. This is quite reasonable on
Note that in an ER-K graph, the average degree is 10, and the degree distribution is uniform. Therefore, the optimization techniques for popular vertices (including FN-Cache and FN-Approx) are not necessary.

Figure 12 shows the vertex degree distribution of the Skew-K graphs. We see that the vertex degree distribution of Skew-1 is essentially a gaussian distribution centered at 100. This is because the edges in Skew-1 are uniformly randomly generated. When $S > 1$, the vertex degree distribution of Skew-S can be seen as a combination of the gaussian distribution centered at $100S$.

### 4.5 Efficiency and Scalability on WeC-K Graphs

In this subsection, we study the efficiency and scalability of Fast-NodeVec solutions on the WeC-K graphs. Unlike the ER-K graphs, the degree distribution in the WeC-K graphs is not uniform. As shown in Table 1, the maximum vertex degree is much (about 10–27 times) larger than the average vertex degree. Therefore, we expect the optimization techniques of FN-Cache and FN-Approx to be beneficial.

Figure 10 shows the execution times of FN-Base, FN-Cache, and FN-Approx for WeC-K graphs and for two sets of Node2Vec $(p, q)$ parameters. We see that FN-Cache achieves a factor of $1.03$–$1.13$ improvements over FN-Base, and FN-Approx achieves a factor of $1.21$–$1.54$ improvements over FN-Base. This confirms our expectation. In the next subsection, we will further study the relationship between the skewness of the graphs and the impact of FN-Cache and FN-Approx on execution time improvements.

Figure 11 shows the scalability of FN-Base on WeC-K graphs. We see that FN-Base scales linearly while the number of vertices increases from $2^{20}$ to $2^{26}$.

### 4.6 In-Depth Analysis Using Skew-K Graphs

Finally, we use the Skew-K graphs to analyze the relationship between graph characteristics and the benefits of our proposed optimization techniques.

Figure 13 shows the vertex degree distribution of the Skew-K graphs. We see that the vertex degree distribution of Skew-1 is essentially a gaussian distribution centered at 100. This is because the edges in Skew-1 are uniformly randomly generated. When $S > 1$, the vertex degree distribution of Skew-S can be seen as a combination of the gaussian distribution.
Figure 14: Memory space consumption of FN-Base for Skew-K graphs, where $K = 2, \ldots, 5$.

As $S$ increases, the benefits of FN-Cache and FN-Approx over FN-Base become larger. As $S$ grows from 1.78 to 5, the speedup of FN-Cache over FN-Base grows from 1.04x to 2.68x when $p = 0.5, q = 2$, and from 1.09x to 2.66x when $p = 2, q = 0.5$. The speedup of FN-Approx over FN-Base grows from 1.45x to 17.2x when $p = 0.5, q = 2$, and from 1.41x to 17.1x when $p = 2, q = 0.5$.

To better understand the results, we study the memory space consumption of FN-Base for processing the Skew-K graphs, as shown in Figure 14. We see that as $S$ increases, the memory space consumed by messages constitutes an increasingly larger portion of the total space used.

Combining the results in Figure 12, Figure 13 and Figure 14 we see that as $S$ increases, the vertex degree distribution is more and more skewed. A greater many vertices have large numbers of neighbors. Vertices with larger degrees also tend to be sampled more frequently in the random walks. This leads to larger memory space allocated for processing NEIG messages. Consequently, optimizations for popular vertices, including FN-Cache and FN-Approx, become more effective when $S$ is larger.

5. CONCLUSION

Node2Vec is a state-of-the-art feature learning method that generates high-quality vector representations for the purpose of employing classical machine learning methods in graph analysis. However, we find that existing Node2Vec implementations have significant difficulties in supporting large-scale graphs. The C++ and Python reference implementations of Node2Vec are limited by the resource of a single machine. An existing Node2Vec solution on the Spark big data platform has poor result quality and incurs large run-time overhead. In this paper, we aim to efficiently support Node2Vec on graphs with billions of vertices using a mid-sized cluster of machines.

We propose and evaluate Fast-Node2Vec, a family of efficient Node2Vec random walk algorithms. Fast-Node2Vec employs GraphLite, a Pregel-like graph computation framework, in order to avoid the overhead of read-only RDDs and I/O-intensive shuffle operations in Spark. It computes the transition probabilities of Node2Vec random walks on demand, thereby reducing the memory space required for storing all the transition probabilities, which is often much larger than the total memory size in the mid-sized cluster for large-scale graphs as shown in our evaluation. Moreover, we also propose and evaluate a set of techniques (e.g., FN-Cache and FN-Approx) to improve the efficiency of handling large-degree vertices. Experimental results show that Compared to Spark-Node2Vec, fast-Node2Vec solutions achieve 7.7–122x speedups speedups. Compared to the baseline Fast-Node2Vec, FN-Cache and FN-Approx achieve up to 2.66x and 17.2x speedups.

In conclusion, our proposed Fast-Node2Vec solutions can successfully support Node2Vec computation on graphs with billions of vertices on a 12-node machine cluster. This means that researchers with moderate computing resources can exploit Node2Vec for employing classical machine learning algorithms on large-scale graphs.

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