Limited Random Walk Algorithm for Big Graph Data Clustering

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Abstract—Graph clustering is an important technique to understand the relationships between the vertices in a big graph. In this paper, we propose a novel random-walk-based graph clustering method. The proposed method restricts the reach of the walking agent using an inflation function and a normalization function. We analyze the behavior of the limited random walk procedure and propose a novel algorithm for both global and local graph clustering problems. Previous random-walk-based algorithms depend on the chosen fitness function to find the clusters around a seed vertex. The proposed algorithm tackles the problem in an entirely different manner. We use the limited random walk procedure to find attracting vertices in a graph and use them as features to cluster the vertices. According to the experimental results on the simulated graph data and the real-world big graph data, the proposed method is superior to the state-of-the-art methods in solving graph clustering problems. Since the proposed method uses the embarrassingly parallel paradigm, it can be efficiently implemented and embedded in any parallel computing environment such as a MapReduce framework. Given enough computing resources, we are capable of clustering graphs with millions of vertices and hundreds millions of edges in a reasonable time.

Index Terms—Graph Clustering, Random Walk, Big Data, Community Finding, Parallel Computing

1 INTRODUCTION

Graph data are important data types in many scientific areas, such as social network analysis, bioinformatics, and computer and information network analysis. Big graphs are normally heterogeneous. They have such non-uniform structures that edges between vertices in a group are much denser than edges connecting vertices in different groups. Graph clustering (also named as “community detection” in the literature) algorithms aim to reveal the heterogeneity and find the underlying relations between vertices. This technique is critical for understanding the properties, predicting dynamic behavior and improving visualization of big graph data.

Graph clustering is a computationally challenging and difficult task, especially for big graph data. Many algorithms have been proposed over the last decades [1]. The criteria-based approaches try to optimize clustering fitness functions using different optimization techniques. Newman defined a modularity measurement based on the probability of the link between any two vertices. He applied a greedy search method to minimize this modularity fitness function in order to partition a graph into clusters [2]. Blondel and Clauset used the same fitness function but combined it with other optimization techniques [3], [4], [5]. Spielman and Teng opted the graph conductance measurement as the fitness function [6]. Other than criteria-based methods, spectral analysis has also been widely adapted in this area [7], [8]. Random-walk-based methods tackle the problem from a different angle [9], [10]. These methods use the Markov chain model to analyze the graph. Each vertex represents a state and the links indicate transitions between the states. The probability values that are distributed among the states (vertices) reveal the graph structure.

In recent years, the size of graph data has grown dramatically. Furthermore, most graphs are highly dynamic. It is very challenging or even intractable to partition the whole graph in real-time. Very often, people are only interested in finding the cluster that contains a seed vertex. This problem is called local clustering problem [6], [11], [12]. For example, from an end user’s perspective, finding the closely connected friends around him or her is more important than revealing the global user clusters of a large social network. It is unnecessary to explore the whole graph structure for this problem. Recently, random walk methods have gained great attention on this local graph clustering problem, since a walk started from the seed vertex is more likely to stay in the cluster where the seed vertex belongs. Comparing to the criteria-based methods, the random-walk-based methods are capable of extracting local information from a big graph without the knowledge of the whole graph data. In [13], [14], [15], a random walk is first applied to find important vertices around the seed vertex. Then a sweep stage is involved to select the vertices that minimize the conductance of the candidate clusters.

The accuracy of any criteria-based clustering method (or those combined with the random walk procedures) is greatly affected by the chosen clustering fitness function. Furthermore, most local clustering algorithms use the criteria that are more suitable for the global graph clustering.
problem. These choices greatly degrade the performance of these algorithms when the graph is big and highly uneven. Also the majority of the graph clustering algorithms are designed in sequential computing paradigm. Therefore, they do not take advantage of modern high-performance computing systems.

In this paper, we propose a novel random-walk-based graph clustering algorithm—the Limited Random Walk (LRW) algorithm. First of all, the LRW algorithm does not rely on any clustering fitness function. Furthermore, the proposed method can efficiently tackle the computational complexity using a parallel programming paradigm. Finally, as a unique property among many graph clustering methods, the LRW can be adapted to both global and local graph clustering in an efficient way.

The rest of the paper is organized as follows: basics of the graph structure and the random walk procedure are explained in Section 2; the LRW procedure is explained and analyzed in Section 3; the proposed LRW algorithm for the global and local graph clustering problems are introduced in Section 4; an extensive set of experiments on the simulated and real graph data, along with both numerical and visual evaluations are given in Section 5; finally, the conclusions and future work are in Section 6.

2 Basic Definitions and the Random Walk Procedure

Let \( G(V, E) \) denote a graph of \( n \) vertices and \( m \) edges, where \( V = \{v_i|i = 1, \ldots, n\} \) is the set of vertices and \( E = \{e_i|i = 1, \ldots, m\} \) is the set of edges. Let \( A \in \mathbb{R}^{n \times n} \) be the adjacency matrix of the graph \( G \) and \( A_{ij} \) are the elements in the matrix \( A \). Let \( D \in \mathbb{R}^{n \times n} \) be the degree matrix, which is a diagonal matrix whose elements on the diagonal are the degrees of each vertex. In this paper, we assume the graph is undirected, unweighted and does not contain self-loops.

Clustering phenomenon is very common in big graph data. A cluster in a graph is a vertex set where the density of the edges inside the cluster is much higher than the density of edges that link the inside vertices and the outside vertices.

Random walk on a graph is a simple stochastic procedure. At the initial state, we let an agent stay on a chosen vertex (seed vertex). At each step, the agent randomly picks a neighboring vertex and moves to it. We repeat this movement and study the probability that the agent lands on each vertex.

Let \( x^{(t)} \) denote the probability that the agent is on vertex \( v_i \) after step \( t \), where \( i = 1, 2, \ldots, n \). \( x^{(0)}(i) \) is the probability of the initial state. Let \( s \) be the seed vertex. We have \( x^{(0)}(s) = 1 \), and \( x^{(0)}(i) = 0 \) for \( i \neq s \). Let \( x^{(t)} = [x^{(t)}(1), x^{(t)}(2), \ldots, x^{(t)}(n)]^T \) be the probability vector, where the superscript \( T \) denotes the transpose of a matrix or a vector. By the definition of the probability, it is easy to see that \( \sum_{i=1}^{n} x^{(t)}(i) = 1 \) or \( \|x^{(t)}\|_1 = 1 \).

The random walk procedure is equivalent to a discrete-time stationary Markov chain process. Each vertex is corresponding to a state in the Markov chain and each edge indicates a possible transition between the two states. The Markov transition matrix \( P \) can be obtained by normalizing the adjacency matrix to have each column sum up to 1, e.g.

\[
P_{ij} = \frac{A_{ij}}{\sum_{k=1}^{n} A_{kj}}
\]

or

\[
P = AD^{-1}
\]

Other forms of the transition matrix \( P \) can also be used, for example the lazy random walk transition matrix in which \( P = \frac{1}{2}(I + AD^{-1}) \). Given the transition matrix \( P \), we can calculate \( x^{(t+1)} \) from \( x^{(t)} \) using the equation:

\[
x^{(t+1)} = Px^{(t)}.
\]

A closed walk is a walk on a graph where the ending vertex is same as the seed vertex. The period of a vertex is defined as the greatest common divisor of the lengths of all closed walks that start from this vertex. We say a graph is aperiodic if all of its vertices have periods of 1.

For an undirected, connected and aperiodic graph, there exists an equilibrium state \( \pi \), such that \( \pi = P\pi \). This state is unique and irrelevant to the starting point. By iterating Eq. \( 3 \), \( x^{(t)} \) converges to \( \pi \). More details about the Markov chain process and the equilibrium state can be found from [16].

3 Limited Random Walk Procedure

3.1 Definitions

We first define the transition matrix \( P \). We assign the same probability to the transition that the walking agent stays in the current vertex and the transition that it moves to any neighboring vertex. We add an identity matrix to the adjacency matrix and then normalize the result to have each column sum to 1. The transition matrix can be written as

\[
P = (I + A)(I + D)^{-1}.
\]

Comparing to the transition matrix in Eq. \( 2 \), this is similar to adding self-loops to the graph. But we increase the degree of each vertex by 1 instead of 2. This modification fixes the periodicity problem that the graph may have. It greatly improves the algorithm’s stability and accuracy in graph clustering.

At each walking step the probability vector \( x^{(t)} \) is computed using Eq. \( 3 \). Note that, in general, elements in \( x^{(t)} \) that are around the seed vertex are non-zeros and the rest are zeros. So we do not need the full transition matrix to calculate the probability vector for the next step.

Starting from the seed vertex, a normal random walk procedure will eventually explore the whole graph. To reveal a local graph structure, different techniques can be used to limit the scope of the walks. In [10] and [13], the random walk function is defined as

\[
x^{(t+1)} = \alpha x^{(0)} + (1 - \alpha) Px^{(t)},
\]

where \( \alpha \) is called the teleport probability. The idea is that there is a certain probability that the walking agent will teleport back to the seed vertex and continue walking.

Inspired by the Markov Clustering Algorithm (MCL) algorithm [2], we adapt the inflation and normalization operation after each step of the transition. The inflation operation is an element-wise super-linear function—a function
that grows faster than a linear function. Here we use the power function

\[ f(x) = [x_1^r, x_2^r, \ldots, x_n^r]^T, \]

where the exponent \( r > 1 \).

Since \( x \) indicates the probability that the agent hits each vertex, \( x \) must be normalized to have a sum of 1 after the inflation operation. The normalization function is defined as

\[ g(x) = \frac{x}{||x||_1}, \]

where \( ||x||_1 = \sum_{i=1}^{n} |x_i| \) is the \( L_1 \) norm of the vector \( x \). Since \( x_i \geq 0 \) and \( \sum_{i=1}^{n} x_i = 1 \), Eq. (7) can also be written in a vector form as

\[ g(x) = \frac{x}{x^T \cdot 1}. \]

where \( 1 = [1, 1, \ldots, 1]^T \). The inflation and normalization operation enhance large values and depress small values in the vector \( x \).

We call this procedure the Limited Random Walk (LRW) procedure. The procedure limits the agent to walk around the neighborhood of the seed vertex, especially if there is a clear graph cluster boundary.

The MCL algorithm simulates flow within a graph. It uses the inflation and normalization operation to enhance the flow within a cluster and reduce the flow between clusters. The MCL procedure is a time-inhomogeneous Markov Chain in which the transition matrix varies over time. The MCL algorithm starts the random walk from all vertices simultaneously—there are \( n \) agents walking on the graph at the same time. The walking can only continue after all agents have completed a walking step and the result probability matrix has been inflated and normalized. Unlike in the MCL algorithm, the LRW procedure is a time-homogeneous Markov Chain. We initiate random walk from a single seed vertex, and do the inflation on the probability values of this walking agent. This design has many advantages. First, it avoids unnecessary walks since the graph structure around the seed vertex may be exposed by a single walk. Second, the procedure is suitable for the local clustering problems because it does not require the whole graph data. Third, if multiple walks are required, each walk procedure can be executed independently. Thus the algorithm is fully parallelizable.

The LRW procedure involves a nonlinear operation, thus it is difficult to analyze its properties on a general graph model. Next we study the equilibrium of the LRW procedure. Later, we will use these properties to analyze the LRW procedure on general graphs.

### 3.2 Equilibrium of the LRW procedure

We first prove the existence of equilibrium of the LRW procedure. Let \( X \) be the set of values of the probability vector \( x \). We have

\[ X = \{(x_1, x_2, \ldots, x_n) | 0 \leq x_1, x_2, \ldots, x_n \leq 1 \text{ and } x_1 + x_2 + \cdots + x_n = 1 \}. \]

The LRW procedure defined by Eqs. (3)–(7) is a function that maps \( X \) to itself. Let \( \mathcal{L} : X \to X \), such that

\[ \mathcal{L}(x) = g(f(Px)). \]
The other ongoing process during the LRW procedure is the contracting process. During this process, the probability values of the visited vertices contract to some vertices. Since the graph is usually heterogeneous, some vertices (and groups of vertices) will receive higher probability values as the procedure continues. The inflation operation further enhances this contracting effect. The degrees of a vertex and its surrounding vertices determine whether the probability values concentrate to or diffuse from these vertices. Some vertices, normally the center of a star structure, receive larger probability values than others. We call these vertices feature vertices since they can be used to represent the structure of a graph.

Because the density of edge inside a cluster is higher than that of linking the nodes inside and outside the cluster, the probability that a walking agent visits nodes outside the cluster is small. Thus, the LRW procedure will find feature vertices that the seed vertex belongs to. We can use these vertices as features to cluster the vertices.

The larger the inflation exponent \( r \) is, the faster the algorithm converges to the feature vertices. The LRW procedure tries to find the feature vertices that are near the seed vertex. However, if \( r \) is too large, the probability values concentrate to the nearest feature vertex (or the seed vertex itself) before the graph is sufficiently explored. If \( r \) is too small, the probability values will concentrate to the feature vertices that may belong to other clusters. The performance of the LRW algorithm depends on choosing a proper inflation exponent \( r \). From this aspect, it is similar to the MCL algorithm. In practice, \( r \) is normally chosen between 1 and 2 and the value 2 was found to be suitable for most graphs.

### 4 Limited Random Walk for Graph Clustering Problems

#### 4.1 Global Graph Clustering Problems

In this section we use the proposed LRW procedure in global graph clustering problems. Our algorithm is divided into two phases—graph exploring phase and cluster merging phase. To improve the performance on big graph data, we also introduce a multi-stage strategy.

#### 4.1.1 Graph Exploring Phase

In the graph exploring phase, the LRW procedure is started from several seed vertices. At each iteration, the agent moves one step as defined in Eq. 6. Then the probability vector \( x \) is inflated by Eq. 6 and normalized by Eq. 7. The iteration stops when the probability vector \( x \) converges or the predefined maximum number of iterations is reached. Let \( x^{(s,i)} \) denote the final probability vector of a random walk that was started from the seed vertex \( v_i \). As described in the previous section, the LRW procedure explores the vertices that are close to the seed vertex. Thus, the vector \( x^{(s,i)} \) has non-zero elements only on these neighboring vertices.

Algorithm 1 illustrates the graph exploring from a seed vertex set \( Q \). Note that for small graph data, we can set the seed vertex set \( Q = V \) (i.e. the whole graph). In such case, the LRW procedure is executed on every vertex of the graph and the multi-stage strategy is not used.

**Algorithm 1** Limited random walk graph exploring from a vertex set

**given** adjacency matrix \( A \) of the graph \( G(V, E) \), the seed vertex set \( Q \), the exponent \( r \) of the inflation function \( 6 \), maximum number of iterations \( T_{max} \), a small value \( \epsilon \) to limit the number of visited vertices, and a small value \( \xi \) for the termination condition

**initialize** the transition matrix \( P \) by Eq. 8

**for each** vertex \( i \) in the vertex set \( Q \)

1) initialize \( x^{(0,i)} \) such that \( x_k^{(0,i)} = \begin{cases} 1 & k = i \\ 0 & \text{otherwise} \end{cases} \) and \( t = 1 \)
2) repeat if \( t < T_{max} \)
   a) \( x^{(t,i)} = P x^{(t-1,i)} \)
   b) if \( x_k^{(t,i)} < \epsilon \) set \( x_k^{(t,i)} \) to 0
   c) \( x_k^{(t,i)} = f(x_k^{(t,i)}) = \left(\frac{x_k^{(t,i)}}{\sum_{j} x_j^{(t,i)}}\right)^r \)
   d) \( x_k^{(t,i)} = \frac{x_k^{(t,i)}}{\|x^{(t,i)}\|_1} \)
   e) if \( \|x^{(t,i)} - x^{(t-1,i)}\|_2 < \xi \), exit the loop
3) output \( x^{(s,i)} \) as the feature vector \( x^{(s,i)} \) for vertex \( i \)

Note that the threshold \( \epsilon \) limit the number of nonzero elements in the probability vector \( x \). It is easy to prove that the number of nonzero elements in \( x^{(s,i)} \) is less than \( 1/\epsilon \). A larger \( \epsilon \) eliminates very small values in \( x^{(s,i)} \) and prevent unnecessary computing efforts. However, \( \epsilon \) does not impose a limit on the largest cluster we can find. Further, the choice of \( \epsilon \) has little impact on the final clustering results because either the LRW procedure finds the most dominant feature vertices in a cluster or the small clusters are merged in the cluster merging phase.

#### 4.1.2 Cluster Merging Phase

After the graph has been explored, we will find the clusters in the cluster merging phase. We treat each \( x^{(s,i)} \) as the feature vector for the vertex \( v_i \). Vertices belonging to the same cluster have feature vectors that are close to each other. Any unsupervised clustering algorithm, such as k-means or single linkage clustering method, can be applied to find the desired number of \( k \) clusters. Because of the computational complexity of these clustering algorithms, we design a fast merging algorithm that can efficiently cluster vertices according to their feature vectors.

Each element \( x_j^{(s,i)} \) in \( x^{(s,i)} \) is the probability value of the stationary state that the walking agent hits the vertex \( v_j \) when the seed vertex is \( v_i \). The feature vector \( x^{(s,i)} \) is determined by the graph structure of the cluster that the initial vertex \( v_i \) belongs to. Thus, vertices in the same cluster should have very similar feature vectors. We first find the vertex that has the largest value in the vector \( x^{(s,i)} \). Suppose \( m = \arg \max_j x_j^{(s,i)} \), we call \( v_m \) the attractor vertex of vertex \( v_i \). Grouping vertices by their attractor vertex can be done in a fast way (complexity of \( O(1) \)) using a dictionary data structure. After the grouping, each vertex is assigned to a cluster that is identified by the attractor vertex. However, it is possible that some vertices in one cluster do not belong
to the same attractor vertex. This may happen when the cluster is large and the edge density in the cluster is low. We then apply the following cluster merging algorithm to handle this overclustering problem.

The vertices that have large values, which determined by a threshold relative to \( x_m^{s,i} \), in \( x_m^{s,i} \) are called significant vertices for vertex \( v_i \). If two vertices have large enough overlaps of their significant vertices, they should be grouped into the same cluster. From this observation, we first collect significant vertices for the found clusters. Then we merge clusters if their significant vertices overlap more than a half. Details of determining the significant vertices and merging clusters are given in

Note that the attractor vertex and the significant vertices are always in the same cluster as the seed vertex. This is very useful when we use the multi-stage graph strategy.

Algorithm 2 shows the details of the merging phase of the LRW algorithm. Note that, for small graph data, we can do LRW procedure on every vertex of the graph. So the seed vertex set \( Q = V \) and the initial clustering dictionary \( D \) to be empty.

Algorithm 2 LRW cluster merging phase

| given feature vectors \( x_i^{s,i} \) of the seed vertex set \( Q \), where \( i \in Q \), threshold \( \tau \) such that \( 0 < \tau < 1 \), and initial clustering dictionary \( D \) |

| for each feature vector \( x_i^{s,i} \) where \( i \in Q \) |

| 1) find \( m = \arg \max_j (x_j^{s,i}) \) and add \( i \) to an empty vertex set \( S \) |

| 2) find all \( j \) such that \( x_j^{s,i} > \tau \cdot x_m^{s,i} \) and add them to an empty vertex set \( F \) |

| 3) if \( D \) does not contain the key \( m \) |

| a) add the pair \( \langle S, F \rangle \) as the value that associated with the key \( m \) to dictionary \( D \) |

| else |

| a) find the value \( \langle S_m, F_m \rangle \) that is associated with the key \( m \) |

| b) add \( i \) to set \( S_m \) and merge \( F \) to \( F_m \) by \( F_m = F_m \cup F \) |

| c) update the value \( \langle S_m, F_m \rangle \) of the key \( m \) in the dictionary \( D \). |

Algorithm 3 Global graph clustering algorithm using multi-stage strategy

| given adjacency matrix \( A \) of the graph \( G(V,E) \), the exponent \( r \) for the inflation function \( \eta \), threshold value \( \eta \), maximum number of iterations \( T_{max} \) and a small enough value \( \epsilon \) |

| initialize the transition matrix \( P \) by Eq. 4, vertex set \( B = V \) and clustering dictionary \( D = \emptyset \) |

| while \( B \) is not empty |

| 1) generate a vertex set \( Q \subset B \) by randomly select vertices from \( B \) |

| 2) do the graph exploring from the vertex set \( Q \) using algorithm 1 to get feature vectors \( x_i^{s,i} \) for \( i \in Q \) |

| 3) given \( x_i^{s,i} \) and \( D \), do the graph cluster merging using algorithm 2 to update the clustering dictionary \( D \) |

| 4) for each key \( m \) in \( D \), merge the feature vertex set \( F_m \) to the cluster vertex set \( S_m, S_m = S_m \cup F_m \) |

| 5) get clustered vertex set \( R = \bigcup_{m \in D} S_m \) |

| 6) let \( B = B \setminus R \) |

| for each key \( m \) in \( D \), output \( S_m \) as the clustering result |

4.2 Local Graph Clustering Problems

For the local graph clustering problems, the LRW procedure can efficiently find the cluster from a given seed vertex. To achieve this, we first perform graph exploring from the seed vertex in the same way as described in Section 4.1.1. Let \( x \) be the probability vector after the graph exploration. If a probability value in \( x \) is large enough, the corresponding vertex is assigned the local cluster without further computation. Similar to the global graph clustering algorithm, we use a relative threshold \( \eta \) that is related to the maximum value in \( x \). Vertices whose probability values are greater than \( \eta \cdot \max \left( x \right) \) are called significant vertices. The significant vertices are assigned to the local cluster directly. A small value of \( \eta \) will reduce the computational complexity, but may decrease the accuracy of the algorithm. Suitable values of \( \eta \) were experimentally found to be between 0.3 and 0.5.

The vertices with low probability values can either be outside of the cluster or inside the cluster but with relatively low significance. Unlike [6, 11, 12], which involve a sweep operation and a cluster fitness function, we do another round of graph exploring from these insignificant
vertices. After the second graph exploring is completed, we apply the cluster merging algorithm described in Section 4.1.2.

Algorithm 4 presents the LRW local clustering algorithm.

Algorithm 4 LRW local graph clustering algorithm

given graph \( G(V, E) \), seed vertex \( v \) and a threshold value \( \eta \), where \( 0 < \eta < 1 \)

1) do graph exploration starting from the seed vertex \( v \) as described in algorithm 1 and get the feature vector \( x^{(s,v)} \)
2) find vertices in \( x^{(s,v)} \) for which \( x^{(s,v)}_i > 0 \) and collect the vertices in to set \( S \)
3) find \( m = \arg \max_j \left( x_j^{(s,v)} \right) \)
4) split the set \( S \) into two sets \( S_1 \) and \( S_2 \) such that \( S_1 = \left\{ j | x_j^{(s,v)} \geq \eta x_m^{(s,v)} \right\} \) and \( S_2 = \left\{ j | x_j^{(s,v)} < \eta x_m^{(s,v)} \right\} \)
5) for each vertex in \( S_2 \) do graph exploration to get feature vectors \( x^{(s,j)} \), where \( i \in S_2 \)
6) do clustering merging according to the feature vectors of the vertex \( v \) and the vertices in \( S_2 \) as described in algorithm 2 and find the cluster \( S_3 \) that contains the seed vertex \( v \)
7) return \( S_1 \cup S_3 \)

4.3 Computational Complexity

We first analyze the computational complexity of the LRW algorithm for the global graph clustering problem. We assume the graph \( G(V, E) \) has clusters. Let \( \bar{n}_c \) be the average cluster size—the number of vertices in the cluster, and \( C \) is the number of clusters. We have \( \bar{n}_c \cdot C = n \). Note \( C \ll n \). The most time-consuming part of the algorithm is the graph exploring phase. For each vertex, every iteration involves a multiplication of the transition matrix \( P \) and the probability vector \( x \). The LRW procedure visits not only the vertices in the cluster but also a certain amount of vertices close to the cluster. Let \( \gamma \) be the coefficient that indicates how far the LRW procedure explores the graph before it converges. Notice the maximum number of nonzero elements in a probability vector is \( 1/\epsilon \). Let \( J \) denote the number of vertices that the LRW procedure visits in each iteration, thus \( J = \min (\gamma \bar{n}_c, \frac{1}{\epsilon}) \). Thus the transition step at each iteration has complexity of \( O(J \bar{n}_c) \). The inflation and normalization steps, which operate on the probability vector \( x \), have the complexity of \( O(J) \). Let \( K \) be the number of iterations for the LRW procedure to converge. So, the computational complexity for a complete LRW procedure on each vertex is \( O(KJ \bar{n}_c) \). For a global clustering problem when performing the LRW procedure on every vertex, the graph exploration phase has a complexity of \( O(KJ \bar{n}_c n) \). In the worst case, the algorithm has a complexity of \( O(n^3) \). This is an extremely rare case and it only happens when the graph is small; does not have a cluster structure; and the edge density is high. This worst case scenario is identical to the MCL algorithm [3]. Notice that the variables \( J \) and \( K \) have upper bounds and \( \bar{n}_c \) is determined by the graph structure, the algorithm has a complexity of \( O(n) \) for big graph data.

The computational complexity of the cluster merging phase involves merging clusters that were found using the attractor vertices. This merging requires \( \binom{C}{2} \) sets comparison operations, where \( C \) is the number of clusters found by the attractor vertices. The complexity of this phase is roughly \( O(C^2) \). This does not impose a significant impact to the overall complexity of the algorithm, since \( C \ll n \). The time spent in this phase is often negligible. Experiments show that the clusters found using the attractor vertices are close to the final results. For applications where speed is more important than accuracy, the cluster merging phase can be left out.

When the LRW algorithm is used in local graph clustering problem, the first graph exploration (started from the seed vertex) has a complexity of \( O(KJ \bar{n}_c) \). After the first graph exploration, there are \( LJ \) vertices to be further explored, where \( L \) is related to the threshold \( \eta \) and \( L < 1 \). The overall complexity of the LRW local clustering algorithm is thus \( O(LKJ^2 \bar{n}_c) \).

The LRW algorithm is a typical example of embarrassingly parallel paradigm. In the graph exploring phase, each random walk can be executed independently. Therefore it can be entirely implemented in a parallel computing environment such as a high-performance computing system. The time spent for graph exploring phase decreases roughly linearly with respect to the number of available computing resources. The two-phase design also fits the MapReduce programming model and can easily be adapted into any MapReduce framework [17].

5 EXPERIMENTS

The LRW algorithm uses the following parameters: inflation exponent \( r \), maximum number of iterations \( T_{max} \), small value \( \epsilon \), merging threshold \( \tau \) and local clustering threshold \( \eta \). In practice, except the inflation exponent \( r \), the values of the other parameters have little impact to the final results. The inflation power \( r \) should be chosen according to the density of the graph. A sparse graph should use a smaller value of \( r \), though \( r = 2 \) is suitable for most real world graphs. In our experiments, we chose \( r = 2 \) unless otherwise specified. The other parameters have been set as: \( T_{max} = 100, \epsilon = 10^{-5} \) and \( \tau = \eta = 0.3 \). We will show the impact of some parameters in Section 5.4.

5.1 Simulated Data for Global Graph Clustering Problem

We first show the performance of the LRW algorithm using simulated graph data. The simulated graph is generated using the Erdoes-Renyi model [18] with some modifications to generate clusters. Using the ground truth of the cluster structure, we can evaluate the performance of graph clustering algorithms. This kind of simulated data are widely used in the literature [2], [19], [20], [21].

The graphs are generated by the model \( G(n, p, c, q) \) where \( c \) is the number of clusters, \( n \) is the number of vertices, \( p \) is the probability of the link between two vertices, and \( q = d_{in}/d_{out} \) is the parameter that indicates the strength of the cluster structure, where \( d_{in} \) is the expected number of edges linking one vertex to other vertices inside the same cluster, and \( d_{out} \) is the expected number of edges linking a given vertex to other vertices in other clusters. Larger
$q$ indicates stronger cluster structure. When $q = 1$, each vertex has equal probability that it links to vertices that are inside and outside of the cluster—the graph has a very weak cluster structure. Let $d$ be the expected degree of a vertex. So, $d = d_{in} + d_{out} = p(n - 1)$. We use this model to generate graphs that consist of $c$ clusters and each cluster has the same number of vertices. For each pair of vertices, we link them with the probability $\frac{\text{deg}(c-1)}{n(n-1)c}$ if they belong to the same cluster, and the probability of $\frac{\text{deg}(n-c)}{n(n-1)c}$ if they belong to different clusters.

We use the normalized mutual information (NMI) to evaluate the clustering result against the ground truth [22, 23]. We first calculate the confusion matrix where each row is a cluster found by the clustering algorithm and each column is a cluster in the ground truth. The entries in the confusion matrix are the cardinality of the intersect set of the $i$-th row and the $j$-th column. Let $N_{ij}$ be the value of the $i$-th row and $j$-th column, $N_{i\cdot}$ the sum of the $i$-th row, $N_{j\cdot}$ the sum of the $j$-th column, $N$ the total number of vertices, $C_A$ the number of clusters that the clustering algorithm found (number of rows), and $C_G$ the number of clusters in the ground truth (number of columns). The NMI is calculated as follows:

$$NMI = \frac{-2 \sum_{i=1}^{C_A} \sum_{j=1}^{C_G} N_{ij} \log \left( \frac{N_{ij} N / N_{i\cdot} N_{j\cdot}}{N_{i\cdot} / N \cdot C_G} \right)}{\sum_{i=1}^{C_A} N_{i\cdot} \log \left( \frac{N_{i\cdot} / N}{N} \cdot C_G \right) + \sum_{j=1}^{C_G} N_{j\cdot} \log \left( \frac{N_{j\cdot} / N}{N} \cdot C_G \right)},$$

where $0 \leq NMI \leq 1$.

If the clustering algorithm returns the exact same cluster structure as the ground truth, $NMI = 1$. Notice, NMI is not a symmetric evaluation metric. If an algorithm assigns all vertices into one cluster ($C_A = 1$), then NMI value is 0. On the other hand if an algorithm assigns each vertex to its own cluster ($C_A = N$), then $NMI > 0$.

We generated graphs by choosing $n = 128$ and $d = 16$. The number of the generated clusters is 4 and each cluster contains 32 vertices. We varied the ratio $q$ and evaluated the performance of the LRW algorithm against Girvan-Newman (GN) [21], Louvain [3], Infomap [24] and MCL [2] algorithms. Two simulated graphs are shown in Fig. 1, where the clusters are colored differently and the graphs are visualized by force-directed algorithms.

Fig. 1. Simulated graphs. (a) $q = 4$, (b) $q = 1.22$

The comparative results are given in Table 1, where the number of clusters found by the algorithms are placed between parentheses.

| $q$ | GN | Louvain | Infomap | MCL | LRW |
|-----|----|---------|---------|-----|-----|
| 4.0 | 0.975 (4) | 1.0 (4) | 1 (4) | 1 (4) | 1.0 (4) |
| 3.0 | 1 (4) | 1.0 (4) | 1 (4) | 1 (4) | 1.0 (4) |
| 2.33 | 0.950 (4) | 1.0 (4) | 1 (4) | 0.860 (7) | 1.0 (4) |
| 1.86 | 0.900 (4) | 1.0 (4) | 1 (4) | 0.478 (95) | 1.0 (4) |
| 1.5 | 0.890 (4) | 1.0 (4) | 0 (1) | 0.453 (119) | 0.975 (4) |
| 1.22 | 0.593 (4) | 0.771 (5) | 0 (1) | 0.444 (128) | 0 (1) |
| 1 | 0.232 (4) | 0.304 (7) | 0 (1) | 0.444 (128) | 0 (1) |

From the results, Louvain the best performing algorithm and LRW algorithm comes as the second. It can be seen that the LRW algorithm can find the correct structure if the graph has a strong clustering structure. When the clustering of a graph into clusters even though the cluster structure is weak. We use real graph data to evaluate the performance of the LRW algorithm on heterogeneous graphs. Details of the experiments and the results are in Section 5.3.

### 5.2 Simulated Data for Local Graph Clustering Problems

In this section, we compare the LRW algorithm with other local clustering algorithms. The test graphs are generated using the protocol defined in [20]. To simulate the data that are close to real world graphs, the vertex degree and the cluster size are chosen to follow the power law. Each test graph contains 2048 nodes. The vertex degree has the minimum value of 16 and the maximum value of 128. The minimum and maximum cluster size are 16 and 128, respectively. Similar to the previous section, the inbound-outbound ratio $q$ defines the strength of the cluster structure.

The competing algorithms are criteria-based algorithms that optimize a fitness function using either the greedy search or the simulated annealing optimization method. Let $C$ be the cluster that contains the seed vertex. $\bar{C} = V \setminus C$ is the complement vertex set of $C$. Let function $a(\cdot)$ be the total degree of a vertex set, that is

$$a(S) = \sum_{i \in S, j \in V} A_{ij},$$

where $A_{ij}$ are the entries of the adjacency matrix. The cut of the cluster $\bar{C}$ is defined as

$$c(C) = \sum_{i \in C, j \in \bar{C}} A_{ij}.$$

The following are the definitions of the fitness functions. Cheeger constant (conductance):

$$f(C) = \frac{c(C)}{\min \left( a(C), a(\bar{C}) \right)}$$

| $q$ | GN | Louvain | Infomap | MCL | LRW |
|-----|----|---------|---------|-----|-----|
| 4.0 | 0.975 (4) | 1.0 (4) | 1 (4) | 1 (4) | 1.0 (4) |
| 3.0 | 1 (4) | 1.0 (4) | 1 (4) | 1 (4) | 1.0 (4) |
| 2.33 | 0.950 (4) | 1.0 (4) | 1 (4) | 0.860 (7) | 1.0 (4) |
| 1.86 | 0.900 (4) | 1.0 (4) | 1 (4) | 0.478 (95) | 1.0 (4) |
| 1.5 | 0.890 (4) | 1.0 (4) | 0 (1) | 0.453 (119) | 0.975 (4) |
| 1.22 | 0.593 (4) | 0.771 (5) | 0 (1) | 0.444 (128) | 0 (1) |
| 1 | 0.232 (4) | 0.304 (7) | 0 (1) | 0.444 (128) | 0 (1) |
Normalized cut:

\[ f(C) = \frac{c(C)}{a(C)} + \frac{c(C)}{a(C)} \]  

(15)

Inverse relative density:

\[ f(C) = \frac{|E| - a(C) + c(C)}{a(C) - c(C)} \]  

(16)

Different local clustering algorithms are used to find the cluster that contains the seed vertex. The Jaccard index is used to evaluate the performance of each algorithm. Let \( C \) be the set of vertices that an algorithm finds and \( T \) be the ground truth cluster that contains the seed vertex. The Jaccard index is defined as

\[ J = \frac{|C \cap T|}{|C \cup T|} \]  

(17)

We generated 10 test graphs for each inbound-outbound ratio \( q \). From each generated graph, we randomly picked 20 vertices as seeds. For each algorithm and each inbound-outbound ratio \( q \), we computed the Jaccard index for each seed and took the average of the 200 Jaccard indices. The results are shown in Table 2 where “Che” stands for the Cheeger constant (conductance) fitness function; “NCut” stands for the normalized cut fitness function; “IRD” stands for the inverse relative density; the ending letter “G” stands for the greedy search method; and the ending letter “S” stands for the simulated annealing method.

| \( q \) | CheG | CheS | NCutG | NCutS | IRDG | IRDS | LRW |
|-------|------|------|-------|-------|------|------|------|
| 4.0   | 0.753| 0.840| 0.752 | 0.820 | 0.753| 0.830| 0.945|
| 3.0   | 0.671| 0.812| 0.671 | 0.801 | 0.671| 0.798| 0.927|
| 2.33  | 0.668| 0.774| 0.668 | 0.758 | 0.668| 0.776| 0.880|
| 1.86  | 0.593| 0.650| 0.593 | 0.681 | 0.593| 0.684| 0.823|
| 1.5   | 0.492| 0.630| 0.493 | 0.629 | 0.492| 0.609| 0.660|
| 1.22  | 0.444| 0.544| 0.437 | 0.549 | 0.444| 0.529| 0.504|
| 1     | 0.298| 0.410| 0.296 | 0.452 | 0.298| 0.424| 0.295|

From the results, the LRW algorithm greatly outperforms other methods when the graph has a clear cluster structure.

5.3 Real World Data

In this section, we evaluate the performance of the LRW algorithm on some real world graph data.

5.3.1 Zachary’s Karate Club

We first do clustering analysis on the Zachary’s karate club graph data [25]. This graph is a social network of friendship in a karate club in 1970. Each vertex represents a club member and each edge represents the social interaction between the two members. During the study, the club split into two smaller ones due to the conflicts between the administrator and the coach. The graph data have been regularly used to evaluate the performance of the graph clustering algorithms [21], [24], [26]. The graph contains 34 vertices and 78 edges. We applied the LRW algorithm on this graph and the result shows two clusters that are naturally formed. Fig. 2 shows the clustering result, where clusters are illustrated using different colors.

As the figure shows, the LRW algorithm finds the two clusters of the Zachary’s karate club. Actually the two clusters perfectly match the ground truth—how the club was split in 1970.

Clustering results of GN, Louvain, Infomap and MCL algorithms are given in supplementary material.

5.3.2 Ego-Facebook Graph Data

The second data we used is the ego-Facebook graph data [27]. The social network website Facebook allows users to organize their friends into “circles” or “friends lists” (for example, friends who share common interests). This data was collected from volunteer Facebook users for researchers to develop automatic circle finding algorithms. Ego-network is the network of an end user’s friends. The ego-Facebook graph is a combination of ego-networks from 10 volunteer Facebook users. There are 4039 vertices and 88234 edges in the graph.

We applied the LRW, GN [21], Louvain [3], Infomap [24] and MCL [9] graph clustering algorithms to this data. To compare the results, we generated the ground truth clustering by combining the vertices in the “circles” of each volunteer user. So, the ground truth contains 10 clusters. If a vertex appears in the circles of more than one volunteer, we assign the vertex to all of these ground truth clusters. We evaluated the number of clusters and the NMI values of the results that each competing algorithm generates.

We also calculated the mean conductance (MC) value of the clustering results. The conductance value of a cluster is calculated using Eq. [14] We then take the mean of all the conductance values of the clusters that an algorithm finds. The smaller MC value shows better clustering results. Note that MC tends to favor smaller number of clusters in general. If the number of clusters are roughly same, MC values give good evaluation of the clustering results. It is also worth noting that MC value is capable of evaluating clustering algorithms without the ground truth. We shall use this metric in later experiments where the ground truth is not available.

The MC scores, NMI scores and the number of clusters found by each algorithm are reported in Table 3. A bold font indicates the best score among all competing algorithms.
The vertices are located using a force-directed algorithm and colored according to their associated clusters. These clustered graphs are given in the supplementary material for subjective evaluation.

The reactome and the infectious graphs have low density. We chose the inflation exponent \( r = 1.2 \) to prevent overclustering the data. For other graph data, the default value \( r = 2 \) is used.

### 5.4 The Sensitivity Analysis of the Parameters

The proposed LRW algorithm depends on a number of parameters to perform global and local graph clustering. In this section, we perform the sensitivity analysis on the parameters.

We use both simulated and real-world graphs in our experiments. Test graph G1, G2 and G3 are similar to those used in Section 5.1 except that we vary the density of each graph. The expected degree \( d \), which is a measure of the graph density, of graph G1, G2 and G3 are 12, 16 and 20 respectively and \( q \) is set to be 1.86 for all test graphs. Test graph G4 is generated in the same way as described in Section 5.2. The ego-Facebook graph data in Section 5.3.2 is used as an example of real-world graphs. We performed global graph clustering on these test graphs using the LRW algorithm with different parameters. NMI scores are used to evaluate the performance of the algorithm. The experiments using simulated graph data were repeated 10 times and the average NMI scores and the average number of clusters are reported.

As described in Section 3.3, the most important parameter of the LRW algorithm is the inflation exponent \( r \). We first set \( T_{\text{max}} = 100, \epsilon = 10^{-5}, \tau = 0.3 \) and vary the inflation exponent \( r \). Table 6 shows NMI scores and the number of clusters reported by the LRW algorithm with different values of \( r \).

The test results show that the performance the LRW algorithm is sensitive to the density of the test graphs. A large inflation exponent \( r \) may overcluster the data as the results on graph G1 and G2 shows. It can be easily noticed that the LRW algorithm is not sensitive to the choice of \( r \) for test graph G4 and the ego-Facebook graph. These graphs, and
almost all real-world graphs, are more heterogeneous than the simulated graphs G1, G2 and G3. The LRW algorithm performs better on this type of graph since the attractor vertices and significant vertices are more stable on these graphs.

The parameter $T_{\text{max}}$ sets a limit on the number of iterations for the LRW procedure to converge. According to our experiments, value 100 is large enough to ensure the convergence of almost all cases. For example, only 3 out of 88,234 LRW procedures do not converge within 100 iterations on the ego-Facebook graph. A few exceptional cases has no impact on the final clustering results. The parameter $\epsilon$ is used to remove small values in the probability vector thus decrease the computational complexity. It has no impact on the final clustering result as long as the value is small enough, for example $\epsilon < 10^{-4}$.

We also conducted the experiments by varying the threshold value $\tau$ from 0.1 to 0.5. The NMI scores and the number of clusters found by the LRW algorithm with different $\tau$ values are almost identical to those in Table 6. This indicates that the choice of $\tau$ has very little impact on the clustering performance.

According to these results, one only needs to choose a proper inflation exponent $r$ to use the LRW algorithms. Other parameters can be chosen freely from a wide range of reasonable values. $r = 2$ is suitable for most of graphs and is preferable because of the computational advantage.

### 5.5 Big graph data

In this section, we apply the LRW algorithm on real-world big graph data and show the computational advantage of its parallel implementation. The test graphs were received from the SNAP graph data collection [34], [35]. These graphs are from major social network services and E-commerce companies. We use the high quality communities that either created by users or the system as ground truth clusters. The details of the high quality communities are described in [35]. The Rand Index is used to evaluate the results of the proposed clustering algorithm. To generate positive samples, we randomly picked 1000 pairs of vertices, where the vertices in each pair come from the same cluster in the ground truth. Negative samples consist of 1000 pairs of vertices, where the vertices from each pair come from different clusters in the ground truth. The Rand Index is defined as

$$RI = \frac{TP + TN}{N},$$

where $TP$ is the number of true positive samples, $TN$ is the number of true negative samples, and $N$ is the total number of samples.

Table 7 shows the size of the test graphs, the time spent on the graph exploration phase, the number of CPU cores and the amount of memory used for graph exploration, the time spent on cluster merging phase, the number of clusters that the LRW algorithm finds and the Rand Index of the clustering results. In this experiment, multiple CPU cores were used for graph exploration and one CPU core was used for clustering merging. Note that the competing algorithms used in previous sections cannot complete this task due to the large size of the data.

Table 6 shows that the LRW algorithm is able to find clusters from large graph data with a reasonable computing time and memory resource. The Rand Index values indicate that the clusters returned by the LRW algorithm match well the ground truth. The time spent on the graph exploration phase is inversely proportional to the number of CPU cores. Computational time can be further reduced if more computing resources are available. The proposed algorithm can efficiently handle graphs with millions of nodes and hundreds of millions of edges. For even larger graphs that exceed the memory limit for each computing process, a mechanism that retrieves part of the graph from a central storage can be used. Since the LRW procedure is capable of exploring a limited number of vertices that are near a seed vertex, the algorithm can cluster much larger graphs if such a mechanism is implemented.

### 6 Conclusions

In this paper, we proposed a novel random-walk-based graph clustering algorithm, the so-called LRW. We studied the behavior of the LRW procedure and developed the LRW algorithms for both global and local graph clustering problems. The proposed algorithm is fundamentally different from previous random-walk-based algorithms. We use the LRW procedure to find attracting vertices and use them as features to cluster vertices in a graph. The performance of the LRW algorithm was evaluated using simulated graphs and real-world big graph data. According to the results, the proposed algorithm is superior to other well-known methods.

The LRW algorithm can be efficiently used in both global and local graph clustering problems. It finds clusters from a big graph data by only locally exploring the graph. This is important for extreme large data that may not even fit in a single computer memory. The algorithm contains two phases—the graph exploring phase and the cluster merging phase. The graph exploring phase is the most critical part and also the most time-consuming part of the algorithm. This phase can be implemented in embarrassingly parallel paradigm. The algorithm can easily be adapted to any MapReduce framework.
From our experiments, we also noticed the limitation of the LRW algorithm. First, when used as a global clustering algorithm, the computational complexity can be high, especially when the graph cluster structure is weak. This is due to the fact that the graph may be analyzed multiple times during the graph exploration phase, if we perform the LRW procedure from every vertex of the graph. However, using the multi-stage strategy can dramatically reduce the computation time. Second, if the cluster structure is obscured, the LRW algorithm may return the whole graph as one cluster—though this behavior is desired in many cases.

The experiments show that the performance of the proposed LRW graph clustering algorithm is not sensitive to any parameter except the inflation exponent r, especially when the graph is not heterogeneous. For future research, we will further improve the LRW algorithm so that it can optimally select the inflation function that best suits the problem at hand.

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### TABLE 7

Clustering Performance of Real-world Big Graph Data

|                      | com-Amazon | com-Youtube | com-LiveJournal | com-Orkut |
|----------------------|------------|-------------|-----------------|-----------|
| nodes                | 334,863    | 1,134,890   | 3,997,962       | 3,072,441 |
| edges                | 925,872    | 2,987,624   | 34,681,189      | 117,185,083 |
| CPU cores for graph exploration | 12         | 96          | 96              | 96        |
| memory per CPU core  | 4G         | 4G          | 8G              | 8G        |
| graph exploration (in hours) | 0.83      | 3.08        | 17.4            | 24.0      |
| cluster merging (in hours) | 0.20      | 1.34        | 9.44            | 2.53      |
| clusters             | 37,473     | 170,569     | 381,246         | 165,624   |
| Rand Index           | 0.908      | 0.755       | 0.951           | 0.751     |
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