`MLN-Subdue`: Substructure Discovery In Homogeneous Multilayer Networks

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Abstract: Substructure discovery is a well-researched problem for graphs (both simple and attributed) for knowledge discovery. Recently, multilayer networks (or MLNs) have been shown to be better suited for modeling complex datasets that have multiple entity and relationship types. However, the MLN representation brings new challenges in finding substructures due to the presence of layers, and substructure discovery methods for MLNs are currently not available.

This paper proposes a substructure discovery algorithm for homogeneous MLNs using the decoupling approach. In HoMLNs, each layer has same or a common subset of nodes but different intralayer connectivity. This algorithm has been implemented using the Map/Reduce framework to handle arbitrarily large layers and to improve the response time through distributed and parallel processing. In the decoupled approach, each layer is processed independently (without using any information from other layers) and in parallel and the substructures generated from each layer are *combined after each iteration* to generate substructures that *span layers*. The focus is on the correctness of the algorithm and resource utilization based on the number of layers. The proposed algorithm is validated through extensive experimental analysis on large real-world and synthetic graphs with diverse graph characteristics.

1 MOTIVATION

Mining has been traditionally performed on transactional data whether it is clustering, classification, or identifying frequent itemsets. For applications where there is an inherent relationship, graphs offer better representation for the modeling of data. As a result, mining techniques were extended to graph models. Graphs can also be used to model relationships among multiple object types and relationships in a variety of applications such as chemical compounds, virus propagation, electrical and road transportation networks, web analysis, etc. In particular, with graph models where each vertex corresponds to an entity and each edge corresponds to a relationship between two entities, the problem of finding frequent patterns becomes one of discovering subgraphs that occur frequently or compress the graph or forest better.

Substructure discovery (Cook and Holder, 1993) was developed as a main memory algorithm for graph models when data sizes were not very large. However, with the advent of social networks and the Internet, graph sizes have grown significantly, necessitating alternative approaches to substructure discovery.

Why Multilayer Networks (MLNs)? As graphs become larger (in terms of the number of nodes and edges) and complex (in terms of the number of entity types and relationships), modeling the data using a representation that preserves the structure and semantics of data becomes important. A model that is also amenable to efficient analysis is another issue to reckon with. From these perspectives, MLNs offer distinct advantages.

Simple graphs are unable to capture the complexity of data and its semantics although a large number of analysis algorithms exist for them. Attributed graphs can handle additional complexity with multiple edges, but lack analysis algorithms. MLNs, as a network of networks, offer separation of semantics (as individual layers) and flexibility of analysis (when decoupling approach (Santra et al., 2017b; Santra et al., 2017a) is used) using desired subsets of layers. In addition, extant simple graph analysis algorithms can be leveraged in the decoupling approach.

If MLNs are used for modeling, each layer in the MLN represents a different relationship, either be-

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tween the *same* type of entities within a layer (intralayer edges), or across layers between *different* types of entities (interlayer edges). The advantages of modeling data using MLNs are discussed in (Boccaletti et al., 2014; Santra et al., 2017b; Kivelä et al., 2013). However, with the use of MLNs, the challenge is to extend graph analysis algorithms, be it community, centrality, or substructure detection, to the new representation.

Depending on the types of entities, multiple layers can be defined for the same (or a subset of) entity type or different entity types. MLNs can be of three different types: Homogeneous, Heterogeneous, and Hybrid. Homogeneous Multilayer Networks (HoMLNs) are used to model multiple distinct relationships existing between the *same type of entities*. Each set of *intralayer* edges represent one particular type of relationship, and the *interlayer* edge sets are implicit, as the same set of nodes are present in every layer. For example, the same set of actors can be connected based on co-acting, similar average rating, and similar movie genres they work in forming three different layers as shown in Figure 1 (a). Relationships among different types of entities are modeled through Heterogeneous Multilayer Networks (or HeMLNs), as shown in Figure 1 (b). The *interlayer* edges here are explicitly represented to demonstrate the relationship across layers. For example, there can be edges between the author layer and paper layer, if an author has written that paper. Finally, for data that includes multiple relationships within and across different types of entity sets, a combination of homogeneous and heterogeneous multilayer networks can be used, called Hybrid Multilayer Networks (or HyMLNs), as shown in Figure 1 (c).

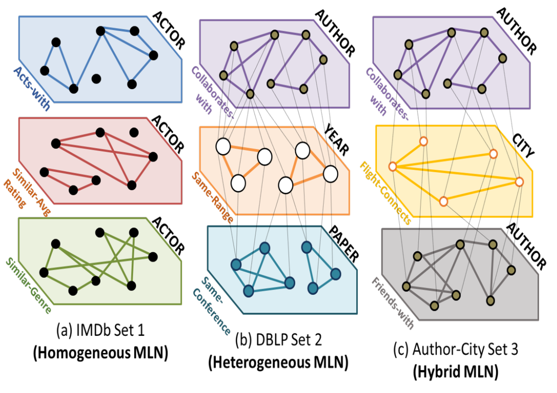


Figure 1: Examples of MLN Types.

Why Map/Reduce? We have used the Map/Reduce paradigm as an example of the distributed and parallel processing approach. Without loss of generality, any other paradigm (e.g., Spark) can be used in its stead without modifying the overall approach.

Problem Statement: The problem addressed in this paper is finding interesting and frequent substructures in a given Homogeneous Multilayer Network (HoMLN) using the decoupling approach proposed in (Santra et al., 2017a; Santra et al., 2017b; Santra et al., 2022) to leverage its advantages. This amounts to not converting the MLN into a single graph, but still getting the same result as if the MLN was processed as a single graph.

The main challenge here is to use the substructures generated for each layer **independently** and in parallel to compose them to compute the *missing* substructures that span multiple layers correctly and efficiently. To the best of our knowledge, there are no MLN substructure discovery algorithms. However, the rationale for using the decoupling approach is that existing algorithms from the literature(Cook and Holder, 1993; Das and Chakravarthy, 2015) can be used effectively for **each layer**. When these algorithms are used to find substructures in each layer independently, many substructures that span layers will be missing as shown in Figure 2.

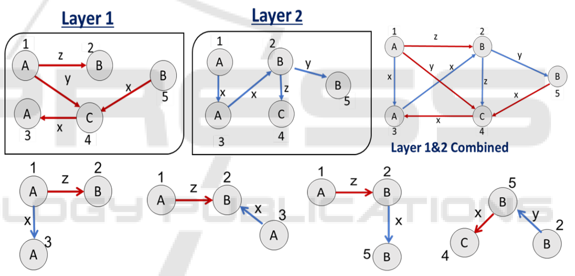


Figure 2: Substructures that span layers - only combined graph can generate them (color coded).

Approaches for MLN Substructure Discovery: MLNs can be processed for various types of analyses (community detection, substructure discovery etc.) Alternative approaches are listed below with a brief explanation.

1. Traditional Aggregation Approach: In this approach, layers of a MLN are conflated into a single graph. Boolean AND or OR aggregation can be used to reduce a HoMLN to a simple graph and find substructures correctly for a given multilayer network. The aggregation process can be costly (depending on the number of layers) and the resulting graph can be large (for OR composition). As a result, substructure discovery time can be significantly greater than that of a single layer. This approach also restricts parallelization as each layer cannot be processed in parallel. The loss in MLN structure, due to aggregation, also makes it difficult to drill-down results without maintaining extensive mapping. Finally, for processing a subset of layers, separate aggregation is required – making the approach less flexible and inefficient.

2. Decoupling-Based Approach: It is a "divide and conquer" approach for analyzing multilayer networks. The goal is to find substructures in each layer independently and then use a *separate* **composition function** to combine the results to generate what is missing for that analysis (e.g., community, centrality, substructure, motif, etc.) The decoupling-based approach used in this paper to address the substructure discovery problem is described along with a figure (Figure 5) in Section 4.

3. Holistic Approach: In this approach, neither the MLN is aggregated nor the decoupling approach is used. An algorithm is developed from scratch (as available graph analysis algorithms cannot be used as in the previous two approaches), keeping the structure and semantics intact. However, a new algorithm need to be developed for each analysis making this approach complex as the algorithm needs to traverse back and forth across layers. This approach has been used for coherent clusering in (Boden et al., 2012)

We use the decoupling-based approach in this paper as it is efficient and extant analysis algorithms (there are several of them depending on the analysis) can be used. The main challenge to be addressed is the development of the composition function and establishing its correctness (soundness and completeness.) Also, evaluating the efficiency of this approach as compared to the aggregation approach (used as GT or ground truth for validation.)

The contributions of this paper are:

- Adapting the **decoupling approach** for substructure discovery
- **Developing Map/Reduce approach** for substructure discovery
- **Composition algorithm** for HoMLN substructure discovery
- **Establishing the empirical correctness** of the composition algorithm
- **Extensive experimental analysis with diverse synthetic and real-world datasets**

This paper is organized as follows. Section 2 discusses related work. Section 3 discusses the preliminaries for substructure discovery using Map/Reduce. Section 4 details the adaptation of the decoupling approach for iteration-based substructure discovery. Section 5 discusses the composition algorithm and its correctness. Section 6 discusses the Map/Reduce approach for distributed and parallel computation on MLN. Section 7 provides experimental analysis. Conclusions are in Section 8.

2 RELATED WORK

SUBDUE (Cook and Holder, 1993; Ketkar et al., 2005) was developed as a main-memory substructure discovery algorithm. It performs a computationally constrained *beam* search where substructures of increasing size are generated iteratively and evaluated using the Minimum Description Length (or MDL) (Rao and Lu, 1992) metric. The algorithm begins with all substructures of size one (i.e., an edge), and in each iteration expands the instances by one neighboring edge in all possible ways. After each iteration, the top *beam* (parameter specified) substructures are carried over to the next iteration. Best substructures are output based on the size and other parameters specified.

Due to the limitations of the main-memory approach, the disk-based approach (Wang et al., 2005) stores the data on disks and stages chunks of data to memory as needed. The graph is indexed to speed up retrieval. However, this approach needs to marshal data between the disk and main memory buffer, and its performance can be very sensitive to buffer size, replacement policies, hit ratios, etc. To overcome the pitfalls of the disk-based approach, a database management system (or DBMS) was used to store the graph and SQL for substructure discovery(Padmanabhan and Chakravarthy, 2009). This takes advantage of the buffer management and optimization provided by the DBMS. Although scalability was achieved to graphs of over a million nodes and edges, use of self-joins on large relations for substructure expansion seems to have made it difficult to go beyond due to computation resulting in unacceptable response time. Also, it appears that the removal of duplicate substructures required sorting columns in row-based Relational DBMS, making it expensive in terms of the number of joins needed.

As the graph sizes grew further with the advent of social networks and the Internet, graphs had to be partitioned to deal with the increasing sizes. As a result scalable parallel computing algorithms had to be developed. Map/Reduce (Das and Chakravarthy, 2015; Das and Chakravarthy, 2018) and other architectures were used to address the problem of substructure discovery on a large graph by dividing the graph into smaller partitions and then combining the results across partitions. In addition to substructure discovery, partitioning of graphs has been explored in other research as well (Yang et al., 2012).

With multilayer networks being used for modeling large complex datasets, there is a need for substructure discovery algorithms on MLNs. A clustering algorithm (Boden et al., 2012) for finding clusters in a multilayer graph has been proposed using the holistic approach described earlier. Similarly, another algorithm (Liu and Wong, 2008) has been proposed to find quasi-cliques to find all one-dimensional clusters in a single layer, which are then used to find multi-dimensional clusters. The focus of this work is to find clusters of vertices that are densely connected by edges with similar edge labels in a subset of graph layers.

This paper differs from the above in that we are proposing a decoupling-based algorithm for substructure discovery that gives the same results as the ground truth. It is also efficient as compared with the algorithm used for GT. Further, it uses Map/Reduce to process each layer and for composition providing better scalability than extant approaches.

3 TERMINOLOGY USED

Graphs are input as text files and this section indicates input formats for `MLN-Subdue` as well as some terminology needed for understanding the paper.

Input Graph Representation: For substructure discovery, labeled graphs are used where vertex and edge labels are not assumed to be unique, but all vertex IDs are unique. The input graph is represented as an unordered list of 1-edge substructures where each edge is represented as a 5-element tuple <*edge label, source vertex id, source vertex label, destination vertex id, destination vertex label*>. The input graph is stored in an ASCII file with a 1-edge substructure in each line. If needed, graphs in other formats are converted to this format.

Adjacency List: Adjacency list of a vertex ID is the set of edges that are incident (both outgoing and incoming) on that vertex ID. The adjacency list is used to expand a substructure from each vertex ID in that substructure using an edge from the adjacency list. Each 1-edge expansion becomes a separate substructure. This allows an n-edge substructure to be expanded into a number of (n+1)-edge substructures in an iteration.

Substructure Expansion: Starting from 1-edge, substructures of increasing size are generated systematically in each iteration using the adjacency list. As the goal is to discover *interesting* substructures of any size, systematic graph expansion is critical to the process. Expansion is done on each substructure *independently* as indicated above. Expansion is unconstrained, i.e., each substructure independently grows into a number of larger substructures in each iteration. This *independent expansion* leads to the generation of duplicate substructures which must be removed to ensure correctness. A substructure is represented as a (lexicographically) ordered list of edges.

Canonical Instances for Duplicate Elimination: Lexicographic ordering of edges in a substructure is used to identify duplicates. Each edge in a substructure is ordered based on edge label, then source vertex label, then destination vertex label, and finally source and destination vertex IDs. If any of the values match, the comparison moves forward to the next component, else the ordering is performed. A substructure can be uniquely represented using the lexicographic order of 1-edge components. This is called a canonical k-edge instance. Intuitively, two duplicate k-edge substructures must have the same ordering of labels and vertex IDs when converted to canonical k-edge instance[1]. Figure 3 shows an example of duplicate substructures generated by two **different** substructure instances during independent expansion and how they are detected as duplicates using their canonical instances.

Canonical Substructures for Graph Isomorphism: Isomorphs in a graph have the same graph structure in terms of vertex and edge labels as well as connectivity, but differ in vertex IDs. In contrast, duplicates have the same vertex IDs. After duplicate elimination, we need to identify isomorphs to count their occurrences. We need to convert canonical instances of substructures to *canonical substructures* using relative ordering of vertex IDs. Intuitively, in the canonical form, two isomorphic substructures have the **same relative ordering** of vertex numbers. To identify isomorphs, the canonical instance is converted into a canonical substructure. This is done by replacing each vertex ID with their relative positions in the instance starting from 1. The inclusion of these relative positions is critical for differentiating the connectivity of the instances. Figure 4 shows an example of how canonical substructure is created from the canonical instance. It can be seen that the isomorphs have different canonical instances. Using the above technique, the relative positioning of vertex Ids (2, 5, 4) for the canonical instance 1 and (7, 10, 9) for the canonical instance 2 are converted to (1, 2, 3). Hence we can

[1]Substructures and substructures instances are used interchangeably when the meaning is clear from the context. However, substructure instances are converted into relative ordering of vertex IDs, termed canonical substructures, which are used for detecting substructure isomorphs.

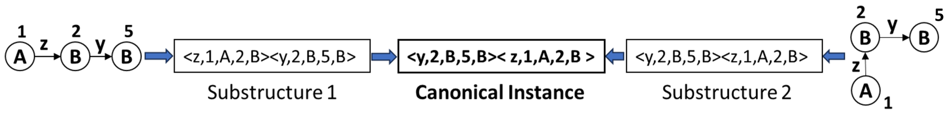


Figure 3: Duplicate substructure identification using canonical instances.

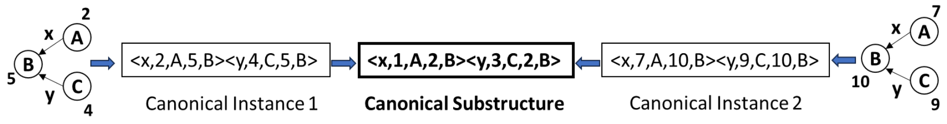


Figure 4: Graph isomorphism and canonical substructures.

identify isomorphs using canonical substructures.

Metrics for Ranking: Many metrics are used to rank substructures based on isomorphs. Frequency of isomorphic substructures is one such metric (higher the frequency, the better the substructure.) Another widely used information-theoretic metric is the Minimum Description Length (or MDL (Rao and Lu, 1992)). MDL calculates the importance of a substructure on how well it compresses the entire graph/forest. A substructure that compresses the graph better is considered an *interesting and repetitive* substructure. When MDL is used, an MRN (Most Restrictive Node)(Bringmann and Nijssen, 2008; Elseidy et al., 2014) metric is used to count non-overlapping instances. But overlapping instances have also been used to compute frequency and MDL for each substructure.

4 DECOUPLING APPROACH

Multilayer networks consist of multiple layers of simple graphs where each layer represents a relationship between entities in that graph. However, most algorithms convert a MLN (or a subset of it) into a simple graph using aggregation (Domenico et al., 2014) and/or projection techniques (Berenstein et al., 2016) to use extant algorithms. However, this leads to loss of structure, semantics, and information from the final analysis results (Kivelä et al., 2013; De Domenico et al., 2014). For the other end, existing single graph algorithms cannot be directly used for the holistic approach described earlier. In this paper, the decoupling-based approach has been used which preserves the structure and semantics of MLNs (Santra et al., 2017a; Pavel et al., 2023) while performing analysis on complex datasets without losing any information. It is also shown to be efficient (Santra et al., 2017a).

The network decoupling approach has been illustrated with respect to substructure discovery in HoMLNs (focus of the paper) in Figure 5, where each

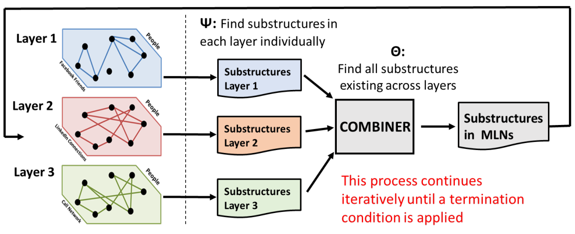


Figure 5: Substructure Discovery: Decoupling Approach.

layer has the same set of nodes but different edge connectivity. It consists of two functions: analysis (Ψ) and composition (Θ). Using the analysis function, each layer in the network is analyzed independently (and in parallel) to obtain the layer substructures. Then, the partial results from any two (or more) layers are combined and processed by the composition function to produce substructures that span participating layers. This is done for each iteration as substructure discovery is an iterative algorithm. This composition can be binary or n-ary. If binary, it can be repetitively applied to *n* layers using previously generated results. This approach allows parallel analysis of each layer to improve efficiency (Santra et al., 2017a). Further, due to the layer-wise analysis, each graph is likely to be small, which requires less memory for computing layer-wise results. Each layer is also analyzed **only once**, and the existing single graph algorithms can be used for that. The results obtained are then used by the composition function. In addition, this approach is application-independent.

In this approach, the major challenge is to develop the composition algorithm (Ψ) which is sound and complete in generating missing substructures that span layers. It is known from earlier work that substructure generation in each layer is sound and complete.

5 ALGORITHM DESIGN

Substructure discovery in single (simple and attributed) graphs is an iterative process, where inter-

Algorithm 1: **`MLN-Subdue`**: Substructure Discovery Algorithm for Homogeneous Multilayer Networks.

```
Require:
    Input: Substructures of size $k$ for $k^{th}$ iteration
    Output: Top beam substructures (intralayer & interlayer) of size $k+1$
 1: Load Adjacency list for each layer
 2: for each substructure of size $k$ in MLN:
 3:     Expand each k-edge substructure by one edge in all directions in each layer
 4:     Eliminate Duplicates using canonical representation in each layer
 5: end for
 6: for each expanded $k+1$ edge substructure:
 7:     Group all the expanded substructures from each layer based on vertex ID
 8:     Apply Combine-MLN recursive function to form $k+1$ edge interlayer substructures from k+1 edge intralayer substructures
 9:     Eliminate duplicates generated during combination
10: end for
11: for all the canonical instances in the MLN:
12:     Count the frequency of all substructures using isomorphism
13: end for
14: Apply metric Frequency or MDL
15: Apply beam heuristic to determine top-beam substructures and send their instances to be used the next iteration // Specify beam as required
16: Increment k by 1 for next iteration
17: Goto Step 1 for the next iteration
```

esting (k+1)-edge substructures are generated in the k^{th} iteration after a multi-step process – independent substructure instance expansion, conversion to canonical form, duplicate elimination, substructure counting & metric evaluation, ranking based on graph isomorphism, and finally, retaining top *beam* substructures to be used for the next iteration. For using the divide-and-conquer-based decoupling approach, the main task during the k^{th} iteration is to figure out how to systematically use the *beam k-edge* substructures and composed substructures (from the previous iteration) to generate next *beam* (k+1)-edge substructures correctly and completely. Thus, in case of MLNs, the challenge is to perform the substructure discovery (from expansion to substructure ranking) synergistically using what is generated in the layer-wise analysis phase and what is composed in the previous iteration.

Algorithm 1 presents the composition algorithm to discover interesting substructures in HoMLNs. The major steps are discussed below:

Expansion (Layer-wise): In the k^{th} iteration, all instances of the *beam k*-edge substructures, generated in the previous iteration, are used (for k = 1, all edges in the layer are used.) In each layer, using the adjacency list for that layer, each substructure instance is expanded *independently* by adding one incident edge (both in and out) to generate as many $(k+1)$-edge substructure instances using the adjacency list (**Lines 1 & 2** of Algorithm 1). However, this unconstrained expansion generates *local (layer-wise)* duplicates, which are identified using canonical ordering (as outlined in Section 3) and are eliminated (**Line 4**).

Composing Layer-wise Substructures: This step generates substructure instances similar to the expansion in layers, but uses a substructure from one layer and edges from a *different* layer which are termed *composed interlayer* substructures. To achieve this, first the expanded substructure instances generated from each layer are *grouped* based on a shared vertex ID (**Line 7**) as vertex IDs are the same in all layers of HoMLNs. This brings together the substructure instances from all layers that have a shared vertex ID. Then, a recursive call (***Combine-MLN***) is made (with two parameters: **set of layers**, and **size of the substructure**) to combine the intralayer substructures from different layers sharing a common vertex ID, to generate $(k+1)$-edge substructures that span multiple layers (**Line 8**). Here, the recursive call performs a systematic exploration of all combination possibilities to generate a $(k+1)$-edge substructure from m layers using the layer-wise substructures of size (k+1). This is applied on all vertices.

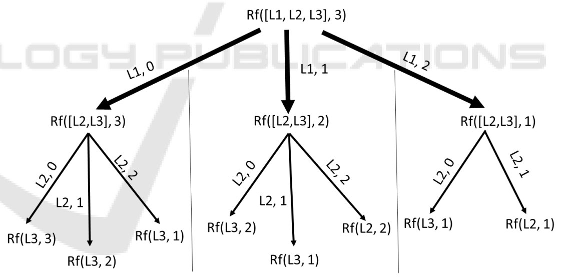


Figure 6: Combination possibilities of generating a 3-edge interlayer substructure.

Figure 6 shows an example of the combinatorial possibilities applied by the ***Combine-MLN*** recursive function, where the set of layers is [L1, L2, L3] and the substructure size is 3. For example, one possibility is to choose 2 edges from L1 and 1 edge from either L2 or L3 (the rightmost subtree) or 1 edge from L1, one edge from L2, and 1 edge from L3 (middle subtree.) Also, this composition stage ensures that only connected composed substructures are generated.

Figure 7 illustrates the working of ***Combine-MLN*** on a 2-layer MLN. For each layer we show all the 2-edge substructures. When we apply the ***Combine-MLN*** function on each Vertex id of the graph as shown above, we find all the substructures of size

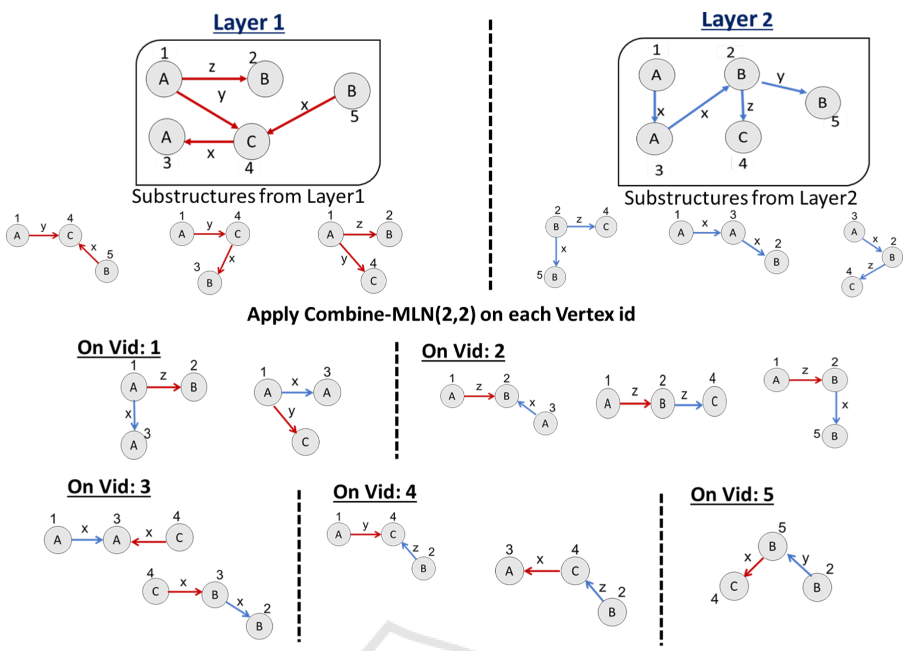

Layer 1
Layer 2
Substructures from Layer1
Substructures from Layer2
Apply Combine-MLN(2,2) on each Vertex id
On Vid: 1
On Vid: 2
On Vid: 3
On Vid: 4
On Vid: 5

Figure 7: Generating composed interlayer substructures by combining intralayer substructures on shared vertex id.

2, which exist across layers. The parameters of Combine-MLN function here is (2,2), which means there are 2 layers and the required size of the substructure is 2.

Duplicate Elimination: The previous step leads to the generation of duplicate instances (e.g., from figure 6, the center branch would be generated while expanding on each of the three layers, L1, L2, and L3.) As the composed substructures are cast into the canonical form, duplicates are identified and removed (**Line 9**).

Frequency Counting: Exact isomorphs are used to detect identical substructures, as two isomorphic substructures have the same relative ordering of the vertex IDs and have same vertex and edge labels. Canonical instances follow the lexicographic ordering, hence it is easy to generate *k*-edge canonical substructures using the relative ordering of unique vertex ID in the order of their appearance in the canonical instance. All the instances are grouped based on their canonical form and their frequency is counted (**Line 12**).

Application of Metric: To restrict the future expansion to high quality substructures, a metric – either MDL or frequency – is used to determine the importance of a particular substructure (**Line 14**). The *beam* parameter (user specified with a default) is used as a heuristic to ensure only the top *beam* substructures based on the metric score will be passed on to the next iteration, thereby restricting the expansion of less important substructures (**Line 15**).

Using the proposed algorithm, top substructures of size *k+1* that exist within and across layers in the k^{th} iteration are generated. Algorithm 1 is applied iteratively to find substructures of the desired size.

6 MAP/REDUCE IMPLEMENTATION

The different components of the proposed Algorithm 1 (layer-wise substructure expansion and duplicate elimination followed by composition, and duplicate elimination again in each iteration) have been implemented using an iterative two-chained Map/Reduce architecture. In the first Map/Reduce job, the mapper performs the expansion of substructures and duplicate elimination in each layer, and the reducer performs the composition to generate substructures that span layers and removes the duplicates from the composed substructures. In the second job, the mapper converts *all* substructure instances into canonical isomorphic instances to count frequency and emits isomorphs as key. The reducer applies the metric and outputs the top-*beam* substructures (intralayer and spanning layers) to be used as candidates for expansion in the next iteration. Figure 8 shows the overall workflow of substructure discovery in a HoMLN using the Map/Reduce framework.

Expansion by Mapper 1: Substructure instances

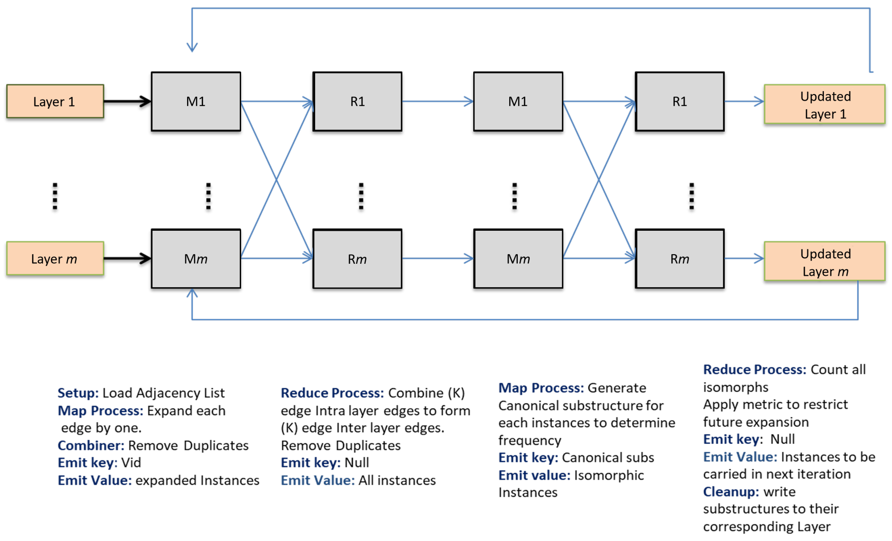

Layer 1
Layer *m*
M1
Mm
R1
Rm
M1
Mm
R1
Rm
Updated Layer 1
Updated Layer *m*
Setup: Load Adjacency List
Map Process: Expand each edge by one.
Combiner: Remove Duplicates
Emit key: Vid
Emit Value: expanded Instances
Reduce Process: Combine (K) edge Intra layer edges to form (K) edge Inter layer edges. Remove Duplicates
Emit key: Null
Emit Value: All instances
Map Process: Generate Canonical substructure for each instances to determine frequency
Emit key: Canonical subs
Emit value: Isomorphic Instances
Reduce Process: Count all isomorphs
Apply metric to restrict future expansion
Emit key: Null
Emit Value: Instances to be carried in next iteration
Cleanup: write substructures to their corresponding Layer

Figure 8: Map/Reduce workflow of **MLN-Subdue** (including composition).

Table 1: Dataset description.

Purpose	Dataset	#Nodes	#Edges
Correctness	Synthetic (SUBGEN)	10K	20K
Correctness	Synthetic (SUBGEN)	100K	800K
Scalability	LiveJournal	3.9M	34.8M
Scalability	Orkut	3.87M	114.8M
Varying Density	Synthetic (SUBGEN)	2K	1M, 1.9M, 2.9M, 3.9M

with their respective layer number are read as mapper input, one at a time. The adjacency list for the layer is loaded using the setup function. For the k^{th} iteration, the input is a k-edge canonical instance. Each instance is expanded by one edge at a time using the adjacency list. The mapper emits the vertex ID as key, and expanded instances as values. As the expansion process is unconstrained, duplicates are generated, which are removed using a combiner. In this version, since each layer is processed by a mapper (even as multiple map tasks based on the block size), all duplicates can be eliminated by the combiner.

Composition in Reducer 1: Each reducer receives a list of expanded substructure instances as values, grouped on the vertex ID as the key. The recursive function (Combine-MLN) is used to combine all $(k+1)$-edge substructures from the mapper outputs to generate $(k+1)$-edge spanning substructures using edges from multiple layers. All substructures, both intralayer and spanning layers, are then emitted to the next Map/Reduce job as input to generate canonical substructures to determine graph isomorphism. The key is null, and the value is the substructure instance.

Identifying Isomorphs in Mapper 2: Creating canonical substructures from instances requires a hash table to identify the relative positioning of each vertex. The mapper receives all the substructure instances as input, and canonical substructure is generated for every instance. The mapper emits the canonical substructure as the key and the corresponding substructure instance as the value.

Ranking and Emitting top-*beam* Instances in Reducer 2: The reducer receives substructure instances across mappers grouped on canonical substructure. The *beam* value is used to rank the best *beam* substructures in a hash map. This is done by calculating the MDL value for each canonical substructure, and storing the top *beam* substructures with the highest MDL values, emitting only their respective instances in order to restrict future expansion to high-ranking substructures in the next iteration. The reducer emits the $(k+1)$-edge substructure instances and layer IDs as the values in the k^{th} iteration, which are then fed into Mapper 1 of the next iteration as input.

7 EXPERIMENTAL ANALYSIS

Experimental Setup: All experiments have been performed using Java with Hadoop on Comet cluster at SDSC (San Diego Supercomputer Center). The

Comet cluster has 1944 nodes and each node has 24 cores (built on two 12-core Intel Xeon E5 2.5 GHz processors) with 128 GB memory, and 320GB SSD for local scratch space.

Dataset Description: Experiments were done on several real-world and synthetic datasets (as shown in Table 1) of varying sizes to establish the correctness, speedup, and scalability of the approach. Subgen[2], an artificial graph generator was used to generate synthetic graphs as it allows the embedding of substructures with user-defined frequency in a larger single graph. To generate HoMLN datasets from each base single graph, edges were randomly distributed across multiple layers among the same set of nodes.

Empirical Correctness: For a given HoMLN with multiple layers, the ground truth is generated by first aggregating the MLN into a single graph by taking the *union* of edges (Boolean OR) and then executing SUBDUE(Ketkar et al., 2005). Both the proposed algorithm and SUBDUE for different HoMLNs generated the same set of substructures with correct frequency, thus *establishing the correctness of the approach empirically*.

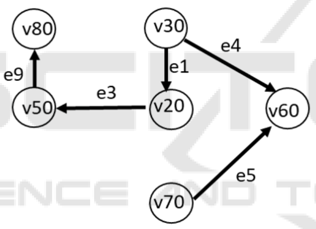


Figure 9: Example 5-edge Embedded Substructure.

However, SUBDUE being a main memory approach failed to execute on large graphs with more than 100K vertices & 800K edges. So, to verify the correctness on large graphs, synthetic graphs were generated having substructures embedded with a user-defined frequency, the goal being to *find the same substructures with the same frequency*. A 5-edge embedded substructure, shown in figure 9, was embedded with a frequency of 1000 in a graph of size 100K vertices & 800K edges. The exact substructure was found with the same frequency (of 1000) using the proposed algorithm, which empirically validates the correctness of the proposed algorithm for this dataset.

Several such experiments were conducted with different embedded graph sizes and frequencies.

Effect of Layer Generation Schemes: This set of experiments is performed using the synthetic dataset of size 400K vertices & 1.2 million edges with embedded substructures. Two partitioning schemes were used: random and edge-based, to verify the correctness of the algorithm and its effect on response time. Random scheme partitions a graph into l layers by distributing edges randomly. Nodes are same in all l layers. Edge-based partitioning, on the other hand, creates layers containing all edges having the same edge label. Multiple edge labels can be in a layer in edge-based partitioning.

[2]https://ailab.wsu.edu/subdue/

Table 2: Edge distribution for different layer generation schemes.

Layers	Random	Edge-Based
Layer 1	399903	351360
Layer 2	399730	478441
Layer 3	400637	370469

Table 2 shows the edge distributions for both partitioning schemes. Notice that the distribution remains even for random partitioning, but becomes skewed for edge-based as there can be edge labels with higher frequency going into a single layer, making it uneven. Figure 10 shows the total time taken by both of the partitioning schemes. There is no substantial difference in the total response time as it more or less remains the same. So, the numbers are drilled-down into and the Map and Reduce times are inspected to understand them clearly.

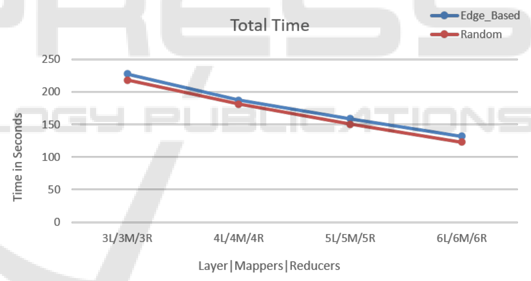


Figure 10: Total response time for partitioning schemes.

As seen in Figure 11, the total map time for edge-based partitioning is significantly higher as compared to the total map time for random partitioning. The reason being, as the edge distribution is skewed, some mappers end up processing more data for edge-based partitioning, contributing to more computation time. On the other hand, total time taken by the reducers does not change as the data processed by each reducer remains the same, because all the substructures in the reducer are grouped based on their vertex IDs and edge labels have no effect on them.

The same embedded substructures were found for both partitioning schemes, indicating that the algorithm is not affected by the connectivity of the graph.

Scalability of Approach: Without altering the graph size, an increase in the number of processors is typi-

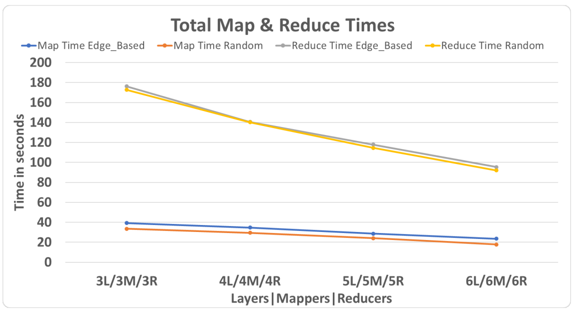


Figure 11: Map & Reduce times using multiple partitioning schemes.

cally beneficial for mining. So, this set of experiments was performed on LiveJournal (Leskovec and Krevl, 2014a) and Orkut (Leskovec and Krevl, 2014b) data to determine the speedup and effectiveness of the algorithm as the number of processors was increased. This has been showcased using 3 scenarios:

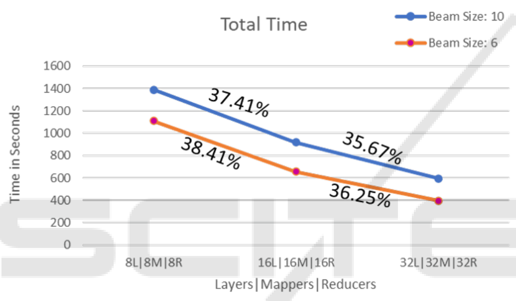


Figure 12: Speedup achieved on LiveJournal data.

Scenario 1: **Same number of mapper and reducer nodes as layers:** For this scenario, all the layers are processed in parallel with the same number of mapper and reducer nodes. Results in Figure 12 show a speedup of over 35% for the LiveJournal dataset when the number of layers, mappers, & reducers are increased from 8 to 16, and again from 16 to 32. As the same dataset is partitioned into more layers and processed by greater number of processors, it leads to smaller partitions and less computation in each processor. This reduction in computation cost contributes to the speedup achieved. Moreover, as the number of layers and reducers are doubled, the data received by each reducer node gets halved, but the mining cost in the 1st reduce job also increases, as the height of the tree grows with the increase in number of layers (as there are composed substructures that span more layers and the **number of combinations** for the recursive procedure ***Compose-MLN*** increases), leading to a higher number of possible interlayer combinations.

Figure 12 also shows that the total time taken when *beam* size is set to 10 is more as compared to *beam* size 6. This is because *as the beam size increases, the number of substructures carried forward in each iteration increases (illustrated in Table 3)*, resulting in more data being processed by each processor.

Table 3: Number of substructures generated in each iteration with *beam* 10 and 6 for the LiveJournal data.

Iterations	Beam 10	Beam 6
1	2836928	2836928
2	3929240	3172184
3	4593864	3628496
4	5249968	3849008
5	5346152	4004984
6	5716984	4128496

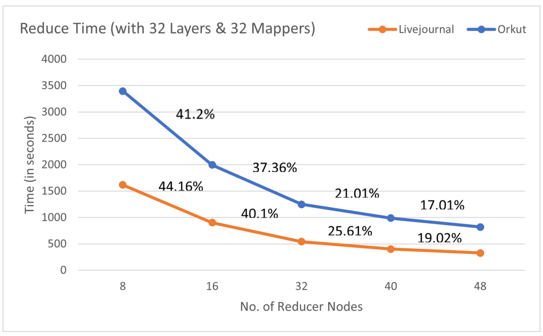
Orkut and LiveJournal datasets were used for the next two scenarios with 32 layers (Figures 13a, 13b.) The purpose is to understand the importance of mappers vs. reducers with respect to the work/computation done during the algorithm.

Scenario 2: **Changing *only* the number of reducer nodes:** In this scenario, the number of mapper nodes is fixed at 32, and the number of reducer nodes is varied to see the effect of reducers on response time.

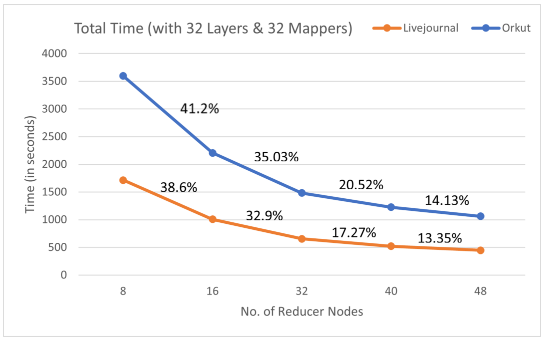
Figure 13a initially shows a high percentage of speedup for both LiveJournal and Orkut in the reduce phase when the number of reducer nodes is increased from 8 to 16 to 32. But after that, the speedup starts to plateau, with the percentage improvement reducing significantly when going from 32 to 40 and then to 48 nodes. So, *merely adding more reducer nodes beyond a certain number does not keep improving speedup*, as the overhead (e.g., reducer setup & cleanup) increases. Orkut takes more absolute time than LiveJournal, as it has more than 3 times the number of edges for a similar number of vertices, leading to more expansion and combination possibilities. In contrast to the reduce time, total time is shown in Figure 13b. This speedup is similar to the reduce time (except in absolute values) indicating that all the speedup comes from the reducers. This matches the work done in the reducers as explained in Section 6 and validates the need for more reducers. Remember, composition is happening in the reducer of job 1 and counting all isomorphs and metric computation is happening in the reducer of job 2.

Scenario 2 clearly indicates that the mappers take less time overall as compared to the reducers. Hence, **distributing reduce computation among more reducers has a significant effect on the speedup** which is exemplified in scenario 3 below.

Scenario 3: **Changing *only* the number of mapper nodes:** Here, the number of reducer nodes is fixed at 32, and the number of mapper nodes is varied to inspect the effect of mappers on response time.

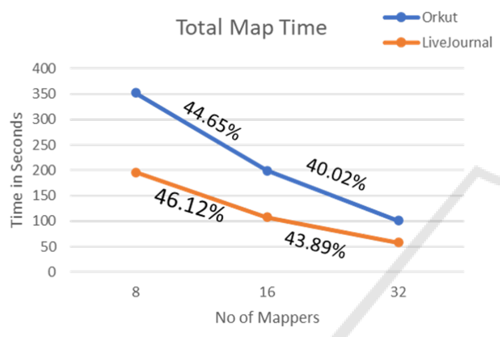


(a) Effect on Reduce Phase Time.

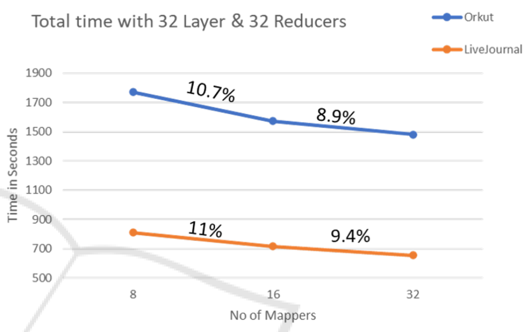


(b) Effect on Overall Map/Reduce Time.

Figure 13: Speedup comparison by varying only the number of reducer nodes.



(a) Effect on Map Phase Time.



(b) Effect on Overall Map/Reduce Time.

Figure 14: Speedup comparison on varying only the number of mapper nodes.

In Figure 14a, significant speedup is seen in the **map time** as the number of mapper nodes is increased from 8 to 16 to 32. But the total time shown in Figure 14b is distinctly different from the one we see in Figure 13b. **Total time speedup** has reduced significantly due to much smaller portion of the computation being distributed. **This, again, clearly indicates that there is not much computation in the mappers to effectively distribute them to improve the overall Map/Reduce performance.** In both jobs in the chain, the reducers are doing heavy lifting in this architecture. *From Scenarios 2 and 3, it can be inferred that for this algorithm, prioritizing an increase in the number of reducers over mappers is more beneficial, as the reduce phase has a greater effect on total execution time.*

Effect of Graph Density: Connectivity of graphs also influences the performance of substructure discovery due to large number of substructures generated during expansion. We categorize graphs as dense to sparse, where the number of vertices is fixed but the number of edges vary along the spectrum ranging from a completely connected graph to a very sparsely connected graph. This experiment was performed on a graph with 2K vertices, but varying densities from 25% (1M edges) to 100% (3.9M edges) on 4 layers using 4 mapper nodes and 4 reducer nodes to see the effect of connectivity of graphs on response time.

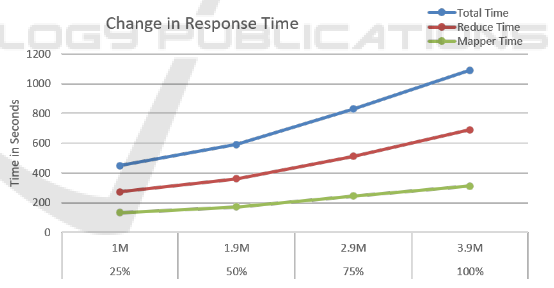


Figure 15: Effect of graph density on response time.

The results in Figure 15 show that with *dense graphs*, where each vertex is connected to more vertices on average, *the computation cost increases as there are more expansions which leads to more map time and more combinations of intralayer edges in the reducer contributing to more reduce time. This further confirms that more time is spent in the reducer in this algorithm as compared to the mapper.*

8 CONCLUSIONS

This paper proposes a scalable substructure discovery algorithm for HoMLNs using the decoupling-based strategy. A generic Map/Reduce algorithm was introduced for the parallel processing of layers and then composing the results, again, using a Map/Reduce framework. The basic components of substructure discovery - substructure expansion, *combining substructures from each layer to generate substructures spanning layers (composition function)*, duplicate elimination, and counting isomorphic substructures - were incorporated into the Map/Reduce framework. Empirical correctness was established. Extensive experimental analysis was performed on diverse synthetic and real-world graph datasets.

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