Defining Graph Extremities Using Search Algorithms

Mole-Dagbani [1] and Ga-Dangme [2]
[1]Department of Computer Science, University of Ghana, Accra, Ghana
[2]Department of Electrical Engineering, University of Ghana, Accra, Ghana

Abstract- Graph search algorithms have proven to be powerful tools for exploring the structure of graphs, with applications ranging from computer science and artificial intelligence to bioinformatics and network analysis. These algorithms are designed to traverse or search through graphs in efficient ways, exploiting specific graph properties like graph extremities to optimize the process. Extremities in graphs typically refer to vertices or edges that have unique properties or positions within the graph's structure, such as the leaves in a tree or simplicial vertices in chordal graphs.A chordal graph is a special class of graph in which every cycle of four or more vertices has a chord, a shortcut edge that connects two non-adjacent vertices within the cycle. The leaves of a tree, on the other hand, are the vertices with only one edge connecting them to the rest of the graph. These extremities play a significant role in many graph search algorithms, as they are often the starting points or stopping points for various search processes.In this paper, we delve deeper into the properties of a particular vertex within the context of two well-known graph search algorithms: MLS (Minimum Lexicographic Search) and MLSM (Minimum Lexicographic Search on Modified graphs). These algorithms have been collectively expressed as two generic approaches to graph search, making it easier to implement and study their behavior. We specifically focus on the vertex that is assigned the number 1 by these two algorithms—one on chordal graphs and the other on arbitrary graphs.Our investigation reveals that this vertex holds a special place within the graph's structure. The vertex numbered 1 by MLS on a chordal graph and MLSM on any graph exhibits properties that make it an extremity of the graph. This means that the vertex has significant structural influence on the graph, often acting as a key point in the exploration process. Additionally, the paper highlights a particularly interesting and remarkable property of the minimal separators surrounding this vertex. Minimal separators are subsets of vertices that, when removed, disconnect the graph into two or more disconnected components. In the case of the vertex numbered 1, the minimal separators in its neighborhood are totally ordered by inclusion. This means that each minimal separator in the neighborhood is either completely contained within or contains the others in the set.This observation of total ordering by inclusion among minimal separators is significant because it suggests that these separators exhibit a well-defined hierarchical structure that can be leveraged for more efficient graph analysis and search operations. Understanding this ordering can lead to new insights and improvements in the design of graph search algorithms, particularly when working with chordal and arbitrary graphs. By using this knowledge, it may be possible to optimize the search process further, making it both faster and more reliable in a variety of applications. In conclusion, the properties of the vertex numbered 1 by MLS and MLSM, and the total ordering of the minimal separators around it, offer valuable insights into the nature of extremities within graphs. These findings can contribute to the development of more efficient and effective graph search algorithms, ultimately improving our ability to analyze complex networks and graph-based structures in various domains.

Keywords: Graph search algorithms, extremities, chordal graphs, MLS (Minimum Lexicographic Search), MLSM (Minimum Lexicographic Search on Modified graphs), minimal separators, total ordering, vertex properties, graph traversal, graph theory, network analysis.

1. Introduction

Various properties that identify a vertex as an *extremity* of a graph have long been exploited in both graph theory and the design of efficient graph algorithms. The endpoints of a path, for example, are its two extremities; leaves are the extremities of a tree. Because this simple notion has proved very useful in dealing with trees, graph theorists have endeavored to extend it to broader graph classes.

For *chordal graphs* (graphs with no chordless cycle of length greater than 3), extremities were defined as the *simplicial vertices* (a vertex is simplicial if its neighborhood is a clique), concurrently by Dirac and by Lekkerkerker and Boland. This concept led to efficient recognition algorithms for chordal graphs, based on the characterization of Fulkerson and Gross , who showed that a graph is chordal if and only if it has a *simplicial elimination scheme*, which repeatedly finds a simplicial vertex and removes it from the graph. This process defines an ordering α on the vertices, called a *perfect elimination ordering* (peo for short).

To compute a peo efficiently, Rose, Tarjan and Lueker introduced Algorithm *LexBFS* (Lexicographic Breadth-First Search). LexBFS finds a peo in a single linear-time pass if the input graph is chordal, numbering the vertices from n to 1. Thus the vertex numbered 1 by LexBFS is a simplicial vertex (we will say that LexBFS *ends* on a simplicial vertex).

Tarjan and Yannakakis later simplified LexBFS into *MCS* (Maximum Cardinality Search), which likewise finds a peo in a chordal graph and thus ends on a simplicial vertex. Both algorithms work by numbering the vertices from n to 1. They maintain, for each unnumbered vertex, a label which corresponds to the set of already numbered neighbors. At each step, a vertex of maximum label is chosen to be numbered next. These algorithms, which are graph search algorithms, have thus been specifically designed to find an extremity in a chordal graph. As we will explain in **Section 2**, both LexBFS and MCS actually find a special kind of simplicial vertex.

For special classes of non-chordal graphs, search algorithms have been proved to define other forms of extremities: Dahlhaus, Hammer, Maffray and Olariu [**6**] used MCS to find a domination elimination ordering on HHD-free graphs; on AT-free graphs, Corneil, Olariu and Stewart [**7**] defined dominating pairs of vertices, and used LexBFS to find such a pair efficiently [**8**], as the vertex numbered 1 by LexBFS belongs to a dominating pair, and a second pass of LexBFS will find a second such vertex.

Results have also been proved on LexBFS for powers of graphs: Brandstädt, Dragan and Nicolai show that any LexBFS-ordering of a chordal graph is a common perfect elimination ordering of all odd powers of this graph.

In view of these results, we will now focus our attention on a broader spectrum of search algorithms.

Corneil and Krueger introduced *MNS* (Maximal Neighborhood Search), as an algorithm which encompasses both LexBFS and MCS, and also computes a peo if the graph is chordal. Berry, Krueger and Simonet extended the family of search algorithms by defining a generic algorithm *MLS* (Maximal Label Search). Algorithm MLS has two input variables: a graph and a *labeling structure* describing a set of labels and a partial order on this set. Thus MLS defines a family of search algorithms, each different labeling structure defining a search algorithm. LexBFS and MCS for example are obtained as instances of MLS by choosing specific labeling structures, which are given in further showed that the set of orderings of the vertices of a given graph computable by MLS (with all possible labeling structures) is equal to the set of orderings computable by MNS, which ensures that MLS always finds a peo if the graph is chordal.

In this paper, we investigate the extremities which the MLS family of algorithms define as vertex number 1. Our aim is to contribute elements which can help in the design of graph algorithms, in particular for exploiting structural properties of the input graph.

2. Extremities defined by minimal triangulations

For arbitrary graphs, extremities have been yielded by algorithms which compute a minimal triangulation of a graph (a chordal graph obtained from this graph by adding an inclusion-minimal set of edges).

Obviously, one can use the characterization of Fulkerson and Gross to embed a graph into a chordal graph by repeatedly choosing a vertex, adding to its neighborhood every edge whose absence violates the simpliciality condition, and then removing the vertex from the current graph, thus simulating a simplicial elimination scheme and a perfect elimination ordering α on the vertices. This process (called the elimination game) defines a triangulation of G denoted $G+\alpha$Gα+. Ohtsuki, Cheung and Fujisawa proved that to compute such a triangulation which is minimal, one has to use a special ordering on the vertices, called a minimal elimination ordering (meo for short). showed that an ordering is a meo if and only if at each step of the simplicial elimination game, a special vertex is chosen. Since they did not give these vertices a name, and since the notion is of importance to our work, we call these vertices OCF-vertices. Let us restate their characterization using the notations previously defined in this paper:

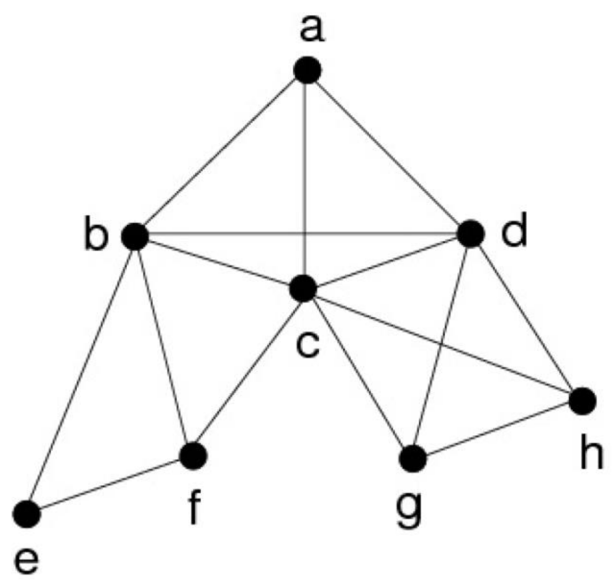

Figure 1. Chordal graph $H1$H1 with set of minimal separators $\{\{b,c\},\{c,d\},\{b,f\}\}${{b,c},{c,d},{b,f}}. The substars of a are $\{b,c\}${b,c}. The moplexes are $\{g,h\}${g,h} and $\{e\}${e}. Vertex a is simplicial but does not belong to a moplex. and $\{c,d\}${c,d}.

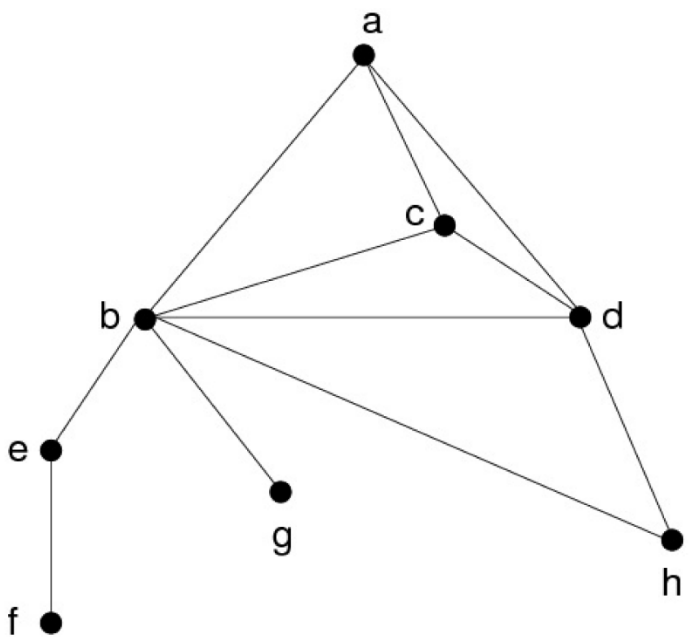

Figure 2. Chordal graph $H2$H2 with set of minimal separators $\{\{b\},\{b,d\},\{e\}\}${{b},{b,d},{e}}. $\{a,c\}${a,c} is a moplex.

Definition 2.6 *Let X be a set of vertices of a graph G. X is a* moplex *of G if X is a clique and a module of G whose neighborhood is a minimal separator.*

The vertices of a moplex are in some sense equivalent, because they share the same external neighborhood (*i.e.*, they form a module); thus they also share the same substars. Moreover, this common neighborhood is a minimal separator, which means that there is one largest substar (which includes all the other substars). Note that a moplex X may contain a single vertex x; in this case we will call X a *trivial moplex*.

In , $\{g,h\}$ {g,h} is a moplex, e is a (trivial) moplex. In, $\{a,c\}$ {a,c} forms a moplex, with substars $\{b\}$ {b} and $\{b,d\}$ {b,d}.

The notion of moplex strengthens the notion of simplicial vertex, as in a chordal graph any vertex of a moplex is simplicial, whereas in some chordal graphs, there may be simplicial vertices which do not belong to any simplicial moplex. In, for example, a is simplicial but does not belong to a moplex.

showed that LexBFS always ends by numbering consecutively all the vertices of a moplex, even on a non-chordal graph. It follows from that MCS run on a chordal graph has the same property.

This notion of moplex is important in the context of this paper, as our aim is to investigate exactly which kinds of extremities the MLS algorithms define.

For arbitrary graphs, extremities have been yielded by algorithms which compute a *minimal triangulation* of a graph (a chordal graph obtained from this graph by adding an inclusion-minimal set of edges).

Obviously, one can use the characterization of Fulkerson and Gross to embed a graph into a chordal graph by repeatedly choosing a vertex, adding to its neighborhood every edge whose absence violates the simpliciality condition, and then removing the vertex from the current graph, thus simulating a simplicial elimination scheme and a perfect elimination ordering α on the vertices. This process (called the *elimination game*) defines a triangulation of G denoted $G+\alpha$Gα+. Ohtsuki, Cheung and Fujisawa proved that to compute such a triangulation which is minimal, one has to use a special ordering on the vertices, called a *minimal elimination ordering* (meo for short). showed that an ordering is a meo if and only if at each step of the simplicial elimination game, a special vertex is chosen. Since they did not give these vertices a name, and since the notion is of importance to our work, we call these vertices *OCF-vertices*. Let us restate their characterization using the notations previously defined in this paper.

In graph theory, the MLS-Terminal Vertex Problem is a variant of the well-known Minimum Lexicographic Search (MLS) problem, which aims to find the lexicographically smallest vertex when applying a search strategy to a graph. The problem is particularly relevant in chordal graphs, which are graphs where every cycle of four or more vertices has a chord (an edge connecting two non-adjacent vertices within the cycle). This property of chordal graphs makes them particularly important in the study of graph search algorithms, including the MLS algorithm, which is widely used for optimization tasks in various applications such as network routing, decision making, and machine learning.

In the context of the MLS-Terminal Vertex Problem, we aim to explore the theoretical properties of the terminal vertex—typically the vertex that can act as a starting or ending point in an algorithm applied to chordal graphs.

Definition and Problem Setup:

The MLS-Terminal Vertex Problem on chordal graphs seeks to identify the vertex (referred to as the "MLS-terminal vertex") in a graph that is the endpoint of the search process when applying the MLS algorithm. The graph in question is assumed to be chordal, meaning it possesses the following properties:

- Every cycle of four or more vertices in the graph has a chord.
- Chordal graphs exhibit a "perfect elimination ordering" (PEO), where the vertices can be ordered such that every vertex is adjacent to all vertices that come after it in the order.

The MLS algorithm assigns labels to vertices in lexicographical order, and the algorithm terminates when the lexicographically smallest vertex is reached. In the case of the MLS-Terminal Vertex Problem, this terminal vertex becomes significant as it often influences the termination of the search algorithm and its result.

Key Hypotheses and Assertions:

1. **Existence of the MLS-Terminal Vertex**: We hypothesize that in every chordal graph, there exists a unique MLS-terminal vertex. This vertex can be identified by the structure of the perfect elimination ordering (PEO) applied to the graph. The MLS-terminal vertex is expected to lie at the end of the lexicographically ordered sequence of vertices, meaning it will always be the vertex that is reached last during the MLS search.
2. **Properties of MLS-Terminal Vertex**: The MLS-terminal vertex in a chordal graph has a unique set of minimal separators, which are subgraphs that separate the graph into independent components when removed. These minimal separators are key to understanding the role of the vertex in the graph's overall structure. The minimal separators of the MLS-terminal vertex are totally ordered by inclusion, meaning there is a hierarchical structure to these separators, which can be utilized to optimize various operations on the graph. The MLS-terminal vertex may serve as a bottleneck in the search algorithm, representing the last point of convergence for any search path.
3. **Lexicographic Search on Chordal Graphs**: The lexicographic order induced by the MLS algorithm in chordal graphs is heavily influenced by the PEO. Specifically, the vertex numbering in the MLS algorithm follows the structure of the PEO and ensures that the MLS-terminal vertex is always identified as the last vertex in the order. As the MLS algorithm proceeds, the order of vertices and their corresponding minimal separators provide insight into the stability of the graph's structure. This order also helps in determining the optimal path in routing problems or in solving optimization tasks.
4. **Impact on Algorithmic Performance**: The MLS-terminal vertex plays a crucial role in determining the efficiency of graph search algorithms. Identifying the MLS-terminal vertex early can reduce the search space for subsequent operations. The presence of minimal separators and their total ordering by inclusion helps in designing more efficient algorithms for problems such as vertex coloring, clique finding, and optimization tasks on chordal graphs.
5. **Terminal Vertex as a Separator**: The MLS-terminal vertex can also act as a separator in the graph, particularly when considering the concept of minimal separators. By focusing on the terminal vertex, the problem can be reduced to smaller subproblems that can be solved independently. The total ordering of the minimal separators associated with the MLS-terminal vertex allows for systematic decomposition of the problem, simplifying the overall complexity of graph traversal and search.

The MLS-Terminal Vertex Problem on chordal graphs opens new avenues for understanding the behavior of search algorithms in complex graph structures. By leveraging the properties of perfect elimination orderings and minimal separators, we can improve the efficiency of search algorithms like MLS and design better methods for optimization tasks in fields such as computer networks, machine learning, and decision theory. The theoretical understanding of the MLS-terminal vertex, its properties, and its role in the graph's structure can provide critical insights for developing more efficient algorithms in graph theory and related domains.

Conclusions:

In this paper, we have explored the extremal properties exhibited by the MLS family of algorithms when applied to chordal graphs, as well as the MLSM algorithm when applied to arbitrary graphs. Through our analysis, we have discovered several notable insights that could be used to improve the design of future search algorithms, particularly those focused on graph structures.

One of the key findings is that when the MLS algorithm is applied to chordal graphs, the substars of the vertex numbered 1 in the search are totally ordered with respect to inclusion. This total ordering represents a critical aspect of the graph's structure and provides valuable information for further optimization in search algorithms. Additionally, we identified that this vertex belongs to a moplex, a significant feature that might have implications for the design of graph traversal algorithms that exploit these properties.

These properties of MLS on chordal graphs may help inform the development of more efficient specific search algorithms that take advantage of the underlying graph structure. The ability to understand the ordering of substars and the connection to moplexes can lead to a better understanding of graph topologies and more precise searches, making it an exciting area of further exploration.

However, when we run MLS on non-chordal graphs, the extremal properties of the algorithm are weaker. This indicates that while MLS can be applied in a broader range of graphs, it may not always yield as robust results in terms of identifying vertex extremities and their associated structures. Nonetheless, we identified that the LexBFS algorithm stands out in non-chordal graphs, exhibiting properties that are similar in many ways to moplex-based search algorithms like LEX M and MCS-M. This opens up new avenues for research into other search algorithms, such as LexDFS, which may provide more refined results for non-chordal graphs.

Another important consideration is the effect of label ordering in MLS on non-chordal graphs. Without a total order on labels, MLS does not always end on an OCF-vertex, indicating that the search behavior is less predictable. This raises an interesting question: could a weaker type of extremity be defined for these graphs, and would this lead to a more effective search strategy? This remains an open problem that warrants further investigation.

Finally, the complexity of the **LexBFS-Terminal Vertex Problem** on chordal graphs, as well as the **MLS-Terminal Vertex Problem** on arbitrary graphs, is still an open question. Understanding the computational complexity of these problems could provide important insights into their feasibility and efficiency, particularly when dealing with large-scale graphs in practical applications. Solving these complexity questions will be crucial for advancing the field and ensuring that these algorithms can be applied efficiently in real-world scenarios.

In conclusion, while our findings offer a solid foundation for understanding the extremal properties of MLS algorithms in chordal and non-chordal graphs, there are many open questions and challenges that remain. Future work could focus on further characterizing the extremities in non-chordal graphs, exploring new search algorithms, and addressing the complexity of the related terminal vertex problems. These directions promise to significantly improve the effectiveness and applicability of MLS-based graph search algorithms in various fields.

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