A UNIFIED VIEW OF GRAPH SEARCHING*

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Abstract. Graph searching is perhaps one of the simplest and most widely used tools in graph algorithms. Despite this, few theoretical results are known about the vertex orderings that can be produced by a specific search algorithm. A simple characterizing property, such as is known for LexBFS, can aid greatly in devising algorithms, writing proofs of correctness, and showing impossibility results. This paper unifies our view of graph search algorithms by showing simple, closely related characterizations of various well-known search paradigms, including BFS and DFS. Furthermore, these characterizations naturally lead to other search paradigms, namely, maximal neighborhood search and LexDFS.

Key words. graph searching, graph traversal, depth-first search, breadth-first search, LexBFS

AMS subject classifications. 05C85, 68R10, 68W05

DOI. 10.1137/050623498

1. Introduction. Graph searching is fundamental. Most graph algorithms employ some mechanism for systematically visiting all vertices and edges in the given graph. After choosing an initial vertex, a search of a connected graph visits each of the vertices and edges of the graph such that a new vertex is visited only if it is adjacent to some previously visited vertex. At any point there may be several vertices that may possibly be visited next; this generic graph search does not specify which vertex to choose. The breadth-first search (BFS) and depth-first search (DFS) algorithms are the traditional strategies for determining the next vertex to visit (see [7] for a recent overview of these searches). BFS traverses an untraversed edge incident with the least recently visited vertex, whereas DFS traverses an untraversed edge incident with the most recently visited vertex. Both searches were used in the 19th century to solve maze traversals. More recently, DFS, as popularized by Tarjan [14], has been used for such problems as graph connectivity, planarity, topological ordering, and strong connectivity of digraphs. Applications of BFS include shortest path problems, network flows, and recognition of various graph classes.

In the mid 1970s, Rose, Tarjan, and Lueker [11] introduced a variant of BFS for determining perfect elimination orderings in chordal graphs. Their lexicographic breadth-first search (LexBFS) has garnered much attention recently and has become an important search algorithm used for recognition of various graph families, diameter approximation, and finding key structures in certain graph classes [3]. One of the key points regarding LexBFS, and one of the reasons for its usefulness, is that there is a very simple characterization of LexBFS orderings. This characterization is critical to the proofs of correctness of various algorithms. In light of the power of such a tool, it is somewhat surprising that the traditional searches of BFS and DFS are not known to have similar characterizations. Other than LexBFS, only the maximum cardinality search (MCS) of Tarjan and Yannakakis [15] has a known characterization [1].

^{*}Received by the editors January 28, 2005; accepted for publication (in revised form) March 26, 2008; published electronically July 25, 2008. This work was supported by the Natural Sciences and Engineering Research Council of Canada (NSERC) and the Ontario Graduate Scholarship Program. http://www.siam.org/journals/sidma/22-4/62349.html

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To provide a common underpinning for viewing graph searches, we examine what is meant by a "generic graph search." We describe a graph search similarly to Tarjan [14]. Given a possibly disconnected graph G whose vertices are initially unexplored, we start from some vertex s of G and choose one of its edges to follow. Traversing this edge leads to a new vertex. We continue, at each step selecting an untraversed edge leading from a vertex already reached. Traversing this edge leads either to a new vertex or to one previously reached. Whenever we run out of edges leading from old vertices, we choose some new unreached vertex and begin again from there. Each edge is traversed exactly once, and we eventually reach all vertices in the graph. How we choose amongst all the edges we may next traverse determines the type of search we perform (i.e., whether it is a BFS or a DFS). The order in which we reach the vertices exhibits very different properties depending on this selection rule.

From a characterization point of view, we concentrate on the following situation. Suppose in the ordering of vertices we have three vertices, a, b, and c, where a was reached before b, which was reached before c, and we have an edge ac present in our graph, but the edge ab is absent (see Figure 1.1). The question is, "how could vertex b have been chosen before vertex c by our search?" With what we know so far about this situation, it seems that c should have been chosen before b. What can we infer about the graph such that the search could have chosen b before c?

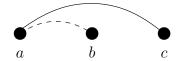


Fig. 1.1. A curious triple of vertices in a search ordering.

In the case of LexBFS, the answer is known. There must exist another vertex d chosen earlier than a such that db is an edge, but dc is not an edge of G [11, 8]. In fact, Brandstädt, Dragan, and Nicolai [1] showed that this condition is a characterization of a vertex ordering being generated by LexBFS.

Experience with LexBFS has shown that such a characterizing property is instrumental in the applicability of the search to various problems. For example, the LexBFS characterization is fundamental in proving that the reverse of a LexBFS ordering of a chordal graph is a perfect elimination ordering [11]. Furthermore, many of the recent LexBFS-based algorithms use multiple sweeps of LexBFS to reveal structure of the given graph (see [3] for several examples). Each subsequent search uses information from the previous sweep(s) to break ties of which vertex to visit next. The related proofs of correctness rely heavily on the LexBFS characterization. The characterization can also be used to show that there is some LexBFS ordering that certifies a graph as being cocomparability, even though we don't know how to find it efficiently [4].

In light of this simple characterization result for LexBFS (and similar results for MCS) and recognizing its usefulness, it is somewhat surprising that it appears that this question has never been asked regarding the more traditional search paradigms of BFS and DFS. In section 2 we further explore the question "how could b have been chosen before c by a graph search?" We present answers to this question for each of the known search paradigms and show that those answers in fact characterize the vertex orderings realizable by the graph search. We will also introduce two new search paradigms, a depth-first version of LexBFS we call LexDFS, and a generalization we

call maximal neighborhood search (MNS). To illustrate the usefulness of these new characterizations, we examine in section 3 which searches of a given graph G are valid searches of powers of G. In particular, we would like to obtain a search ordering of G^k without the necessity of computing G^k (i.e., in time linear in the size of G). We conclude with some remarks about the impact of these new characterizations and their extension to other areas.

1.1. Notation and definitions. We now define some notation to facilitate our discussion. We let G = (V, E) be a graph on vertex set V and edge set E. We will assume, for simplicity, that all graphs in this paper are connected and undirected; extension of our results to disconnected graphs is straightforward. Let n = |V|. We define $\sigma = (v_1, \ldots, v_n)$ to be a linear ordering of V, which will typically be the left-toright order in which we number the vertices in a search. We let $\sigma_i = (v_1, \ldots, v_i)$ be a prefix of the ordering σ for $1 \le i \le n$. We use the notation $\sigma(i) = v_i$ and $\sigma^{-1}(v_i) = i$ to refer to a specific vertex in σ . The ordering σ implicitly imposes a total order on V; we say $v_1 <_{\sigma} v_2 <_{\sigma} \cdots <_{\sigma} v_n$ and omit the subscript σ when the ordering is clear. We let $G_i = G[v_1, \ldots, v_i]$ be the subgraph of G induced on a prefix of σ , and let $N_H(v)$ be the neighborhood of v in a subgraph H of G. When referring to searches, $s = v_1$ is the start vertex.

A graph is said to be *chordal* if every cycle of length at least 4 has at least one chord. A vertex is *simplicial* in a graph G if its neighborhood is a clique in G. An ordering (v_1, \ldots, v_n) of V is a *perfect elimination ordering* of G if v_i is simplicial in G_i . A graph is chordal if and only if it has a perfect elimination ordering [6]. A graph is *bipartite* if its vertex set can be partitioned into two disjoint sets X, Y such that all edges are of the form xy for some $x \in X$ and $y \in Y$. A graph is *chordal bipartite* if it is bipartite and every cycle of length at least 6 has a chord. The *complement* of a graph G = (V, E), written $\overline{G} = (V, \overline{E})$, is defined by $\overline{E} = \{xy : x, y \in V \text{ with } x \neq y \text{ and } xy \notin E\}$. The kth power of a graph G, written $G^k = (V, E^k)$, for some positive integer k, is obtained from G by including an edge between every pair of vertices that are of distance at most k in G (hence G^1 is precisely G itself).

We draw particular attention to the fact that the search algorithms in this paper generate vertex orderings from left to right. In many applications it may be useful to reverse the ordering generated by search, and some of the LexBFS literature considers this reversal as part of the search algorithm.

2. Characterizing graph search.

2.1. Generic search. We begin by formalizing the generic search idea, similar to Tarjan's description in [14], and present it as Algorithm 1. We use a generic "set" data structure S to store the candidate vertices we may next visit during our search. We note that we impose no selection criteria on which member of S we choose in line 3 beyond that it must be in S.

We call any ordering of V that can be generated by Algorithm 1 a search ordering of the graph G. As an example, we notice that (1,6,2,3,4,5) is not a valid search ordering of the 3-sun in Figure 2.1, whereas (1,2,4,3,5,6) is a valid search ordering of this graph. The reader will notice that this search ordering is neither a BFS nor a DFS, which is permissible by the generic selection criterion in line 3. We may opt to use a more restrictive data structure to obtain other properties for our search, such as replacing set S with a queue to obtain BFS. Note also that, as stated, a given vertex may be added to S multiple times as each of its neighbors is numbered. How S deals with this can change the nature of the search. For example, using a variant of a stack

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ALGORITHM 1: Generic search.

input: a graph G = (V, E) and start vertex s \in V
output: an ordering \sigma of V

1 S \leftarrow \{s\}
2 for i \leftarrow 1 to n do
3 | pick and remove an unnumbered vertex v from S
4 | \sigma(i) \leftarrow v // This assigns to v the number i
5 | foreach unnumbered vertex w adjacent to v do
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add w to S

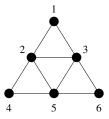
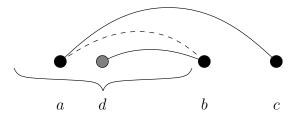


Fig. 2.1. The 3-sun, used as an example for our graph searches.

where the add operation moves a vertex to the top of the stack if that vertex was added previously will yield DFS.

We now proceed to answer the fundamental question raised above about our search orderings: how could b have been chosen before c? We give a simple answer, which turns out to be the characterizing property of search orderings.



(S): Given an ordering σ of V, if a < b < c and $ac \in E$ and $ab \notin E$, then there exists a vertex d < b such that $db \in E$.

We note that (S) makes no statement to the relative order of a and d in σ . It simply says that there must be a vertex adjacent to b visited sometime earlier than b in σ . We will now show that (S) characterizes search orderings. That is to say that any ordering that the generic search algorithm can produce has this property, and that any vertex ordering with this property can be produced by the generic search algorithm when we break ties suitably.

THEOREM 2.1. For an arbitrary graph G, an ordering σ of V is a search ordering of G if and only if σ has property (S).

Proof. For the forward direction, suppose σ is an ordering generated by Algorithm 1. Let a < b < c be a triple of vertices in σ with $ac \in E$ and $ab \notin E$. At the point when b is chosen, both b and c must be in S. Since b is in S, some neighbor of b must have already been chosen; call this neighbor d. Thus d < b and $db \in E$. Since the triple a < b < c was arbitrary, property (S) holds on σ .

For the converse, suppose $\sigma = (v_1, \dots, v_n)$ is an ordering respecting property (S). Suppose for contradiction that (v_1, \dots, v_{i-1}) can be obtained by Algorithm 1, but (v_1, \dots, v_i) cannot, for some $i, 1 < i \le n$. That is, v_i is the first vertex in σ that cannot be chosen next by the algorithm. Consider the next iteration of the algorithm after choosing v_{i-1} . Since v_i cannot be chosen next, $v_i \notin S$. Let u be a vertex that the algorithm may choose next. Then u must be in S. Let w be the neighbor of u which caused u to be added to S. Since $v_i \notin S$, we know that $wv_i \notin E$. By applying property (S) to the vertex triple $w < v_i < u$, we know there exists a vertex $d < v_i$ with $dv_i \in E$. Hence $v_i \in S$, contradicting our assumption that v_i could not be chosen by Algorithm 1.

In fact, the perceptive reader will note that vertex c is irrelevant when restricting our attention to connected graphs. However, the presence of c is required when extending to more general settings.

2.2. BFS. We now proceed to the familiar BFS algorithm. BFS is a restriction of generic search in that we use a queue to determine which vertex we may choose next at our selection step. BFS does not, however, determine which order to push the neighbors of a numbered vertex onto the queue (see LexBFS in section 2.3 for a search that does). Algorithm 2 should be familiar to most readers.

Algorithm 2: Breadth-first search (BFS).

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input: a graph G = (V, E) and start vertex s \in V output: an ordering \sigma of V

1 initialize queue to \{s\}

2 for i \leftarrow 1 to n do

3 | dequeue v from beginning of queue

4 | \sigma(i) \leftarrow v // This assigns to v the number i

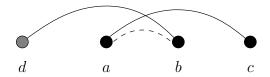
5 | foreach unnumbered vertex w adjacent to v do

6 | if w is not already in queue then

7 | enqueue w to end of queue
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We mention that (1, 2, 3, 4, 5, 6) is a valid BFS ordering of the 3-sun in Figure 2.1. Note that (1, 2, 3, 6, 5, 4) is not a BFS ordering of this graph, though it does give a distance layering of the graph with respect to vertex 1.

We key in on our central question: How could b have been chosen before c in a BFS? The answer is a simple restriction to the answer we found for generic search.



(B): Given an ordering σ of V, if a < b < c and $ac \in E$ and $ab \notin E$, then there exists a vertex d < a such that $db \in E$.

This property is merely property (S) with the added restriction that d < a. Interestingly, we find that this is sufficient to characterize all BFS orderings.

Theorem 2.2. For an arbitrary graph G, an ordering σ of V is a BFS ordering of G if and only if σ has property (B).

Proof. For the forward direction, suppose σ is a BFS ordering. Let a < b < c be a triple of vertices in σ with $ac \in E$ and $ab \notin E$. If b was removed from (and thus placed on) the queue before c, it must have a neighbor d that was numbered at least as early as a. Since a does not have b as a neighbor, d must be earlier than a.

For the reverse direction, suppose for contradiction that $\sigma = (v_1, \ldots, v_n)$ is an ordering satisfying property (B) such that (v_1, \ldots, v_{i-1}) can be produced by BFS, but (v_1, \ldots, v_i) cannot, for some $i, 1 < i \le n$. That is, v_i cannot be chosen next by any valid execution of BFS on G. Let u be a vertex that may be chosen next by some execution of BFS. Since u is dequeued in this extension, it must have been enqueued when some neighbor v_j with j < i was previously numbered. Then $v_j v_i \notin E$; otherwise some valid execution of BFS can enqueue v_i before u. Applying (B) to the triple $v_j < v_i < u$, there must exist a vertex $d < v_j$ with $dv_i \in E$. Thus v_i is enqueued before, and dequeued before, u, contradicting our assumption above.

To illustrate an application of this property, we now prove the correctness of a generalization of a well-known technique for extracting a shortest s, w-path (for arbitrary w) given an ordering with property (B) starting with s. For notation, when given a vertex ordering σ of V and a subset $T \subseteq V$, we say $\sigma|_T$ is the restriction of σ to T.

COROLLARY 2.3. Let σ be an arbitrary ordering of the vertices of a graph G, and let H = G[T] be a connected induced subgraph of G such that $\sigma|_T$ satisfies (B). Suppose s is the first vertex in $\sigma|_T$, and let $w = w_0$ be an arbitrary vertex in T. For i > 0, define w_i to be the leftmost (in $\sigma|_T$) neighbor of w_{i-1} , until s is reached. Then $(s = w_k, \ldots, w_1, w_0 = w)$ is a shortest s, w-path in H.

Proof. Suppose, for contradiction, that $(s = w_k, \ldots, w_1, w_0 = w)$ is not a shortest s, w-path in H. Let $(s = x_{k'}, \ldots, x_1, x_0 = w)$ be a shorter s, w-path, with k' < k. Note that $x_{k'} < w_{k'}$. Choose the smallest i > 0 such that $x_i < w_i$. Then $w_{i-1} \le x_{i-1}$. Since $x_i x_{i-1} \in E$ and w_i is the leftmost neighbor of w_{i-1} , we know that $x_i w_{i-1} \notin E$ (and thus $w_{i-1} \ne x_{i-1}$). Consider the triple $x_i < w_{i-1} < x_{i-1}$. Since $x_i x_{i-1} \in E$ but $x_i w_{i-1} \notin E$, property (B) applied to $\sigma|_T$ says there is a vertex d in T such that $d < x_i$ with $dw_{i-1} \in E$. This contradicts w_i being the leftmost neighbor of w_{i-1} , and hence our original path was in fact shortest. \square

2.3. LexBFS. In the studies of LexBFS, the answer to our key question, property (LB) below, has long been exploited as a useful characterization of LexBFS orderings. For completeness, we present the traditional LexBFS labeling algorithm as Algorithm 3.

As an example, consider Algorithm 3 on the graph in Figure 2.1 from the start vertex 1. The ordering (1, 2, 3, 5, 4, 6) is a valid LexBFS ordering of the 3-sun. Note that once 1, 2, 3 are picked, 5 must be chosen over 4 since $label(5) = \{4, 3\}$ while

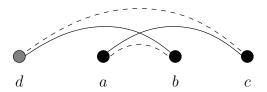
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Algorithm 3: Lexicographic breadth-first search (LexBFS).
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input: a graph G = (V, E) and start vertex s \in V output: an ordering \sigma of V

1 assign the label \epsilon to all vertices
2 label(s) \leftarrow \{n+1\}
3 for i \leftarrow 1 to n do
4 | pick an unnumbered vertex v with lexicographically largest label
5 | \sigma(i) \leftarrow v // This assigns to v the number i
6 foreach unnumbered vertex w adjacent to v do
7 | append (n-i) to label(w)
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 $label(4) = \{4\}$. This ordering is also a BFS ordering of the 3-sun, but the BFS ordering (1, 2, 3, 4, 5, 6) is not a LexBFS ordering.

We now restate the answer to our key question for LexBFS.



(LB): Given an ordering σ of V, if a < b < c and $ac \in E$ and $ab \notin E$, then there exists a vertex d < a such that $db \in E$ and $dc \notin E$.

This property says that if we choose b before c, but there is an earlier vertex a that would normally pull c before b, then there must be an even earlier vertex d that caused b to be pulled ahead of c. Though this has long been known to be a property of LexBFS orderings [11, 8], the reverse direction showing (LB) characterizes LexBFS orderings has only recently been shown [1].

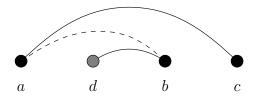
THEOREM 2.4 (see [11, 8, 1]). For an arbitrary graph G, a vertex ordering σ is a LexBFS ordering of G if and only if σ has property (LB).

Remarkably, the requirement of dc not being an edge is the only difference between lexicographic and traditional BFS. We obtain the immediate corollary, without any mention of the respective algorithms, that a LexBFS ordering is a BFS ordering, since (B) subsumes (LB).

2.4. DFS. We now turn our attention to DFS DFS is very different from BFS in that it progresses forward through the graph as much as possible, backtracking only when necessary, whereas BFS first systematically explores close vertices before venturing out to the far reaches of the graph. One also notes that DFS produces two vertex orderings: a discovery ordering, which is the order vertices are first visited, and a finishing ordering, indicating the order in which each vertex's neighborhood is fully explored with all incident edges traversed and causing a backtracking step. In this paper we concentrate on the discovery orderings of DFSs, though we note an interesting relationship between the two orderings in section 4.

We start by presenting a DFS algorithm exploiting a stack data structure to store candidate vertices to visit next. We present DFS as Algorithm 4 in a style similar to our generic search algorithm in section 2.1. We note that line 6 would typically be included in the push operation of a suitable stack-type data structure, but we include the step here in our algorithm for clarity.

We again concentrate on our key question: If given a DFS ordering with a < b < c with ac an edge but ab not an edge, how could DFS have chosen b over c? The answer is property (D), which we will show characterizes DFS orderings.



(D): Given an ordering σ of V, if a < b < c and $ac \in E$ and $ab \notin E$, then there exists a vertex d with a < d < b such that $db \in E$.

Algorithm 4: Depth-first search (DFS).

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\begin{array}{c} \textbf{input} : \textbf{a graph } G = (V, E) \ \textbf{and start vertex } s \in V \\ \textbf{output:} \ \textbf{an ordering } \sigma \ \textbf{of } V \\ \textbf{1 initialize } stack \ \textbf{to } \{s\} \\ \textbf{2 for } i \leftarrow 1 \ to \ n \ \textbf{do} \\ \textbf{3} \quad \text{pop } v \ \textbf{from top of } stack \\ \textbf{4} \quad \sigma(i) \leftarrow v \quad // \ \textbf{This assigns to } v \ \textbf{the number } i \\ \textbf{5} \quad \textbf{for each } unnumbered \ vertex \ w \ adjacent \ to \ v \ \textbf{do} \\ \textbf{6} \quad \text{if } w \ already \ in \ stack \ \textbf{then } \text{remove } w \ \text{from } stack \\ \textbf{7} \quad \text{push } w \ \textbf{on top of } stack \\ \end{array}
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Notice that this property restricts (S) only in that d must also appear to the right of a. We contrast this with BFS property (B), where d was to the left of a. In this sense, DFS is the opposite search paradigm to BFS.

THEOREM 2.5. For an arbitrary graph G, an ordering σ of V is a DFS ordering of G if and only if σ has property (D).

Proof. For the forward direction, suppose σ is an ordering produced by DFS. Suppose we have a triple of vertices a < b < c in σ with $ac \in E$ and $ab \notin E$. Since b is numbered (and $b \neq s$, the initial vertex), b must have been pushed on the stack when one of its neighbors was previously numbered. Let d be the rightmost neighbor of b appearing before b in σ . Then d < b and $d \neq a$. Suppose d < a. Since a was numbered after d, c is pushed on the stack above b. As there are no other neighbors of b before b is numbered, c is higher on the stack than b and must be numbered before b, a contradiction. Thus we must have a < d, and property (D) holds.

Now for the reverse direction, suppose $\sigma = (v_1, \ldots, v_n)$ is an ordering respecting property (D). Suppose (v_1, \ldots, v_{i-1}) can be obtained by DFS, but (v_1, \ldots, v_i) cannot. That is, v_i is the first vertex in σ that cannot be chosen next by DFS. Let u be a vertex that DFS may choose next. Then $v_i < u$. Let v_j be the rightmost vertex in σ_{i-1} such that $v_j u \in E$ (that is, v_j is the parent vertex of u in the DFS-tree). Then $v_j v_i \notin E$ (otherwise v_i could be chosen next) and, more generally, $v_k v_i \notin E$ for all k, $j \leq k < i$. By applying property (D) to the triple $v_j < v_i < u$, we know there exists a vertex d between v_j and v_i such that $dv_i \in E$, a contradiction to v_i being ineligible to be chosen next.

We can apply (D) repeatedly to obtain the following simple corollary.

COROLLARY 2.6. Given a graph G and an arbitrary DFS ordering σ of V, if a < b < c and $ac \in E$, then there exists a path P from a to b whose vertices increase in σ . That is, there exists an a,b-path $P = (a = d_k, \ldots, d_1, d_0 = b)$ in G with $\sigma^{-1}(d_i) < \sigma^{-1}(d_{i-1})$ for each $d_i \in P \setminus \{b\}$.

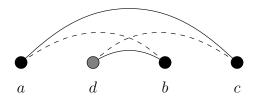
Most previous results regarding DFS rely on properties of the DFS-tree. The DFS-tree T is defined on the vertices of G and includes exactly those edges traversed to number a new vertex. Formally, $v_iv_j \in E(T)$ with i < j if and only if $i = \max\{k \mid v_kv_j \in E(G) \text{ and } k < j\}$. We say u is the parent of v in v if v if v if v if v in v if v if v is an ancestor of v if there is a path from v to v all of whose edges go from parent to child. We say two vertices are related if one is an ancestor of the other.

Many data structure textbooks (for example, [2]) mention the following fundamental property of DFS (which follows from Corollary 2.6).

(D2): In a DFS-tree of an undirected graph, the two endpoints of each back (non-tree) edge are related.

Consider a back edge uv in a DFS-tree. The four-vertex condition (D) is stronger than (D2) in that it says all vertices between u and v (inclusive) are related to u.

2.5. LexDFS. Looking at the relationship between BFS and LexBFS, one naturally asks whether there is a "lexicographic analogue" for DFS. We have noted that LexBFS enforces the requirement of " $dc \notin E$ " on top of BFS. It is natural to question whether a similar requirement makes sense for DFS. We state this restriction of property (D) below.



(LD): Given an ordering σ of V, if a < b < c and $ac \in E$ and $ab \notin E$, then there exists a vertex d with a < d < b such that $db \in E$ and $dc \notin E$.

We turn to the task of devising an algorithm that realizes this property. Considering our 3-sun example in Figure 2.1, once vertices 1 and 2 are chosen, the only way to avoid violating (LD), and hence the only valid ordering, is (1,2,3,5,6,4). Clearly this is a DFS ordering, and we observe that the DFS ordering (1,2,4,5,6,3) violates (LD). The LexBFS ordering (1,2,3,5,4,6) is also disallowed.

These examples suggest that our algorithm should choose vertices that are adjacent to as many vertices we have more recently numbered as possible. As it is to be related to LexBFS, our algorithm should also be in some sense similar to our LexBFS algorithm. (We discuss the property that actually relates LexBFS and LexDFS in section 2.6.) We present Algorithm 5 as our LexDFS algorithm.

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Algorithm 5: Lexicographic depth-first search (LexDFS).
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\begin{array}{l} \textbf{input} : \text{a graph } G = (V, E) \text{ and start vertex } s \in V \\ \textbf{output} \text{: an ordering } \sigma \text{ of } V \\ \textbf{1} \quad \text{assign the label } \epsilon \text{ to all vertices} \\ \textbf{2} \quad label(s) \leftarrow \{0\} \\ \textbf{3} \quad \textbf{for } i \leftarrow 1 \text{ to } n \text{ do} \\ \textbf{4} \quad \text{pick an unnumbered vertex } v \text{ with lexicographically largest label} \\ \textbf{5} \quad \sigma(i) \leftarrow v \quad // \text{ This assigns to } v \text{ the number } i \\ \textbf{6} \quad \text{foreach } unnumbered \text{ vertex } w \text{ adjacent to } v \text{ do} \\ \textbf{7} \quad \text{prepend } i \text{ to } label(w) \\ \end{array}
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Examining Algorithm 5, our answer to the "what is LexDFS?" question becomes quite convincing. There is just one difference between this algorithm and the LexBFS algorithm. For LexDFS, we *prepend* the new digit i to label(w) at line 7, whereas, for LexBFS, we *append* the new label digit n-i. This elementary change converts the algorithm from a BFS into a DFS. We now show that our algorithm correctly defines LexDFS.

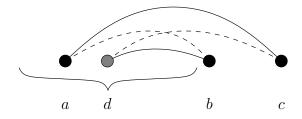
THEOREM 2.7. For an arbitrary graph G, an ordering σ of V is a LexDFS ordering of G if and only if σ has property (LD).

Proof. For the forward direction, suppose σ is an ordering computed by some execution of LexDFS. We define $label_u(v)$ to represent the label assigned to vertex v in this execution immediately before vertex u was numbered. Let a < b < c be a triple of vertices in σ with $ac \in E$ and $ab \notin E$. Since b was numbered before c, $label_b(b) \ge label_b(c)$. We note that the digits in each label appear in decreasing order. Since $\sigma^{-1}(a)$ appears in $label_b(c)$ and does not appear in $label_b(b)$, $label_b(b)$ must include some digit $j > \sigma^{-1}(a)$ which does not appear in $label_b(c)$. Let $d = \sigma(j)$. Then d < b, $db \in E$, and $dc \notin E$. Since $j > \sigma^{-1}(a)$, a < d, and thus property (LD) is satisfied.

Now for the reverse direction, suppose $\sigma = (v_1, \ldots, v_n)$ is an ordering respecting property (LD). Suppose (v_1, \ldots, v_{i-1}) can be obtained by LexDFS, but (v_1, \ldots, v_i) cannot. That is, v_i is the first vertex in σ that cannot be chosen next by LexDFS. Let u be a vertex that LexDFS may choose next. Since u must be chosen over v_i , at this point of execution label(u) must be lexicographically larger than $label(v_i)$: let j be the largest digit in label(u) that is not in $label(v_i)$ (i.e., v_j is the rightmost vertex in σ_{i-1} with $v_ju \in E$ and $v_jv_i \notin E$). By applying property (LD) to the vertex triple $v_j < v_i < u$, we know there exists a vertex d between v_j and v_i such that $dv_i \in E$ and $du \notin E$. Then $\sigma^{-1}(d)$ is in $label(v_i)$ but not in label(u). Since $v_j < d$, $label(v_i)$ is in fact larger than label(u), a contradiction to v_i being ineligible to be chosen next.

When examining a new search algorithm, we should concern ourselves with its implementation. Algorithm 5 does not immediately have a linear-time implementation using those ideas used for LexBFS. The partitioning idea exploited for LexBFS cannot efficiently be applied to LexDFS (leading to an $O(m \log n)$ time bound), as its depth-first properties can pull in an arbitrary vertex to be the next to be numbered. We refer to [10] for an $O(\min\{n^2, m \log n\})$ implementation; recently an $O(m \log \log n)$ implementation has been discovered [13] employing van Emde Boas trees to keep track of the relative lexicographic order of unnumbered vertices. It is an open question whether there is a linear-time implementation of LexDFS.

2.6. Maximal neighborhood search. We now consider the question of "what fact relates LexBFS and LexDFS?" What useful property does this nonedge dc give us? Equivalently, we ask what type of search we get when adding the restriction $dc \notin E$ to the generic search property (S). We formalize our discussion around this property.



(M): Given an ordering σ of V, if a < b < c and $ac \in E$ and $ab \notin E$, then there exists a vertex d with d < b and $db \in E$ and $dc \notin E$.

Surprisingly, this property has already been used in the literature. Tarjan and Yannakakis [15] mentioned that both MCS (where at each step we choose a vertex that is adjacent to the maximum number of vertices previously numbered) and LexBFS respect our property (M) (which [15] calls "P"), and they showed that any ordering

with property (M) is the reverse of a perfect elimination ordering of a chordal graph. But the paper does not consider whether there is a natural search algorithm that is characterized by this property. We answer that question here by introducing maximal neighborhood search (MNS) as Algorithm 6.

The idea behind MNS is simple: at each step, pick a vertex whose neighborhood in the part of the graph already explored is maximal (with respect to set inclusion). This is a straightforward generalization of the LexBFS, LexDFS, and MCS algorithms. We obtain each of these searches from Algorithm 6 by further specifying how to order incomparable neighborhoods. For LexBFS, we choose a vertex adjacent to as many earliest chosen vertices as possible. For LexDFS, we choose a vertex adjacent to as many most recently chosen vertices as possible. For MCS, we choose a vertex whose neighborhood has maximum cardinality.

```
Algorithm 6: Maximal neighborhood search (MNS)
```

We now show that the vertex orderings produced by Algorithm 6 are characterized by property (M).

THEOREM 2.8. For an arbitrary graph G, an ordering σ of V is an MNS ordering if and only if σ has property (M).

Proof. For the forward direction, suppose σ is an MNS ordering. Suppose a < b < c is a triple in σ that violates (M). That is, $ac \in E$ and $ab \notin E$, yet there is no vertex d < b with $db \in E$ and $dc \notin E$. Consider the point in the execution when $b = v_i$ is chosen. Then $N_{G_{i-1}}(b) \subsetneq N_{G_{i-1}}(c)$, so b could not have been chosen next by MNS, a contradiction. Hence (M) must hold for σ .

For the converse, suppose $\sigma = (v_1, \ldots, v_n)$ is an ordering respecting property (M). Suppose (v_1, \ldots, v_{i-1}) can be obtained by MNS, but (v_1, \ldots, v_i) cannot; that is, v_i is the first vertex in σ that cannot be chosen next by MNS. Then there must be another vertex u with $N_{G_{i-1}}(u) \supseteq N_{G_{i-1}}(v_i)$. Let $x \in N_{G_{i-1}}(u) - N_{G_{i-1}}(v_i)$ (such an x must exist). We apply (M) to the triple $x < v_i < u$, giving a vertex $d < v_i$ with $dv_i \in E$ and $du \notin E$. This contradicts $N_{G_{i-1}}(u) \supseteq N_{G_{i-1}}(v_i)$, and hence our assumption that v_i could not be chosen by MNS was incorrect.

Thus, for chordal graphs, every MNS ordering is the reverse of a perfect elimination ordering. A natural question is whether every perfect elimination ordering of a chordal graph is the reverse of an MNS ordering. This question is studied by Shier [12] and answered in the negative: the reverse of many perfect elimination orderings are not search orderings, and thus cannot be found by MNS. However, [12] shows how to generalize search orderings by considering connected components in the unvisited portion of the graph to capture the entire family of perfect elimination orderings.

3. Application to powers of graphs. All searches give a certain amount of insight into a graph's structure, including the insight gained from our four-vertex characterizations. At times we wish to use this insight to gain information about some graph arising from a given graph via some function. Examples of such functions include the graph's complement, some power of the graph, the line graph, or the product or join of the graph. Often, we want to obtain insight into the structure of a derived graph without incurring the possibly large cost of computing the function.

Search is often a convenient and efficient way to do this. For example, it has been previously noted that a LexBFS ordering (and thus a BFS ordering) of the complement of a graph can be found without computing the complement, given a slight modification of the standard LexBFS algorithm [9]. Dahlhaus, Gustedt, and McConnell [5] have shown how to find a DFS ordering of the complement of a graph in time linear in the original graph. We can use such results to obtain information about the derived graph (such as whether the graph's complement is chordal) more efficiently than actually computing the derived graph.

In this section, we consider the problem of computing some type of search ordering of some power of the graph, but without resorting to computing that power. One possibility is to compute a search ordering of the original graph, and ask whether it is a search ordering of the power. We will show that the aforementioned search characterizations are invaluable in obtaining straightforward proofs of both positive and negative results for this problem.

We start with the simple question of whether a BFS ordering of a graph remains a BFS ordering for all powers of a graph.

THEOREM 3.1. For any graph G, every BFS ordering of G is a BFS ordering of G^k for all $k \geq 1$.

Proof. Let σ be a BFS ordering of G. The theorem is trivially satisfied when k=1. For k>1, we assume for induction that σ is a BFS ordering for all powers of G strictly less than k and consider σ on G^k . Suppose a < b < c is a triple in σ on G^k with $ac \in E^k$ and $ab \notin E^k$.

If a < b < c is such a triple in σ on G^{k-1} , then by (B) and our induction hypothesis, there exists a vertex d < a with $db \in E^{k-1} \subseteq E^k$, hence satisfying (B) on G^k .

Suppose instead that a < b < c is not such a triple in σ on G^{k-1} . Then $ac \notin E^{k-1}$. But then there must be a vertex e with $ae \in E^{k-1}$ and $ec \in E$. Since $ab \notin E^k$ but $ae \in E^{k-1}$, we must have $eb \notin E$. We have 3 cases for the position of e in σ relative to a and b.

Case 1. e < a. In σ on G, since $ec \in E$ and $eb \notin E$, we apply (B) to the triple e < b < c, giving us a vertex d < e < a such that $db \in E \subseteq E^k$, satisfying (B) on G^k .

Case 2. a < e < b. We first consider σ on G. We know that $ec \in E$ and $eb \notin E$, so by applying (B) to the triple e < b < c, we get a vertex d < e such that $db \in E$. If d < a, we're done; otherwise, we have a < d. Since $db \in E$ but $ab \notin E^k$, we must have $ad \notin E^{k-1}$. We apply (B) and our inductive hypothesis to the triple a < d < e in σ on G^{k-1} , giving us a vertex $d_2 < a$ such that $d_2d \in E^{k-1}$. Since $d_2d \in E^{k-1}$ and $db \in E$, d_2 and b are of distance at most k in G. Thus $d_2b \in E^k$, satisfying (B) on G^k .

Case 3. b < e. In σ on G^{k-1} , since $ae \in E^{k-1}$ and $ab \notin E^{k-1}$, we apply (B) and our inductive hypothesis to the triple a < b < e, giving us a vertex d < a with $db \in E^{k-1} \subseteq E^k$, satisfying (B) on G^k .

In each case, we show the existence of a vertex d < a with $db \in E^k$, and hence (B) is satisfied by σ on G^k . Thus σ is a BFS ordering of G^k .

While a BFS ordering survives through the powers of a graph, and clearly generic search orderings also survive, one naturally wonders about DFS. We now show that a DFS ordering of G is not necessarily a DFS ordering in a given power of G. Again, the characterizing property of DFS will play an crucial role in our proof.

THEOREM 3.2. For every $k \geq 2$, there exists a graph G such that no DFS ordering of G is a DFS ordering of G^k .

Proof. Fix $k \geq 2$. We first show the existence of a graph G such that no DFS ordering starting from a distinguished start vertex s is a DFS ordering of G^k .

Let G be the graph consisting of two vertices s and r connected by three paths of length k + 1. This graph is diagrammed in Figure 3.1.

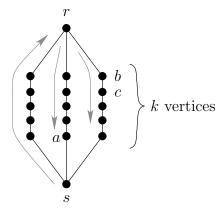


Fig. 3.1. Given k, a graph G where no DFS from s is a DFS of G^k . The possible DFS path through G is shown in gray.

Let σ be an arbitrary DFS ordering of G starting from s. The DFS will proceed from s along one of the three paths to reach r. From r, the DFS will follow a second path towards s to reach a adjacent to s. As s is already discovered, the DFS will recurse back to r and travel the third path towards s. Let s be the first vertex visited on this third path, and let s be the next vertex on the path.

Thus, in σ , we have s < r < a < b < c. Moreover, b appears in σ immediately following a (when a is reached, all neighbors of a are already numbered, so DFS recurses to r, where b must be the next vertex to be numbered).

Now consider σ in G^k . One easily verifies that a and c are of distance k in G, and a and b are of distance k+1 in G. Hence $ac \in E^k$ and $ab \notin E^k$. But since a and b are next to each other in σ , there can be no vertex between a and b. Therefore, the triple a < b < c violates the condition (D). Hence σ cannot be a DFS ordering of G^k .

To prove the theorem, we consider two copies of G joined at s by an edge: call this graph G'. Consider any DFS ordering σ' of G': it may start in either copy of G, possibly at s itself. We observe that if σ' starts in one copy of G, σ' restricted to the other copy of G appears as a DFS ordering of G starting at s. Following the argument above, we can identify three vertices a < b < c in the second copy of G.

We note that no vertex from the other copy of G is within distance k of b, and thus there can be no edge ab in $(G')^k$. The triple a < b < c violates (D) as above, so σ' is not a DFS of $(G')^k$. Since σ' was chosen arbitrarily, no DFS ordering of G' can be a DFS ordering of $(G')^k$.

Failing for DFS, one may wonder about LexBFS. Brandstädt, Dragan, and Nicolai [1] have shown that the reverse of a LexBFS ordering of a chordal graph G is a common

perfect elimination ordering of all odd powers of G. One may be tempted to think that a LexBFS ordering of a chordal graph is a LexBFS ordering of the odd powers, but we show this is not the case.

THEOREM 3.3. For each $k \geq 2$, there exists a chordal graph G such that no LexBFS ordering of G is a LexBFS ordering of G^k .

Proof. Let $k \geq 2$ be fixed. If k is even, we consider the graph G_k in Figure 3.2(a); otherwise, if k is odd, we consider the graph H_k in Figure 3.2(b). We note that each of these graphs is chordal. We will show that no LexBFS ordering of the graph starting from vertex 1 will be a LexBFS ordering of the kth power, then join two copies of the graph at vertex 1 to prove the theorem for a LexBFS ordering starting from an arbitrary vertex.

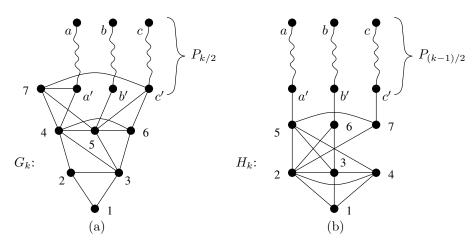


Fig. 3.2. Constructions for (a) k even and (b) k odd, where no LexBFS ordering starting from 1 is a LexBFS ordering of G^k .

Suppose k is even. We note that any LexBFS ordering σ of the graph G_k which starts at 1 must have 7 < a' < b' < c'. Then a < b < c in σ . We examine the triple a < b < c in G_k . We note that $ac \in E(G_k^k)$ since $d_{G_k}(a,c) = 2(k/2-1)+2=k$, and $ab \notin E(G_k^k)$ since $d_{G_k}(a,b) = 2(k/2-1)+3=k+1$. It is easy to check that there is no vertex d < a with $db \in E(G_k^k)$ and $dc \notin E(G_k^k)$: any vertex left of a within distance k of b in G_k must be within distance k of c. Thus property (LB) is violated in G_k^k , showing σ is not a LexBFS ordering of G_k^k .

Now suppose k is odd. Considering the graph in Figure 3.2(b), we note that any LexBFS ordering σ of H_k that starts at 1 must have a' < b' < c'. Then a < b < c in σ . We note that $d_{H_k}(b',3) = 2$ and $d_{H_k}(c',3) = 3$, and $d_{H_k}(b',6) = 1$ and $d_{H_k}(c',6) = 3$, but for all other vertices x < a' in σ , $d_{H_k}(b',x) \ge d_{H_k}(c',x)$. We examine the triple a < b < c in H_k . We have $ac \in E(H_k)$, since $d_{H_k}(a,c) = 2(\frac{k-1}{2}-1)+3=k$, and $ab \notin E(H_k)$, since $d_{H_k}(a,b) = 2(\frac{k-1}{2}-1)+4=k+1$. But since all vertices d < a in σ within distance k of b are also within distance k of c, there is no candidate vertex d to satisfy property (LB) for a,b,c. Thus σ is not a LexBFS ordering of H_k .

To complete the proof, we construct a graph G consisting of two copies of G_k if k is even (respectively, two copies of H_k if k is odd), with the vertices labeled 1 in each copy joined by an edge. Any LexBFS ordering of G when restricted to at least one of the copies of G_k (or H_k) will appear as a LexBFS ordering with start

vertex 1. Applying the argument above will identify vertices a < b < c that violate property (LB) in G^k , completing our proof.

We note that the graph in Figure 3.2(b) is in fact strongly chordal. A graph is strongly chordal if it is chordal and every cycle $C = (x_1, \ldots, x_{2k})$ of even length has a chord $x_i x_j$ where the distance between the endpoints x_i and x_j in C is odd. An immediate corollary of Theorem 3.4 is that for each $k \geq 1$, there exists a strongly chordal graph G such that no LexBFS ordering of G is a LexBFS ordering of G^{2k+1} .

LexBFS does, however, work for a particular class of graphs, as shown by the next theorem.

THEOREM 3.4. Let G be a chordal bipartite graph. If σ is a LexBFS ordering of G, then σ is a LexBFS ordering of the graph G^2 .

Proof. Let σ be a LexBFS ordering of a chordal bipartite graph G = B(X, Y, E). Let l(x) denote the BFS layer of x in σ ; l(x) = 0 if x is the first vertex of σ . We first state a few simple facts.

FACT 1. If $x \in X$ and $xy \in E$, then $y \in Y$.

FACT 2. If $x \in X$ and $xy \in E^2 - E$, then $y \in X$.

FACT 3. If $x \in X$, $y \in Y$, and $z \in X$, then l(x) = l(y) + 2i - 1 = l(z) + 2j for some (possibly negative) integers i, j.

FACT 4. If there is some induced P_5 a, b, c, d, e with l(a) = l(e) = l(b) - 1 = l(d) - 1 = l(c) - 2, then there exists an induced C_{2k} , $k \ge 3$, in G.

To prove our theorem, suppose we have a < b < c with $ac \in E^2$ and $ab \notin E^2$. We will show the existence of a vertex z < a with $zb \in E^2$ and $zc \notin E^2$.

Case 1. $ac \in E$. By (LB) on a < b < c, there is a d < a with $db \in E$ and $dc \notin E$. If $dc \notin E^2$, d satisfies the theorem. So assume $dc \in E^2 - E$. Since $ab \notin E^2$, we must have $da \notin E$. By Facts 2 and 3, and since $l(d) \le l(a) = l(c) - 1$, we have l(d) = l(c) - 2. By (LB) on d < a < b, there is an e < d with $ea \in E$ and $eb \notin E$. Since l(e) = l(d), $ed \notin E$. By (LB) on e < d < a, there must be some f < e with $fd \in E$, $fa \notin E$ and l(f) = l(d) - 1 = l(c) - 3. Thus $fb \in E^2$ and $fc \notin E^2$, satisfying our requirement.

Case 2. $ac \notin E$. Then there is some d with $da, dc \in E$; choose the leftmost (in σ) such d. Since $ab \notin E^2$, $db \notin E$. We have 4 cases for the position of d relative to a, b, and c.

Case 2.1. c < d. By (LB) on a < c < d, there is an e < a with $ec \in E$ and $ed \notin E$. Since d is leftmost, $ea \notin E$. By (LB) on e < a < c, there is an f < e with $fa \in E$ and $fc \notin E$. Then f, a, d, c, e is an induced P_5 such that Fact 4 gives us an induced cycle of length at least 6, contradicting G being chordal bipartite.

Case 2.2. b < d < c. By (LB) on a < b < d, there is an e < a with $eb \in E$ and $ed \notin E$. Since $ab \notin E^2$, $ea \notin E$. For generality, we discard our assumptions that b < d and $ed \notin E$. Now, by (LB) on e < a < b, there is some f < e with $fa \in E$ and $fb \notin E$, which means l(f) = l(a) - 1 = l(c) - 3. If $fe \in E$, then $fb \in E^2$ and since $fc \notin E^2$, f satisfies the theorem. Otherwise $fe \notin E$, so applying (LB) to f < e < a gives us a g < f with $ge \in E$, $ga \notin E$. Since $l(g) \le l(f) = l(c) - 3$, we know $gc \notin E^2$, so g fulfills the theorem since $gb \in E^2$.

Case 2.3. a < d < b. By (LB) on d < b < c, there is some e < d with $eb \in E$ and $ec \notin E$. Since $ab \notin E^2$, $ea \notin E$. If e < a, we are in the generalized Case 2.2 above, and can find a vertex g to satisfy the theorem. When a < e, we can apply (LB) to a < e < d to give an f < a with $fe \in E$, $fd \notin E$. Thus $fb \in E^2$ and f satisfies the theorem unless there exists some g with $fg, gc \in E$. Suppose such a g exists. Then l(f) = l(g) - 1 = l(c) - 2 and $dg \notin E$. If $ag \notin E$, then a, d, c, g, f forms a P_5 and

Fact 4 gives us an induced cycle of length at least 6, contradicting G being chordal bipartite. Thus $ag \in E$ and d < g (since d is leftmost). By (LB) on f < d < g, there is an h < f with $hd \in E$ and $hg \notin E$. Then l(h) = l(f) and $hf \notin E$. But then f, g, c, d, h is a P_5 such that Fact 4 gives us an induced cycle of length at least 6, contradicting G being chordal bipartite. Thus no such g can exist, and f satisfies the theorem.

Case 2.4. d < a. By (LB) on d < b < c, there is an e < d with $eb \in E$, $ec \notin E$. Then l(e) = l(b) - 1 = l(c) - 1, so $ec \notin E^2$, thus completing the proof.

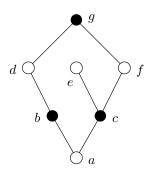


Fig. 3.3. A bipartite graph with a LexBFS ordering that is not a LexBFS ordering of the square.

Note that this theorem cannot be strengthened to bipartite graphs, as shown by the graph in Figure 3.3. Call this graph B. The ordering $\sigma=(a,b,c,d,e,f,g)$ is clearly a LexBFS ordering of B; however, the triple of vertices d < e < f violates property (LB) in B^2 . We have $df \in E^2$ and $de \notin E^2$, but every vertex in σ left of d that is adjacent to e in B^2 is also adjacent to f in B^2 . Attaching a second copy of B via an edge at a ensures no LexBFS ordering of the graph is a LexBFS ordering of its square.

4. Concluding remarks. We have examined six different search algorithms from the perspective of our key question: If a search visits a vertex a before b before c, and there is an edge ac but no edge ab, how could the search have visited b before c? In this examination, we have discovered characterizing properties for the classic breadth-first and depth-first searches, and introduced a new class of maximal neighborhood searches. We summarize the characterizations of the six search paradigms and the hierarchy they form in Figure 4.1.

From this picture, one might be tempted to conjecture that the set of LexBFS orderings of a graph might be exactly the intersection of the set of MNS orderings and the set of BFS orderings. Clearly any LexBFS ordering must be both a BFS ordering and an MNS ordering, but the converse does not hold. For example, the ordering (3,1,2,5,4) is both a BFS ordering and an MNS ordering of the gem in Figure 4.2, but is not a LexBFS ordering of this graph. Similarly for DFS, (1,2,3,4,5) is both a DFS ordering and an MNS ordering of this graph, but not a LexDFS ordering.

We mentioned that the DFS algorithm produces two different orderings of the vertices of a graph: the discovery ordering and the finishing ordering. The following proposition relates these two orderings in the case of undirected graphs.

PROPOSITION 4.1. For an arbitrary undirected graph G, an ordering σ of V is the reverse of a DFS finishing ordering if and only if σ has property (D).

In other words, for undirected graphs, every ordering is the reverse of a finishing

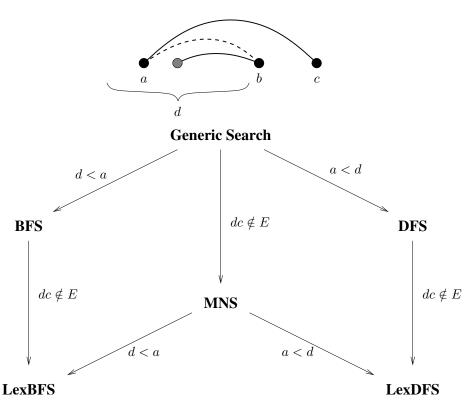


Fig. 4.1. Summary of search characterizations. For example, vertex ordering σ is a LexDFS ordering if and only if σ satisfies the condition for generic search together with $dc \notin E$ and a < d.

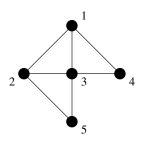


Fig. 4.2. The gem, used as an example to distinguish sets of orderings.

ordering if and only if it is a discovery ordering. Note that a similar proposition does not hold for LexDFS.

Though we have concentrated on simple graphs in this paper, these ideas can easily be extended to more general environments. Our characterizations make no mention of multiple edges, but are equally applicable to searches on multigraphs. A search ordering implicitly imposes an orientation on the edges of a simple graph: it is straightforward to apply the same ideas to directed graphs to obtain similar characterizations. We can also extend such characterizations beyond graphs: these ideas also hold for searches on hypergraphs. We refer to [10] for details.

Such characterizing properties can be a very powerful and useful tool for studying graphs. Beyond giving us a better understanding of how a search reveals the structure

of a graph, it allows us to employ (and analyze) multiple sweeps of a search to gather additional information about a graph. Multisweep LexBFS has recently been applied to a variety of problems [3], resulting in very simple, and in many cases intuitive, algorithms. Will the results presented in this paper lead to multisweep algorithms involving other searches or combinations of different searches?

Acknowledgments. We wish to thank the anonymous referees for their valuable comments on the paper; in particular, one referee noticed Proposition 4.1 and kindly allowed us to include it in the paper. We also thank Marty Golumbic for his careful reading of an earlier draft of the paper.

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