Systems of Graph Formulas and their Equivalence to Alternating Graph Automata

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Graph-based modeling plays a fundamental role in many areas of computer science. In this paper, we introduce systems of graph formulas with variables for specifying graph properties; this notion generalizes the graph formulas introduced in earlier work by incorporating recursion. We show that these formula systems have the same expressive power as alternating graph automata, a computational model that extends traditional finite-state automata to graphs, and allows both existential and universal states. In particular, we provide a bidirectional translation between formula systems and alternating graph automata, proving their equivalence in specifying graph languages. This result implies that alternating graph automata can be naturally represented using logic-based formulations, thus bridging the gap between automata-theoretic and logic-based approaches to graph language specification.

1 Introduction

Graph-like structures are ubiquitous in computer science and beyond. In many cases, they need to fulfill application-dependent structural properties that have to be specified and checked. In the literature, such properties have been called global [18] if they concern graph regions of unbounded size, like connectedness or the existence of cycles. In this paper, we relate two mechanisms for specifying global graph properties: systems of graph formulas and alternating graph automata.

Graph expressions based on the notion of graph concatenation by Engelfriet and Vereijken [16] have been introduced in [10, 8]. They resemble ordinary regular expressions and define a class of graph languages which can be shown to be equal to the class of graph languages accepted by finite graph automata. In [11], we have used graph expressions to introduce a more powerful notion of graph formulas. Rather than being a special case of formulas in predicate logic such as monadic second-order logic [7], the structure of our formulas corresponds to that of the nested graph conditions by Habel and Pennemann [19, 23]. However, the basic building blocks are graph expressions in the former case rather than graph morphisms as in the latter case. Graph properties specified by graph formulas are in the polynomial hierarchy PH.

On the one hand, graph formulas can be translated to the alternating graph automata introduced in [12]. This was shown in [11], thus proving that the latter are at least as powerful as the former. On the other hand, from [12] alternating graph automata are known to be capable of describing PSPACE-complete graph properties. Together with the aforementioned fact that graph formulas can only capture graph properties in the polynomial hierarchy, this shows that alternating graph automata are strictly more powerful than graph formulas, provided that $PH \neq PSPACE$.

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Intuitively, the reason for this difference in power is that each graph formula has a fixed number of quantifier alternations as each formula syntactically resembles a tree. In contrast, alternating graph automata can be cyclic, thus implementing unbounded quantifier depth.

In this paper we extend graph formulas to systems of graph formulas with variables, similar to Flick who extended nested graph conditions to recursively nested graph conditions [17]. Also similar to Mezei and Wright's notion of systems of language equations [22], such a system consists of a finite set of variables, each of which is mapped to a graph formula. Intuitively, each variable represents the set of graphs that satisfy the associated formula. Since every formula may itself contain variables, the system may be cyclic. This leads us to define its semantics as a least fixed point.

After preliminary definitions in Section 2 and a recap of alternating graph automata in Section 3, we define systems of graph formulas and their semantics in Section 4, where we also show that this semantics coincides with that of graph formulas in the acyclic case (Lemma 4.6). Furthermore, we establish a useful normal form of systems of graph formulas. Using this normal form, we finally prove the main result of this paper in Section 5: systems of graph formulas are precisely as powerful as alternating graph automata (Theorem 5.3). As a running example, we specify the language of all graphs that have a Hamiltonian cycle, which cannot be specified by recursively nested conditions [17, p. 143].

2 Preliminaries

We let \mathbb{N} denote the set of non-negative integers and [n] the set $\{1,\ldots,n\}$ for all $n \in \mathbb{N}$. A^* denotes the set of all finite sequences over a set A; the empty sequence is denoted by ε . For a sequence $s \in A^*$, [s] denotes the set of all members of A occurring in s. For a binary relation $\leadsto \subseteq A \times B$, we write $\not\leadsto$ for its complement, i.e., for $a \in A$ and $b \in B$, $a \not\leadsto b$ holds if and only if $a \leadsto b$ does not.

We consider edge-labeled hypergraphs (which we simply call graphs), i.e., edges are attached to sequences of nodes. To be able to concatenate graphs in the way originally proposed by Engelfriet and Vereijken [16], we supply each graph with two sequences of distinguished nodes, its front and rear interfaces. As in [9], we require these sequences to be free of repetitions.

A ranked set $(\mathscr{S}, rank)$ consists of a finite set \mathscr{S} of elements and a function $rank \colon \mathscr{S} \to \mathbb{N}$, which assigns a rank to each element $a \in \mathscr{S}$. The pair $(\mathscr{S}, rank)$ is usually identified with \mathscr{S} , keeping rank implicit. For $k \in \mathbb{N}$, we let $\mathscr{S}^{(k)} = \{a \in \mathscr{S} \mid rank(a) = k\}$.

Definition 2.1 (Graph) Let Σ be a ranked set of symbols. A graph over Σ is a tuple $G=(\dot{G},\bar{G},att_G,lab_G,front_G,rear_G)$, where \dot{G} and \bar{G} are disjoint finite sets of nodes and edges, respectively, $att_G\colon \bar{G}\to \dot{G}^*$ attaches sequences of nodes to edges, $lab_G\colon \bar{G}\to \Sigma$ labels edges with symbols so that $|att_G(e)|=rank(lab_G(e))$ for every edge $e\in \bar{G}$, and the repetition-free node sequences $front_G,rear_G\in \dot{G}^*$ are the front and the front and the front interface, respectively.

The *type* of a graph G is $(|front_G|, |rear_G|)$. The set of all graphs of type (m, n) is denoted by $\mathbb{G}_{\Sigma}^{(m,n)}$. Furthermore, $\mathbb{G}_{\Sigma}^m = \bigcup_{n \in \mathbb{N}} \mathbb{G}_{\Sigma}^{(m,n)}$ and $\mathbb{G}_{\Sigma} = \bigcup_{m,n \in \mathbb{N}} \mathbb{G}_{\Sigma}^{(m,n)}$. A subset $\mathscr{L} \subseteq \mathbb{G}_{\Sigma}$ is called a *graph language*, and if $\mathscr{L} \subseteq \mathbb{G}_{\Sigma}^{(m,n)}$, then it is a graph language of type (m,n).

A permutation graph is a graph G with $\bar{G} = \emptyset$ and $\dot{G} = [front_G] = [rear_G]$. If, furthermore, $front_G = rear_G$ and $|\dot{G}| = n$, then G is an identity graph (on n nodes) and is denoted by Id_n .

Definition 2.2 (Graph Concatenation [16]) Let $G \in \mathbb{G}^{(i,k)}_{\Sigma}$ and $H \in \mathbb{G}^{(k,j)}_{\Sigma}$. We assume for simplicity that $rear_G = front_H$, $\dot{G} \cap \dot{H} = [rear_G] = [front_H]$, and $\bar{G} \cap \bar{H} = \varnothing$. (Otherwise, appropriate isomorphic copies of G and H are used.) The (typed) concatenation $G \cdot H$ of G and G is the graph G such that $\dot{C} = \dot{G} \cup \dot{H}$, $\dot{C} = \bar{G} \cup \bar{H}$, $att_C = att_G \cup att_H$, $lab_C = lab_G \cup lab_H$, $front_C = front_G$, and $rear_C = rear_H$. Thus, $C \in \mathbb{G}^{(i,j)}_{\Sigma}$.

Note that $G \cdot H$ is defined on concrete graphs if the assumptions in Definition 2.2 are satisfied, but is otherwise only defined up to isomorphism. To avoid unnecessary technicalities, we usually assume without mentioning that the former is indeed the case.

We will need to find frontal subgraphs of a graph and to cut them off in order to define the semantics of alternating graph automata and systems of graph formulas in the next sections.

Definition 2.3 (Frontal Subgraphs and Cutting Them Off) A graph $G \in \mathbb{G}^{(i,k)}_{\Sigma}$ is a *frontal subgraph* of $H \in \mathbb{G}^{(i,j)}_{\Sigma}$ if

- $\dot{G} \subseteq \dot{H}$,
- $\bar{G} \subseteq \bar{H}$ with $lab_G(e) = lab_H(e)$ and $att_G(e) = att_H(e)$ for all $e \in \bar{G}$,
- $front_G = front_H$, and
- for all $v \in \dot{G}$, $v \in [rear_H]$ implies $v \in [rear_G]$.

Then, *cutting* G *off* H yields the graph $H \ominus G$, which is obtained from H by removing all nodes in $\dot{G} \setminus [rear_G]$, as well as all edges that are either in \bar{G} or attached to a node in $\dot{G} \setminus [rear_G]$. In the resulting graph, $rear_G$ becomes the front interface and $rear_H$ becomes the rear interface.

Example 2.1 Figure 1 shows graphs G and G' of type (2,1), from which frontal subgraphs F and F' of type (2,2) are cut off, yielding the results R, R', and R''. Nodes with the same name (written inside the circle) correspond to each other in subgraph relations.

Figure 1: Cutting off frontal subgraphs.

Our graphical conventions for drawing graphs are as follows. Binary edges like the ones in this example are drawn as arrows. Edges of other ranks are drawn as boxes connected to their attached nodes by lines. If there is more than one edge label, labels are ascribed to the arrows or written inside the boxes, or we may distinguish differently labeled edges by drawing them in different styles. Throughout the paper, we reserve the binary special edge label _, the "invisible label", to mean "unlabeled". Graphs over { _, } are called *unlabeled graphs*.

Front and rear interface nodes are connected with double lines to the left and right border, respectively, of the graph. Both sequences are ordered from top to bottom. The graph F, for instance, thus has type (2,2).

Note that even though F and F' are isomorphic, they are different frontal subgraphs of G', leading to different results $R' = G' \ominus F$ and $R'' = G' \ominus F'$. Another fact worth noting is that cutting F and F' off G' also removes the other edge attached to node a, which would otherwise dangle. Thus, \ominus is not the inverse of graph concatenation.

A basic property of the cut operation is that it is compatible with graph concatenation:

Fact 2.4 For all graphs G, Γ, Γ' of appropriate types, it holds that $(G \ominus \Gamma) \ominus \Gamma' = G \ominus (\Gamma \cdot \Gamma')$.

3 Alternating Graph Automata

We now recall the definition of alternating graph automata of [5, 12].

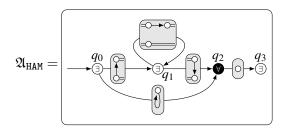


Figure 2: An alternating graph automaton accepting graphs containing a Hamiltonian cycle.

Definition 3.1 An alternating graph automaton over Σ is given by $\mathfrak{A} = (\Sigma, Q, \Delta, q_0, Q_{\forall})$ where

- Σ is a ranked set of edge labels,
- Q is a ranked set of states,
- $\Delta \subseteq \bigcup_{m,n\in\mathbb{N}} \left(Q^{(m)} \times \mathbb{G}^{(m,n)}_{\Sigma} \times Q^{(n)}\right)$ is the set of *transitions*,
- $q_0 \in Q$ is the *initial state*, and
- $Q_{\forall} \subseteq Q$ is the subset of *universal states*.

The set $Q \setminus Q_{\forall}$ of *existential* states is denoted by Q_{\exists} . A *permutation cycle* of \mathfrak{A} is a non-empty sequence $\delta_1 \delta_2 \cdots \delta_n \in \Delta^*$ where $\delta_i = (q_i, \Gamma_i, q_i')$, Γ_i is a permutation graph, and $q_i' = q_{(i \bmod n)+1}$ for each $i \in [n]$.

Example 3.1 Figure 2 shows an example of an alternating graph automaton. In such illustrations of alternating graph automata, they are drawn as transition diagrams. The dangling incoming arrow indicates the initial state q_0 , and transitions (q, Γ, q') are drawn as arrows from q to q' with the graph Γ drawn on it. The interior of existential states is white with a small inscribed \exists , and that of universal states is black with a small inscribed \forall .

In [12], the semantics of alternating graph automata is defined by means of their *configuration graphs*. In this paper, we will apply this approach not only to alternating graph automata, but also to define the semantics of systems of graph formulas (in Section 4). For this, we now introduce *evaluation graphs*, a slightly more abstract version of configuration graphs.

Evaluation graphs have existential and universal nodes which, when instantiated to the case of alternating graph automata, will correspond to configurations of the automaton in existential and universal states, respectively. Iteratively, each node receives a truth value as the disjunction or conjunction, respectively, of the truth values of its successors. This process starts at the nodes which do not have outgoing edges, whose truth values are either false (for existential nodes) or true (for universal ones). Since the graph may contain cycles, the truth values at some nodes may remain indeterminate.

Definition 3.2 (Evaluation Graph and Truth Assignment Evolution) An *evaluation graph* is an unlabeled graph in which every node is classified as either *universal* or *existential*. Given such an evaluation graph E, we let Ass_E denote the set of all partial functions $\alpha : \dot{E} \to \{true, false\}$ assigning truth values to (some of) the nodes in E. A truth assignment $\alpha \in Ass_E$ evolves (directly) into the truth assignment $\alpha' \in Ass_E$ given as follows, for all $c \in \dot{E}$: if

- (1) c is universal and
 - (1.1) has only outgoing edges to nodes $c' \in \dot{E}$ such that $\alpha(c') = true$ or
 - (1.2) has an outgoing edge to some $c' \in \dot{E}$ such that $\alpha(c') = false$, or
- (2) c is existential and
 - (2.1) has only outgoing edges to nodes $c' \in \dot{E}$ such that $\alpha(c') = false$ or

(2.2) has an outgoing edge to some $c' \in \dot{E}$ such that $\alpha(c') = true$

then

$$\alpha'(c) = \begin{cases} true & \text{in cases (1.1) and (2.2)} \\ false & \text{in cases (1.2) and (2.1)}. \end{cases}$$

If none of the conditions (1.1)–(2.2) is satisfied, then $\alpha'(c) = \alpha(c)$.

The function that maps every truth assignment to the one it evolves into is denoted by Evo_E , i.e., in the case above $\alpha' = Evo_E(\alpha)$.

Let α_{\perp} be the completely undefined truth assignment. It is shown in [12] (for configuration graphs, but the proof is the same) that the sequence $(Evo_E^i(\alpha_{\perp}))_{i\in\mathbb{N}}$ has a fixed point, in the following denoted by $Evo_E^*(\alpha_{\perp})$. More precisely, for truth assignments α and α' , let $\alpha \sqsubseteq \alpha'$ if $\alpha'(c) = \alpha(c)$ for all $c \in \dot{E}$ such that $\alpha(c)$ is defined. Then the following holds:

Fact 3.3 (Part of [12, Lemma 1]) For every evaluation graph E, the fixed point $\alpha_E^* = Evo_E^*(\alpha_\perp)$ exists and it is the smallest fixed point of Evo_E with respect to \sqsubseteq .

Intuitively, $\alpha_E^* = Evo_E^*(\alpha_\perp)$ is the "most undefined" fixed point of Evo_E . We now recall configuration graphs from [12], a particular type of evaluation graphs.

Definition 3.4 (Configuration Graph) A *configuration* of an alternating graph automaton $\mathfrak{A} = (\Sigma, Q, \Delta, q_0, Q_{\forall})$ is a pair $(q, G) \in \bigcup_{m \in \mathbb{N}} (Q^{(m)} \times \mathbb{G}_{\Sigma}^m)$. It is *universal* if q is, and *existential* otherwise. There is a *(transition) step* $(q, G) \vdash_{\Delta} (q', G')$ if there is a transition $(q, \Gamma, q') \in \Delta$ such that (an isomorphic copy of) Γ is a frontal subgraph of G and $G' = G \ominus \Gamma$.

The *configuration graph* of $\mathfrak A$ for an input graph $G_0 \in \mathbb G^{rank(q_0)}_{\Sigma}$ is the smallest graph $CG_{\mathfrak A}(G_0)$ over configurations containing the *initial configuration* (q_0,G_0) and, for each configuration (q,G) that it contains and each step $(q,G) \vdash_{\Delta} (q',G')$, the node (q',G') and an edge from (q,G) to (q',G') representing this step.

Obviously, configuration graphs are evaluation graphs. Hence, the semantics of alternating graph automata can be defined using Fact 3.3, as follows.

Definition 3.5 (Languages Accepted by Alternating Graph Automata) Let $\mathfrak{A} = (\Sigma, Q, \Delta, q_0, Q_{\forall})$ be an alternating graph automaton. An input graph $G_0 \in \mathbb{G}^{rank(q_0)}_{\Sigma}$ is *accepted* by \mathfrak{A} if $\alpha_K^*(q_0, G_0) = true$ and is *rejected* by \mathfrak{A} if $\alpha_K^*(q_0, G_0) = false$, where K is the configuration graph of \mathfrak{A} for G.

The lower (upper) language accepted by $\mathfrak A$ is the set $\underline{L}(\mathfrak A)$ (the set $\overline{L}(\mathfrak A)$, resp.) of all graphs $G_0 \in \mathbb G^{rank(q_0)}_{\Sigma}$ accepted (not rejected, resp.) by $\mathfrak A$.

Note that every state q without outgoing transitions can be considered as accepting or rejecting, depending on whether it is universal or not. This is because, for every configuration $c \in K$ which does not have outgoing edges in K, by the definition of Evo_K it holds that $Evo_K(\alpha)(c) = true$ if c is universal (by case (1.1)), and $Evo_K(\alpha)(c) = false$ if c is existential (by case (2.1)), for every assignment α . In particular, this is the case for c = (q, G) if q has no outgoing transitions at all.

If α_K^* is a total function for all input graphs in $\mathbb{G}_{\Sigma}^{rank(q_0)}$, we have $\underline{L}(\mathfrak{A}) = \overline{L}(\mathfrak{A})$. Then we say that $L(\mathfrak{A}) = \underline{L}(\mathfrak{A})$ is the *language accepted by* \mathfrak{A} . As explained in [12], a sufficient condition for this is that \mathfrak{A} does not have permutation cycles. Then each configuration graph is a directed acyclic graph (DAG) and the construction of α_K^* as the fixed point of $Evo_K^0(\alpha_\perp), Evo_K^1(\alpha_\perp), Evo_K^2(\alpha_\perp), \ldots$ can be replaced by a simple recursive evaluation of $\alpha_K^*(c)$ for all $c \in K$.

As shown in [12, Theorem 2] alternating graph automata can accept graph languages that are PSPACE-complete.

Example 3.2 The automaton shown in Figure 2 detects whether a graph contains a Hamiltonian cycle or not, basically by checking whether there is a cycle in the graph such that there are no more nodes. It does this in the following way: Using the transitions from state q_0 via q_1 to q_2 , the automaton finds and follows a cycle of at least two binary edges. Using the transition from state q_0 directly to q_2 instead, it finds a single loop. In both cases the automaton ignores all other edges connected to nodes of the cycle (by cutting them off). The automaton accepts the graph if it finds no more nodes after reaching q_2 . Otherwise it reaches the rejecting state q_3 , so it rejects the graph.

4 Graph Expressions and Systems of Graph Formulas

We now define graph expressions and, based on them, systems of graph formulas with variables. Similarly to ordinary regular expressions for string languages, graph expressions construct graph languages from singleton languages by means of union, concatenation, and Kleene star as operators.

Definition 4.1 (Graph Expressions) Let $i, j, k \in \mathbb{N}$.

- $\bullet \ \ \text{The (typed) concatenation of } \mathscr{L} \subseteq \mathbb{G}_{\Sigma}^{(i,k)} \ \text{and} \ \mathscr{M} \subseteq \mathbb{G}_{\Sigma}^{(k,j)} \ \text{is} \ \mathscr{L} \cdot \mathscr{M} = \{G \cdot H \mid G \in \mathscr{L}, H \in \mathscr{M}\}.$
- The (*Kleene*) star \mathscr{L}^* of $\mathscr{L} \subseteq \mathbb{G}^{(i,i)}_{\Sigma}$ is the smallest graph language containing Id_i and, for all graphs $G \in \mathscr{L}$ and $H \in \mathscr{L}^*$, the graph $G \cdot H \in \mathscr{L}^*$.

The set $\mathbb{E}_{\Sigma}^{(i,j)}$ of graph expressions ex of type (i,j) over Σ and the languages L(ex) they denote are defined inductively, as follows:

- 1. $\varnothing \in \mathbb{E}_{\Sigma}^{(i,j)}$ with $L(\varnothing) = \varnothing$.
- 2. If $G \in \mathbb{G}_{\Sigma}^{(i,j)}$, then $G \in \mathbb{E}_{\Sigma}^{(i,j)}$ with $L(G) = \{G\}$.
- 3. If $ex_1, ex_2 \in \mathbb{E}_{\Sigma}^{(i,j)}$, then $ex_1 \oplus ex_2 \in \mathbb{E}_{\Sigma}^{(i,j)}$ with $L(ex_1 \oplus ex_2) = L(ex_1) \cup L(ex_2)$.
- 4. If $ex_1 \in \mathbb{E}^{(i,j)}$ and $ex_2 \in \mathbb{E}^{(j,k)}_{\Sigma}$, then $ex_1 \odot ex_2 \in \mathbb{E}^{(i,k)}_{\Sigma}$ with $L(ex_1 \odot ex_2) = L(ex_1) \cdot L(ex_2)$.
- 5. If $ex \in \mathbb{E}_{\Sigma}^{(i,i)}$, then $ex^{\circledast} \in \mathbb{E}_{\Sigma}^{(i,i)}$ with $L(ex^{\circledast}) = L(ex)^*$.

Note that graph concatenation is associative. For $\mathscr{L} \subseteq \mathbb{G}_{\Sigma}^{(i,i)}$, we may also abbreviate the *n*-fold iterated concatenation of \mathscr{L} with itself by \mathscr{L}^n , i.e., $\mathscr{L}^0 = \{Id_i\}$ and $\mathscr{L}^{n+1} = \mathscr{L} \cdot \mathscr{L}^n$ for $n \in \mathbb{N}$.

Example 4.1 (Paths and Cycles) The following graph expressions specify a path from the front node to a node attached to a unary edge labeled L, and a cycle in a graph (with empty front interface), respectively.

$$\mathsf{Path} = \textcircled{\$} \odot \textcircled{\blacksquare} \mathsf{Cycle} = \textcircled{\blacksquare} \mathsf{Cycle} =$$

In examples, \circledast binds stronger than \odot , and \odot binds stronger than \oplus .

Definition 4.2 (System of Graph Formulas with Variables) For $m \in \mathbb{N}$ and ranked sets Σ and X of edge labels and variables, respectively, the set $\mathscr{F}^m_{\Sigma,X}$ of graph formulas with variables (formulas for short) of type m over Σ and X is defined inductively as follows:

- (1) $true, false \in \mathscr{F}^m_{\Sigma,X}$;
- (2) $X^{(m)} \subseteq \mathscr{F}_{\Sigma X}^m$;
- (3) if $ex \in \mathbb{E}_{\Sigma}^{(m,i)}$ and $fo \in \mathscr{F}_{\Sigma,X}^i$, then $\exists (ex,fo) \in \mathscr{F}_{\Sigma,X}^m$ and $\forall (ex,fo) \in \mathscr{F}_{\Sigma,X}^m$;
- (4) if $fo, fo' \in \mathscr{F}^m_{\Sigma,X}$, then $\neg fo \in \mathscr{F}^m_{\Sigma,X}$, $fo \land fo' \in \mathscr{F}^m_{\Sigma,X}$, and $fo \lor fo' \in \mathscr{F}^m_{\Sigma,X}$.

A formula fo is called *conjunctive* when fo = true, when it has the form $fo = fo' \land fo''$, or the form $fo = \forall (ex, fo')$. In all other cases, fo is called *disjunctive*.

We let $\mathscr{F}_{\Sigma,X} = \bigcup_{m \in \mathbb{N}} \mathscr{F}_{\Sigma,X}^m$ denote the set of all formulas over Σ and X.

A system of graph formulas with variables (formula system for short) is a function $F: X \to \mathscr{F}_{\Sigma,X}$ such that $F(x) \in \mathscr{F}_{\Sigma,X}^m$ for all $x \in X^{(m)}$.

We will use the classification of formulas into conjunctive and disjunctive formulas later on when defining formula configurations.

In the following, unless explicitly stated otherwise, we assume fixed ranked sets Σ and X of edge labels and variables, respectively.

Note that those formulas which can be built without using case (2) in Definition 4.2, are precisely the graph formulas without variables as they are defined in [11]. In other words, the latter set is a strict subset of the formulas considered here.

Before formalizing the semantics of formula systems, we define the special case of *acyclic* formula systems.

Definition 4.3 (Acyclic formula system) Given a *formula system* $F: X \to \mathscr{F}_{\Sigma,X}$, the *dependency graph* D_F of F is an unlabeled graph defined as follows: Its node set is $\dot{D}_F = X$, and there is an edge from $u \in X$ to $v \in X$ whenever v appears as a variable in F(u). The formula system F is *acyclic* if D_F is acyclic.

We now define the semantics of formula systems. A natural approach would be to define the semantics inductively based on the structure of the formulas. However, this is challenging because a formula may directly or indirectly depend on the variable to which it is assigned within the system, potentially creating cyclic dependencies. For traditional systems of language equations as introduced in the seminal paper by Mezei and Wright [22] such dependencies do not pose problems as there is a least fixed point, i.e., there is a smallest assignment of languages to the variables (with respect to set inclusion) such that the language equations are fulfilled. This is due to the monotonicity of the involved operations. Here, such monotonicity is lacking, essentially because formulas may contain negations.

To deal with this situation, we adopt an approach similar to that used for alternating graph automata. Specifically, we define the semantics in terms of *formula configuration graphs*, a specialized form of evaluation graphs. This approach allows us to define the general semantics through the fixed points of truth value assignments.

Definition 4.4 (Formula Configuration Graph (FCG)) A *formula configuration* is a triple (fo, G, sign) where $fo \in \mathscr{F}^m_{\Sigma,X}$, $G \in \mathbb{G}^m_{\Sigma}$, and $sign \in \{pos, neg\}$. It is called *universal* if sign = pos and fo is conjunctive, or sign = neg and fo is disjunctive. Otherwise, it is said to be *existential*.

Given a formula system $F: X \to \mathscr{F}_{\Sigma,X}$, there is a $step\ (fo,G,sign) \rhd_F (fo',G',sign')$ from the formula configuration (fo,G,sign) to (fo',G',sign') in the following cases, for all $\emptyset \in \{\lor,\land\}$, $Q \in \{\lor,\exists\}$, and $x \in X$:

- $(\neg fo, G, sign) \triangleright_F (fo, G, \overline{sign})$ where $\overline{pos} = \text{neg and } \overline{\text{neg}} = \text{pos}$,
- $(fo_1 \otimes fo_2, G, sign) \triangleright_F (fo_1, G, sign)$ and $(fo_1 \otimes fo_2, G, sign) \triangleright_F (fo_2, G, sign)$,
- $(Q(ex,fo),G,sign) \triangleright_F (fo,G \ominus P,sign)$ for all frontal subgraphs $P \in L(ex)$ of G, and
- $(x,G,sign) \triangleright_F (F(x),G,sign)$.

Given a formula system $F: X \to \mathscr{F}_{\Sigma,X}$ and a variable $x \in X$, the formula configuration graph (FCG for short) of F at x for an input graph $G_0 \in \mathbb{G}^m_\Sigma$ is the smallest graph $FCG_{F,x}(G_0)$ over formula configurations containing the *initial configuration* (x, G_0, pos) and, for each formula configuration $(f_0, G, sign)$ that it contains and each step $(f_0, G, sign) \triangleright_F (f_0', G', sign')$, the node $(f_0', G', sign')$ and an edge from $(f_0, G, sign)$ to $(f_0', G', sign')$ representing this step.

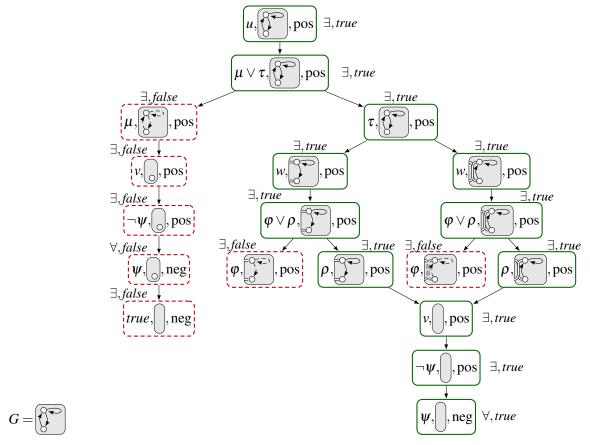


Figure 3: A graph

Figure 4: The formula configuration graph $FCG_{H,u}(G)$

Note that the FCG is finite for any formula system *F* and variable *x*.

Example 4.2 Let $\Sigma = \{ \subseteq \}$ with $rank(\subseteq) = 2$, and let $X = \{u, v, w\}$, where each variable has rank 0. We define the formula system $H: X \to \mathscr{F}_{\Sigma,X}$ by:

$$H(u) = \overrightarrow{\exists \left(\overrightarrow{0}, v \right)} \vee \overrightarrow{\exists \left(\overrightarrow{0}, w \right)}, \qquad H(v) = \neg \overrightarrow{\exists \left(\overrightarrow{0}, true \right)}, \qquad H(w) = \overrightarrow{\exists \left(\overrightarrow{0}, w \right)} \vee \overrightarrow{\exists \left(\overrightarrow{0}, v \right)}.$$

We name subformulas μ , τ , ψ , φ , and ρ for reference in Figure 4.

The intuitive semantics of H is as follows: the variable u defines graphs that either consist of a node with a loop followed by a subgraph described by v (subformula μ), or a graph that starts with an edge and continues with a subgraph described by w (subformula τ). The variable w is satisfied by graphs that either start with an edge and are recursively followed by another w graph (subformula φ), or graphs that connect the two front interface nodes with a single edge followed by a subgraph satisfying v (subformula φ). Finally, v is satisfied if there are no nodes left in the graph. All in all, u specifies graphs that contain a Hamiltonian cycle.

Figure 4 shows the formula configuration graph $FCG_{H,u}(G)$ for the graph G shown in Figure 3. The labels next to the configurations indicate whether they are universal (\forall) or existential (\exists) . The indicated truth values will become relevant in Example 4.3. Note that the formula configuration graph $FCG_{H,u}(G)$ is acyclic, in contrast to H itself, which is cyclic.

Since every FCG K is an evaluation graph, we can once again use Definition 3.2 to describe how truth values assigned to formula configurations evolve from an initial assignment. By Fact 3.3, the most undefined fixed point, denoted by α_K^* , exists. Following the approach in Definition 3.5, we thus define:

Definition 4.5 (Languages Accepted by Formula Systems) Given a formula system $F: X \to \mathscr{F}_{\Sigma,X}$ and a variable $x \in X$, an input graph $G_0 \in \mathbb{G}_{\Sigma}^m$ is *accepted* by F at x if $\alpha_K^*(x, G_0, pos) = true$ and is *rejected* by F at x if $\alpha_K^*(x, G_0, pos) = false$, where K is the formula configuration graph of F at x.

The lower language accepted by F at x is the set $\underline{L}_x(F)$ of all graphs $G_0 \in \mathbb{G}_{\Sigma}^m$ accepted by F at x, and the upper language accepted by F at x is the set $\overline{L}_x(F)$ of all graphs $G_0 \in \mathbb{G}_{\Sigma}^m$ not rejected by F at x.

In the special case where α_K^* is a total function for all input graphs in \mathbb{G}_{Σ}^m , we have $\underline{L}_x(F) = \overline{L}_x(F)$. Then we say that $L_x(F) = \underline{L}_x(F)$ is the *language accepted by F at x*.

Note the difference between this definition and Definition 3.5: While an automaton has a particular state designated as its initial state, no particular variable is singled out as "initial" in a formula system. Therefore, there is not a single pair of upper and lower languages defined by a formula system, but each variable is associated with its own pair of languages. To put it in another way, specifying a pair of upper and lower languages by a formula system requires us to additionally say which variable we are considering.

Example 4.3 Continuing Example 4.2, let $K = FCG_{H,u}(G)$. The truth value assigned by α_K^* is specified for each configuration in Figure 4. Since K is acyclic, the function α_K^* is total, and $G \in \underline{L}_u(H) \cap \overline{L}_u(H)$.

Let us now demonstrate that the semantics of graph formulas without variables, as defined in [11], coincides with the semantics of acyclic formula systems.

Every variable $x \in X$ occurring in an acyclic formula system F can be identified with an acyclic formula $F^*(x)$ in the sense of [11], namely the one obtained by taking F(x) and recursively replacing every occurrence of a variable x' in it by $F^*(x')$. Conversely, every formula fo in the sense of [11] can be written as the acyclic formula system $F(x) = \varphi$ with only one variable x. In other words, acyclic formula systems do indeed coincide with the graph formulas of [11]. The following lemma shows that the semantics of acyclic formula systems coincides with the inductive semantics definition of graph formulas in [11]:

Lemma 4.6 For each acyclic formula system $F: X \to \mathscr{F}_{\Sigma,X}$ and each variable $x \in X$, it holds that $\underline{L}_x(F) = \overline{L}_x(F) = \{G \mid G \vDash_F x\}$ where the satisfaction relation $\vDash_F \subseteq \mathbb{G}_{\Sigma}^m \times \mathscr{F}_{\Sigma,X}^m$ is defined by induction as follows. It is the smallest relation such that the following hold for every graph $G \in \mathbb{G}_{\Sigma}^m$ (where $fo, fo' \in \mathscr{F}_{\Sigma,X}$ and $x \in X$):

- (1) $G \vDash_F true$.
- (2) $G \vDash_F \exists (ex, fo) \text{ if } G \ominus P \vDash_F fo \text{ for some frontal subgraph } P \in L(ex) \text{ of } G.$
- (3) $G \vDash_F \forall (ex, fo) \text{ if } G \ominus P \vDash_F fo \text{ for all frontal subgraphs } P \in L(ex) \text{ of } G.$
- (4) $G \vDash_F \neg fo \text{ if } G \not\vDash_F fo.$
- (5) $G \vDash_F fo \land fo'$ if $G \vDash_F fo$ as well as $G \vDash_F fo'$.
- (6) $G \vDash_F fo \lor fo'$ if $G \vDash_F fo$ or $G \vDash_F fo'$ (or both).
- (7) $G \vDash_F x$ if $G \vDash_F F(x)$.

The definition of the satisfaction relation in this lemma is a straightforward extension of [11, Definition 7], which defines satisfaction of graph formulas without variables. Lemma 4.6 simply adds case (7) and defines the satisfaction of variables by the satisfaction of the assigned formula.

Proof. Let $F: X \to \mathscr{F}_{\Sigma,X}$ be an acyclic formula system, $x \in X$ a variable, and $G_0 \in \mathbb{G}_{\Sigma}^{rank(x)}$ a graph. Define $K = FCG_{F,x}(G_0)$ as the FCG of F at x for G_0 .

We first show that K is acyclic. Suppose, for contradiction, that K contains a cycle. By the definition of the step relation \triangleright_F in Definition 4.4, such a cycle must include formula configurations (y, G, sign) and $(F(y), G, sign) \in K$ such that

$$(y, G, sign) \triangleright_F (F(y), G, sign) \triangleright_F^* (y, G, sign)$$

for some $y \in X$. This implies that the dependency graph D_F of F contains a cycle involving y, contradicting the assumption that F is acyclic. This proves that K is acyclic.

For each formula configuration $c = (fo, G, sign) \in K$, we prove by induction on the length of the longest path starting at c that

$$\alpha_K^*(c) = \begin{cases} true & \text{if } sign = \text{pos and } G \vDash_F fo, \text{ or } sign = \text{neg and } G \not\vDash_F fo, \\ false & \text{otherwise.} \end{cases}$$
 (1)

For the base case, consider a configuration c with no outgoing edges. Then fo must be of the form true, false, $\exists (ex, fo')$, or $\forall (ex, fo')$. We analyze the case $fo = \forall (ex, fo')$; the others follow similarly.

Since $fo = \forall (ex, fo')$, the configuration c is universal if sign = pos and existential if sign = neg, by Definition 4.4. The fact that c has no outgoing edges means that G has no frontal subgraph in L(ex), which implies $G \vDash_F fo$ by case (3). Furthermore, by Definition 3.2 the absence of edges leaving c means that $\alpha_K^*(c) = true$ if sign = pos and $\alpha_K^*(c) = false$ if sign = neg. Hence, equation (1) holds for c in both cases.

For the inductive step, assume that c has at least one successor configuration c' with $c \triangleright_F c'$, and that (1) holds for all such c'. By Definition 4.4, fo must be one of $fo \in X$, $\exists (ex, fo')$, $\forall (ex, fo')$, $\neg fo'$, $fo' \land fo''$, and $fo' \lor fo''$. In each case, either sign = pos or sign = neg, and either $G \vDash_F fo$ or $G \nvDash_F fo$. We analyze two representative cases: $fo = \forall (ex, fo')$ and $fo = \neg fo'$, both with sign = pos and $G \vDash_F fo$; the remaining cases follow similarly.

- Case $fo = \neg fo'$, sign = pos, and $G \models_F fo$. Since $fo = \neg fo'$, the only successor configuration is c' = (fo', G, neg). Since $G \models_F fo$, we have $G \not\models_F fo'$, so the induction hypothesis gives $\alpha_K^*(c') = true$. By Definition 3.2, this implies $\alpha_K^*(c) = true$, as required by equation (1).
- Case $fo = \forall (ex, fo')$, sign = pos, and $G \vDash_F fo$. By assumption, $G \vDash_F fo$. This can only be the case if $G \ominus P \vDash_F fo'$ holds for all frontal subgraphs $P \in L(ex)$. By Definition 4.4, each successor configuration of c is of the form $c' = (fo', G \ominus P, pos)$. By the induction hypothesis, $\alpha_K^*(c') = true$ for all such c', and by Definition 3.2 this implies $\alpha_K^*(c) = true$, as required by equation (1), because c is universal.

Since equation (1) holds for all configurations in K, it particularly holds for the initial configuration (x, G_0, pos) of K. Consequently,

$$\alpha_K^*(x, G_0, pos) = \begin{cases} true & \text{if } G_0 \vDash_F x, \\ false & \text{if } G_0 \not\vDash_F x. \end{cases}$$

Thus, $G_0 \vDash_F x$ if and only if $G_0 \in L_x(F)$, completing the proof.

Note that, as one would expect, by Definition 4.5 the semantics of disjunction and conjunction of formulas is both commutative and associative. This follows directly from the fact that FCGs contain no information about the order of arguments of disjunctions and conjunctions, i.e., interchanging them

results in the same FCG. Thus, given a (finite) set $FO = \{fo_1, \dots, fo_n\}$ of formulas, we can express their disjunction and conjunction using the standard notations

$$\bigvee_{fo \in FO} fo = fo_1 \lor fo_2 \lor \cdots \lor fo_n, \quad \text{and} \quad \bigwedge_{fo \in FO} fo = fo_1 \land fo_2 \land \cdots \land fo_n$$

as shorthands for sequences of binary disjunctions and conjunctions, respectively.

In the next section we will show that formula systems have the same expressive power as alternating graph automata. To facilitate that proof, but also because it is of independent interest, we now develop a normal form of formula systems which we call *shallow normal form*. The result states that every formula system F can be brought into a structurally simpler normal form F' over a larger set of variables X' such that, for all $x \in X'$, every proper sub-formula of F(x) is a variable.

Theorem 4.7 (Shallow Normal Form) For each formula system $F: X \to \mathscr{F}_{\Sigma,X}$ there is a formula system $F': X' \to \mathscr{F}_{\Sigma,X'}$ with $X' \supseteq X$ such that

- 1. $\underline{L}_x(F') = \underline{L}_x(F)$ and $\overline{L}_x(F') = \overline{L}_x(F)$ for all $x \in X$, and
- 2. for every $x \in X'$, F'(x) has one of the following forms, where $G \in \mathbb{G}_{\Sigma}$ and $x', x'' \in X'$:

true, false,
$$x' \vee x''$$
, $x' \wedge x''$, $\exists (G, x')$, and $\forall (G, x')$.

The proof of the existence of the shallow normal form makes use of an auxiliary lemma.

Lemma 4.8 Call a graph expression *non-permuting* if it has no sub-expression of the form ex^{\circledast} such that L(ex) contains a permutation graph. Then every graph expression has an equivalent non-permuting graph expression.

Proof. Denote by $P^{(i)}$ the set of all permutation graphs of type (i,i). We show the following statement by structural induction: for every graph expression $ex \in \mathbb{E}^{(i,j)}_{\Sigma}$, there is a non-permuting graph expression $ex_0 \in \mathbb{E}^{(i,j)}_{\Sigma}$ such that $L(ex_0) = L(ex) \setminus P^{(i)}$. This proves the lemma because the set P of permutation graphs in L(ex) is finite, say $P = \{\pi_1, \dots, \pi_k\}$, and thus $ex_0 \oplus \pi_1 \oplus \dots \oplus \pi_k$ is a non-permuting graph expression equivalent to ex.

The induction is straightforward: if $ex = G \in \mathbb{G}^{(i,j)}_{\Sigma}$ then $ex_0 = G$ unless G is a permutation graph, in which case $ex_0 = \varnothing$. If $ex = ex' \oplus ex''$ then $ex_0 = ex'_0 \oplus ex''_0$, where ex'_0 and ex''_0 are obtained from ex' and ex'' using the induction hypothesis. If $ex = ex' \odot ex''$ then $ex_0 = (ex'_0 \odot ex'') \oplus (ex' \odot ex''_0)$. Finally, if $ex = (ex')^{\circledast}$ and $\{\pi_1, \ldots, \pi_k\}$ is the set of permutation graphs in L(ex) then

$$ex_0 = \Pi \odot ex'_0 \odot (\Pi \odot ex'_0)^{\circledast} \odot \Pi$$

where $\Pi = \pi_1 \oplus \cdots \oplus \pi_k$.

Correctness follows immediately from the relevant definitions, especially the fact that the concatenation of graphs G and G' is a permutation graph if and only if both G and G' are.

Proof of Theorem 4.7. The construction of the shallow normal form F' of F proceeds in two steps. First we remove negations by "pushing negations down" through the formulas. Second, we repeatedly decompose formulas into smaller ones.

For the first step, let \bar{x} be a fresh copy of each variable $x \in X$, and extend F by adding the equation $F(\bar{x}) = \neg F(x)$ for every $x \in X$. Clearly, this does not affect any of the languages accepted or rejected at the original variables x because no F(x), $x \in X$, contains one of the new variables. Consequently, the

language accepted (rejected) at \bar{x} is the language rejected (accepted, respectively) at x, for every $x \in X$. In the following, we let $\bar{X} = \{\bar{x} \mid x \in X\}$ and $\bar{\bar{x}} = x$ for all $x \in X$.

Now, as long as the formula system obtained in this way still contains negations, pick any subformula of the form $\neg fo$ and replace it by

$$\begin{cases} fo' & \text{if } fo = \neg fo' \\ \neg fo' \ \bar{\otimes} \ \neg fo'' & \text{if } fo = fo' \otimes fo'' \text{ for some } \otimes \in \{\lor, \land\}, \text{ where } \bar{\lor} = \land \text{ and } \bar{\land} = \lor \\ \bar{Q}(ex, \neg fo') & \text{if } fo = Q(ex, fo') \text{ for some } Q \in \{\exists, \forall\}, \text{ where } \bar{\exists} = \forall \text{ and } \bar{\forall} = \exists \\ \bar{x} & \text{if } fo = x \in X \cup \bar{X}. \\ \bar{fo} & \text{if } fo \in \{true, false\}, \text{ where } \bar{true} = false \text{ and } \bar{false} = true \end{cases}$$

Obviously, this transformation procedure terminates after a finite number of steps and results in a formula system without occurrences of \neg .

Using the standard rules of predicate logic (in particular deMorgan's rules) and the relation between the languages accepted and rejected at x and \bar{x} , it can be verified in a straightforward manner that each of the transformation steps preserves those languages, and thus by induction the languages accepted and rejected by the resulting formula system at each $x \in X$ are preserved as well. In the following, second step of the transformation to normal form, we can thus assume without loss of generality that the original system F does not contain negations.

Next, we transform the formula system iteratively until it is in shallow normal form. In doing so, we may keep equations of the form F'(x) = x', because such an equation can obviously be replaced by $F'(x) = x' \wedge x'$ without affecting the most undefined fixed point α^* .

If F is is not yet in shallow normal form, pick an $x \in X$ such that F(x) is not as required. We decompose F(x) by introducing one or two fresh variables and replacing the equation for F(x) by two or more equations. For all $x' \in X \setminus \{x\}$ we let F'(x') = F(x'). We distinguish the relevant cases, where x_1 and x_2 are fresh variables of appropriate types.

If $F(x) = fo_1 \otimes fo_2$ with $\emptyset \in \{ \vee, \wedge \}$ and $\{ fo_1, fo_2 \} \nsubseteq X$, we let $F'(x) = x_1 \otimes x_2$ and $F'(x_i) = fo_i$ for $i \in [2]$.

If
$$F(x) = Q(G,fo)$$
 with $Q \in \{\exists, \forall\}$, $G \in \mathbb{G}_{\Sigma}$, and $fo \notin X$, let $F'(x) = Q(G,x_1)$ and $F'(x_1) = fo$.

Finally, let F(x) = Q(ex, fo) where $Q \in \{\exists, \forall\}$ and $ex \notin \mathbb{G}_{\Sigma}$. By Lemma 4.8, we may assume without loss of generality that ex is non-permuting. This case has a number of sub-cases depending on the structure of ex, as follows.

If $ex = ex_1 \oplus ex_2$, we define

$$F'(x) = \begin{cases} x_1 \lor x_2 & \text{if } \mathsf{Q} = \exists \\ x_1 \land x_2 & \text{if } \mathsf{Q} = \forall \end{cases} \text{ and } F'(x_i) = \mathsf{Q}(ex_i, fo) \text{ for } i \in [2].$$

If $ex = ex_1 \odot ex_2$, we define $F'(x) = Q(ex_1, x_1)$ and $F'(x_1) = Q(ex_2, fo)$, which is semantically equivalent by Fact 2.4.

If $ex = ex_1^{\circledast}$, we define

$$F'(x) = \begin{cases} x_1 \lor x_2 & \text{if } Q = \exists \\ x_1 \land x_2 & \text{if } Q = \forall \end{cases} \quad F'(x_1) = fo \quad \text{and} \quad F'(x_2) = Q(ex_1, x)$$

again making use of Fact 2.4.

This construction can only be repeated a finite number of times (bounded from above by the sum of the sizes of the formulas F(x)) because in each step the sum of the sizes of those formulas which violate normal form is reduced by one.

For the correctness proof of the construction, we need to show that every step of the transformation preserves the languages at each of the original variables. Rather than showing this in detail for each case, we look at one example case because the rest is similar. We consider the least obvious one of the cases, namely F(x) = Q(ex,fo) where $ex = ex_1^{\circledast}$. Assume that $Q = \forall$ (the case $Q = \exists$ is dual and thus follows by the same arguments) and consider FCGs $FCG_{F,x_0}(G_0)$ and $FCG_{F',x_0}(G_0)$, respectively, for some input graph G_0 .

In the rest of the proof, we denote the set of all frontal subgraphs of a graph G by FG(G).

Now, consider a configuration $\kappa = (x, G, sign)$ in $FCG_{F,x_0}(G_0)$. By the definition of $FCG_{F,x_0}(G_0)$, κ has the unique successor $(\forall (ex,fo),G,sign)$. In turn, the successors of that configuration are all (fo,G',sign) such that $G' \in NEXT$, where

$$NEXT = \{G \ominus \Gamma \mid \Gamma \in FG(G) \cap L(ex)\}.$$

Since $ex = ex_1^\circledast$ and NEXT is finite, there is some $k \in \mathbb{N}$ such that $NEXT = NEXT_0 \cup \cdots \cup NEXT_k$ where $NEXT_0 = \{G\}$ and $NEXT_{i+1} = \{G' \ominus \Gamma \mid G' \in NEXT_i, \ \Gamma \in FG(G') \cap L(ex_1)\}$ for all $i \in \mathbb{N}$. Note that, since $L(ex_1)$ does not contain permutation graphs, each $G' \ominus \Gamma$ in this construction is strictly smaller than G'.

 $FCG_{F',x_0}(G_0)$ differs from $FCG_{F,x_0}(G_0)$ in that the edges from κ to (fo,G',sign) $(G'\in NEXT)$ are replaced by a more complex structure. Since

$$F'(x) = \begin{cases} x_1 \lor x_2 & \text{if } \mathsf{Q} = \exists \\ x_1 \land x_2 & \text{if } \mathsf{Q} = \forall \end{cases} \quad F'(x_1) = fo \quad \text{and} \quad F'(x_2) = \mathsf{Q}(ex_1, x),$$

this structure is defined recursively, as follows: For every graph $G' \in NEXT_i$ such that $FCG_{F',x_0}(G_0)$ contains the configuration $\kappa' = (x, G', sign)$ (the initial case being $\kappa' = \kappa$), there is an edge from κ' to $(x_1 \land x_2, G', sign)$ and there are edges from the latter to $(x_1, G', sign)$ and $(x_2, G', sign)$. These have the unique successors (fo, G', sign) and $(\forall (ex_1, x), G', sign)$, respectively. Of these, the former is in $FCG_{F',x_0}(G_0)$ (the recursive construction stops) whereas the latter has all (x, G'', sign) as successors such that $G'' \in NEXT_{i+1}$. The fact that G'' is strictly smaller than G' ensures that the subgraph of $FCG_{F',x_0}(G_0)$ created in this way is a DAG whose leaves are precisely the elements of NEXT, i.e., the successors of (fo, G', sign) in $FCG_{F,x_0}(G_0)$. It follows that $\alpha^*_{FCG_{F',x_0}(G_0)}(\kappa') = \alpha^*_{FCG_{F,x_0}(G_0)}(\kappa)$, as claimed.

5 Expressive Power of Formula Systems

In this section, we investigate the expressive power of formula systems and establish their equivalence to alternating graph automata. Specifically, we show that every alternating graph automaton can be transformed into a formula system that yields the same upper and lower languages. Conversely, we construct an alternating graph automaton for any given formula system F in shallow normal form and any $x \in X$, such that the languages accepted and rejected by F at x are precisely those accepted and rejected, respectively, by the automaton.

Lemma 5.1 Let $\mathfrak{A} = (\Sigma, Q, \Delta, q_0, Q_{\forall})$ be an alternating graph automaton. Define the function $F: Q \to \mathscr{F}_{\Sigma,O}$ by

$$F(q) = \begin{cases} \bigwedge_{(q,\Gamma,q') \in \Delta} \forall (\Gamma,q') & \text{if } q \in Q_{\forall}, \\ \bigvee_{(q,\Gamma,q') \in \Delta} \exists (\Gamma,q') & \text{otherwise} \end{cases}$$
 (2)

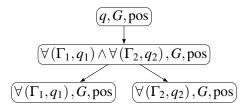


Figure 5: Formula configuration $(q, G, pos) \in \dot{K}'$ and (some of) its successors in K'.

for each state $q \in Q$. Then F is a formula system and the following equivalences hold:

$$\underline{L}(\mathfrak{A}) = \underline{L}_{q_0}(F)$$
 and $\overline{L}(\mathfrak{A}) = \overline{L}_{q_0}(F)$.

Proof. Let \mathfrak{A} and F be as described in the lemma, and consider a graph $G_0 \in \mathbb{G}^{rank(q_0)}_{\Sigma}$. Define $K = CG_{\mathfrak{A}}(G_0)$ and $K' = FCG_{F,q_0}(G_0)$ to be the configuration graph of \mathfrak{A} and the formula configuration graph of F at G_0 , respectively, both constructed for the input graph G_0 . Clearly, F is a formula system since $F(G) \in \mathscr{F}^m_{\Sigma,O}$ for every G0.

Next, we show that every configuration $(q,G) \in K$ also appears in K' as (q,G,pos) . This is proven by induction on the length of the shortest path from the initial configuration (q_0,G_0) to (q,G) in K. For the base case, the claim holds trivially since $(q_0,G_0,\operatorname{pos})$ is the initial configuration of K'. For the inductive step, assume that (q,G) and (q',G') are configurations in K such that $(q,G) \vdash_{\Delta} (q',G')$, and assume, as the induction hypothesis, that $(q,G,\operatorname{pos}) \in K'$. Further, let q have exactly $n \in \mathbb{N}$ outgoing transitions $(q,\Gamma_1,q_1),\ldots,(q,\Gamma_n,q_n) \in \Delta$. Consequently, there exists an index $i \in [n]$ and a frontal subgraph P of G such that $q'=q_i$, Γ_i is isomorphic to P, and $G'=G \ominus P$. We now consider the case where q is universal; the existential case follows analogously. Since $F(q)=\bigwedge_{i\in [n]}\forall(\Gamma_i,q_i)$, the configuration (q,G,pos) in K' has $(F(q),G,\operatorname{pos})$ as its only successor. This configuration, in turn, has successor configurations $(\forall(\Gamma_j,q_j),G,\operatorname{pos})$ in K' (along with possibly some intermediate configurations) for all $j\in [n]$. An example for n=2 is shown in Figure 5. As a result, $(\forall(\Gamma_i,q_i),G,\operatorname{pos})\triangleright_F(q',G',\operatorname{pos})$, which implies that $(q',G',\operatorname{pos})\in K'$, completing the induction.

By a very similar argument, we can show that every formula configuration $(q, G, pos) \in \dot{K}'$ also appears in \dot{K} as (q, G).

Next, we examine the most undefined fixed points α_K^* and $\alpha_{K'}^*$ for K and K', respectively. First, observe that for every formula configuration $(q,G,\operatorname{pos})\in K'$, we have $\alpha_{K'}^*(q,G,\operatorname{pos})=\alpha_{K'}^*(F(q),G,\operatorname{pos})$, since $(F(q),G,\operatorname{pos})$ is the only successor of (q,G,pos) in K'.

Now consider any formula configuration $(F(q), G, pos) \in \dot{K}'$. We focus on the case where q is universal, i.e., $F(q) = \bigwedge_{i \in [n]} \forall (\Gamma_i, q_i)$ for some $n \in \mathbb{N}$; again, the existential case is analogous. The configuration (F(q), G, pos) is the root of a subtree in K' whose leaves are the formula configurations $(\forall (\Gamma_i, q_i), G, pos)$ for each $i \in [n]$. Figure 5 illustrates this structure for n = 2. All nodes in this tree are universal.

As shown earlier, every step $(q,G) \vdash_{\Delta} (q',G')$ in K corresponds to a step $(\forall (\Gamma_i,q_i),G,\operatorname{pos}) \triangleright_F (q',G',\operatorname{pos})$ in K', and the reverse correspondence also holds. This establishes that the evolution of truth values in K and K' results in fixed points α_K^* and $\alpha_{K'}^*$ such that $\alpha_K^*(q,G) = \alpha_{K'}^*(q,G,\operatorname{pos})$ for all configurations $(q,G) \in \dot{K}$, and in particular for the initial configurations, yielding

$$\alpha_{K}^{*}(q_{0},G_{0})=\alpha_{K'}^{*}(q_{0},G_{0},\mathrm{pos}),$$

which completes the proof.

¹For simplicity, we also write $\alpha_K^*(c) = \alpha_{K'}^*(c')$ if both $\alpha_K^*(c)$ and $\alpha_{K'}^*(c')$ are undefined.

Example 5.1 Consider the alternating graph automaton in Figure 2 with the set $Q = \{q_0, q_1, q_2, q_3\}$ of states. Its equivalent formula system $F: Q \to \mathscr{F}_{\Sigma,O}$ is defined by:

$$q_0 \mapsto \exists \left(\overbrace{0}, q_2 \right) \lor \exists \left(\overbrace{0}, q_1 \right) \quad q_1 \mapsto \exists \left(\overbrace{0}, q_1 \right) \lor \exists \left(\overbrace{0}, q_2 \right) \quad q_2 \mapsto \forall \left(\overbrace{0}, q_3 \right) \quad q_3 \mapsto \mathit{false}$$

Note that $F(q_2)$ and $F(q_3)$ can be combined to $F(q_2) = \forall (\bigcirc, false)$, which is equivalent to H(v) in Example 4.2. This shows that Example 4.2 indeed specifies the language of all graphs with a Hamiltonian cycle.

To prove the converse, namely that alternating graph automata are at least as expressive as formula systems, we show that every formula system can be transformed into an equivalent alternating graph automaton. Since every formula system can be transformed into shallow normal form, it is sufficient to consider only formula systems in this normal form.

Lemma 5.2 Let $F: X \to \mathscr{F}_{\Sigma,X}$ be a formula system in shallow normal form, and let $x_0 \in X$ be any variable. Define the alternating graph automaton $\mathfrak{A} = (\Sigma, Q, \Delta, q_0, Q_{\forall})$ with Q = X, $q_0 = x_0$, $Q_{\forall} = \{x \in X \mid F(x) \text{ is conjunctive}\}$, and Δ being the smallest set such that:

- $(x, Id_m, x'), (x, Id_m, x'') \in \Delta$ for each $x \in X^{(m)}$ such that F(x) is of the form $x' \vee x''$ or $x' \wedge x''$.
- $(x, \Gamma, x') \in \Delta$ for each $x \in X$ such that F(x) is of the form $\forall (\Gamma, x')$ or $\exists (\Gamma, x')$.

Then, the following equalities hold:

$$\underline{L}(\mathfrak{A}) = \underline{L}_{x_0}(F)$$
 and $\overline{L}(\mathfrak{A}) = \overline{L}_{x_0}(F)$.

Proof. Let F, x_0 , and $\mathfrak A$ be as described in the lemma. Now construct the formula system $F': X \to \mathscr F_{\Sigma,X}$ from $\mathfrak A$ as described in Lemma 5.1. Note that both F and F' are defined for the same set X of variables. The following equality follows immediately from the construction of $\mathfrak A$ and the definition of F' by (2), for each $x \in X$:

$$F'(x) = \begin{cases} \exists (Id_m, x') \lor \exists (Id_m, x'') & \text{if } F(x) = x' \lor x'' \\ \forall (Id_m, x') \land \forall (Id_m, x'') & \text{if } F(x) = x' \land x'' & \text{where } m = rank(x). \end{cases}$$

$$F(x) = \begin{cases} \exists (Id_m, x') \lor \exists (Id_m, x'') & \text{if } F(x) = x' \lor x'' \\ F(x) & \text{otherwise} \end{cases}$$

$$(3)$$

Note that each graph formula $fo \in \mathscr{F}^m_{\Sigma,X}$ is semantically equivalent to both $\exists (Id_m,fo)$ and $\forall (Id_m,fo)$. This is easy to see when considering the formula configurations

$$(\exists (Id_m,fo),G,sign)$$
 and $(\forall (Id_m,fo),G,sign)$

for any graph $G \in \mathbb{G}^{(m)}_{\Sigma}$ and $sign \in \{pos, neg\}$. For both, (fo, G, sign) is their only successor configuration in any FCG E, and hence

$$\alpha_F^*(\exists (Id_m, fo), G, sign) = \alpha_F^*(\forall (Id_m, fo), G, sign) = \alpha_F^*(fo, G, sign),$$

showing the equivalence of fo, $\exists (Id_m, fo)$ and $\forall (Id_m, fo)$. Consequently, the equality (3) can be reduced to F' = F, which completes the proof.

Lemma 5.1 and Lemma 5.2 establish a bidirectional correspondence between alternating graph automata and formula systems. In particular, they show that any alternating graph automaton can be transformed into an equivalent formula system, and conversely, any formula system, if it is in shallow normal form, can be translated into an equivalent alternating graph automaton. Since every formula system can be transformed into this normal form, this leads to the main result of this paper:

Theorem 5.3 Formula systems and alternating graph automata are of equal expressive power.

6 Summary and Related Work

We have introduced systems of graph formulas which extend the graph formulas of [11] by an element of recursion, using a mechanism related to the systems of language equations introduced by Mezei and Wright [22]. Our main result is that these formula systems have the same expressive power as the alternating graph automata proposed in [12]. By results proved in the latter paper this implies that the graph languages that can be specified by formula systems are in PSPACE and include some PSPACE-complete languages. Since we know from [11] that graph formulas on their own (without variables) can only specify languages in the polynomial hierarchy PH, it follows that formula systems are more powerful than graph formulas unless PSPACE = PH.

Our notion of formula systems is related to the extension of the widely known nested graph conditions of Rensink, Habel, and Pennemann [24, 19, 23] by Flick, termed "recursively nested" [17], which can specify certain non-local graph conditions such as being acyclic or a tree. However, they cannot specify conditions whose definition, e.g., demands the existence of certain cycle-free or disjoint paths. Hamiltonicity, for example, cannot be specified by recursively nested conditions, which is possible with our formula systems. In fact, Hamiltonicity can even be specified by a single graph formula without any variable, as shown in [11].

While there has been work on finite graph-processing automata [26, 21, 3, 20, 2, 1, 6], we are only aware of two papers on *alternating* graph automata: (1) The automata of Bruggink *et al.* [5] appear to be weaker than ours, as discussed in [12, Example 5]. (2) The automata of Brandenburg and Skodinis [4] allow to specify graph languages that can be defined by node replacement [15], more precisely languages of undirected node-labelled graphs defined by boundary NCE grammars. In a universal configuration (q, G) of their automata, with ongoing transitions $(q, \Gamma_1, q_1) \dots (q, \Gamma_k, q_k)$, cutting the occurrences of Γ_1 to Γ_k off G must result in pairwise unconnected remainder graphs $R_1 \dots R_k$ so that the automaton can proceed with configurations (q_1, R_1) to (q_k, R_k) in parallel. This seems rather obscure, since such steps require a global check of the remainder graph, which contradicts the common understanding of automata.

Monadic second-order (MSO) logic on graphs is an extremely well-studied formalism for specifying graph languages; see [7] and the multitude of references therein. While also being a logic formalism, our formula systems are fundamentally different: MSO logic is an instance of predicate logic whereas the formulas introduced in [11] and extended in the current paper are based on the idea of analyzing a graph by repeatedly matching and cutting off (frontal) subgraphs. Investigating the relation between the two formalisms could be an interesting avenue for future work, our current conjecture being that they are incomparable with respect to their expressive power.

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