Computations of graph polynomials by *fly-automata*

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Overview

We give algorithms based on MSO (Monadic Second-Order) logic and automata that will help to compute MSO-definable polynomials for graphs of bounded tree-width or clique-width.

We use infinite automata, called *fly-automata,* that *compute* their transitions. Their inputs are finite algebraic terms denoting graphs.

The functions to compute are, typically, for φ MSO:

#(X,Y).φ(X,Y) := number of pairs (X,Y) that satisfy φ(X,Y) in graph G,

Sp(X,Y).φ(X,Y) := set of pairs ($|X|$, $|Y|$) for (X,Y) satisfying φ(X,Y) in graph G,

MSp(X,Y).φ(X,Y) := multiset of pairs ($|X|$, $|Y|$) for (X,Y) satisfying φ(X,Y) in graph G, (1)

Max(X).φ(X) := max cardinality of X that satisfies φ(X) in G.

Sat(X,Y).φ(X,Y) := set of pairs (X,Y) that satisfy φ(X,Y) in G.

(1) : Cf. counting generalized colorings (Kotek, Makowsky, Zilber).

FPT algorithms are known for the first 4 cases and FPT ones in the size of the result for the last one (Grohe et al.).

Contradicting a common statement, automata can be used for that : we give a theoretical framework and report about implementation.

Relevance to graph polynomials

All classical graph polynomials are, in some sense, MSO-definable (Makowsky).

Examples : Matching polynomial

$M(G,u) := \Sigma\, m(G,k).\, u^{k}$

m(G,k) is the number of k-matchings in G (sets of k pairwise disjoint edges) = $\#(X).\, \varphi_k(X)$, where $\varphi_k(X)$ says that X is a set of k pairwise disjoint edges (FO-definable for each k).

Sokal's multivariate polynomial, subsumes Tutte's.

$Z(G,u,\mathbf{x}_E) := \sum u^{k(A)} . \mathbf{x}_A$

summation is over all sets of edges $A = \{a1,..., ap\}$,

x_{ai} is an undeterminate indexed by edge ai,

$\mathbf{x}_A := x_{a1} ... x_{ap}$ (commutative product)

$k(A)$:= number of connected components of $G[A]$.

We have $\{k(A)\} = Sp(X). \varphi(X,A)$ where

$\varphi(X,A)$ says that X has 1 vertex in each con. comp. of $G[A]$.

The chromatic polynomial of G is $Z(G,u, x_e := -1)$

For Tutte's polynomial $T(G,u,v)$, we have

$$(u-1)^{k(G)}.(v-1)^n . T(G,u,v) = Z(G,(u-1)(v-1), x_e := v-1)$$

Tutte's polynomial

$T(G,u,v) := \Sigma\, t_{i,j} \,.\, u^{i} \,.\, v^{j}$

$t_{i,j}$ is the number of spanning trees of *internal activity* i and *external activity* j, relative to a linear order on edges (from each term defining G, we have such an order).

An MSO formula $\varphi(X,Y,Z)$, where X,Y are sets of edges, is such that, if

$MSp(X,Y,Z).\varphi(X,Y,Z) = \ldots + p.(k,i,j) + \ldots$

then :

$T(G,u,v) = \ldots + p.u^{i} v^{j} + \ldots$

$\varphi(X,Y,Z)$ says that X is a spanning tree T and Y, *resp.* Z are the internally, *resp.* externally active edges of G wrt T. (This counting works because Y and Z are uniquely determined from X.)

Multivariate interlace polynomial (B.C., 2008)

$C(G,u,v, \mathbf{x}_V, \mathbf{y}_V) := \sum \mathbf{x}_A . \mathbf{y}_B . u^{f(A,B)} . v^{g(A,B)}$

$G\Lambda B$:= G where the loops at the vertices in B are toggled,

$f(A,B) := rk(G\Lambda B[A \cup B])$ and $g(A,B) := |A \cup B| - f(A,B)$,

rk(H):= rank over GF(2) of the adjacency matrix of graph H.

The rank of H is Max(X). $\varphi(X)$ for an MSO formula $\varphi(X)$ written with the even cardinality set predicate Even(Y). (As graphs are ordered, this predicate is MSO-definable).

Graphs are defined by algebraic terms and processed by automata on these terms.

Our graph parameter is *clique-width* (cwd(.)) and the terms denoting graphs are those from which clique-width is defined because :

- it is easier to handle than (the very popular) tree-width (twd(.)) for constructing automata, and it is more powerful: bounded tree-width implies bounded clique-width,
- it is defined in terms of elementary graph operations, hence is easier than the equivalent notion of rank-width,
- it works equally well on directed graphs.

- We can handle edge quantifications via incidence graphs:

  If $G = (V_G, edg_G(.,.))$ then $Inc(G) := (V_G \cup E_G, inc_G(.,.))$

  where : $inc_G(u,e) : \Leftrightarrow$ u is an end of e.

MSO formulas over Inc(G) can use quantifications on edge sets of G and express more properties.

Proposition (T.Bouvier) : $twd(G) \leq k \implies cwd(Inc(G)) \leq k+3$.

Hence, no exponential jump.

The system AUTOGRAPH (by Irène Durand) and the corresponding theory [B.C.&I.D.: *Automata for the verification of monadic second-order graph properties*, J. Applied Logic, 10 (2012) 368-409] are based on clique-width.

Using automata

Theorem [B.C.]: For every k, every MSO graph property P can be checked by a *finite* automaton, which recognizes the terms that:

(1) are written over the finite set F_k of operations that generate the graphs of *clique-width* at most k, and

(2) define a graph satisfying P.

However, these automata are *much much* too large to be tabulated.

Our remedy: We use fly-automata (in French "automates programmés"), whose states and transitions are described and not tabulated. Only the transitions necessary for a particular input term are computed, "on the fly".

As states are not listed, a fly-automaton can use an infinite set of states. It can recognize sets of words or terms that are not monadic second-order definable : the language $a^n b^n$, the terms of arbitrary clique-width defining regular graphs (all vertices of same degree).

It can compute values: the number of p-colorings, or of "acyclic" p-colorings of a graph (the graph induced by any two color classes is acyclic).

We can construct fly-automata in uniform ways from logical formulas. In this way, we develop a *theory* of (some aspects of) *dynamic programming*.

Review of definitions

Definition 1 : Monadic Second-Order Logic

First-order logic extended with (quantified) variables
denoting subsets of the domains.

MSO (expressible) properties : transitive closure, properties of paths,
connectedness, planarity (via Kuratowski), p-colorability.

Examples of formulas for $G = (V_G , edg_G(.,.))$, undirected

G is 3-colorable :

$$\exists X,Y \, (X \cap Y = \varnothing \; \wedge$$
$$\forall u,v \, \{ edg(u,v) \Rightarrow$$
$$[(u \in X \Rightarrow v \notin X) \wedge (u \in Y \Rightarrow v \notin Y) \wedge$$
$$(u \notin X \cup Y \Rightarrow v \in X \cup Y) \;]$$
$$\})$$

G is not connected :

$\exists Z\ (\ \exists x \in Z\ \wedge\ \exists y \notin Z\ \wedge\ (\forall u,v\ (u \in Z\ \wedge\ edg(u,v) \Rightarrow v \in Z)\ )$

Transitive and reflexive closure : **TC**(R, x, y) :

$\forall\ Z\ \{$ "Z is R-closed" $\wedge\ x \in Z\ \Rightarrow y \in Z\ \}$

where "Z is R-closed" is defined by :

$\forall u,v\ (u \in Z\ \wedge\ R(u,v) \Rightarrow v \in Z)$

The relation R can be defined by a formula as in :

$\forall x,y\ (x \in Y\ \wedge\ y \in Y \Rightarrow$ **TC**("$u \in Y\ \wedge v \in Y \wedge edg(u,v)$", x, y)

expressing that G[Y] is connected (Y is free in R).

Reference : B.C. & J. Engelfriet *: Graph structure and monadic second-order logic,* Cambridge University Press, 2012

Definition 2 : Clique-width

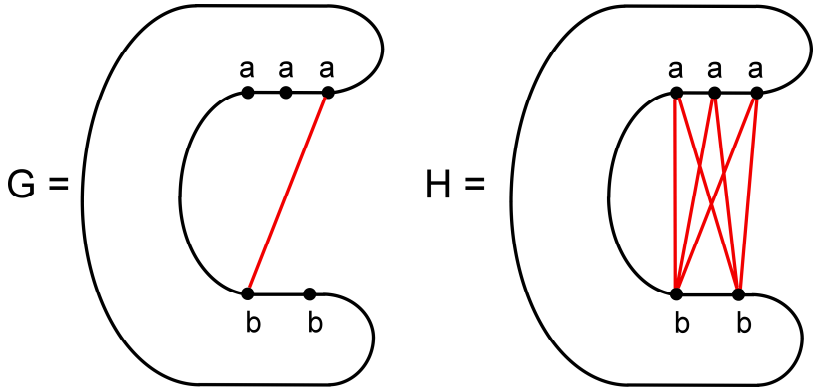
Defined from graph operations. Graphs are simple, directed or not, and labelled by *a* , *b* , *c, ...* . A vertex labelled by *a* is called an *a-vertex*.

One binary operation: *disjoint union* : $\oplus$

Unary operations: (1) edge addition denoted by $Add_{a,b}$

$Add_{a,b}$(G) is G augmented with undirected edges between every *a*-vertex and every *b*-vertex.

The number of added edges depends on the argument graph.



H = $Add_{a,b}$(G) ; only 5 new edges added

Directed edges can be defined similarly.

(2) Vertex relabellings :

$Relab_{a \to b}(G)$ is G with every *a*-vertex is made into a *b*-vertex

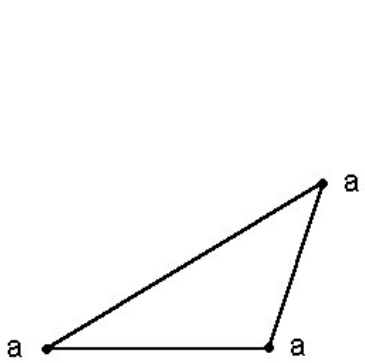
Nullary operations for basic graphs with a single vertex **a**, labelled by *a*.

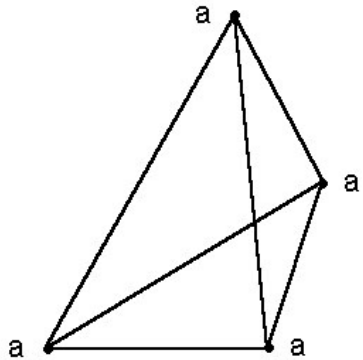
Definition: A graph G has clique-width $\leq$ k (denoted by cwd(G))

$\Leftrightarrow$ G = G(t), defined by a term t using $\leq$ k labels.

Example : Cliques have clique-width 2.

K_n is defined by t_n where t_{n+1} = $Relab_{b \to a}(Add_{a,b} (t_n \oplus \mathbf{b}))$





New definition 3 : Fly-automaton (FA)

A = < F, Q, δ, Out >

F : finite or countable (effective) signature (set of operations),

Q : finite or countable (effective) set of states (integers, pairs of integers, finite sets of integers: states are encoded by finite words, integers are in binary),

Out : Q → D , computable (D : effective domain,a recursive set of words),

δ : computable (bottom-up) transition function.

Nondeterministic case : δ is *finitely multi-valued*.

This automaton defines a computable function : T(F) → *D*

(or : T(F) → *P*(*D*) if it is not deterministic)

If *D* = { *True, False* }, it defines a decidable property, equivalently, a decidable subset of T(F).

Deterministic computation of a nondeterministic FA :

bottom-up computation of *finite* sets of states (classical simulation of the determinized automaton): these states are the useful ones of the *determinized automaton*; these sets are *finite* because the transition function is *finitely multivalued*.

To be defined later : *Enumerating computation*.

Example : The number of accepting runs of a nondeterministic automaton.

Let $A = < F, Q, \delta,$ Acc $>$ be finite, nondeterministic.

Then $\#A := < F, [\, Q \rightarrow \mathbf{N}\,], \delta^{\#},$ Out $>$

$[\, Q \rightarrow \mathbf{N}\,]$ = the set of total functions : $Q \rightarrow \mathbf{N}$

$\delta^{\#}$ is easy to define such that the state reached at position

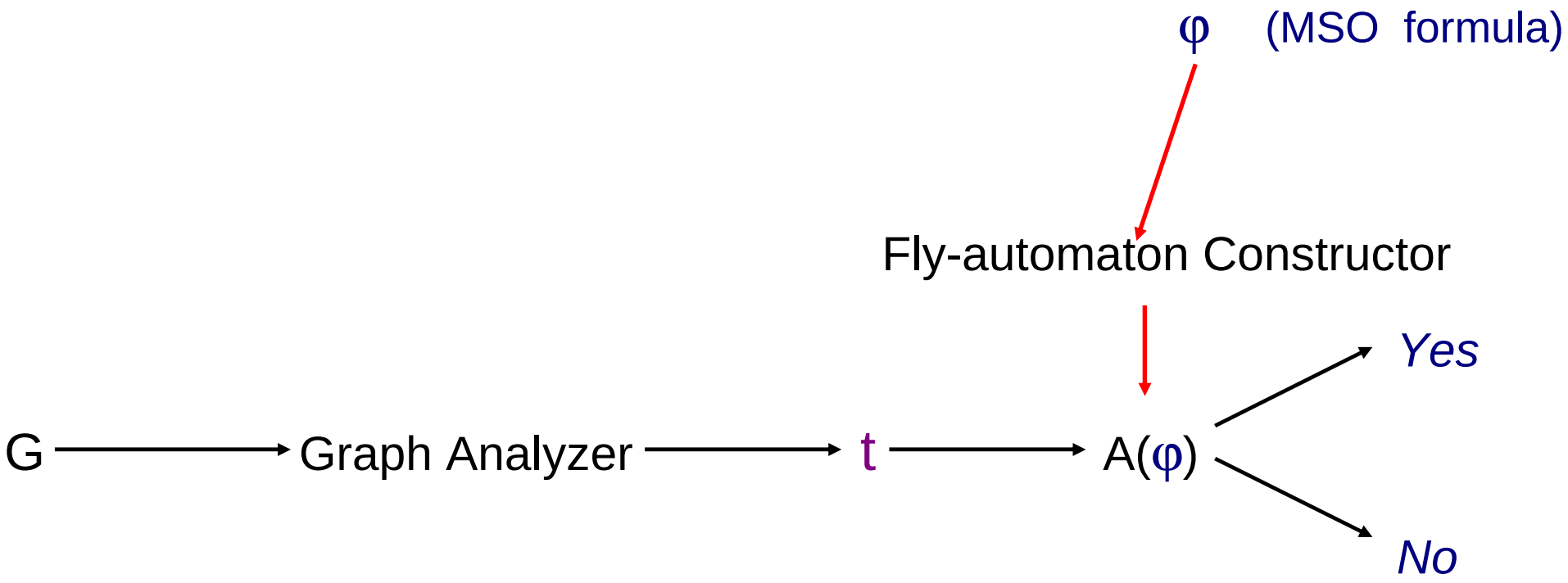
u in the input term is the function σ such that $\sigma(q)$ is

the number of runs reaching q at u.

Out(σ) is the sum of $\sigma(q)$ for q in Acc.

$\#A$ is a fly-automaton obtained by a *generic construction* that extends to the case of infinite fly-automata.

The algorithmic MSO meta-theorem through *fly-automata*



A(φ) is an *infinite fly-automaton* over the countable set F of all graph operations that define clique-width. The time taken by A(φ) depends on the number of labels that occur in t), not only on the size of G or t.

Fly-automata that check graph properties

How to construct them ?

(1) Direct construction for a well-understood graph property or

(2) Inductive construction based on the structure of an MSO formula;

a *direct* construction is anyway needed for atomic formulas;

logical connectives are handled by *transformations* of automata :

products, projection (making them nondeterministic), determinization (for negation).

Example of a direct construction : Connectedness.

The state at position u in term t is the *set of types (sets of labels)* of the connected components of the graph G(t/u). For k labels (k = bound on clique-width), the set of states has size $\leq 2 \wedge 2^k$.

Proved lower bound : $2 \wedge 2^{k/2}$.

→ Impossible to compile the automaton (to list its transitions) .

Example of a state : q = { {a}, {a,b}, {b,c,d}, {b,d,f } }, (a,b,c,d,f : labels).

Some transitions :

$Add_{a,c}$: q ⟶ { {a,b,c,d}, {b,d,f } },

$Relab_{a \to b}$: q ⟶ { {b}, {b,c,d}, {b,d,f } }

Transitions for ⊕ : union of sets of types.

Note : Also state (p,p) if G(t/u) has ≥ 2 connected components, all of type p.

We can allow fly-automata with *infinitely* many states and, also, with *outputs* : numbers, finite sets of tuples of numbers, etc.

Example continued : For computing the number of connected components, we use states such as :

q = { ({a}, 4), ({a,b}, 2), ({b,c,d},2), ({b,d,f },3) },

where 4, 2, 2, 3 are the numbers of connected components of respective types {a}, {a,b}, {b,c,d}, {b,d,f }.

Computation time of a fly-automaton

F : all (*cwd*) graph operations, F_k : those using labels 1, …, k.

On term $t \in T(F_k)$ defining G(t) with n vertices, if a fly-automaton takes time bounded by :

$(k + n)^c$ → it is a P-FA (a polynomial-time FA),

$f(k).n^c$ → it is an FPT-FA,

$a.n^{g(k)}$ → it is an XP-FA.

The associated algorithm is, respectively, polynomial-time, FPT or XP for clique-width as parameter.

Recognizability Theorem [B.C & I.D.] : For each MSO property P, one can construct a single infinite FPT-FA over F (the operations that generate all graphs) that recognizes the terms $t \in T(F)$ such that P(G(t)) holds.

For each k, its restriction to the *finite* signature F_k (the operations that generate graphs of cwd $\leq$ k) is a finite automaton.

Consequences : (1) The same automaton (the same *model-checking program*) can be used for all graphs (of any clique-width).

(2) It can be implemented in non-trivial cases.

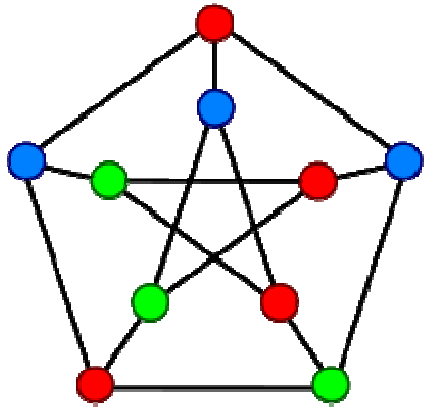
Some experiments using FA (by Irène Durand)

Number of 3-colorings of the 6 x 90 "modified" grid of clique-width 8 in 1 min. 9 sec. (modified with diagonals on the squares of the first column).

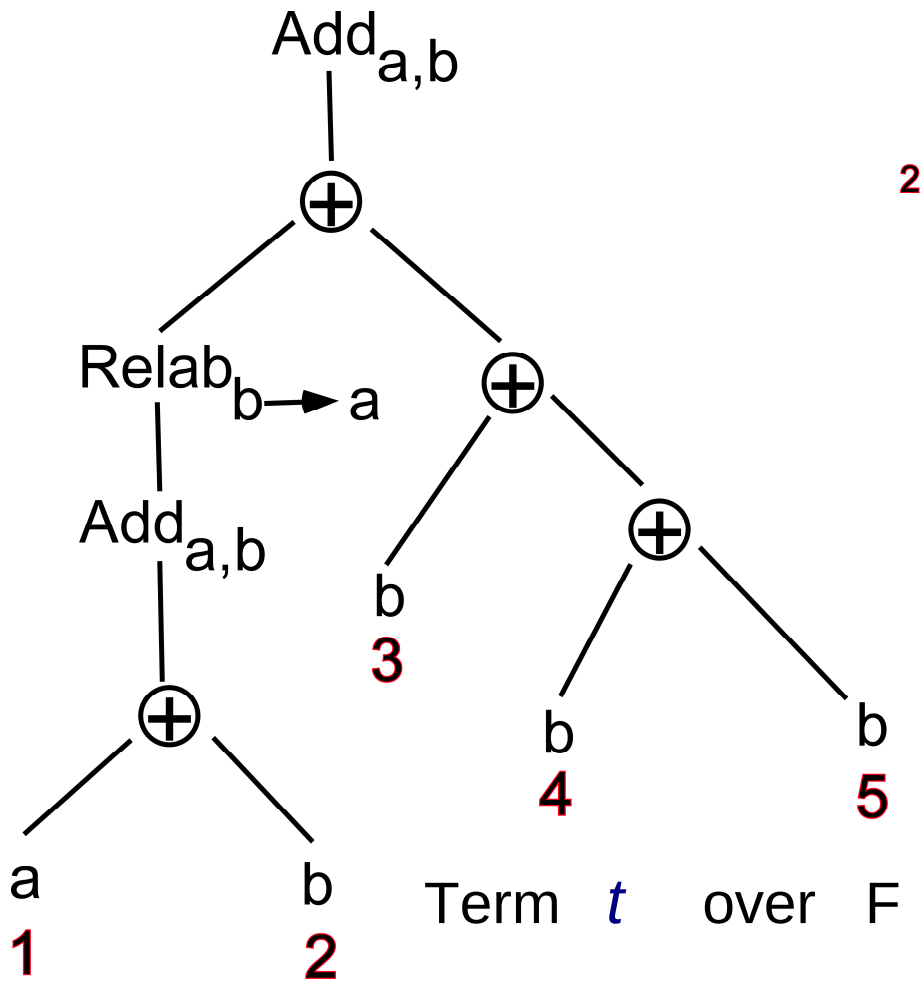
For the similar 6 x 250 grid : < 6 min. ; for 6 x 360 : < 9 min.

4-*acyclic*-colorability of the Petersen graph (clique-width 5) in 1.5 min., from a term in $T(F_6)$.

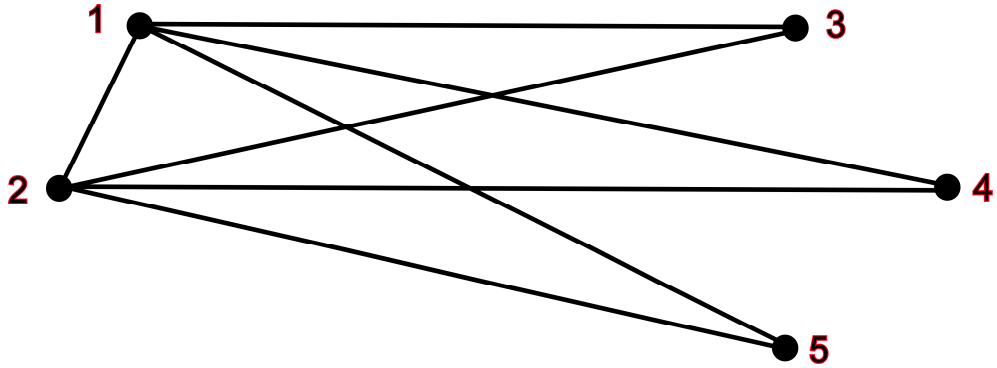
(3-colorable but not acyclically; **red** and **green** vertices induce a cycle).



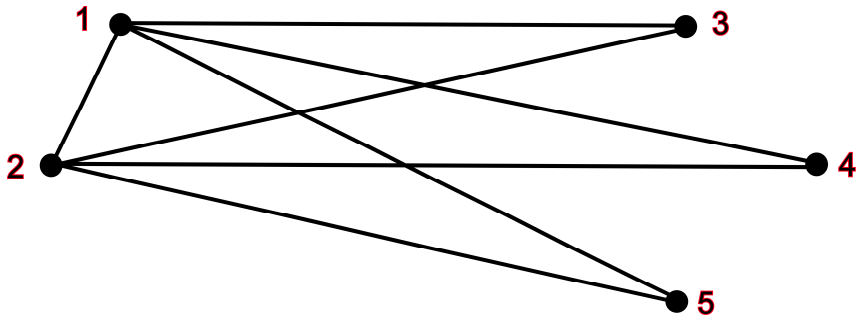
Existential quantifications and nondeterminism

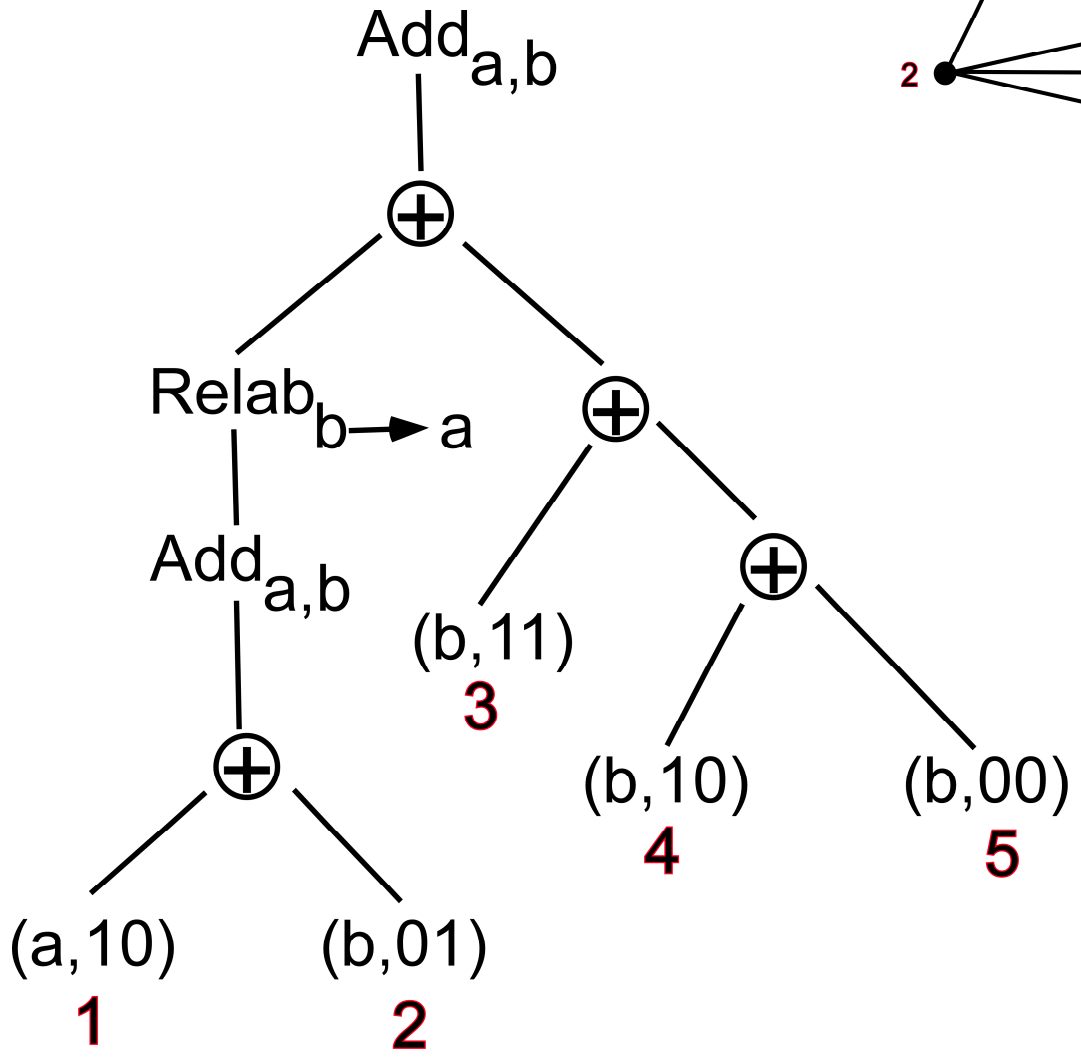


Term t over F



Graph G(t)





$V_1 = \{1,3,4\}, \; V_2 = \{2,3\}$

Term $t*(V_1,V_2)$ over $F^{[2]}$ ([2] because of 2 Booleans).

Consider a property $\exists X,Y.\ \varphi(X,Y)$ to be checked on graph G(t).

We construct a deterministic automaton A over $F^{[2]}$ recognizing the terms $t*(X,Y)$ such that $G(t*(X,Y)) \mathrel{!}= \varphi(X,Y)$.

We delete the Booleans in the nullary symbols of $F^{[2]}$: we obtain a nondeterministic automaton B over F (called a projection : A → B).

The different runs of B correspond to trying the different possible pairs (X,Y) when looking for a satisfying one.

B recognizes the terms t such that $G(t) \mathrel{!}= \exists X,Y.\ \varphi(X,Y)$.

By an induction on φ, we construct for each $\varphi(X_1,\ldots,X_n)$ a FA $A(\varphi(X_1,\ldots,X_n))$ that recognizes:

$$L(\varphi(X_1,\ldots,X_n)) := \{ t * (V_1,\ldots,V_n) \in \mathbf{T}(F^{(n)}) \ / \ (G(t), V_1,\ldots,V_n) \models \varphi \}$$

Quantifications: Formulas are written without $\forall$

$$L(\exists X_{n+1} . \varphi(X_1, ..., X_{n+1})) = pr(L (\varphi(X_1, ..., X_{n+1}))$$

$$A(\exists X_{n+1} . \varphi(X_1, ..., X_{n+1})) = pr(A (\varphi(X_1, ..., X_{n+1}))$$

where pr is the *projection* that eliminates the last Boolean;

→ a *non-deterministic* automaton $B = pr(A (\varphi(X_1, ..., X_{n+1}))$.

Determinized runs of B defined by deterministic FAs C

For $\exists \underline{X}.P(\underline{X})$: the state of C at position u is

{ state *q* of B / some run reaches *q* at position u }

For # $\underline{X}.P(\underline{X})$: the state of C at position u is

{ (*q*,m) / m = the number of runs that reach *q* at u }

equivalently, the corresponding multiset of states *q*, cf. $\exists \underline{X}.P(\underline{X})$

For Sp$\underline{X}.P(\underline{X})$: the state of C at position u is

{ (*q*,S) / S = the set of tuples of cardinalities of

the "components of $\underline{X}$ below u" that yield *q* at u }.

For MSp$\underline{X}.P(\underline{X})$: S is the corresponding multiset.

For MinCard X.P(X) : the state of C at position u is

{ (*q*, s) / s = the minimum cardinality of "X below u" that yields *q* at u }.

SatX.P(X) := the set of all tuples X that satisfy P(X),

the state of C at position u is

{ (*q*, S) / S = the set of all tuples below u that yield *q* }

A common presentation for all this cases:

We call the component s in a state (q,s) is an attribute of q.

An attribute s of q at u collects *certain* information about *all* the runs that yield q at u. Computations of attributes correspond to variants of the basic determinization: they use, according to the cases :

Set union (for basic determinization)

Union of multisets, (for counting runs)

Selection of minimal number or minimal set (e.g. for inclusion),

A **+** B where A and B are sets of numbers,

etc…

Distributive algebras offer a formal setting (see B.C., I.Durand, *Theoret. Comput. Sci* **619** (2016)).

Optimizations : How to avoid intermediate computations that do not contribute to the final result.

Theorem (Flum and Grohe) : One can compute Sat$\underline{X}$.P($\underline{X}$) in time f(k).(n+ size of the result) where cwd(G) $\leq$ k and n is the size of the term.

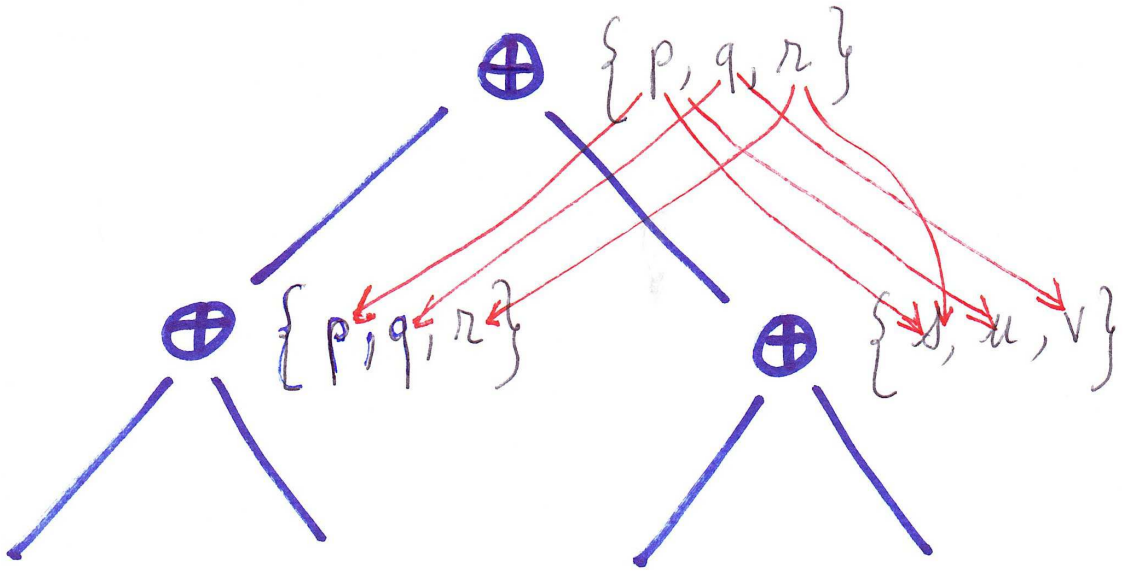
The bottom-up inductive computation must “know” that certain states will not belong to any accepting run on the considered term.

Method : 3 pass algorithm

1 : determinized bottom-up run keeping pointers showing how states are obtained from others,

2 : top-down run starting from the accepting states at the root and marking the *useful states*,

3 : bottom-up computation of attributes only for the useful states.



$\oplus[p, s] \rightarrow p$

$\oplus[p, u] \rightarrow p$

$\oplus[q, v] \rightarrow q$

$\oplus[r, s] \rightarrow r$

This 3-pass algorithm is applicable for all our computations of attributes.

Example : Checking that a graph has a unique 3-coloring.

1st method : expressing that in MSO : possible but cumbersome.

2nd method : computing the total number of 3-colorings: we want result 6 (assume the graph is not 2-colorable) : OK but lengthy.

3rd method : "optimized" counting with reporting Failure if a useful intermediate result shows that more than 6 coloring will be found.

This is applicable to : $\exists!\ \underline{X}.P(\underline{X})$ for every MSO property P.

Enumeration techniques

Enumeration of accepting states

- stopping as soon as one is obtained
- less space but more time for checking negation (failure to recognition),
- listing the assignments $\underline{X}$ satisfying $\varphi(\underline{X})$: we maintain with each state, at each position, its “origin”: the partial assignment that produced it.

If an Error state is found in a partially constructed run, we abort its completion.

Enumerators

An *enumerator* is a triple E = (D, *reset, next*) where D is an effective (countable) set, *reset* and *next* are two programs guaranteed to terminate. E defines a finite list List(E) of elements of D.

List(E) may contain repetitions,

next produces one more element or reports “end of list”,

reset reinitializes the program *next.*

Remark : Enumerators can be extended to produce infinite lists.

Basic enumerators : For each nullary a, E_a produces the list of states q (not Error) arising from a (by the nondeterministic automaton B that checks $\exists \underline{X}.\varphi(\underline{X})$ and that is obtained from the deterministic automaton A checking $\varphi(\underline{X})$, by deleting the sequences of Booleans w in the nullary symbols (a,w) of the signature $F^{[p]}$ of A).

Alternatively, $\underline{E}_a$ produces the list of pairs (q,w) : we keep track of the w that produced q (its “origin”).

Transforming and combining enumerators.

Making a copy of E : $copy_u(E)$ indexed by u, a position of the given term.

Making E into nr(E), nonredundant: produces the same elements without repetitions (nr(E) uses the list of already generated elements).

Applying a unary function h : D → D'

If E enumerates elements of D, then $h \circ E$ produces the images by h of the elements of List(E).

Cartesian product.

If E enumerates elements of D, E' elements of D', we want to list the pairs (d,d') where $d \in \text{List}(E) = d_1, \ldots,\ d' \in \text{List}(E') = d'_1, \ldots$

Possible orders:

"Line order" (lexico) : $(d_1, d'_1), (d_1, d'_2), \ldots, (d_2, d'_1), (d_2, d'_2), \ldots$

"Column order" : $(d_1, d'_1), (d_2, d'_1), \ldots, (d_1, d'_2), (d_2, d'_2), \ldots$

"Diagonal order" : $(d_1, d'_1),\ (d_1, d'_2), (d_2, d'_1),$

$(d_1, d'_3), (d_2, d'_2), (d_3, d'_1), \ldots..$

$E\ x_{Line}\ E'$, $E\ x_{Col}\ E'$, $E\ x_{Diag}\ E'$ realize these enumerations.

Given a term t and an automaton A that checks $\varphi(\underline{X})$, one builds a (big) enumerator E_t by combining basic ones with Cartesian compositions, $h_O(.)$ and possibly nr(.).

If t=f(s), then $E_t = h_O(E_s)$ where h is based on transitions for f.

If t=f(s,s'), then $E_t = h_O(E_s \times E_{s'})$ where h is similar.

Running E_t by calling its *next* component iteratively produces the desired list (unless the system lacks of memory).

The system AUTOGRAPH (by I. Durand)

(1) Fly-automata for basic graph properties :

Clique, Stable (no edge), Link(X,Y), NoCycle,

Connectedness, *Regularity*, Partition(X, Y, Z), etc…

and functions :

#Link(X,Y)= number of edges between X and Y,

Maximum degree.

Procedures for combining fly-automata, corresponding to logical constructions : $\wedge$, $\vee$, negation, $\exists \underline{X}.\ \varphi(\underline{X})$.

Procedures to build automata that compute functions:

#$\underline{X}.\varphi(\underline{X})$: the number of tuples $\underline{X}$ that satisfy $\varphi(\underline{X})$ in the input term (hence, in the associated graph),

Sp$\underline{X}.\varphi(\underline{X})$: the spectrum = the set of tuples of cardinalities of the components of the $\underline{X}$ that satisfy $\varphi(\underline{X})$, etc…

Enumeration: construction of an enumerator from a term and a fly-automaton.

These constructions are "uniform" with respect to the input automata.

Some tests

Checking colorability of grids 6 x M of clique-width 8.

M	2-col. det	2-col. enum	3-col. det	3-col. enum
7	0.03 s	6 s	10 s	6 s
8	0.03 s	9 s	Fails	9 s
20	0.2 s	3 min	Fails	3 min

Counting 2-colorings : for M = 200, in 2 seconds (2).

Counting 3-colorings : for M= 5, in 3 seconds (6 204 438).

Fails for M = 6.

Works for M = 360 for modified grids.

Enumerating 3-colorings :

M = 20 : Construction of enumerator in 3 minutes

Then, first result in 0.5 second.

Conclusion

These algorithms are based on fly-automata, that can be quickly constructed from logical descriptions (and basic automata)

→ flexibility.

The system AUTOGRAPH implements these constructions. Tests have been made for colorability and connectedness problems.