FIRST-ORDER AUTOMATA

Nicola Gigante Free University of Bozen-Bolzano, Italy iFM² April 19, 2024 Udine, Italy Model-checking and other verification techniques for **finite-state** systems have been extremely successful in the past decades.

However, many real-world scenarios require reasoning over infinite-state systems.

Infinite-state specification and verification

There are many infinite-state formalisms around.

- timed automata [AD94]
- hybrid automata [Alu+92]
- recursive state machines [Alu+05; BMP10]
- visibly pushdown languages [AM04]
- operator-precedence languages [Dro+17]
- FIFO machines [BZ83]
- counter machines [Woj99]
- Petri nets [Mur89; JK09]
- data-aware systems [DLV19; CGM13; Ghi+23]
- automata over infinite alphabets [Seg06; IX19]
- register automata [KF94]

And many logics to talk about them.

- precedence oriented temporal logic [CMP22]
- metric temporal logics [Koy90; LVR22; AH94]
- temporal logics with concrete domains [DQ21]
- temporal logics with arithmetics [Fel+23; Cim+20]
- separation logic [CYO01; BK18; Man20]
- constrained horn clauses [GB19]
- logics on data words [Boj+06; DLN07]
- signal temporal logic [MN04]
- first-order temporal logics [Kon+04]

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First-order temporal logics are expressive formalisms to specify properties of infinite-state systems:

- badly undecidable, however;
- used mostly in really tailored fragments or in knowledge representation applications where reasoning is not the main task;

Question

Can we make them **practical**, as a specification language for **verification** tasks, while maintaining a substantial fraction of its **expressive power**?

In the finite-state setting, **automata** have played the crucial role of the algorithmic powerhorse of verification and model checking.

Question

Can we define a similar tool for **first-order** temporal logic?

High-level overview of the talk:

- recap on propositional and first-order temporal logics
- past results: LTL modulo theories
- current directions: first-order automata
- conclusions

FIRST-ORDER TEMPORAL LOGICS

Let us recap the main concepts of Linear Temporal Logic:

- modal logic interpreted over discrete linear orders
- traditionally, infinite linear orders
- recently, finite models gained attention [DV13]





p and q hold



tomorrow p and q hold



eventually p and q hold



p and q hold always



p holds **until** q holds









weak tomorrow



In FOLTL we mix classical first-order logic with LTL temporal operators.

$$\forall x \exists y \operatorname{\mathsf{G}}(p(x) \to \operatorname{\mathsf{F}}(q(x, y))) \qquad \operatorname{\mathsf{G}}(\forall xy (p(x, y) \to \widetilde{\operatorname{\mathsf{X}}}p(x, y+1)))$$
$$\forall x \operatorname{\mathsf{X}}\neg p(x) \land \operatorname{\mathsf{X}}\exists x p(x)$$

FOLTL is interpreted over sequences of first-order structures.

- possibly over multisorted signatures;
- first-order features interpreted over the current structure;
- temporal operators to move from one structure to another;
- the **domain** of each sort is arbitrary but **constant** throughout the sequence.

FOLTL is famous for being highly undecidable, but, for a fragment F such that:

- the underlying FO fragment is decidable; and
- temporal formulas are monodic;
 - only one free variable inside temporal operators;
- constants in the signature are considered rigid;
- then FOLTL(F) is decidable [HWZ00]

Are there decidable fragments of FO?

- monadic fragment
- Bernays-Schönfinkel-Ramsey fragment $(\exists^*\forall^*/=)$
- Ackermann fragment $(\exists^* \forall \exists^*)$
- Gödel-Kalmár-Schütte fragment (∃*∀∀∃*)
- Skolem fragment
- two-variable fragment
- guarded fragment
- separated fragment
- combinations of the above in multi-sorted signatures
- many description logics are decidable FO fragments in disguise

See [Voi19] for a detailed survey.

THE PAST: LTL MODULO THEORIES

There have been many developments in the world of first-order theorem proving.

- many good solvers (SPASS, Vampire, E, etc.);
- not specific to decidable fragments, however.

Can we use these as a foundation of FOLTL reasoning? Yes.

See e.g., TSPASS, a solver for monodic first-order temporal logic

However, the monodic temporal fragment is limited for applications.

Imagine modeling an update query on an SQL database:

update R set x = x - 1 where x > 0

In FOLTL, it can become something like:

$$\forall k \forall x \left(\begin{array}{c} \left(R(k,x) \land x > 0 \to \mathsf{X}(\neg R(k,x) \land R(k,x-1)) \right) \\ \land \left(R(k,x) \land x \leqslant 0 \to \mathsf{X}R(k,x) \right) \end{array} \right)$$

We need to accept dealing with semi-decidability.

There is another approach at **first-order** reasoning:

- satisfiability modulo theories
- **bottom-up** approach:
 - let's add to SAT solvers bits of tractable first-order reasoning step by step
- SMT solvers are strong at quantifier-free reasoning over specific theories useful for program verification
 - linear integer arithmetics/real arithmetics
 - arrays
 - bitvectors
 - constrained Horn clauses
 - algebraic data types
- sometimes quantification works, as well

 LTL_{f}^{MT} is a sweet spot in the specification of infinite-state properties. [IJCAI 22]



- let Σ be a first-order signature and T a Σ -theory
- LTL_{f}^{MT} is interpreted over finite words of *T*-structures
- predicates and function symbols are rigid
- constants are **non-rigid**, *i.e.*, change over time
 - this is not covered by existing decidability results about FOLTL

• terms can refer to the value of constants at the next or previous state.

 $t \coloneqq c \mid x \mid f(t_1, \ldots, t_n) \mid \bigcirc c \mid \bigcirc c \mid \triangleleft c \mid \triangleleft c$

$$\begin{split} \lambda &\coloneqq p(t_1, \dots, t_n) \mid \neg \lambda \mid \lambda \lor \lambda \mid \lambda \land \lambda \mid \exists x \lambda \mid \forall x \lambda \\ \varphi &\coloneqq \lambda \mid \neg \varphi \mid \phi \lor \phi \mid \phi \land \phi \mid X \phi \mid \widetilde{X} \phi \mid Y \phi \mid Z \phi \\ \mid \phi \cup \phi \mid \phi \land \varphi \mid \phi \land \phi \mid \phi \land \phi \mid \phi \land \phi \end{split}$$

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• terms can refer to the value of constants at the **next** or **previous** state.

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$$G(a = 2b) \qquad (a < b) \cup (b = 0) \qquad G(a > 5) \land F(a = 0)$$
$$G(\exists x (a = 2x))$$
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$$a = 0 \land ((\bigcirc a = a + 1) \cup a = 42)$$
$$b = 1 \land G(\bigcirc b = b + 1 \land a = 2b)$$
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$$a = 0 \land ((\bigcirc a = a + 1) \lor a = 42)$$
$$b = 1 \land \mathsf{G}(\bigcirc b = b + 1 \land a = 2b)$$
$$\mathsf{G}(p(a) \to \widetilde{\mathsf{X}}p(\triangleleft a + 1))$$

 LTL_{f}^{MT} is **undecidable**, but:

- it is semi-decidable
- so we can get something useful, sometimes:
 - models of satisfiable formulas
 - counterexamples of specifications over bugged systems
- moreover, we have some interesting decidable fragments [ECAI 23]
- why finite traces?
 - on infinite traces, LTL^{MT} is not even semi-decidable.

(MC) Formulas over LRA where all **iteration conditions** are **monotonicity constraints**, *i.e.*, variable-to-variable or variable-to-constant comparisons, *e.g.*:

 $a < 0 \land b = 1 \land ((\bigcirc b > b \land \bigcirc a \leqslant a) \lor a = b)$

(IPC) Formulas over LIA where all iteration conditions are integer periodicity constraints, e.g.:

$$(b \equiv_3 a) \cup (a > 42) \land \mathsf{F}(a + b = c)$$

Iteration conditions:

- α in $\alpha \cup \beta$
- $\blacksquare \beta in \alpha R \beta$

(BL) **Bounded lookback** formulas, that generalize the above two by requiring that cross-state interaction is restricted to finitely many steps back. What does it mean?









$$a < 0 \land b = 1 \land ((\bigcirc b > b \land \bigcirc a \leqslant a) \lor a = b)$$



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$$a < 0 \land b = 1 \land ((\bigcirc b > b \land \bigcirc a \leqslant a) \lor a = b)$$



(NCS) Formulae without cross-state comparisons, *i.e.*, without any $\bigcirc c$, $\odot c$, *e.g.*:

$$(a > b \cup a + b = 2c) \land \mathsf{G}(a + b > 0)$$

(FX) Formulas where the only temporal operators are F, X, and \widetilde{X} , *e.g.*:

 $\mathsf{F}(p(\bigcirc a) \land \mathsf{X}(\neg p(a))) \land \mathsf{XF}(r(a, b) \lor r(\bigcirc a, b))$

The SAT encoding of Reynolds' tableau can be extended to an **SMT encoding** for LTL_f^{MT} .

- implemented in our BLACK solver¹ for arithmetic theories;
- given to off-the-shelf SMT solvers such as Z3 [MB08], cvc5 [Bar+22], etc.

¹https://www.black-sat.org

Which systems can we verify LTL_{f}^{MT} formulas on?

Knowledge-base driven Dynamic Systems (KDS):

infinite-state transition systems

$$D = \langle \mathsf{K}, I(X), T(X, X'), F(X) \rangle$$

- states are structures over the first-order theory K
- I(X), T(X, X'), F(X) are arbitrary first-order formulas over the theory K
 - initial states satisfying I(X)
 - **final** states satisfying F(X)
 - **transition relation** expressed by T(X, X')

Let *D* be a KDS and ϕ an LTL^{MT} formula:

- all the executions of a KDS D can be represented by an LTL_f^{MT} formula ψ_D
- **model-checking** of ϕ over *D* reduces to **satisfiability** of:

 $\gamma \equiv \psi_D \wedge \neg \phi$

- if γ is satisfiable, the specification does not hold and the model is a counterexample
- if γ is **unsatisfiable**, the specification is valid over D
- this needs non-rigid predicates: only semi-decidable!

Test setting:

- simulation of a company hiring process
- nondeterministic transitions:
 - dependent on arithmetic constraints
 - acting on unbounded relational data
- minimal length of the counterexamples dependent over scalable parameter N
- two modelings of the same system:
 - P₁ employs arithmetic constraints
 - P₂ avoids arithmetics, simulates constraints by other means
- two different properties for each variant



$$\begin{split} \varphi_s^1 &\equiv \mathsf{G}(x_{state} = \textit{final} \to 2x_{under} > x_{winners}) \\ \varphi_\ell^1 &\equiv \mathsf{G}\begin{pmatrix} x_{state} = \textit{app} \to \\ F(x_{state} = \textit{final} \land 2x_{under} > x_{winners}) \end{pmatrix} \end{split}$$

Results:

- 5 minutes timeout reached at N = 70
- exponential growth
 - but could be much worse, the problem is undecidable!
- liveness property not harder than the safety one
- system with explicit arithmetics faster to verify



THE PRESENT: FIRST-ORDER AUTOMATA

 LTL_{f}^{MT} is limited in many ways:

- many complex systems need evolving predicates;
- nesting of quantifiers and temporal operators is often essential
- we want to approach **full** FOLTL.

In the finite-state setting, automata are essential:

- operational counterpart of temporal logics
- basis of many algorithms and techniques

We want a class of automata for FOLTL.

What may an infinite-state first-order automaton look like?

- **states**: first-order structures over a state signature Γ ;
- **letters**: first-order structures over an alphabet signature Σ ;
- initial states: a class of Γ-structures;
- final states: a class of Γ-structures;
- **transition**: a relation between:
 - a Γ-structure (source state),
 - a Σ-structure (letter), and
 - another Γ-structure (dest. state).

But this is algorithmically untractable.

A **finite-state** automaton:

$$A = \langle \Sigma, Q, Q_0, \Delta, F
angle$$

A **symbolic** finite-state automaton:

$$\mathcal{A} = \langle \Sigma, X, I(X), T(X, \Sigma, X'), F(X) \rangle$$

A **finite-state** automaton:

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A symbolic finite-state automaton:

$$\mathcal{A} = \langle \Sigma, X, I(X), T(X, \Sigma, X'), F(X) \rangle$$

A **first-order** automaton:

$$\mathbf{A} = \langle \Sigma, \Gamma, \phi_I, \phi_T, \phi_F \rangle$$

where:

- Σ is the word signature and Γ is the state signature;
- ϕ_I and ϕ_F are Γ -sentences;
- $\phi_{\mathcal{T}}$ is a sentence over $\Gamma \cup \Sigma \cup \Gamma'$.

A first-order automaton:

$$\mathbf{A} = \langle \boldsymbol{\Sigma}, \boldsymbol{\Gamma}, \boldsymbol{\varphi}_{I}, \boldsymbol{\varphi}_{T}, \boldsymbol{\varphi}_{F} \rangle$$

where:

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- $\phi_{\mathcal{T}}$ is a sentence over $\Gamma \cup \Sigma \cup \Gamma'$.

A word (sequence of Σ -structures) $\overline{\sigma} = \langle \sigma_0, \dots, \sigma_{n-1} \rangle$ is accepted iff there is a **trace** (sequence of Γ -structures) $\overline{\rho} = \langle \rho_0, \dots, \rho_n \rangle$ such that:

• $\rho_0 \models \varphi_0;$

•
$$\rho_i \cup \sigma_i \cup \rho'_{i+1} \models \phi_T$$
;

• $\rho_n \models \phi_F$.

A set of first-order words whose structures come from a theory T is a T-language.

A *T*-language is **first-order** *T*-regular if there is a first-order automaton accepting it.

Theorem (Closure properties)

First-order T-regular languages are **closed** by:

- union;
- intersection;
- concatenation;
- Kleene star.

As an example we see how to prove concatenation.

We have two automata $A_1 = \langle \Sigma, \Gamma_1, \varphi_0^1, \varphi_T^1, \varphi_F^1 \rangle$ and $A_2 = \langle \Sigma, \Gamma_2, \varphi_0^2, \varphi_T^2, \varphi_F^2 \rangle$.

We want $A = \langle \Sigma, \Gamma, \varphi_0, \varphi_T, \varphi_F \rangle$ such that $\mathcal{L}(A) = \mathcal{L}(A_1) \cdot \mathcal{L}(A_2)$.

suppose for a moment that \$\phi_T\$ can be an existential second-order sentence;
then, what about:

$$\begin{split} \Phi_{\mathcal{T}} &\equiv (p \wedge \Phi_{\mathcal{T}}^{1} \wedge p') \vee (\neg p \wedge \Phi_{\mathcal{T}}^{2} \wedge \neg p') \vee \\ & \left(p \wedge \neg p' \wedge \Phi_{\mathcal{F}}^{1} \wedge \exists \Gamma'' \left(\Phi_{0}^{2} [\Gamma/\Gamma''] \wedge \Phi_{\mathcal{T}}^{2} [\Gamma/\Gamma''] \right) \right) \end{split}$$

with $\Gamma = \Gamma_1 \cup \Gamma_2 \cup \{p\}$.
$$\Phi_{T} \equiv \exists \Gamma'' \begin{bmatrix} (p \land \Phi_{T}^{1} \land p') \lor (\neg p \land \Phi_{T}^{2} \land \neg p') \lor \\ (p \land \neg p' \land \Phi_{F}^{1} \land (\Phi_{0}^{2}[\Gamma/\Gamma''] \land \Phi_{T}^{2}[\Gamma/\Gamma'']) \end{bmatrix} \end{bmatrix}$$

$$\Phi_{T} \equiv \exists \Gamma'' \begin{bmatrix} (p \land \varphi_{T}^{1} \land p') \lor (\neg p \land \varphi_{T}^{2} \land \neg p') \lor \\ \left(p \land \neg p' \land \varphi_{F}^{1} \land (\varphi_{0}^{2}[\Gamma/\Gamma''] \land \varphi_{T}^{2}[\Gamma/\Gamma'']) \right) \end{bmatrix}$$

Now the predicates in Γ'' can be added to Γ itself:

- the semantics of the automata will require the existence of their interpretation;
- we get back a first-order automaton on an extended state signature.

$$\Phi_{T} \equiv \begin{bmatrix} (p \land \varphi_{T}^{1} \land p') \lor (\neg p \land \varphi_{T}^{2} \land \neg p') \lor \\ (p \land \neg p' \land \varphi_{F}^{1} \land (\varphi_{0}^{2}[\Gamma/\Gamma''] \land \varphi_{T}^{2}[\Gamma/\Gamma'']) \end{bmatrix} \end{bmatrix}$$

Now the predicates in Γ'' can be added to Γ itself:

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Complementation is missing from the picture:

- easy for deterministic automata;
- so **determinization** is the key;
- how to symbolically represent the subset construction of a first-order automaton?
 - we are working on it...

A major feature of automata is that they capture temporal logic.

Can we capture FOLTL with first-order automata?

We need some ingredients.

Definition (Stepped normal form)

Given an FOLTL formula ϕ , the *step normal form* of ϕ , denoted snf(ϕ), is the formula defined recursively as follows:

- $\operatorname{snf}(p(t_1,\ldots,t_n)) = p(t_1,\ldots,t_n)$ and $\operatorname{snf}(t_1 = t_2) = (t_1 = t_2)$;
- $snf(Qx\varphi) = Qx snf(\varphi)$, where $Q \in \{\forall, \exists\}$ and x is a first-order variable;

•
$$\operatorname{snf}(\neg \phi) = \neg \operatorname{snf}(\phi);$$

- $\mathsf{snf}(\varphi_1 \circ \varphi_2) = \mathsf{snf}(\varphi_1) \circ \mathsf{snf}(\varphi_2)$, where $\circ \in \{\land, \lor\}$
- $snf(\circ \varphi) = \circ \varphi$ where $\circ \in \{X, Y, \widetilde{X}, Z\};$
- $\blacksquare \ \mathsf{snf}(\varphi_1 \ U \ \varphi_2) = \mathsf{snf}(\varphi_2) \lor (\mathsf{snf}(\varphi_1) \land \mathsf{X}(\varphi_1 \ U \ \varphi_2));$
- $\operatorname{snf}(\phi_1 \operatorname{R} \phi_2) = \operatorname{snf}(\phi_2) \wedge (\operatorname{snf}(\phi_1) \lor \widetilde{X}(\phi_1 \operatorname{R} \phi_2)).$

Definition (Closure)

The *closure* of a FOLTL sentence φ is the set $C(\varphi)$ defined as follows:

- $\blacksquare \ X\varphi \in C(\varphi);$
- $\psi \in C(\varphi)$ for any subformula ψ of φ (including itself);
- $\blacksquare \text{ for any } \varphi_1 \: U \: \varphi_2 \in \mathsf{C}(\varphi) \text{ we have } \mathsf{X}(\varphi_1 \: U \: \varphi_2) \in \mathsf{C}(\varphi);$
- for any $\varphi_1 R \varphi_2 \in C(\varphi)$ we have $\widetilde{X}(\varphi_1 R \varphi_2) \in C(\varphi)$.

We also define the following subsets of the closure:

$$\begin{split} XS &= \{ xs_{\psi} \mid X\psi \in C(\varphi) \} \\ \widetilde{X}S &= \{ ws_{\psi} \mid \widetilde{X}\psi \in C(\varphi) \} \end{split}$$

where xs_{ψ} and ws_{ψ} are predicates of the arity *n* corresponding to the number of free first-order variables in ψ .

Let ϕ be a FOLTL sentence. The automaton of ϕ is $\mathcal{A}(\phi) = \langle \Sigma, \Gamma, \phi_0, \phi_T, \phi_F \rangle$ where:

- the state signature is $\Gamma = XS \cup \widetilde{X}S$;
- the initial and final conditions are:

$$\begin{split} \varphi_0 &\equiv \mathsf{xs}_{\varphi} \\ \varphi_F &\equiv \bigwedge_{\mathsf{ws}_{\psi} \in \widetilde{\mathsf{XS}}} \forall \overline{\mathsf{x}}.\mathsf{ws}_{\psi}(\overline{\mathsf{x}}) \land \bigwedge_{\mathsf{xs}_{\psi} \in \mathsf{XS}} \forall \overline{\mathsf{x}}.\neg\mathsf{xs}_{\psi}(\overline{\mathsf{x}}) \end{split}$$

• the transition relation is:

$$\varphi_{\mathcal{T}} \equiv \bigwedge_{s_{\psi} \in \mathsf{XS} \cup \widetilde{\mathsf{XS}}} \forall \overline{\mathsf{x}}.[s_{\psi}(\overline{\mathsf{x}}) \leftrightarrow \mathsf{snf}_{\mathcal{S}}'(\psi(\overline{\mathsf{x}}))]$$

Of course checking emptiness of first-order automata is **undecidable**.

However, we can state a semi-algorithm for non-emptiness with some assumptions.

For k > 0, let:

$$\llbracket A \rrbracket_k^F \equiv \Phi_0^0 \wedge \bigwedge_{i=0}^{k-1} \Phi_T^k \wedge \Phi_F^k$$

1:	<pre>procedure NonEmpty(A)</pre>
2:	$k \leftarrow 0$
3:	while true do
4:	if $[\![A]\!]_k^F$ is satisfiable then
5:	return not empty
6:	end if
7:	$k \gets k+1$
8:	end while
9:	end procedure

Recall the result from the literature we cited before.

For a fragment F such that:

- the underlying FO fragment is decidable; and
- temporal formulas are monodic;
 - only one free variable inside temporal operators;
- constants in the signature are considered rigid;
- then FOLTL(F) is decidable [HWZ00]

Can we recover this result from first-order automata? Yes.

- if we follow the encoding we notice that monodic FOLTL sentences translate into automata with monadic state signature Γ;
- monadic predicates are easier to deal with (*e.g.*, monadic FO is decidable);
- we can translate a monadic Γ into a Γ containing only **propositions**;
- emptyness for this kind of automata is decidable (they are almost finite-state).

CONCLUSIONS

Our satisfiability checking tool BLACK is currently being refactored to support full FOLTL through first-order automata.

experimental results soon, maybe another iFM² talk?

Can we go beyond the simple unraveling semi-algorithm shown before?

For better **practical** results we need more **theory**.

Interesting paths we are exploring:

- fixpoint computation based on second-order quantifier elimination [GSS08];
- encoding into constrained Horn clauses [GB19];

We can add **past operators** to FOLTL.

- if we start from pure-past FOLTL sentences, we directly obtain deterministic first-order automata;
- this happens with pure-past LTL as well and is crucial for reactive synthesis;
- 2EXPTIME for LTL, EXPTIME for pure-past LTL, because of this fact;
- can this help with reactive synthesis for FOLTL specifications?

We want first-order temporal logics to become practical tools for infinite-state specification and verification.

- long way ahead;
- little steps already done;
- first-order automata as a reasoning and algorithmic tool;
- many theoretical and algorithmic developments missing yet.

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