Learning Dynamics with Synchronous, Asynchronous and General Semantics

Tony Ribeiro[1], Maxime Folschette[2], Morgan Magnin[1], Olivier Roux[1], Katsumi Inoue[3]

1. Laboratoire des Sciences du Numérique de Nantes, France
2. Univ Rennes, Inria, CNRS, IRISA, IRSET, F-35000 Rennes, France
3. National Institute of Informatics, Tokyo, Japan

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Outline

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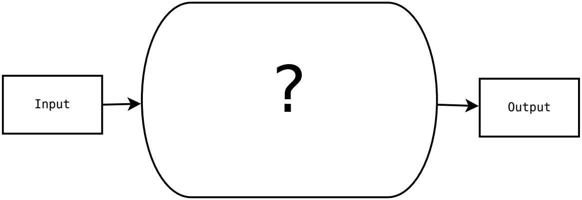
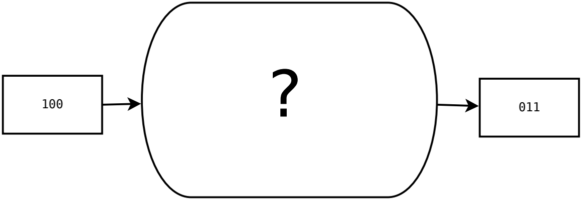
Research area

Idea: given a set of input/output states of a black-box system, learn its internal mechanics.



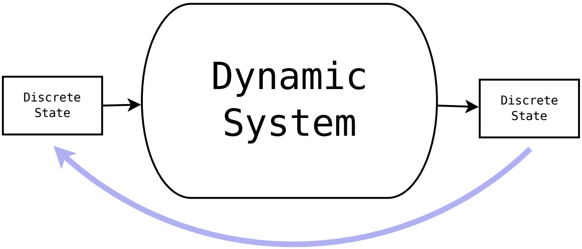
Research area

Discrete system: input/output are vectors of same size which contain discrete values.



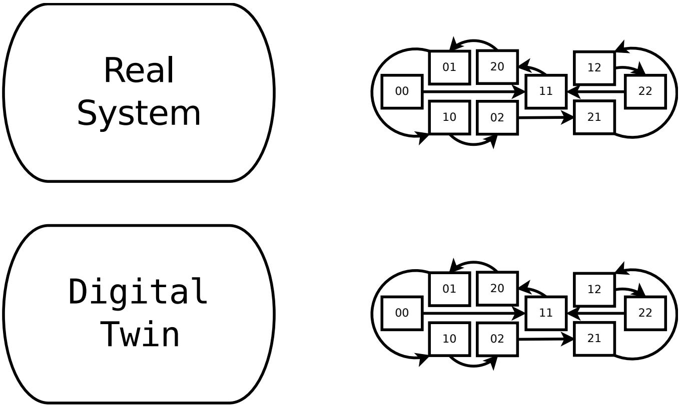
Research area

Dynamic system: input/output are state of the system and output becomes the next input.



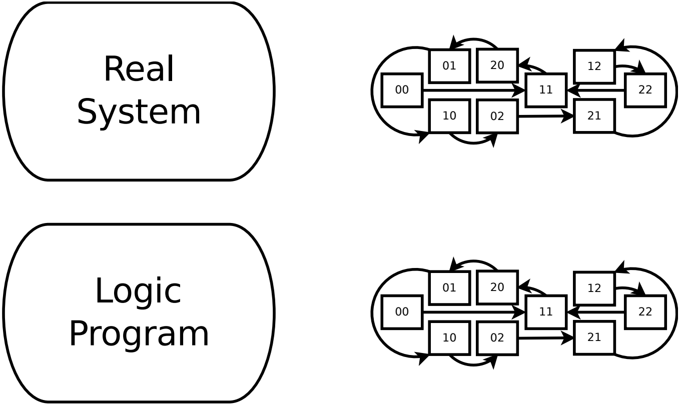
Research area

Goal: produce an artificial system with the same behavior as the one observed, i.e. a digital twin.



Research area

Representation: propositional logic programs with annotated atoms encoding multi-valued variables.

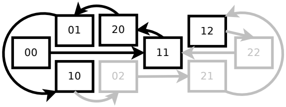


Research area

Method: learn the dynamics of systems from the observations of some of its state transitions.

DATA

?



RESULTS

a(0,T) :- a(2,T-1)
a(1,T) :- a(0,T-1), b(0,T-1).
a(2,T) :- a(1,T-1)
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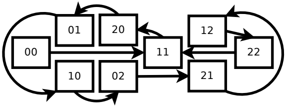
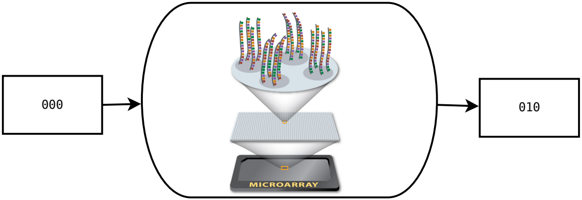


Motivation

Data: time series of genes expression levels in a organic cell.
Goal: model genes interactions to understand their influences.



Example (Possible Applications)

- **Bioinformatics**: Construct gene regulatory networks.
- **Robotics**: Learn action models from robot observations.

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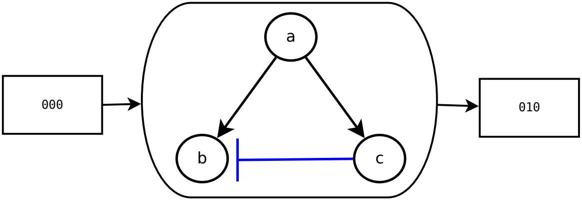

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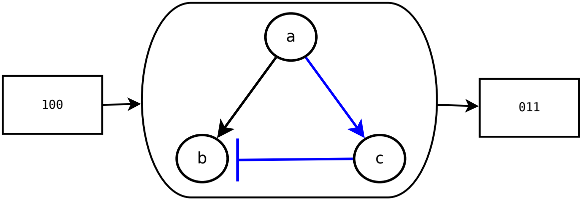

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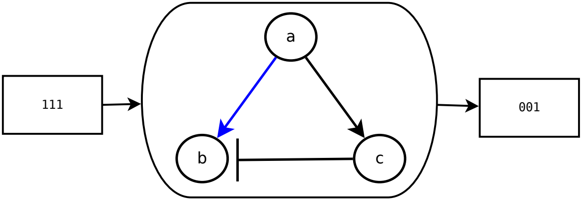

Example (Possible Applications)

- **Bioinformatics**: Construct gene regulatory networks.
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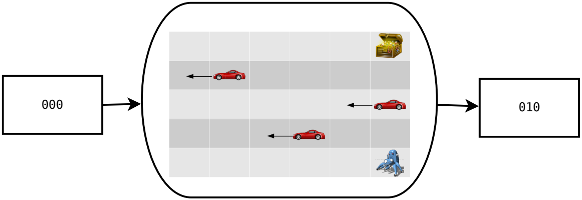
Motivation

Data: observations of environment evolution according to a robot actions.
Goal: produce a predictive model of the environment for action planning.



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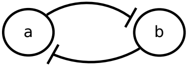
Semantics

Boolean network transitions differ according to the update semantics used.



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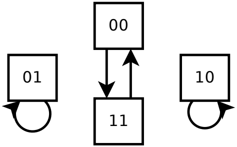
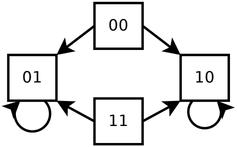
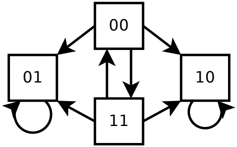


Synchronous



Asynchronous



General

- Synchronous: all variable are updated
- Asynchronous: only one variable is updated
- General: any number of variable can be updated

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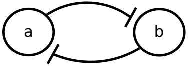

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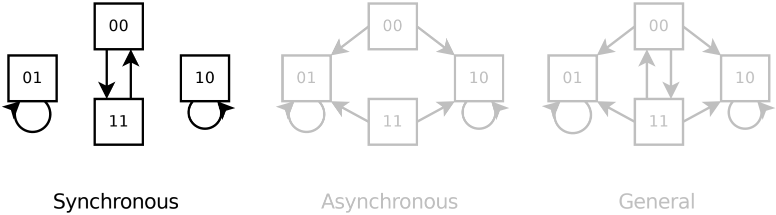

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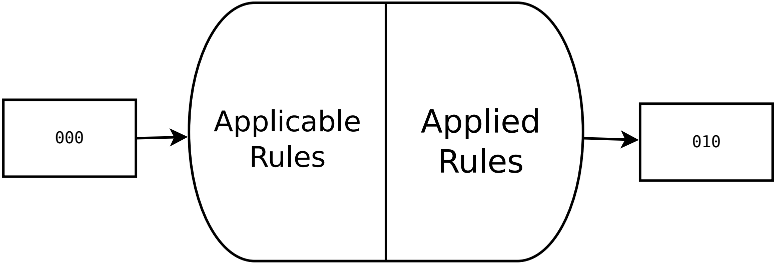
What is a semantics?

For those three semantics atleast its about computing the next state by selecting among applicable local rules the ones that will be applied.



Semantics: what is an applicable rule and what is a valid set of applied rule.

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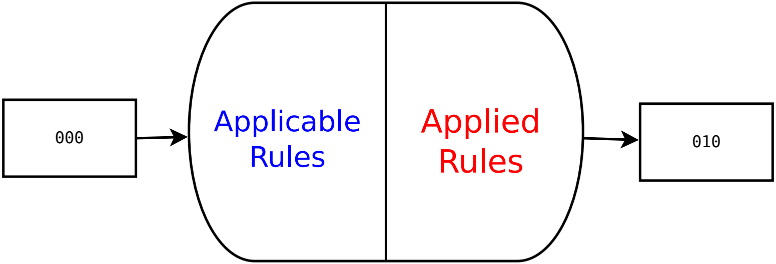

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Learning algorithm intuition: classification problem

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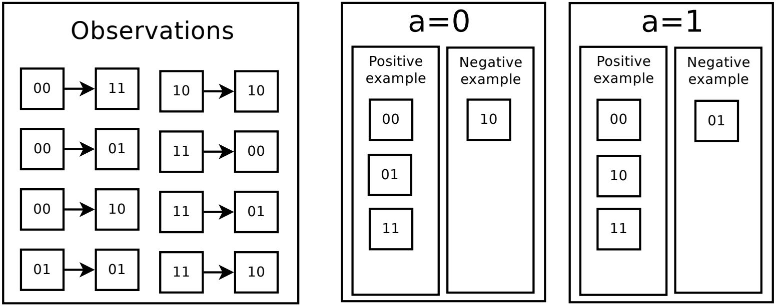

Equivalent to a classification problem: for each variable value, what is a typical state where the variable can takes this value in the next state ?

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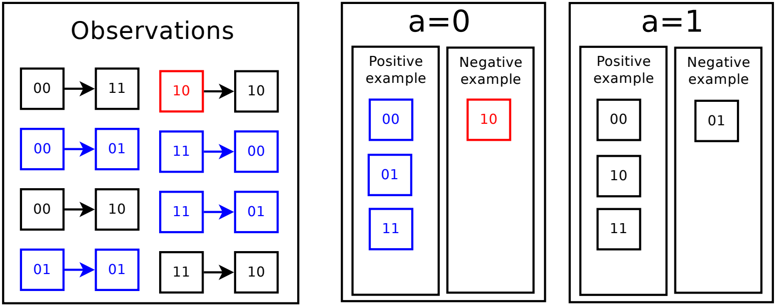

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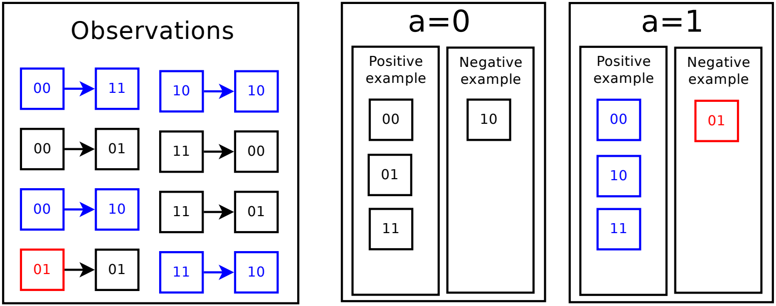

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Outline

Multi-valued Logic ($\mathcal{M}$VL)

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Definition (Atoms)

Let $\mathcal{V} = \{\mathrm{v}_1, \dots, \mathrm{v}_n\}$ be a finite set of $n \in \mathbb{N}$ variables, and dom : $\mathcal{V} \to \mathbb{N}$
The atoms of $\mathcal{M}$VL are of the form v^{val} where $\mathrm{v} \in \mathcal{V}$ and
$val \in [\![0; \mathrm{dom}(\mathrm{v})]\!]$. The set of such atoms is denoted by $\mathcal{A}^{\mathcal{V}}_{\mathrm{dom}}$ or simply $\mathcal{A}$.

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Definition (Rules)

A $\mathcal{M}$VL rule R is defined by:

$$R = \mathrm{v}_0^{val_0} \leftarrow \mathrm{v}_1^{val_1} \wedge \cdots \wedge \mathrm{v}_m^{val_m} \quad (1)$$

where $\forall i \in [\![0; m]\!], \mathrm{v}_i^{val_i} \in \mathcal{A}$ are atoms in $\mathcal{M}$VL.

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Left-hand side is called the head of R and is denoted $h(R) := \mathrm{v}_0^{val_0}$.

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$\mathrm{var}(h(R)) := \mathrm{v}_0$ denotes the variable that occurs in $h(R)$.

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Right-hand side is called the body of R, written $b(R) := \{\mathrm{v}_1^{val_1}, \dots, \mathrm{v}_m^{val_m}\}$

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A *multi-valued logic program* ($\mathcal{M}$VLP) is a set of $\mathcal{M}$VL rules.

Rules Properties

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Definition (Rule Domination)

Let R_1, R_2 be two $\mathcal{M}\mathrm{VL}$ rules. R_1 dominates R_2, written $R_2 \leq R_1$ if $h(R_1) = h(R_2)$ and $b(R_1) \subseteq b(R_2)$.

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Proposition (Double domination is equality)

If $R_1 \leq R_2$ *and* $R_2 \leq R_1$ *then* $R_1 = R_2$.

Rules with the most general bodies dominate the other rules.
These are the rules we want since they cover the most general cases.

Dynamical System Modeling

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Definition (Transitions)

We write $\mathcal{S}$ to denote the set of all discrete states, and a couple of states $(s, s') \in \mathcal{S}^2$ is called a transition.

Dynamical System Modeling

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Definition (Rule-state matching)

Let $s \in \mathcal{S}$. The $\mathcal{M}\mathrm{VL}$ rule R matches s, written $R \sqcap s$, if $b(R) \subseteq s$.

When matching a state, a rule can be used to realize a transition.

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A rule R realizes the transition (s, s'), written $s \xrightarrow{R} s'$, if $R \sqcap s, h(R) \in s'$.

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Definition (Program realization)

A $\mathcal{M}\mathrm{VLP}$ P realizes (s, s'), written $s \xrightarrow{P} s'$, if
$\forall \mathrm{v} \in \mathcal{V}, \exists R \in P, \mathrm{var}(h(R)) = \mathrm{v} \wedge s \xrightarrow{R} s'$.
It realizes $T \subseteq \mathcal{S}^2$, written $\overset{P}{\hookrightarrow} T$, if $\forall (s, s') \in T, s \xrightarrow{P} s'$.

Desired Properties

In the following, for all sets of transitions $T \subseteq \mathcal{S}^2$, we denote:
$\mathrm{fst}(T) := \{s \in \mathcal{S} \mid \exists (s_1, s_2) \in T, s_1 = s\}$.

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Definition (Conflicts)

A $\mathcal{M}\mathrm{VL}$ rule R conflicts with a set of transitions $T \subseteq \mathcal{S}^2$ when $\exists s \in \mathrm{fst}(T), \big(R \sqcap s \land \forall (s, s') \in T, h(R) \notin s'\big)$.

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Definition (Concurrent rules)

Two $\mathcal{M}\mathrm{VL}$ rules R and R' are concurrent when
$R \sqcap R' \wedge \mathrm{var}(h(R)) = \mathrm{var}(h(R')) \wedge h(R) \neq h(R')$.

Definition (Complete program)

A $\mathcal{M}\mathrm{VLP}$ P is complete if $\forall s \in \mathcal{S}, \forall \mathrm{v} \in \mathcal{V}, \exists R \in P, R \sqcap s \wedge \mathrm{var}(h(R)) = \mathrm{v}$.

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Let $s \in \mathrm{fst}(T)$, a program consistent with T will only realize the transitions $(s, s') \in T$.

Optimal $\mathcal{M}$VLP

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Definition (Suitable program)

Let $T \subseteq \mathcal{S}^2$. A $\mathcal{M}$VLP P is suitable for T when:

- P is consistent with T, — Cover no negative example
- P realizes T, — Cover all positive example
- P is complete — Cover all state space
- $\forall R$ not conflicting with T, $\exists R' \in P$ s.t. $R \leq R'$. — Cover all hypotheses

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Definition (Optimal program)

If in addition, $\forall R \in P$, all the rules R' belonging to a $\mathcal{M}$VLP suitable for T are such that $R \leq R'$ implies $R' \leq R$ then P is called optimal.

An optimal program is the set of all rules that are not dominated by any consistent rules. Contains all minimal hypotheses

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Proposition

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Yeah ! And this property is the starting point of the learning algorithm.

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$P_{\mathcal{O}}(\emptyset) = \{\mathrm{v}^{val} \leftarrow \emptyset \mid \mathrm{v}^{val} \in \mathcal{A}\}$.

Yeah ! And this property is the starting point of the learning algorithm.

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Let $T \subseteq \mathcal{S}^2$. If P is a $\mathcal{M}$VLP suitable for T, then
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Optimal $\mathcal{M}$VLP

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Let $T \subseteq \mathcal{S}^2$. The $\mathcal{M}$VLP optimal for T is unique and denoted $P_{\mathcal{O}}(T)$.

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We can obtain the optimal program from any suitable program by simply removing the dominated rules.

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How to make a minimal modifications of a $\mathcal{M}\mathrm{VLP}$ in order to be suitable with a new set of transitions?

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Thus, a $\mathcal{M}\mathrm{VLP}$ can be revised to only realizes given transitions from s.

Definition (Program least revision)

Let P be a $\mathcal{M}\mathrm{VLP}$, $s \in \mathcal{S}$ and $T \subseteq \mathcal{S}^2$ such that $\mathrm{fst}(T) = \{s\}$. Let $R_P := \{R \in P \mid R \text{ conflicts with } T\}$. The least revision of P by T is $L_{\mathrm{rev}}(P, T) := (P \setminus R_P) \cup \bigcup_{R \in R_P} L_{\mathrm{spe}}(R, s)$.

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Guess what? Least revision can conserves suitability :)

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Theorem

Let $s \in \mathcal{S}$ *and* $T, T' \subseteq \mathcal{S}^2$ *such that* $|\mathrm{fst}(T')| = 1 \land \mathrm{fst}(T) \cap \mathrm{fst}(T') = \emptyset$. $L_{\mathrm{rev}}(P_{\mathcal{O}}(T), T')$ *is a* $\mathcal{M}\mathrm{VLP}$ *suitable for* $T \cup T'$.

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In association with previous results it gives a method to iteratively compute $P_{\mathcal{O}}(T)$ for any $T \subseteq \mathcal{S}^2$, starting from $P_{\mathcal{O}}(\emptyset)$.

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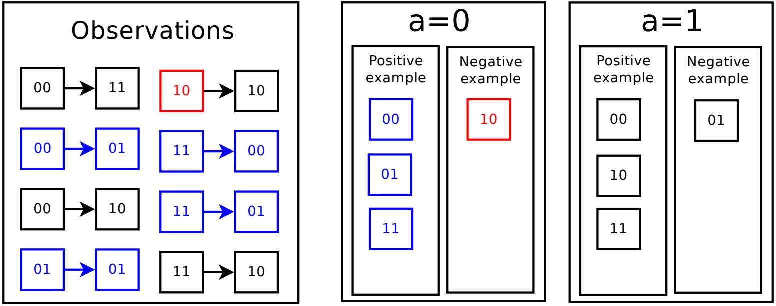

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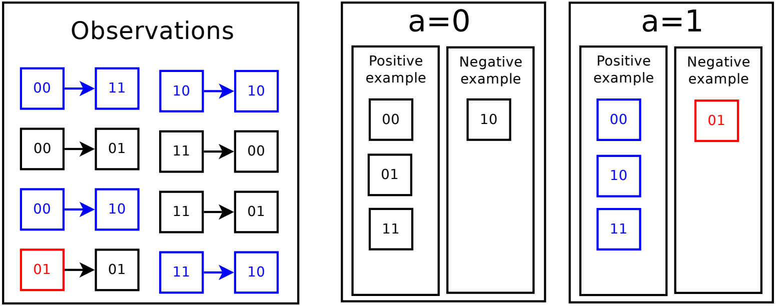

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OUTPUT: $P_{\mathcal{O}}(T) := P$.

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Definition (Semantics)

Let $\mathcal{A}^{\mathcal{V}}_{\mathsf{dom}}$ be a set of atoms and $\mathcal{S}$ the corresponding set of states. A semantics (on $\mathcal{A}^{\mathcal{V}}_{\mathsf{dom}}$) is a function that associates, to each complete $\mathcal{M}\mathrm{VLP}$ P, a set of transitions $T \subseteq \mathcal{S}^2$ so that: $\mathrm{fst}(T) = \mathcal{S}$. Equivalently, a semantics can be seen as a function of $(\mathrm{c}\text{-}\mathcal{M}\mathrm{VLP} \rightarrow (\mathcal{S} \rightarrow \wp(\mathcal{S}) \setminus \emptyset))$ where $\mathrm{c}\text{-}\mathcal{M}\mathrm{VLP}$ is the set of complete $\mathcal{M}\mathrm{VLP}$s and $\wp$ is the power set operator.

Definition (Synchronous semantics)

The synchronous semantics $\mathcal{T}_{syn}$ is defined by:

$$\mathcal{T}_{syn} : P \mapsto \{(s, s') \in \mathcal{S}^2 \mid s' \subseteq \{h(R) \in \mathcal{A} \mid R \in P, R \sqcap s\}\}$$

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Semantic free modeling

Finally, we can state that the definitions and method developed in the previous section are independent of those three semantics.

Theorem (Semantics-free correctness)

Let P be a $\mathcal{M}\mathrm{VLP}$ such that P is complete.

- $\mathcal{T}_{syn}(P) = \mathcal{T}_{syn}(P_{\mathcal{O}}(\mathcal{T}_{syn}(P)))$,
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Whatever the semantic which produced T, given the optimal $\mathcal{M}$VLP of T we can reproduce exactly T with the same semantic.

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And **GULA** can learn such an optimal $\mathcal{M}\mathrm{VLP}$ from T.

Theorem (GULA Termination, soundness, completeness, optimality)

Let $T \subseteq \mathcal{S}^2$. The call **GULA**$(\mathcal{A}, T)$ *terminates and* **GULA**$(\mathcal{A}, T) = P_{\mathcal{O}}(T)$.

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Victory! In theory, but how does it scale in practice?

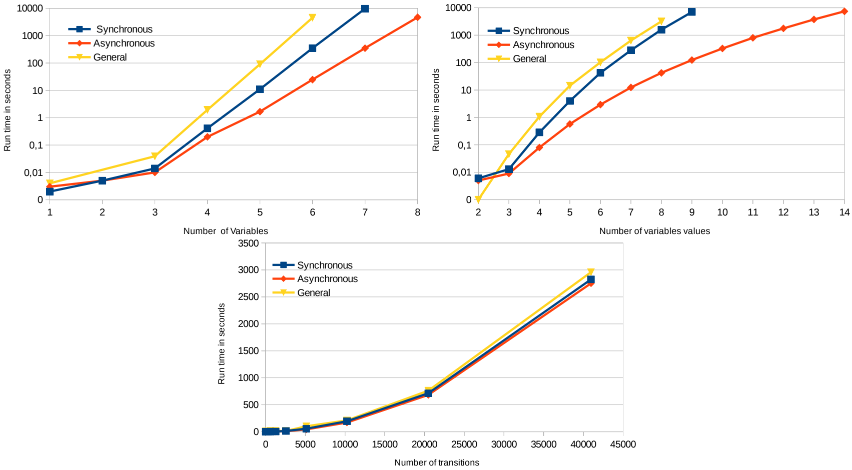
Outline

Evaluation

Theorem (**GULA** Complexity)

Let $T \subseteq \mathcal{S}^2$ be a set of transitions, $n := |\mathcal{V}|$ be the number of variables of the system and $d := \max(\text{dom}(\mathcal{V}))$ be the maximal number of values of its variables. The worst-case time complexity of **GULA** *when learning from T belongs to $\mathcal{O}(|T|^2 + 2n^3 d^{2n+1} + 2n^2 d^n)$ and its worst-case memory use belongs to $\mathcal{O}(d^{2n} + 2d^n + nd^{n+2})$.*

Evaluation



Evaluation of **GULA**'s scalability w.r.t. number of variables (top left), number of variables values (top right) and number of input transitions (bottom).

Evaluation

Semantics	Mammalian (10)	Fission (10)	Budding (12)	Arabidopsis (15)
Synchronous	1.84s / 1,024	1.55s / 1,024	34.48s / 4,096	2,066s / 32,768
Asynchronous	19.88s / 4,273	19.18s / 4,217	523s / 19,876	T.O. / 213,127
General	928s / 34,487	1,220s / 29,753	T.O. / 261,366	T.O. / $>$ 500,000

Run time of **GULA** (run time in seconds / number of transitions as input) for Boolean network benchmarks up to 15 nodes for the three semantics.

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New contribution

Conclusion

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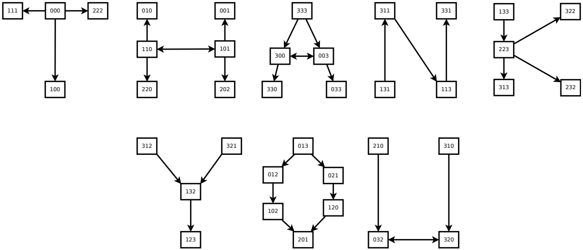
- One algorithm to learn them all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