

Bioss-IA 2020 Workshop

GULA: Learning (From Any) Semantics of a Biological Regulatory Network

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Joint work with Morgan MAGNIN (ECN + LS2N + NII)
and Katsumi INOUE (NII + SOKENDAI + Tokyo Tech)

2020-11-24

Introduction

Learn interaction rules from the dynamical transitions

- LFIT: **synchronous** semantics, deterministic (Boolean)
[Inoue, Ribeiro, Sakama, *Machine Learning Jour.*, 2014]
- LFkT: **synchronous** semantics, with memory (Boolean)
[Ribeiro, Magnin, Inoue, Sakama, *Frontiers in Bioeng. and Biotech.*, 2015]
- LUST: **synchronous** semantics, non-deterministic
[Martinez, Ribeiro, Inoue, Alenya, Torras, *ICLP*, 2015.]
- ACEDIA: **synchronous** semantics, continuous domains
[Ribeiro, Turret, Folschette, +5, *ILP*, 2017]
- **GULA: synchronous, asynchronous, general** semantics
[Ribeiro, Folschette, Magnin, Roux, Inoue, *ILP*, 2018]

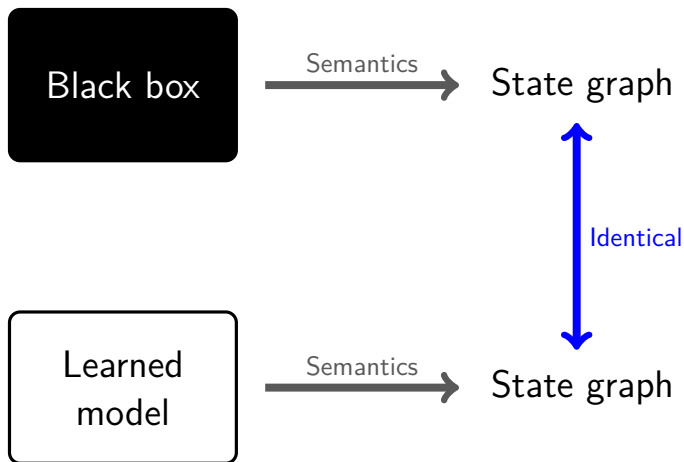
Content of this presentation: improvements on GULA

- Define the scope of “learnable” semantics
- Learn the rules of the semantics itself
- ...and more!

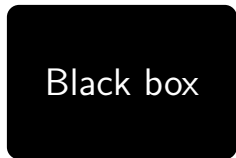
Introduction



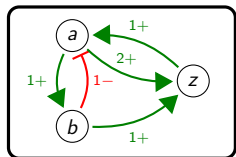
Introduction



Introduction



State graph



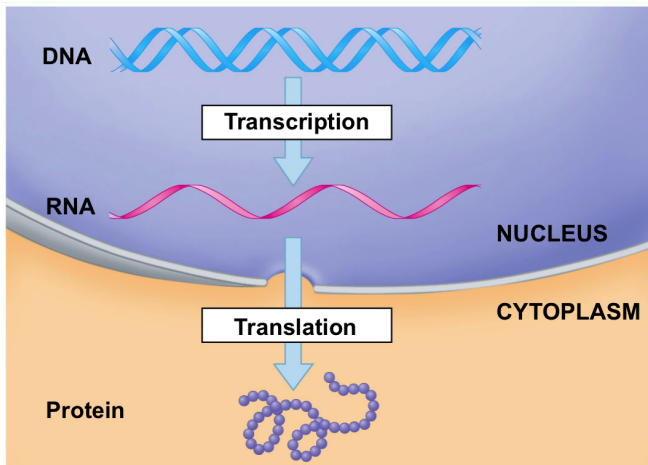
State graph



Identical

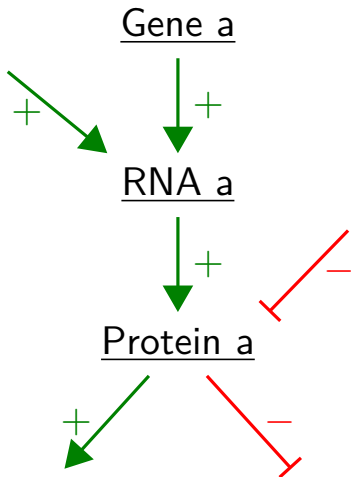
Discrete Networks

Preliminary Abstraction

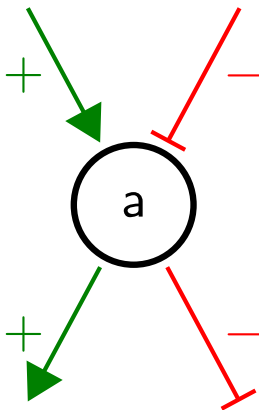


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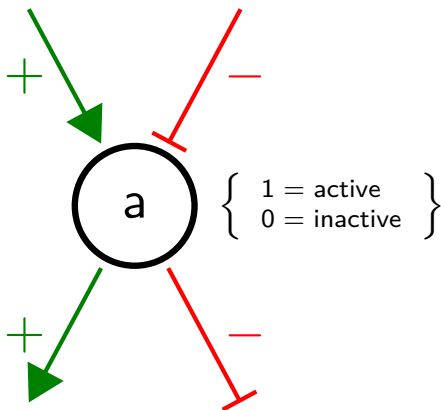
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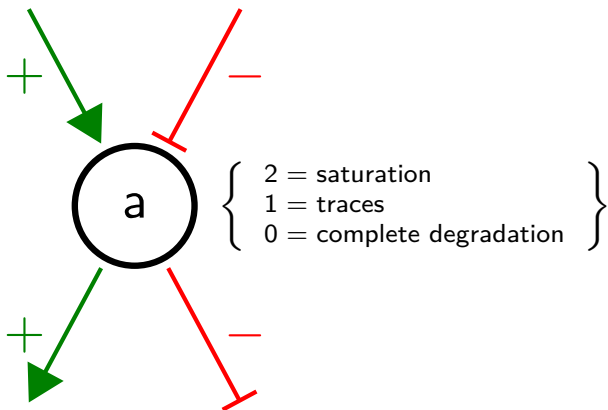
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Preliminary Abstraction



Discrete Networks / Thomas Modeling

[Kauffman, *Journal of Theoretical Biology*, 1969]

[Thomas, *Journal of Theoretical Biology*, 1973]

- A set of components $N = \{a, b, z\}$
- A discrete domain for each component $\text{dom}(a) = \llbracket 0; 2 \rrbracket$
- Discrete parameters / evolution functions $f^a : \mathcal{S} \rightarrow \text{dom}(a)$
- Signs & thresholds on the edges (redundant) $a \xrightarrow{2+} z$

	a	f^b	z	b	f^a	a	b	f^z
(a)	0	0	0	0	1	0	0	0
	1	1	0	1	0	0	1	0
	2	1	1	0	1	1	0	0
			1	1	2	1	1	0
						2	0	0
						2	1	1

(a)

(z)

(b)

Semantics = From this information, what are the next possible state(s)?

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(b)

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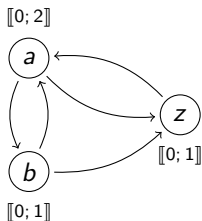
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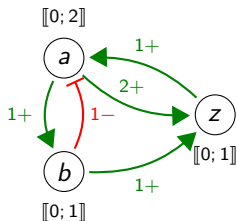
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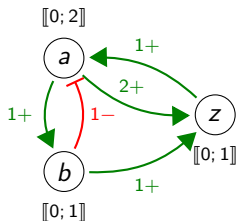
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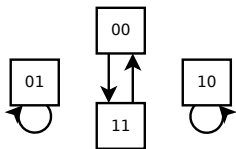
Semantics

State transitions differ according to the update semantics used

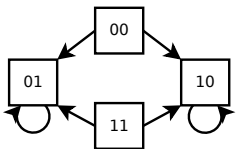


$f(a) := \text{not } b.$

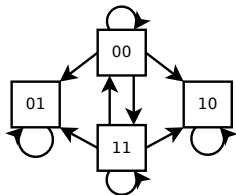
$f(b) := \text{not } a.$



Synchronous



Asynchronous

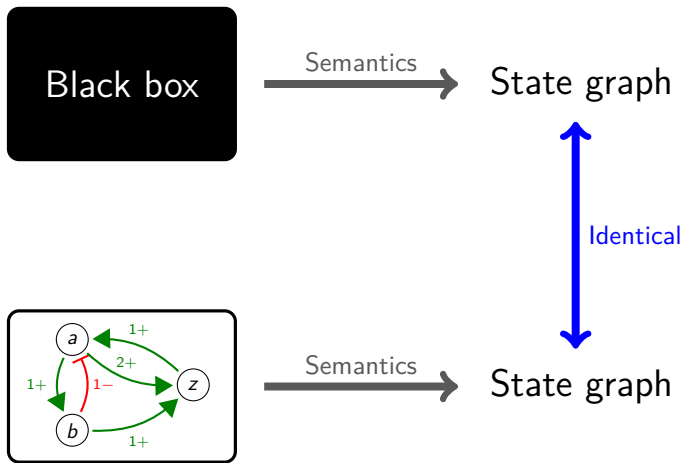


General

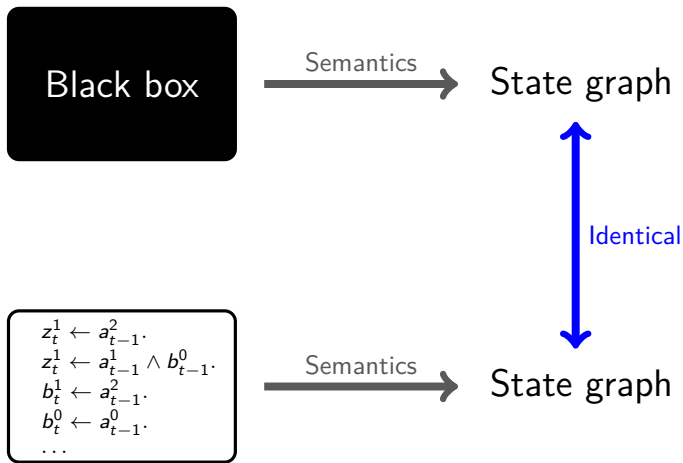
- **Synchronous:** all variables are updated
- **Asynchronous:** only one variable is updated
- **General:** any number of variables can be updated

Logic Programs

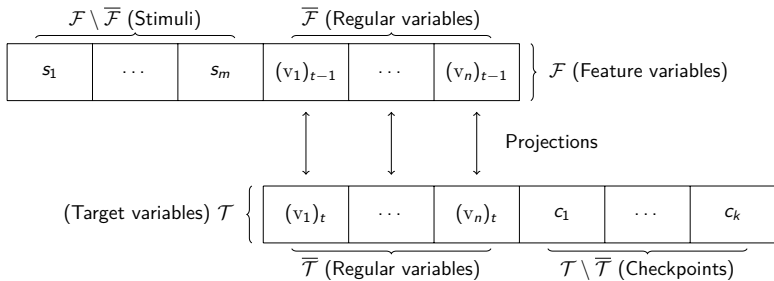
Principle of the Learning



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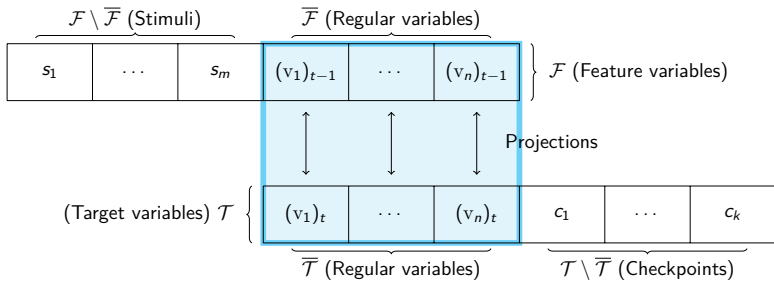


Feature & Target Variables



- **Feature variables** = causes
- **Target variables** = consequences
- Stimuli = known inputs
- Checkpoints = known outputs

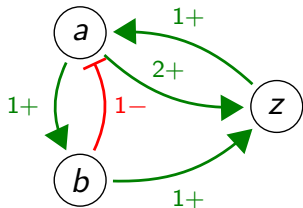
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Discrete Model as a Logic Program

Discrete model:



+ Discrete parameters
or evolution functions

Logic program:

$$b_t^1 \leftarrow a_{t-1}^1.$$

$$b_t^1 \leftarrow a_{t-1}^2.$$

$$b_t^0 \leftarrow a_{t-1}^0.$$

$$z_t^1 \leftarrow a_{t-1}^2 \wedge b_{t-1}^1.$$

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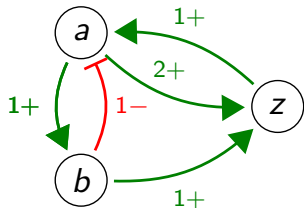
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etc...

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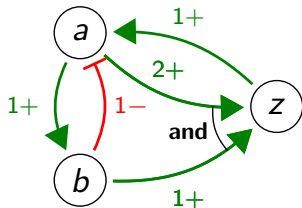
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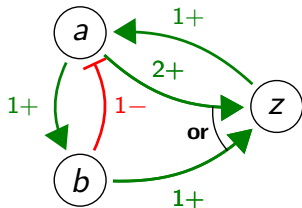
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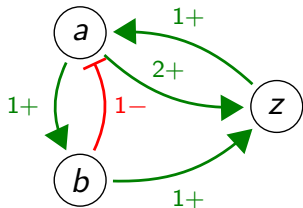
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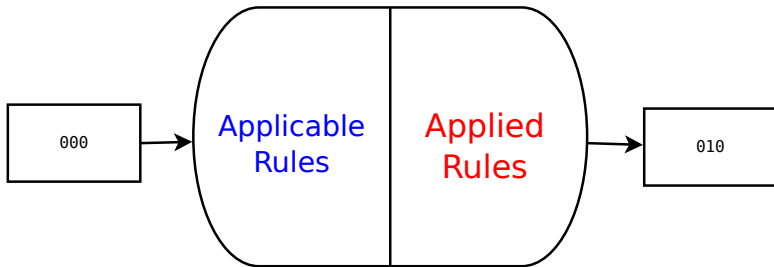
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Learning

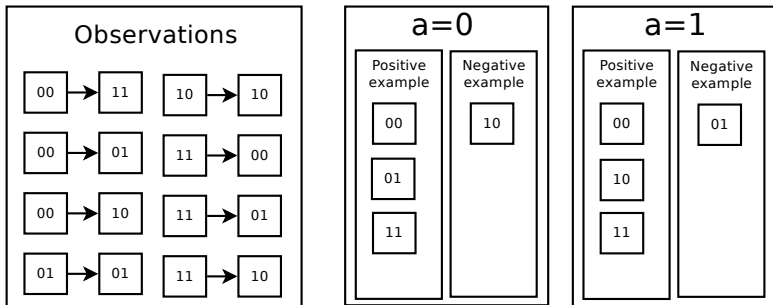
Semantics-Free Learning

Semantics = computing the next state by selecting, among **applicable** local rules, the ones that will be **applied**.



Learning Intuition: Classification Problem

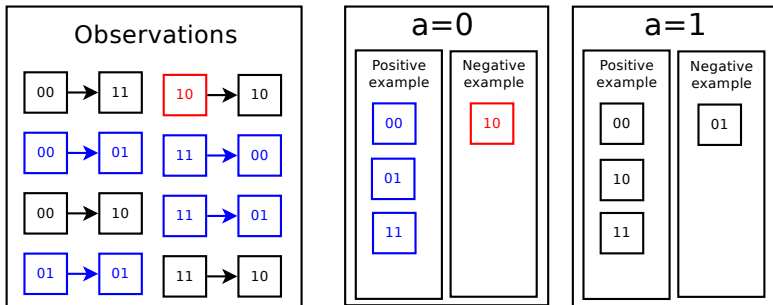
What is an **applicable** rule? The **conditions** so that a variable **can** take a certain value in next state.



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

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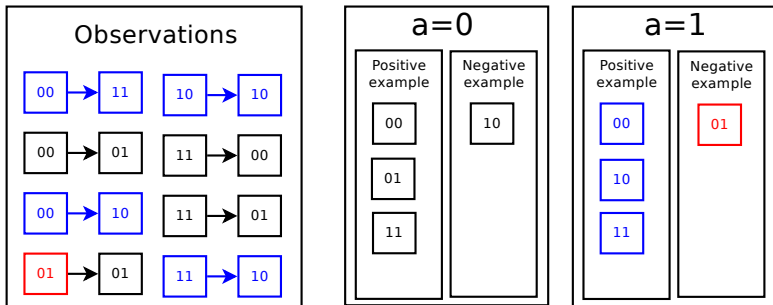
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What is an **applicable** rule? The **conditions** so that a variable **can** take a certain value in next state.



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

GULA = General Usage LFIT Algorithm

Input: a set of transitions (feature \rightarrow target)

Output: a program that respects:

- **Consistency:** the program allows no negative examples
- **Realization:** the program covers all positive examples
- **Completeness:** the program covers all the state space
- **minimality** of the rules (most general bodies)

Method: start from most general rules and **specialize** iteratively.

Least Specialization

Ensure consistency of a rule:

$$\underbrace{V_0^{val_0}}_{\text{head}} \leftarrow \underbrace{V_1^{val_1} \wedge V_2^{val_2} \wedge \dots \wedge V_n^{val_n}}_{\text{body}}.$$

→ Used when a rule matches a negative example s : $body \subseteq s$.

→ Add **one** condition to $body$ that prevents matching s .

Examples:

$$\left. \begin{array}{l} a_t^1 \leftarrow \top. \\ b_t^0 \leftarrow a_{t-1}^0. \\ ch^2 \leftarrow a_{t-1}^0 \wedge b_{t-1}^1 \wedge st^1. \end{array} \right\} \begin{array}{l} \text{all match } (a_{t-1}^0, b_{t-1}^1, st^1) \\ \rightarrow \text{how to specialize each one?} \end{array}$$

Suppose $\text{dom}(a_{t-1}) = \text{dom}(b_{t-1}) = \{0, 1\}$ and $\text{dom}(st) = \{0, 1, 2\}$.

The Least Specialization of $a_t^1 \leftarrow \top$. is:

$$\rightarrow \{ a_t^1 \leftarrow a_{t-1}^1. ; a_t^1 \leftarrow b_{t-1}^0. ; a_t^1 \leftarrow st^0. ; a_t^1 \leftarrow st^2. \}$$

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→ \emptyset

GULA: General Usage LFIT Algorithm

GULA: INPUT: a set of transitions T .

Initialize $P = \emptyset$

For each existing target atom v^{val}

- Extract all states from which no transition to v^{val} exist:
 $Neg_{v^{val}} := \{s \mid \nexists (s, s') \in T, v^{val} \in s'\}$
- Initialize $P_{v^{val}} := \{v^{val} \leftarrow \top.\}$
- For each state $s \in Neg_{v^{val}}$
 - Replace each rule that matches s by its least specializations
 - Remove all dominated rules, that is, that are not the most general:
 $head(R) = head(R')$ and $body(R) \subseteq body(R')$
- $P := P \cup P_{v^{val}}$

OUTPUT: $P_O(T) := P$ the optimal program of T .

Formally proved: Compatible with transitions generated in **synchronous**, **asynchronous** and **general** semantics.

Also proved: Compatible with a wider class of “learnable” semantics.

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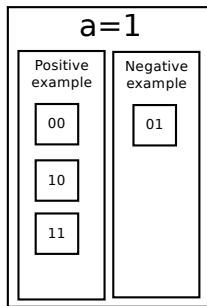
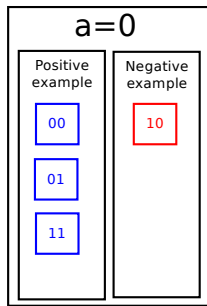
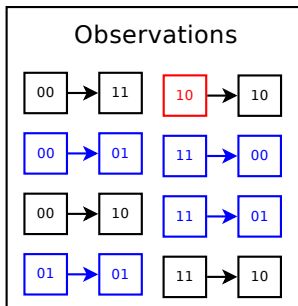
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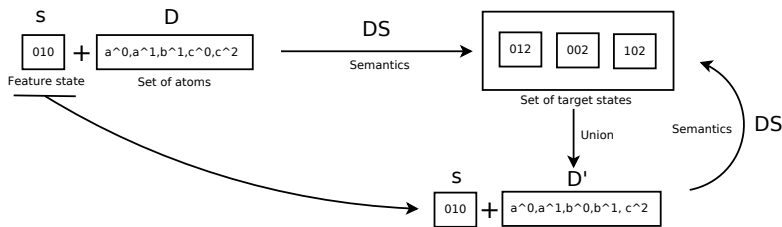
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Learnable Semantics: Pseudo-Idempotent

→ Consider a function DS that maps a **feature state** and a **set of target atoms** to a **set of target states**

→ Such that given the **same state** and the **union of its output**, it produces the **same result** (pseudo-idempotent)



→ A program gives possible target values (D)

→ A semantics gives which combinations are possible ($DS(s, D)$)

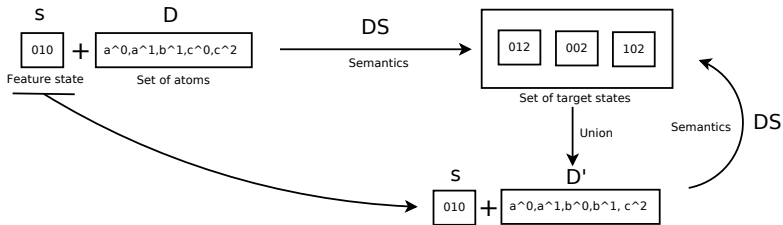
→ If the semantics produces the same states given those local values, then **GULA** learns a programs equivalent to the original one under this semantics:

$$DS(s, D) = DS(s, D') \implies DS(P) = DS(GULA(DS(P)))$$

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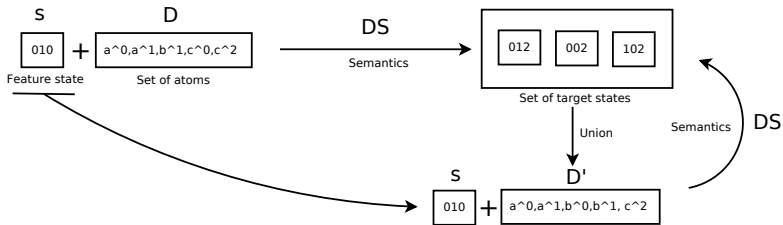
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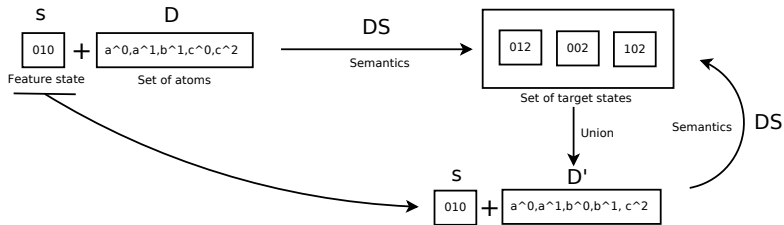
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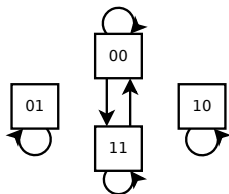
What if we don't know the semantics?

Three examples of arbitrary semantics:

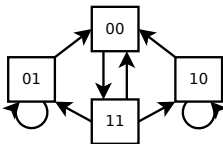


$f(a) := \text{not } b.$

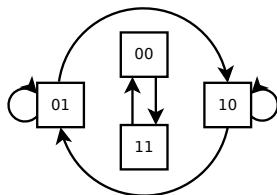
$f(b) := \text{not } a.$



All or nothing change



Degradation

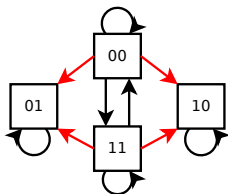


Inverse all values

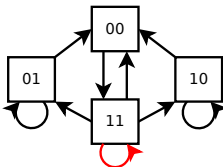
How can we learn a program able to reproduce such behavior?

What is impossible?

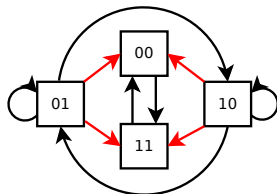
If we use the program learned by **GULA** with the synchronous semantics, we observe **spurious** transitions, which were not in the observations:


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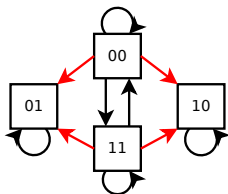
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How to prevent these **impossible** transitions?

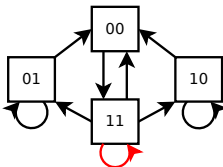
We need "impossibility rules": **constraints!**

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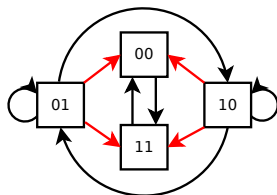
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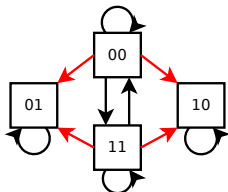


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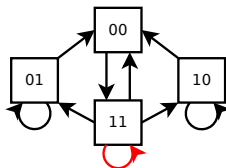
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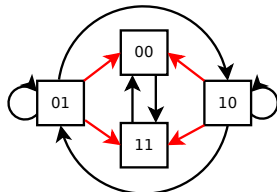
Classification Modeling of Impossibility



All or nothing change

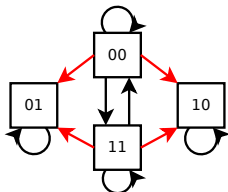


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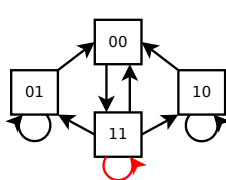


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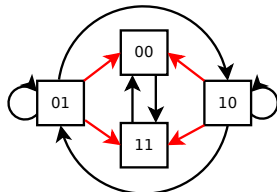
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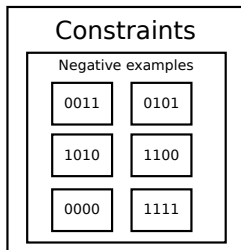
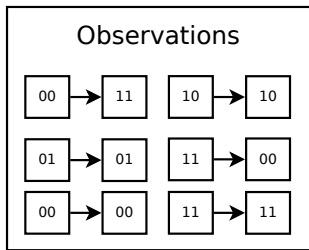
All or nothing change



Degradation



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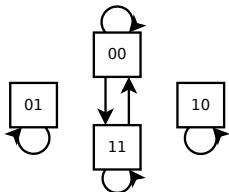


Learning Any Semantics Dynamics

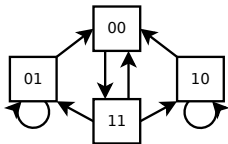
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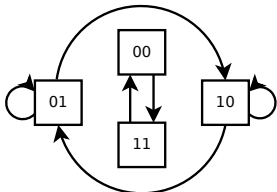
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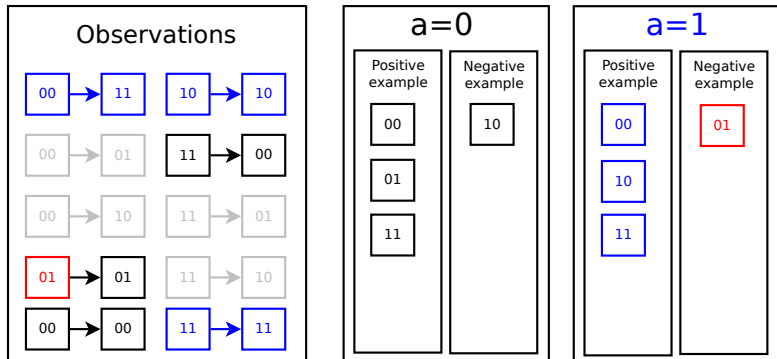
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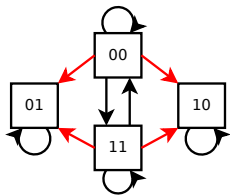
```

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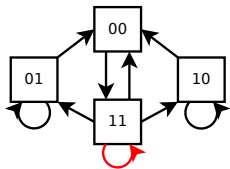
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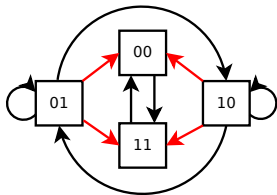
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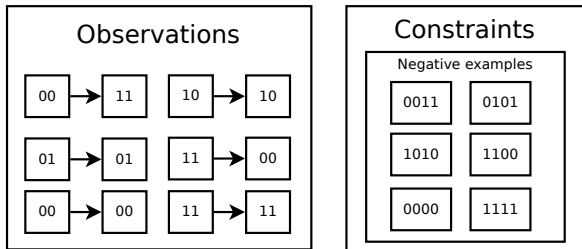
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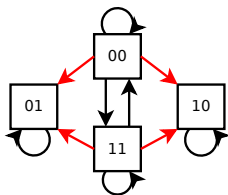
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- **OUTPUT:** $P \cup P'$ which exactly reproduces T , under the **constrained synchronous semantics**

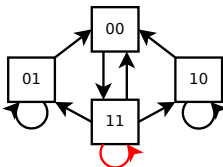
Examples of learned programs



All or nothing change

```

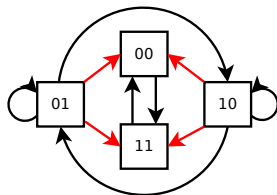
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Degradation

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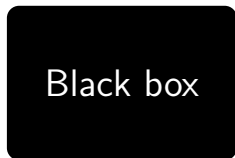
Inverse all values

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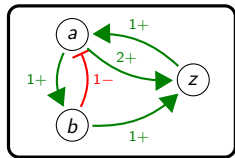
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```

Learning Time Series

Potential Usage

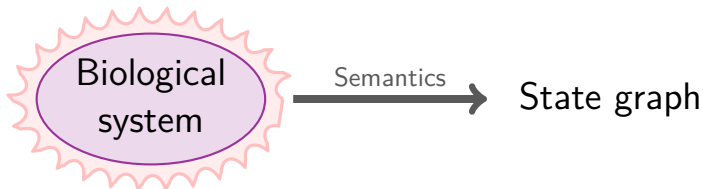


State graph

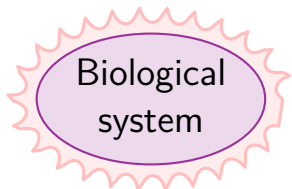


State graph

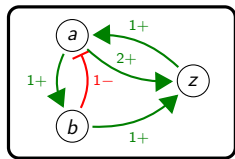
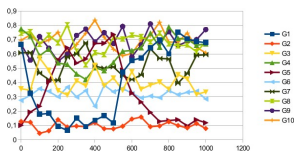
Potential Usage



Potential Usage



Behavior →



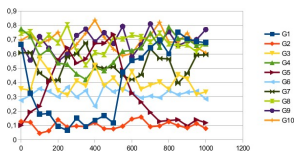
Semantics →

State graph

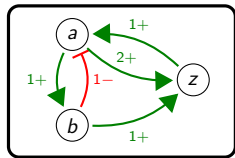
Potential Usage



Behavior →



Discretization



Semantics →

State graph

Scalability of GULA

Run time of **GULA** for 9 to 18 nodes Boolean networks for the three semantics: run time in seconds for 25%/50%/75%/100% of the transitions as input, and total number of transitions.

Benchmark	size	synchronous	asynchronous	general
arellano_rootstem	9	2s/1.8s/0.9s/0.3s/512	2.4s/1.4s/1.1s/0.2s/1,940	1.1s/0.5s/0.3s/0.3s/11K
davidich_yeast	10	16s/10s/4s/0.6s/1,024	12s/6s/4s/0.5s/4,364	3s/1.5s/1s/0.9s/39K
faure_cellcycle	10	15s/10s/4s/0.8s/1,024	12s/5.6s/4.7s/0.6s/4,273	4s/1.2s/0.9s/0.9s/31K
fission_yeast	10	16s/10s/4.8s/0.8s/1,024	12s/5.8s/4.6s/0.4s/4,157	3.6s/1.2s/1s/0.8s/34K
mammalian	10	14.8s/11s/4.8s/0.8s/1,024	12s/5.7s/3.4s/0.6s/4,273	3.4s/1.4s/1s/0.9s/31K
budding_yeast	12	564s/194s/61s/3.7s/4,096	216s/107s/85s/2.6s/20K	51s/14s/5.9s/4.1s/260K
n12c5	12	468s/200s/64s/2.8s/4,096	213s/103s/144s/1.3s/30K	4.7s/6s/8.6s/11s/1,122K
tournier_apoptosis	12	369s/164s/54s/2.7s/4,096	199s/98s/94s/2s/22K	26s/6.7s/4.6s/4.6s/358K
dinwoodie_stomatal	13	-/748s/221s/6.1s/8,192	-/548s/628s/4s/53K	70s/18s/15s/18s/1.5M
multivalued	13	-/406s/6s/8,192	-/565s/765s/4.9s/49K	61s/18s/13s/13s/1M
saadatpour_guardcell	13	-/757s/219s/6s/8,192	-/575s/638s/4.2s/53K	68s/17s/15s/18s/1.5M
arabidopsis	15	-/-/53s/32K	-/-/50s/213K	-/352s/123s/103s/7M
dinwoodie_life	15	-/-/37s/32K	-/-/30s/245K	-/352s/240s/256s/20M
randomnet_n15k3	15	-/-/51s/32K	-/-/31s/262K	731s/219s/226s/280s/22M
irons_yeast	18	-/-/653s/262K	-/-/324s/2M	memory out

Exponential w.r.t variables/values but faster if more observations.

Runtime is not a problem with **PRIDE**, a polynomial approximation.

Polynomial Approximation: PRIDE

PRIDE = Polynomial Relational Inference of Discrete Events

Input: a set of transitions (feature \rightarrow target)

Output: a program that respects:

- **Consistency:** The program allows no negative examples
- **Realization:** The program covers all positive examples
- ~~Completeness:~~ ~~The program covers all the state space~~
- **Minimality** of the rules (most general bodies)

Method:

- Keep only one specialization according to a non-matched positive example.
- Use greedy search to minimize rules.

Learning Semantics is exponential

Run time of **Synchronizer** for 6 to 10 nodes Boolean networks for the three semantics: run time in seconds for 25%/50%/75%/100% of the transitions as input, and total number of transitions.

Benchmark	size	synchronous	asynchronous	general
n6s1c2	6	0.2s/0.3s/0.2s/0.1s/64	2.5s/4.4s/3.6s/1s/230	9s/6s/2.9s/0.5s/1,039
n7s3	7	1.6s/3.1s/2.5s/0.3s/128	32s/35s/26s/5s/451	139s/68s/21s/6s/2,243
randomnet_n7k3	7	5.9s/16s/19s/6.6s/128	25s/47s/32s/5.4s/394	133s/93s/45s/9.9s/1,580
xiao_wnt5a	7	0.96s/1.4s/1s/0.2s/128	11s/21s/12s/3s/324	25s/14s/7s/1.1s/972
arellano_rootstem	9	86s/83s/40s/2.6s/512	-/-/-/145s/1,940	-/-/-/41s/11,472
davidich_yeast	10	-/796s/363s/28s/1,024	-/-/-/622s/4,364	-/-/-/-/38,720
faure_cellcycle	10	-/-/558s/31s/1,024	-/-/-/865s/4,273	-/-/-/-/30,971
fission_yeast	10	-/-/478s/36s/1,024	-/-/-/662s/4,157	-/-/-/-/33,727
mammalian	10	-/-/598s/33s/1,024	-/-/-/841s/4,273	-/-/-/-/30,971

Prediction Power of GULA/PRIDE

Evaluate quality of rules:

- Prediction of each variable possible value
- Learn from partial observations (group by initial state / random)
- Prediction from unseen states ($train \cap test = \emptyset$)

Method:

- Use **GULA/PRIDE** to learn two programs: P and \bar{P}
- P : classic program that say when a target atom is possible
- \bar{P} : a kind of anti-program that say when a target atom is not possible
- Rules are weighted by the number of observations they match
- Probabilities can be obtain from the most matching rule/anti-rule

Predicting probabilities of a_t^0 from $\langle a_{t-1}^1, b_{t-1}^1, c_{t-1}^1, st^1 \rangle$

P :

$$(105) : a_t^0 \leftarrow b_{t-1}^0.$$

$$(42) : a_t^0 \leftarrow b_{t-1}^1 \wedge c_{t-1}^1.$$

$$(12) : a_t^0 \leftarrow c_{t-1}^1 \wedge st^1.$$

\bar{P} :

$$(81) : a_t^0 \leftarrow b_{t-1}^0.$$

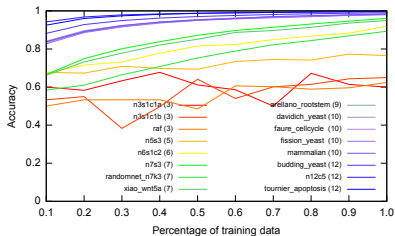
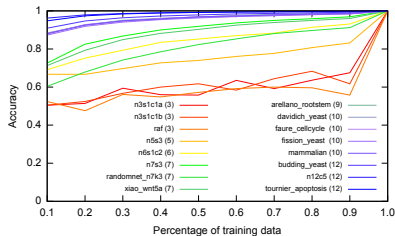
$$(61) : a_t^0 \leftarrow a_{t-1}^1 \wedge c_{t-1}^0.$$

$$(30) : a_t^0 \leftarrow a_{t-1}^1 \wedge st^1.$$

Prediction: $0.5 + 0.5 \times \frac{42-30}{42+30} = 0.58$

Accuracy: mean absolute error VS Ground truth: 0 : 0.58, 1 : 0.42

Prediction power

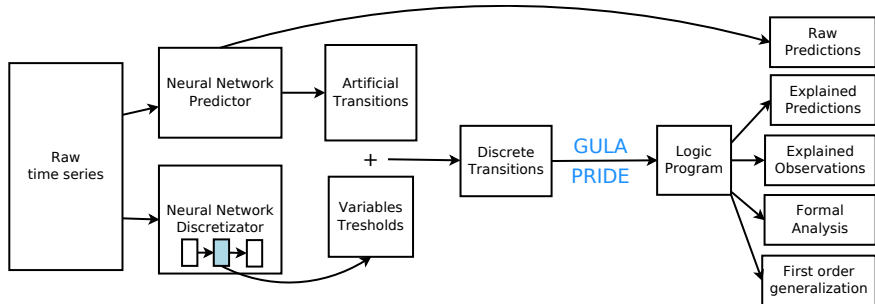


Partial initial states

Partial transitions

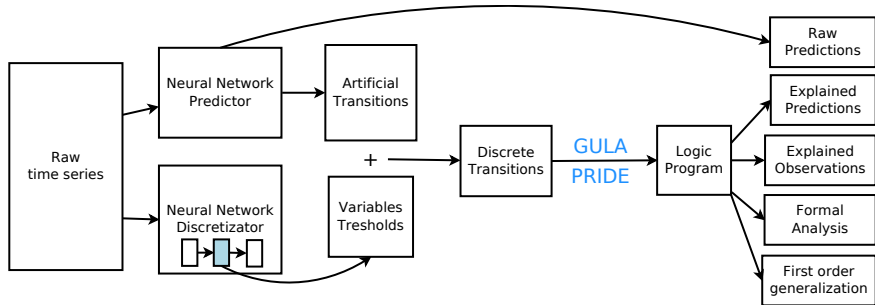
Figure: Accuracy of the models learned by **GULA** when predicting possible target variable values from unseen states: (left) experiment 1, with a complete set of input transitions from a partial number of initial states; and (right) experiment 2, with a potentially incomplete set of input transitions from an incomplete set of initial states.

Outlook: GULA/PRIDE Workflow



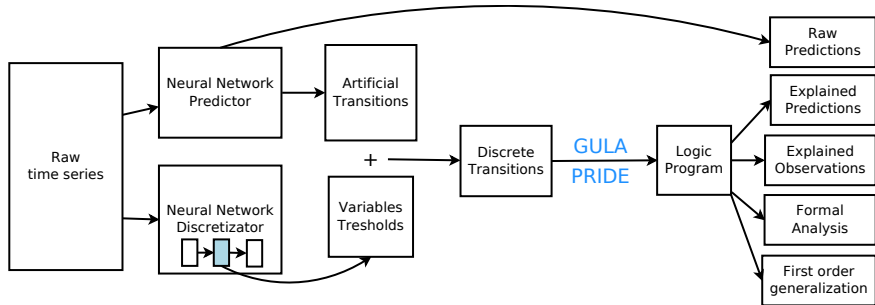
- Pre-process: Use statistical ML for data augmentation/noise tolerance
- Pre-process: Automatic discretization using hand-made NN layer
- Post-process: Weight rules for predictions
- Post-process: First order generalization to simplify explanations

Outlook: GULA/PRIDE Workflow



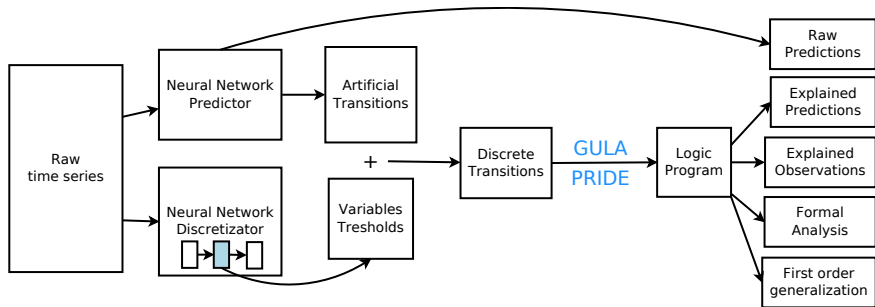
- Pre-process: Use statistical ML for **data augmentation/noise tolerance**
- Pre-process: **Automatic discretization** using hand-made NN layer
- Post-process: Weight rules for **predictions**
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Outlook: GULA/PRIDE Workflow



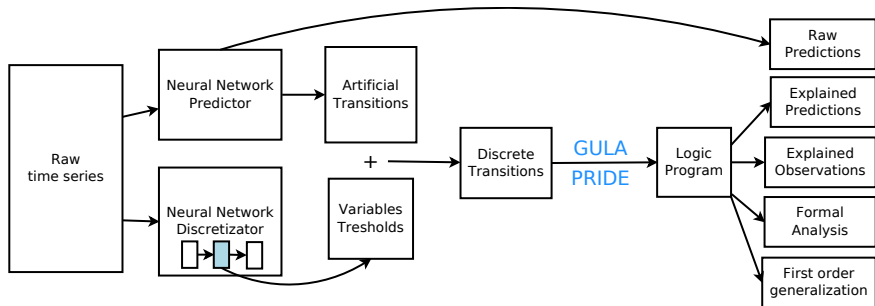
- Pre-process: Use statistical ML for **data augmentation/noise tolerance**
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Outlook: GULA/PRIDE Workflow



- Pre-process: Use statistical ML for **data augmentation/noise tolerance**
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Outlook: GULA/PRIDE Workflow



- Pre-process: Use statistical ML for **data augmentation/noise tolerance**
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Conclusion

Logic rules \Leftrightarrow networks interactions \Leftrightarrow automata transitions

Learning of the structure of a model

1-step learning algorithm by successive refinements

Independent of the semantics

Proved for pseudo-idempotent semantics

→ Includes synchronous, asynchronous, general semantics

Outlooks

- Automatic learning of time series data (noise, discretization, ...)
- Learning probabilistic models
- Improve explainability (first order, post-processing)
- Optimizations (parallelization, approximations)

Thank you

All algorithms are open-source at:

<https://github.com/Tony-sama/pylfit>

Our questions:

- How to automatically and meaningfully discretize?
- Do you know a metrics to evaluate prediction on sets of states?
- Do you have datasets to apply GULA/PRIDE on?

Your questions?

References

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- René Thomas. [Boolean formalization of genetic control circuits](#). *Journal of Theoretical Biology*, volume 42, n. 3, pages 563–85, 1973.
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- Tony Ribeiro, Maxime Folschette, Morgan Magnin, Olivier Roux, Katsumi Inoue. [Learning Dynamics with Synchronous, Asynchronous and General Semantics](#). *The 27th International Conference on Inductive Logic Programming (ILP)*, Ferrara, Italy, 2018.

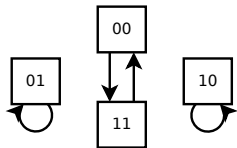
Characterization of Classical Semantics

The three semantics can be detected by checking the following properties.

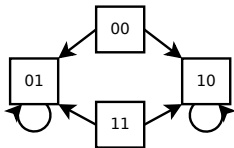


$f(a) := \text{not } b.$

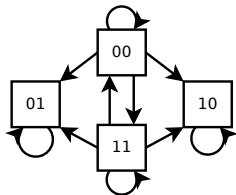
$f(b) := \text{not } a.$



Synchronous



Asynchronous



General

Synchronous:

$$\forall (s, s_1), (s, s_2) \in T, \forall s_3 \in \mathcal{S}^T, s_3 \subseteq s_1 \cup s_2 \implies (s, s_3) \in T.$$

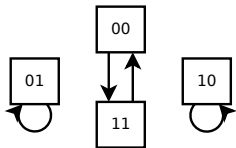
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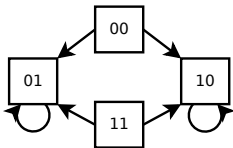


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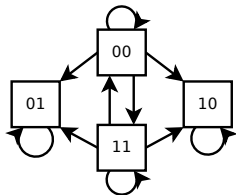
$f(b) := \text{not } a.$



Synchronous



Asynchronous



General

Asynchronous: $\forall (s, s') \in T, \text{sp}_{\mathcal{F} \rightarrow \mathcal{T}}(s) \not\subseteq s', ((s, s'') \in T, \text{sp}_{\mathcal{F} \rightarrow \mathcal{T}}(s) \subseteq s'' \implies (s, s') \notin T) \wedge ((s, s') \in T \implies |\text{sp}_{\mathcal{F} \rightarrow \mathcal{T}}(s) \setminus s'| = 1).$

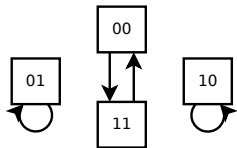
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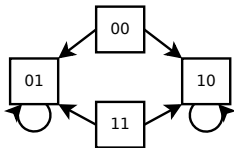


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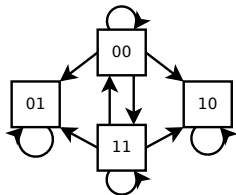
$f(b) := \text{not } a.$



Synchronous



Asynchronous



General

General:

$$\forall (s, s_1), (s, s_2) \in T, \forall s_3 \in \mathcal{S}^T, s_3 \subseteq \text{sp}_{\mathcal{F} \rightarrow \mathcal{T}}(s) \cup s_1 \cup s_2 \implies (s, s_3) \in T.$$

Pseudo-Idempotent Semantics

Definitions:

- $\mathcal{A}_{\mathcal{T}}$ = all feature atoms
- $\mathcal{S}^{\mathcal{F}}$ = all states on feature atoms
- $\mathcal{S}^{\mathcal{T}}$ = all states with target atoms
- $\text{Ccl}(s, P)$ = set of heads of rules in P that match s
- $P_{\mathcal{O}}(P)$ = optimal program (learned by GULA)

Theorem 2 (Pseudo-idempotent Semantics and Optimal \mathcal{DMVLP})

Let DS be a dynamical semantics.

For all P a \mathcal{DMVLP} , if:

$\exists \text{pick} \in (\mathcal{S}^{\mathcal{F}} \times \wp(\mathcal{A}_{\mathcal{T}}) \rightarrow \wp(\mathcal{S}^{\mathcal{T}}) \setminus \{\emptyset\})$ so that

- 1 $\forall s \in \mathcal{S}^{\mathcal{F}}, \forall D \subseteq \mathcal{A}_{\mathcal{T}}, \text{pick}(s, \bigcup_{s' \in \text{pick}(s, D)} s') = \text{pick}(s, D)$ and
- 2 $\forall s \in \mathcal{S}^{\mathcal{F}}, (DS(P))(s) = \text{pick}(s, \text{Ccl}(s, P)),$

then: for all P a \mathcal{DMVLP} , $DS(P_{\mathcal{O}}(DS(P))) = DS(P)$.