Learning any memory-less discrete semantics for dynamical systems represented by logic programs

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Abstract

Learning from interpretation transition (LFIT) automatically constructs a model of the

Contributions

- Algorithm to learn a discrete model from its stage graph
- Independant of the semantics for a defined class of memoryless semantics
- Heuristic for noisy/incomplete data

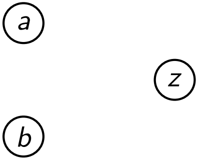
Outline

General Definitions

Discrete Networks / Thomas Modeling

[Kauffman, *Journal of Theoretical Biology*, 1969]
[Thomas, *Journal of Theoretical Biology*, 1973]

- A set of components $N = \{a, b, z\}$



Discrete Networks / Thomas Modeling

[Kauffman, *Journal of Theoretical Biology*, 1969]
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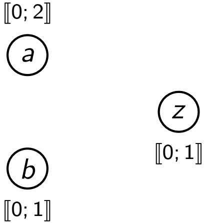
- A set of components $N = \{a, b, z\}$
- A discrete domain for each component $\text{dom}(a) = [\![0; 2]\!]$



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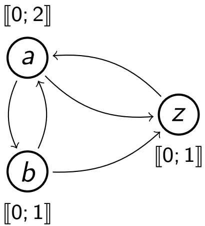
- A set of components $N = \{a, b, z\}$
- A discrete domain for each component $\mathrm{dom}(a) = [\![0; 2]\!]$
- Discrete parameters / evolution functions $f_a : \mathcal{S} \to \mathrm{dom}(a)$



a	f_b
0	0
1	1
2	1

z	b	f_a
0	0	1
0	1	0
1	0	1
1	1	2

a	b	f_z
0	0	0
0	1	0
1	0	0
1	1	0
2	0	0
2	1	1

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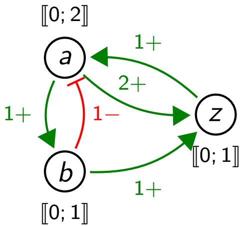
- Signs & thresholds on the edges (redundant) $a \xrightarrow{2+} z$



a	f_b
0	0
1	1
2	1

z	b	f_a
0	0	1
0	1	0
1	0	1
1	1	2

a	b	f_z
0	0	0
0	1	0
1	0	0
1	1	0
2	0	0
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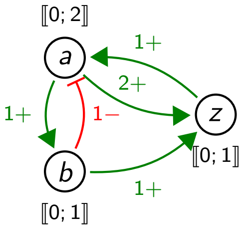

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a	b	f_z
0	0	0
0	1	0
1	0	0
1	1	0
2	0	0
2	1	1

Semantics = From this information, what are the possible next states?

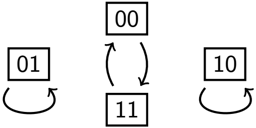
Semantics

$f_a = \neg b$ $\qquad$ $f_b = \neg a$

b	f_a
0	1
1	0

a	f_b
0	1
1	0

State transitions differ according to the update semantics used:



Synchronous

- **Synchronous**: all variables are updated

Semantics

$f_a = \neg b$ $f_b = \neg a$

b	f_a
0	1
1	0

a	f_b
0	1
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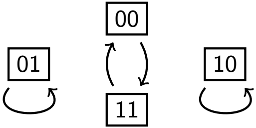

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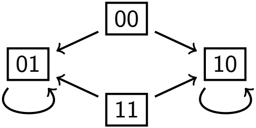

Asynchronous

- **Synchronous**: all variables are updated
- **Asynchronous**: only one variable is updated

Semantics

$f_a = \neg b$ $\qquad$ $f_b = \neg a$

b	f_a
0	1
1	0

a	f_b
0	1
1	0

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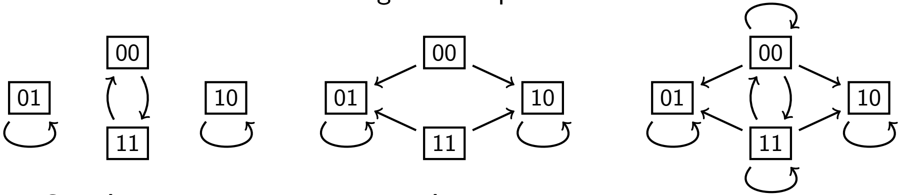
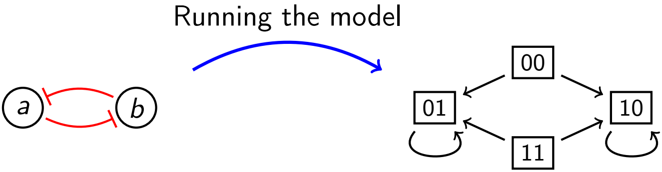


Synchronous **Asynchronous** **General**

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

Learning from the State Graph



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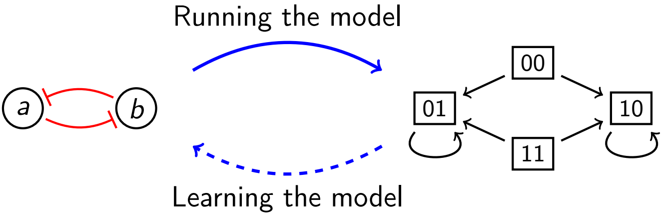

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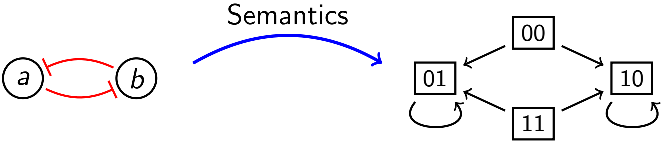

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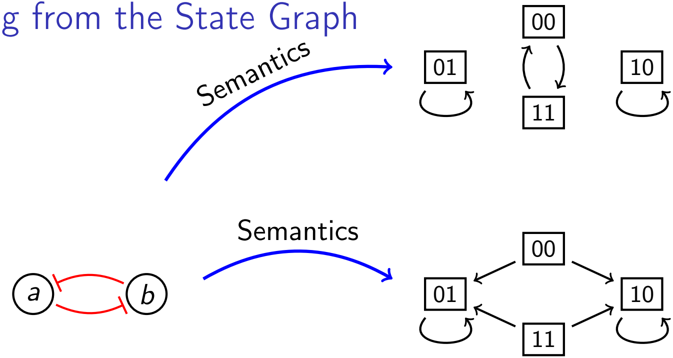

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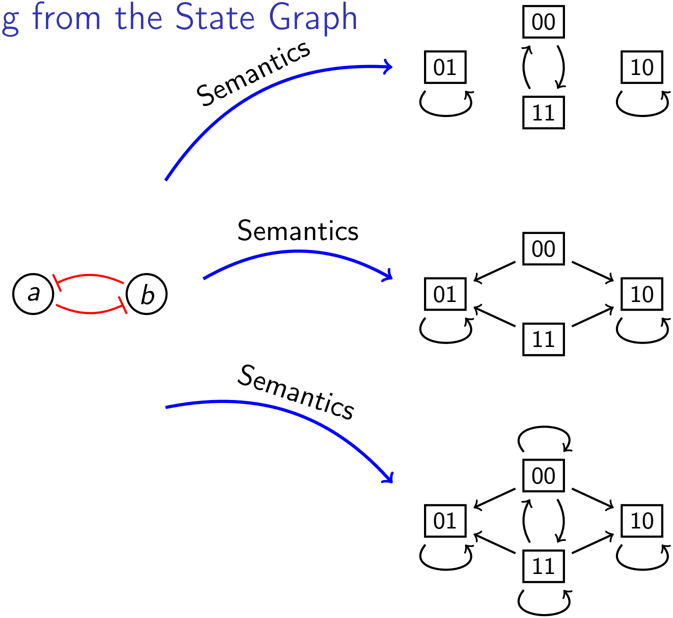

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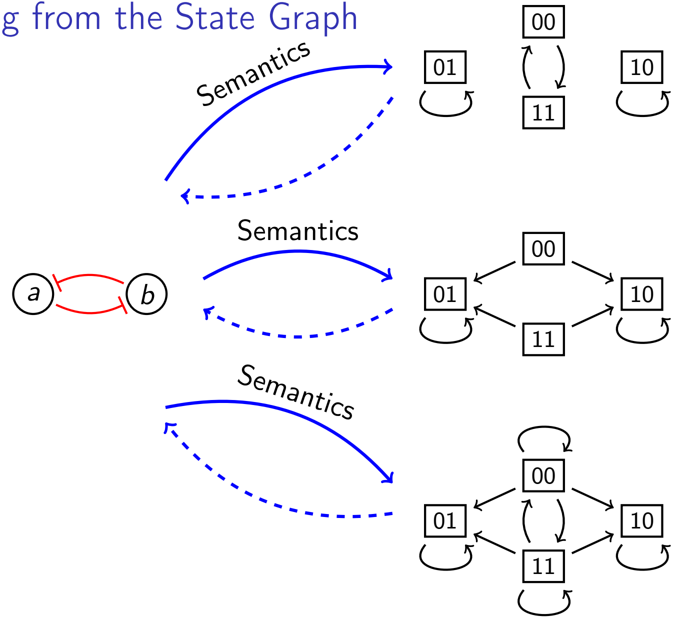

Logic Rules

LFIT learns a logic program, which is a set of logic rules.
It is an alternative representation of biological networks.

$$a_1 \leftarrow a_0, b_0, c_2.$$

If a and b are at level 0 and c is at level 2, then a can change its value to 1.

$$a_1 \leftarrow c_2.$$

Whenever c is at level 2, a can change its value to 1.

$$a_1 \leftarrow .$$

a can change its value to 1 anytime.

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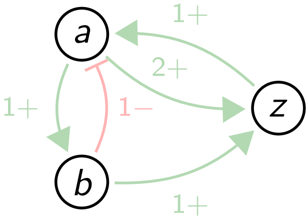
Discrete Models as Logic Programs

Discrete model:



Logic program:

Discrete Models as Logic Programs

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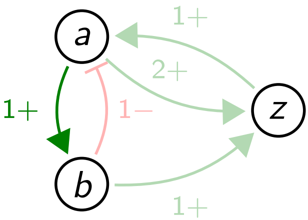
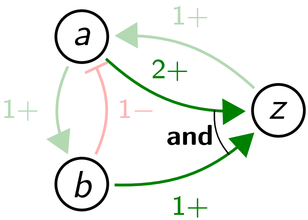


Logic program:

$b_1 \leftarrow a_1.$
$b_1 \leftarrow a_2.$
$b_0 \leftarrow a_0.$

Discrete Models as Logic Programs

Discrete model:



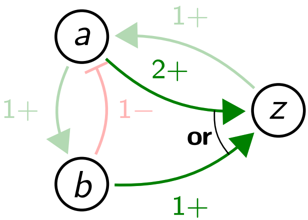
Logic program:

$b_1 \leftarrow a_1.$
$b_1 \leftarrow a_2.$
$b_0 \leftarrow a_0.$

$z_1 \leftarrow a_2 \wedge b_1.$
$z_0 \leftarrow a_0.$
$z_0 \leftarrow a_1.$
$z_0 \leftarrow b_0.$

Discrete Models as Logic Programs

Discrete model:



Logic program:

$b_1 \leftarrow a_1.$
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$b_0 \leftarrow a_0.$

$z_1 \leftarrow a_2.$
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$z_0 \leftarrow a_1 \wedge b_0.$
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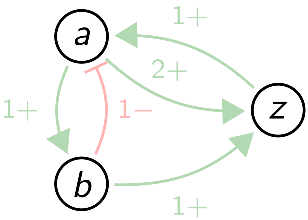
Discrete Models as Logic Programs

Discrete model:



$<$

Expressivity

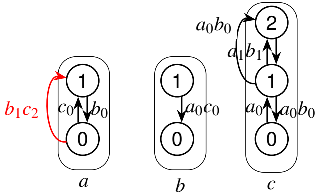
Logic program:

$b_1 \leftarrow a_1.$
$b_1 \leftarrow a_2.$
$b_0 \leftarrow a_0.$

$z_1 \leftarrow a_2.$
$z_1 \leftarrow b_1.$
$z_0 \leftarrow a_1 \wedge b_0.$
$z_0 \leftarrow a_0 \wedge b_0.$

AANs as Logic Programs

Asynchronous automata network:



Picture: [Soh et al., CMSB'2023]

Logic program:

$b_1 \leftarrow a_1.$

$b_1 \leftarrow a_2.$

$b_0 \leftarrow a_0.$

$z_1 \leftarrow a_2.$

$z_1 \leftarrow b_1.$

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AANs as Logic Programs

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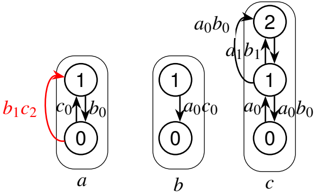

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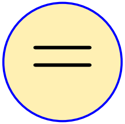

Expressivity

Logic program:

$b_1 \leftarrow a_1.$

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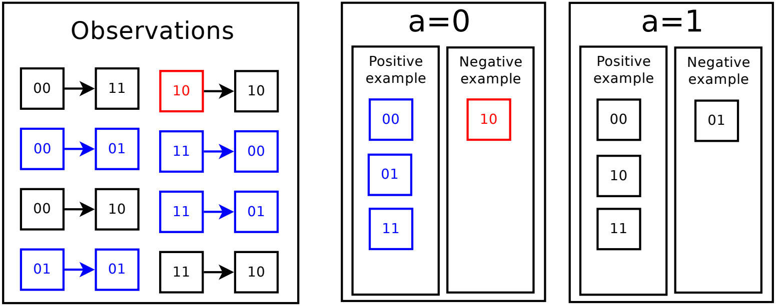
$z_0 \leftarrow a_1 \wedge b_0.$

$z_0 \leftarrow a_0 \wedge b_0.$

Learning From Interpretation Transition (LFIT)

Learning Algorithm Intuition: Classification Problem

Learn applicable rules: conditions so that a variable **can** take a certain value in next state.



Equivalent to a **classification problem**: What is a typical state where a can take value 0 in the next state ? Here: when a_0 or b_1 is present.

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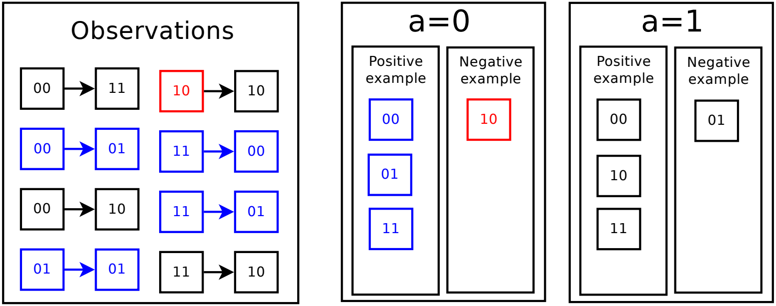

Equivalent to a **classification problem**: What is a typical state where a can take value 0 in the next state ? Here: when a_0 or b_1 is present.

That is: $a_0 \leftarrow a_0.$ $a_0 \leftarrow b_1.$

Presentation of GULA

GULA = General Usage LFIT Algorithm

Input: a set of transitions $(s_1 \rightarrow s_2)$

Output: a logic 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 conditions)

Compatible with semantics that use the specifications of the model
This includes the synchronous, asynchronous and general semantics

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

Specialization by Minimal Refinements

Suppose:

- a and b have two levels $\{0, 1\}$ and c has three levels $\{0, 1, 2\}$
- the current program contains the following rules regarding a_1:

$$a_1 \leftarrow c_2. \qquad\qquad a_1 \leftarrow b_1.$$

- from state $\langle a_1, b_0, c_2 \rangle$, a_1 is never observed in the next states.

Minimal refinement to make the rules inapplicable in this state:

Specialization by Minimal Refinements

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$$a_1 \leftarrow a_0, c_2.$$
$$a_1 \leftarrow b_1, c_2.$$
$$a_1 \leftarrow c_2, c_0.$$
$$a_1 \leftarrow c_2, c_1.$$

$$a_1 \leftarrow b_1.$$

(No change)

Specialization by Minimal Refinements

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Minimal refinement to make the rules inapplicable in this state:

$$a_1 \leftarrow a_0, c_2.$$
$$a_1 \leftarrow b_1, c_2.$$

$$a_1 \leftarrow b_1.$$

(More general)

Specialization by Minimal Refinements

Suppose:

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Minimal refinement to make the rules inapplicable in this state:

$$a_1 \leftarrow a_0, c_2. \qquad\qquad a_1 \leftarrow b_1.$$

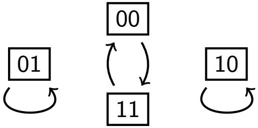
Example: Synchronous Semantics

$f_a = \neg b$

b	f_a
0	1
1	0

$f_b = \neg a$

a	f_b
0	1
1	0



Synchronous

$// \ f_a = \neg b$

$a_0 \leftarrow b_1$

$a_1 \leftarrow b_0$

$// \ f_b := \neg a$

$b_0 \leftarrow a_1$

$b_1 \leftarrow a_0$

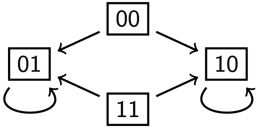
Example: Asynchronous Semantics

$f_a = \neg b$

b	f_a
0	1
1	0

$f_b = \neg a$

a	f_b
0	1
1	0



Asynchronous

// $f_a = \neg b$

$a_0 \leftarrow b_1$

$a_1 \leftarrow b_0$

// $f_b = \neg a$

$b_0 \leftarrow a_1$

$b_1 \leftarrow a_0$

// Default rules

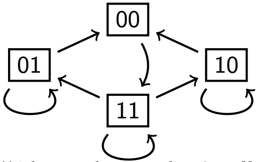
$a_0 \leftarrow a_0$

$a_1 \leftarrow a_1$

$b_0 \leftarrow b_0$

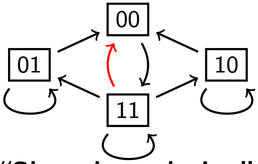
$b_1 \leftarrow b_1$

Learning the semantics with constraints



“Slow degradation”

Learning the semantics with constraints



"Slow degradation"

// $f_a = \neg b$
$a_0^t \leftarrow b_1^{t-1}.$
$a_1^t \leftarrow b_0^{t-1}.$

// $f_b = \neg a$
$b_0^t \leftarrow a_1^{t-1}.$
$b_1^t \leftarrow a_0^{t-1}.$

// Conservation rules
$a_1^t \leftarrow a_1^{t-1}.$
$b_1^t \leftarrow b_1^{t-1}.$

// Degradation
$a_0^t \leftarrow a_1^{t-1}.$
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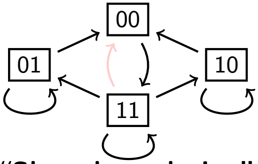
Learning the semantics with constraints



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// Degradation
$a_0^t \leftarrow a_1^{t-1}.$
$b_0^t \leftarrow b_1^{t-1}.$

// Constraints
$\bot \leftarrow a_0^t, b_0^t, a_1^{t-1}, b_1^{t-1}.$

Results

- **Algorithm that allows to learn the network**
  - Structure of the model
  - Under the form of a logic program
- **Directly works for a class of memoryless semantics**
  - Characterization of applicable semantics
- Usable to learn from other semantics as well
  - By using constraints to learn the semantics along with the model

Limitations:

- Exponential complexity
- What if the data is **incomplete** or **noisy**?

A Heuristic on LFIT

Weighted Likeliness/Unlikeliness Rules

- Use the algorithm twice to learn two logic programs:
  - likeliness rules: what is possible
  - unlikeliness rules: what is impossible
- Weight each rule by the number of observations it matches

Statistical overlay $\Rightarrow$ usable on **noisy datasets**

Likeliness rules	**Unlikeliness rules**
$(3, a_0 \leftarrow b_1)$	$(30, a_0 \leftarrow c_1)$
$(15, a_1 \leftarrow b_0)$	$(5, a_1 \leftarrow c_0)$
$\vdots$	$\vdots$

Using Weighted Likeliness/Unlikeliness Rules

Explainable predictions:

- Compare weights of applicable likeliness/unlikeliness rules
- Ratio of highest weights $\Rightarrow$ **probability** P
- Rules with highest weights $\Rightarrow$ **explanation** E

$$\text{predict} : (atom, state) \mapsto (P, E)$$

Likeliness rules	**Unlikeliness rules**
$(3, a_0 \leftarrow b_1)$	$(30, a_0 \leftarrow c_1)$
$(15, a_1 \leftarrow b_0)$	$(5, a_1 \leftarrow c_0)$

Using Weighted Likeliness/Unlikeliness Rules

Explainable predictions:

- Compare weights of applicable likeliness/unlikeliness rules
- Ratio of highest weights ⇒ **probability** P
- Rules with highest weights ⇒ **explanation** E

$$\text{predict} : (atom, state) \mapsto (P, E)$$

Likeliness rules

$(3, a_0 \leftarrow b_1)$

$(15, a_1 \leftarrow b_0)$

Unlikeliness rules

$(30, a_0 \leftarrow c_1)$

$(5, a_1 \leftarrow c_0)$

$\text{predict}(a_1, \langle a_1, b_0, c_0 \rangle) = (0.75, ((15, a_1 \leftarrow b_0), (5, a_1 \leftarrow c_0))) \Rightarrow$ Likely

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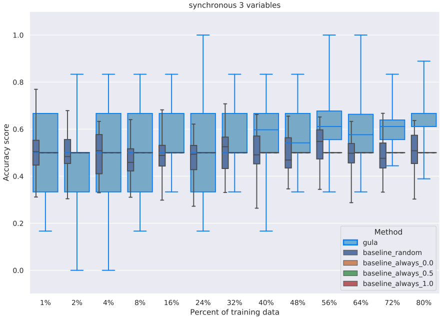
Likeliness rules	**Unlikeliness rules**
$(3, a_0 \leftarrow b_1)$	$(30, a_0 \leftarrow c_1)$
$(15, a_1 \leftarrow b_0)$	$(5, a_1 \leftarrow c_0)$

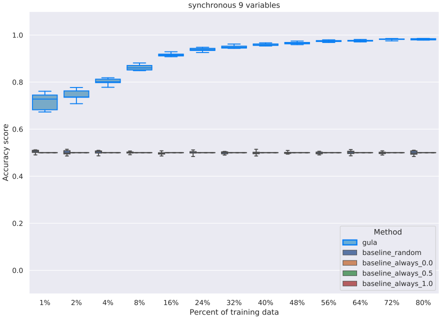
$\text{predict}(a_1, \langle a_1, b_0, c_0 \rangle) = (0.75, ((15, a_1 \leftarrow b_0), (5, a_1 \leftarrow c_0))) \Rightarrow$ Likely

$\text{predict}(a_0, \langle a_1, b_1, c_1 \rangle) = (0.09, ((3, a_0 \leftarrow b_1), (30, a_0 \leftarrow c_1))) \Rightarrow$ Unlikely

Prediction power



3 variables



9 variables

Training data = X% of transitions
Tested against unseen states (not in the training data)

Conclusion

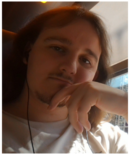
Conclusion

- **Learn** the network with LFIT (theory)
  - When not "learnable", learn the semantics with constraints
- **Heuristics** to tackle real data (practice)
  - Good results with 10% of the transitions

Outlooks:

- PRIDE: polynomial algorithm that "misses" some explanations
- Learn from the Most Permissive semantics
- Application to real data (marine phytoplankton)

Thanks



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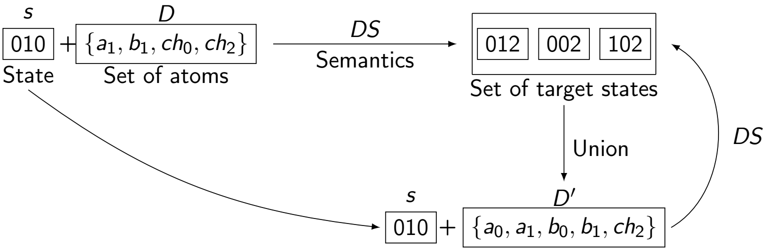
- pyLFIT Python library: `https://github.com/Tony-sama/pylfit`
- About PRIDE: Tony Ribeiro, Maxime Folschette, Morgan Magnin and Katsumi Inoue. **Polynomial Algorithm For Learning From Interpretation Transition**. Poster at the *1st International Joint Conference on Learning & Reasoning*. October 2021, Online. `https://hal.science/hal-03347026v1`
- Application to phytoplankton: Omar Iken, Maxime Folschette and Tony Ribeiro. **Automatic Modeling of Dynamical Interactions Within Marine Ecosystems**. Poster in the *1st International Joint Conference on Learning & Reasoning*. October 2021, Online. `https://hal.science/hal-03347033v1`

Pseudo-idempotent semantics

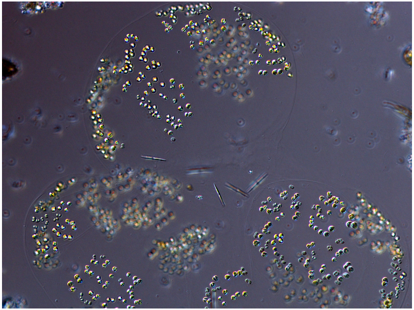
GULA can model observations from any pseudo-idempotent semantics.

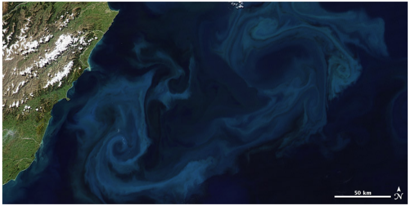


$$\longrightarrow DS(s, D) = DS\Big(s, \bigcup_{s' \in DS(s,D)} s'\Big)$$

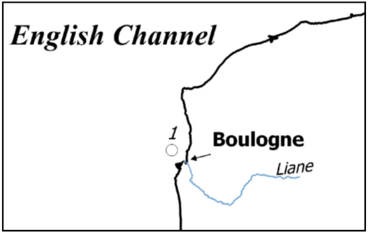
where DS is the dynamical semantics, and D is set of heads of rules of a multi-valued logic program that match the sate s.

Phytoplankton Blooms





SRN Dataset



https://www.seanoe.org/data/00397/50832/

Sampling location	Sampling date	Taxon	Value	Sampling depth
001-P-015	1992-05-18	CHLOROA	6.0	Surface (0-1m)
006-P-001	2019-12-02	Chaetoceros	1000.0	Surface (0-1m)
002-P-007	1994-05-25	Pleurosigma	100.0	Surface (0-1m)
002-P-030	2005-10-19	SALI	34.83	Surface (0-1m)
006-P-007	2015-09-28	Guinardia delicatula	11400.0	Surface (0-1m)

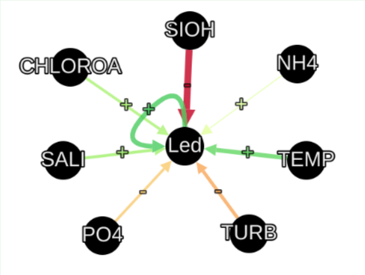
Environmental variables (7) Phytoplankton species (12)

Global Influences

Process: Search and count patterns in rules that characterize an activation/inhibition
Hypotheses: Monotonous influences & same threshold for all variables
Result: Score $[-1;+1]$ between each pair of variables (no threshold)

Influences on phytoplankton specie `Led`:

Variable	Positive	Negative	Global
`PO4`	$+0$	-58	-0.36
`SALI`	$+71$	-4	$+0.42$
`CHLOROA`	$+84$	-22	$+0.39$
`SIOH`	$+3$	-161	-0.98
`NH4`	$+25$	-5	$+0.12$
`TEMP`	$+106$	-5	$+0.63$
`TURB`	$+10$	-87	-0.48



$$\text{global\_influence}(\texttt{PO4} \to \texttt{Led}) = \frac{+0 + (-58)}{161} = -0.36$$