Learning Dynamical Interactions Within Marine Ecosystems with LFIT

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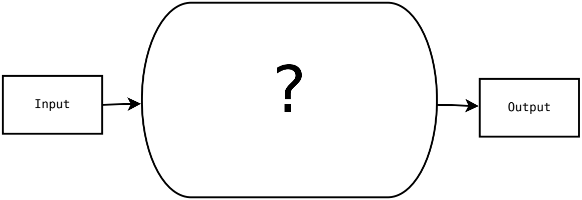
4th February 2022, Bioss, Online

Outline

Outline

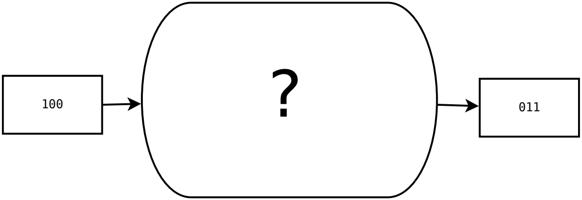
Research area

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



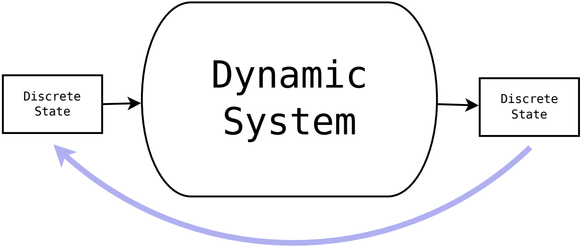
Research area

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



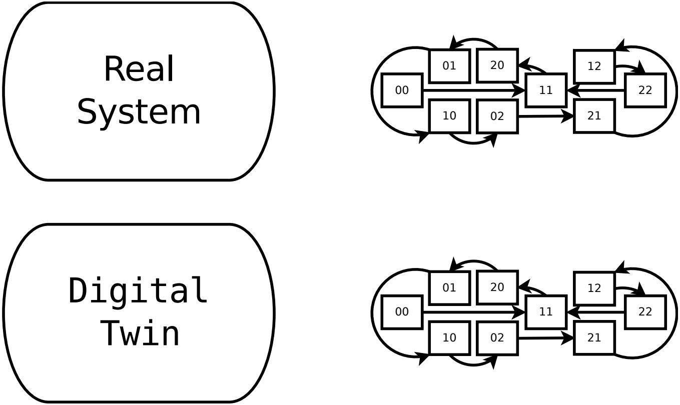
Research area

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



Research area

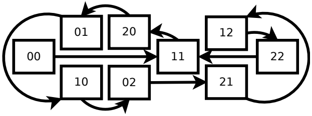
Goal: produce an artificial system with the same behavior as the one observed, i.e., a digital twin.



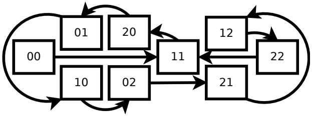
Research area

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

Real System



Logic Program

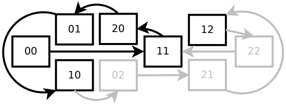


Research area

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).
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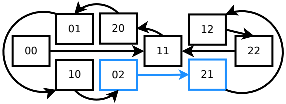
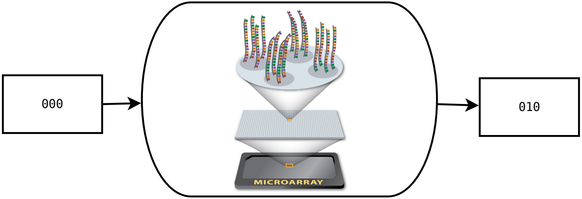


Motivation

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



Example (Possible Applications)

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

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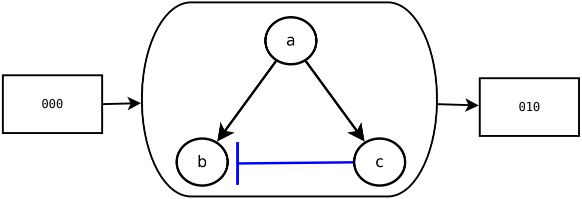

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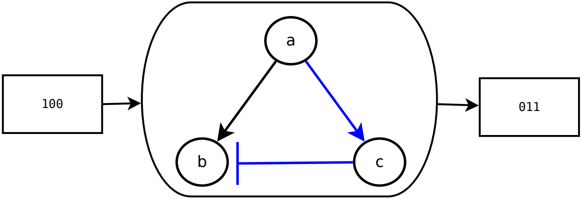

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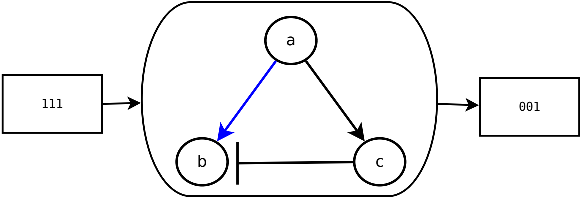
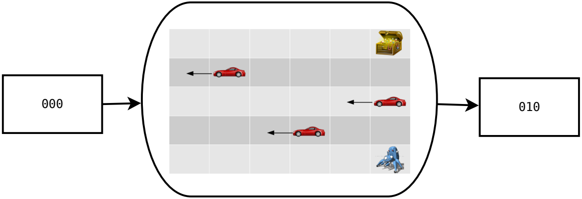


Example (Possible Applications)

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

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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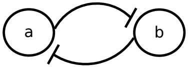
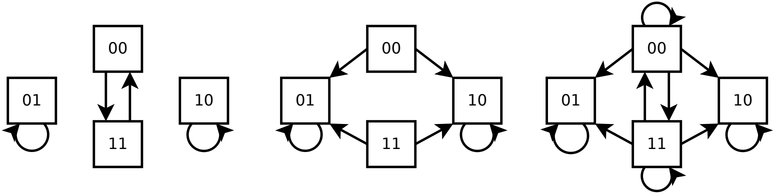
Outline

Dynamical Semantics

Boolean network transitions differ according to the update semantics used.



f(a) := not b.
f(b) := not a.



Synchronous   Asynchronous   General

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

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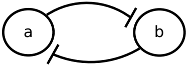

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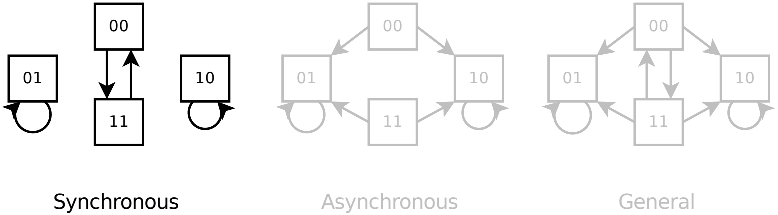

- Synchronous: all variables are updated
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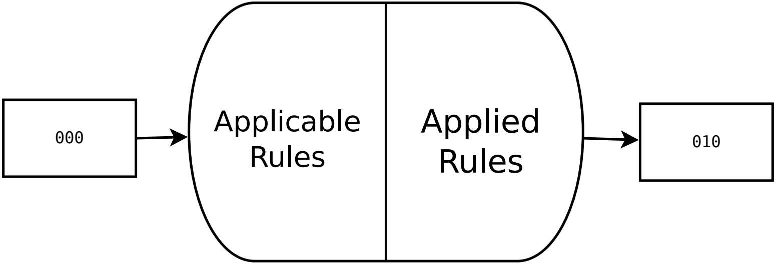
What is a semantics?

For those three semantics at least, it is 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.

The three semantics that are considered here differ on the selection but share the same definition of what is an applicable rule.

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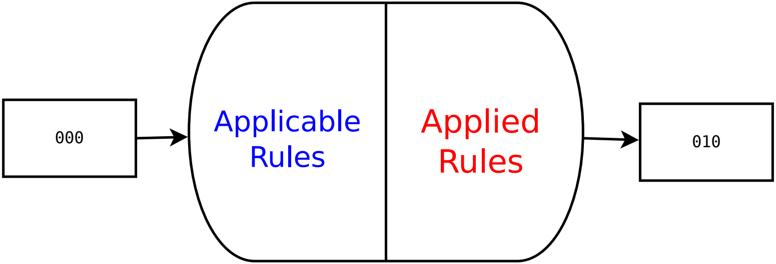

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Learning algorithm intuition: classification problem

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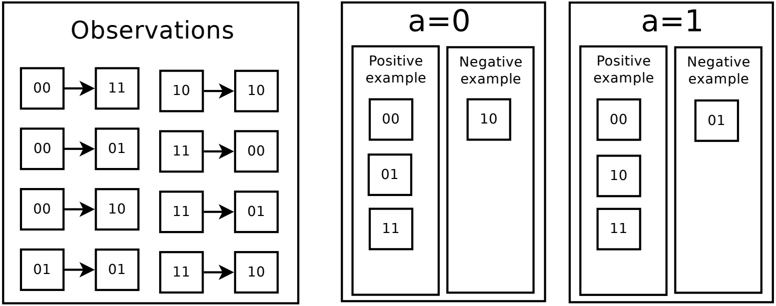

Equivalent to a classification problem: for each value of a variable, what is a typical state where the variable can takes this value in the next state ?

Learning algorithm intuition: classification problem

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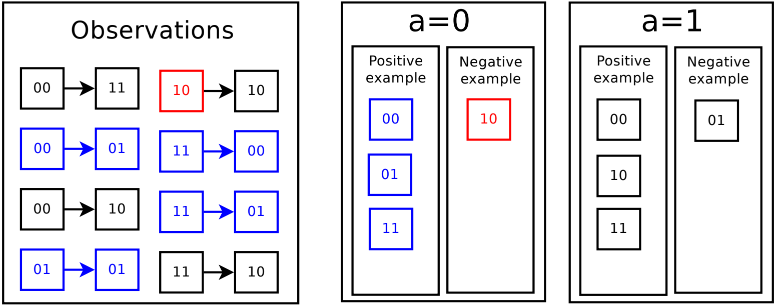

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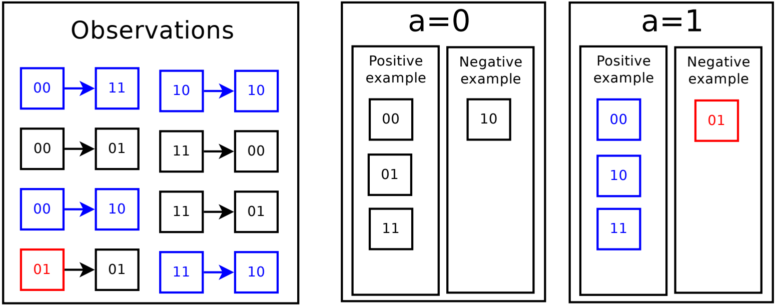

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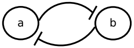
General Usage LFIT Algorithm (**GULA**) ouptut



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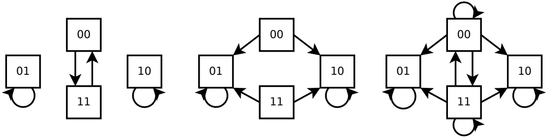

Synchronous	Asynchronous	General
// f(a) := not b	// f(a) := not b	// f(a) := not b
$a_t^0 \leftarrow b_{t-1}^1$	$a_t^0 \leftarrow b_{t-1}^1$	$a_t^0 \leftarrow b_{t-1}^1$
$a_t^1 \leftarrow b_{t-1}^0$	$a_t^1 \leftarrow b_{t-1}^0$	$a_t^1 \leftarrow b_{t-1}^0$
// f(b) := not a	// f(b) := not a	// f(b) := not a
$b_t^0 \leftarrow a_{t-1}^1$	$b_t^0 \leftarrow a_{t-1}^1$	$b_t^0 \leftarrow a_{t-1}^1$
$b_t^1 \leftarrow a_{t-1}^0$	$b_t^1 \leftarrow a_{t-1}^0$	$b_t^1 \leftarrow a_{t-1}^0$
	// Default rules	// Default rules
	$a_t^0 \leftarrow a_{t-1}^0$	$a_t^0 \leftarrow a_{t-1}^0$
	$a_t^1 \leftarrow a_{t-1}^1$	$a_t^1 \leftarrow a_{t-1}^1$
	$b_t^0 \leftarrow b_{t-1}^0$	$b_t^0 \leftarrow b_{t-1}^0$
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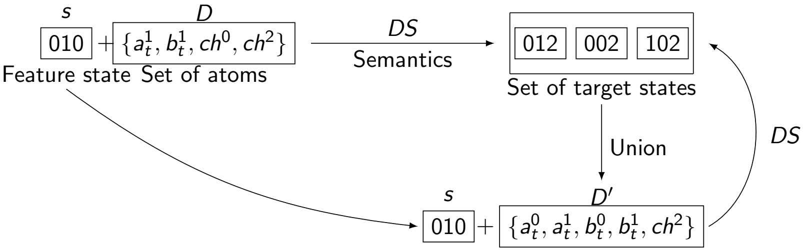
Pseudo-idempotent semantics

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 the head of rules of a multi-valued logic program that match the sate s.

Heuristic Model for Real Data

Modeling:

- Use GULA to learn two logic programs: possibilities/impossibilities.
- Weight each rule by the number of observations it matches.

Prediction:

- Likeliness: combine weight of matching possibility/impossibility rules
- Explanation: the rules used for the prediction

Example

Likeliness rules
$(3, a^0 \leftarrow b^1)$
$(15, a^1 \leftarrow b^0)$
...

Unlikeliness rules
$(30, a^0 \leftarrow c^1)$
$(5, a^1 \leftarrow c^0)$
...

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$(3, a^0 \leftarrow b^1)$	$(30, a^0 \leftarrow c^1)$
$(15, a^1 \leftarrow b^0)$	$(5, a^1 \leftarrow c^0)$
...	...

$predict(target, feature\_state) = (\text{proba, explanations})$

$predict(a^0, \{a^1, b^1, c^1\}) = (0.5, (0, None), (0, None))$ Unconclusive

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$(15, a^1 \leftarrow b^0)$	$(5, a^1 \leftarrow c^0)$
...	...

$predict(a^0, \{a^1, b^1, c^1\}) = (1.0, (3, a^0 \leftarrow b^1), (0, None))$ Possible

$predict(a^1, \{a^0, b^1, c^0\} = (0.0, (0, None), (5, a^1 \leftarrow c^0)$ Impossible

Heuristic Model for Real Data

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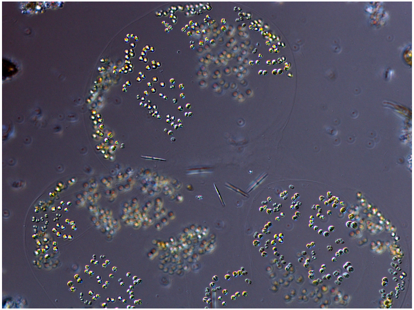
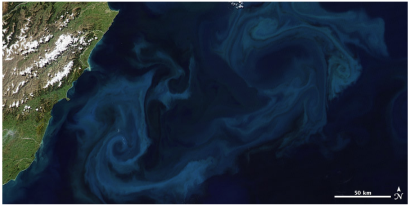
$(15, a^1 \leftarrow b^0)$	$(5, a^1 \leftarrow c^0)$
...	...

$predict(a^1, \{a^1, b^1, c^0\} = (0.75, (15, a^1 \leftarrow b^0), (5, a^1 \leftarrow c^0)$ Likely
$predict(a^0, \{a^1, b^1, c^0\} = (0.09, (3, a^0 \leftarrow b^1), (30, a^0 \leftarrow c^1)$ Unlikely

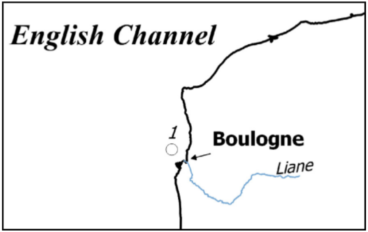
Outline

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 (12)

Applying *LFIT*

Input

- 253 training transitions
- 53 testing transitions
- Features = Phytoplankton + Envir^t
- Targets = Phytoplankton

Output

- Run time = 2.35s (PRIDE)
- 1683 likeliness rules
- 1981 unlikeliness rules
- Model accuracy: **0.670**

Prediction example for phytoplankton specie `Cha`, in a given state:

- Level 0 with 5.3% probability (Non-deterministic dynamics $\Rightarrow$ Total $\neq$ 100%)
  - 1 match for $Cha(0) \leftarrow SALI(0), TEMP(0), TURB(1), Cha(0), Dit(0).$
  - 18 anti-matches for $Cha(0) \leftarrow TURB(1), Nit(2).$
- Level 1 with 87.5% probability
  - 7 matches for $Cha(1) \leftarrow SALI(0), TURB(1), Nit(2).$
  - 1 anti-match for $Cha(1) \leftarrow SALI(0), TEMP(0), TURB(1), Cha(0), Dit(0).$
- Level 2 with 2.6% probability
  - 1 match for $Cha(2) \leftarrow TEMP(0), Dit(0), Par(1), Pss(0), Thn(1).$
  - 37 anti-matches for $Cha(2) \leftarrow SALI(0), TURB(1).$

Model Improvement

Process: For each rule in the program, replace the body with a subset and weight this new rule on the dataset

Expectations: Noise removal, accuracy improvement, simpler rules

Likeliness rule: $Cha(0) \leftarrow CHLOROA(0), TEMP(1), Cha(0), Gud(2).$

Replace body with...	correct	wrong
$CHLOROA(0), TEMP(1), Cha(0), Gud(2)$	1	0
$CHLOROA(0), Cha(0), Gud(2)$	10	4
$TEMP(1), Cha(0)$	18	5
$Gud(2)$	25	2

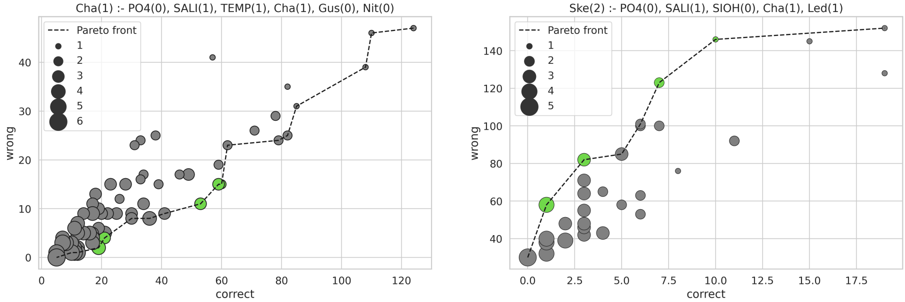
Unlikeliness rule: $Cha(0) \leftarrow Par(1), Dit(1), TEMP(0), Cha(1).$

Replace body with...	correct	wrong
$Par(1), Dit(1), TEMP(0), Cha(1)$	0	1
$Par(1), TEMP(0), Cha(1)$	3	12
$Dit(1), Cha(1)$	5	11
$Cha(1)$	11	66

Model Improvement

Pareto frontier

- For likeliness rules : maximize correct and minimize wrong weights
- For unlikeliness rules : maximize wrong and minimize correct weights



Accuracy improvement: 0.670 → **0.716**

Likeliness rules: 1683 → **1609**

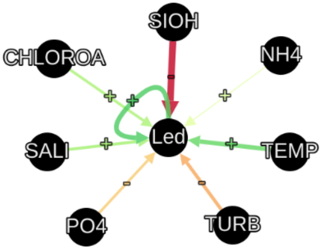
Unlikeliness rules: 1981 → **1405**

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)

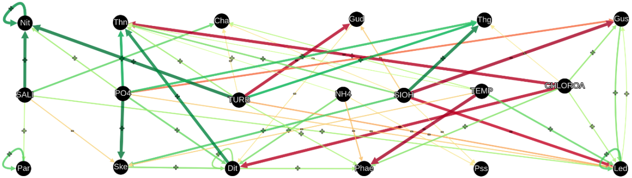
Example: **Influences** on phytoplankton specie `Led`:

Feature	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

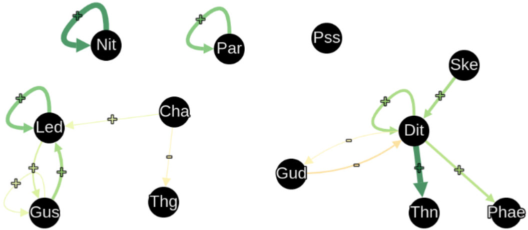


$$\text{global\_influence}(\texttt{PO4} \rightarrow \texttt{Led}) = \frac{+0+(-58)}{161} = -0.36$$

Result

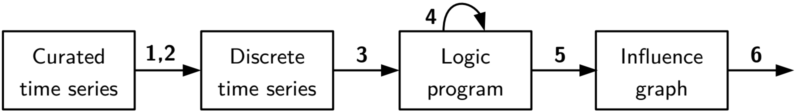


Global influence graph (biotic and abiotic interactions)



Biotic interactions (between phytoplankton only)

Conclusion



- **1** Data cleaning
- **2** Discretization ★
- **3 LFIT**

- **4** Rules improvement with Pareto front ★
- **5** Influence graph extraction ★
- **6** TODO: Validation & Exploitation ★

★ = Still work to do!

Special thanks:

- Sébastien Lefebvre — Professor of ecology, Université de Lille
  Laboratoire d'Océanologie et de Géosciences (Wimereux)
- Omar Iken — Master student in Data Science

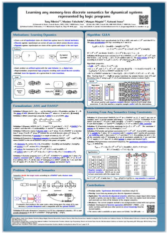
We are looking for PhD candidates!
Potential PhD thesis funding by Université de Lille
Please contact Cédric Lhoussaine or Maxime Folschette

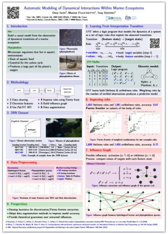
Outline

Conclusions

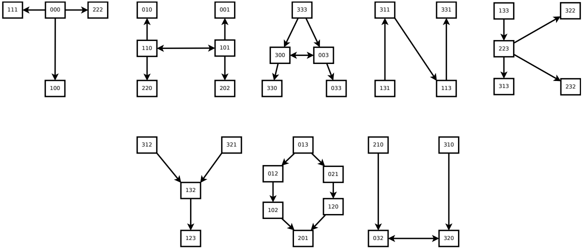
- **Previous works:** Synchronous deterministic transitions only.
- **Novelty:** Learn from any memory-less discrete dynamical semantics.
- **Application:** Explain observed dynamics as simple logic rules.
- **Collaboration:** Learn biotic influences from a marine ecosystem.
- **Outlook:** Heuristic to extract more knowledge from learned programs.
- Source code (Python) available as open source on Github.

Manuscript





Source Code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