Polynomial Algorithm For Learning From Interpretation Transition

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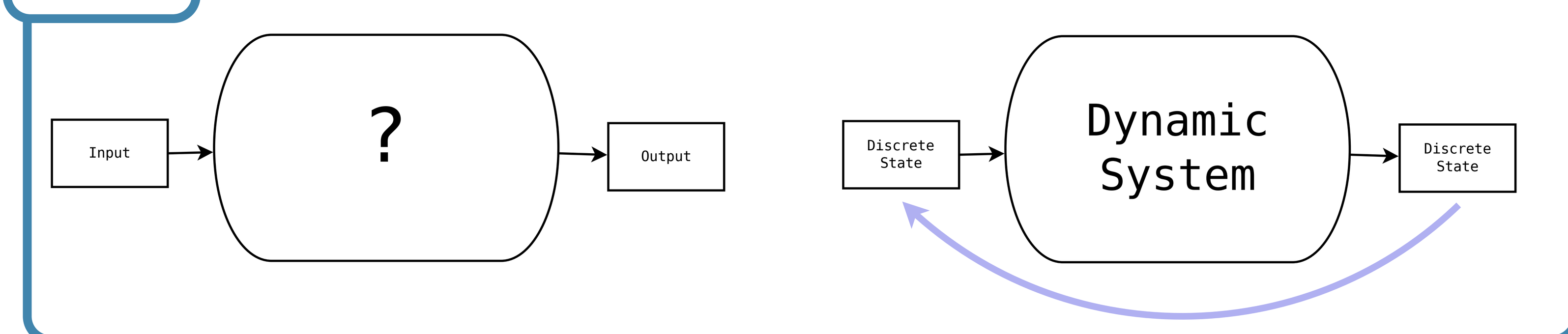
Motivations: Learning Dynamics

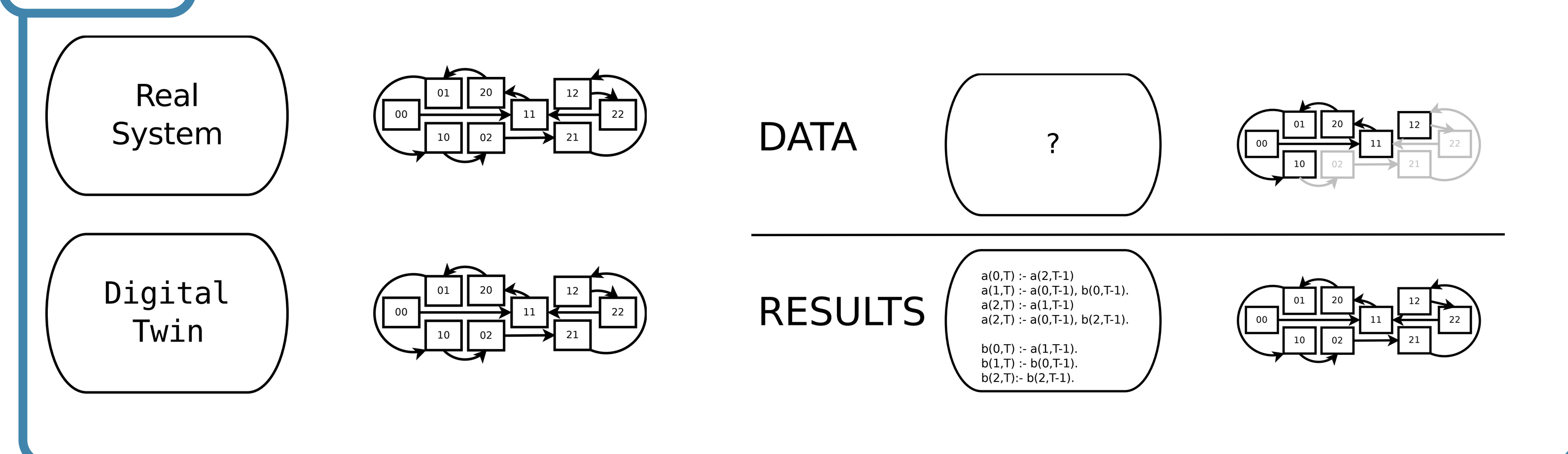
- Given a set of input/output states of a black-box system, learn its internal mechanics.
- **Discrete system**: input/output are vectors of same size which contain discrete values.
- **Dynamic system**: input/output are states of the system and output is the next input.

Problem



- **Goal:** produce an artificial system with the same behavior, i.e., a digital twin.
- **Representation:** propositional logic programs encoding multi-valued discrete variables.
- **Method:** learn the dynamics of a system from its state transitions.

Goal



Formalization: $\mathcal{MVL}$ and $\mathcal{DMVLP}$

Definition 1 (Atoms). *Let $\mathcal{V} = \{v_1, \dots, v_n\}$ be a finite set of $n \in \mathbb{N}$ variables, and* $\mathrm{dom} : \mathcal{V} \to \mathbb{N}$. *The atoms of $\mathcal{MVL}$ (denoted $\mathcal{A}$) are of the form v^{val} where $v \in \mathcal{V}$ and $val \in [\![0; \mathrm{dom}(v)]\!]$.*

Definition 2 (Multi-valued logic program). *A $\mathcal{MVLP}$ is a set of $\mathcal{MVL}$ rules:*

$$\underbrace{v_0^{val_0}}_{head} \leftarrow \underbrace{v_1^{val_1} \wedge v_2^{val_2} \wedge v_3^{val_3} \wedge \dots \wedge v_m^{val_m}}_{body}$$

Definition 3 (Dynamic $\mathcal{MVLP}$). *Let $\mathcal{T} \subset \mathcal{V}$ and $\mathcal{F} \subset \mathcal{V}$ such that $\mathcal{F} = \mathcal{V} \setminus \mathcal{T}$. A $\mathcal{DMVLP}$ P is a $\mathcal{MVLP}$ such that $\forall R \in P, \mathrm{var}(\mathrm{head}(R)) \in \mathcal{T}$ and $\forall v^{val} \in \mathrm{body}(R), v \in \mathcal{F}$.*

Definition 4 (Discrete state). *A discrete state s on $\mathcal{T}$ (resp. $\mathcal{F}$) of a $\mathcal{DMVLP}$ is a function from $\mathcal{T}$ (resp. $\mathcal{F}$) to $\mathbb{N}$. $\mathcal{S}^{\mathcal{T}}$ (resp. $\mathcal{S}^{\mathcal{F}}$) denote the set of all discrete states of $\mathcal{T}$ (resp. $\mathcal{F}$).*

Definition 5 (Transition). *A transition is a couple of states $(s, s') \in \mathcal{S}^{\mathcal{F}} \times \mathcal{S}^{\mathcal{T}}$.*

Definition 6 (Semantics). *A dynamical semantics is a function $\mathcal{DMVLP} \to (\mathcal{S}^{\mathcal{F}} \to \wp(\mathcal{S}^{\mathcal{T}}) \setminus \{\emptyset\})$ where $\mathcal{DMVLP}$ is the set of $\mathcal{DMVLP}$s and $\wp$ is the power set symbol.*

- R_1 dominates R_2, written $R_1 \geq R_2$, if $head(R_1) = head(R_2)$ and $body(R_1) \subseteq body(R_2)$.
- R matches $s \in \mathcal{S}^{\mathcal{F}}$, written $R \sqcap s$, if $body(R) \subseteq s$.
- R realizes the transition $(s, s') \in \mathcal{S}^{\mathcal{F}} \times \mathcal{S}^{\mathcal{T}}$, if $R \sqcap s$ and $head(R) \in s'$.
- R conflicts with $T \subseteq \mathcal{S}^{\mathcal{F}} \times \mathcal{S}^{\mathcal{T}}$ if $\exists (s, s') \in T, \big(R \sqcap s \wedge \forall (s, s'') \in T, head(R) \notin s''\big)$.

Definition 7 (Suitable program). *Let $T \subseteq \mathcal{S}^{\mathcal{F}} \times \mathcal{S}^{\mathcal{T}}$. A $\mathcal{DMVLP}$ P is suitable for T when: P is complete, consistent with T, realizes T and $\forall R$ not conflicting with T, $\exists R' \in P$ s.t. $R \geq R'$. If, in addition, $\forall R \in P$, all the rules R' belonging to a $\mathcal{MVLP}$ suitable for T are such that $R \geq R'$ implies $R' \geq R$, then P is unique, called optimal and denoted $P_{\mathcal{O}}(T)$.*

Problem: Combinatorial Explosion

GULA and **PRIDE**:

- In [2] we proposed an Algorithm (**GULA**) to learn $P_{\mathcal{O}}(T)$ but with exponential complexity.
- We introduce the heuristic algorithm **PRIDE** which trades the completeness of **GULA** for a polynomial complexity. **PRIDE** learns a subset of $P_{\mathcal{O}}(T)$ that is sufficient to realize T.

Run Time

System variables (n)	7	9	10	12	13	15	18	23
GULA run time	0.027s	0.157s	0.49s	2.62s	5.63s	T.O.	T.O.	T.O.
PRIDE run time	0.005s	0.02s	0.06s	0.37s	0.484s	1.55s	6.39s	32.43s

Average run time of **GULA** and **PRIDE** when learning Boolean networks of PyBoolNet [3] from at most 10,000 transitions with a time-out (T.O.) of 1,000 seconds.

PRIDE performances allow to learn more complex systems and drastically reduce computation time on smaller ones.

Algorithm: PRIDE

Theorem 1 (Consistent Rule Always exists). *Let $T \subseteq \mathcal{S}^{\mathcal{F}} \times \mathcal{S}^{\mathcal{T}}$, $(s, s') \in T$ and $v^{val} \in s'$. The rule $R = v^{val} \leftarrow s$ is consistent with T and realizes (s, s').*

Theorem 2 (Irreducible Rules are Optimal). *Let R be a rule consistent with a set of transitions $T \subseteq \mathcal{S}^{\mathcal{F}} \times \mathcal{S}^{\mathcal{T}}$. If $\forall R' \in \{\mathrm{head}(R) \leftarrow \mathrm{body}(R) \setminus \{v^{val}\} \mid v^{val} \in \mathrm{body}(R)\}$, R' conflicts with T, then $\nexists R'' \neq R$ consistent with T such that $R'' \geq R$ and thus, $R \in P_{\mathcal{O}}(T)$.*

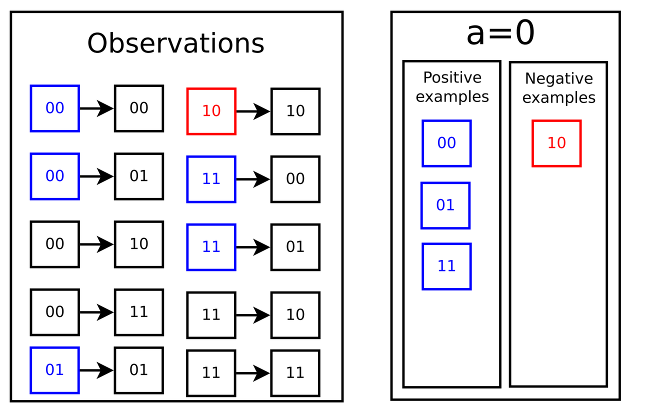
Idea:

- Consider positives/negatives examples of occurrence of a target atom v^{val} in T
- We can find a rule $R \in P_{\mathcal{O}}(T)$ to explain each positive example s
- Starting from $v^{val} \leftarrow s$, remove body atoms until conflict is not avoidable

Algorithmic properties:

- It is faster to start from $v^{val} \leftarrow \emptyset$: specialise it until consistency and then generalise
- Adding only the atoms of s ensures to matches s, in the worst case we obtain $v^{val} \leftarrow s$
- The more variables in the system, the more generalization is avoided

PRIDE



Algorithm 1 PRIDE$(\mathcal{A}, T, \mathcal{F}, \mathcal{T})$

```
INPUT : A set of atoms A, a set of transitions T ⊆ S^F × S^T, two sets of variables F and T.
OUTPUT: A DMVLP P ⊆ P_O(T) s.t. P realizes T
for each v^val ∈ A such that v ∈ T do
    // 1) Extract positives and negatives examples
    Pos_v^val := {s ∈ S^F | ∃(s, s') ∈ T, v^val ∈ s'}
    Neg_v^val := {s ∈ S^F | ∄(s, s') ∈ T, v^val ∈ s'}
    // 2) Generate the rules of v^val that are in P_O(T) and that match each state of Pos_v^val
    while Pos_v^val ≠ ∅ do
        pick pos ∈ Pos_v^val
        R := search(v^val, pos, Neg_v^val)
        // Clean other positives examples covered
        Pos_v^val := Pos_v^val \ {s | s ∈ Pos_v^val, R⊓s}
        P = P ∪ {R}
return P
```

Algorithm 2 search$(v^{val}, pos, Neg_{v^{val}})$

```
INPUT : An atom v^val ∈ A, a state pos ∈ S^F and a set of states Neg_v^val ⊂ S^F.
OUTPUT: A MVL rule R ∈ P_O(T) s.t. R ⊓ pos
R := v^val ← ∅
// Specialize R until consistency with Neg_v^val
for each neg ∈ Neg_v^val do
    if R ⊓ neg then
        pick c ∈ (pos \ neg)
        R := head(R) ← body(R) ∪ {c}
// Generalize R while keeping consistency
for each c ∈ body(R) do // Test each condition
    R' := head(R) ← body(R) \ {c}
    conflict := false
    for each neg ∈ Neg_v^val do
        if R' ⊓ neg then // Necessary condition
            conflict := true; BREAK
    if conflict == false then // R' is valid
        R := R'
return R
```

We extract positive and negatives examples (feature states) of each target atom occurrence. Rules should match a positive and no negative while being irreducible.

Implementation: Python Library and User API

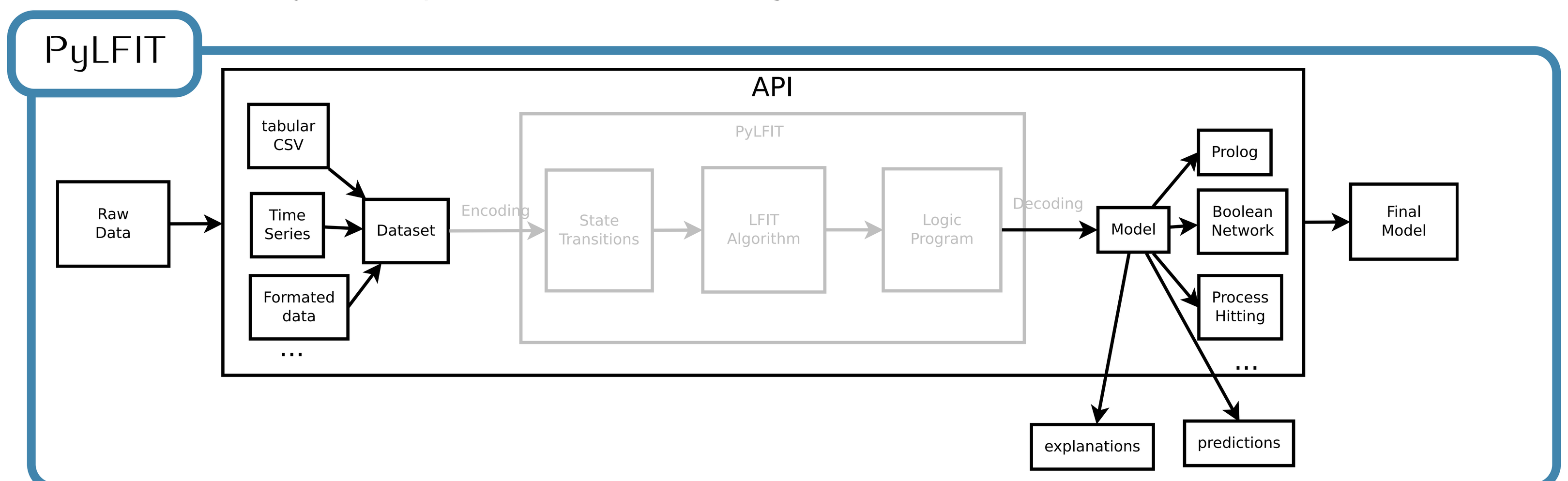
PyLFIT Library

- Open source Python library: `pip install pylfit`
- Contains all LFIT algorithms and a simple user API
- Built-in data/model conversion/usage

User API

- Load raw data from different formats into a Dataset object
- Choose desired model type and run corresponding LFIT algorithm
- Use model object for predictions and analysis, or convert it to other formats

PyLFIT



Predictions:

- $\mathcal{DMVLP}$ and $\mathcal{CDMVLP}$ (constraints) can be used to predict possible target states
- $\mathcal{WDMVLP}$ models both possibility and impossibility, it also adds weights to rules w.r.t. observations to allow probabilistic predictions of target atom occurrence in a transition

$\mathcal{WDMVLP}$

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

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

- The API provides metrics to evaluate prediction accuracy and quality of explanation rules

Summary

- The polynomiality of **PRIDE** is obtained at the cost of completeness over $P_{\mathcal{O}}(T)$.
- Still, the program learned can reproduce all observations and provides minimal explanation for each of them in the form of optimal rules.
- The source code is available as open source on github and pypi.org (see QR code).
- A user-friendly API allows to easily use LFIT algorithms on different kinds of datasets and is already being used in several research collaborations [4].

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[2] Tony Ribeiro, Maxime Folschette, Morgan Magnin, Olivier Roux, Katsumi Inoue: Learning dynamics with synchronous, asynchronous and general semantics. In: International Conference on Inductive Logic Programming. pp. 118–140. Springer (2018)
[3] Hannes Klarner, Adam Streck, Heike Siebert: PyBoolNet: a Python package for the generation, analysis and visualization of Boolean networks. *Bioinformatics* 33(5), 770–772 (2016).
[4] Alfonso Ortega, Julian Fiérrez, Aythami Morales, Zilong Wang, Tony Ribeiro: Symbolic AI for XAI: Evaluating LFIT Inductive Programming for Fair and Explainable Automatic Recruitment. WACV (Workshops) 2021: 78-87