On the Design of PSyKI: a Platform for Symbolic Knowledge Injection into Sub-Symbolic Predictors

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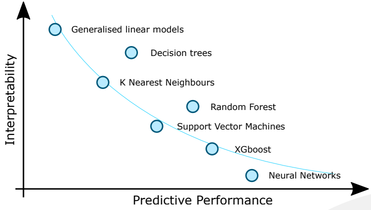
1. Motivation & Context
2. Design overview
3. Use case and example
4. Conclusions & future works

Context

- Most of modern ML predictors are black-boxes [Lipton, 2018]
  - interpretability vs performance trade-off



⇒ Dual (not exclusive) approaches to tackle the problem:

- ! symbolic knowledge extraction (SKE)
- ! symbolic knowledge injection (SKI)

- Binding of inductive and deductive reasoning

Motivation

- More and more ML applications in critical domains
  - e.g. medicine, finance, law
  - ⇒ Prevent predictors to become black-boxes
    - symbolic knowledge is used to guide predictors during learning
      - ⇒ predictors do not violate or violate less the prior knowledge
- Overcome the performances of ML state-of-the-art solutions
  - e.g. accuracy, learning time, need for less training data
- Fill the lack of public and usable implementation of SKI algorithms

Contribution

Contributions of the work

- Elicit common steps of SKI workflow algorithms from literature
- Implementation of a Python library for usage and development of SKI algorithms
  - ⇒ that supports the key phases of the SKI workflow
  - ⇒ with interoperability for PSyKE [Sabbatini et al., 2021] and 2ppy

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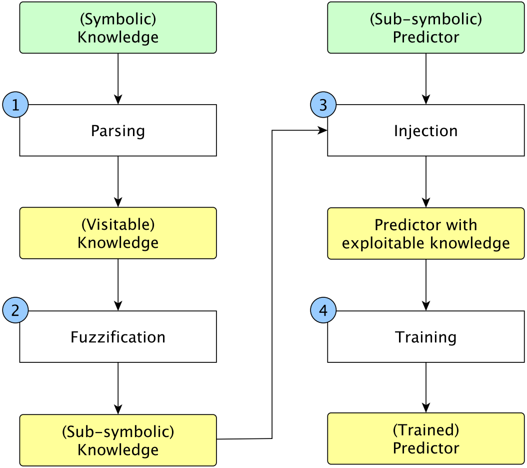
Modelling

Common SKI workflow steps from literature
[Besold et al., 2017, Xie et al., 2019, Calegari et al., 2020]

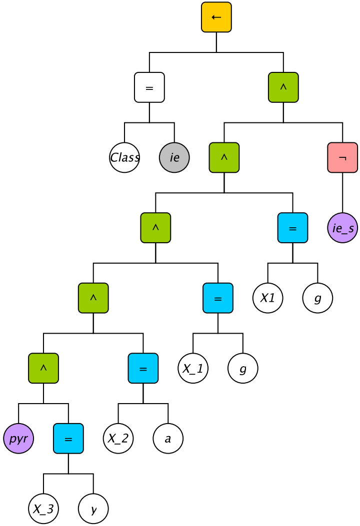
1. Knowledge is commonly provided using a logic formalism
   e.g. first order logic, knowledge graph, propositional logic, etc.
2. Symbolic knowledge is somehow encoded into a sub-symbolic form
3. Ad-hoc methods to inject the sub-symbolic knowledge into a predictor
   e.g. modifying the loss function, structuring the architecture, etc.
4. Training (virtually always required)

General SKI workflow



1 – Parsing

$$
\begin{aligned}
&\mathit{class}(X_{-30}, \ldots, X_{30}, \mathit{ie}) \leftarrow \\
&\qquad \mathit{pyramidine\text{-}rich}(\ldots) \land \\
&\qquad X_{-3} = y \land \\
&\qquad X_{-2} = a \land \\
&\qquad X_{-1} = g \land \\
&\qquad X_{1} = g \land \\
&\qquad \neg(\mathit{ie\text{-}stop}(\ldots))
\end{aligned}
$$



2 – Fuzzification

Formula	Continuous interpretation
$[\![\neg\phi]\!]$	$1 - [\![\phi]\!]$
$[\![\phi \wedge \psi]\!]$	$min\{[\![\phi]\!], [\![\psi]\!]\}$
$[\![\phi \vee \psi]\!]$	$max\{[\![\phi]\!], [\![\psi]\!]\}$
$[\![\phi = \psi]\!]$	$[\![\neg(\phi \neq \psi)]\!]$
$[\![\phi \neq \psi]\!]$	$\lvert[\![\phi]\!] - [\![\psi]\!]\rvert$
$[\![\phi > \psi]\!]$	$max\{0, [\![\phi]\!] - [\![\psi]\!]\}$
$[\![\phi \geq \psi]\!]$	$[\![(\phi > \psi) \vee (\phi = \psi)]\!]$
$[\![\phi < \psi]\!]$	$max\{0, [\![\psi]\!] - [\![\phi]\!]\}$
$[\![\phi \leq \psi]\!]$	$[\![(\phi < \psi) \vee (\phi = \psi)]\!]$
$[\![\phi \Rightarrow \psi]\!]$	$min\{1, 1 - [\![\psi]\!] + [\![\phi]\!]\}$
$[\![\phi \Leftarrow \psi]\!]$	$min\{1, 1 - [\![\phi]\!] + [\![\psi]\!]\}$
$[\![\phi \Leftrightarrow \psi]\!]$	$min\{1, 1 - \lvert[\![\phi]\!] - [\![\psi]\!]\rvert\}$
$[\![\mathrm{expr}(\bar{X})]\!]$	$\mathrm{expr}([\![\bar{X}]\!])$
$[\![\mathtt{true}]\!]$	1
$[\![\mathtt{false}]\!]$	0
$[\![X]\!]$	x
$[\![\mathrm{k}]\!]$	k
$[\![p(\bar{X})]\!]^{**}$	$[\![\psi_1 \vee \ldots \vee \psi_k]\!]$
$[\![class(\bar{X}, \mathrm{y}_i) \leftarrow \psi]\!]$	$[\![\psi]\!]^*$

* encodes the value for the i^{th} output

** assuming p is defined by k clauses of the form:
$p(\bar{X}) \leftarrow \psi_1, \ \ldots, \ p(\bar{X}) \leftarrow \psi_k$

$$class(X_{-30}, \ldots, X_{30}, ie) \leftarrow$$
$$X_{-3} = y \ \wedge$$
$$X_{-2} = a \ \wedge$$
$$X_{-1} = g \ \wedge$$
$$X_1 = g$$

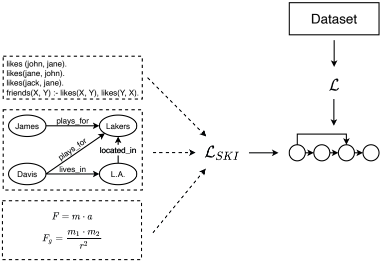
$$\downarrow$$

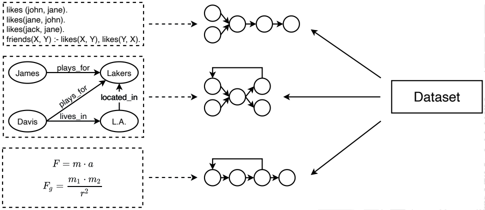
$$min\{min\{min\{1 - |X_{-3} - y|, 1 - |X_{-2} - a|\}, 1 - |X_{-1} - g|\}, 1 - |X_1 - g|\}$$

3 – Injection

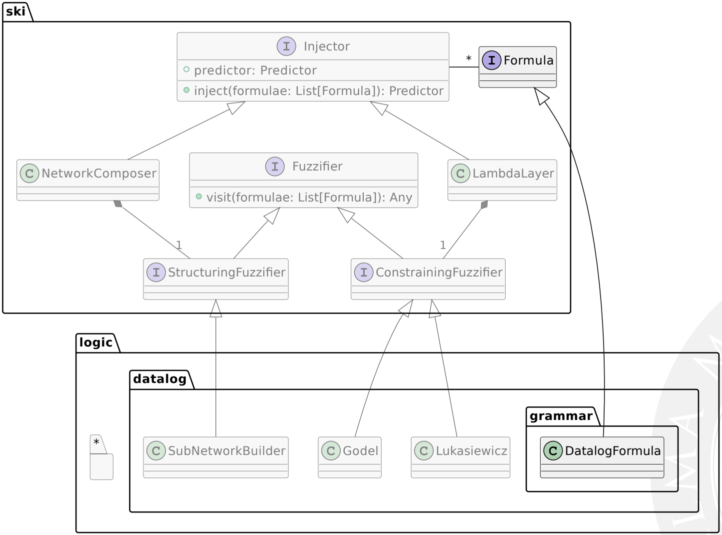
Usually injection is performed

- by adding a cost factor to the loss function [Tresp et al., 1992]
- by structuring the predictor [Ballard, 1986, Towell et al., 1990]

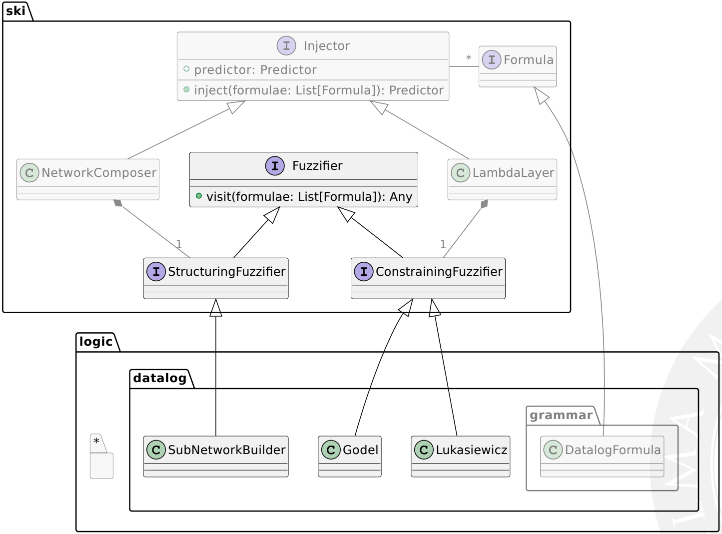




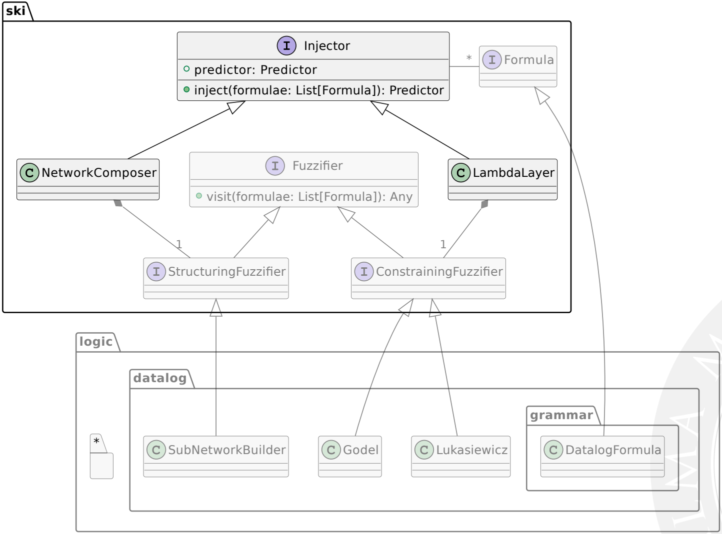
PSyKI high level class diagram



PSyKI high level class diagram



PSyKI high level class diagram



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Use case and example

Splice junction dataset and knowledge from UCI [Dua and Graff, 2017]

```
EI-stop ::- @-3 'TAA'.
EI-stop ::- @-3 'TAG'.
EI-stop ::- @-3 'TGA'.
EI-stop ::- @-4 'TAA'.
EI-stop ::- @-4 'TAG'.
EI-stop ::- @-4 'TGA'.
EI-stop ::- @-5 'TAA'.
EI-stop ::- @-5 'TAG'.
EI-stop ::- @-5 'TGA'.

IE-stop ::- @1 'TAA'.
IE-stop ::- @1 'TAG'.
IE-stop ::- @1 'TGA'.
IE-stop ::- @2 'TAA'.
IE-stop ::- @2 'TAG'.
IE-stop ::- @2 'TGA'.
IE-stop ::- @3 'TAA'.
IE-stop ::- @3 'TAG'.
IE-stop ::- @3 'TGA'.

pyramidine-rich :- 6 of (@-15 'YYYYYYYYYY').

EI :- @-3 'MAGGTRAGT', not(EI-stop).

IE :- pyramidine-rich, @-3 'YAGG', not(IE-stop).
```

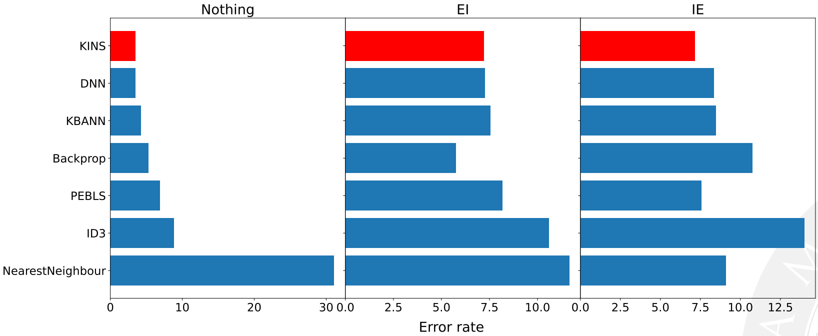
```
Class, Id, DNA-sequence

EI,ATRINS-DONOR-521,CCAGCTGCAT...AGCCAGTCTG
EI,ATRINS-DONOR-905,AGACCCGCCG...GTGCCCCCGC
EI,BABAPOE-DONOR-30,GAGGTGAAGG...CACGGGGATG
...
IE,ATRINS-ACCEPTOR-701,TTCAGCGGCC...GCCCTGTGGA
IE,ATRINS-ACCEPTOR-1678,GGACCTGCTC...GGGGGCTCTA
IE,BABAPOE-ACCEPTOR-801,GCGGTTGATT...AAGATGAAGG
...
N,AGMKPNRSB-NEG-1,CAAAAGAACA...CAAGGCTACA
N,AGMORS12A-NEG-181,AGGGAGGTGT...GGGCATGGGG
N,AGMORS9A-NEG-481,TGGTCAATTC...TCTTGCTCTG
...
```

Code snippet

General script to perform injection

```python
from psyki.logic.datalog.grammar.adapters.antlr4 import get_formula_from_string
from psyki.ski.injectors import NetworkComposer

# ...

# Symbolic knowledge
with open(filename) as file:
    rows = file.readlines()
# 1 - Parsing
knowledge = [get_formula_from_string(row) for row in rows]

predictor = build_NN()
# 2 and 3 - Fuzzification and injection
injector = InjectorX(predictor)
predictor_with_knowledge = injector.inject(knowledge)

# 4 - Training
predictor_with_knowledge.fit(train_x, train_y)
```

Results


Nothing
EI
IE
KINS
DNN
KBANN
Backprop
PEBLS
ID3
NearestNeighbour
0
10
20
30
0.0
2.5
5.0
7.5
10.0
0.0
2.5
5.0
7.5
10.0
12.5
Error rate

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Conclusions & future works

Summing up

Relevant contributions of this work:

- detecting main steps of SKI workflow
- implementation of a Python library that
  - provide already existing SKI algorithms
  - support the development of new algorithms

Future works

Some future research directions

- training predictors combining SKE and SKI
- implementation of the most successful SKI algorithms

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