

Symbolic Knowledge Injection via PSyKI

A tutorial

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- 1 What and Why
- 2 Background
- 3 PSyKI
- 4 Tutorial
- 5 Discussion



Next in Line...

1 What and Why

2 Background

3 PSyKI

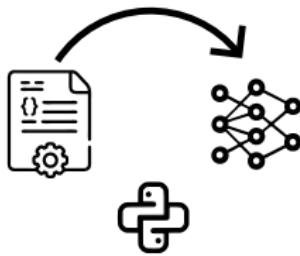
4 Tutorial

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What

PSyKI: a (Python) platform for symbolic knowledge injection



GitHub Repository

<https://github.com/psykei/psyki-python>
(please star us :)

Main papers

- [Magnini et al., 2022b]



Why SKI?

There are several benefits:

- prevent the predictor to become a black-box!;
- reduce learning time;
- reduce the data size needed for training;
- improve predictor's accuracy;
- build a predictor that behave as a logic engine.



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Symbolic Knowledge Injection I

Key insights:

- Altering ML predictors . . .
- . . . to make they comply to user-provided knowledge . . .
- . . . which is represented in symbolic form

Symbolic Knowledge Injection II

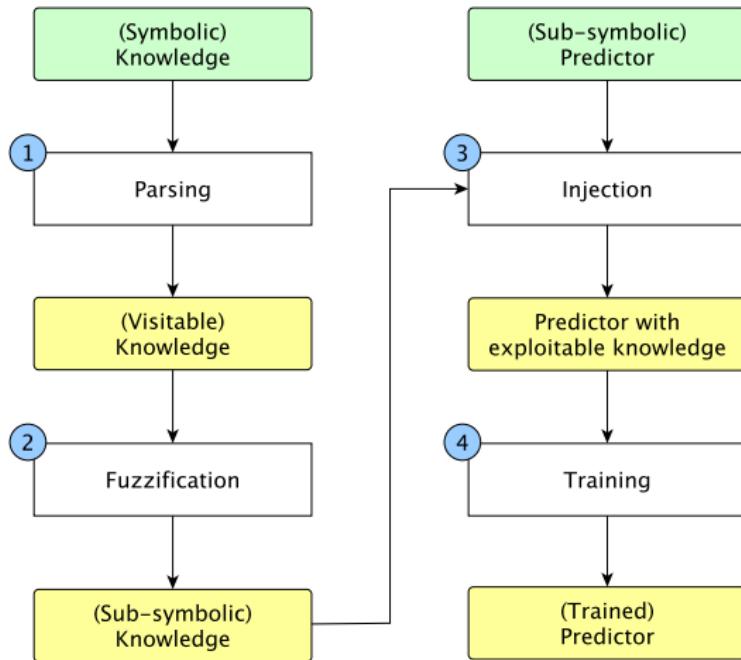
We define SKI as:

any **algorithmic** procedure affecting how **sub-symbolic predictors** draw their inferences in such a way that predictions are either **computed** as a function of, or made **consistent** with, some **given symbolic knowledge***.

* a wide definition that includes the vast majority of the works surveyed in [Besold et al., 2017, Xie et al., 2019, Calegari et al., 2020].

Symbolic Knowledge Injection III

General workflow:



What does 'symbolic' actually mean? I

According to [van Gelder, 1990], **symbolic** representations of knowledge

- involves a **set of symbols**,
- which can be combined (e.g., concatenated) in (possibly) **infinitely many ways**,
- following precise **syntactical** rules, and
- where both elementary symbols and any admissible combination of them can be assigned with **meaning**
ie **each** symbol can be mapped into some entity from the domain at hand.

Notable example

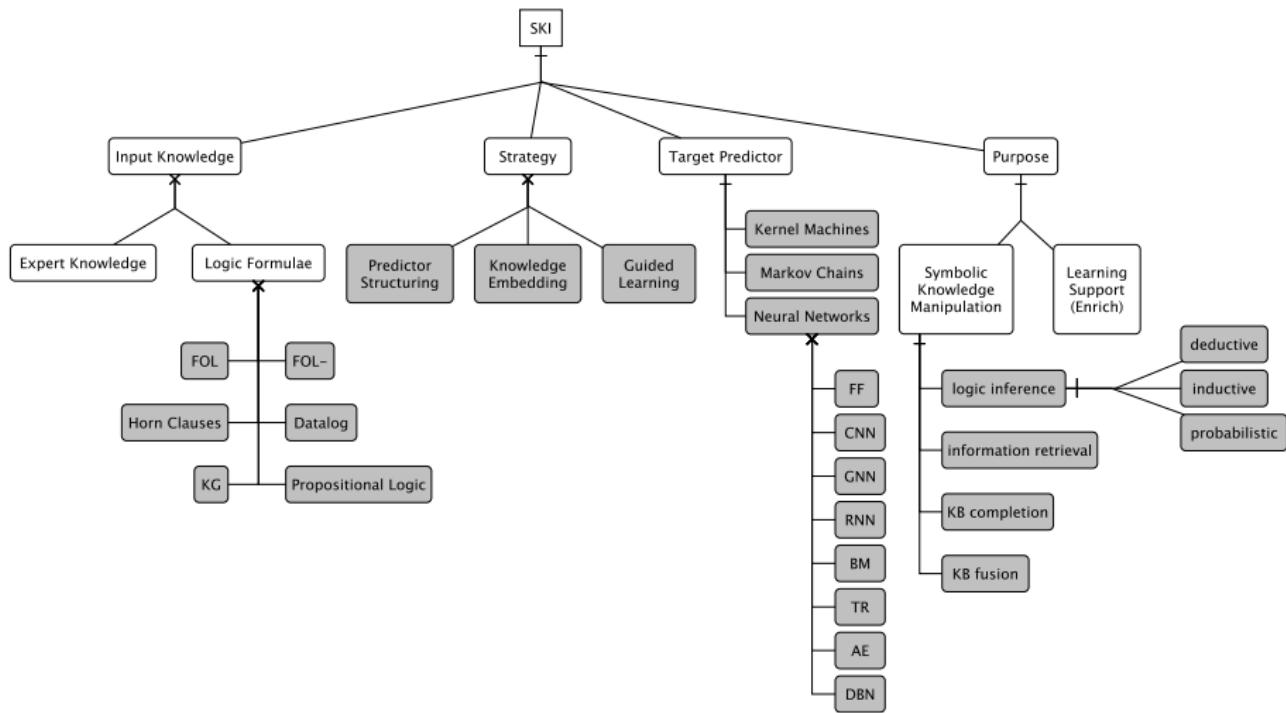
- formal logic

What does 'symbolic' actually mean? II

Opposite notion: **distributed** representations

- where symbols **alone** have no meaning
- unless it is considered along with its **neighbourhood**
ie any other symbol which is **close** (according to some notion of closeness)

Taxonomy of SKI methods I



Taxonomy of SKI methods II

- **input knowledge** how is the knowledge to-be-injected represented?
 - commonly, some sub-set of first-order logic (FOL)
- **target predictor** which predictors can knowledge be injected into?
 - mostly, neural networks
- **strategy** how does injection actually work?
 - **guided learning** the input knowledge is used to **guide the training process**
 - **structuring** the **internal** composition of the predictor is **(re-)structured** to reflect the input knowledge
 - **embedding** the input knowledge is **converted** into numeric array form
- **purpose** why is knowledge injected in the first place?
 - **knowledge manipulation** improve / extend / reason about symbol knowledge—subsymbolically
 - **learning support** improve the sub-symbolic predictor (e.g. speed, size, etc.)

Next in Line...

1 What and Why

2 Background

- Focus on input knowledge

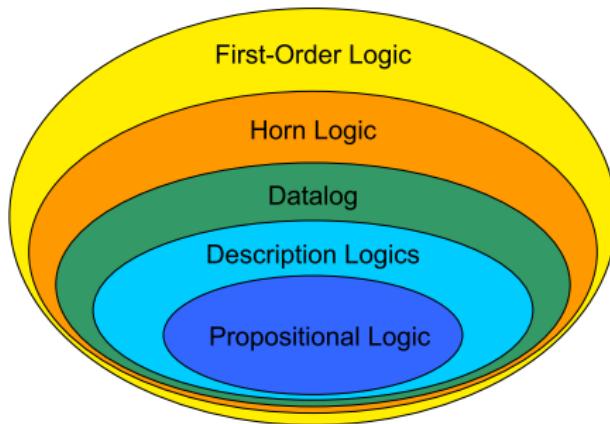
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About Logic I

How to represent knowledge?



- *expressiveness–tractability trade-off* [Levesque and Brachman, 1987, Brachman and Levesque, 2004]

About Logic II

In practice, virtually all SKI algorithms deal with:

- **datalog**;
- description logics (a.k.a. **knowledge graph**, KG);
- **propositional logic** (PL).



First Order Logic I

Overview

- FOL is extremely flexible and expressive
 - variables, quantifiers, structured terms, negation, logic connectives
- one can use **recursion** to define recursive structures;
 - possibly, **intensionally**—i.e. without **extensively** describing everything
- maybe too “powerful” for canonical NN
 - most NN are essentially DAG
 - training via backpropagation^[Baldi and Sadowski, 2016] requires no cycles
→ recursion not supported

First Order Logic II

Example of FOL knowledge base (Peano numbers)

natural(zero)

$\forall X : \text{natural}(X) \rightarrow \text{natural}(\text{successorOf}(\text{var}X))$

Horn Clauses (\approx Prolog) I

Overview

- sub-set of FOL with:
 - implicit quantifiers
 - limited set of logic connectives
- still supports recursion
- nice expressiveness–tractability trade-off
 - often exploited to design/realise automatic reasoning

Horn Clauses (\approx Prolog) II

Example of Horn clauses (Peano numbers)

natural(zero)

natural(successorOf(varX)) ← natural(X)

Datalog I

Overview

- sub-set of Horn clauses with **no recursion**
- good for SKI!

Peano numbers in Datalog

- cannot be represented!
 - (as they require recursion)

Description Logics (\approx Knowledge Graphs) I

Overview

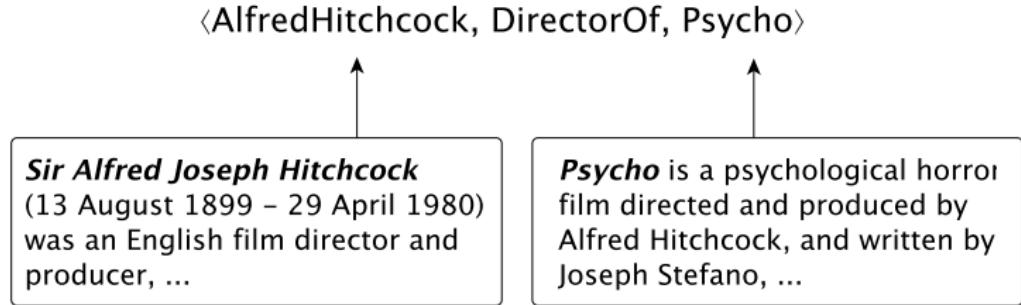
- Very restricted subset of FOL
 - only constants, variables and n -ary predicates with $n \leq 2$;
- Everything is represented via collections of triplets of the form:

$$\langle a \ f \ b \rangle \text{ or } f(a, b)$$

where a, b are entities, and f is a (binary) relationship

- essentially, directed graph:
 - nodes (i.e. entities) represent individuals,
 - edges (i.e. relationships) represent relations among individuals;

Description Logics (\approx Knowledge Graphs) II



Propositional Logic I

Overview

- The simplest subset of FOL
 - no quantifiers, no terms, no n -ary predicates with $n > 0$
 - essentially, just Boolean algebra
- low expressiveness, but easy to work with.



Propositional Logic II

Example

$big_petal \wedge average_sepal \rightarrow virginica.$

$big_petal \wedge \neg average_sepal \rightarrow versicolor.$

$big_petal \rightarrow setosa.$

$average_sepal \equiv (3 \leq SepalWidth < 5)$

$big_petal \equiv (PetalLength > 3)$

Next in Line...

1 What and Why

2 Background

- Focus on strategy

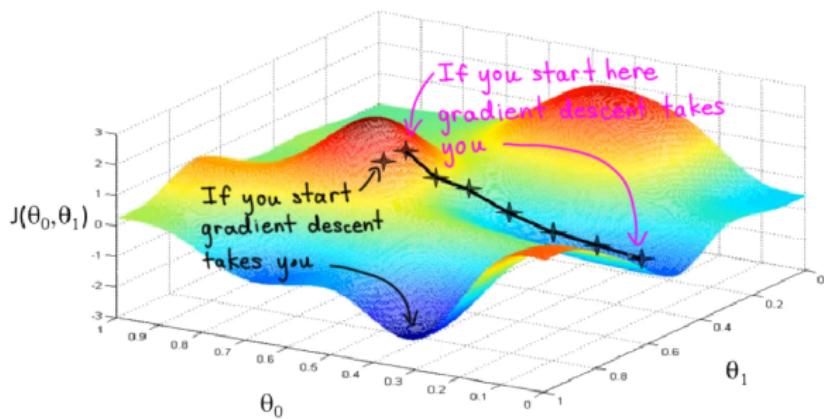
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Strategy 1: Guided Learning I



- learning is essentially an **optimization** process
- ... often performed via **gradient descent**
ie minimising a **loss function**

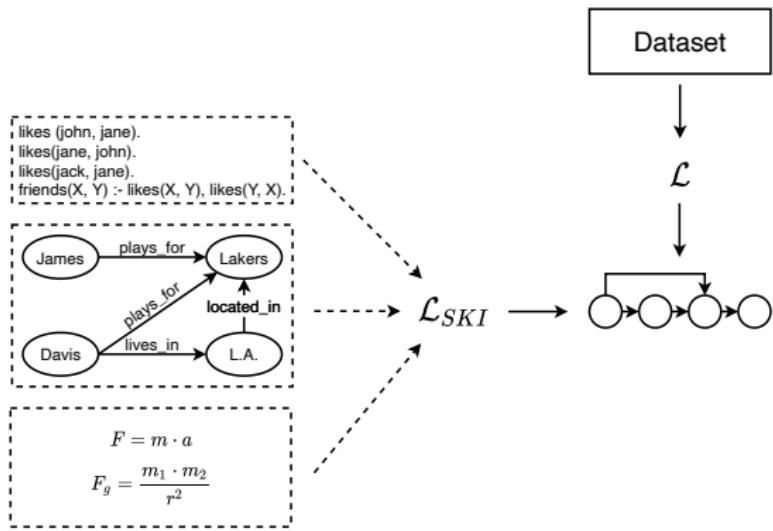
Strategy 1: Guided Learning II

SKI via Guided Learning

- ① Input knowledge is converted into a **cost factor**
ie the more the knowledge is violated, the higher the cost
 - ② The loss function is altered to **include** that cost factor
eg as a simple additive regularisation factor
 - ③ The predictor is then trained **as usual**
- Training minimises both the predictors' **error** and **inconsistency** w.r.t. knowledge



Strategy 1: Guided Learning III



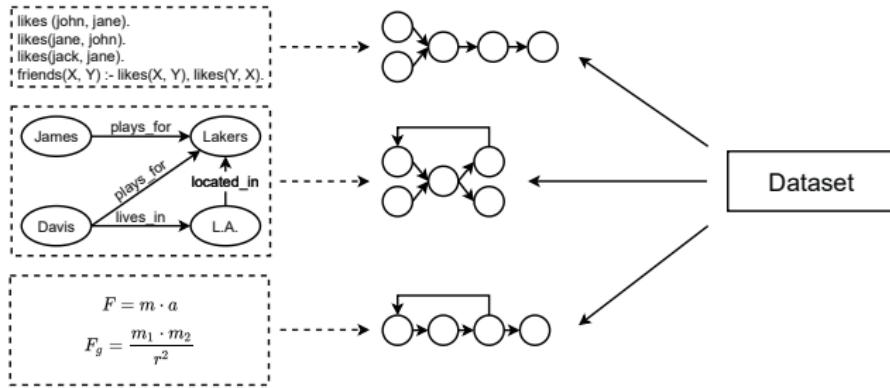
Strategy 2: Structuring I

SKI via Guided Learning

- The predictor's inner architecture is shaped to "mimic" the knowledge
 - Shaping is predictor-dependent
 - eg for neural networks, this means creating **ad-hoc layers**
 - where small groups of neurons are used to compute pieces of a formula
- The predictor directly exploits the knowledge during inference



Strategy 2: Structuring II



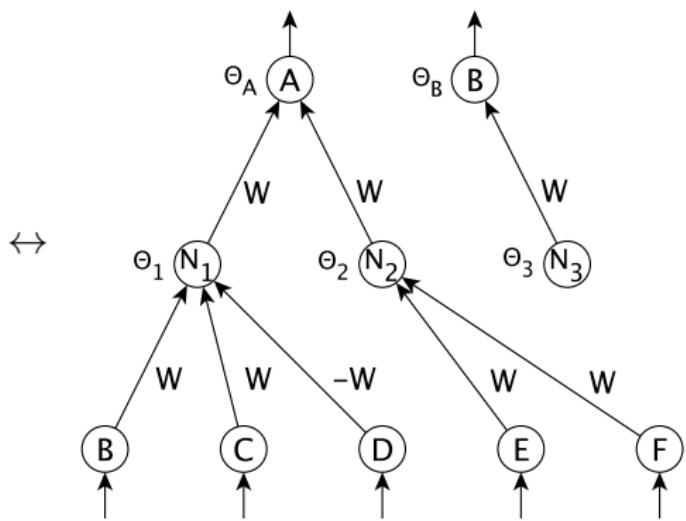
Strategy 2: Structuring III

Example:

$$A \leftarrow B \wedge C \wedge \neg D.$$

$$A \leftarrow E \wedge F.$$

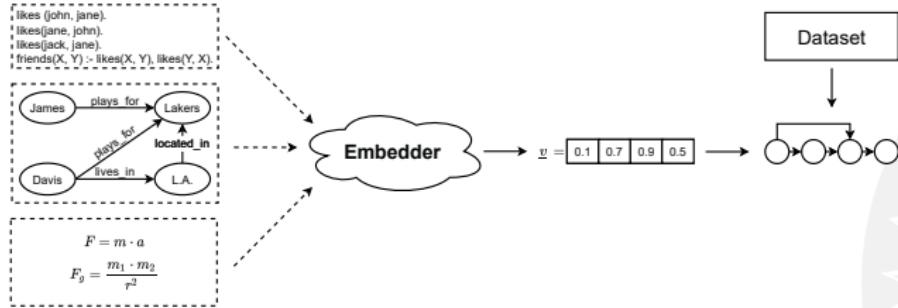
$$B \leftarrow \text{true}.$$



Strategy 3: Embedding I

SKI via Guided Learning

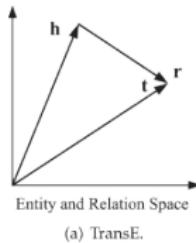
- Input knowledge is converted into numeric tensor(s)
 - These are used as the training set for an ordinary learning process
- The predictor is trained and used 'as usual'



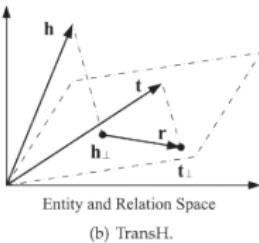
Strategy 3: Embedding II

Example: knowledge graph embedding [Wang et al., 2017]

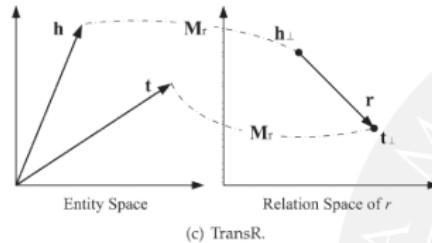
- **entities** and **relations** are embedded into continuous vector spaces;
- scoring function $f_r(h, t)$ defined on each fact (h, r, t) to measure its plausibility;



(a) TransE.

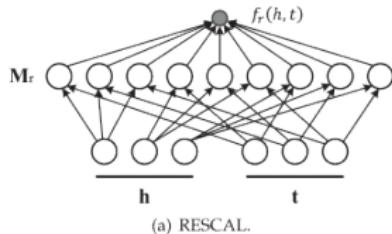


(b) TransH.

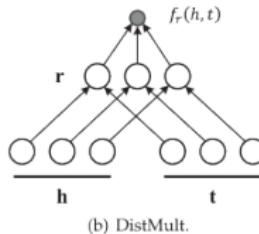


(c) TransR.

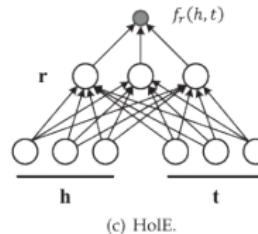
Strategy 3: Embedding III



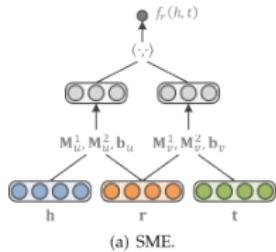
(a) RESCAL.



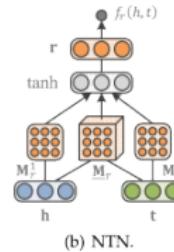
(b) DistMult.



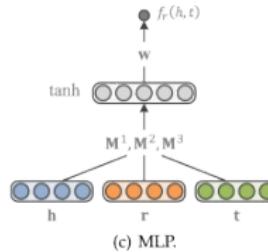
(c) HolE.



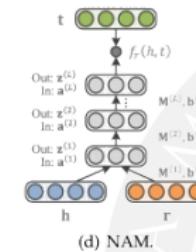
(a) SME.



(b) NTN.



(c) MLP.



(d) NAM.

Next in Line...

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- Example algorithms

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Knowledge Injection via Network Structuring [Magnini et al., 2022a]

KINS

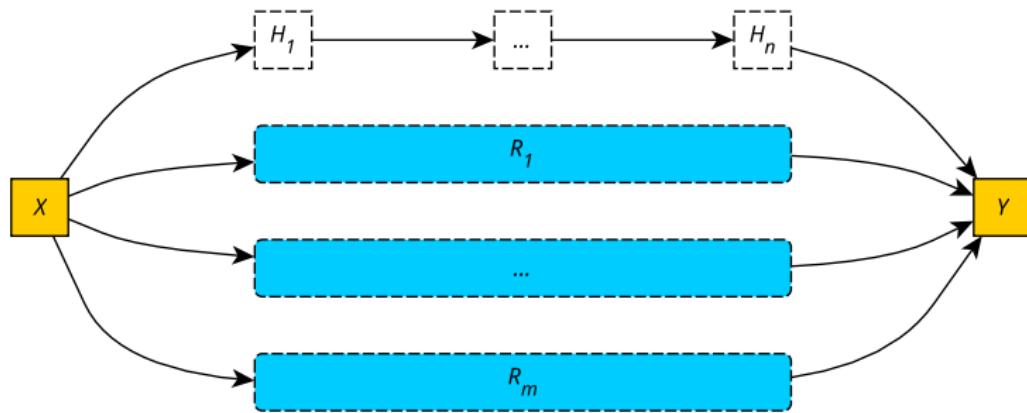
purpose → learning support;

target predictor → neural networks;

strategy → structuring;

input logic → stratified Datalog with negation.

Knowledge Injection via Network Structuring [Magnini et al., 2022a] //



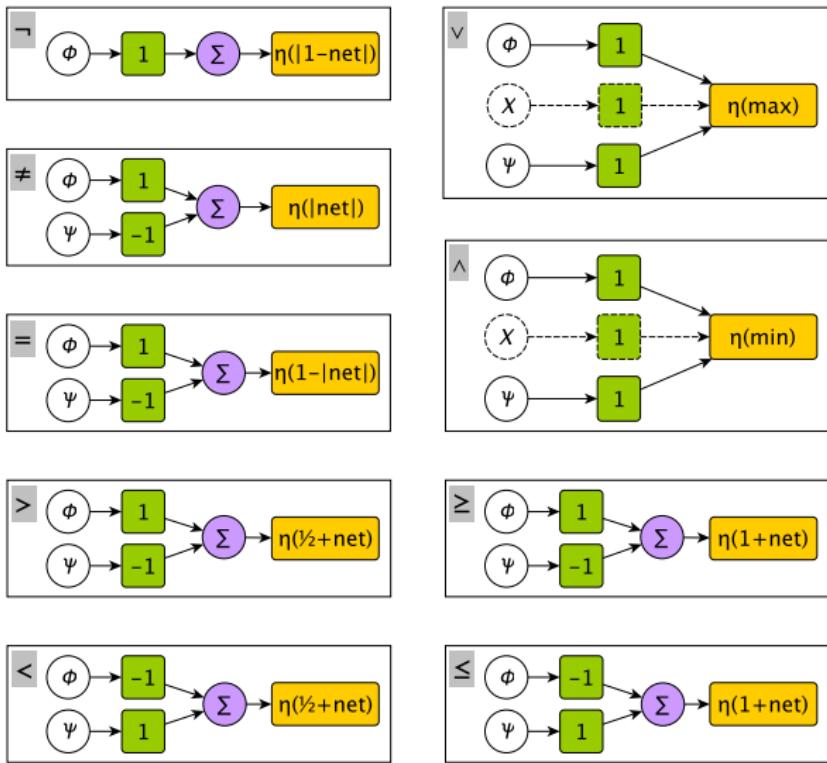
Knowledge Injection via Network Structuring [Magnini et al., 2022a] III

Formula	C. interpretation	Formula	C. interpretation
$\llbracket \neg \phi \rrbracket$	$\eta\{1 - \llbracket \phi \rrbracket\}$	$\llbracket \phi \leftarrow \psi \rrbracket$	$\eta\{\min\{1, 1 - \llbracket \phi \rrbracket + \llbracket \psi \rrbracket\}\}$
$\llbracket \phi \wedge \psi \rrbracket$	$\eta\{\min\{\llbracket \phi \rrbracket, \llbracket \psi \rrbracket\}\}$	$\llbracket \phi \leftrightarrow \psi \rrbracket$	$\eta\{\min\{1, 1 - \llbracket \phi \rrbracket - \llbracket \psi \rrbracket \}\}$
$\llbracket \phi \vee \psi \rrbracket$	$\eta\{\max\{\llbracket \phi \rrbracket, \llbracket \psi \rrbracket\}\}$	$\llbracket \text{expr}(\bar{X}) \rrbracket$	$\text{expr}(\llbracket \bar{X} \rrbracket)$
$\llbracket \phi = \psi \rrbracket$	$\eta\{\llbracket \neg(\phi \neq \psi) \rrbracket\}$	$\llbracket \text{true} \rrbracket$	1
$\llbracket \phi \neq \psi \rrbracket$	$\eta\{ \llbracket \phi \rrbracket - \llbracket \psi \rrbracket \}$	$\llbracket \text{false} \rrbracket$	0
$\llbracket \phi > \psi \rrbracket$	$\eta\{\max\{0, \llbracket \phi \rrbracket - \llbracket \psi \rrbracket\}\}$	$\llbracket X \rrbracket$	x
$\llbracket \phi \geq \psi \rrbracket$	$\eta\{\llbracket (\phi > \psi) \vee (\phi = \psi) \rrbracket\}$	$\llbracket k \rrbracket$	k
$\llbracket \phi < \psi \rrbracket$	$\eta\{\max\{0, \llbracket \psi \rrbracket - \llbracket \phi \rrbracket\}\}$	$\llbracket p(\bar{X}) \rrbracket^{**}$	$\llbracket \psi_1 \vee \dots \vee \psi_k \rrbracket$
$\llbracket \phi \leq \psi \rrbracket$	$\eta\{\llbracket (\phi < \psi) \vee (\phi = \psi) \rrbracket\}$	$\llbracket \text{class}(\bar{X}, y_i) \leftarrow \psi \rrbracket$	$\llbracket \psi \rrbracket^*$
$\llbracket \phi \rightarrow \psi \rrbracket$	$\eta\{\min\{1, 1 - \llbracket \psi \rrbracket + \llbracket \phi \rrbracket\}\}$		

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

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

Knowledge Injection via Network Structuring [Magnini et al., 2022a] IV



Knowledge Injection via Lambda Layer [Magnini et al., 2022c]

KILL

purpose → learning support;

target predictor → neural networks;

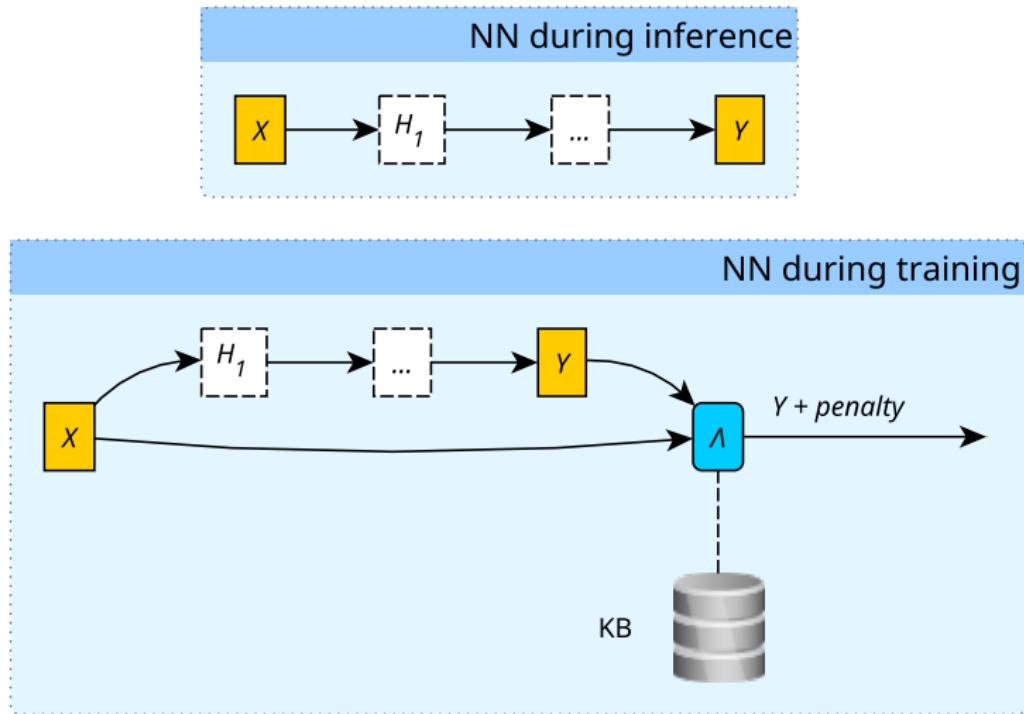
strategy → guided learning;

input logic → stratified Datalog with negation.

Knowledge Injection via Lambda Layer

[Magnini et al., 2022c]

II



Knowledge Injection via Lambda Layer

[Magnini et al., 2022c] III

Formula	C. interpretation	Formula	C. interpretation
$\llbracket \neg \phi \rrbracket$	$\eta(1 - \llbracket \phi \rrbracket)$	$\llbracket \phi \leq \psi \rrbracket$	$\eta(\llbracket \phi \rrbracket - \llbracket \psi \rrbracket)$
$\llbracket \phi \wedge \psi \rrbracket$	$\eta(\max(\llbracket \phi \rrbracket, \llbracket \psi \rrbracket))$	$\llbracket \text{class}(\bar{X}, y_i) \leftarrow \psi \rrbracket$	$\llbracket \psi \rrbracket^*$
$\llbracket \phi \vee \psi \rrbracket$	$\eta(\min(\llbracket \phi \rrbracket, \llbracket \psi \rrbracket))$	$\llbracket \text{expr}(\bar{X}) \rrbracket$	$\text{expr}(\llbracket \bar{X} \rrbracket)$
$\llbracket \phi = \psi \rrbracket$	$\eta(\llbracket \phi \rrbracket - \llbracket \psi \rrbracket)$	$\llbracket \text{true} \rrbracket$	0
$\llbracket \phi \neq \psi \rrbracket$	$\llbracket \neg(\phi = \psi) \rrbracket$	$\llbracket \text{false} \rrbracket$	1
$\llbracket \phi > \psi \rrbracket$	$\eta(0.5 - \llbracket \phi \rrbracket + \llbracket \psi \rrbracket)$	$\llbracket X \rrbracket$	x
$\llbracket \phi \geq \psi \rrbracket$	$\eta(\llbracket \psi \rrbracket - \llbracket \phi \rrbracket)$	$\llbracket k \rrbracket$	k
$\llbracket \phi < \psi \rrbracket$	$\eta(0.5 + \llbracket \phi \rrbracket - \llbracket \psi \rrbracket)$	$\llbracket p(\bar{X}) \rrbracket^{**}$	$\llbracket \psi_1 \vee \dots \vee \psi_k \rrbracket$

* encodes the penalty for the i^{th} neuron

** assuming predicate p is defined by k clauses of the form:

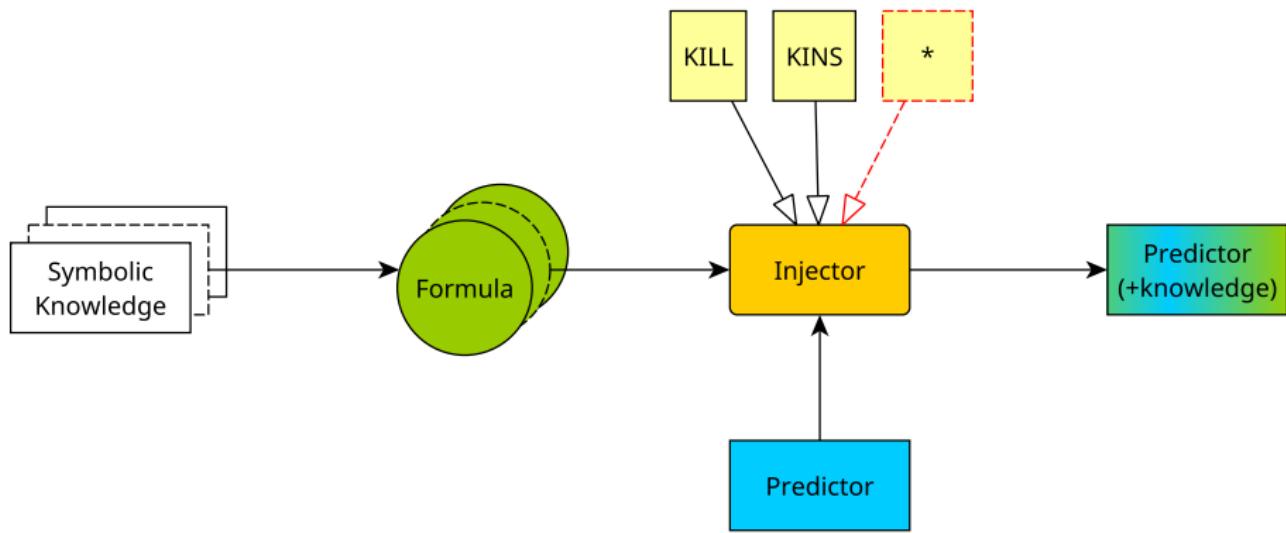
$$p(\bar{X}) \leftarrow \psi_1, \dots, p(\bar{X}) \leftarrow \psi_k$$

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Overall Design I



Overall Design II

Key components:

injector: any entity capable of injecting knowledge into a sub-symbolic predictor

- it simply alters/reconfigures the predictor...
- ... which should be trained after the injector operates

predictor: the partially-trained classifier/regressor where knowledge should be injected into

- untrained is ok too

formula: formal representation of the symbolic knowledge to be injected

- e.g. in Prolog or FOL syntax

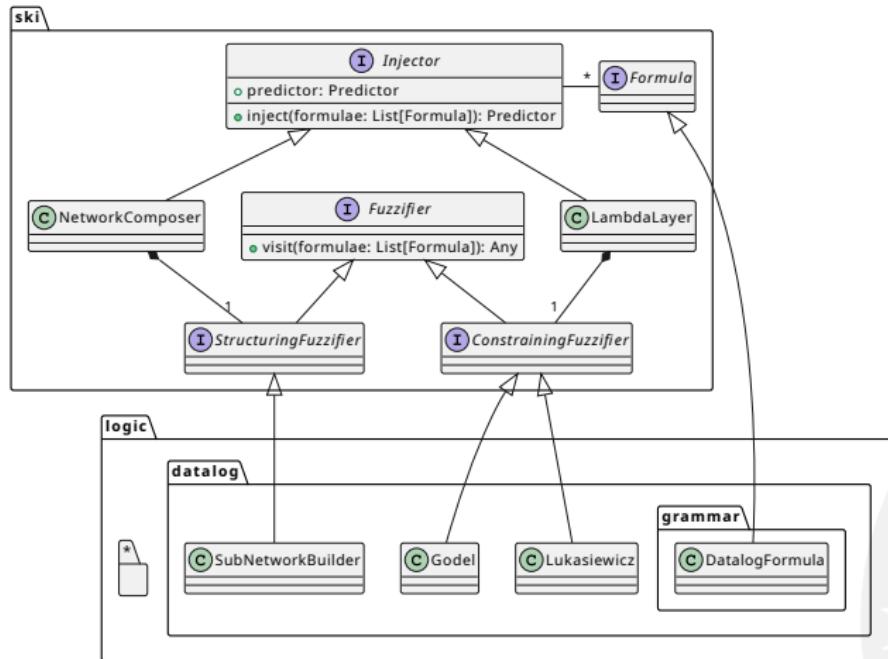
Overall Design III

Unified API for SKI

- 1 interface for Injector, several implementations
 - eg KILL, KINS, etc.
- 1 interface for Formula, several implementations
 - eg FOL, Datalog, etc.
- 1 interface for Predictor, several implementations
 - eg NN, kNN, DT



API Design I



API Design II

Remarks

- The user only needs to know:
 - the particular injector to exploit (and its parameters)
 - the particular parser to decode logic rules

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Tutorial

Two ways to reproduce the tutorial:

GitHub Repository (long way)

<https://github.com/pikalab-unibo/prima-tutorial-2022>

DockerHub Images (quick way)

<https://hub.docker.com/r/pikalab/prima-tutorial-2022/tags>

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• From GitHub

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How to set the tutorial up from GitHub I

Environmental pre-requisites

- Python **3.9.x**
- JDK ≥ 11
- Git

- ❶ `git clone
https://github.com/pikalab-unibo/prima-tutorial-2022`
- ❷ `cd prima-tutorial-2022`
- ❸ `pip install -r requirements.txt`
- ❹ `jupyter notebook`

How to set the tutorial up from GitHub II

- ⑤ Your browser should automatically open showing the following page:



The screenshot shows a Jupyter Notebook interface with the title "Jupyter". At the top, there are tabs for "Files", "Running", and "Clusters", along with "Out" and "Logout" buttons. Below the tabs is a toolbar with "Duplicate", "Rename", "Move", "Download", "View", "Edit", and a refresh icon. To the right of the toolbar are "Upload" and "New" dropdown menus. A search bar is also present. The main area displays a file list with the following details:

Name	Last Modified	File size
data	7 ore fa	
knowledge	7 ore fa	
psyke-tutorial.ipynb	7 ore fa	25.9 kB
<input checked="" type="checkbox"/> psyki-tutorial.ipynb	7 ore fa	47.4 kB
Dockerfile	7 ore fa	620 B
publish-m1.sh	7 ore fa	349 B
README.md	7 ore fa	107 B
requirements.txt	7 ore fa	62 B
setup.py	7 ore fa	3.23 kB
utils.py	7 ore fa	1.43 kB

- ⑥ open the `psyki-tutorial.ipynb` notebook
⑦ listen to the speaker presenting the tutorial =)

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How to set the tutorial up via Docker I

Environmental pre-requisites

- Docker

①

DOCKER_IMAGE=

$$\begin{cases} \text{pikalab/prima-tutorial-2022:latest} \\ \text{pikalab/prima-tutorial-2022:latest}-\text{apple-m1} \end{cases}$$

② docker pull \$DOCKER_IMAGE

- in case of lacking Internet access:

```
docker image load -i /path/to/local/image/file.tar
```

③ docker run -it -rm -name prima-tutorial-ske-ski -p 8888:8888 \$DOCKER_IMAGE

④ Some textual output such as the following one should appear:

How to set the tutorial up via Docker II

```
1 [I 09:51:46.940 NotebookApp] Writing notebook server cookie secret to /root/.local/
2 share/jupyter/runtime/notebook_cookie_secret
3 [I 09:51:47.159 NotebookApp] Serving notebooks from local directory: /notebook
4 [I 09:51:47.159 NotebookApp] Jupyter Notebook 6.5.2 is running at:
5 [I 09:51:47.159 NotebookApp] http://cb0a3641caf0:8888/?token=2
6 b02d31671c6ad9e9cf8e036eb6962d3592af9cfdd5e60bd
7 [I 09:51:47.159 NotebookApp] or http://127.0.0.1:8888/?token=2
8 b02d31671c6ad9e9cf8e036eb6962d3592af9cfdd5e60bd
9 [I 09:51:47.160 NotebookApp] Use Control-C to stop this server and shut down all
10 kernels (twice to skip confirmation).
11 [C 09:51:47.162 NotebookApp]
12
13 To access the notebook, open this file in a browser:
14   file:///root/.local/share/jupyter/runtime/nbserver-7-open.html
15 Or copy and paste one of these URLs:
16   http://cb0a3641caf0:8888/?token=2
17     b02d31671c6ad9e9cf8e036eb6962d3592af9cfdd5e60bd
18 or http://127.0.0.1:8888/?token=2b02d31671c6ad9e9cf8e036eb6962d3592af9cfdd5e60bd
```

How to set the tutorial up via Docker III

- ⑤ Copy-paste into your browser any link of the form:

`http://cb0a3641caf0:8888/?token=TOKEN`

- ⑥ Your browser should now be showing the following page:



- ⑦ open the `psyki-tutorial.ipynb` notebook
- ⑧ listen to the speaker presenting the tutorial =)

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Notable Remarks

- knowledge bases should express relations about input–output pairs
- embedding implies extensional representation of knowledge
 - guided learning, and structuring support intensional knowledge
- propositional knowledge implies binarising the I/O spaces



Current Limitations

- support for regression is preliminary
- recursive data structures are not supported
- recursive clauses are not supported
- extensional representation cost storage
 - not always possible
- guided learning works poorly with lacking data



Future research activities

- foundational: address recursion
- practical: address regression
- is SKI possible outside the NN domain?



Symbolic Knowledge Injection via PSyKI

A tutorial

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November 16, 2022

References |

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A theory of local learning, the learning channel, and the optimality of backpropagation.
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DOI:10.1016/j.neunet.2016.07.006.
- [Besold et al., 2017] Besold, T. R., d'Avila Garcez, A. S., Bader, S., Bowman, H., Domingos, P. M., Hitzler, P., Kühnberger, K., Lamb, L. C., Lowd, D., Lima, P. M. V., de Penning, L., Pinkas, G., Poon, H., and Zaverucha, G. (2017).
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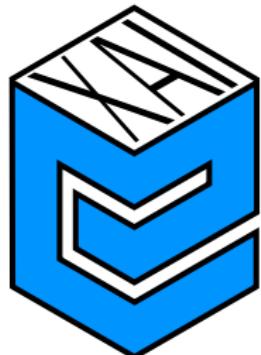
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EXPECTATION



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