Towards Explainability in Knowledge Enhanced Neural Networks

Data Science Master Thesis

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FONDAZIONE BRUNO KESSLER

UNIVERSITÀ DEGLI STUDI DI PADOVA

Outline

1. Introduction and motivations
2. Knowledge Enhanced Neural Networks (KENN)
3. **Contributions:** Experiments on collective classification
4. **Contributions:** Extracting explanations from KENN
5. Conclusions

Deep NNs have several flaws. For example:

- They are **data hungry**:
  - With few data, learning is not possible, even for simple logical reasoning tasks;
  - This motivates **Neural Symbolic Integration (NeSy)**.

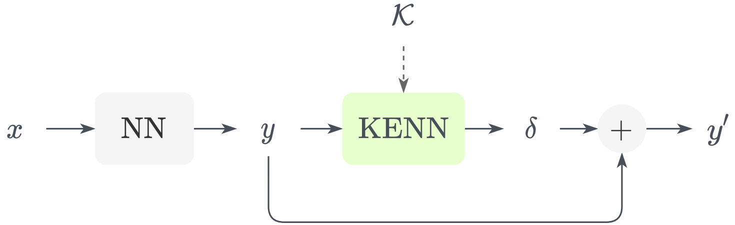
Introduction

Deep NNs have several flaws. For example:

- They are **data hungry**:
  - With few data, learning is not possible, even for simple logical reasoning tasks;
  - This motivates **Neural Symbolic Integration (NeSy)**.
- They are **black boxes**:
  - Predictions are not explainable, might lead to lack of trust in AI applications;
  - This motivates the research field of **Explainable AI (XAI)**.

Knowledge Enhanced Neural Networks

KENN[1] consists in a residual layer designed to improve the predictions of a base NN, by using logical prior knowledge, consisting in a set of FOL formulas $\mathcal{K}$.



[1] Daniele, Alessandro, and Luciano Serafini. "Knowledge enhanced neural networks." Pacific Rim International Conference on Artificial Intelligence. Springer, Cham, 2019.

Basic Terminology

Definition (The Language)

Our language will be a function-free first order language $\mathcal{L}$, defined by:

- A set of **constants**: $\mathcal{C} = \{a_1, \ldots, a_{|\mathcal{C}|}\}$;
- A set of **predicates**: $\mathcal{P} = \{P_1, \ldots, P_{|\mathcal{P}|}\}$;

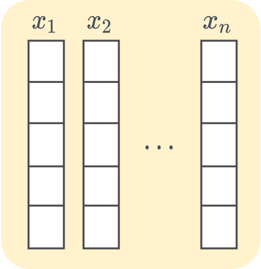
Definition (Clause)

A clause c is a formula expressed a disjunction of literals:

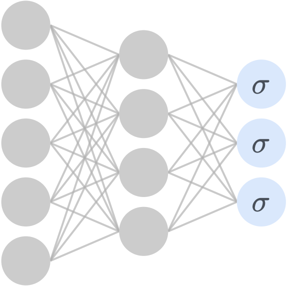
$$c := \bigvee_{i=1}^{k} l_i, \quad l_i \neq l_j \quad \forall i \neq j$$

Language Semantic

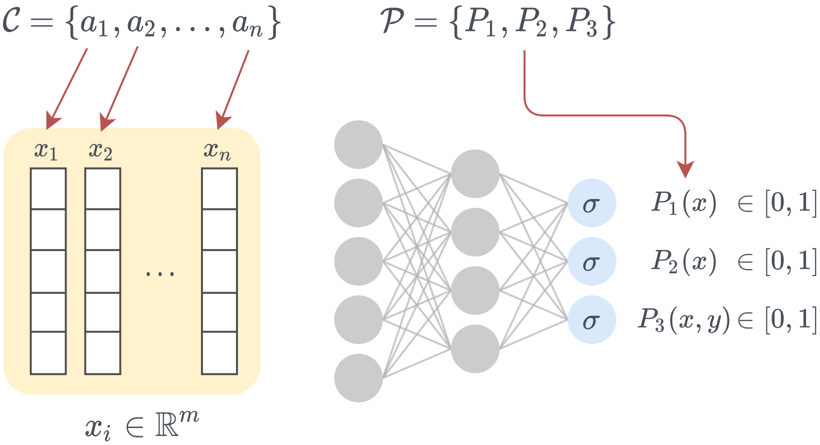
$$\mathcal{C} = \{a_1, a_2, \ldots, a_n\} \qquad \mathcal{P} = \{P_1, P_2, P_3\}$$



$x_i \in \mathbb{R}^m$



Language Semantic



KENN: Intuition

Given the vector of predictions of the NN y, KENN computes the final vector of predictions as follows:

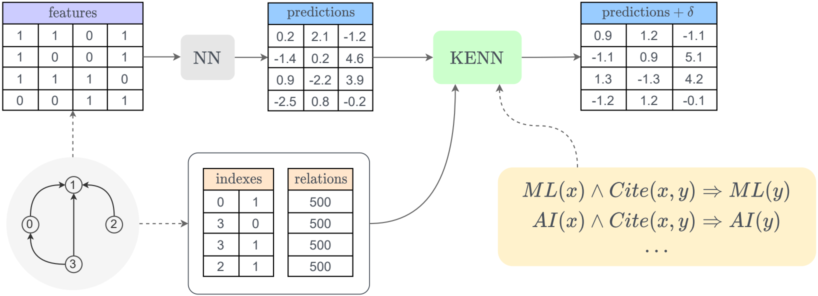
$$y' = y + \sum_{c \in \mathcal{K}} w_c \cdot \delta^c$$

where, for each $c \in \mathcal{C}$:

- δ^c improves the truth value of c, keeping $\|\delta^c\|_2$ minimal;
- $w_c \in \mathbb{R}$ is the **clause weight**, a learnable parameter that quantifies the importance of clause c.

Citeseer Experiments

- We tested KENN on a Collective Classification task;
- The **Citeseer Dataset** was used: citation network with 4732 citations (edges) between 3312 papers (nodes);
- The task is to predict the topic of each paper (6 possible topics).



Comparison with previous literature

- We also provide a comparison with two other NeSy models:
  - **Semantic Based Regularization**[2];
  - **Relational Neural Machines**[3];

[2] Diligenti, Michelangelo, Marco Gori, and Claudio Sacca. "Semantic-based regularization for learning and inference." Artificial Intelligence 244 (2017): 143-165.

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- The main evaluation metric is the **relative improvement** over the base NN accuracy;
- Same experiments are performed over different sizes of the training set.

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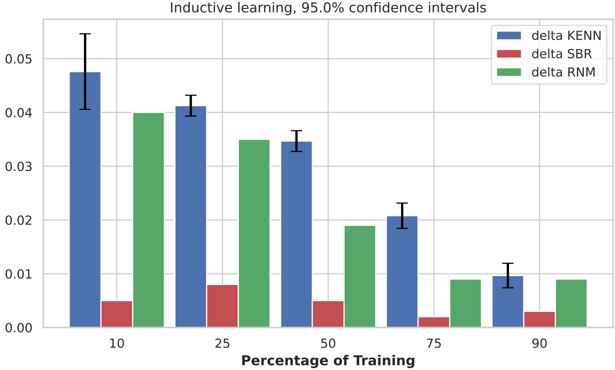
Results


Inductive learning, 95.0% confidence intervals
delta KENN
delta SBR
delta RNM
0.00
0.01
0.02
0.03
0.04
0.05
10
25
50
75
90
Percentage of Training

Results

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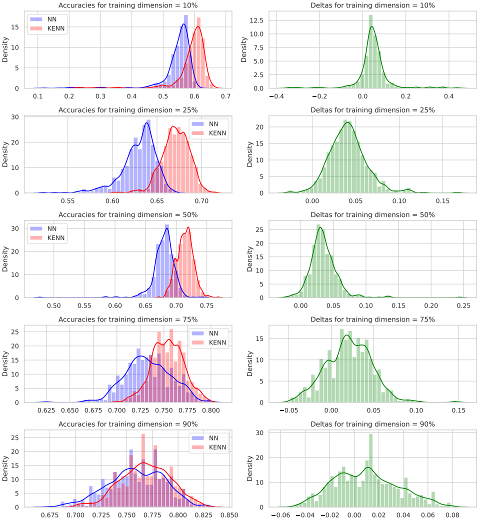
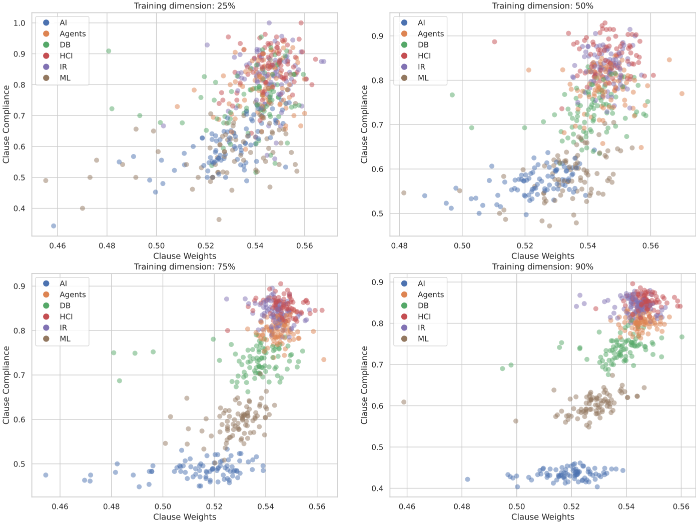


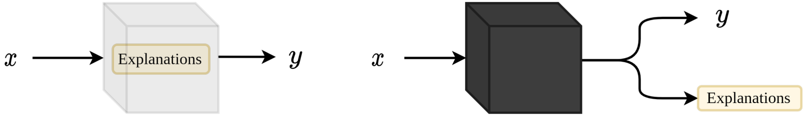
Clause Weights Learning



Explainability

In XAI, two main paradigms for explainability are distinguished:

- **Transparency**
- **Post-hoc explainability**



Explainability in KENN

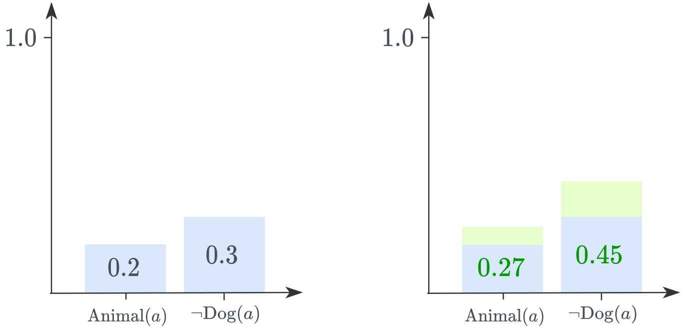
KENN can be considered a **partially transparent** model:

- A KENN layer will always be based on the prediction of a base NN, which will always be an inherently opaque model;
- On the contrary, everything happening inside the KENN layer is transparent;
- The explanations will only regard the knowledge enforcement stage.

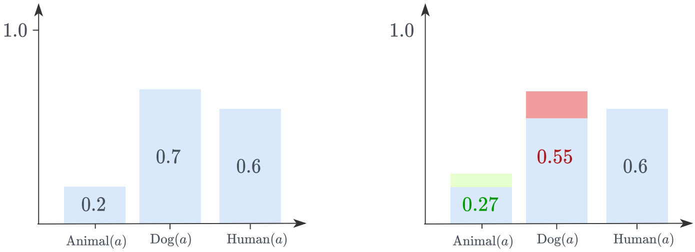
Local explanations from a single clause

$$\neg \, \mathrm{Dog}(a) \vee \mathrm{Animal}(a)$$

$$\neg\,\mathsf{Dog}(a) \lor \mathsf{Animal}(a)$$



$\neg \, \mathsf{Dog}(a) \lor \mathsf{Animal}(a)$



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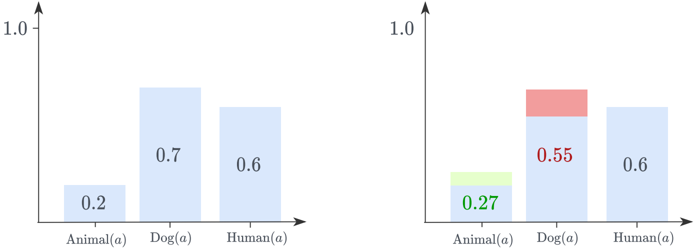

Since the NN was confident that a is not an Animal, the truth value for a being a dog should decrease.

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  - if, and where those clauses provided a positive or negative contribution;
  - if and where there is any conflict between the formulas inside $\mathcal{C}$.

Improvement Score

Given $\mathcal{C} \subseteq \mathcal{K}$, the improvement score quantifies the positive (or negative) contribution of $\mathcal{C}$ for sample x and is defined as follows:

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$IS(x_1, \mathcal{C}) = -1.2$	$IS(x_2, \mathcal{C}) = 5.4$	$IS(x_3, \mathcal{C}) = 1.4$	$IS(x_4, \mathcal{C}) = -3.3$	$IS(x_5, \mathcal{C}) = 0.1$

Evaluation metrics

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$\big\downarrow$ sort

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Evaluation metrics

Disagreement Score

We first define the disagreement vector:

$$DV(x, \mathcal{C}) = \sum_{c \in \mathcal{C}} |\delta_c| - \left| \sum_{c \in \mathcal{C}} \delta_c \right| .$$

Starting from $DV(x, C)$ we can finally define the disagreement score for a specific subset of predicates $\hat{\mathcal{P}} \subseteq \mathcal{P}$:

$$DS(x, \mathcal{C}, \hat{\mathcal{P}}) = \sum_{i \in \hat{\mathcal{P}}} DV(x, \mathcal{C})_i .$$

Conclusions

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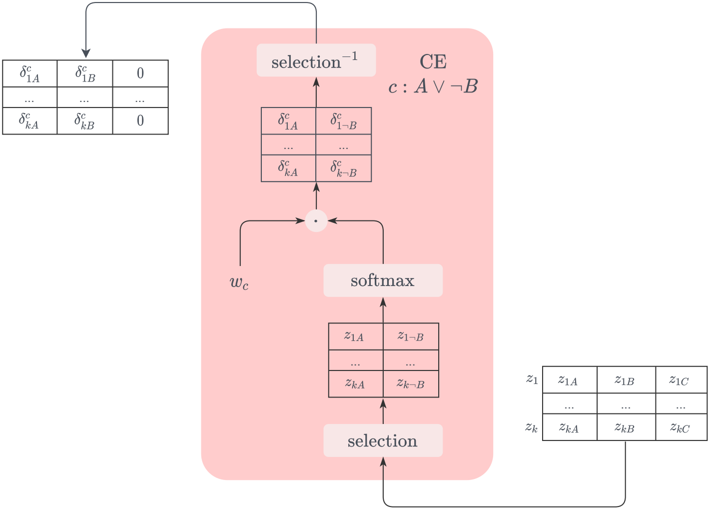
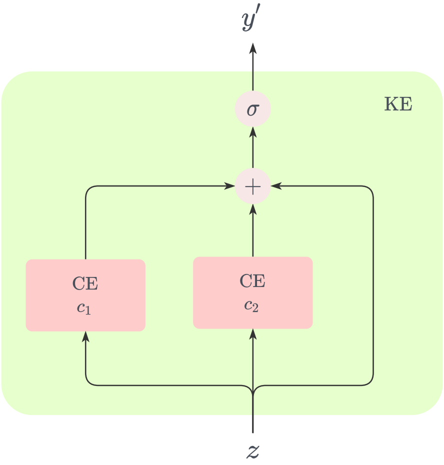
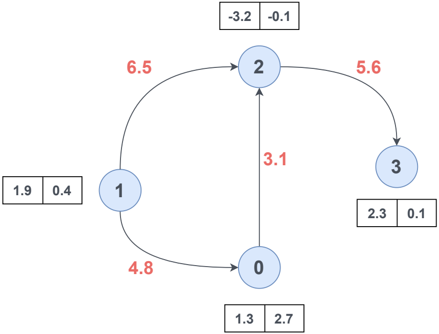
1. Experimental results show that KENN outperforms other NeSy methods for the collective classification task;
2. Further experiments show a correlation between the clause weights and the satisfaction of the clause in the training data;
3. KENN is inherently a transparent NN layer: explanations can be easily extracted in a understandable and human readable form;
4. We proposed two evaluation metrics which can be used for debugging purposes.

Thank you for your attention


selection^{-1}
CE
$c : A \vee \neg B$
δ^c_{1A} δ^c_{1B} 0
... ...
δ^c_{kA} δ^c_{kB} 0
δ^c_{1A} $\delta^c_{1\neg B}$
... ...
δ^c_{kA} $\delta^c_{k\neg B}$
$\cdot$
w_c
softmax
z_{1A} $z_{1\neg B}$
... ...
z_{kA} $z_{k\neg B}$
selection
z_1 z_{1A} z_{1B} z_{1C}
... ...
z_k z_{kA} z_{kB} z_{kC}

Appendix: Knowledge Enhancer





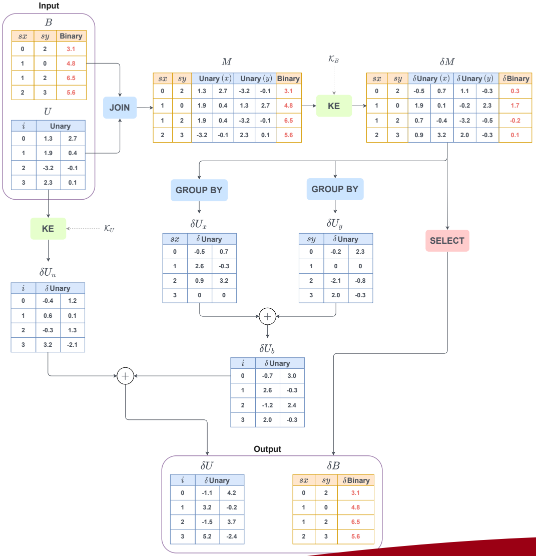
U

i	Unary	
0	1.3	2.7
1	1.9	0.4
2	-3.2	-0.1
3	2.3	0.1

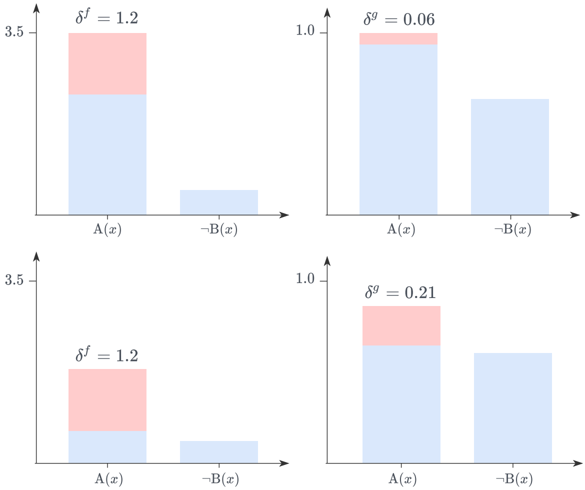
B

sx	sy	Binary
0	2	3.1
1	0	4.8
1	2	6.5
2	3	5.6

Appendix: KENN for relational data



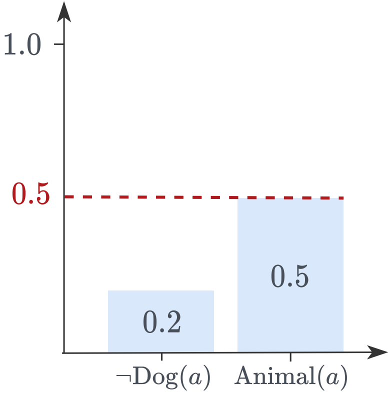
Appendix: preactivations vs activations



Example: truth value of a clause

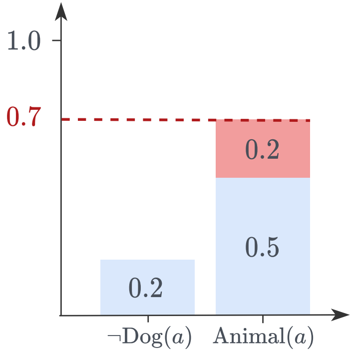
$$z = (0.5, 0.8, 0.3) \xrightarrow[c\,:\,\neg\,\mathrm{Dog}(a)\,\vee\,\mathrm{Animal}(a)]{\text{selection}} z_c = (0.2, 0.5)$$

Example: truth value of a clause



$\perp_{\max}(0.2, 0.5) = \max(0.2, 0.5) = 0.5$

Increasing satisfaction of a single clause



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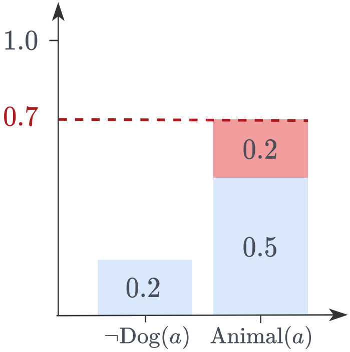

$$\delta_s^{w_c}(z_c) = w_c \cdot \mathrm{softmax}(z_c)$$