Compositional Relational Machines

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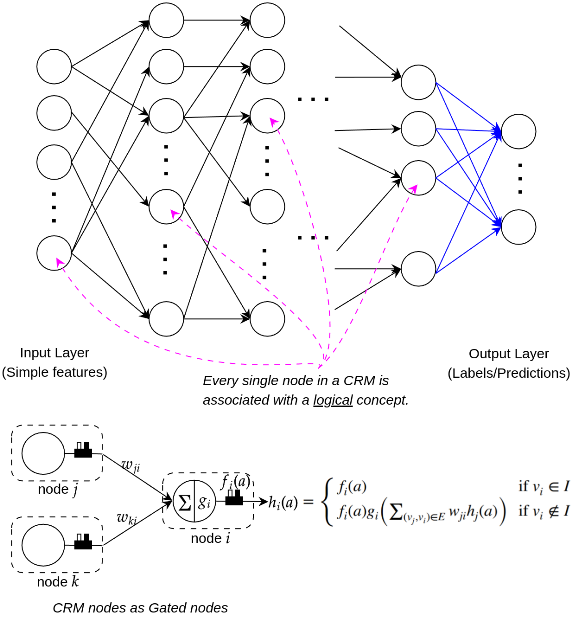


Input Layer
(Simple features)
Every single node in a CRM is associated with a logical concept.
Output Layer
(Labels/Predictions)
node j
node k
node i
w_{ji}
w_{ki}
Σ g_i
$f_i(a)$
$h_i(a) = \begin{cases} f_i(a) & \text{if } v_i \in I \\ f_i(a) g_i\left(\sum_{(v_j,v_i)\in E} w_{ji} h_j(a)\right) & \text{if } v_i \notin I \end{cases}$
CRM nodes as Gated nodes

Relational Features

A relational feature takes a clausal form:

$$C : \forall X \ (p(X) \leftarrow \exists \boldsymbol{Y} \ Body(X, \boldsymbol{Y}))$$

or,

$$C : (p(X) \leftarrow Body(X, \boldsymbol{Y}))$$

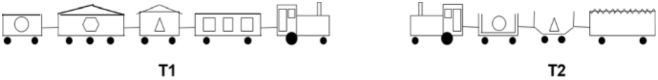
Here,

$$\begin{aligned} p(X) &: \text{Head literal} \\ Body(X, \boldsymbol{Y}) &: \text{Conjunction of body literals} \end{aligned}$$

Assumption: C is not self-recursive. We call C a "feature-clause".

Feature clauses

Let's look at the classic trains problem:



Some feature-clauses for trains:

$$C_1 : p(X) \leftarrow (has\_car(X, Y), short(Y))$$
$$C_2 : p(X) \leftarrow (has\_car(X, Y), short(Y), closed(Y))$$
$$C_3 : p(X) \leftarrow (has\_car(X, Y), has\_car(X, Z), short(Y), closed(Z))$$

The predicates *has_car*/2, *short*/1, *closed*/1, etc. are defined as part of the background knowledge (B) about trains.

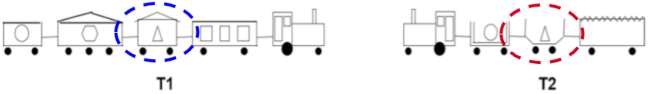
Feature functions

A feature function is defined, for $X = a$ as:

$$f_{C,B}(a) = \begin{cases} 1 & \text{if } B \cup (C\{X/a\}) \models p(a) \\ 0 & \text{otherwise} \end{cases}$$

Simply, for a feature-clause C_i, we refer to the corresponding feature-function as $f_i(X)$.

Example:

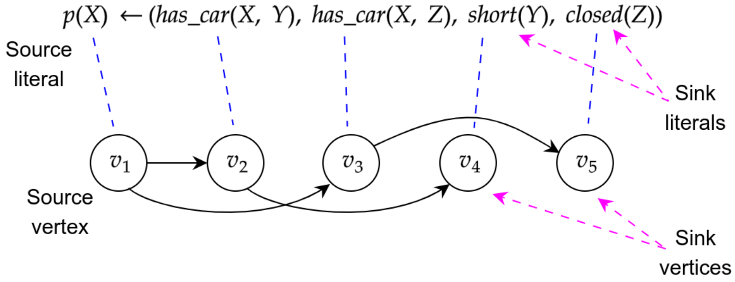


Some feature functions are:

$$f_1(t_1) = 1, f_2(t_1) = 1, f_2(t_2) = 0.$$

Ordered Clause and Clause-dependency Graph

Ordered Clause: We impose an ordering of the literals in a clause. If C is a clause of the form $\lambda_1 \leftarrow \lambda_2, \ldots, \lambda_k$, then the ordered clause is: $\langle C \rangle = \langle \lambda_1, \lambda_2, \ldots, \lambda_k \rangle$.



Simple feature-clause: A feature-clause with a single sink literal [1].

ρ-derivation of feature-clauses (Composition)

Example 1:

$$\begin{aligned} p(X) \leftarrow\ & has\_car(X,\ Y), short(Y), \\ & has\_car(X,\ Z), closed(Z), \\ & Y = Z \end{aligned}$$

$$\uparrow$$

$$\boxed{\rho_1}$$

$$\uparrow$$

$$\begin{aligned} p(X) \leftarrow\ & has\_car(X,\ Y), short(Y), \\ & has\_car(X,\ Z), closed(Z) \end{aligned}$$

$$\uparrow$$

$$\boxed{\rho_2}$$

$$C1: \ p(X) \leftarrow has\_car(X, Y), short(Y) \qquad C2: \ p(X) \leftarrow has\_car(X, Z),\ closed(Z)$$

ρ-derivation of feature-clauses (Composition)

Example 2:

$$p(X) \leftarrow has\_car(X, U),\ has\_car(X, V),\ smaller(U, V),\ has\_car(X, Y), short(Y),\ U = V,\ U = Y$$

$$\uparrow \boxed{\rho_1} \uparrow$$

$$p(X) \leftarrow has\_car(X, U),\ has\_car(X, V),\ smaller(U, V),\ has\_car(X, Y), short(Y),\ U = V$$

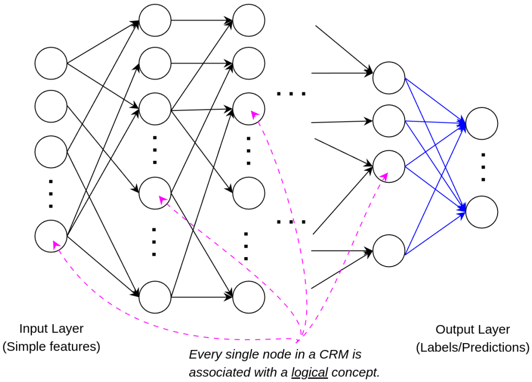
$$\uparrow \boxed{\rho_1} \uparrow$$

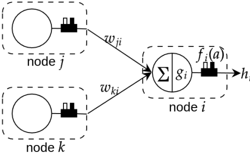
$$p(X) \leftarrow has\_car(X, U),\ has\_car(X, V),\ smaller(U, V),\ has\_car(X, Y), short(Y)$$

$$\uparrow \boxed{\rho_2}$$

$$\mathrm{C1}:\ p(X) \leftarrow has\_car(X, Y), short(Y) \qquad \mathrm{C2}:\ p(X) \leftarrow has\_car(X, U),\ has\_car(X, V),\ smaller(U, V)$$

CRM



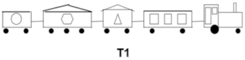


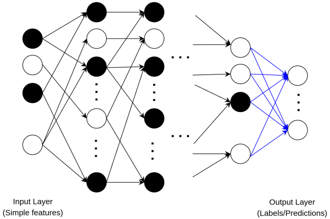
$$h_i(a) = \begin{cases} f_i(a) & \text{if } v_i \in I \\ f_i(a) g_i\left(\sum_{(v_j, v_i) \in E} w_{ji} h_j(a)\right) & \text{if } v_i \notin I \end{cases}$$

CRM nodes as Gated nodes

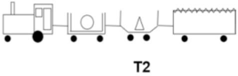
CRM

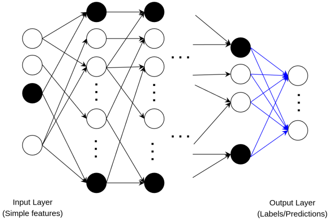
Relational instance 1:





Relational instance 2:





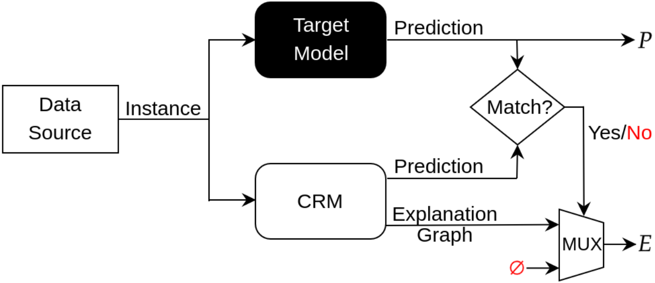
Empirical Evaluation

Experimental setup:

- Machine: 64GB RAM, 12 Intel Xeon CPUs
- Languages: Prolog (Aleph), PyTorch
- Feature-clauses:
  - No. of body literals: 2
  - Min. support: 10
  - Min. precision: 0.5
- Composition depth of CRMs: 3
- Activation function in CRM nodes: `ReLU`
- Optimiser: Adam (learning rate=0.001)
- Expl. Graph: Layer-wise Relevance Propagation (LRP)

Empirical Evaluation

Two aspects: (a) Predictive fidelity, (b) Explanatory fidelity



<ins>Explanation</ins>: Constructed by back-tracing the top activations in each layer of the deep neural network.

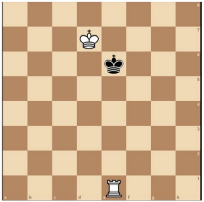
Empirical Evaluation

(A) Synthetic datasets (Trains and Chess)

- Target theory (model) known

Trains

Chess

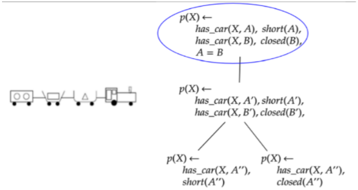


- Results

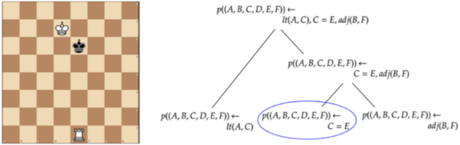
Dataset	Fidelity			
	CRM		Baseline	
	Pred.	Expl.	Pred.	Expl.
Trains	1.0	1.0	0.5	0.4
Chess	1.0	0.9	0.7	0.7

Empirical Evaluation

- Some explanations generated by the CRM:



Train t_1 (With the substitution $\{X/t1\}$)



Board $(d, 7, e, 1, e, 6)$ (With the substitution $\{A/d, B/7, \ldots, F/6\}$)

<u>Target theory:</u> Train X has a car Y and Y is short and closed.

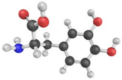
<u>Target theory:</u> White Rook and Black King are on the same file (column).

- CRM also generates "buggy" explanations for the chess problems: Most of these are close to or more-specific than the correct theory.

Empirical Evaluation

(B) Real datasets (drug design: NCI GI50; $n = 10$)

- Target theory is NOT known. BotGNNs are used as the target models [*Dash et al., MLJ, 2022*].

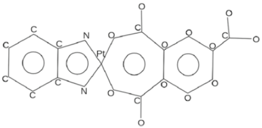
( , Pos)

- Results: Predictive fidelity

Dataset	CRM	Baseline
786_0	0.77	0.53
A498	0.79	0.59
A549_ATCC	0.85	0.63
ACHN	0.73	0.58
BT_549	0.78	0.51
CAKI_1	0.81	0.69
CCRF_CEM	0.82	0.68
COLO_205	0.77	0.53
DLD_1	0.90	1.00
DMS_114	0.89	0.91
Avg.	0.81 (0.05)	0.66 (0.17)

Empirical Evaluation

- An explanation generated by CRM:



$p(X) \leftarrow$
$\quad has\_struc(X, A, B, hetero\_aromatic),$
$\quad lteq(B, 7),$
$\quad has\_struc(X, C, D, amine),$
$\quad lteq(D, 2),$
$\quad has\_struc(X, E, F, oxide),$
$\quad lteq(F, 7)$

$p(X) \leftarrow$
$\quad has\_struc(X, A, B, amine),$
$\quad lteq(B, 2),$
$\quad has\_struc(X, C, D, oxide),$
$\quad lteq(D, 7)$

$p(X) \leftarrow$
$\quad has\_struc(X, A, B, hetero\_aromatic),$
$\quad lteq(B, 7)$

$p(X) \leftarrow$
$\quad has\_struc(X, A, B, amine),$
$\quad lteq(B, 2)$

$p(X) \leftarrow$
$\quad has\_struc(X, A, B, oxide),$
$\quad lteq(B, 7)$

Empirical Evaluation

Some additional predictive comparisons:

Dataset	Predictive accuracy				
	CRM	GNN	DRM (500)	CILP++	Baseline
786_0	0.66 (0.01)	0.69 (0.01)	0.69 (0.01)	0.67 (0.01)	0.55 (0.01)
A498	0.67 (0.01)	0.72 (0.01)	0.70 (0.01)	0.66 (0.01)	0.52 (0.01)
A549_ATCC	0.64 (0.01)	0.67 (0.01)	0.70 (0.01)	0.60 (0.01)	0.51 (0.01)
ACHN	0.64 (0.01)	0.70 (0.01)	0.70 (0.01)	0.64 (0.01)	0.51 (0.01)
BT_549	0.66 (0.01)	0.68 (0.01)	0.70 (0.01)	0.65 (0.01)	0.53 (0.01)
CAKI_1	0.63 (0.01)	0.68 (0.01)	0.66 (0.01)	0.64 (0.01)	0.54 (0.01)
CCRF_CEM	0.65 (0.01)	0.71 (0.01)	0.71 (0.01)	0.68 (0.01)	0.63 (0.01)
COLO_205	0.60 (0.01)	0.69 (0.01)	0.67 (0.01)	0.66 (0.01)	0.56 (0.01)
DLD_1	0.69 (0.02)	0.69 (0.02)	0.70 (0.02)	0.72 (0.02)	0.69 (0.02)
DMS_114	0.68 (0.02)	0.74 (0.02)	0.75 (0.02)	0.75 (0.02)	0.76 (0.02)

GNN: Dash et al., MLJ, 2022.
DRM: Dash et al., ICANN, 2019.

CILP++: Franca et al., MLJ, 2014.

Concluding Remarks

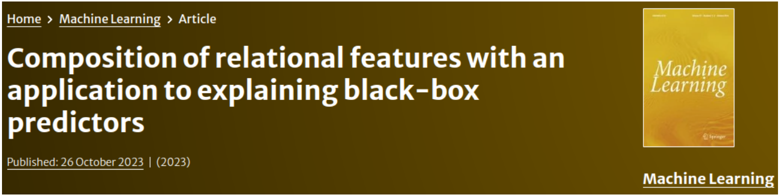
We make 3 contributions in this work:

- Conceptual: Provide conceptual basis of relational features, development of composition operators, and prove their completeness.
- Implementation: Use the concepts to construct a "explanable" deep neural network, called CRM in which each neuron has an associated logical concept.
- Application: Demonstrate predictive and explanatory potential of CRMs.

We are currently working on:

- CRMs as high-quality standalone predictors;
- Fast learning of large-CRMs for real-world problems.

Thank you!



Full Paper: Machine Learning, 2023

Code: `https://github.com/tirtharajdash/CRM`

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