

Composition of Relational Features with an Application to Explaining Black-Box Predictors

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Abstract Three key strengths of relational machine learning programs like those developed in Inductive Logic Programming (ILP) are: (1) The use of an expressive subset of first-order logic that allows models that capture complex relationships amongst data instances; (2) The use of domain-specific relations to guide the construction of models; and (3) The models constructed are human-readable, which is often one step closer to being human-understandable. The price for these advantages is that ILP-like methods have not been able to capitalise fully on the rapid hardware, software and algorithmic developments fuelling current developments in deep neural networks. In this paper, we treat relational features as functions and use the notion of generalised composition of functions to derive complex functions from simpler ones. Motivated by the work of McCreath and Sharma (McCreath and Sharma, 1998a; McCreath, 1999) we formulate the notion of a set of M-simple features in a *mode language* M and identify two composition operators (ρ_1 and ρ_2) from which all possible complex features can be derived. We use these results to implement a form of “explainable neural network” called Compositional Relational Machines, or CRMs. CRMs are labelled directed-acyclic graphs. The vertex-label for any vertex j in the CRM contains a feature-function f_j and an continuous activation function g_j . If j is a “non-input” vertex, then f_j is the composition of features associated with vertices in the direct predecessors of j . Our focus is on CRMs in which input vertices (those without any direct predecessors) all have M-simple features in their vertex-labels. We provide a randomised procedure for constructing the structure of such CRMs, and a procedure for esti-

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mating the parameters (the w_{ij} 's) using back-propagation and stochastic gradient descent. Using a notion of explanations based on the compositional structure of features in a CRM, we provide empirical evidence on synthetic data of the ability to identify appropriate explanations; and demonstrate the use of CRMs as 'explanation machines' for black-box models that do not provide explanations for their predictions.

Keywords Explainable Neural Networks, Relational Features, Inductive Logic Programming, Neuro-Symbolic Learning

1 Introduction

It has long been understood that choice of representation can make a significant difference to the efficacy of machine-based induction. A seminal paper by [Quinlan \(1979\)](#) demonstrates the increasing complexity of models constructed for a series of problems defined on a chess endgame, using a fixed representation consisting of 25 features (called properties in the paper). These features were identified manually (by him), and captured relations between the pieces and their locations in the endgame. Commenting on the increasing complexity of the models, he concludes:

“This immediately raises the question of whether these and other properties used in the study were appropriate. The answer is that they were probably not; it seems likely that a chess expert could develop more pertinent attributes . . . If the expert does his job well the induction problem is simplified; if a non-expert undertakes the definition of properties (as was the case here) the converse is true.”

Although Quinlan assumed the representation would be identified manually, the possibility of automatic identification of an appropriate representation was already apparent to [Amarel \(1968\)](#) a decade earlier: “An understanding of the relationship between problem formulation and problem solving efficiency is a prerequisite for the design of procedures that can automatically choose the most ‘appropriate’ representation of a problem (they can find a ‘point of view’ of the problem that maximally simplifies the process of finding a solution)”. In fact, by ‘choose’ what is probably meant is ‘construct’, if we are to avoid kicking Feigenbaum’s famous knowledge-acquisition bottleneck down the road from extracting models to extracting representations.

It has also been known that one way to construct representations automatically is through the use of neural networks. But extraction and re-use of these representations for multiple tasks have become substantially more common only recently, with the routine availability of specialised hardware. This has allowed the construction of networks in which adding layers of computation is assumed to result in increasingly complex representations (10s of layers are now common, but 100s are also within computational range). In principle, while a single additional layer is all that is needed (due to the Universal approximation theorems for neural networks ([Hornik et al., 1989](#); [Cybenko, 1989](#); [Pinkus, 1999](#))), it is thought that the main benefit of the additional layers lies in constructing representations that are multiple levels of abstractions, allowing more efficient modelling. There are however 3 important issues that have surfaced: (1) Automatic construction of abstractions in this way requires a lot of data, often 100s of 1000s of examples;

(2) The kinds of neural networks used for constructing abstractions depend on the type of data. For example, certain kinds of networks are used for text, others for images and so on: there is apparently no single approach for representation learning that can automatically adjust to the data type; and (3) The internal representations of data are opaque to human-readability, making it difficult to achieve the kind of understanding identified by Amarel.

Recent results with neural-based learning suggest the possibility of viewing representation learning as program synthesis. Of particular interest are methods like Dreamcoder (Ellis et al., 2021) that automatically construct programs for generating data, given some manually identified primitive functions represented in a symbolic form (Dreamcoder uses λ -expressions for the primitive functions). A combination of generative and discriminative network models is used to direct the hierarchical construction of higher-level functions by compositions of lower-level ones. Compositions are generated and assessed for utility in interleaved phases of generate-and-test (called “Dream” and “Wake” phases), until the neural-machinery arrives at a small program, consisting the sequential composition of primitive- and invented functions. The final result is some approximation to the Bayesian MAP program for generating the data provided, assuming a prior preference for small programs. There are good reasons to look at this form of program-synthesis as a mechanism for automated representation learning: (a) Empirical results with programs like Dreamcoder show that it is possible to identify programs with small numbers of examples (the need for large numbers of examples is side-stepped by an internal mechanism for generating data in the Dream phase); (b) In principle, the symbolic language adopted for primitive functions (λ -expressions) and the mechanism of function composition is sufficiently expressive for constructing programs for data of any type; (c) The intermediate representations have clearly defined interpretations, based on functional composition. There are however some shortcomings. First, the primitive functions have to be manually identified. Secondly, the construction of new representations requires a combinatorial discrete search that is usually less efficient than those based on continuous-valued optimisation. Thirdly, the representation of λ -expressions, although mathematically powerful, can prove daunting as a language for encoding domain-knowledge or for interpreting the results. Finally, the Dreamcoder-like approach for representation learning has only been demonstrated on very simple generative tasks of a geometric nature.

In this paper, we partially address these shortcomings by drawing on, and extending some results on representation developed in the area of Inductive Logic Programming (ILP). The main contributions of this paper are as follows:

- (a) **Conceptual** We develop the conceptual basis for a class of ‘simple’ relational features using a well-known specification language in ILP (mode-declarations). Additionally, we develop composition operators for deriving more complex relational features, and prove some completeness properties that apply to the use of the operators;
- (b) **Implementation** We use the concepts developed to specify and implement a form of neural network called Compositional Relational Machines, or CRMs. An important feature of these networks is that each node is identified with a clearly defined relational feature. This allows us to associate structured ‘explanations’ with each node in the network;

(c) **Application** We present empirical results on 2 synthetic data that demonstrate the ability of CRMs to construct appropriate explanations; and results on using CRMs to act as ‘explanation machines’ for a state-of-the-art black-box predictor on 10 real-world datasets.

The rest of the paper is organised as follows: In [Section 2](#) we provide a conceptual framework for relational features and their compositions. We use this framework to implement CRMs in [Section 3](#). We provide empirical evaluation of CRMs as explanation machines in [Section 4](#). Related work of immediate relevance to this paper are presented in [Section 5](#). Concluding remarks are in [Section 6](#). The paper has several appendices that act as supporting material.

2 Relational Features and their Composition

In this paper, we are principally interested in specifying and combining *relational features*. For us, a k -ary relational feature will be a function with k terms as arguments. We will specify such a feature by $f : \mathcal{A}_1 \times \mathcal{A}_2 \times \dots \times \mathcal{A}_k \rightarrow \mathcal{B}$, where $\mathcal{A}_1, \mathcal{A}_2, \dots, \mathcal{A}_k, \mathcal{B}$ are some sets. For the most part in this paper, we will restrict ourselves to $k = 1$ and $\mathcal{B} = \{0, 1\}$, although the results here can be generalised. We will denote this setting as $f : \mathcal{A} \rightarrow \{0, 1\}$, for some set \mathcal{A} . A relational feature is defined in 2 steps. First, we represent the conditions under which the feature takes the value 1 using a clause of the form:¹

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

or, simply:

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

to mean the quantification as shown earlier. Here, the fixed predicate symbol $p(X)$ is called the *head* of C , and $\text{Body}(X, \cdot)$ —the *body* of clause C —is a conjunction of literals l_2, l_3, \dots, l_k containing some existentially quantified variables collectively represented here as \mathbf{Y} . We assume the body of C does not contain a literal of the form $p(\cdot)$ (that is, C is not self-recursive) and call clauses like these *feature-clauses*.² The clausal representation does not tell us how to obtain the value (0 or 1) of the feature itself for any $X = a$. For this we assume an additional set of clausal formulae B (“background”) which does not contain any occurrence of the predicate-symbol $p/1$ and define the *feature-function* associated with the clause C as follows. Let θ_a denote the substitution $\{X/a\}$ for $a \in \mathcal{A}$. Then:

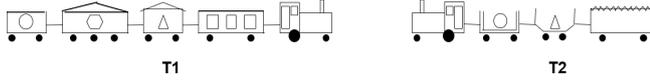
$$f_{C,B}(a) = \begin{cases} 1 & \text{if } B \cup (C\theta_a) \models p(a) \\ 0 & \text{otherwise} \end{cases}$$

¹ See [Appendix A](#) for a summary of logical syntax and concepts needed for this paper. We assume a logic with equality ($=/2$).

² This clause is equivalent to the disjunct $l_1 \vee \neg l_2 \vee \dots \vee \neg l_k$. It will sometimes also be written as the set of literals $\{l_1, \neg l_2, \dots, \neg l_k\}$. The literals can contain predicate symbols representing relations: hence the term “relational”. The requirement that all feature-clauses have the same predicate symbol $p/1$ in the head is a convenience that will be helpful in what follows. It may be helpful to read the symbol $p/1$ as a proposition defined on X .

In general, given feature-clauses C_1, C_2, \dots, C_j we will write $f_{C_i, B}(\cdot)$ as $f_i(\cdot)$ ($1 \leq i \leq j$), when the context is obvious. If $f_i(x) = 1$ for $x = a$, we will say “the feature f_i is true for $x = a$ ”.

Example 1 An early example of a problem requiring relational features was the problem of discriminating amongst goods trains (Michalski, 1980), which has subsequently served as a touchstone for the construction and use of relational features (see for example, the “East-West Challenge” (Michie et al., 1994)). In its original formulation, the task is to distinguish eastbound trains from westbound ones using properties of the carriages and their loads (the engine’s properties are not used), using pictorial descriptions like these (**T1** is eastbound and **T2** is westbound):



Examples of feature-clauses are:

$$\begin{aligned} C_1 &: p(X) \leftarrow (has_car(X, Y), short(Y)) \\ C_2 &: p(X) \leftarrow (has_car(X, Y), closed(Y)) \\ C_3 &: p(X) \leftarrow (has_car(X, Y), short(Y), closed(Y)) \\ C_4 &: p(X) \leftarrow (has_car(X, Y), has_car(X, Z), short(Y), closed(Z)) \end{aligned}$$

Here, we will assume that predicates like $has_car/2$, $short/1$, $closed/1$, $long/1$, $has_load/3$, etc., are defined as part of the background B , and capture the situation shown diagrammatically. That is,

$$\begin{aligned} B = \{ & has_car(t1, c1.1), has_car(t1, c1.2), \dots \\ & long(c1.1), closed(c1.1), has_load(c1.1, square, 3), \dots \\ & has_car(t2, c2.1), has_car(t2, c2.2), \dots \}. \end{aligned}$$

Then the corresponding feature-function values are:

$$\begin{aligned} f_{C_1, B}(t1) &= f_1(t1) = 1; f_1(t2) = 1; \\ f_{C_2, B}(t1) &= f_2(t1) = 1; f_2(t2) = 1; \\ f_{C_3, B}(t1) &= f_3(t1) = 1; f_3(t2) = 0; \\ f_{C_4, B}(t1) &= f_4(t1) = 1; f_4(t2) = 1. \end{aligned}$$

Although not used in this paper, feature-clauses need not be restricted to descriptions of single objects. An example of a feature-clause about train-pairs for example is:

$$C_5 : p((X1, X2)) \leftarrow (has_length(X1, L1), has_length(X2, L2), L1 \geq L2).$$

(The corresponding feature-function will then also be defined over pairs of objects.)

We intend to describe a mechanism for automatically enumerating feature-clauses like these, as well as mechanisms for combining simpler feature-clauses to give more complex ones. We start with some preliminary definitions needed.

2.1 Preliminaries

It will be necessary for what follows to assume an ordering over literals in a feature-clause.

Definition 1 (Ordered Clause) Let C be a feature-clause with 1 head literal and $k - 1$ body literals. We assume an ordering over the literals that maps the set of literals in the clause to a sequence $\langle C \rangle = \langle \lambda_1, \lambda_2, \lambda_3, \dots, \lambda_k \rangle$, where λ_1 is the head literal and the $\lambda_2, \dots, \lambda_k$ are literals in the body of the feature-clause.

Definition 2 (Ordered Subclause) Let $\langle C \rangle = \langle \lambda_1, \lambda_2, \lambda_3, \dots, \lambda_k \rangle$ be an ordered clause. Then an ordered subclause $\langle C' \rangle$ is any clause $\langle \lambda'_1, \lambda'_2, \dots, \lambda'_j \rangle$ where $\lambda'_1 = \lambda_1$ and $\langle \lambda'_2, \dots, \lambda'_j \rangle$ is a sub-sequence of $\langle \lambda_2, \dots, \lambda_k \rangle$.

From now on, we will use the term “ordered clause” to emphasise an ordering on the literals is assumed. For simplicity, we will assume that the intended ordering is reflected in a left-to-right reading of the clause. Given an ordered clause, it is possible to recover trivially the set of literals constituting the feature-clause. We use $Set(\langle C \rangle) = Set(\langle \lambda_1, \dots, \lambda_k \rangle) = \{\lambda_1, \neg\lambda_2, \dots, \neg\lambda_k\}$. Usually, we will further use the set-notation interchangeably with $\lambda_1 \leftarrow \lambda_2, \dots, \lambda_k$ to denote the feature-clause C .

2.2 Feature-Clauses in a Mode Language

The field of Inductive Logic Programming (ILP) has extensively used the idea of a *mode language* to specify a set of acceptable clauses.³ We use this approach here to specify the set of feature-clauses. We provide details of mode-declarations and the definition of a mode-language based on such declarations in [Appendix B](#). We need the following concepts from the Appendix: (a) type-names and their definitions; (b) set of mode declarations and clauses in the mode-language; (c) input term of type γ in some literal; and (d) output term of type γ in some literal. With these notions in place, we will require the mode-language for specifying feature-clauses to satisfy the following constraints:

- MC1. The set of modes M contains exactly one mode-declaration for every predicate occurring in a feature-clause;
- MC2. All modes in M for predicates which appear in the body of a feature-clause contain at least 1 “input” argument; and
- MC3. If $\mu = modeh(p) \in M$, then p is an unary predicate and $modeb(p)$ does not occur in M .

These constraints extend to p/k if the features are defined over a product-space. We note that the restriction MC1 is more strict than the mode language allowed by ILP implementations like Progol ([Muggleton, 1995](#)) or Aleph ([Srinivasan, 2001](#)). Effectively, it prevents a predicate being called in multiple ways, which is allowed

³ The notion of associating *modes* for predicates has its origins in typed logics and functional programming. Even in ILP, modes are not the only way of specifying acceptable sets of clauses; they are used here as they provide a straightforward way of specifying the notion of *simple features* that follows in a later section.

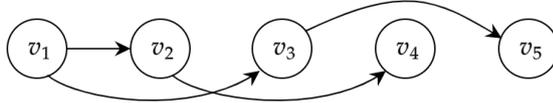
in logic programming languages like Prolog. Here, to achieve the same effect, we will need to use different predicate symbols for each mode of call. Now, variables (and ground-terms) are constrained by the type-restrictions. Given a set of mode-declarations, feature-clauses in the mode-language are therefore more constrained than we have presented thus far.⁴ Henceforth we will use M is a set of “constrained mode-declarations” to mean that M satisfies MC1–MC3.

The categorisation of variables in a literal as being inputs or outputs allows a natural association of an ordered clause with a graph.

Definition 3 (Clause Dependency-Graph) Let M be a set of constrained mode-declarations and T be a set of type definitions for the type-names in M . Let $\langle C \rangle$ be an ordered clause $(\lambda_1 \leftarrow \lambda_2, \dots, \lambda_k)$ in the mode-language $\mathcal{L}_{M,T}$ (see [Appendix B](#)). The clause dependency-graph $G_M(\langle C \rangle)$ associated with $\langle C \rangle$ is the labelled directed graph (V, E, ψ) defined as follows:

- $V = \{v_1, v_2, \dots, v_k\}$;
- for each i , $\psi(v_i) = \lambda_i$;
- $(v_i, v_j) \in E$ iff:
 - $i = 1, 2 \leq j \leq k$, and there exists a variable X such that λ_i has X as an input variable of type γ in M and λ_j has X as an input variable of type γ in M ; or
 - $1 < i < j$, λ_i has an output variable X of type γ in M and X occurs in λ_j as an input variable of type γ in M .

Example 2 Let us assume the set of mode-declarations M contain at least the following: $\{ \text{modeh}(p(+train)), \text{modeb}(\text{has_car}(+train, -car)), \text{modeb}(\text{short}(+car)), \text{modeb}(\text{closed}(+car)) \}$ where $train$ and car are type-names, with definitions in T . The ordered clause $p(X) \leftarrow (\text{has_car}(X, Y), \text{has_car}(X, Z), \text{short}(Y), \text{closed}(Z))$ is in the mode-language $\mathcal{L}_{M,T}$. The clause dependency-graph for this ordered clause is given below and ψ is defined as follows: $\psi(v_1) = p(X)$, $\psi(v_2) = \text{has_car}(X, Y)$, $\psi(v_3) = \text{has_car}(X, Z)$, $\psi(v_4) = \text{short}(Y)$, $\psi(v_5) = \text{closed}(Z)$.



Remark 1 We note the following about the clause dependency-graph:

- The clause dependency-graph for an ordered clause is a directed acyclic graph. This is evident from the definition: if $(v_i, v_j) \in E$ then $i < j$.
- The clause dependency-graph for an ordered clause is unique.

Given a set of modes M we introduce the notion M -simple clauses in a manner similar to ([McCreath, 1999](#)).

⁴ That is, a feature-clause of the form $\forall X(p(X) \leftarrow \exists \mathbf{Y} \text{Body}(X, \mathbf{Y}))$ should be read as $\forall X \in \Lambda [p(X) \leftarrow \exists \mathbf{Y} \in \mathbf{\Lambda} \text{Body}(X, \mathbf{Y})]$ where Λ and $\mathbf{\Lambda}$ informally denote the sorts of X and the \mathbf{Y} 's. For simplicity, we will not refer to the type-restrictions on variables and terms when we say that a feature-clause is in a mode-language. The restrictions are taken as understood, and to be enforced during inference.

Definition 4 (Source- and Sink- Vertices and Literals) Given a set of constrained mode-declarations M , type-definitions T , and an ordered clause $\langle C \rangle$ in $\mathcal{L}_{M,T}$, let $G_M(\langle C \rangle) = (V, E, \psi)$ be the clause dependency-graph of $\langle C \rangle$. A vertex $v \in V$ is said to be a sink vertex if there is no outgoing edge from v . The corresponding literal, $\psi(v)$, is called a sink literal. A vertex $v \in V$ is said to be a source vertex if there is no incoming edge to v . The corresponding literal, $\psi(v)$, is called a source literal.

Example 3 The clause in [Example 2](#) has one source vertex v_1 and two sink vertices: v_4 and v_5 . Correspondingly, there is one source literal $p(X)$, and two sink literals: $short(Y)$, $closed(Y)$.

Remark 2 Let M satisfy MC1–MC3. Then:

- The clause dependency-graph of any ordered clause in $\mathcal{L}_{M,T}$ will have exactly 1 source-vertex v_1 (and exactly 1 source-literal).
- For every vertex v in the clause dependency-graph, there exists at least one path from v_1 to v . Also the union of all the paths from v_1 to v will be a directed acyclic graph and this is unique. We will denote this directed acyclic graph by $DAG_{\langle C \rangle}(v)$.
- For every vertex v in the clause dependency-graph, either v will be a sink vertex or it will be on a path from the source vertex (v_1) to a sink vertex.

Of these the third observation is not obvious. Suppose a vertex v is not a sink vertex. Then it will have at least one outgoing edge from it. By following outgoing edges forward, we will end in a sink vertex. If $v \neq v_1$, then there is at least one incoming edge to v . By following incoming edges backward, we will end in a source vertex. Since there is only one source vertex, this will be v_1 . So v will be a sink vertex or it will be on a path from v_1 to a sink vertex.

Definition 5 (M-Simple Feature-Clause) Given a set of constrained mode-declarations M , type-definitions T , an ordered feature-clause $\langle C \rangle$ in the mode-language $\mathcal{L}_{M,T}$ is said to be an M-simple feature-clause, or simply a M-simple clause iff the clause dependency-graph $G_M(\langle C \rangle)$ has exactly one sink literal.

Example 4 We continue [Example 2](#). The ordered clauses $p(X) \leftarrow has_car(X, Y)$, $short(Y)$ and $p(X) \leftarrow has_car(X, Y)$ are M-simple clauses as both have only one sink literal $short(Y)$ and $has_car(X, Y)$ respectively. The ordered clause $p(X) \leftarrow has_car(X, Y), short(Y), closed(Y)$ is not a M-simple clause as it has two sink literals $short(Y)$ and $closed(Y)$.

Definition 6 (Maximal M-simple subclause) Given a set of constrained mode-declarations M , type-definitions T , an ordered clause $\langle C' \rangle$ in the mode-language $\mathcal{L}_{M,T}$ is said to be a maximal M-simple subclause of an ordered clause $\langle C \rangle$ in $\mathcal{L}_{M,T}$ iff: (a) $\langle C' \rangle$ is an ordered subclause of $\langle C \rangle$; and (b) there is an isomorphism from the clause dependency-graph $G_M(\langle C' \rangle)$ to $DAG_{\langle C \rangle}(v)$ for some sink vertex v in $G_M(\langle C \rangle)$.

Example 5 Continuing [Example 2](#), the ordered clause $p(X) \leftarrow has_car(X, Y), short(Y)$ is a maximal M-simple subclause of $p(X) \leftarrow has_car(X, Y), short(Y), closed(Y)$. The ordered clause $p(X) \leftarrow has_car(X, Y)$ is not a maximal M-simple subclause of $p(X) \leftarrow has_car(X, Y), short(Y), closed(Y)$.

Definition 7 (Basis) Let M be a set of constrained mode-declarations, T be a set of type-definitions, $\langle C \rangle$ be an ordered clause in the mode-language $\mathcal{L}_{M,T}$. Then $Basis(\langle C \rangle) = \{ \langle C' \rangle \mid \langle C' \rangle \text{ is a maximal } M\text{-simple subclause of } \langle C \rangle \}$.

Example 6 The basis for $p(X) \leftarrow has_car(X, Y), has_car(X, Z), short(Y), closed(Z)$ is $\{p(X) \leftarrow has_car(X, Y), short(Y), p(X) \leftarrow has_car(X, Z), closed(Z)\}$.

Remark 3 For given an ordered clause C in $\mathcal{L}_{M,T}$, $Basis(\langle C \rangle)$ is unique. Moreover, if the number of sink vertices in the clause dependency-graph of $\langle C \rangle$ is k , then $|Basis(\langle C \rangle)| = k$.

Lemma 1 (Basis Lemma) Let M be a set of constrained mode-declarations, T be a set of type-definitions. Let $\langle C \rangle$ be an ordered clause in the mode-language $\mathcal{L}_{M,T}$ with k sink-literals. If $Basis(\langle C \rangle) = \{\langle S_1 \rangle, \langle S_2 \rangle, \dots, \langle S_k \rangle\}$ then $\bigcup_{i=1}^k S_i = C$.

Proof Let $G_M(\langle C \rangle) = (V, E, \psi)$ be the clause dependency-graph for the ordered clause $\langle C \rangle$ and $Basis(\langle C \rangle) = \{\langle S_1 \rangle, \langle S_2 \rangle, \dots, \langle S_k \rangle\}$. We prove $\bigcup_{i=1}^k S_i \subseteq C$ and $C \subseteq \bigcup_{i=1}^k S_i$. We consider first $\bigcup_{i=1}^k S_i \subseteq C$. Assume the contrary. That is, there exists some $l \in \bigcup_{i=1}^k S_i$ but $l \notin C$. Since l is a literal in $\bigcup_{j=1}^k S_j$, then $l \in S_j$ for some j . Since every $\langle S_j \rangle$ is an ordered subclause of $\langle C \rangle$, by definition every literal in S_j occurs in C . Therefore $l \in C$ which is a contradiction.

Next we consider $C \subseteq \bigcup_{i=1}^k S_i$. Let l be a literal in C . There exists a vertex v_j in the clause dependency-graph $G_M(\langle C \rangle)$ such that $\psi(v_j) = l$. Either v_j is a sink vertex or not a sink vertex in $G_M(\langle C \rangle)$. If it is a sink vertex, then there exists a maximal M -simple subclause $\langle S_j \rangle$ with v_j as a sink vertex. Hence l is in S_j . If v_j is not a sink vertex, then it will be on the path from v_1 to some sink vertex v_m (see [Remark 2](#)). Then the directed acyclic sub-graph $DAG_{\langle C \rangle}(v_m)$ will have this vertex v_j . Since v_m is a sink vertex, there exists a maximal M -simple subclause $\langle S_m \rangle$ with v_m as a sink vertex and there is an isomorphism between the clause dependency-graph $G_M(\langle S_m \rangle)$ and $DAG_{\langle C \rangle}(v_m)$. Hence $l \in S_m$. So in both cases l is in $\bigcup_{i=1}^k S_i$. Hence $C \subseteq \bigcup_{i=1}^k S_i$. ■

Let M be a set of constrained mode-declarations, and T be a set of type definitions. Let M' be M extended with an additional mode-declarations allowing body-literals of the form $+\gamma = +\gamma$ (that is, M' allows equality between variables of the same type γ , if this is not already allowed in M); the definition of $=/2$ is provided by axioms of the equality logic. For more details see [Appendix A](#). We note that if the ordered clause $\langle C \rangle$ is in $\mathcal{L}_{M,T}$, then $\langle C \rangle$ is in $\mathcal{L}_{M',T}$.

We define operators ρ_1, ρ_2 as follows:

1. Let $\langle C \rangle$ be in $\mathcal{L}_{M',T}$ s.t. $\langle C \rangle : p(X) \leftarrow Body(X, \mathbf{Y})$. Then $\rho_1(\langle C \rangle) = \{ p(X) \leftarrow Body(X, \mathbf{Y}), Y_1 = Y_2 \mid Y_1, Y_2 \text{ are output variables of the same type in } Body \}$;
2. Let $\langle C_1 \rangle, \langle C_2 \rangle$ be in $\mathcal{L}_{M',T}$ s.t. $\langle C_1 \rangle : p(X) \leftarrow Body_1(X, \mathbf{Y}_1)$ and $\langle C_2 \rangle : p(X) \leftarrow Body_2(X, \mathbf{Y}_2)$. Then $\rho_2(\langle C_1 \rangle, \langle C_2 \rangle) = \{ p(X) \leftarrow Body_1(X, \mathbf{Y}_1), Body_2(X, \mathbf{Y}_2) \}$

These operators allows us to establish a link between the derivability of clauses in $\mathcal{L}_{M',T}$ using $\{\rho_1, \rho_2\}$ and clauses in $\mathcal{L}_{M,T}$.

Definition 8 (Derivation of Feature-Clauses) Let M be a set of mode-declarations, and M' be an extension of M as above. Let T be a set of type-definitions, and

$\Omega \subseteq \{\rho_1, \rho_2\}$. Let Φ be a set of feature-clauses in $\mathcal{L}_{M',T}$. A sequence of feature-clauses $\langle C_1 \rangle, \langle C_2 \rangle, \dots, \langle C_n \rangle$ is said to be a derivation sequence of $\langle C_n \rangle$ from Φ using Ω iff each clause $\langle C_i \rangle$ in the sequence is either : (a) an instance of an element of Φ such that no variables other than X occur earlier in this sequence; or (b) an element of the set $\rho_1(\langle C_j \rangle)$ ($j < i$), if $\rho_1 \in \Omega$; or (c) an element of the set $\rho_2(\langle C_j \rangle, \langle C_k \rangle)$ ($j, k < i$), if $\rho_2 \in \Omega$. We will say $\langle C_n \rangle$ is derivable from Φ using Ω if there exists a derivation sequence of $\langle C_n \rangle$ from Φ using Ω .

Example 7 Let us assume the set of mode-declarations M contain the following:

$$\{ \text{modeh}(p(+train)), \text{modeb}(\text{has_car}(+train, -car)), \text{modeb}(\text{short}(+car)), \\ \text{modeb}(\text{closed}(+car)), \text{modeb}(\text{smaller}(+car, +car)) \},$$

where *train* and *car* are type-names, with definitions in T . Here is a derivation sequence of

$$p(X) \leftarrow \text{has_car}(X, U), \text{has_car}(X, V), \text{smaller}(U, V), U = V, \\ \text{has_car}(X, Y), \text{short}(Y), U = Y$$

from

$$\{ p(X) \leftarrow \text{has_car}(X, Y), \text{short}(Y), \\ p(X) \leftarrow \text{has_car}(X, U), \text{has_car}(X, V), \text{smaller}(U, V) \}$$

using $\{\rho_1, \rho_2\}$.

1	$p(X) \leftarrow \text{has_car}(X, U), \text{has_car}(X, V), \text{smaller}(U, V)$	Given
2	$p(X) \leftarrow \text{has_car}(X, U), \text{has_car}(X, V), \text{smaller}(U, V), U = V$	$1, \rho_1, U, V$
3	$p(X) \leftarrow \text{has_car}(X, Y), \text{short}(Y)$	Given
4	$p(X) \leftarrow \text{has_car}(X, U), \text{has_car}(X, V), \text{smaller}(U, V), U = V, \\ \text{has_car}(X, Y), \text{short}(Y)$	$2, 3, \rho_2$
5	$p(X) \leftarrow \text{has_car}(X, U), \text{has_car}(X, V), \text{smaller}(U, V), U = V, \\ \text{has_car}(X, Y), \text{short}(Y), U = Y$	$4, \rho_1, U, Y$

It is useful to define the notion of a ρ -derivation graph from a set of feature-clauses Φ .

Definition 9 (ρ -derivation graph given Φ) Let $\gamma = (V, E, \phi)$ be a labelled DAG with vertices V , edges E and vertex-labelling function ϕ . Let $Pred(v)$ denote the set of immediate predecessors of any $v \in V$. Let \mathcal{F}_M be a set of feature-clauses given modes M and $I \subseteq \mathcal{F}_M$. Let Φ be a set of feature-clauses in $\mathcal{L}_{M',T}$. Then γ is a ρ -derivation graph given Φ iff:

- For each vertex $v_i \in V$, $\phi(v_i) = C_i$, where $C_i \in \mathcal{F}_M$;
- $0 \leq |Pred(v)| \leq 2$ for all $v \in V$;
- For each $v \in V$:
 - If $Pred(v) = \emptyset$ then $\phi(v) \in \Phi$;
 - If $Pred(v) = \{u\}$ then $\phi(v) \in \rho_1(\phi(u))$;
 - If $Pred(v) = \{u_1, u_2\}$ then $\phi(v) \in \rho_2(\phi(u_1), \phi(u_2))$

Since we are only concerned with ρ_1, ρ_2 in this paper, we will usually call this the derivation graph given Φ or even just the derivation graph, when Φ is understood.

Remark 4 We note that ρ_1 and ρ_2 preserve equivalence, in the following sense:

- If $C' \equiv C$ then $\rho_1(C) \equiv \rho_1(C')$; and
- If $C'_1 \equiv C_1$ and $C'_2 \equiv C_2$ then $\rho_2(C_1, C_2) \equiv \rho_2(C'_1, C'_2)$

Here, equivalence across sets has the usual conjunctive meaning. That is, for sets A, B , $A \equiv B$ iff $\bigwedge_{x \in A} x \equiv \bigwedge_{y \in B} y$. Two ordered clauses $\langle C_1 \rangle$ and $\langle C_2 \rangle$ are equivalent iff the $Set(\langle C_1 \rangle)$ is equivalent to the $Set(\langle C_2 \rangle)$.

Definition 10 (Closure) Let Φ be a set of feature-clauses and $\Omega \subseteq \{\rho_1, \rho_2\}$. We define the closure of Φ using Ω as the set of ordered clauses $\langle C \rangle$ which has a derivation sequence from Φ using Ω . We use $Closure_\Omega(\Phi)$ to denote the closure of Φ using Ω .

We will say θ is a type-consistent substitution if for every variable U , the substitution $U/t \in \theta$ (that is, $\theta(U) = t$), then U, t have the same type in M . It follows that if θ is a type-consistent substitution for variables in an ordered clause $\langle C \rangle$ in $\mathcal{L}_{M, T}$ and $\theta(u) = \theta(v)$ for u, v in $\langle C \rangle$, then u, v have the same type in M .

Lemma 2 (Derivation Lemma) Given M, M' and $\Omega = \{\rho_1, \rho_2\}$ as before. Let $\langle C \rangle$ be an ordered clause in $\mathcal{L}_{M, T}$, with head $p(X)$. Let S be a set of ordered M -simple clauses in $\mathcal{L}_{M, T}$, with heads $p(X)$ and all other variables of clauses in S standardised apart from each other and from C . If there exists a substitution θ s.t. $Basis(\langle C \rangle) \subseteq S\theta$ then there exists an ordered clause $\langle C' \rangle$ in $\mathcal{L}_{M', T}$ such that $\langle C' \rangle$ is equivalent to $\langle C \rangle$ and derivable from S using Ω .

Proof See [Appendix C](#). ■

Remark 5 Let $\langle C_1 \rangle, \langle C_2 \rangle, \dots, \langle C_n \rangle$ be a derivation from a set of ordered clauses S using $\{\rho_1, \rho_2\}$. Also, for any clause $\langle C_i \rangle$ in the derivation sequence, let f_i denote the corresponding feature-function as defined in [Section 2](#) using background knowledge B . Let a denote a data-instance. We note the following consequences for $1 \leq i < j \leq n$:

1. C_i subsumes C_j ;⁵
2. If $f_i(a) = 0$ then $f_j(a) = 0$;
3. If $f_j(a) = 1$ then $f_i(a) = 1$; and
4. If $\langle C_{i+1} \rangle \in \rho_1(\langle C_i \rangle)$, $f_i(a) = 1$ and $f_{i+1}(a) = 0$ then there exists a clause C'_{i+1} s.t. $C_i \equiv C_{i+1} \vee C'_{i+1}$ and $f_{B, C'_{i+1}}(a) = 1$

(1) follows straightforwardly since for any $\langle C_i \rangle$, subsequent clauses in the derivation only result in the addition of literals (that is, $C_i \subset C_j$ for $i < j$). For (2), we note that since $C_i \subset C_j$ and both C_i, C_j have the same head literal ($p(X)$) we can take $C_i = \forall(p(X) \vee l_1 \vee \dots \vee l_k)$ and $C_j = \forall(p(X) \vee l_1 \vee \dots \vee l_k \vee l_{k+1} \vee \dots \vee l_m)$. If $f_i(a) = 0$ then $B \cup C_i \not\models p(a)$. That is, there exists some interpretation I that is a model for $B \cup C_i$

⁵ Here subsumption is used in the sense described by [Plotkin \(1972\)](#). That is, representing clauses as sets of literals, clause C subsumes clause D iff there exists a substitution θ s.t. $C\theta \subseteq D$.

s.t. $p(a)$ is false in I . If I is a model for $B \cup C_i$ then it is a model for C_i . Further, if I is a model for C_i and $p(a)$ is false in I then I is a model for $\forall(l_1 \vee \dots \vee l_k)$. But then I is a model for $C_j = \forall(p(X) \vee l_1 \vee \dots \vee l_k \vee l_{k+1} \vee \dots \vee l_m)$. Thus I is a model for $B \cup C_j$ and not a model for $p(a)$. That is, $B \cup C_j \not\models p(a)$ and $f_j(a) = 0$. (3) follows from the fact that if C_i subsumes C_j then $C_i \models C_j$ (Gottlob, 1987). Therefore, if $B \cup C_j \models p(a)$ then $B \cup C_i \models p(a)$. That is, if $f_j(a) = 1$ then $f_i(a) = 1$. For (4), let $C_i : p(X) \leftarrow \text{Body}_i(X, \mathbf{Y})$. Then $C_{i+1} : p(X) \leftarrow \text{Body}_i(X, \mathbf{Y}), Y_i = Y_j$ for $y_{i,j} \in \mathbf{Y}$. Since $f_i(a) = 1$ and $f_{i+1}(a) = 0$, it must be the case that $Y_i = Y_j$ does not hold for $x = a$. Let $C'_{i+1} : p(X) \leftarrow \text{Body}_i(X, \mathbf{Y}), Y_i \neq Y_j$. It is evident that, $f_{B, C'_{i+1}}(a) = 1$ and $C_i \equiv C_{i+1} \vee C'_{i+1}$.

A specialised form of derivation results from the repeated use of ρ_2 first, followed by the repeated use of ρ_1 . We call this form of derivation a *linear derivation*. We describe this next (relevant proofs are in Appendix D).

Definition 11 (Linear Derivation of Feature-Clauses) Let M be a set of mode-declarations, and M' be an extension M as earlier. Let T be a set of type-definitions. Let Φ be a set of feature-clauses in $\mathcal{L}_{M', T}$ and ρ_1, ρ_2 be the operators defined earlier. A sequence of feature-clauses $\langle C_1 \rangle, \langle C_2 \rangle, \dots, \langle C_n \rangle$ is said to be a linear derivation sequence of $\langle C_n \rangle$ from Φ using $\{\rho_1, \rho_2\}$ iff there exists j such that $1 \leq j \leq n$ and:

- For $i \leq j$:
 - Clause $\langle C_i \rangle$ in the sequence is either an element of Φ or an element of the set $\rho_2(\langle C_{i-1} \rangle, \langle C_k \rangle)$ where $\langle C_k \rangle \in \Phi$ and $k < i$.
- For $i > j$:
 - Clause $\langle C_i \rangle$ is an element of the set $\rho_1(\langle C_{i-1} \rangle)$.

We will say $\langle C_j \rangle$ is linearly derivable from Φ using $\{\rho_2\}$; and C_n is linearly derivable from Φ using $\{\rho_1, \rho_2\}$.

Example 8 We continue Example 7. Below is a linear derivation sequence of

$$p(X) \leftarrow \text{has_car}(X, U), \text{has_car}(X, V), \text{smaller}(U, V), \\ \text{has_car}(X, Y), \text{short}(Y), U = V, U = Y$$

from

$$\{ p(X) \leftarrow \text{has_car}(X, Y), \text{short}(Y), \\ p(X) \leftarrow \text{has_car}(X, U), \text{has_car}(X, V), \text{smaller}(U, V) \}$$

using $\{\rho_1, \rho_2\}$.

1	$p(X) \leftarrow \text{has_car}(X, U), \text{has_car}(X, V), \text{smaller}(U, V)$	Given
2	$p(X) \leftarrow \text{has_car}(X, Y), \text{short}(Y)$	Given
3	$p(X) \leftarrow \text{has_car}(X, U), \text{has_car}(X, V), \text{smaller}(U, V), \\ \text{has_car}(X, Y), \text{short}(Y)$	1, ρ_2
4	$p(X) \leftarrow \text{has_car}(X, U), \text{has_car}(X, V), \text{smaller}(U, V), \\ \text{has_car}(X, Y), \text{short}(Y), U = V$	3, ρ_1, U, V
5	$p(X) \leftarrow \text{has_car}(X, U), \text{has_car}(X, V), \text{smaller}(U, V), \\ \text{has_car}(X, Y), \text{short}(Y), U = V, U = Y$	4, ρ_1, U, Y

There is no way to derive the clause $p(X) \leftarrow \text{has_car}(X, U), \text{has_car}(X, V), \text{smaller}(U, V), U = V, \text{has_car}(X, Y), \text{short}(Y), U = Y$ using linear derivation from the given set, but we can derive an equivalent clause $p(X) \leftarrow \text{has_car}(X, U), \text{has_car}(X, V), \text{smaller}(U, V), \text{has_car}(X, Y), \text{short}(Y), U = V, U = Y$ using linear derivation. We would like to point out that the positions of equality literal $U = V$ in the first clause and the second clause are different.

Lemma 3 (Linear Derivation Lemma) *Given M, M' and a set of ordered clauses Φ . If an ordered clause $\langle C \rangle$ is derivable from Φ using $\{\rho_1, \rho_2\}$ then there exists an equivalent ordered clause $\langle C' \rangle$ and it is linearly derivable from Φ using $\{\rho_1, \rho_2\}$.*

Proof See [Appendix D](#). ■

Feature-clauses and their composition using the ρ -operators provide the tools for the development of a particular kind of neural network that we describe next.

3 Compositional Relational Machines (CRMs)

Formally, a CRM is defined as follows:

Definition 12 (CRM) A CRM is a 7-tuple $(V, I, O, E, \phi, \psi, h)$ where:

- V denotes a set of vertices;
- $I \subseteq V$ is a set of “input” vertices;
- $O \subseteq V$ is a set of “output” vertices;
- $E \subseteq \{(v_i, v_j) : v_i, v_j \in V, v_i \notin O, v_j \notin I\}$;
- A vertex-labelling function $\phi : V \rightarrow \mathcal{F}_M \times \mathcal{G}$, where \mathcal{F}_M is the set of feature-clauses given a set of modes M ; and \mathcal{G} denotes a set of activation functions.⁶
In this paper, we will further assume, if $v \in I$ then we restrict $\phi(v) = (\cdot, \mathbf{1})$, where $\mathbf{1}(\cdot) = 1$;
- An edge labelling function $\psi : E \rightarrow \mathbb{R}$, assigns some real-valued labels to edges in the graph; and
- $h : \mathbb{R}^{|O|} \rightarrow \mathbb{R}^n$ is a computation function, for some fixed n

such that (V, E, ϕ') is a derivation graph ([Definition 9](#)) given Φ where $\phi'(v) = C$ if $\phi(v) = (C, \cdot)$ and $\Phi = \{\phi'(v) \mid v \in I\}$.

We note 2 important features of CRMs: (1) Each vertex has a feature-clause associated with it; and (2) Edges between vertices in a CRM are required to satisfy the constraints on edges imposed by a derivation graph. That is, the only edges allowed are those that result from ρ_1 or ρ_2 operations on the feature-clauses associated with the vertices.

3.1 CRMs as Explainable Neural Networks

We describe a use of CRMs as a form of neural network capable of generating logical explanations relevant to its prediction. The architecture of the neural network is inspired by Turing’s idea of unorganised machines ([Turing, 1948](#)) (see

⁶ We assume activation functions in \mathcal{G} are $\mathbb{R} \rightarrow \mathbb{R}$.

Figure 1). Each “neuron” has 2 parts, implementing the vertex-label specification of a CRM’s node: (i) An arithmetic part that is concerned with the g -function in the CRM’s vertex-label; and (ii) A logical part that acts as a switch, depending on the feature-clause associated with the CRM’s vertex-label. We call neurons in such a network “arithmetic-logic neurons” or ALNs for short.

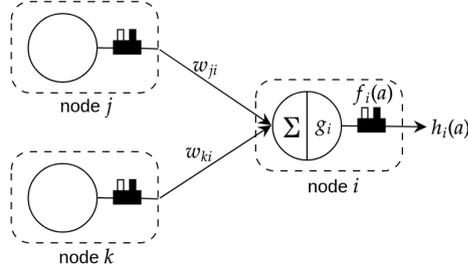


Fig. 1: A neural network implementation of a CRM inspired by Turing’s gated neural networks (Turing, 1948). A neuron n_i corresponds to a vertex v_i in the CRM, with vertex-label $\psi(v_i) = (C_i, g_i)$. In the figure, n_i is connected to neurons n_j and n_k , implying (v_j, v_i) and (v_k, v_i) are in the edge-set of the CRM. f_i (correctly $f_{C_i, B}$) is the feature-function obtained from the feature-clause C_i (see Section 2), and acts as a gate. For a data instance a , $g_i(w_{ji}h_j(a) + w_{ki}h_k(a))$ passes through the gate if and only if $f_i(a) = 1$. In general, $h_i(a)$ is thus $g_i(\sum_{k \in \text{Pred}(n_i)} w_{ki}h_k(a))$ or 0, where $\text{Pred}(n_i)$ is the set of immediate predecessors of n_i in the neural network.

In the rest of the paper, we will use “CRM” synonymously with this form of neural-network implementation. The 7-tuple defining a CRM $(V, I, O, E, \phi, \psi, h)$ corresponds to the following aspects of the neural implementation: (a) The structure of the network is defined by V, I, O, E , and ϕ ; (b) The parameters of the network are defined by ψ ; and (c) the computation of the network is defined by h . We consider each of these in turn.

3.1.1 Structure Selection

Procedure 1 is an enumerative procedure for obtaining a 5-tuple (V, I, O, E, ϕ) , given a set of feature-clauses Φ . For simplicity, the procedure assumes a single activation function g .

Procedure 1 has an important practical difficulty:

- We are interested in a class of CRMs that can be constructed using a set of M-simple feature-clauses $\{C_1, \dots, C_n\}$. Now, it may be impractical to obtain all possible M-simple feature-clauses in a mode-language. Even if this were not the case, it may be impractical to derive all non-simple clauses in the manner shown in Procedure 1.

Procedure 2 describes a randomised implementation to address this. The procedure also uses the result in the Linear Derivation Lemma (Lemma 3 in Section 2) to construct a CRM structure that first uses the ρ_2 operator, followed by the ρ_1 operator.

Procedure 1: (ConstructCRM) Depth-bounded construction of a CRM's structure

Input: A set $\tilde{\Phi}$ of feature-clauses $\{C_1, C_2, \dots, C_n\}$ with heads $p(X)$ and all other variables are standardised apart from each other; an activation function g ; and a bound d on the depth of composition

Output: A CRM structure

- 1 $I = \{v_1, v_2, \dots, v_n\}$;
- 2 $V = I$;
- 3 $E = \emptyset$;
- 4 **for** $i = 1$ **to** n **do**
- 5 $\phi(v_i) = (C_i, \mathbf{1})$
- 6 **for** $j = 1$ **to** d **do**
- 7 $V_{j,1} = \{(C', v) : v \in V, \phi(v) = (C, \cdot), C' = \rho_1(C)\}$;
- 8 $V_{j,2} = \{(C', v_1, v_2) : v_1, v_2 \in V, \phi(v_1) = (C_1, \cdot), \phi(v_2) = (C_2, \cdot), C' = \rho_2(C_1, C_2)\}$;
- 9 Let V_1 be a set of new vertices v s.t. there exists $(C', v') \in V_{j,1}$ and $\phi(v) = (C', g)$;
- 10 Let V_2 be a set of new vertices v s.t. there exists $(C', v_1, v_2) \in V_{j,2}$ and $\phi(v) = (C', g)$;
- 11 Let $V' = V_1 \cup V_2$;
- 12 $V = V \cup V'$;
- 13 $E = E \cup \{(v_1, v) : (C, v_1) \in V_{j,1}, \phi(v) = (C, g)\} \cup \{(v_1, v), (v_2, v) : (C, v_1, v_2) \in V_{j,2}, \phi(v) = (C, g)\}$;
- 14 $O = \{v : v \in V, \nexists v' \text{ s.t. } (v, v') \in E\}$;
- 15 **return** (V, I, O, E, ϕ)

In the rest of the paper, we will use the term *Simple CRM* to denote a CRM constructed by either [Procedure 1](#) or [Procedure 2](#) in which the input clauses C_1, C_2, \dots, C_n are M-simple feature-clauses.

3.1.2 Parameter Estimation

[Procedure 2](#) does not completely specify a CRM. Specifically, neither the edge-labelling ψ nor h are defined. We now describe a procedure that obtains a ψ given the partial-specification returned by [Procedure 2](#) and a pre-specified h suitable for the usual task of using the neural network for function approximation. That is, given a partial specification of an unknown function $\delta : \mathcal{A} \rightarrow \mathcal{Y}$ in the form of sample data $D = \{(a_i, y_i)\}_1^N$. We want the the neural network to construct an approximation $\hat{\delta} : \mathcal{A} \rightarrow \mathcal{Y}$ that is reasonably consistent with D . In order to estimate the goodness of the approximation, we need to define a *loss* function, that computes the penalty of using $\hat{\delta}$. We will take $\hat{\delta}$ to be synonymous with h , the computation function of the CRM. Recall $h : \mathbb{R}^{|O|} \rightarrow \mathbb{R}^n$ for some fixed n . In this paper, we will therefore take $\mathcal{Y} = \mathbb{R}^n$ and define h in the usual manner adopted by neural networks, namely as a function of “local” computations performed at each of the O vertices of the CRM.

Definition 13 (Local Computation in a CRM) Let (V, I, O, E, ϕ, ψ) be a partially-specified CRM, where $O = \{o_1, o_2, \dots, o_k\}$. For each vertex $v_i \in V$ let $\phi(v_i) = (C_i, g_i)$ and for each edge (v_i, v_j) $\psi((v_i, v_j)) = w_{ij}$. Let f_i denote f_{C_i} . For any $a \in \mathcal{A}$ we define $h_i : \mathcal{A} \rightarrow \mathbb{R}$ as follows:

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

Procedure 2: (RandomCRM) Randomised construction of a CRM structure, with linear derivation of feature-clauses.

Input: A set Φ of feature-clauses $\{C_1, C_2, \dots, C_n\}$ with heads $p(X)$ and all other variables are standardised apart from each other; an activation function g ; a sample size s ; bounds d_{ρ_1}, d_{ρ_2} on the depth of application of the ρ_1 and ρ_2 operators

Output: A CRM structure

```

1  $I = \{v_1, v_2, \dots, v_n\}$ ;
2  $V_0 = I$ ;
3  $V = V_0$ ;
4  $E = \emptyset$ ;
5 for  $i = 1$  to  $n$  do
6    $\phi(v_i) = (C_i, \mathbf{1})$ ;
7 for  $j = 1$  to  $d_{\rho_1} + d_{\rho_2}$  do
8    $V_j = \emptyset$ ;
9    $E_j = \emptyset$ ;
10  if  $j \leq d_{\rho_2}$  then
11     $op = \rho_2$ ;
12  else
13     $op = \rho_1$ ;
14  for  $i = 1$  to  $s$  do
15    if  $op = \rho_2$  then
16      Sample a vertex  $v_1$  from  $I$  using a uniform distribution and sample a
17      vertex  $v_2$  from  $V_{j-1}$  using the uniform distribution;
18      Create a vertex  $v'$  such that  $\phi(v') = (C', g)$  where  $C' = \rho_2(C_1, C_2)$ ,
19       $\phi(v_1) = (C_1, g)$  and  $\phi(v_2) = (C_2, g)$ ;
20       $V_j = V_j \cup \{v'\}$ ;
21       $E_j = E_j \cup \{(v_1, v'), (v_2, v')\}$ ;
22    else
23      Sample a vertex  $v$  from  $V_{j-1}$  using the uniform distribution;
24      Create a vertex  $v'$  such that  $\phi(v') = (C', g)$  where  $C' = \rho_1(C)$  and
25       $\phi(v) = (C, g)$ ;
26       $V_j = V_j \cup \{v'\}$ ;
27       $E_j = E_j \cup \{(v, v')\}$ ;
28     $V = V \cup V_j$ ;
29     $E = E \cup E_j$ ;
30   $O = \{v : v \in V, \nexists v' \text{ s.t. } (v, v') \in E\}$ ;
31 return  $(V, I, O, E, \phi)$ ;
```

Then $\hat{\delta}(a) = h(h_{o_1}(a), \dots, h_{o_k}(a))$.

For a multi-class classification task, function h computes the probability distribution over the classes, for example, a **softmax** function. Similarly, for a regression task, h computes a real number, for example, a **linear** function.

Procedure 3 estimates the parameters of the neural network using a standard weight-update procedure based on stochastic gradient descent (SGD) (Rumelhart et al., 1986; Goodfellow et al., 2016), given the structure obtained from **Procedure 2**, a pre-defined computation function h , and a loss function L .

3.1.3 Predictions and Explanations

We denote the prediction of a CRM $\gamma = (V, I, O, E, \phi, \psi, h)$ by $\hat{\delta}(a) = h(h_{o_1}(a), \dots, h_{o_k}(a))$, where $O = \{o_1, \dots, o_k\}$ and the h_{o_i} are as defined in [Definition 13](#).

Procedure 3: (TrainCRM) Parameter estimation of a CRM, given its structure, using stochastic gradient descent (SGD). The training is done until some stopping criterion is reached, which refers to the condition when the number of training epochs reaches some pre-specified maximum value.

Input: A CRM structure $\gamma = (V, I, O, E, \phi)$, a dataset $D = \{(a_i, y_i)\}_1^N$, where $a_i \in \mathcal{A}$ and $y_i \in \mathbb{R}^n$, a computation function $h : \mathbb{R}^{|O|} \rightarrow \mathbb{R}^n$, a loss function $L : \mathbb{R}^n \times \mathbb{R}^n \rightarrow \mathbb{R}$.

Output: A CRM

- 1 Let $O = \{o_1, \dots, o_k\}$;
 - 2 Initialise ψ ;
 - 3 **while** *stopping criterion is not met* **do**
 - 4 Randomly draw an instance (a_i, y_i) from D ;
 - 5 Let $\hat{y}_i = h(h_{o_1}(a), \dots, h_{o_k}(a))$ (see [Definition 13](#));
 - 6 $Error = L(y_i, \hat{y}_i)$;
 - 7 Update ψ using SGD to minimise $Error$;
 - 8 **return** $(V, I, O, E, \phi, \psi, h)$;
-

The association of feature-clauses with every vertex of the CRM allows us to construct “explanations” for predictions. For this we introduce the notion of ancestral graph of a vertex and explanation graph of an output vertex in a CRM.

Definition 14 (Ancestral Graph of a Vertex) Let $\gamma = (V, I, O, E, \phi, \psi, h)$ be a CRM. The set of ancestors of a vertex $v \in V$ in γ , denoted by $Ancestors(v, \gamma)$, is defined as follows:

$$Ancestors(v, \gamma) = \begin{cases} \{v\} & \text{if } v \in I \\ \bigcup_{(u,v) \in E} Ancestors(u, \gamma) \cup \{v\} & \text{otherwise} \end{cases}$$

The ancestral graph of a vertex v in γ is (V', E') where $V' = Ancestors(v, \gamma)$ and $E' = \{(u', u'') : u', u'' \in V', (u', v'') \in E\}$.

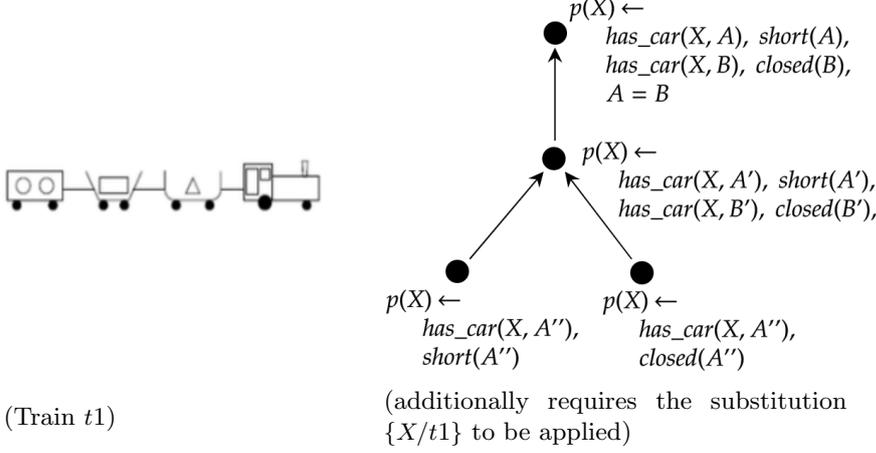
Definition 15 (Explanation Graph) Let $\gamma = (V, I, O, E, \phi, \psi, h)$ be a CRM, and $a \in \mathcal{A}$ be a data instance. Let $O = \{o_1, \dots, o_k\}$ and let $\hat{\delta}(a) = h(h_{o_1}(a), \dots, h_{o_k}(a))$ be the prediction of the CRM for a . For $o_i \in O$, let C_i be the feature-clause associated with o_i (that is, $\phi(o_i) = (C_i, \cdot)$). Let f_i be the corresponding feature-function (as defined in [Section 2](#)), and (V', E') be an ancestral graph of o_i in γ . Then the explanation graph of a from vertex o_i , denoted by $Explain_{\gamma, o_i}(a)$, is as follows:

$$Explain_{\gamma, o_i}(a) = \begin{cases} (V', E', \phi') & \text{if } f_i(a) = 1 \\ \emptyset & \text{otherwise} \end{cases}$$

where $\phi' : V' \rightarrow \mathcal{F}_M$ is a vertex-labelling function. $\phi'(v) = C\theta_a$, where θ_a the substitution $\{X/a\}$ for the variable X in the head literal and $\phi(v) = (C, \cdot)$.

Remark 6 $Explain_{\gamma, o_i}(a)$ consists of a (labelled) tree of feature-clauses extracted from the derivation graph of feature-clauses. The root of the tree is the feature-clause at o_i and sub-trees contain simpler feature-clauses. If the CRM is a Simple CRM, then the leaves of the explanation-tree are M-simple feature-clauses.

Example 9 In the Trains problem, suppose the data instance is the train shown on the left below. The explanation graph, associated with an output vertex of the CRM is shown on the right.



By definition, we know that the feature-function value associated with $p(t_1) \leftarrow has_car(t_1, A), short(A), has_car(t_1, B), closed(B)$ has the value 1. Also, we know that feature-function values with all other clauses in the explanation will also be 1.

The notion of an explanation graph from a vertex extends naturally to the explanation graph from a set of vertices which we do not describe here. It will be useful in what follows to introduce the notion of a feature-clause being “contained in an explanation graph”.

Definition 16 (Feature-clause Containment) Let γ be a CRM, o be an output vertex of γ , Let a be a data instance, Let $Explain_{\gamma,o}(a) = (V, E, \alpha)$, and $F_{\gamma,o}(a) = \{\alpha(v) \mid v \in V\}$ be the set of feature-clauses in the explanation graph. We will say a feature-clause C is contained in $Explain_{\gamma,o}(a)$, or $C \sqsubseteq Explain_{\gamma,o}(a)$ iff there exists $C' \in F_{\gamma,o}(a)$ s.t. $C\theta_a \equiv C'$ (where $\theta_a = \{X/a\}$, is a substitution for the variable X in the head of C).

(This naturally extends to the containment of a set of clauses.)

Example 10 The feature-clause $C : p(X) \leftarrow has_car(X, Y), short(X), closed(X)$ is contained in the explanation graph shown for train t_1 in [Figure 6](#) because:

- $F_{\gamma,o}(t_1) = \{C_1, C_2, C_3, C_4\}$ where:
 - $C_1 : p(t_1) \leftarrow (has_car(t_1, A), short(A), has_car(t_1, B), closed(B), A = B)$;
 - $C_2 : p(t_1) \leftarrow (has_car(t_1, A'), short(A'), has_car(t_1, B'), closed(B'))$;
 - $C_3 : p(t_1) \leftarrow (has_car(t_1, A''), short(A''))$; and
 - $C_4 : p(t_1) \leftarrow (has_car(t_1, A''), closed(A''))$
- With $\theta_a = \{X/t_1\}$, $C\theta_a = (p(t_1) \leftarrow (has_car(t_1, A), short(A), closed(A)))$; and
- $C\theta_a \equiv C_1$

Explanatory Fidelity

Explanatory fidelity refers to how closely the CRM’s explanation matches the “true explanation”. Of course, in practice, explanatory fidelity will be a purely notional concept, since the true explanation will not be known beforehand. However it is useful for us to calibrate the CRM’s explanatory performance when it is used for problems where true explanations are known (the synthetic problems considered in experiments below are in this category).

For a prediction $\hat{\delta}(h_{o_1}(a), \dots, h_{o_k}(a))$ by a CRM, suppose we have a relevance ordering over the output vertices o_1, \dots, o_k . Let o^* be the most relevant vertex in this ordering. Then we will call the explanation graph from o^* as the *most-relevant explanation graph* for a given the CRM.⁷

For a classification task, we use clause containment and the most-relevant explanation graph to arrive at a notion of explanatory fidelity of a CRM to a set of feature-clauses \mathcal{T}_c that are known to be ‘acceptable’ feature-clauses for class c (if no such acceptable clauses exist for class c , then $\mathcal{T}_c = \emptyset$). Let γ be a CRM used to predict the class-labels for a set of data-instances. For any instance a , let o^* denote the most relevant output vertex of the CRM. We will say that a data instance a is consistently explained iff: (i) the CRM predicts that a has the class-label c ; and (ii) there exists a $C \in \mathcal{T}_c$ s.t. $C \sqsubseteq \text{Explain}_{\gamma, o^*}(a)$; and (iii) for $c' \neq c$, there does not exist $C' \in \mathcal{T}_{c'}$ s.t. $C' \sqsubseteq \text{Explain}_{\gamma, o^*}(a)$.

Given a set of data-instances E , let CE denote the set of instances in E explained consistently and IE denote the set of instances in E not explained consistently. Then the explanatory fidelity of the CRM (correctly, this is only definable w.r.t. the \mathcal{T}_c ’s) is taken to be $\frac{|CE|}{|CE|+|IE|}$, provided $(|CE|+|IE|) \neq 0$ (and undefined otherwise).

3.2 CRMs as Explanation Machines

CRMs can be used as ‘explanation machines’ for black-box predictors that do not intrinsically include an explanatory component. The approach, sometimes called *post hoc* explanation generation, is shown in [Figure 2](#).

To assess the utility of using the CRM in this manner, we will change the usual assessment of predictive accuracy to one of ‘predictive fidelity’, which refers to how closely the CRM matches the prediction of the target model.

4 Empirical Evaluation of CRMs as Explanation Machines

4.1 Aims

We consider two kinds of experiments with Simple CRMs:

⁷ In implementation terms, one way to obtain such a relevance ordering over output vertices of the CRM is to use the $h_i(\cdot)$ values for vertices in O to select a vertex o^* that has the highest magnitude (this is the same as selecting the best vertex after one iteration of the layer-wise relevance propagation, or LRP ([Binder et al., 2016](#)), procedure).

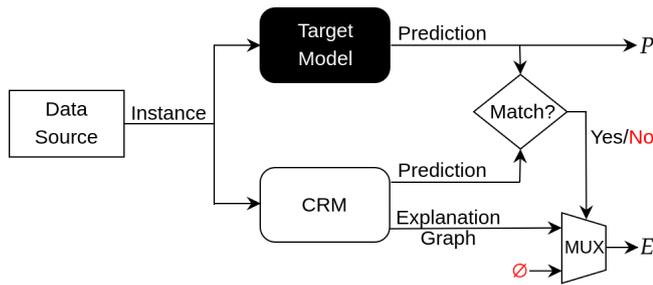


Fig. 2: Using a CRM as an explanation machine. The target model is a “black box” that does not have an explanatory output. The CRM model is trained using training data labelled with the prediction from the black box (and not the ‘true label’). The multiplexer (MUX) selects between the CRM’s explanation graph and the “empty” explanation \emptyset depending on whether the CRM’s prediction does or does not match the target model’s prediction. By using the setup as shown here, we are able to get a prediction P and a corresponding explanation E .

Synthetic data. Using tasks for which both target-model predictions and acceptable feature-clauses are available, we intend to investigate the hypothesis that: (a) Simple CRMs can construct models with high predictive fidelity to the target’s prediction; and (b) Simple CRMs have high explanatory fidelity to the set of acceptable feature-clauses.

Real data. Using real-world datasets, for which we have predictions from a state-of-the-art black-box target model, we investigate the hypothesis that Simple CRMs can construct models with high predictive fidelity to the target’s prediction. We also provide illustrative examples of using the CRM to provide explanations for the predictions.

We clarify what is meant by ‘acceptable feature-clauses’ for the synthetic data in [Section 4.3](#). For real data, the target-model is the state-of-the-art (SOTA, which in this case is a graph-based neural network). That is, the CRM is being used here to match the SOTA’s predictions (and not the ‘true value’), and to provide proxy explanations. No acceptable feature-clauses are known for classes in the real data.⁸

4.2 Materials

4.2.1 Data and Background Knowledge

Synthetic Data. We use two well-known synthetic datasets. The first dataset is the “Trains” problem of discriminating between eastbound (class = +) and westbound trains (class = -) ([Michalski, 1980](#)). The original data consists only of 10 instances (5 in each class). We generate a dataset of 1000 instances with a class-distribution of approximately 50% + and 50% -, using the data

⁸ The CRM can of course be used to predict the true value directly. We will comment on this later, but that is not the primary goal of the experiment here.

generator (Michie et al., 1994). We use 700 instances as training data and 300 instances as test-data. The second dataset consists of the task of discriminating between illegal (class = +) and legal (class = -) chess positions in the King-Rook-King endgame (Bain, 1994; Michie, 1976). The class-distribution is approximately 33% + and 67% -. We use 10000 instances of board-positions as training data and 10000 instances as test-data. Examples of + instances are showed pictorially in Figure 3.

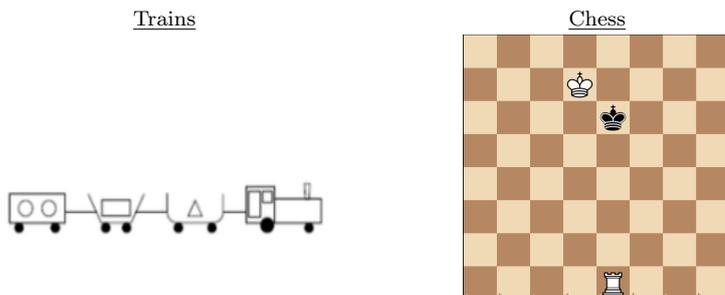


Fig. 3: Pictorial examples of positive instances in the synthetic data. The actual data are logical encodings of examples like these. The instance on the left is an example of a train classified as “eastbound” (+). The instance on the right is of a board position classified as “illegal” (+), given that it is White’s turn to move. For both problems, we have a target model that is complete and correct. We also know a set of feature-clauses that are acceptable as explanations for instances that are correctly predicted as +.

Real Data. Our real data consists of 10 datasets obtained from the NCI⁹. Each dataset represents extensive drug evaluation with the concentration parameter GI50, which is the concentration that results in 50% growth inhibition of cancer cells (Marx et al., 2003). A summary of the dataset is presented in Figure 4. Each relational data-instance in a dataset describes a chemical compound (molecule) with atom-bond representation: a set of bond facts. The background knowledge consists of logic programs defining almost 100 relations for various functional groups (such as amide, amine, ether, etc.) and various ring structures (such as aromatic, non-aromatic etc.). There are also higher-level domain-relations that determine presence of connected, fused structures. Some more details on the background knowledge can be seen in these recent studies: (Dash et al., 2021, 2022).

4.2.2 Algorithms and Machines

We use the ILP system Aleph (Srinivasan, 2001) for constructing the feature-clauses. The CRMs are implemented using PyTorch (Paszke et al., 2019). The

⁹ The National Cancer Institute (<https://www.cancer.gov/>)

# of datasets	Avg. # of instances	Avg. # of atoms per instance	Avg. # of bonds per instance	% of positives
10	3018	24	51	50–75 Avg.= 57

Fig. 4: Summary of the NCI-50 datasets (Total no. of instances is approx. 30,200). The graph neural network predictor described in (Dash et al., 2021) is taken as the target model. No acceptable feature-clauses are known for these tasks.

parameter learning of CRMs has been done with the autograd engine available within PyTorch for the implementation of backpropagation. Our implementation of Layerwise-Relevance Propagation (LRP) is based on (Bach et al., 2015; Binder et al., 2016).

The CRM implementation and all our experiments are conducted on a workstation running with Ubuntu (Linux) operating system, 64GB main-memory, and a CPU running with 12 Intel Xeon processors.

4.3 Method

The experiments are in two parts: an investigation on synthetic data to examine the predictive performance and explanatory fidelity of CRMs; and an investigation on real data, to compare the predictive performance of CRMs against state-of-the-art deep networks. Some examples of explanations are also provided for the explanations generated by a CRM on real data. We describe the method used for each part in turn.

4.3.1 Experiments with Synthetic Data

For both synthetic datasets, we have access to symbolic descriptions of the true concepts involved. The ‘target model’ in each case is taken to be equivalent to a classifier that labels instances consistent with the corresponding true concept. This allows us to judge the fidelity of explanations generated. The method used in each case is straightforward:

For each problem:

- (a) Construct the dataset D of instances labelled by the target model;
- (b) Generate a subset of M -simple feature-clauses in the mode-language for the problem;
- (c) Randomly split D into training and test samples;
- (d) Construct a CRM using Procedure 2 with the M -simple features. The weights for the CRM are obtained using the training data and the SGD-based weight-update steps described in Procedure 3 (see below for additional details);
- (e) Obtain an estimate of the predictive and the explanatory fidelity of the CRM using the test data (again, see below for details).

The following additional details are relevant to the method just described:

- For both datasets, the composition depth of CRMs is at most 3. Also, the mode-declarations for Chess allow the occurrence of equalities in M-simple features (see [Appendix F](#)), additional compositions using ρ_1 are not used in this problem;
- We use the rectified linear (`relu`) activation function for the local computation in the neurons of the internal (hidden) layers of the CRMs.
- We use Adam optimiser ([Kingma and Ba, 2015](#)) to minimise the training cross-entropy loss between the true classes and the predicted classes by the network;
- We provide as input feature-clauses only a subset of all possible M-simple feature-clauses. The subset is constrained by the following: (i) At most 2 body literals; (ii) Minimum support of at least 10 instances¹⁰; and (iii) Minimum precision of at least 0.5. All subsequent feature-clauses obtained by composition are also required to satisfy the same support and precision constraints. The learning rate for the Adam optimiser is set to 0.001 while keeping other hyperparameters to their defaults within PyTorch;
- The number of training epochs is set to 5 for the Trains dataset and 10 for the Chess dataset;
- Both synthetic problems are binary classification tasks. We call the classes + and – for convenience. Predictive fidelity is estimated in the usual manner, namely as the proportion of correctly predicted test-instances;
- Explanatory fidelity is estimated as described in [Section 3.1.3](#). For this, we need to pre-define sets of feature-clauses that are acceptable in explanations. For the synthetic datasets, we are able to identify sets of acceptable feature-clauses from the literature: These feature-clauses are obtained from a target model that is known to be complete and correct (see ([Michie et al., 1994](#)) for the target model for Trains and ([Bain, 1994](#)) for Chess). The acceptable clauses in \mathcal{T}_+ are as follows:

Problem	Acceptable Feature Clause
Trains	$p(X) \leftarrow has_car(X, Y), short(X), closed(X)$
Chess	$p((A, B, C, D, C, E)) \leftarrow true$ $p((A, B, C, D, E, D)) \leftarrow true$ $p((A, B, A, B, C, D)) \leftarrow true$ $p((A, B, C, D, E, F)) \leftarrow adj(A, E), adj(B, F)$

In Trains, the feature clauses apply to descriptions of trains. For Chess these are descriptions of the board in an endgame. The board is a 6-tuple that denotes the file and rank of the position of the White King, White Rook and Black King, respectively. In all cases $\mathcal{T}_- = \emptyset$. Explanatory fidelity will be estimated by checking clause-containment of the feature-clauses above in the explanation graph for the most-relevant output vertex of the CRM (see [Section 3.1.3](#));

- The acceptable feature-clause for the Trains is a direct rewrite of the function used to generate the labels. For Chess, the (set of) feature-clauses are direct

¹⁰ In principle, increasing the number of input clauses will increase the size (width and breadth) of the CRM (measured by the number of layers and neurons in each layer of the CRM). Furthermore, since complex features are more specific than the features represented by simple clauses, the coverage of the complex features (that is, instances for which the features have the value 1) will usually be lower than those of simple clauses. Thus, if we restrict complex features to those having a positive coverage of at least p , simple features will have also have a coverage of at least p . Thus, simple features with a lower positive coverage will not be part of any connection in the CRM, and therefore need not appear in the inputs.

rewrites of an approximate symbolic description taken from (Srinivasan et al., 1992). These approximate description isn't identical to the correct description, but is very closely related to it (the approximation differ from the correct description only in about 40 of 10,000 cases). For our purposes therefore, high explanatory fidelity, w.r.t. the set of feature-clauses shown, will taken to be sufficient; and

- We provide a baseline comparison for predictive fidelity against a ‘majority class’ predictor. A baseline comparison is also provided for explanatory fidelity against random selection of a feature-clause from the set of feature-clauses associated with the output vertices of the CRM that have a feature-function value of 1 for the data instance being predicted.

4.3.2 Experiments with Real Data

For the real-world datasets, the current state-of-the-art predictions are from a Graph Neural Network (GNN) constructed using the background knowledge described earlier (Dash et al., 2022). However, the GNN model constitutes a black-box model, since it does not produce any explanations for its predictions. We investigate equipping this black-box model with CRM model for explanation. The method is as follows:

For each problem:

- (a) Construct the dataset D consisting of problem instances and their predictions of the target model;
- (b) Generate a subset of M -simple feature-clauses in the mode-language for the problem. The restrictions used for synthetic data are used to constrain the subset;
- (c) Construct a CRM using Procedure 2 with the M -simple features and the dataset D . The weights for the CRM are obtained using the training data used by the state-of-the-art methods and the SGD-based weight-update procedure; and
- (d) Obtain the predictive fidelity of the CRM model to the predictions of the target model.

The following additional details are relevant:

- As with the synthetic data, the compositional depth for the CRMs is set to 3. Again, we do not use ρ_1 operations, since the mode-declarations allow equalities. The constraints on input feature-clauses is the same as those used for synthetic data;¹¹
- The CRM implementation is the same as the one used for synthetic data. We perform a grid-search of the learning rate for the Adam optimiser using the parameter grid: $\{0.01, 0.001, 0.005, 0.0001\}$. The total number of training epochs is 10, with early-stopping mechanism (Prechelt, 1998) with a patience period of 3;

¹¹ Our choice for the compositional depth of 3 is also loosely-based on our previous work on Deep Relational Machines (DRMs: (Dash et al., 2018)). However, we note that a depth higher than 3 will increase the complexity of a CRM (due to increase in number of layers and neurons), which might result in better predictive performance of a CRM. We expect that in practice the depth bound will be treated as a hyperparameter and subject to the usual forms of hyperparameter optimisation.

- As with the synthetic data, we provide a baseline comparison against the ‘majority class’ predictor;
- Unlike the synthetic data, no pre-defined set of acceptable feature-clauses exists, and therefore no estimate of explanatory fidelity is possible. Correspondingly, there is no baseline provided either.

4.4 Results

Figure 5 tabulates the results used to compute estimates of predictive and explanatory fidelity on synthetic and real data. The main details in these tabulations are these: (a) For the synthetic data, Simple CRMs models able to match the target’s prediction perfectly (predictive fidelity of 1.0); (b) The high explanatory fidelity values show that for instances labelled +, the maximal explanation for the most-relevant vertex contains at least 1 clause from the set of acceptable feature-clauses; and for instances labelled –, the maximal explanation of the most relevant vertex does not contain any clauses from the target theory; and (c) On the real datasets predictive fidelity of CRMs is reasonably high: suggesting that about 81% of the time, the CRM’s prediction will match that of the state-of-the-art model.

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

(a) Synthetic data

Dataset	Pred. Fidelity	
	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
CAKL1	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)

(b) Real data

Fig. 5: Estimates of fidelity for Simple CRMs on the synthetic datasets and real datasets. Explanatory fidelity is assessable on synthetic data since we have access to the “correct” explanation. Baseline for prediction is the majority class predictor. For explanations, Baseline refers to random selection of a feature-clause from the set of feature-clauses associated with the output vertices of the CRM with function value 1 for the data instance being predicted by the majority class predictor.

We now turn to examine the results in greater detail.

4.4.1 Predictive Fidelity

Although we obtain perfect predictive fidelity to the target model on synthetic data, fidelity on the real datasets clearly has room for improvement. Improvements in fidelity are possible simply by considering ensembles of CRMs, obtained simply due to the sampling variation arising in Step (c) (refer [Section 4.3.2](#)). Below, we tabulate changes in predictive fidelity on 1 of the real-world problems (786_0), using a sample consisting of upto 3 CRMs. With multiple CRMs, for a data-instance to be correctly predicted it is sufficient for any one of the CRMs to predict the same class as the target-model. Recall the primary purpose of the CRM is to explain the target-model’s prediction in terms of its feature-clauses. Any CRM that matches the target-model’s prediction can be used to explain the prediction. More on this under “Explanation” below.

No. of CRMs	Predictive Fidelity
1	0.75
2	0.83
3	0.85

4.4.2 Explanatory Fidelity

For the synthetic datasets we show below in [Figure 6](#) a representative + instance (shown pictorially for ease of understanding), along with the predictions of both target and the CRM. The last column shows an acceptable feature-clause along with a stylised English translation. In both instances, an equivalent form of the acceptable feature-clause is contained in the CRM’s explanation graph.

For the Chess data, the CRM’s explanatory fidelity is less than 1. This means that there are instances for which the CRM’s explanation graph does not contain an acceptable feature-clause. We discover 19 different kinds of ‘buggy’ explanations are found by the CRM: a full listing is in [Appendix F](#). Here we provide illustrative instances of two kinds of errors: those that are close to the correct explanation; and those that are an artifact of the specific data instance being explained (see [Figure 7](#)). Besides these, in many cases, we find explanation errors arise from the fact that definitions in background knowledge of file and rank adjacency hold when ranks and files are the same (that is, if A and B are ranks (or files) and $A = B$, then $adj(A, B)$ is true).¹² In many instances inconsistent explanations result from feature-clauses contain literals that use equality instead of adjacency (that is, the CRM’s explanation contains $A = E$, rather than $adj(A, E)$: see [Section F.2](#) in [Appendix F](#)). However, even accounting for this, the CRM’s explanations can be more specific than the correct explanation; and in some cases, incorrect (an example of each is shown in [Figure 7](#)).

What about explanations on real data? At this point, we do not have any independent source of acceptable feature-clauses for this data. We nevertheless show a representative example of the explanation for a test-instance (see [Figure 8](#)).

¹² M. Bain, the author of the background definitions, confirms that this is the intended meaning of the $adj/2$ predicate for this problem (personal communication).

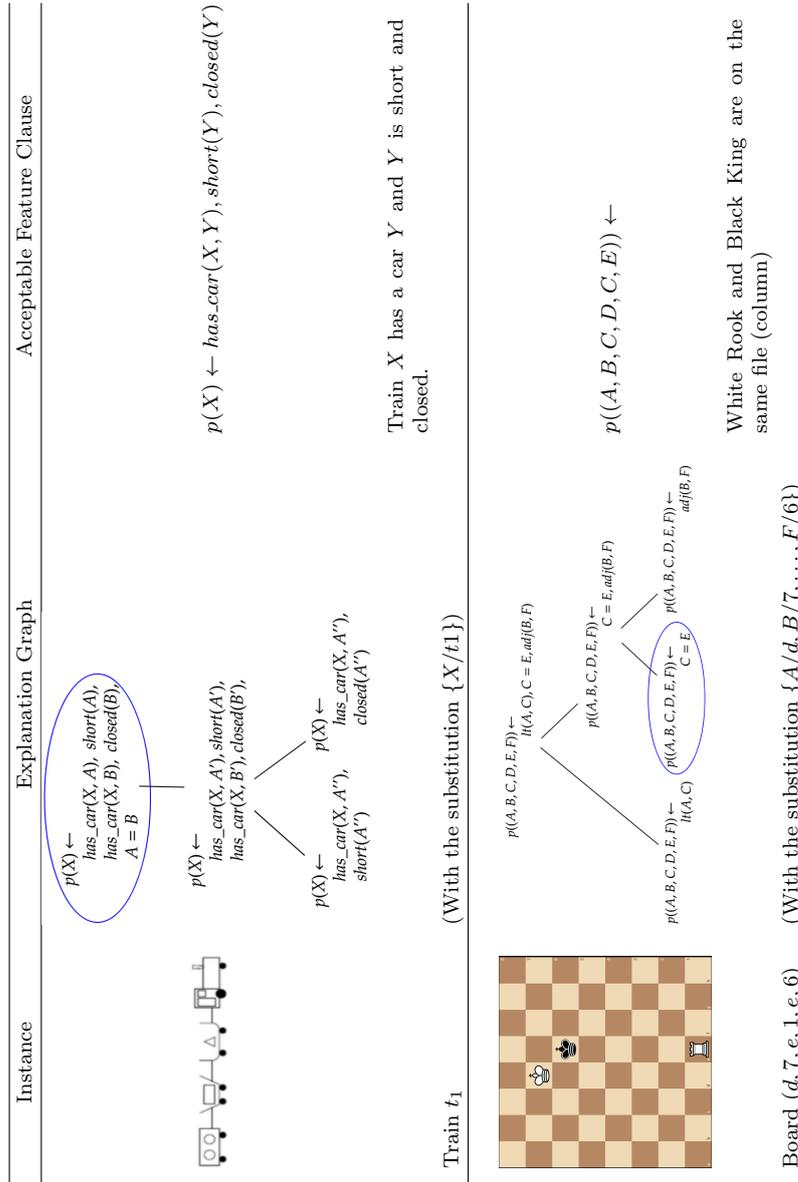


Fig. 6: Explanations from the CRMs for a + prediction by both target-model and the CRM for two instances in the synthetic data. In both cases, the CRM’s explanation graph contains an acceptable feature-clause (circled).

We close this examination by drawing the reader’s attention to an important aspect of a CRM’s explanation. The feature-clauses are defined in terms of relations provided as prior knowledge. This makes them potentially intelligible to a person familiar with the meanings of these relations. This makes it easier-in

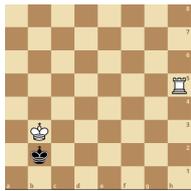
Instance	Explanation Graph	Acceptable Feature-Clause
	$ \begin{array}{l} p(A, B, C, D, E, F) \leftarrow \\ \quad \text{adj}(A, E), h(C, E), \text{adj}(B, F) \\ \swarrow \quad \searrow \\ p(A, B, C, D, E, F) \leftarrow \quad p(A, B, C, D, E, F) \leftarrow \\ \quad \text{h}(C, E), \text{adj}(B, F) \\ \swarrow \quad \searrow \\ p(A, B, C, D, E, F) \leftarrow \quad p(A, B, C, D, E, F) \leftarrow \quad p(A, B, C, D, E, F) \leftarrow \\ \quad \text{adj}(A, E) \quad \text{h}(C, E) \quad \text{adj}(B, F) \end{array} $	$ p((A, B, C, D, E, F)) \leftarrow \\ \text{adj}(A, E), \text{adj}(B, F) $
	$ \begin{array}{l} p(A, B, C, D, E, F) \leftarrow \\ \quad \text{h}(A, C), \text{h}(F, B), \text{adj}(B, F) \\ \swarrow \quad \searrow \\ p(A, B, C, D, E, F) \leftarrow \quad p(A, B, C, D, E, F) \leftarrow \\ \quad \text{h}(A, C) \quad \text{h}(F, B), \text{adj}(B, F) \\ \swarrow \quad \searrow \\ p(A, B, C, D, E, F) \leftarrow \quad p(A, B, C, D, E, F) \leftarrow \quad p(A, B, C, D, E, F) \leftarrow \\ \quad \text{h}(A, C) \quad \text{h}(F, B) \quad \text{adj}(B, F) \end{array} $	

Fig. 7: Examples where the target model and the CRM’s prediction are both +, but the CRM’s explanation graph does not contain an acceptable feature-clause. For simplicity, we do not show the substitutions for $A \dots F$.

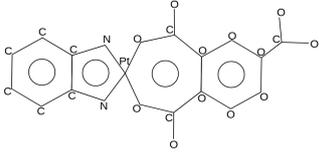
Instance	Explanation Graph
	$ \begin{array}{l} p(X) \leftarrow \\ \quad \text{has_struc}(X, A, B, \text{hetero_aromatic}), \\ \quad \text{lteq}(B, 7), \\ \quad \text{has_struc}(X, C, D, \text{amine}), \\ \quad \text{lteq}(D, 2), \\ \quad \text{has_struc}(X, E, F, \text{oxide}), \\ \quad \text{lteq}(F, 7) \\ \swarrow \quad \searrow \\ p(X) \leftarrow \quad p(X) \leftarrow \\ \quad \text{has_struc}(X, A, B, \text{amine}), \quad \text{has_struc}(X, A, B, \text{amine}), \\ \quad \text{lteq}(B, 2), \quad \text{has_struc}(X, C, D, \text{amine}), \quad \text{has_struc}(X, C, D, \text{amine}), \\ \quad \text{lteq}(D, 2), \quad \text{lteq}(D, 7) \\ \swarrow \quad \searrow \quad \searrow \\ p(X) \leftarrow \quad p(X) \leftarrow \quad p(X) \leftarrow \\ \quad \text{has_struc}(X, A, B, \text{hetero_aromatic}), \quad \text{has_struc}(X, A, B, \text{amine}), \quad \text{has_struc}(X, A, B, \text{oxide}), \\ \quad \text{lteq}(B, 7) \quad \text{lteq}(B, 2) \quad \text{lteq}(B, 7) \end{array} $

Fig. 8: A CRM explanation for a prediction on the real data. The class-label predicted by both CRM and the black-box model for this data instance is +.

principle at least—to perform a human-based assessment of the feature-clauses in the explanation graph (this is apparent from the ‘debugging’ of explanations that we have been to accomplish with the Chess data).

4.4.3 Additional Results: CRMs as Prediction Machines

The tabulations of fidelity and the subsequent assessments above provide a measure of confidence in the use of CRMs as explanation machines. But it is evident that CRMs can be used as ‘white-box’ predictors in their own right. We provide an indicative comparison of a CRM predictor against the state-of-the-art predictors (for the real-data, the prediction is by majority-vote from an ensemble of 3 CRMs):

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)
CAKL1	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)

Fig. 9: Predictive performance comparison of an ensemble of 3 Simple CRMs against some leading black-box predictors. The numbers are estimates of predictive accuracy obtained on test data. The number in parentheses is the estimated standard deviation. The techniques being compared are: GNN, the graph-based neural network approach described in (Dash et al., 2022); DRM (500), is a form of MLP called a Deep Relational Machine that has, as input, Boolean feature-vectors resulting from a stochastic selection of 500 relational features (Dash et al., 2019); and CILP++, an MLP that has input Boolean feature-vectors resulting from an exhaustive feature construction technique called Bottom-Clause Propositionalisation (França et al., 2014). Baseline is the majority class predictor.

The results in Figure 9 indicate that Simple CRMs perform approximately as well as CILP++ (França et al., 2014), but are worse than either the GNN (Dash et al., 2022) or DRM (Dash et al., 2019). However, Figure 9 are best treated as preliminary. Variations in CRMs arise in Procedure 2 purely due to sampling, of course. However, the CRM obtained is also affected by the following: (1) The subset constraints on support and precision all feature-clauses in the CRM; (2) bounds on the depth of compositions ρ_2 followed by ρ_1 operators; (3) The number of feature-clauses drawn in each layer of the CRM. Additional variation can arise from the initialisation of weights for the SGD-based estimation of parameters. This suggests that substantially more experimentation is needed to see if the predictive performance of Simple CRMs can be improved. We note also that the DRM uses substantially more complex features than the Simple CRM, and that CILP++ constructs substantially more features than the Simple CRM (anywhere between 30,000 to 50,000 compared to about 330 M-simple features for the CRMs). Of

course none of GNN, DRM or CILP++ have any intrinsic mechanism of associating explanations with their prediction.

5 Related Work

We note first that ρ_1 and ρ_2 are closely related to the notion of refinement operators which have been studied extensively in ILP, in the context of the search through a hypothesis space (see (Tamaddoni-Nezhad and Muggleton, 2009; Nienhuys-Cheng et al., 1997)). Our motivation in this paper is, however, in the use of these operators to derive relational features. Consequently, we describe connections to related work in 3 categories: conceptual work on relational features; implementation and applied work on propositionalisation in ILP; and work on explainable deep networks.

On the conceptual understanding of relational features, perhaps the most relevant single summary is in (Saha et al., 2012). There the authors identify several feature-classes, based on somewhat similar notions of source- and sink-literals. The relationship between the different classes in that paper is shown in Figure 10(a). The relationship to these sets of the class of M-simple feature-clauses, denoted here as F_M , is shown in Figure 10(b) (see Appendix E for more details).

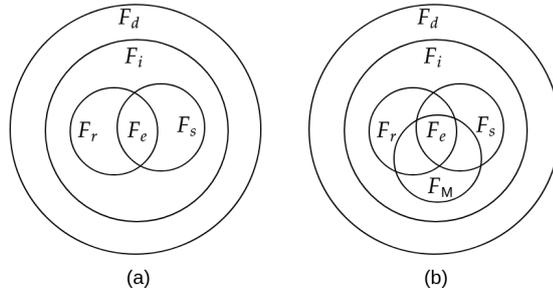


Fig. 10: The feature classes proposed in (Saha et al., 2012): (a) and the relationship to the class of M-simple features (b).

Simple clauses in (McCreath, 1999) and the corresponding set of features in F_s are restricted to determinate predicate-definitions.¹³ Results in (McCreath, 1999) show that features from F_s can be used to derive the subset of feature-clauses in F_d that only contain determinate predicate-definitions. There is no such restriction imposed on F_M and all clauses in F_d (and therefore all other classes shown) can be derived using some composition of ρ_1 and ρ_2 . No corresponding operators or completeness results are known for F_r .

Relational features have been shown to be an extremely effective form of learning with relational objects (Kramer et al., 2001; Lavrač et al., 2021). Methods that construct and use relational features, guided by some form of mode-declarations can be found in (Srinivasan and King, 1999; Lavrač et al., 2002; Ramakrishnan

¹³ Informally, a *determinate* predicate is one whose definition encodes a function. That is, for a given set of values for input arguments, there is exactly one set of values for output arguments.

et al., 2007; Joshi et al., 2008; Specia et al., 2009; Faruque et al., 2012; Saha et al., 2012; França et al., 2014; Vig et al., 2017; Dash et al., 2018). Of these, the features in Lavrač et al. (2002) are from the feature class F_r . There are no reports on the class of features used in the other reports, although the procedures for obtaining the features suggest that they are not restricted to any specific sub-class (that is, they are simply from F_d). Given our results on derivation of features in F_d from features in F_M , and the class-inclusions shown, we would expect at least some features in a super-class would require additional composition operations to those in a sub-class. In terms of a CRM structure, we would expect features in F_i , for example, would usually be associated with vertices at a greater depth than those in F_r . Empirical results tabulated for some statistical learners in (Saha et al., 2012) suggest that relational features from the class F_i were most useful for statistical learners. If this empirical trend continues to hold, then we would expect the performance of CRMs to improve as depth increases (and features in F_i are derived), and then to flatten or decrease (as features in $F_d \setminus F_i$ are derived).

The development and application of CRMs is most closely related to the area of *self-explainable* deep neural networks (Alvarez Melis and Jaakkola, 2018; Angelov and Soares, 2020; Ras et al., 2022). The structure of the CRM enforces a meaning to each node in the network, and in turn, we have shown here how to extract one form of explanation from these meanings. A different kind of neural network, also with meanings associated nodes is described in (Sourek et al., 2018). Those networks are also explainable, although not in the manner described here. In (Srinivasan et al., 2019), a symbolic proxy-explainer is constructed using ILP for a form of multi-layer perceptron (MLP) that uses as input values of relational features. The features there drawn from the class F_d , and the explanations are logical rules constructed by ILP using the feature-definitions provided to the MLP. There are at least two important differences to the explanations constructed there and the ones obtained with a CRM: (i) The rules constructed in (Srinivasan et al., 2019) effectively only perform the ρ_2 operation on relational features. This can result in a form of incompleteness: some features in F_d cannot be represented by the rules, unless they are already included as input to the MLP; and (ii) The structuring of explanations in (Srinivasan et al., 2019) requires relevance information: here, the structuring is from usual functional (de)composition.

6 Conclusion

It has been long-understood in machine learning that the choice of representation can make a significant difference to the performance and efficiency of a machine learning technique. Representation is also clearly of relevance when we are interested in constructing human-understandable explanations for predictions made by the machine learning technique. A form of machine learning that has paid particular attention to issues of representation is the area of Inductive Logic Programming (ILP). A form of representation that has been of special interest in ILP is that of a *relational feature*. These are Boolean-valued functions defined over objects, using definitions of relations provided as prior- or background knowledge. The use of relational features forms the basis of an extremely effective form of ILP called *propositionalisation*. This obtains a Boolean-vector description of objects in the data, using the definition of the relational features and the background

knowledge. Despite the obvious successes of propositionalisation, surprising little is known, conceptually, about the space of relational features. In this paper, we have sought to address this by examining relational features within a mode-language M , introduced in ILP within the setting of mode-directed inverse entailment (Muggleton, 1995). Within a mode-language, we identify the notion of M -simple relational features, and two operations ρ_1 and ρ_2 that allows us to compose progressively more complex relational feature in the mode-language. In the first half of the paper, we show that ρ_1 and ρ_2 are sufficient to derive all relational features within a mode-language M . This generalises a previous result due to McCreath and Sharma (1998b), which was restricted to determinate definitions for predicates in the background knowledge, albeit starting from a different definition of simple features to that work.

In the second half of the paper, we use the notion of M -simple features and the composition operators ρ_1 and ρ_2 to construct a kind of deep neural network called a Compositional Relational Machine, or CRM. A special aspect of CRMs is that we are able to associate a relational feature with each node in the network. The structure of the CRM allows us to identify further how the feature at the node progressively decomposes into simpler features, until an underlying set of M -simple features are reached. This corresponds well to the intuitive notion of a structured explanation, that is composed of increasingly simpler components. We show how this aspect of CRMs allows them to be used as “explanation machines” for black-box models. Our results on synthetic and real-data suggest that CRMs can reproduce target-predictions with high fidelity; and the explanations constructed on synthetic data suggest that CRM’s explanatory structure usually also contains an acceptable explanation.

We have not explored the power of CRMs as “white-box” predictors in their own right, but early results suggest that it may be possible to obtain CRMs with good predictive accuracy. Although still significantly lower than the state-of-the-art, we believe this can change. We have also not explored other forms of CRMs, both simpler and more elaborate. For example, the identification of M -simple features and their subsequent compositions using the ρ -operators suggests an even simpler CRM structures than that used here. It is possible for example, simply to obtain all possible compositions to some depth, and use a Winnow-like parameter estimation (Littlestone, 1988) to obtain a self-explainable linear model. Equally, more complex CRMs are possible by incorporating weights on the M -simple features (this could be implemented simply by changing the activation function at the input nodes of the network). Taking this one step further, it is possible to associate weights with all the relational features, which will allow the use of the inference machinery of probabilistic logic programs (De Raedt et al., 2019). We think an investigation of these other kinds of compositional relational machines would contribute positively to the growing body of work in human-intelligible machine learning.

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Declaration

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Data and code availability All data and codes used in our research can be found at: <https://github.com/tirtharajdash/CRM>.

Authors' contributions AS and AB conceived and worked on the conceptual parts related to simple features and their composition, and the specification of CRMs. TD conceived and worked on the implementation of CRMs as gated neural networks. AS and TD conceived and worked on the application of CRMs to synthetic- and real-data. DS was involved in some parts of the implementation of CRMs.

Appendices

A Logic Terminology

In this section we cover only terminology used in the paper, and further confined largely to logic programming. For additional background and further terminology see (Lloyd, 2012; Chang and Lee, 2014; Nilsson, 1991; Muggleton and de Raedt, 1994). The summary below is adapted from (Srinivasan et al., 2019).

A language of first order logic programs has a vocabulary of constants, variables, function symbols, predicate symbols, logical implication ‘ \leftarrow ’, and punctuation symbols. A function or predicate can have a number of arguments known as *terms*. Terms are defined recursively. A constant symbol (or simply “constant”) is a term. A variable symbol (or simply “variable”) is a term. If f is an m -ary function symbol, and t_1, \dots, t_m are terms, then the function $f(t_1, \dots, t_m)$ is a term. A term is said to be *ground* if it contains no variables.

We use the convention used in logic programming when writing clauses. Thus, predicate, function and constant symbols are written as a lower-case letter followed by a string of lower- or upper-case letters, digits or underscores (‘_’). Variables are written similarly, except that the first letter must be upper-case. This is different to the usual logical notation, where predicate-symbols start with upper-case, and variables start with lower-case: however the logic programming syntax is useful for the implementation of CRMs. Usually, predicate symbols will be denoted by symbols like p, q, r , etc., and symbols like X, Y, Z to denote variables. If p is an n -ary predicate symbol, and t_1, \dots, t_n are terms, then the predicate $p(t_1, \dots, t_n)$ is an atom. Predicates with the same predicate symbol but different arities are distinguished by the notation p/n where p is a predicate of arity n .

A literal is either an atom or the negation of an atom. If a literal is an atom it is referred to as a positive literal, otherwise it is a negative literal. A clause is a disjunction of the form $A_1 \vee \dots \vee A_i \vee \neg A_{i+1} \vee \dots \vee \neg A_k$, where each A_j is an atom. Alternatively, such a clause may be represented as an implication (or “rule”) $A_1, \dots, A_i \leftarrow A_{i+1}, \dots, A_k$. A definite clause $A_1 \leftarrow A_2, \dots, A_k$ has exactly one positive literal, called the *head* of the clause, with the literals A_2, \dots, A_k known as the *body* of the clause. A definite clause with a single literal is called a *unit* clause, and a clause with at most one positive literal is called a Horn clause. A set of Horn clauses is referred to as a logic program. It is often useful to represent a clause as a set of literals.

A *substitution* θ is a finite set $\{v_1/t_1, \dots, v_n/t_n\}$ mapping a set of n distinct variables v_i , $1 \leq i \leq n$, to terms t_j , $1 \leq j \leq n$ such that no term is identical to any of the variables. A substitution containing only ground terms is a *ground* substitution. For substitution θ and clause C the expression $C\theta$ denotes the clause where every occurrence C of a variable from θ is replaced by the corresponding term from θ . If θ is a ground substitution then $C\theta$ is called a ground clause. Since a clause is a set, for two clauses C, D , the set inclusion $C\theta \subseteq D$ is a partial order called *subsumption*, usually written $C \theta$ -subsumes D and denoted by $C \preceq D$. For a set of clauses S and the subsumption ordering \preceq , we have that for every pair of clauses $C, D \in S$, there is a least upper bound and greatest lower bound, called, respectively, the least general generalisation (lgg) and most general unifier (mgu)

of C and D , which are unique up to variable renaming. The subsumption partial ordering on clauses enables the definition of a lattice, called the *subsumption lattice*.

We assume the logic contains axioms allowing for inference using the equality predicate $=/2$. This includes axioms for reflexivity ($\forall x(x = x)$), and substitution ($\forall x(\phi(x) \wedge (x = y) \rightarrow \phi(y))$).

B Mode Language

We borrow some of the following definitions from (Dash et al., 2022). The definition of $\lambda\mu$ sequence is simplified as we are dealing only with feature clauses here and all other definitions are same as in (Dash et al., 2022).

Definition 17 (Term Place-Numbering) Let $\pi = \langle i_1, \dots, i_k \rangle$ be a sequence of natural numbers. We say that a term τ is in place-number π of a literal λ iff: (1) $\pi \neq \langle \rangle$; and (2) τ is the term at place-number $\langle i_2, \dots, i_k \rangle$ in the term at the i_1^{th} argument of λ . τ is at a place-number π in term τ' : (1) if $\pi = \langle \rangle$ then $\tau = \tau'$; and (2) if $\pi = \langle i_1, \dots, i_k \rangle$ then τ' is a term of the form $f(t_1, \dots, t_m)$, $i_1 \leq m$ and τ is in place-number $\langle i_2, \dots, i_k \rangle$ in t_{i_1} .

Definition 18 (Type-Names and Type-Definitions) Let Γ be a set of types and \mathbb{T} be a set of ground-terms. For $\gamma \in \Gamma$ we define a set of ground-terms $T_\gamma = \{\tau_1, \tau_2, \dots\}$, where $\tau_i \in \mathbb{T}$. We will say a ground-term τ_i is of type γ if $\tau_i \in T_\gamma$, and denote by T_Γ the set $\{T_\gamma : \gamma \in \Gamma\}$. T_Γ will be called a set of type-definitions.

Definition 19 (Mode-Declaration)

- (a) Let Γ be a set of type names. A mode-term is defined recursively as one of: (i) $+\gamma$, $-\gamma$ or $\#\gamma$ for some $\gamma \in \Gamma$; or (ii) $\phi(mt'_1, mt'_2, \dots, mt'_j)$, where ϕ is a function symbol of arity j , and the mt'_k s are mode-terms.
- (b) A mode-declaration μ is of the form $modeh(\lambda')$ or $modeb(\lambda')$. Here λ' is a ground-literal of the form $p(mt_1, mt_2, \dots, mt_n)$ where p is a predicate name with arity n , and the mt_i are mode-terms. We will say μ is a *modeh*-declaration (resp. *modeb*-declaration) for the predicate-symbol p/n . In general there can be several *modeh* or *modeb*-declarations for a predicate-symbol p/n . We will use $ModeLit(\mu)$ to denote λ' .
- (c) μ is said to be a mode-declaration for a literal λ iff λ and $ModeLit(\mu)$ have the same predicate symbol and arity.
- (d) Let τ be the term at place-number π in μ . We define

$$ModeType(\mu, \pi) = \begin{cases} (+, \gamma) & \text{if } \tau = +\gamma \\ (-, \gamma) & \text{if } \tau = -\gamma \\ (\#, \gamma) & \text{if } \tau = \#\gamma \\ unknown & \text{otherwise} \end{cases}$$

- (e) If μ is a mode-declaration for literal λ , $ModeType(\mu, \pi) = (+, \gamma)$ for some place-number π , τ is the term at place π in λ , then we will say τ is an input-term of type γ in λ given μ (or simply τ is an input-term of type γ). Similarly we define output-terms and constant-terms.

We will also say that mode μ contains an input argument of type γ if there exists some term-place π of μ s.t. $ModeType(\mu, \pi) = (+, \gamma)$. Similarly for output arguments.

Definition 20 ($\lambda\mu$ -Sequence) Assume a set of type-definitions T_Γ , modes M . Let $\langle C \rangle = \langle l_1, \neg l_2, l_3, \dots, \neg l_k \rangle$ be an ordered clause. Then $\langle (\lambda_1, \mu_1), (\lambda_2, \mu_2), \dots, (\lambda_k, \mu_k) \rangle$ is said to be a $\lambda\mu$ -sequence for $\langle C \rangle$ iff it satisfies the following constraints:

Match. (i) $\lambda_i = l_i$; (ii) For $j = 1, \dots, k$, μ_j is a mode-declaration for λ_j s.t. $\mu_j = modeh(\cdot)$ ($j = 1$) and $\mu_j = modeb(\cdot)$ ($j > 1$).

Terms. (i) If τ is an input- or output-term in λ_j given μ_j , then τ is a variable in λ_j ; (ii) Otherwise if τ is a constant-term in λ_j given μ_j then τ is a ground term.

Types. (i) If there is a variable v in both λ_i, λ_j then the type of v in λ_i given μ_i is the same as the type of v in λ_j given μ_j ; (ii) If τ is a constant-term in λ_i and the type of τ in λ_i given μ_i is γ , then $\tau \in T_\gamma$.

Ordering. (i) If τ is an input-term in λ_j given μ_j and $j > 1$ then there is an input-term τ in λ_1 given μ_1 ; or there is an output-term τ in λ_i ($m < i < j$) given μ_i . (ii) If τ is an output-term in λ_1 given μ_1 , then τ is an output-term of some λ_i ($1 < i \leq k$) given μ_i .

Definition 21 (Mode-Language) Assume a set of type-definitions T and modes M . The mode-language $\mathcal{L}_{M,T}$ is $\{\langle C \rangle : \text{either } C = \emptyset \text{ or there exists a } \lambda\mu\text{-sequence for } \langle C \rangle\}$.

C Proof of the Derivation Lemma

Lemma 2 (Derivation Lemma) Given M, M' and $\Omega = \{\rho_1, \rho_2\}$ as before. Let $\langle C \rangle$ be an ordered clause in $\mathcal{L}_{M,T}$, with head $p(X)$. Let S be a set of ordered M -simple clauses in $\mathcal{L}_{M,T}$, with heads $p(X)$ and all other variables of clauses in S standardised apart from each other and from C . If there exists a substitution θ s.t. $Basis(\langle C \rangle) \subseteq S\theta$ then there exists an ordered clause $\langle C' \rangle$ in $\mathcal{L}_{M',T}$ such that $\langle C' \rangle$ is equivalent to $\langle C \rangle$ and derivable from S using Ω .

Proof We prove this in 3 parts:

1. We first show: if $Basis(\langle C \rangle) \subseteq S\theta$, then θ is a type-consistent substitution for clauses in S .

Let $Basis(\langle C \rangle) = \{\langle C_1 \rangle, \dots, \langle C_k \rangle\}$ and $S' = \{\langle S_1 \rangle, \dots, \langle S_k \rangle\} \subseteq S$. Without loss of generality, let $\langle S_i \rangle \theta = \langle C_i \rangle$. Let $\theta = \{Y_1/t_1, Y_2/t_2, \dots, Y_n/t_n\}$ where the Y_i are variables in S and the t_i are terms in $Basis(\langle C \rangle)$. In general, the t_i 's are variables, constants, or functional terms. Let t_j be a constant. Suppose clause S_i has the variable Y_j in some location in S_i and clause C_i has the constant t_j in the corresponding location. Since both S_i and C_i are in $\mathcal{L}_{M,T}$, this is only possible if there are multiple mode-declarations for the corresponding literals in S_i and C_i . But constraint MC2 (in [Section 2.2](#)) ensures that there is exactly one mode-declaration for any literal. Therefore t_i cannot be a constant. Reasoning similarly, t_i cannot be a functional term. Therefore t_i has to be a variable in C_i . Since Y_j and t_j are in the

same locations for some literal l in S_i and C_i , and there is only one mode-declaration for l in M , it follows that the types of Y_j and t_j must be the same.

2. If there exists a type-consistent substitution θ for clauses in S , then there is an ordered clause $\langle C'' \rangle$ in $Closure_{\{\rho_2\}}(S)$ s.t. $C''\theta \equiv C$.

Let us fix an ordering among the simple clauses in S : S_1, \dots, S_k , where $S_i = p(X) \leftarrow Body_i(X, \mathbf{Y}_i)$. Let us define a sequence of ordered clauses $\langle C_1 \rangle, \langle C_2 \rangle, \dots, \langle C_k \rangle$ where $\langle C_1 \rangle$ is $\langle S_1 \rangle$, and $\langle C_i \rangle$ is in $\rho_2(\langle C_{i-1} \rangle, \langle S_i \rangle)$ for $i = 2$ to k . It is easy to see that the above sequence is a derivation sequence of $\langle C_k \rangle$ from $\{\langle S_1 \rangle, \langle S_2 \rangle, \dots, \langle S_k \rangle\}$ using $\{\rho_2\}$. That is, $\langle C_k \rangle$ is in $Closure_{\{\rho_2\}}(S)$. $\langle C_k \rangle$ is of the form $p(X) \leftarrow Body_1(X, \mathbf{Y}_1), Body_2(X, \mathbf{Y}_2), \dots, Body_k(X, \mathbf{Y}_k)$. That is $C_k = \bigcup_{i=1}^k S_i$. Since $S\theta = Basis(\langle C \rangle)$, then $C = \bigcup_{i=1}^k S_i\theta$. Let $\langle C'' \rangle = \langle C_k \rangle$. That is, $C''\theta = C$. Hence $C''\theta \equiv C$. Also, since θ is a type-consistent substitution for clauses $S_i \in S$, and $C'' = \bigcup_i S_i$, θ is a type-consistent substitution for C'' .

3. From above $\langle C'' \rangle$ and θ , we construct an ordered clause $\langle C' \rangle$ in $\mathcal{L}_{M', T}$ s.t. $\langle C' \rangle$ is in $Closure_{\{\rho_1\}}(\{\langle C'' \rangle\})$ and $C''\theta \equiv C'$.

Let $\langle C'' \rangle = (p(X) \leftarrow Body(X, \mathbf{Y}))$, and $\theta = \{Y_1/Y'_1, \dots, Y_l/Y'_l\}$. It is easy to see that θ induces an equivalence relation on the variables in C'' . Variables Y_i and Y_j are in the same equivalence class if both variables map to the same variable Y'_m . For each equivalence class $[U]$, we earmark one element in the class as representative of the class. This element is denoted by $rep([U])$. Let C'' be $p(X) \leftarrow Body(X, \mathbf{Y})$. Let us fix an order among the variables occurring in $\langle C'' \rangle$: Y_1, Y_2, \dots, Y_l . Consider the following sequence of ordered clauses $\langle C_0 \rangle, \langle C_1 \rangle, \dots, \langle C_l \rangle$ where $\langle C_0 \rangle = \langle C'' \rangle$, and $\langle C_i \rangle = p(X) \leftarrow Body(X, \mathbf{Y}), Y_1 = rep([Y_1]), Y_2 = rep([Y_2]), \dots, Y_l = rep([Y_l])$. The above sequence is a derivation of $\langle C_l \rangle$ from $\langle C'' \rangle$ using only ρ_1 . That is $\langle C_l \rangle$ is in $Closure_{\{\rho_1\}}(\{\langle C'' \rangle\})$. Let $\langle C' \rangle$ be $\langle C_l \rangle$ and it is of the form $p(X) \leftarrow Body(X, \mathbf{Y}), Y_1 = rep([Y_1]), \dots, Y_l = rep([Y_l])$. It is easy to see that $\langle C' \rangle \in \mathcal{L}_{M', T}$. We now show $C''\theta \equiv C'$. Let $\theta = \theta'' \circ \theta'$, where $\theta'' = \{Y_1/rep([Y_1]), \dots, Y_l/rep([Y_l])\}$ and $\theta' = \{rep([Y_1])/Y'_1, \dots, rep([Y_l])/Y'_l\}$.¹⁴ The variables $rep([Y_i])$ are in S and the variables Y'_i are in C . Since the variables in S are standardised apart from the variables in C , θ' is a renaming substitution. Therefore $C''\theta' \equiv C''$. Therefore $C''\theta \equiv C''\theta''$. By the substitution axiom in the equality logic $C''\theta'' \equiv C'$. Therefore $C''\theta \equiv C'$.

From (1)–(3) above, the result follows. \blacksquare

D Properties of Derivations using ρ_1, ρ_2

Lemma 4 (Reordering Lemma) *Given M, M' and a set of ordered clauses Φ . If an ordered clause $\langle C \rangle$ is derivable from Φ using $\{\rho_1, \rho_2\}$ then: (a) there is a derivation*

¹⁴ Correctly, θ' and θ'' have to be functions. It is evident that θ'' is a function, since each variable maps to the representative of its equivalence class. We argue informally that θ' is a function as follows. If Y_i and Y_j are in the same equivalence class, then $rep([Y_i])$ and $rep([Y_j])$ are the same variables. But according to our θ' , they are mapped to Y'_i and Y'_j . One might think θ' is not a function. But the variables in the same equivalence class are mapped to same variable. So Y'_i is the same as Y'_j and hence θ' is a function.

for $\langle C_j \rangle$ from Φ using $\{\rho_2\}$; (b) there is a derivation for $\langle C_k \rangle$ from $\{\langle C_j \rangle\}$ using $\{\rho_1\}$; and (c) $\langle C \rangle$ is equivalent to $\langle C_k \rangle$.

Proof Let us assume there is a derivation τ for $\langle C \rangle$ from Φ using $\{\rho_1, \rho_2\}$. There exists an ordered clause $\langle C_k \rangle$ equivalent to $\langle C \rangle = p(X) \leftarrow l_1, l_2, \dots, l_j, l_{j+1}, l_{j+2}, \dots, l_k$ such that

- the sequence of literals l_1, \dots, l_j can be split into $Body(X, Y_1), \dots, Body(X, Y_m)$ such that $p(X) \leftarrow Body(X, Y_i) \in \Phi$ for each $i = 1, \dots, m$, and
- l_{j+1}, \dots, l_k are equality predicates introduced using ρ_1 operator in the derivation τ . Let $\langle C_j \rangle$ be $p(X) \leftarrow Body(X, Y_1), \dots, Body(X, Y_m)$.

It is easy to see that there is derivation τ_1 for $\langle C_j \rangle$ from Φ using ρ_2 operator. Now we can apply ρ_1 operator on $\langle C_j \rangle$ repeatedly to derive $\langle C_k \rangle$. ■

Lemma 5 *Given M, M' and a set of ordered clauses Φ . If an ordered clause $\langle C \rangle$ is derivable from Φ using $\{\rho_2\}$ then it is linearly derivable from Φ using $\{\rho_2\}$.*

Proof Let us assume that $\langle C \rangle$ is derivable from Φ using $\{\rho_2\}$. Hence there exists a derivation sequence ξ of ordered clauses $\langle C_1 \rangle, \langle C_2 \rangle, \dots, \langle C_n \rangle$ from Φ using $\{\rho_2\}$ and $\langle C_n \rangle = \langle C \rangle$. Now we use mathematical induction to prove that for each $1 \leq i \leq n$, there exists a linear derivation of $\langle C_i \rangle$ from Φ using $\{\rho_2\}$.

Base step: Case $n = 1$ is easy as $\langle C_1 \rangle$ should be in Φ and hence there is a linear derivation for $\langle C_1 \rangle$ from Φ using $\{\rho_2\}$.

Induction step: We assume there exists a linear derivation for $\langle C_i \rangle$ from Φ using $\{\rho_2\}$ for each $i < j$ (induction hypothesis) and prove that there exists a linear derivation for $\langle C_j \rangle$. The clause $\langle C_j \rangle$ occurs in the derivation sequence ξ . There are two cases to be considered: it is in Φ or it is in $\rho_2(\langle C_l \rangle, \langle C_m \rangle)$ where $l, m < j$. If $\langle C_j \rangle$ is in Φ , there exists a linear derivation sequence for $\langle C_j \rangle$ from Φ (just the one step derivation containing itself). Now we prove the claim for the second case. Since $l, m < j$, by induction hypothesis, there exist linear derivation sequences ξ_l for $\langle C_l \rangle$ and ξ_m for $\langle C_m \rangle$ from Φ using $\{\rho_2\}$. Let $\langle C'_1 \rangle, \langle C'_2 \rangle, \dots, \langle C'_k \rangle$ be the clauses in Φ and occurring in ξ_m . Now consider the following sequence ξ_j containing $\xi_l, \langle C'_1 \rangle, \langle C''_1 \rangle, \langle C'_2 \rangle, \langle C''_2 \rangle, \dots, \langle C'_k \rangle, \langle C''_k \rangle$ where $\langle C''_1 \rangle \in \rho_2(\langle C_l \rangle, \langle C'_1 \rangle)$ and $\langle C''_a \rangle \in \rho_2(\langle C''_{a-1} \rangle, \langle C'_a \rangle)$ for $a = 2$ to k . It is easy to see that ξ_j is a linear derivation sequence for $\langle C_j \rangle$ from Φ using ρ_2 . Hence there exists a linear derivation sequence for $\langle C_n \rangle$ from Φ using $\{\rho_2\}$. ■

Now the linear derivation lemma (re-stated below) can be easily proved by combining the above two lemmas.

Lemma 3 (Linear Derivation Lemma) *Given M, M' and a set of ordered clauses Φ . If an ordered clause $\langle C \rangle$ is derivable from Φ using $\{\rho_1, \rho_2\}$ then there exists an equivalent ordered clause $\langle C' \rangle$ and it is linearly derivable from Φ using $\{\rho_1, \rho_2\}$.*

E Relationship of M-Simple Feature-Clauses to Known Feature Classes

We note the following about the sets of feature-clauses in Figure 10(b) and the set F_M of M-simple feature clauses:

The set F_d . This is identical to the set of ordered feature-clauses in the mode-language M;

The set F_i . This set is defined based on a given mode language M (but without constraints MC–MC3). An ordered feature clause $\langle C \rangle$ is in F_i iff the number of connected components after removing the source vertex (corresponding to the head literal) from the clause dependency graph of $\langle C \rangle$ is exactly one. Since the clause dependency graph of a clause in F_M has exactly one sink literal and any vertex in that graph has a path to that sink vertex (Remark 2). So the number of connected components after removing the source vertex is one. Hence $F_M \subseteq F_i$. It is easy to see that $F_i \not\subseteq F_M$ (see the counterexample given for $F_s \subseteq F_M$).

The set F_s . This set is defined based on the class of *simple* clauses identified by McCreath (1999) who proposed *simple clauses*. We note:

1. Feature-clause definitions in F_s do not refer to a mode-language. The clause dependency-graph is constructed using a procedure described in (McCreath, 1999), and is based on the re-occurrence of variables (without any reference to input or output variables or types). M-simple feature-clauses require a mode-language, with the constraints MC1–MC3;
2. $F_M \not\subseteq F_s$. For example assume a mode language $p(+int), q(+int, -int), r(+int)$ and the feature-clause $p(X) \leftarrow q(X, X), r(X)$. The clause dependency-graph of this clause has only one sink vertex and so it is in F_M . But this is not in F_s since the directed graph associated with this clause has two sink literals.
3. $F_s \not\subseteq F_M$. For example assume a mode language $p(+int), q(+int, -int), r(+int, -int)$ and the feature-clause $p(X) \leftarrow q(X, Y), r(X, Y)$. This is in F_s , but is not in F_M . The clause dependency-graph described in this paper doesn't have an edge between the vertices for q and r resulting in two sink vertices. But the dependency graph constructed in (McCreath, 1999) will have an edge between the vertices for q and r because of the shared variable y .

The set F_r . The set F_r consist of feature-clauses designed for *subgroup discovery* in relational data (Lavrač et al., 2002). Then:

1. Feature-clauses in F_r do require a mode-language, and we can construct a clause dependency-graph as described here. The clause dependency-graph for feature-clauses in F_r have exactly one component, and all new existential variables introduced by a source literal appear in source or sink literals.
2. $F_M \not\subseteq F_r$. For example assume a mode language $p(+int), q(+int, -int)$ and the clause $p(X) \leftarrow q(X, Y)$. This is a M-simple clause but not in F_r as the existential variable introduced at the source literal q but it is not appearing later.
3. $F_r \not\subseteq F_M$. For example assume a mode language $p(+train), has_car(+train, -car), short(+car), closed(+car)$ and the clause $p(X) \leftarrow has_car(X, Y), short(Y), closed(Y)$. This is not M-simple clause there are two sink literals in it but it is in F_r .

F Additional Details Relevant to the Experiments

F.1 Examples of Mode Declarations and Simple Feature-Clauses

Figure 11–Figure 13 show examples of mode declarations used for the experiments. Also shown are examples of M-simple feature-clauses constructed automatically from the mode-declarations.

Modes	M-simple feature clauses
<code>modeh(p(+tr))</code>	$p(A) \leftarrow has_car(A, B)$
<code>modeb(short(+car))</code>	$p(A) \leftarrow has_car(A, B), short(B)$
<code>modeb(closed(+car))</code>	$p(A) \leftarrow has_car(A, B), closed(B)$
<code>modeb(long(+car))</code>	$p(A) \leftarrow has_car(A, B), long(B)$
<code>modeb(open_car(+car))</code>	$p(A) \leftarrow has_car(A, B), open_car(B)$
<code>modeb(double(+car))</code>	$p(A) \leftarrow has_car(A, B), double(B)$
<code>modeb(jagged(+car))</code>	$p(A) \leftarrow has_car(A, B), jagged(B)$
<code>modeb(shape(+car, #shape))</code>	$p(A) \leftarrow has_car(A, B), shape(B, u_shaped)$
<code>modeb(load(+car, #shape, #int))</code>	$p(A) \leftarrow has_car(A, B), shape(B, rectangle)$
<code>modeb(wheels(+car, #int))</code>	$p(A) \leftarrow has_car(A, B), shape(B, hexagon)$
<code>modeb(has_car(+tr, -car))</code>	$p(A) \leftarrow has_car(A, B), wheels(B, 3)$
	$p(A) \leftarrow has_car(A, B), wheels(B, 2)$
	$p(A) \leftarrow has_car(A, B), load(B, circle, 3)$
	$p(A) \leftarrow has_car(A, B), load(B, rectangle, 3)$
	$p(A) \leftarrow has_car(A, B), load(B, hexagon, 3)$
	$p(A) \leftarrow has_car(A, B), load(B, circle, 2)$
	\vdots

Fig. 11: Examples of mode-definitions and simple feature-clauses for the Trains problem.

F.2 Debugging Inconsistent Explanations from the CRM

For the Chess problem, 1044 instances (out of 10,000) are inconsistently explained. That is, the explanation graph from the most relevant output vertex does not contain an acceptable feature-clause. Further examination reveals: (a) for all 1044 instances, the predictions made by the CRM are correct; (b) a majority (1033/1044) of the inconsistently instances are + examples for which the White King and Black King are on adjacent files and ranks (the corresponding acceptable feature-clause is $p((A, B, C, D, E, F)) \leftarrow adj(A, E), adj(B, F)$). We find there are 19 distinct ‘buggy explanations’ produced by the CRM for the inconsistently explained data. The corresponding feature-clauses at the ‘root’ in the explanation graph are listed in Figure 14 (for simplicity, we do not show the simpler features and the full graph structure):

Modes	M-simple feature clauses
<code>modeh(p((+wkfile,+wkrank,+wrfile, +wrrank,+bkfile,+bkrank)))</code>	$p((A, B, C, D, E, F)) \leftarrow C = E$
<code>modeb(lt(+wkfile,+wkrank))</code>	$p((A, B, C, D, E, F)) \leftarrow B = D$
<code>modeb(lt(+wkrank,+bkrank))</code>	$p((A, B, C, D, E, F)) \leftarrow B = F$
<code>modeb(lt(+wkrank,+wkrank))</code>	$p((A, B, C, D, E, F)) \leftarrow D = F$
<code>modeb(lt(+wrrank,+wkrank))</code>	$p((A, B, C, D, E, F)) \leftarrow \text{adj}(A, C)$
<code>modeb(lt(+wrrank,+bkrank))</code>	$p((A, B, C, D, E, F)) \leftarrow \text{adj}(A, E)$
<code>modeb(lt(+bkrank,+wkrank))</code>	$p((A, B, C, D, E, F)) \leftarrow \text{adj}(C, E)$
<code>modeb(lt(+bkrank,+wrrank))</code>	$p((A, B, C, D, E, F)) \leftarrow \text{adj}(B, D)$
<code>modeb(lt(+wkfile,+wrfile))</code>	$p((A, B, C, D, E, F)) \leftarrow \text{adj}(B, F)$
<code>modeb(lt(+wkfile,+bkfile))</code>	$p((A, B, C, D, E, F)) \leftarrow \text{adj}(D, F)$
<code>modeb(lt(+wrfile,+wkfile))</code>	$p((A, B, C, D, E, F)) \leftarrow \text{lt}(A, C)$
<code>modeb(lt(+wrfile,+bkfile))</code>	$p((A, B, C, D, E, F)) \leftarrow \text{lt}(C, A)$
<code>modeb(lt(+bkfile,+wkfile))</code>	$p((A, B, C, D, E, F)) \leftarrow \text{lt}(A, E)$
<code>modeb(lt(+bkfile,+wrfile))</code>	$p((A, B, C, D, E, F)) \leftarrow \text{lt}(E, A)$
<code>modeb(adj(+wkrank,+wrrank))</code>	$p((A, B, C, D, E, F)) \leftarrow \text{lt}(C, E)$
<code>modeb(adj(+wkrank,+bkrank))</code>	$p((A, B, C, D, E, F)) \leftarrow \text{lt}(E, C)$
<code>modeb(adj(+wrrank,+bkrank))</code>	$p((A, B, C, D, E, F)) \leftarrow \text{lt}(B, D)$
<code>modeb(adj(+wkfile,+wrfile))</code>	$p((A, B, C, D, E, F)) \leftarrow \text{lt}(D, B)$
<code>modeb(adj(+wkfile,+bkfile))</code>	$p((A, B, C, D, E, F)) \leftarrow \text{lt}(B, F)$
<code>modeb(adj(+wrfile,+bkfile))</code>	$p((A, B, C, D, E, F)) \leftarrow \text{lt}(F, B)$
<code>modeb((+wkrank = +wrrank))</code>	$p((A, B, C, D, E, F)) \leftarrow \text{lt}(D, F)$
<code>modeb((+wkrank = +bkrank))</code>	$p((A, B, C, D, E, F)) \leftarrow \text{lt}(F, D)$
<code>modeb((+wrrank = +bkrank))</code>	$p((A, B, C, D, E, F)) \leftarrow A = E$
<code>modeb((+wkfile = +wrfile))</code>	$p((A, B, C, D, E, F)) \leftarrow C = E$
<code>modeb((+wkfile = +bkfile))</code>	$p((A, B, C, D, E, F)) \leftarrow B = D$
<code>modeb((+wrfile = +bkfile))</code>	$p((A, B, C, D, E, F)) \leftarrow B = F$
	$p((A, B, C, D, E, F)) \leftarrow D = F$
	$p((A, B, C, D, E, F)) \leftarrow \text{adj}(A, C)$
	$p((A, B, C, D, E, F)) \leftarrow \text{adj}(A, E)$
	$p((A, B, C, D, E, F)) \leftarrow \text{adj}(C, E)$
	\vdots

Fig. 12: Examples of mode-definitions and simple feature-clauses for the Chess problem.

Modes	M-simple feature clauses
<code>modeh(class(+mol, +class))</code>	<code>p(A) ← has_struct(A, B, C, amine), gteq(C, 1)</code>
<code>modeb(symbol(+mol, +atomid, +atomid, #bondtype))</code>	<code>p(A) ← has_struct(A, B, C, ammonium_ion), gteq(C, 1)</code>
<code>modeb(bond(+mol, -atomid_1, -atomid_2, #atomtype, #atomtype, #bondtype))</code>	<code>p(A) ← has_struct(A, B, C, benzene_ring), gteq(C, 1)</code>
<code>modeb(atom(+mol, -atomid, #element))</code>	<code>p(A) ← has_struct(A, B, C, benzene_ring), gteq(C, 2)</code>
<code>modeb(has_struct(+mol, -atomids, -length, #structype))</code>	<code>p(A) ← has_struct(A, B, C, benzene_ring), gteq(C, 3)</code>
<code>modeb(connected(+mol, +atomids, +atomids))</code>	<code>p(A) ← has_struct(A, B, C, benzene_ring), gteq(C, 4)</code>
<code>modeb(fused(+mol, +atomids, +atomids))</code>	<code>p(A) ← has_struct(A, B, C, benzene_ring), gteq(C, 5)</code>
<code>modeb(gteq(+length, #length))</code>	<code>p(A) ← has_struct(A, B, C, benzene_ring), gteq(C, 6)</code>
<code>modeb(lteq(+length, #length))</code>	<code>p(A) ← has_struct(A, B, C, conjug_base_car), gteq(C, 1)</code>
<code>modeb((+atomid = +atomid))</code>	<code>p(A) ← has_struct(A, B, C, conjug_base_car), gteq(C, 2)</code>
<code>modeb((+atomidids = +atomidids))</code>	<code>p(A) ← has_struct(A, B, C, conjug_base_car), gteq(C, 3)</code>
<code>modeb((+length = +length))</code>	<code>p(A) ← has_struct(A, B, C, diazo_group), gteq(C, 1)</code>
	<code>p(A) ← has_struct(A, B, C, diazo_group), gteq(C, 2)</code>
	<code>p(A) ← has_struct(A, B, C, dithio_ester_car), gteq(C, 1)</code>
	<code>p(A) ← has_struct(A, B, C, dithio_ester_car), gteq(C, 2)</code>
	<code>p(A) ← has_struct(A, B, C, dithio_ester_car), gteq(C, 3)</code>
	<code>:</code>

Fig. 13: Examples of mode-definitions and simple feature-clauses for the NCI problem.

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1. $p((A, B, C, D, E, F)) \leftarrow \text{adj}(B, F), \text{lt}(D, B), \text{adj}(C, E)$
 2. $p((A, B, C, D, E, F)) \leftarrow \text{adj}(D, F), B = D, \text{lt}(A, E)$
 3. $p((A, B, C, D, E, F)) \leftarrow \text{adj}(A, E), \text{lt}(A, C), \text{lt}(F, D)$
 4. $p((A, B, C, D, E, F)) \leftarrow \text{lt}(E, C), A = C, \text{lt}(B, F)$
 5. $p((A, B, C, D, E, F)) \leftarrow \text{lt}(E, A), A = C, \text{adj}(A, C)$
 6. $p((A, B, C, D, E, F)) \leftarrow \text{lt}(E, A), \text{lt}(D, B), \text{adj}(A, E)$
 7. $p((A, B, C, D, E, F)) \leftarrow B = D, A = C, \text{adj}(A, E)$
 8. $p((A, B, C, D, E, F)) \leftarrow B = F, A = E, \text{lt}(E, C)$
 9. $p((A, B, C, D, E, F)) \leftarrow \text{lt}(A, C), \text{lt}(B, D), \text{adj}(A, C)$
 10. $p((A, B, C, D, E, F)) \leftarrow \text{lt}(D, F), A = E, \text{lt}(E, C)$
 11. $p((A, B, C, D, E, F)) \leftarrow A = E, \text{adj}(D, F), \text{adj}(B, F)$
 12. $p((A, B, C, D, E, F)) \leftarrow \text{lt}(B, F), \text{lt}(E, C), \text{adj}(D, F)$
 13. $p((A, B, C, D, E, F)) \leftarrow \text{adj}(B, D), \text{lt}(E, A), \text{adj}(A, C)$
 14. $p((A, B, C, D, E, F)) \leftarrow \text{adj}(A, E), \text{lt}(C, E), \text{adj}(B, F)$
 15. $p((A, B, C, D, E, F)) \leftarrow A = E, A = C, \text{adj}(B, F)$
 16. $p((A, B, C, D, E, F)) \leftarrow \text{lt}(A, C), \text{lt}(F, B), \text{adj}(B, F)$
 17. $p((A, B, C, D, E, F)) \leftarrow \text{lt}(D, B), \text{lt}(A, E), \text{adj}(A, E)$
 18. $p((A, B, C, D, E, F)) \leftarrow \text{lt}(E, A), A = C, \text{adj}(B, D)$
 19. $p((A, B, C, D, E, F)) \leftarrow \text{adj}(A, E), B = F, \text{lt}(A, E)$
-

Fig. 14: Buggy explanations produced by the CRM for the inconsistently explained data instances from the Chess problem.

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