Unsupervised Neural-Symbolic Integration

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Abstract
Symbolic has been long considered as a language of human intelligence while neural networks have advantages of robust computation and dealing with noisy data. The integration of neural-symbolic can offer better learning and reasoning while providing a means for interpretability through the representation of symbolic knowledge. Although previous works focus intensively on supervised feedforward neural networks, little has been done for the unsupervised counterparts. In this paper we show how to integrate symbolic knowledge into unsupervised neural networks. We exemplify our approach with knowledge in different forms, including propositional logic for DNA promoter prediction and first-order logic for understanding family relationship.

1 Introduction
An interesting topic in AI is integration of symbolic and neural networks, two different information processing paradigms. While the former is the key of higher level of intelligence the latter is well known for a capability of effective learning from data. In the last two decades, researchers have been working on the idea that combination of the two should offer joint benefits [Towell and Shavlik, 1994; Smolensky, 1995; Avila Garcez and Zaverucha, 1999; Valiant, 2006; Garcez et al., 2008; Penning et al., 2011; Franca et al., 2014; Tran and Garcez, 2016].

In previous work, supervised neural networks have been used intensively for the integration based on the analogy of modus ponens inference with symbolic rules and forward passing in neural networks [Towell and Shavlik, 1994; Avila Garcez and Zaverucha, 1999]. In such networks, due to the discriminative structures only a subset of variables can be inferred, i.e. the variables in the left hand of if-then ← formulas. This may limit their use in general reasoning. Unsupervised network, on the other hand, offers more flexible inference mechanism which seems more suitable for symbolic reasoning. Let us consider an XOR example \( z \leftrightarrow (x \oplus y) \). Here, given the truth values of any two variables one can infer the rest. For supervised networks, a class variable must be discriminated from the others and only it can be inferred. An unsupervised network, in contrast, do not require such discrimination.

Encoding symbolic knowledge in an unsupervised neural network needs a mechanism to convert symbolic formulas to the network without loss of generality. In previous work, Penalty logic shows that any propositional formula can be represented in a symmetric connectionist network (SCN) where inference with rules is equivalent to minimising the network’s energy. However, SCN uses dense connections of hidden and visible units which make the inference very computational. Recent work shows that any propositional formula can be represented in restricted Boltzmann machines [Tran, 2017]. Different from Penalty logic, here the RBM is a simplified version of SCN where there is no visible-visible and hidden-hidden connections. This makes inference in RBMs is easier.

Several attempts have been made recently to integrate symbolic representation and RBMs [Penning et al., 2011; Tran and Garcez, 2016]. Despite achieving good practical results they are still heuristic. In this paper, we show how to encode symbolic knowledge in both propositional and first-order forms into the RBM by extending the theory in [Tran, 2017].

The remainder of this paper is organized as follows. Section 2 review the idea of Confidence rule, a knowledge form to represent symbolic formulas in RBMs. In section 3 we show how to encode knowledge into RBMs. Section 4 presents the empirical verification of our encoding approach and Section 5 concludes the work.

2 Confidence Rules: Revisit
A confidence rule [Tran and d’Avila Garcez, 2013; Tran and Garcez, 2016] is a propositional formula in the form:

\[
c : h \leftrightarrow \bigwedge_{t} x_t \land \bigwedge_{k} \neg x_k
\]

where h is called hypothesis, c is a non-negative real value called confidence value. Inference with a confidence rule is to find the model that makes the hypothesis h holds. If there exist a target variable y the inference of such variable will be similar to modus ponens, as shown in Table 1.

An interesting feature of Confidence rules is that one can represent them in an RBM where Gibbs sampling can be seen
Confidence rule inference
\[ y \leftarrow \bigwedge_t x_t \land \bigwedge_k \neg x_k \quad \text{for } \forall t \in T, \forall k \in K \]

Table 1: Confidence rule and Modus ponens
equivalently as maximising the total (weighted) satisfiability
[Tran, 2017]. If a knowledge base is converted into Confidence rules then we can take the advantage of the computation mechanism in such neural networks for efficient inference. The equivalence between confidence rules and an RBM is defined in that the satisfiability of a formula is inversely proportional to the energy of a network:

\[ s_\varphi(x) = -aE_{rank}(x) + b \]

where \( s_\varphi \) is the truth value of the formula \( \varphi \) given an assignment \( x \); \( E_{rank}(x) = \min_h E(x, h) \) is the energy function minimised over all hidden variables; \( a > 0, b \) are scalars.

By using disjunctive normal form (DNF) to present knowledge Confidence rules attract some criticism for practicality since it is more popular to convert a formula to a conjunctive normal form of polynomial size. However we will show that Confidence rules are still very useful in practice. In fact, in such tasks as knowledge extraction, transfer, and integration Confidence rules have been already employed [Penning et al., 2011], [Tran and d’Avila Garcez, 2013] [Tran and Garecez, 2016]. For knowledge integration previous work separates the if-and-only-if symbol in Confidence rules into two if-then rules to encode in a hierarchical networks [Tran and Garecez, 2016]. In this work, we show that such separation is not necessary since any propositional if-then formulas can be efficiently converted to Confidence rules. The details are in the next section.

3 Knowledge Encoding

In many cases background knowledge presents a set of if-then formulas (or equivalent Horn clauses). This section shows how to convert them into Confidence rules for both propositional and first-order logic forms

3.1 Proposition Logic

A propositional if-then formula has the form

\[ c : y \leftarrow \bigwedge_t x_t \land \bigwedge_k \neg x_k \]

which can be transformed to a DNF as:

\[ c : (y \land \bigwedge_t x_t \land \bigwedge_k \neg x_k) \lor \bigvee_t (\neg x_t) \lor \bigvee_k (x_k) \]

and then to the confidence rules:

\[ c : h_y \leftarrow y \land \bigwedge_t x_t \land \bigwedge_k \neg x_k \]

\[ c : h_t \leftarrow \neg x_t \quad \text{for } \forall t \]

\[ c : h_k \leftarrow x_k \quad \text{for } \forall k \]

Encoding these rules into an RBM does not guarantee the equivalence. This is because it violates the condition that the DNF of a formula should have at most one conjunct is true given an assignment [Tran, 2017]. Fortunately this can be solved by grouping \( \neg x_t, x_k \) with a max-pooling hidden unit which results in an RBM with the energy function as:

\[ E = -c \times h_y(y + \sum_t x_t - \sum_k x_k - |T| - 1 + \epsilon) \]

\[ -c \times h_p \max\{\neg x_t + \epsilon, x_k - 1 + \epsilon|t \in T, k \in K\} \]

Here a max pooling hidden unit represents a hypothesis:

\[ h_p \leftrightarrow \bigvee_k h_k \lor \bigvee_t \neg x_t \]

which, in this case, can be written as:

\[ c : h_p \leftrightarrow \bigvee_k \neg x_k \lor \bigvee_t x_t \]

The final set rules are:

\[ c : h_y \leftrightarrow y \land \bigwedge_t x_t \land \bigwedge_k \neg x_k \]

\[ c : h_p \leftrightarrow \bigvee_k \neg x_k \lor \bigvee_t x_t \]

Example 1. Let us consider the formula 5 : \( y \leftarrow x_1 \land \neg x_2 \) which would be converted to DNF as: 5 : \( (y \land x_1 \land \neg x_2) \lor (\neg x_1) \lor (x_2) \), and then to an RBM with the energy function:

\[ E = -5h_1(y + x_1 - x_2 - 1.5) - 5h_2 \max\{x_1 + 0.5, x_2 - 0.5\} \]

Table 2 shows the equivalence between the RBM and the formula.

| x_1 | x_2 | y | s_\varphi | E_{rank} |
|-----|-----|---|---------|--------|
| 0   | 0   | 0 | 1       | -2.5   |
| 0   | 0   | 1 | -2.5    | 1      |
| 0   | 1   | 0 | -2.5    | 0      |
| 0   | 1   | 1 | -2.5    | 1      |
| 0   | 1   | 1 | -2.5    | 0      |
| 1   | 0   | 0 | 1       | -2.5   |
| 1   | 0   | 1 | -2.5    | 1      |
| 1   | 1   | 0 | -2.5    | 0      |
| 1   | 1   | 1 | -2.5    | 0      |

Table 2: Energy of RBM and truth values of the formula 5 : \( y \leftarrow x_1 \land \neg x_2 \) where \( s_\varphi \) is (unweighted) truth values of the formula. This indicates the equivalence between the RBM and the formula as:

\[ s_\varphi(x_1, x_2, y) = -\frac{1}{2.5}E_{rank}(x, y, z) + 0 \]

3.2 First-order Logic

A first order logic formula can also be converted into a set of Confidence rules. First, let us consider a predicate: \( P(x, y) \) which one can present in a propositional DNF as:

\[ \bigvee_{a,b \mid P(a, b) = true} p_{x=a} \land p_{y=b} \land p_{P} \]

where \( (a, b) \) are the models of \( P(x, y) \); \( p_{x=a} \) and \( p_{y=b} \) are the propositions that are true if \( x = a \) and \( y = b \) respectively, otherwise they are false; \( p_{P} \) is the proposition indicating if

\[ \epsilon \quad \text{such as in} \quad [\text{Tran, 2017}] \]

\[ 0 < \epsilon < 1 \]
the value of $P(a,b)$. Each conjunct in this DNF then can be represented as a Confidence rule.

Now, let us consider a first-order formula which we are also able to present in a set of Confidence rules. For example, a clause $\varphi$ as:

$$\forall x,y,z \, \text{son}(x,z) \leftarrow \text{brother}(x,y) \land \text{has_father}(y,z)$$

can be converted into:

$$\bigwedge_{a,b,c|\varphi=true} (p_{x=a} \land p_{y=b} \land p_{z=c} \land p_{\text{son}} \land p_{\text{brother}} \land p_{\text{has_father}}) \lor (\neg p_{x=a} \lor \neg p_{y=b} \lor \neg p_{z=c} \lor \neg p_{\text{brother}} \lor \neg p_{\text{has_father}})$$

If one wants to encode the background knowledge through its samples, for example:

$$\text{son}(\text{James}, \text{Andrew}) \leftarrow \text{brother}(\text{James}, \text{Jen}) \land \text{has_father}(\text{Jen}, \text{Andrew})$$

then we can convert it into confidence rules:

$$c : h_1 \leftrightarrow \text{james} \land \text{jen} \land \text{andrew} \land \text{son} \land \text{brother} \land \text{has_father}$$

In practice, in many cases we are only interested in inferring the predicates therefore we can omit $\neg$-james, $\neg$-jen, $\neg$-andrew from the second rule.

4 Empirical Evaluation

In this section we apply the encoding approaches discussed in the previous section to integrate knowledge into unsupervised networks.

4.1 DNA promoter

The DNA promoter dataset consist of a background theory with 14 logical if-then rules [Towell and Shavlik, 1994]. The rules includes four symbols $\text{contact}$, $\text{minus10}$, $\text{minus35}$, $\text{conformation}$ which are not observed in the data. This is suitable for hierarchical models as shown in previous works [Towell and Shavlik, 1994; Tran and Garcez, 2016]. In this experiment we group the rules using hypothetical syllogism to eliminate the unseen symbols. After that we encode the rules in an RBM following the theory in Section 3.1. The confidence values are selected empirically.

We test the normal RBMs and the RBMs with encoded rule using leave-one-out method, both achieve 100% accuracy. In order to evaluate the effectiveness of our approach we partition the data into nine different training-test sets with number of training samples are 10, 20, 30, 40, 50, 60, 70, 80, 90. All experiments are repeated 50 times and the average results are reported in Figure 1. We perform the prediction using both Gibbs sampling and conditional distribution $P(y|x)$. In particular, Figure 1A shows the prediction results using 1-step Gibbs sampling where the input is fixed to infer the hidden states and then to infer the label unit. In Figure 1B the results show the prediction accuracy achieved by inferring the label unit from the conditional distribution. As we can see, in both cases the integrated RBMs perform better than the normal RBMs on small training sets with number of training sample is less than 60. With larger training sets, the rules are no longer effective since the training samples are adequate to generalise the model to achive 100% accuracy.

In this experiment, we use the approach discussed in Section 3.2 for relation discovery and reasoning tasks with Kinship dataset [Hinton, 1986; Sutskever and Hinton, 2008]. Here given a set of examples about relations we perform two type of reasoning: (1) what is relation between two people, i.e $R(x,y)$; and (2) a person has a relation $R$ with whom, i.e. $R(x,?)$. Previous approaches are using matrices/tensors to represents the relations making it difficult to explain [Sutskever and Hinton, 2008]. In this work, since only predicates are given, we encode the examples for the predicates in an unsupervised network as shown earlier in Section 3.2. This constructs the left part of the integrated model in Figure 2. In the right part, we model the unknown clauses by using a set of hidden units. The idea here is that by inferring the predicates using the encoded rules in the left part we can capture the relationship information, from which the desired relation is inferred by reconstruction of such relationship in the right part. In this experiment, we use auto-encoder [Bengio, 2009] for the right part for the purpose of efficient learning. The whole process is described in Algorithm 1.

4.2 Kinship

Let us take an example where one wants to find the relation between two people $R(Marco, Pierro) = ?$. First, we use the other examples to construct an integrated model as in Figure 2. After that, we train the auto-encoder in the right part using unsupervised learning algorithm, then we extract the relation features from Marco and Pierro as shown in Figure 2.
0% In that table we also show the reconstructed scores for all the relations where son is the correct one.

Algorithm 1

Data: Examples: E, Question: R(a,b)
Result: R
Encode all examples in an RBM: N
Initialise $D = \emptyset$

for each example $R(x, y)$ in $E$
do
$f = \text{INFER}(N,a,y)$
Add $f$ to $D$
end
Train an Auto-Encoder (AE) on $D$
$f = \text{INFER}(N,a,b)$
Reconstruct $f$ using AE
Return $R = \arg \max_{R_f}(\hat{f}_R)$ \Comment{Return the unseen relation where the reconstruction feature have the highest value.}

1: function $\text{INFER}(N, a, b)$
2: \hspace{0.5em} Infer direct relation between $a, b$
3: \hspace{0.5em} Infer possible relations of $a$: $R(a, *)$
4: \hspace{0.5em} Infer possible relations of $b$: $R(*, b)$
5: \hspace{0.5em} $f = \text{concatenation of all relations}$
6: \hspace{0.5em} Return $f$
7: end function

We test the model on answering the question $R(x, y) = ?$ using leave-one-out validation which achieve 100% accuracy. We also use the integrated model to reason about whom one has a relation with. This question may have more than one answer, for example, son(Athar, ?) can be either Christopher or Penelope. We randomly select 10 examples for testing and repeat it for 5 times. If the designate answers are in the top relations with highest reconstructed features then we consider this as correct, otherwise we set it as wrong. The average error of this test is 0%. However, when we increase the number of test samples to 20 and 30 the average errors grow to 2.8% and 6.8% respectively. For comparison, the matrices based approach such as [Sutskever and Hinton, 2008] achieves 0.4%, 1.2%, 2.0% average error rates for 10, 20, 30 test examples respectively. Note that, such approach and many others [Socher et al., 2013] model each relation by a matrix/tensor while in this experiment we share the parameters across all relations. Also, the others use discriminative learning while we use unsupervised learning. The purpose of this is to exemplify the encoding technique we proposed earlier in this paper. Improvement can be achieved if similar methods are employed.

5 Conclusions

The paper shows how to integrate symbolic knowledge into unsupervised neural networks. This work bases on the theoretical finding that any propositional formula can be represented in RBMs [Tran, 2017]. We show that converting background knowledge in the form of if-then rules to Confidence rules for encoding is efficient. In the experiments, we evaluate our approaches for DNA promoter prediction and relationship reasoning to show the validity of the approach.

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| Marco, Pierro | 1.000: has_father | Marco has father who is Pierro |
|---------------|------------------|-------------------------------|
|               | 0.191:has_wife   | Marco has wife                |
|               | 0.191:husband    | Marco is a husband of someone |
|               | 0.191:has_mother | Marco has mother              |
|               | 0.191:father     | Marco is a father of someone  |
|               | 0.191:has_daughter | Marco has daughter         |
|               | 0.191:son        | Marco has is a son of someone |
|               | 0.191:has_son    | Marco has son                 |
|               | 0.191:has_sister | Marco has sister              |
|               | 0.191:brother    | Marco is a brother of someone |

| Marco         | 0.191: has_wife | Pierro has wife               |
|---------------|----------------|-------------------------------|
|               | 0.191:husband  | Pierro is a husband of someone|
|               | 0.191:father   | Pierro is a father of someone |
|               | 0.191:has_daughter | Pierro has daughter     |

| Pierro        | 0.008:wife 0.008:husband 0.001:mother 0.016:father 0.045:daughter 0.252:son 0.005:sister 0.013:brother 0.001:aunt 0.002:uncle 0.003:niece 0.002:nephew |

| Reconstruct (possible relations) | 0.008:wife 0.008:husband 0.001:mother 0.016:father 0.045:daughter 0.252:son 0.005:sister 0.013:brother 0.001:aunt 0.002:uncle 0.003:niece 0.002:nephew |

Table 3: Relation features

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