Deep Logic Networks: Inserting and Extracting Knowledge from Deep Belief Networks

Son N. Tran and Artur S. d'Avila Garcez*

***Abstract*—Developments in deep learning have seen the use of layer-wise unsupervised learning combined with supervised learning for fine-tuning. With this layer-wise approach, a deep network can be seen as a more modular system which lends itself well to learning representations. In this paper we investigate whether such modularity can be useful to the insertion of background knowledge into deep networks, and whether it can improve learning performance when it is available, and to the extraction of knowledge from trained deep networks, and whether it can offer a better understanding of the representations learned by such networks. To this end we use a simple symbolic language - a set of logical rules which we call *confidence rules* - and show that it is suitable for the representation of quantitative reasoning in deep networks. We show by knowledge extraction that confidence rules can offer a low-cost representation for layer-wise networks (or restricted Boltzmann machines). We also show that layer-wise extraction can produce an improvement in the accuracy of Deep Belief Networks. Furthermore, the proposed symbolic characterisation of deep networks provides a novel method for the insertion of prior knowledge and training of deep networks. With the use of this method, a deep neural-symbolic system is proposed and evaluated, with experimental results indicating that modularity through the use of confidence rules and knowledge insertion can be beneficial to network performance.**

***Index Terms*—Neural-Symbolic Integration, Deep Belief Networks, Knowledge Representation and Reasoning, Deep Learning, Knowledge Extraction**

I. Introduction

Knowledge representation and reasoning are two important topics in Artificial Intelligence (AI). Since the early years of AI, researchers have sought to represent knowledge in symbolic form to facilitate automated reasoning and help explain a machine's conclusions much like humans do. The benefits of having a symbolic representation are that knowledge can be verified formally, consolidated into knowledge-bases which can offer insight into the nature of the problem domain, and used to provide explanations for the answers produced by the system e.g. in the form of proofs.

Although symbolic representations have been deployed successfully in many intelligent and multi-agent systems, flexible representations and forms of reasoning are needed that can account for the inherent uncertainty in the problems tackled by AI [1], [2], such as for example handling noise in video and audio data. In such domains, statistical models such as deep networks seem capable of approximating a desired input-output function well purely from data for application in a range of classification tasks. More specifically, a Deep Belief Network (DBN) [3] can be constructed by stacking several generative Restricted Boltzmann Machines (RBMs) [4]. Nevertheless, scientists are still concerned about offering a better understanding of how such complex systems work [5].

Within the area of neural-symbolic computing [6], [7] efforts have been placed on how knowledge can be inserted and extracted from neural-network models [8], [9]. Background knowledge insertion, whenever it is available, is expected to offer an alternative to network pre-training. Knowledge extraction after training is expected to provide explanations [10], [11], [12], [13], [14], as already mentioned. A major challenge which has not been addressed fully yet is how to build an efficient neural-symbolic system capable of capturing the semantic meaning of a domain within a simple representation while supporting flexible inference given large-scale, noisy data, particularly from image, video and audio data.

Results in deep learning [3], [15] have shown that the combination of unsupervised (layer-wise, modular) network training with supervised training (also known as fine-tuning, using back-propagation) over multiple network layers can provide an effective way of learning and representing complex patterns. Bottou [16] argues that modularity should be key to building a reasoning system that combines rich inference and simple manipulations from linked models.

In this paper, we study the effects of modularity on a hierarchical network from a neural-symbolic perspective. We propose and evaluate methods and algorithms for inserting hierarchical knowledge into deep networks, and for knowledge extraction from deep networks following network training [9]. A simple symbolic language for hierarchical knowledge representation, named *confidence rules* [17], [18], [19], is deployed and evaluated. Confidence rules are shown empirically to be suitable for combining symbolic knowledge and quantitative reasoning, including probabilistic inference in deep networks. Each confidence rule is associated with a real number called a *confidence value* c such that a rule of the form $c : \mathsf{h} \leftrightarrow \mathsf{x}_1 \wedge \neg \mathsf{x}_2 \wedge \mathsf{x}_3$ denotes that h holds with confidence c if x_1 holds, x_2 does not hold, and x_3 holds. In order to perform inference under uncertainty dealing with continuous-valued data as well as missing values, an extension of the traditional *modus-ponens* logical inference rule is introduced. A novel and efficient knowledge extraction algorithm is then shown capable of deriving useful confidence rules from DBNs trained directly from data. Finally, we study how to insert prior knowledge into deep networks. In previous work [20], [21], prior knowledge such as local information of image batches was used to improve learning of deep networks. In this paper, we study the effects of inserting hierarchical knowledge into deep networks. We introduce a deep neural-symbolic system

*Garcez and Tran are with the Department of Computer Science, City University London, London, EC1V 0HB, UK e-mail: son.tran.1@city.ac.uk, aag@soi.city.ac.uk

capable of encoding symbolic knowledge into DBNs and leveraging the above inference algorithm to guide and improve learning of the model.

The paper is organised as follows. The next section reviews the related literature in DBNs and neural-symbolic integration. Section III defines confidence rules and shows their relationship with Deep Networks. Section IV proposes and evaluates the general algorithm for extracting symbolic knowledge from RBMs, and extends it to deal with DBNs. Section V shows how prior knowledge in the form of hierarchical confidence rules can be encoded effectively into Deep Networks, and how this can improve learning performance in comparison with DBNs. Section VI concludes the paper and discusses directions for future work.

II. Preliminaries

A. Notation

Matrices and vectors are denoted using boldface capital letters $\mathbf{X}$ and boldface letters $\mathbf{x}$, respectively. A subscript is used to denote an element of a matrix or vector, for example x_{ij} and x_i. A vector $\mathbf{x}_j$ denotes the column j of matrix $\mathbf{X}$. While numerical variables are denoted as x, a logical proposition is denoted as x, and it assumes two possible values: $true$ or $false$, which are equivalent to a binary variable x with values 1 and 0, respectively.

B. Deep Networks

In unsupervised learning, deep networks [3], [22], [15] have been established as a powerful architecture for the learning of features at different levels of abstraction. For example, a Deep Belief Network (DBN) [3] can be constructed by stacking several generative Restricted Boltzmann Machines (RBMs) [4] one on top of another in order to learn better representations of unlabelled data. Shallow generative networks with a single hidden layer such as RBMs have an advantage that inference, i.e. the conditional probability of a unit's state given the states of the other units, can be computed exactly. However, they are limited in their learning to a single level of representation [15]. Deep architectures [23], [20], [3], [24], [25], on the other hand, are connectionist systems that consist of many hidden layers, and therefore are capable of learning representations at multiple levels of abstraction. Even though these deep models are complex in terms of learning, e.g. their cost function is non-convex, research has shown that they can scale better than their shallow counterparts [15].

Formally, one can represent a deep belief network as a hierarchy of network layers $X, H^{(1)}, ..., H^{(L)}$, where X is a visible layer and $H^{(l)}$ ($l = 1 : L$) are hidden layers. Let us consider a network with a single hidden layer (L=1; i.e. a restricted Boltzmann machine [4], [26]). This two-layer connectionist model is characterised by an energy function:

$$E(\mathbf{x}, \mathbf{h}^{(1)}) = -\sum_{ij} x_i w_{ij} h_j^{(1)} - \sum_i a_i x_i - \sum_j b_j h_j^{(1)} \quad (1)$$

where $w_{ij} \in \mathbf{W}$ is the weight between unit i in layer X and unit j in layer $H^{(1)}$, a_i and b_j are the biases of the units in X and $H^{(1)}$, respectively. For learning, one can train the model by maximising the log-likelihood:

$$\log P(\mathbf{x}) = \log \frac{\sum_{\mathbf{h}^{(1)}} e^{-\mathbf{E}(\mathbf{x}, \mathbf{h}^{(1)})}}{Z} \quad (2)$$

where Z is the partition function $Z = \sum_{\mathbf{x}, \mathbf{h}^{(1)}} e^{-E(\mathbf{x}, \mathbf{h}^{(1)})}$.

The gradient of this function, call it $\bigtriangledown\theta$, can be computed as follows:

$$\bigtriangledown\theta = \mathbb{E}\Big[\frac{\partial \mathbf{E}(\mathbf{x}, \mathbf{h}^{(1)}; \theta)}{\partial \theta}\Big]_{\mathbf{h}^{(1)}|x} - \mathbb{E}\Big[\frac{\partial \mathbf{E}(\mathbf{x}, \mathbf{h}^{(1)}; \theta)}{\partial \theta}\Big]_{\mathbf{x}, \mathbf{h}^{(1)}} \quad (3)$$

Here, we get into a common problem in statistical machine learning: even though the first term can be computed exactly, the second term is intractable as the complexity of computing the joint probability $P(\mathbf{x}, \mathbf{h}^{(1)})$ increases exponentially with the size of $\mathbf{x}$ and $\mathbf{h}^{(1)}$. This is typically a serious problem because most real-world applications such as video analysis will have a large number of attributes $\mathbf{x}$. Now, if we generalise the model into a deep network with multiple hidden layers, the problem of intractability worsens with the dependency between hidden layers, to the point that one becomes unable to compute the conditional probability $P(\mathbf{h}^{(l)}|\mathbf{x})$ exactly from the data.

The common way to avoid the above intractability is to learn a deep network layer by layer [3], [24], [27]. To this end, the deep network is used as a stack of several shallow networks, each having a single hidden layer. Training of each layer is performed bottom-up with the focus now turned to how Eq. 2 can be solved approximately. This is called layer-wise pre-training. After that, the fine-tuning phase trains the network as a whole using the parameters which have been initialised by the pre-training phase. In this paper, we are interested in investigating such modularity property and the hierarchical reasoning that takes place within deep networks. Therefore, we focus on layer-wise training as a key component in learning complex models. We exclude the fine-tuning phase from our models, since it can break the modularity of the models by treating them as traditional multi-layer neural networks [15].

C. Neural-Symbolic Systems

Considerable research has been devoted to the integration of symbolic knowledge and connectionist systems [28], [29], [17], [8], [9], [30], [6], [31], [32]. The first reason for this is that symbolic rules can represent knowledge in a formal language and therefore offer a formal semantics to models and systems. The second is that one may find symbolic knowledge helpful when seeking a better understanding of the connectionist models learned or when seeking to add prior knowledge to such models. Furthermore, symbolic knowledge extracted from a connectionist model can be employed as a foundation for some other sub-areas of Artificial Intelligence, e.g. knowledge-based transfer learning [33].

In several circumstances, prior knowledge can be provided by domain experts, frequently in the form of symbolic logic rules. Such a use of *domain knowledge* has been shown capable of improving model learning. In [34], a model named KBANN (Knowledge-Based Artificial Neural Networks) was proposed. KBANN uses multi-layer feedforward networks and a method for encoding rules into the networks to enable learning from data and background knowledge. In [35], the CILP (Connectionist Inductive Logic Programming) system was introduced. Inspired by KBANN, CILP uses logic programming rules applied to recurrent neural networks to achieve an improvement in performance in comparison with KBANN at learning from data and background knowledge.

Symmetrical systems such as Markov networks and recurrent temporal restricted Boltzmann machines also have been used for neural-symbolic integration. In [36], a method is presented for encoding background knowledge into a template Markov network (named Markov Logic Network, MLNs) which is used to create a ground Markov network representing the relationships between all the instances in the data. The idea of representing each formula into a clique of Markov network is similar to that of Penalty Logic which has been proposed to integrate symbolic knowledge and Hopfield networks [32]. The difference is that in MLNs a feature is defined by the number of true groundings of the formulas corresponding to a clique in the template model, while in Penalty Logic [32] a feature is defined by the multiplication of the variables in the clique. In practice, MLNs work well in a variety of relational domains; however, the models learned are not as comprehensible as one would expect from a symbolic model due to the size of the ground Markov network and exponential nature of such grounding. A more recent development in neural-symbolic integration is the Neural-Symbolic Cognitive Agent (NSCA) introduced in [17] in which a model based on recurrent temporal restricted Boltzmann machines (RTRBM) is proposed to represent temporal symbolic knowledge and applied to online learning and reasoning. The NSCA model contains algorithms for learning and extraction of temporal logic rules by sampling the RTRBM. It has been applied successfully to driving assessment and training in simulators.

For decades, neural networks have been used successfully as a learning model, from which symbolic rules can be extracted through the use of knowledge extraction algorithms [29], [8], [9]. However, most extraction algorithms exist for discriminative models which do not support modularity. We argue that the modularity found in deep networks may facilitate knowledge extraction, in particular improving efficiency of extraction from large networks. Most such discriminative extraction approaches treat the class variables as a special type of variable. As a result, the rules which are extracted may be helpful at explaining the relationships between all other variables and the class variables, but not the relationships that might exist among such other variables. For example, suppose a discriminative neural network was trained perfectly to learn the XOR function (denoted by $\oplus$ below) from its truth-table. Discriminative knowledge extraction might produce the rule $x_3 \leftrightarrow x_1 \oplus x_2$, with x_3 as the class variable, but fail to capture equally valid rules $x_1 \leftrightarrow x_2 \oplus x_3$ and $x_2 \leftrightarrow x_1 \oplus x_3$. In what follows, we introduce an efficient method for symbolic knowledge extraction from generative models, specifically RBMs, which can capture such relations. Efficiency is measured by the computational complexity of the rule extraction, as discussed in Section IV, which instead of depending on the combinations of the input vectors (which might be intractable for real-valued inputs or a large number of attributes $\mathbf{x}$), uses the network structure for extraction, depending on the values of the network's weight vectors $\mathbf{W}$ structured hierarchically. Knowledge extraction from DBNs will then be performed layer-by-layer through the extraction of confidence rules from each RBM [18], [19], [17].

III. Confidence Rules

Classical logical reasoning has been found difficult to adapt to account for uncertainty in complex domains, with various non-classical ways of integrating logic and probabilities having been proposed towards this end (for a recent account, c.f. [37]). One way of accounting for uncertainty has been by assigning a real value between 0 and 1 (a probability) to each logical variable so that if, say, x is $false$, given the truth-table shown in Table I, one can conclude that the probability of y being $true$ is 0.5.

In what follows we define confidence rules which will be used for combining symbolic representations and deep networks. Confidence rules support the above form of quantitative inference, useful for reasoning under uncertainty in a way similar to Penalty Logic [32]. In order to perform inference using confidence rules, dealing with continuous data and missing values, we introduce an algorithm that extends the standard *modus-ponens* logical inference rule, as detailed next.

x	y	$(x \leftrightarrow y)$
$false$	$false$	$true$
$false$	$true$	$false$
$true$	$false$	$false$
$true$	$true$	$true$

TABLE I: Truth-table for bi-conditional (if-and-only-if).

A. Confidence Rules

A *confidence rule* is a bi-conditional (if-and-only-if) formula of the form $c : \mathsf{h} \leftrightarrow \mathsf{x}_1 \wedge \cdots \wedge \mathsf{x}_n$, where h is an atomic proposition and each x_i, $1 \leq i \leq n$, is a literal (an atomic proposition or its negation), labelled by a real-valued number c called a *confidence value* [17]. For example, the formula:

$$1.5 : \mathsf{h} \leftrightarrow \mathsf{x}_1 \wedge \neg \mathsf{x}_2 \wedge \mathsf{x}_3 \tag{4}$$

associates hypothesis (hidden unit) h with beliefs (visible units) $\mathsf{x}_1, \mathsf{x}_2, \mathsf{x}_3$ with confidence value 1.5. The *confidence value* as defined in this paper is similar to the *penalty* used by Penalty Logic [32], *formula weights* from Markov Logic Networks [36], and *confidence credibility* used by Neural-Symbolic Cognitive Agents [17]. However, a main difference from all of these is that, in this paper, confidence values are used for quantitative inference by selecting rules for extraction based on their confidence. Specifically, given the confidence values of two formulas, one can quantitatively decide, because of the way that the values will be calculated, which formula should be selected for extraction. In what follows, we describe the inference algorithm for confidence-logic rules.

INFERENCE RULE: INF1

Given:
$c : \mathsf{h} \leftrightarrow \bigwedge_{\forall t \in T} \mathsf{x}_t \wedge \bigwedge_{\forall k \in K} \neg \mathsf{x}_k$
$\alpha_{t'} : \mathsf{x}_{t'}$ where $t' \in T, \alpha_{t'} \in [min, max]$
$\alpha_{k'} : \mathsf{x}_{k'}$ where $k' \in K, \alpha_{k'} \in [min, max]$
Infer:
$\alpha_h : \mathsf{h}$ with $\alpha_h = c \cdot (\sum_{t'} \alpha_{t'} + \sum_{m \neq \forall t'}^{m \in T} \alpha_m - \sum_{k'} \alpha_{k'} - \sum_{m \neq \forall k'}^{m \in K} \alpha_m)$
where $\alpha_m = \frac{min+max}{2}$

B. Hierarchical Inference

Many logic programming systems have hierarchical rules in which *intermediate literals* exist. An intermediate literal is a literal that appears in the antecedent (or body) of some rule and in the consequent (or head) of another rule. For example, in the background theory of the DNA promoter dataset used by [8] (Table II), literals minus_{35}, minus_{10}, $\mathsf{contact}$ and $\mathsf{conformation}$ are intermediate literals. In what follows, we will use the same promoter dataset to exemplify our work. We represent the name of each nucleotide with its position in subscript, e.g. t_{-35} denotes that nucleotide t appears at position -35 in the DNA sequence.

L-1{	minus_{35}	$\leftarrow \mathsf{t}_{-36} \wedge \mathsf{t}_{-35} \wedge \mathsf{g}_{-34} \wedge \mathsf{a}_{-33} \wedge \mathsf{c}_{-32}$
	minus_{10}	$\leftarrow \mathsf{t}_{-12} \wedge \mathsf{a}_{-11} \wedge \mathsf{t}_{-7}$
	$\mathsf{conformation}$	$\leftarrow \mathsf{a}_{-45} \wedge \mathsf{a}_{-44}$
	$\mathsf{conformation}$	$\leftarrow \mathsf{a}_{-44} \wedge \mathsf{a}_{-41}\}$
L-2{	$\mathsf{contact}$	$\leftarrow \mathsf{minus}_{35} \wedge \mathsf{minus}_{10}\ \}$
L-3{	$\mathsf{promoter}$	$\leftarrow \mathsf{contact} \wedge \mathsf{conformation}\}$

TABLE II: Hierarchy of rules used as background knowledge for the promoter DNA dataset; the first four rules appear in level L_1 of the hierarchy, then level L_2, and so on. Each level will be mapped onto a layer of a DBN.

Confidence rules can also be organised into hierarchies, and inference is performed bottom-up: for each subset of rules in the hierarchy, the confidence value of each hypothesis in the subset is inferred, given the confidence value of each belief that is present. This value is then normalised before being used for inference, now as beliefs, at the next level of the hierarchy using another subset of the rules. Here, normalisation is required to maintain correspondence between the propositions in the rules and the units of the RBMs. The following definition formalises this idea.

Definition 3.1: Let $\beta^{(1)}$ be a set of confidence rules relating a set of beliefs $\mathsf{x}_1, \mathsf{x}_2, ...$ and a set of hypotheses $\mathsf{h}_1^{(1)}, \mathsf{h}_2^{(1)}, ...$ Let $\beta^{(2)}$ be a set of confidence rules relating hypotheses $\mathsf{h}_1^{(1)}, \mathsf{h}_2^{(1)}, ...$ and new hypotheses $\mathsf{h}_1^{(2)}, \mathsf{h}_2^{(2)}, ...$ Let $\beta^{(3)}$ be a set of confidence rules relating hypotheses $\mathsf{h}_1^{(2)}, \mathsf{h}_2^{(2)}, ...$ and new hypotheses $\mathsf{h}_1^{(3)}, \mathsf{h}_2^{(3)}, ...$, and so on. We call $\beta^{(1)}, \beta^{(2)}, \beta^{(3)}, ...$ a hierarchical weighted knowledge-base.

Given an input to any sequence $\beta^{(1)}, \beta^{(2)}, ..., \beta^{(i)}$ of a hierarchical weighted knowledge-base, local inference can be carried out and results propagated to $\beta^{(i+1)}$. This type of inference can be seen as an extension of *modus-ponens* to deal with uncertainty through the calculation of confidence values, which allows logical inference to work with real-valued data types through the application of inference rule INF1, as defined above.

Algorithm 1 QUANT_INFERENCE

```
1: Initialise the set of beliefs B in level 1 to $\alpha_i : \mathsf{x}_i^{(1)}$, where each belief has a value $\alpha_i^{(1)}$ ($\alpha_i^{(1)}$ can be seen as the input value of visible unit $x_i$ corresponding to proposition $\mathsf{x}_i$);
2: for $l = 1$ to $L$ do
3:     Initialise the set of beliefs B$_{next}$ at the next level to zero, i.e. $0 : \mathsf{x}_j^{(l+1)}$
4:     for each rule $r$ in level $l$ do
5:         Calculate the confidence value $\alpha$ of the hypotheses in $r$ using INF1;
6:         Normalise $\alpha$;
7:         Increase the confidence value of the beliefs in B$_{next}$ that are associated with the hypotheses in $r$ by the normalised $\alpha$;
8:     end for
9:     Set B = B$_{next}$
10: end for
```

In inference rule INF1, T and K are sets of positive and negative literals, respectively. The *confidence value* α_m of any missing beliefs is the average of an upper-bound and a lower-bound on the normalised *confidence values* in the rule set. For example, given the rule and beliefs:
$1.5 : \mathsf{h} \leftrightarrow \mathsf{x}_1 \wedge \neg \mathsf{x}_2 \wedge \mathsf{x}_3$
$1 : \mathsf{x}_1$, normalised to $[0, 1]$
x_2 is missing
$1 : \mathsf{x}_3$, normalised to $[0, 1]$
one uses $\alpha_2 = 0.5$ to derive h with confidence value $1.5 \times (2 - 0.5) = 2.25$.

In this process, with normalisation bounded by $[min, max]$, if $\neg \mathsf{x}$ has confidence value α then x must have confidence value $min + max - \alpha$. Algorithm 1 specifies the inference process.

IV. Knowledge Extraction from Deep Networks

In this section, we focus on the extraction of knowledge in the form of confidence rules from deep networks. In order to build hierarchies of confidence rules, we employ a layer-wise approach [3], [15] to extract rules from each layer of a deep network. In what follows, we introduce the algorithm for knowledge extraction from RBMs, and then we extend it to deep networks. For ease of presentation, we omit the biases; however, the approach below can be extended easily to include biases.

A. Knowledge Extraction from RBMs

We now propose an algorithm for extracting rules from a trained RBM. For each hidden unit j, a confidence rule is extracted of the form:

$$c_j : \mathsf{h}_j \leftrightarrow \bigwedge_{\forall t \in T} \mathsf{x}_t \wedge \bigwedge_{\forall k \in K} \neg \mathsf{x}_k \quad (5)$$

where x_t and $\neg\mathsf{x}_k$ represent the literals $x_t = 1$ and $x_t = 0$, respectively. The idea behind the extraction algorithm is that it seeks to find the positive and negative literals and confidence values c_j that minimise information loss, according to the following equation:

$$\mathcal{I}_{loss} = \sum_{ij} \|w_{ij} - c_j \mathbb{I}_j(x_i)\|^2 \quad (6)$$

where c_j is the *confidence value* of rule j corresponding to unit j in a hidden layer, and:

$$\mathbb{I}_j(x_i) = \begin{cases} 1 & \text{if literal } \mathsf{x}_i \text{ appear in rule } j \\ -1 & \text{if literal } \neg\mathsf{x}_i \text{ appear in rule } j \\ 0 & \text{otherwise} \end{cases} \quad (7)$$

For ease of notation, let us use $s_{ij} = \mathbb{I}_j(x_i)$, such that Eq. 6 becomes:

$$\mathcal{I}_{loss} = \sum_{ij} \|w_{ij} - c_j s_{ij}\|^2 \quad (8)$$

Since Eq. (8) is quadratic, the *confidence values* can be found by setting the derivatives to zero, as follows.

$$\begin{aligned} &\sum_i 2(w_{ij} - c_j s_{ij}) s_{ij} = 0, \text{ for all } j \\ &\sum_i w_{ij} s_{ij} - c_j \sum_i s_{ij}^2 = 0, \text{ for all } j \end{aligned} \quad (9)$$

From Eq. (9), we obtain:

$$c_j = \frac{\sum_i w_{ij} s_{ij}}{\sum_i s_{ij}^2} \quad (10)$$

Since the value of s_{ij} is in the set $\{-1, 0, 1\}$, we have:

$$\begin{aligned} \|w_{ij} - c_j s_{ij}\|^2 &= \|\text{abs}(w_{ij}) - c_j \frac{s_{ij}}{\text{sign}(w_{ij})}\|^2 = \\ &= \begin{cases} (\text{abs}(w_{ij}) + c_j)^2 & \text{if } s_{ij} \neq \text{sign}(w_{ij}) \\ (\text{abs}(w_{ij}) - c_j)^2 & \text{if } s_{ij} = \text{sign}(w_{ij}) \\ \text{abs}(w_{ij})^2 & \text{if } s_{ij} = 0 \end{cases} \end{aligned} \quad (11)$$

Here, $\text{abs}(w_{ij})$ and $\text{sign}(w_{ij})$ are functions that return, respectively, the absolute value and sign of w_{ij}. Since $(\text{abs}(w_{ij}) + c_j)^2 > (\text{abs}(w_{ij}) - c_j)^2$ and $(\text{abs}(w_{ij}) + c_j)^2 > \text{abs}(w_{ij})^2$, the information loss will be minimised if $s_{ij} = \text{sign}(w_{ij})$ or $s_{ij} = 0$. In particular, $s_{ij} = 0$ will minimise the loss function if and only if:

$$\begin{aligned} &\text{abs}(w_{ij})^2 \leq (\text{abs}(w_{ij}) - c_j)^2 \\ &\frac{c_j}{2} \geq \text{abs}(w_{ij}) \end{aligned} \quad (12)$$

The intention here is that for each rule j, an input x_i with small weight $\text{abs}(w_{ij}) \leq c_j/2$ should not appear in the rule. The rule, therefore, only captures the relations between input variables having *strong connection* through the hidden unit j. From Eq. (10) and Eq. (12), the extraction algorithm below is derived.

Algorithm 2 RBM_EXTRACT

```
Require: An RBM with visible layer V and hidden layer H
 1: for $j = 1$ to the number of hidden units do
 2:     Create rule $r_j$ of the form $c_j : \mathsf{h}_j \leftrightarrow \bigwedge_{w_{tj}>0} \mathsf{x}_t \wedge \bigwedge_{w_{kj}<0} \neg\mathsf{x}_k$
 3:     Create sign matrix $S$ with each $s_{ij} = \text{sign}(w_{ij})$
 4: Do
 5:     $c_j := \frac{\sum_{s_{ij} \neq 0} \text{abs}(w_{ij})}{\sum_i s_{ij}^2}$
 6:     for each $s_{ij} \neq 0$ do
 7:         if $c_j \geq 2 \cdot \text{abs}(w_{ij})$ then
 8:             $s_{ij} := 0$
 9:             Remove $\mathsf{x}_i$ or $\neg\mathsf{x}_i$ from rule $r_j$
10:         end if
11:     end for
12: Until the value of $c_j$ is unchanged
13: end for
```

Suppose an RBM has I visible units and J hidden units. Rule extraction Algorithm 2 has worst-case time complexity $\mathcal{O}(I \times J)$. This is an improvement on searching through the combinations of input vectors, which has worst-case time complexity $\mathcal{O}(2^I)$.

A working example (XOR problem): In this example, we show how confidence rules can be extracted from an RBM trained on the XOR function shown in Table III. An RBM with visible units x_1, x_2, x_3 and 10 hidden units was trained to learn this truth-table using input value 0 to denote truth-value *false*, and input value 1 to denote *true*.

x_1	x_2	x_3
$false$	$false$	$false$
$false$	$true$	$true$
$true$	$false$	$true$
$true$	$true$	$false$

TABLE III: Truth-table for XOR function

In this example, 10 rules exist with antecedents x_1, x_2 and x_3, and consequent h_i, $1 \leq i \leq 10$. The rules extracted from the trained RBM are shown below: Assuming that x_3

$1.340 : \mathsf{h}_1 \leftrightarrow \mathsf{x}_1 \wedge \neg\mathsf{x}_2 \wedge \mathsf{x}_3$	$1.677 : \mathsf{h}_6 \leftrightarrow \neg\mathsf{x}_1 \wedge \mathsf{x}_2 \wedge \mathsf{x}_3$
$2.970 : \mathsf{h}_2 \leftrightarrow \mathsf{x}_1 \wedge \neg\mathsf{x}_2 \wedge \mathsf{x}_3$	$2.544 : \mathsf{h}_7 \leftrightarrow \mathsf{x}_1 \wedge \neg\mathsf{x}_2 \wedge \mathsf{x}_3$
$6.165 : \mathsf{h}_3 \leftrightarrow \neg\mathsf{x}_1 \wedge \mathsf{x}_2 \wedge \mathsf{x}_3$	$7.355 : \mathsf{h}_8 \leftrightarrow \mathsf{x}_1 \wedge \mathsf{x}_2 \wedge \neg\mathsf{x}_3$
$0.158 : \mathsf{h}_4 \leftrightarrow \neg\mathsf{x}_1 \wedge \mathsf{x}_2 \wedge \neg\mathsf{x}_3$	$6.540 : \mathsf{h}_9 \leftrightarrow \neg\mathsf{x}_1 \wedge \neg\mathsf{x}_2 \wedge \neg\mathsf{x}_3$
$2.481 : \mathsf{h}_5 \leftrightarrow \mathsf{x}_1 \wedge \neg\mathsf{x}_2 \wedge \mathsf{x}_3$	$4.868 : \mathsf{h}_{10} \leftrightarrow \neg\mathsf{x}_1 \wedge \neg\mathsf{x}_2 \wedge \neg\mathsf{x}_3$

TABLE IV: Rules extracted from RBM trained on XOR

is a target proposition, one can see by inspecting Table IV that, among the rules with the higher confidence values, x_3 is associated with either $\mathsf{x}_1 \wedge \neg\mathsf{x}_2$ or with $\neg\mathsf{x}_1 \wedge \mathsf{x}_2$. Similarly, $\neg\mathsf{x}_3$ is associated with $\neg\mathsf{x}_1 \wedge \neg\mathsf{x}_2$ or with $\mathsf{x}_1 \wedge \mathsf{x}_2$, as expected. In this case, a rule such as $7.355 : \mathsf{h}_8 \leftrightarrow \mathsf{x}_1 \wedge \mathsf{x}_2 \wedge \neg\mathsf{x}_3$ can be read as: If x_1 is true and x_2 is true then, assuming that h_8 is true, z should be false with confidence 7.355. Notice how in this way any subset of the visible units could have been assumed to be the target proposition.

Given a trained RBM, it is clear that Algorithm 2 would also apply to any subset I of the RBM's visible units. The algorithm could equally be applied from the hidden units to the remaining visible units not in I. In this way, an RBM where the visible units have been split into input and target units can be seen as a single-hidden-layer DBN to which Algorithm 2 is applied twice for the sake of rule extraction. This idea will be explored in detail in the next section. Returning to the XOR example, assuming I=$\{\mathsf{x}_1, \mathsf{x}_2\}$, the following rules can be extracted:

$1.499 : \mathsf{h}_1 \leftrightarrow \mathsf{x}_1 \wedge \neg\mathsf{x}_2$	$1.908 : \mathsf{h}_6 \leftrightarrow \neg\mathsf{x}_1 \wedge \mathsf{x}_2$
$2.782 : \mathsf{h}_2 \leftrightarrow \mathsf{x}_1 \wedge \neg\mathsf{x}_2$	$2.638 : \mathsf{h}_7 \leftrightarrow \mathsf{x}_1 \wedge \neg\mathsf{x}_2$
$6.134 : \mathsf{h}_3 \leftrightarrow \neg\mathsf{x}_1 \wedge \mathsf{x}_2$	$7.375 : \mathsf{h}_8 \leftrightarrow \mathsf{x}_1 \wedge \mathsf{x}_2$
$0.139 : \mathsf{h}_4 \leftrightarrow \neg\mathsf{x}_1 \wedge \mathsf{x}_2$	$6.433 : \mathsf{h}_9 \leftrightarrow \neg\mathsf{x}_1 \wedge \neg\mathsf{x}_2$
$2.582 : \mathsf{h}_5 \leftrightarrow \mathsf{x}_1 \wedge \neg\mathsf{x}_2$	$4.823 : \mathsf{h}_{10} \leftrightarrow \neg\mathsf{x}_1 \wedge \neg\mathsf{x}_2$

$$5.720 : \mathsf{x}_3 \leftrightarrow \mathsf{h}_1 \wedge \mathsf{h}_2 \wedge \mathsf{h}_3 \wedge \neg\mathsf{h}_4 \wedge \mathsf{h}_5 \wedge \mathsf{h}_6 \wedge \mathsf{h}_7 \wedge \neg\mathsf{h}_8 \wedge \neg\mathsf{h}_9 \wedge \neg\mathsf{h}_{10}$$

TABLE V: Rules from part of the RBM trained on XOR

From the above rules, an assignment of truth-values to x_1 and x_2 allows us to derive confidence values for x_3 by applying Inference Rule INF1. In this example, as expected, x_3 will have a high confidence value when either x_1 is $true$ and x_2 is $false$ or vice-versa, but not when both x_1 and x_2 are assigned the same truth-value.

Notice that, if either x_1 or x_2 were chosen as target variable, the same procedure above could be applied, without the need for retraining the RBM. Differently from extraction from supervised models [8], [9], here the target does not have to be chosen in advance and the model retrained for each target.

Low-cost Representation: In RBMs, the state of the hidden units given the state of the visible units can be used as latent features which, in many cases, can improve the training of a classifier. Frequently, the accuracy of, say, a Support Vector Machine (SVM) will improve when it is trained having latent features such as the state of an RBM's hidden units as input, instead of raw data (that is, the state of the RBM's visible units). Let us investigate whether the same holds for confidence rules. Given one's confidence in a set of beliefs, the confidences of the hypotheses referred to by the confidence rules can be inferred using rule of inference INF1. These confidence values can also be used as input to a classifier. In what follows, we compare the performance of RBMs with that of confidence rules on large image data sets. The confidence rules are shown to offer a more compact representation than RBMs.

We compare the performances of the confidence rules and the latent features of the RBM using three datasets: the TiCC handwritten characters, the MNIST handwritten digits, and the Yale faces dataset. All three datasets consist of images with pixel values ranging from 0 to 255, which are then normalised onto the interval [0-1]. Hence, for the purpose of carrying out inference using the rules we convert each pixel value $x_i = \alpha_i$ into a proposition x_i having confidence value α_i. The TiCC dataset consists of $18,189$ training samples, $1,250$ validation samples, and $18,177$ test samples. The MNIST consists of $60,000$ training and $10,000$ test samples. The Yale dataset contains 135 training and 30 test samples. Model selection was performed by running a grid search (except for the Yale dataset) over the learning rates for the RBMs (between 0.001 and 1), and for the SVM, cost (between 0.0001 and 100) and gamma (between 0.0001 and 100), all on a log-scale. On the MNIST dataset, for efficiency, we have used $10,000$ samples for training and $2,000$ samples for validation. Once the best hyper-parameters were selected, the entire set of $60,000$ samples was used for training the best model, as is normally the case, which was then tested on the unseen $10,000$ test samples. The number of hidden units was fixed at 500 (we have also trained an RBM with $1,000$ hidden units which produced a non-statistically significant improvement in performance). The classifier used was an SVM with Gaussian kernel [38].

Table VI contains the test-set accuracies of the SVMs trained using as input the values of the latent variables from the RBMs with 500 and 1,000 hidden units, trained on the three datasets, compared with the accuracies of the SVMs trained using as input the confidence values obtained by applying rule of inference INF1 on the rules extracted by Algorithm 2 from the same RBMs. Each experiment was run 10 times and we report the mean accuracies on the hold-out test sets, along with the standard deviation. The results show that the performance of the rules can be (consistently) almost identical to that of the RBMs. In addition, in the rule set, each (positive or negative) literal can be represented by 1 bit, while in the RBM each weight value must be represented by a double data type (i.e. 64 bits in a 32-bit computer). Therefore, the rules require far less storage memory than the RBMs while still preserving similar performance. Confidence rules can be seen, therefore, as a suitable low-cost representation for RBMs.

B. Knowledge Extraction from DBNs

Following a layer-wise approach [3], [15], a hierarchy of confidence rules can be built for the extraction of rules from DBNs through the repeated application of Algorithm 2. Let us start by considering in more detail the case discussed earlier of a single-hidden-layer DBN created by splitting the visible layer of an RBM into input and target subsets and applying Algorithm 2 twice. This will be followed by the presentation of the general-case algorithm for rule extraction from DBNs.

A working example (DNA promoter problem): The DNA promoter dataset [8] has 106 examples, each consisting of a sequence of 57 nucleotides (either A, T, G or C) from position -50 to $+7$ in the DNA; 53 examples are gene promoters and 53 examples are not. Let us use n_p to denote a nucleotide n at position p, such that $\mathsf{a}_p, \mathsf{t}_p, \mathsf{g}_p, \mathsf{c}_p$ indicate, respectively, that $n_p = A, n_p = T, n_p = G, n_p = C$.

For each variable n_p, a group of 4 visible units was created in the RBM. Two target units were also added, one for $\mathsf{promoter}$ and one for $\neg\mathsf{promoter}$. Five RBMs were trained using 96 examples, each with 10 examples randomly selected from the original 106 for testing. Only three hidden units were used ($\mathsf{h}_1, \mathsf{h}_2, \mathsf{h}_3$); this was sufficient for the networks to achieve 90.67% training set performance on average. By applying Inference Rule INF1 on these rules, all 10 test examples were classified correctly, with $\mathsf{promoter}$ obtaining a higher confidence value than $\neg\mathsf{promoter}$ whenever the DNA sequence was a gene promoter. On average, for the five RBMs, the rules

	TiCC SVM	MNIST SVM	Yale SVM
RBM (J=500)	$94.851\% \pm 0.033$	$98.553\% \pm 0.031$	$95.00\% \pm 2.833$
Confidence rules	$94.711\% \pm 0.072$	$98.530\% \pm 0.040$	$94.333\% \pm 3.865$
RBM (J=1000)	$94.928\% \pm 0.016$	$98.680\% \pm 0.024$	$97.000\% \pm 2.919$
Confidence rules	$94.729\% \pm 0.070$	$98.562\% \pm 0.035$	$96.667\% \pm 1.757$

TABLE VI: Accuracy of SVMs trained on the TiCC, MNIST and Yale datasets using the hidden features of an RBM (with either 500 or 1000 hidden units) as input, compared with accuracy of SVMs trained using as input the confidence values of the hypotheses derived from the rules extracted from the RBMs (c.f. Algorithm 2) by applying inference rule INF1.

extracted (such as the two rules which follow) have achieved a test-set accuracy of $90\% \pm 6.9296$.

$$0.761 : \neg\mathsf{promoter} \leftrightarrow \neg\mathsf{h}_1^{(1)} \wedge \mathsf{h}_2^{(1)} \wedge \neg\mathsf{h}_3^{(1)}$$
$$1.042 : \mathsf{promoter} \leftrightarrow \mathsf{h}_1^{(1)} \wedge \mathsf{h}_3^{(1)}$$

Direct comparisons with other extraction approaches such as MofN [8] and RuleSet [9] would be non-trivial because of the differences in methodology and learning method (supervised vs. unsupervised). Nevertheless, for completeness, we report here the results obtained by those extraction methods on the DNA promoter problem. The MofN approach is reported to have achieved 92.5% accuracy using 10-fold cross-validation, while RuleSet achieved 9 correct classifications out of 10 test set examples on a rule set extracted from a feedforward neural network trained using backpropagation on the remaining 96 examples.

Exploring the DNA promoter experiment more systematically, let us now evaluate empirically the impact of the information loss expected as part of the process of rule extraction. In order to do this, in what follows, we compare the test set accuracy of the rules extracted from the DBN with that of the DBN itself. This evaluation was done for four different partitions of training and test data, as shown in Figures 1 and 2. For each partition, 20 networks were trained using different settings. The figures plot the classification performance of the network model against that obtained by the corresponding rule set. The results indicate a high fidelity of the rules[1].

We now turn our attention to the special nature of certain nodes in the network, as seen in the case of the group-of-four in the DNA promoter problem, and notably when the target nodes are expected to be exclusive (e.g. as part of a softmax target layer in the network). In this case, the rules extracted are expected to follow the conditional distribution:

$$P(\mathbf{y} = o|\mathbf{x}) \propto \prod_j (1 + e^{\sum_i w_{ij}x_i + u_{oj}y_o}) \tag{13}$$

where U is the weight matrix between the label layer Y and the hidden layer H, and $\mathbf{y}$ is a one-hot vector representing the label classes. For example, $\mathbf{y} = o$ represents class o where $y_o = 1$ and $y_{o' \neq o} = 0$. From Eq. (13), the following confidence function can be defined:

$$\mathcal{C}(\mathbf{y} = o, \mathbf{x}) = \sum_j \log(1 + e^{\sum_i w_{ij}x_i} e^{u_{oj}y_o}) \tag{14}$$

[1]Notice that the grid-like arrangement of accuracies in Figure 1(a) and Figure 2(a) is a result of the small number of test samples in such cases (10 samples only)

Algorithm 2 accounts for the first product in the above equation by extracting rules from input I to the hidden layer $\mathsf{h}_j^{(1)}$ (or, more generally, from $\mathsf{h}_j^{(i)}$ to $\mathsf{h}_j^{(i+1)}$). With $\mathbf{y} = o$ expressed as $y_o = 1$, the exponential in the second product in the above equation can be used to normalise the confidence values $\alpha_j^{(1)}$ of $\mathsf{h}_j^{(1)}$, producing:

$$\mathcal{C}(\mathbf{y} = o, \mathbf{x}) \approx \sum_j \log(1 + \alpha_j^{(1)} e^{u_{oj}}) \tag{15}$$

Given Eq. (15), for each hidden unit and hypothesis $\mathbf{y} = o$, one can extract a rule $e^{u_{oj}} : \mathbf{y} = o \leftrightarrow \mathsf{h}_j^{(1)}$, whose confidence value is $e^{u_{oj}}$. By applying Inference Rule INF1 and adding the confidence values of each hypothesis normalised by $f(\alpha) = \log(1 + \alpha)$, one obtains the same confidence values as produced by Eq. (15). Algorithm 3 formalises the resulting rule extraction for such softmax layers.

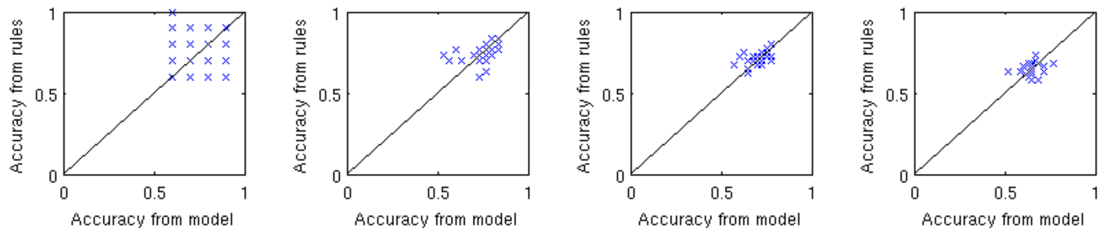
Algorithm 3 TOP_RBM_EXTRACT

```
Require: An RBM with visible layer I, hidden layer H, and
    label layer Y
 1: R = ∅, T=∅
 2: R = RBM_EXTRACT(I,H)
 3: for each hidden unit $j \in$ H and output unit $o \in$ Y do
 4:     Add a rule : $e^{u_{oj}} : \mathbf{y} = o \leftrightarrow \mathsf{h}_j$ to T
 5: end for
 6: return R,T
```

We are now in position to introduce the general algorithm for rule extraction from DBNs, Algorithm 4. It follows a layer-wise approach whereby, for a DBN having n layers, either Algorithm 2 is applied n times or Algorithm 2 is applied $n-1$ times and Algorithm 3 is applied once. We call the first alternative *compact* as it generates fewer rules at the top level of the DBN.

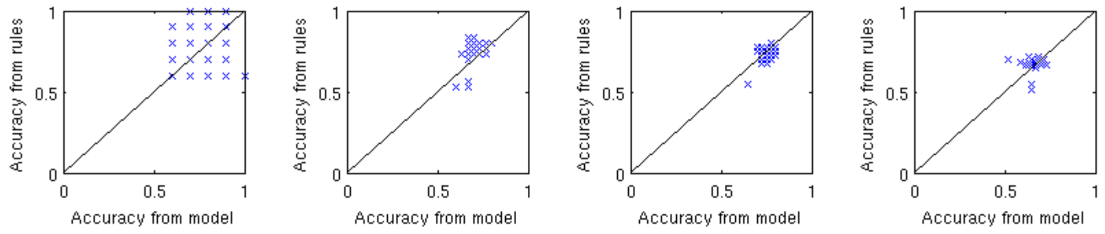
Algorithm 4 DBN_EXTRACT

```
Require: A stack of L RBMs
 1: Create empty rule set R = ∅
 2: for $l = 1$ to $L - 1$ do
 3:     R$^{(l)}$ = RBM_EXTRACT(l,l+1)
 4:     Add R$^{(l)}$ to R
 5: end for
 6: if COMPACT then
 7:     R$^{(L)}$ = RBM_EXTRACT(L,Y)
 8: else
 9:     R$^{(L)}$ = TOP_RBM_EXTRACT(L,Y)
10: end if
11: Add R$^{(L)}$ to R
```



(a) 96-training, 10-test (b) 76-training, 30-test (c) 66-training, 40-test (d) 46-training, 60-test

Fig. 1: Classification performances of RBMs and the extracted rules on DNA promoter dataset



(a) 96-training, 10-test (b) 76-training, 30-test (c) 66-training, 40-test (d) 46-training, 60-test

Fig. 2: Classification performances of DBNs compared with extracted rules on the DNA promoter dataset

Information Loss in Complex Domains: We now test the general method of rule extraction from DBNs (Algorithm 4) on a harder problem, namely the MNIST handwritten digit recognition dataset. This is a difficult problem for rule extraction because the inputs are the values of the pixels in the images to be classified into classes 0, 1, 2,..., 9. The rules are therefore expected to capture the levels of abstraction learned by the DBN, from the raw data through to the class, hopefully identifying useful concepts such as edges and shapes as part of the rule hierarchy. Such image domains are notoriously difficult for symbolic reasoning.

In what follows, we report results using *COMPACT=False* (c.f. Algorithm 4). In this image domain, we found that information loss is larger when *COMPACT=True*. We attribute information loss in this case of the MNIST dataset to the fact that the input data is non-binary, showing more variance than the DNA data evaluated earlier. As a result, in the case of a deep network, information loss may be compounded when inference is applied sequentially through the rule hierarchy (i.e. without sampling). In what follows, we evaluate information loss in more detail.

In Section IV-A, the confidence values of the rules extracted from an RBM were provided as input for training an SVM. In the case of a DBN, the same layer-wise approach would result in each RBM in the hierarchy being trained and rules extracted before the next RBM can be trained. In order to evaluate information loss in DBNs, though, instead of doing the above, we are interested in the extraction of a complete hierarchy of rules from the entire DBN. We have trained 155 DBNs using the standard configuration used by others [3]: 784 input nodes, 500 nodes in the first hidden layer, 1000 nodes in the second hidden layer, and 10 target nodes. We have used the benchmark MNIST data set with $20,000$ training examples, $10,000$ held-out examples used for early stopping validation [39], and $10,000$ test examples. Figure 3 shows for the MNIST data, as done for the DNA promoter data, a comparison between the test-set accuracy of the DBNs (model accuracy) and the test-set accuracy of the extracted rules. As expected, the results indicate more information loss here than in the case of the DNA data, with an average information loss in the rules of 15.3026% ±5.9255 in relation to the DBNs.

The DBNs were trained using learning rate decay and early stopping based on their performance on the validation set (whenever the validation set error increased, a lower learning rate was used for network training). The same can be done using rule sets extracted from the network, as follows: rules are extracted after each epoch of training. Instead of the network, the rules are used to calculate the validation set error. Whenever the validation error increases using the rules, a lower learning rate is used in the training of the network. In this way, the extracted rules are used to trigger the early stopping of the network training. It is expected that, by using the rules for validation, the fidelity of the rules to the final model should increase. Nevertheless, since the time complexity of the extraction of rules from each RBM is $\mathcal{O}(I \times J)$, the computation cost for validation by rules is higher than validation by using the model itself. Figure 4 shows a comparison between the test-set accuracy of the DBNs (model accuracy), now using such rule-based early stopping, and the test-set accuracy of the extracted rules. Now, an average information loss of 9.2519% ±4.2095 is achieved in relation to the DBNs. In comparison with Figure 3, it can be seen that the use of rule-based early stopping produces rule sets with higher fidelity to the network model (i.e. lower information loss). Given the complexity of image domains when it comes to rule extraction, we interpret the results shown in Figure 4 as indicative that the extracted rules can be useful at highlighting certain important relationships in the network models, e.g. if the same or very similar rules are extracted from the various network models. This domain specific analysis is left as future work.

Achieving a higher level of integration between network and rule models at learning may be desirable, as seen e.g. above when extracted rules were used as criterion for the network's early stopping. Such integration can be achieved fully through the provision of algorithms for inserting rules into network models. This will be the topic of discussion for the rest of this paper.

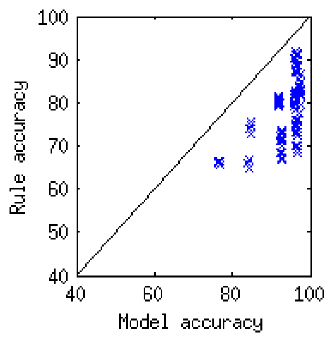


Fig. 3: Comparison between the test-set accuracies of DBNs (model accuracy) and extracted rules on the MNIST dataset.

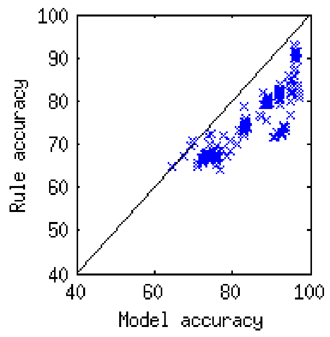


Fig. 4: Comparison between the test-set accuracies of DBNs (model accuracy) and extracted rules using rule-based early stopping on the MNIST dataset.

V. Deep Neural-Symbolic Integration

Having seen how symbolic knowledge can be extracted from DBNs, we now investigate the inverse problem of inserting symbolic knowledge into DBNs to improve network learning using background knowledge. The idea of encoding knowledge into DBNs to improve learning performance is inspired by early work on knowledge-based neural networks [34], [35]. In addition to improving learning time, prior knowledge has been shown capable of improving learning accuracy by allowing knowledge that is not reinforced through learning, but that might nevertheless be relevant, to persist in the network model.

A. Knowledge Encoding

In this section, we propose a method and algorithm for encoding confidence rules into DBNs. We also perform an evaluation of knowledge insertion using both the DNA and MNIST datasets used earlier. This evaluation shows that, as expected, improvements in performance can be achieved with the use of prior knowledge. We argue, therefore, that when prior knowledge is available, the provision of algorithms allowing its use within network models (such as the algorithm introduced in this section) is desirable.

As has been discussed in Section IV, a hierarchical knowledge-base with associated confidence values can offer an appropriate symbolic representation for DBNs. In fact, such a representation has been motivated by the way that DBNs work, as indicated by the way that a hierarchical weighted knowledge-base has been defined (c.f. Definition 3.1).

Example 5.1 and Figure 5 illustrate the main idea behind the encoding algorithm to follow using a simple set of rules. Figure 5 also illustrates how the DBN can be extended to account for learning from data and background knowledge, which is discussed in the sequel.

Example 5.1: (Encoding knowledge) Given a hierarchical set of rules $K^s = \{K^{(1)}, K^{(2)}, K^{(3)}\}$, where:

$$K^{(1)} = \{c_1 : \mathsf{y}_1 \leftrightarrow \mathsf{x}_1 \wedge \neg\mathsf{x}_2; c_2 : \mathsf{y}_2 \leftrightarrow \mathsf{x}_2 \wedge \mathsf{x}_3; c_3 : \mathsf{y}_3 \leftrightarrow \neg\mathsf{x}_3 \wedge \mathsf{x}_4\}$$
$$K^{(2)} = \{c_4 : \mathsf{z}_1 \leftrightarrow \neg\mathsf{y}_1 \wedge \mathsf{y}_2; c_5 : \mathsf{z}_2 \leftrightarrow \mathsf{y}_3\}$$
$$K^{(3)} = \{c_6 : \mathsf{t}_1 \leftrightarrow \mathsf{z}_1 \wedge \mathsf{z}_2\}$$

For a dataset with variables $\{x_1, x_2, x_3, x_4, x_5, t_1, t_2\}$, consider rule $c_1 : \mathsf{y}_1 \leftrightarrow \mathsf{x}_1 \wedge \neg\mathsf{x}_2$. We add a unit y_1 to the hidden layer of the first RBM and set the weights to $w_{11} = c_1, w_{21} = -c_1$. We repeat the process for each rule in $K^{(1)}$, and create random down-weight connections for the units. We then repeat the process for each level of the hierarchy. Finally, we allow the addition of extra hidden nodes with bidirectional random connections to each hidden level. Figure 5 shows the resulting network for hierarchical set K.

Algorithm 5 shows how a hierarchical weighted knowledge-base can be encoded into a DBN. Since the connections in an RBM are bidirectional, while the rules only support bottom-up inference, the confidence values are encoded as *up-weights* in the network, with a set of down-weights with random values being added from the hidden units to the visible units.

B. Learning with Background Knowledge

Let $\mathcal{K}$ be a hierarchical weighted knowledge-base, that is, a hierarchical set of implication rules with *confidence values*, as defined earlier. We have encoded each subset of rules $\mathcal{K}^{(l)}$ at each level of the hierarchy into an RBM and have added more hidden units to it (the number of extra hidden units to add will be investigated empirically). For each RBM, the energy function is:

$$\mathbf{E}(\mathbf{x}, \mathbf{h}) = -\sum_j h_j c_j \sum_i s_{ij} x_i - \sum_{ik} x_i u_{ik} h_k - \sum_i a_i x_i - \sum_k b_k h_k \quad (16)$$

where, $\mathbf{x}$ and $\mathbf{h}$ denote units added by Algorithm 5, associated with background knowledge rules, c_j is the initial *confidence value* of rule j, J denotes the number of rule-encoded units in the hidden layer (corresponding to the number of rules), K is the number of extra units added to the hidden layer, $s_{ij} = 1$ if

Algorithm 5 Rule Encoding Algorithm

```
Require: a hierarchical weighted knowledge-base $K$
1:  for $l = 1$ to $L$ do
2:      Initialise an empty RBM $N^{(l)}$;
3:      for each rule $c_j^{(l)} : \mathsf{h}_j^{(l)} \leftrightarrow \bigwedge_t \mathsf{h}_t^{(l-1)} \wedge \bigwedge \neg \mathsf{h}_k^{l-1)} \in K_l$ do;
4:          Add a unit $j$ to hidden layer $l$;
5:          Set the value of the connection weight $w_{tj}^l$ from node $\mathsf{h}_t^{(l-1)}$ to node $j$ to $c_i$;
6:          Set the value of the connection weight $w_{kj}^l$ from node $\mathsf{h}_k^{(l-1)}$ to node $j$ to $-c_i$;
7:      end for
8:      if $l > 1$ then
9:          Stack $N^{(l)}$ on top of $N^{(l-1)}$;
10:     end if
11: end for
```

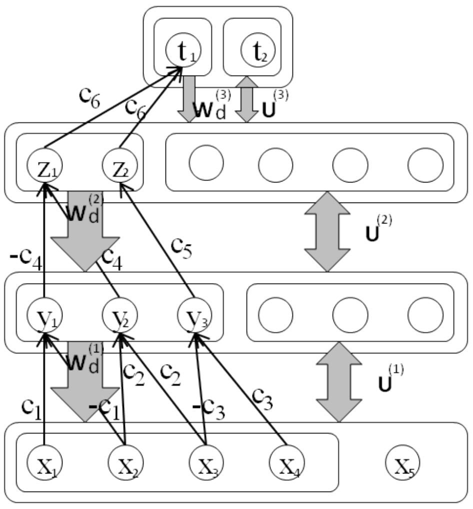


Fig. 5: DBN obtained from hierarchical rule set K from Example 5.1

the encoded weight is positive, $s_{ij} = -1$ if the encoded weight is negative, or $s_{ij} = 0$ if the weight is zero (c.f. Algorithm 5), and $u_{ij} \in U$ is the value of the weights of the extra hidden units (see Figure 5).

The encoded knowledge will be used to guide learning within the neural-symbolic RBMs by maximising the log-likelihood of the parameters given the data and background knowledge. Since the connections in an RBM are bi-directional, while the background knowledge only supports bottom-up inference, we split the connection weights between visible and rule-encoded hidden units. The confidence values were used to define the *up-weights* (W_u), and random values were assigned to the *down-weights* (W_d). The learning algorithm below will, therefore, adapt the parameters that consist of additional connection weights U and the down-weights W_d given the confidence values.

We use Contrastive Divergence [26] to train the networks. The log-likelihood function is given by:

$$\mathcal{L}_{lRBM} = \sum_{\mathbf{x} \in \mathcal{D}} P(\mathbf{x}|\theta = \{U, W_d\}; \mathcal{K}) \qquad (17)$$

The gradient of the log-likelihood function is given by:

$$\Delta u_{ik} = \langle x_i h_k \rangle_0 - \langle x_i h_k \rangle_{\mathcal{K}} \qquad (18)$$

where $\langle . \rangle_{\mathcal{K}}$ is the average over the set of examples given a neural-symbolic network with background knowledge $\mathcal{K}$. We call the learning algorithm below *learning with guidance* because prior knowledge is used to partially fix some upward connections in the network; all other connections, both downward and bi-directional, are allowed to change as part of learning using standard Contrastive Divergence.

Algorithm 6 Learning with Guidance

```
Require: A set of rules $K_l^{(s)}$; input data $X$
1:  Select a number of rules in $K_l^{(s)}$ with the highest confidence values
2:  Encode $K_l^{(s)}$ in hidden units $H^{(s)}$ with up-weights $W_u^{(l)}$ and random down-weights $W_d^{(l)}$
3:  Add extra hidden units $H^{(t)}$ with weights $U^{(l)}$
4:  repeat
5:  % positive stage: assign X to visible layer
6:      $X_{pos} := X$;
7:      $H_{pos} := P(H|X_{pos})$;        $\hat{H}_{pos} \sim P(H|X_{pos})$;
8:      $X_{neg} := P(X|\hat{H}_{pos})$;        $\hat{X}_{neg} \sim P(X|\hat{H}_{pos})$;
9:  % negative stage
10:     $H_{neg} = P(H|\hat{X}_{neg})$;
11:     $W_d^{(l)} = W_d^{(l)} + \eta(\langle X_{pos}^\top H_{pos}^{(s)} - \hat{X}_{neg}^\top H_{neg}^{(s)} \rangle)$
12:     $U^{(l)} = U^{(l)} + \eta(\langle X_{pos}^\top H_{pos}^{(t)} - \hat{X}_{neg}^\top H_{neg}^{(t)} \rangle)$
13: until convergence
```

C. Experiments on DNA Promoter dataset

In this experiment, we use the domain theory provided with the DNA promoter dataset[2] to set up and train a DBN. As before, we use variable n_p to denote a nucleotide at position p such that e.g. a_p represents $n_p = A$. Hence, background knowledge rule $minus_{10} \leftrightarrow n_{-12} = T \wedge n_{-11} = A \wedge n_{-7} = T$ becomes $c : \mathsf{minus}_{10} \leftrightarrow \mathsf{t}_{-12} \wedge \mathsf{a}_{-11} \wedge \mathsf{t}_{-7}$, with arbitrary confidence value c.

We use Algorithm 5 to encode the domain theory into the network and use Algorithm 6 to train each layer greedily as done in standard DBNs. The domain theory is divided into a hierarchical set of rules that is encoded into a 2-layer DBN. We choose two hidden layers because the rule $\mathsf{promoter} \leftrightarrow \mathsf{contact} \wedge \mathsf{conformation}$ consists of variable $\mathsf{conformation}$ at level 2 and $\mathsf{contact}$ at level 3 of the hierarchy. By combining such rules we do not need to create another layer with more intermediate variables[3].

For evaluation, we partition the data into a training, validation and test set. In order to investigate how background knowledge influences learning given different amounts of data, we use different training sets with 10, 30, 50 and 70 samples.

[2]http://archive.ics.uci.edu/ml/datasets/Molecular+Biology+(Promoter+Gene+Sequences)

[3]We merge rules c : $\mathsf{promoter} \leftrightarrow \mathsf{contact} \wedge \mathsf{conformation}$ and c : $\mathsf{contact} \leftrightarrow \mathsf{minus}_{35} \wedge \mathsf{minus}_{10}$ into $c : \mathsf{promoter} \leftrightarrow \mathsf{minus}_{35} \wedge \mathsf{minus}_{10} \wedge \mathsf{conformation}$

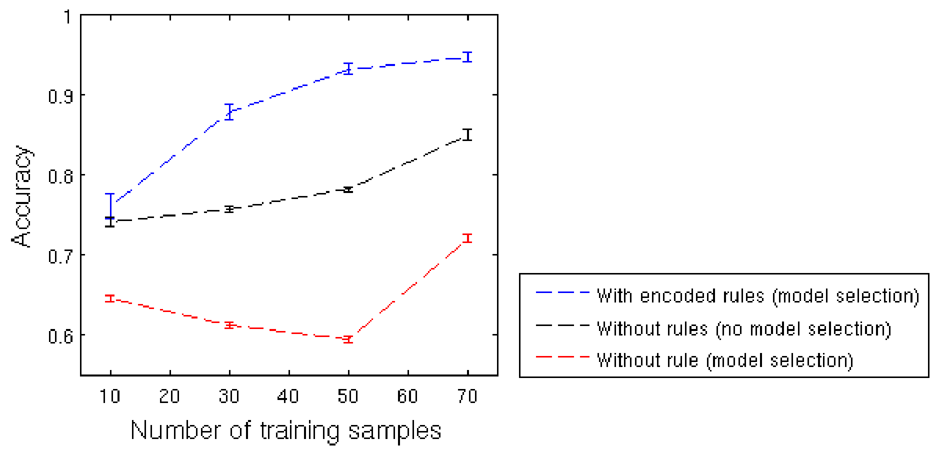


Fig. 6: Test set classification performance of 2-layer standard DBN (red and black lines, with and without model selection), and 2-layer DBN encoded with prior knowledge from the DNA promoter domain theory using training sets with 10, 30, 50 and 70 samples, and 20 test samples.

The validation and test sets are the same for each of the training sets and consist of 16 and 20 samples, respectively. From this experiment, we observe that when using the validation set to select the DBNs without background knowledge, this results in low performance on the test set. For the DBNs encoded with background knowledge, the models selected by the validation set produce good accuracy on the test set. This might happen because the number of hyper-parameters is large compared to the small validation and test sets. Hence, the grid search tends to produce a DBN that overfits the validation set. When background knowledge is encoded into the networks, overfitting is avoided through the use of the rule guidance learning algorithm, which seems to be able to produce a more general model.

In order to make a better comparison between the standard DBN and the encoded DBN, we include in Figure 6 the best accuracy achieved on the test set using the standard DBN without using model selection. The figure shows that with background knowledge to guide the learning, the DBN can achieve a considerable improvement in performance (e.g. up by 15% when the training set has size 50). It also shows that when the training set is larger (70 examples), the standard DBN is able to learn from the data alone the knowledge that had been provided as background theory, and therefore the improvement with prior knowledge is smaller for larger training sets.

D. Experiments on MNIST dataset

In order to evaluate the influence of background knowledge on the MNIST dataset (for which no prior symbolic knowledge is available), we have extracted rules from a network trained on a subset of the data by applying Algorithm 4, and then inserted such rules into a new network for further training and comparison. In the MNIST dataset, there were 20,000 examples for training, 10,000 examples for validation, and 10,000 examples for testing. We have selected 1,000 examples randomly from the training set for training a 2-layer DBN from which rules were then extracted. Such rules were encoded into a new DBN, following the procedure in Section V-A. This new DBN was then trained on the remaining 19,000 examples. Finally, results were compared with those obtained by another DBN trained from scratch on the entire 20,000 examples without any rule insertion.

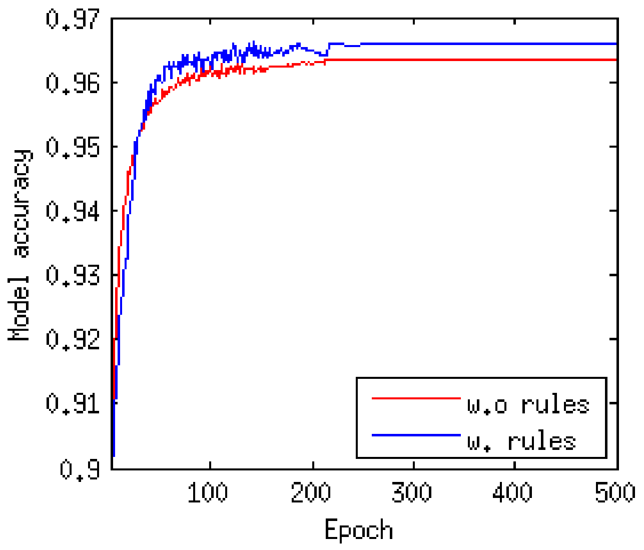


Fig. 7: Test set performance comparison between DBNs trained with and without prior encoding of rules on the MNIST dataset; DBNs with rule encoding achieve slightly higher accuracy faster.

Figure 7 shows that with the encoding of rules, a DBN can achieve a slightly higher accuracy faster than a DBN without rules. This suggests that the network structure may be important. Although there is information loss within the rules extracted from the DBN trained on the 1,000 examples, the DBN set-up with such rules and trained on the remaining 19,000 examples performed slightly better than the DBN trained on the entire 20,000 examples in one goal, which included those 1,000 examples. This indicates that maintaining the structures of the representations learned by deep networks can be beneficial as part of a modular approach to learning. This requires further research.

VI. Conclusion and Future Work

This paper introduced and evaluated algorithms for inserting and extracting knowledge from deep networks. The question of whether modularity can help the integration of learning and reasoning in deep networks has been investigated empirically. A new inference rule for deep networks using *confidence rules* has been proposed, which combines symbolic representation and quantitative reasoning. This inference rule and logical representation was designed to support hierarchical reasoning, and was shown to be an adequate representation for the modular training of deep networks. Knowledge represented by confidence rules can be inserted or extracted from Deep Belief Networks (DBNs). It is shown that in single-layer DBNs, also known as restricted Boltzmann machines (RBMs), confidence rules offer a low-cost representation for the RBMs. The use of a modular, layer-wise approach to knowledge extraction from DBNs is shown to produce information loss at times, notably when the networks are trained on complex image data. Yet, the modular training of networks as part of a cycle of knowledge insertion, learning and extraction can produce an improvement in performance (c.f. Figures 6 and 7). Knowledge encoding into DBNs in the form of confidence rules has been shown to be useful, leading to an improvement in performance following a layer-wise training. The results from this work suggest that there is promise in building a hierarchical reasoning system capable of integrating symbolic and subsymbolic capabilities. With the layer-wise extraction and insertion principle, the work in this paper can be extended to deeper networks. However, for knowledge extraction from very deep networks, as discussed earlier, the use of extracted rules for model selection may not be practical due to an increased computational overhead.

As future work, further domain specific experimental evaluations may be carried out. Of particular interest are applications of multimodal data using very deep networks. Recent research shows a deep semantic mapping between text and images [40] which motivates the use of knowledge extraction from, say, a text modality as relevant for the explanation of context in the image modality. Another direction for future work includes the parallel implementation of the proposed knowledge insertion and extraction algorithms, and its use in the iterative evaluation of very large networks, as part of a cycle of knowledge acquisition and revision. In this process, one may consider the use of recent techniques from high-performance computing which, applied to neural networks, may take advantage of the underlying graph structures to achieve large-scale improvements in performance. These include the local parallel method applied to directed acyclic graphs and the multi-index chained hashing method for fast neuron memory search [41], [42], [43].

References

[1] L. G. Valiant, “Three problems in computer science,” *Journal of the ACM*, vol. 50, no. 1, pp. 96–99, 2003.

[2] J. Y. Halpern, *Reasoning about uncertainty*. Cambridge, Mass., London: MIT Press, 2003. [Online]. Available: http://opac.inria.fr/record=b1100784

[3] G. E. Hinton, S. Osindero, and Y.-W. Teh, “A Fast Learning Algorithm for Deep Belief Nets,” *Neural Comp.*, vol. 18, no. 7, pp. 1527–1554, Jul. 2006.

[4] P. Smolensky, “Information processing in dynamical systems: Foundations of harmony theory,” in *Parallel Distributed Processing: Volume 1: Foundations*. MIT Press, Cambridge, 1986, pp. 194–281.

[5] L. Breiman, “Statistical modeling: The two cultures (with comments and a rejoinder by the author),” *Statistical Science.*, vol. 16, no. 3, pp. 199–231, 08 2001. [Online]. Available: http://dx.doi.org/10.1214/ss/1009213726

[6] A. d’Avila Garcez, L. Lamb, and D. Gabbay, *Neural-Symbolic Cognitive Reasoning*, ser. Cognitive Technologies. Springer, 2009.

[7] A. d’Avila Garcez, L. de Raedt, L. Lamb, R. Miikkulainen, P. Hitzler, T. Icard, T. Besold, P. Foldiak, D. Silver, and K.-U. Kuehnberger, “Neural-symbolic learning and reasoning: Contributions and challenges,” in *AAAI Spring Symposium on Knowledge Representation and Reasoning: Integrating Symbolic and Neural Approaches*, March 2015.

[8] G. G. Towell and J. W. Shavlik, “The extraction of refined rules from knowledge-based neural networks,” in *Machine Learning*, 1993, p. 71101.

[9] A. d’Avila Garcez, K. Broda, and D. Gabbay, “Symbolic knowledge extraction from trained neural networks: A sound approach,” *Artificial Intelligence*, vol. 125, pp. 155–207, 2001.

[10] M. G. Augasta and T. Kathirvalavakumar, “Reverse engineering the neural networks for rule extraction in classification problems,” *Neural Processing Letters*, vol. 35, no. 2, pp. 131–150, 2012. [Online]. Available: http://dx.doi.org/10.1007/s11063-011-9207-8

[11] K. Odajima, Y. Hayashi, G. Tianxia, and R. Setiono, “Greedy rule generation from discrete data and its use in neural network rule extraction,” *Neural Networks*, vol. 21, no. 7, pp. 1020–1028, 2008. [Online]. Available: http://dx.doi.org/10.1016/j.neunet.2008.01.003

[12] R. Setiono, B. Baesens, and C. Mues, “Recursive neural network rule extraction for data with mixed attributes,” *IEEE Trans. Neural Networks*, vol. 19, no. 2, pp. 299–307, 2008. [Online]. Available: http://doi.ieeecomputersociety.org/10.1109/TNN.2007.908641

[13] A. Hara and Y. Hayashi, “Ensemble neural network rule extraction using re-rx algorithm,” in *The 2012 International Joint Conference on Neural Networks (IJCNN), Brisbane, Australia, June 10-15, 2012*, 2012, pp. 1–6. [Online]. Available: http://dx.doi.org/10.1109/IJCNN.2012.6252446

[14] T. A. Etchells and P. J. G. Lisboa, “Orthogonal search-based rule extraction (OSRE) for trained neural networks: a practical and efficient approach,” *IEEE Trans. Neural Networks*, vol. 17, no. 2, pp. 374–384, 2006. [Online]. Available: http://doi.ieeecomputersociety.org/10.1109/TNN.2005.863472

[15] Y. Bengio, P. Lamblin, D. Popovici, and H. Larochelle, “Greedy layer-wise training of deep networks,” in *Advances in Neural Information Processing Systems 19*, B. Scholkopf, J. Platt, and T. Hoffman, Eds. Cambridge, MA: MIT Press, 2007, pp. 153–160.

[16] L. Bottou, “From machine learning to machine reasoning: an essay,” *Machine Learning*, vol. 94, pp. 133–149, January 2014. [Online]. Available: http://leon.bottou.org/papers/bottou-mlj-2013

[17] L. d. Penning, A. S. d. Garcez, L. C. Lamb, and J.-J. C. Meyer, “A neural-symbolic cognitive agent for online learning and reasoning,” in *IJCAI*, 2011, pp. 1653–1658.

[18] Son Tran and A. Garcez, “Logic extraction from deep belief networks,” in *ICML 2012 Representation Learning Workshop*, Edinburgh, Jul. 2012. [Online]. Available: https://sites.google.com/site/representationworkshopicml2012/schedule

[19] S. N. Tran and A. d’Avila Garcez, “Knowledge extraction from deep belief networks for images,” in *IJCAI-2013 Workshop on Neural-Symbolic Learning and Reasoning*, 2013.

[20] Y. Lecun, L. Bottou, Y. Bengio, and P. Haffner, “Gradient-Based Learning Applied to Document Recognition,” *Proceedings of the IEEE*, vol. 86, no. 11, pp. 2278–2324, Nov. 1998.

[21] H. Lee, C. Ekanadham, and A. Y. Ng, “Sparse deep belief net model for visual area v2,” in *Advances in Neural Information Processing Systems*, 2007.

[22] H. Lee, R. Grosse, R. Ranganath, and A. Y. Ng, “Convolutional deep belief networks for scalable unsupervised learning of hierarchical

representations," in *Proceedings of the International Conference on Machine Learning*. New York, NY, USA: ACM, 2009, p. 609616.

[23] Y. LeCun, B. Boser, J. S. Denker, D. Henderson, R. E. Howard, W. Hubbard, and L. D. Jackel, "Backpropagation applied to handwritten zip code recognition," *Neural Computation*, vol. 1, no. 4, pp. 541–551, Dec. 1989.

[24] Y. Bengio, P. Lamblin, D. Popovici, and H. Larochelle, "Greedy layer-wise training of deep networks," in *Proceedings of the International Conference on Machine Learning*, 2007, pp. 153–160.

[25] R. Salakhutdinov, "Learning in markov random fields using tempered transitions," in *Advances in Neural Information Processing Systems*, Y. Bengio, D. Schuurmans, J. Lafferty, C. K. I. Williams, and A. Culotta, Eds., 2009, p. 15981606.

[26] G. E. Hinton, "Training products of experts by minimizing contrastive divergence," *Neural Computation*, vol. 14, no. 8, pp. 1771–1800, Aug. 2002.

[27] R. Salakhutdinov, "Learning deep boltzmann machines using adaptive mcmc." in *Proceedings of the International Conference on Machine Learning*. Omnipress, 2010, pp. 943–950.

[28] R. V. Borges, A. S. d'Avila Garcez, and L. C. Lamb, "Learning and representing temporal knowledge in recurrent networks," *IEEE Transactions on Neural Networks*, vol. 22, no. 12, pp. 2409–2421, 2011.

[29] M. W. Craven and J. W. Shavlik, "Learning symbolic rules using artificial neural networks," in *The Proceedings of International Conference on Machine Learning*. Morgan Kaufmann, 1993, pp. 73–80.

[30] A. d'Avila Garcez, K. Broda, and D. Gabbay, *Neural-Symbolic Learning Systems: Foundations and Applications*, ser. Perspectives in Neural Computing. Springer, 2002.

[31] B. Hammer and P. Hitzler, Eds., *Perspectives of Neural-Symbolic Integration*. Springer, 2007.

[32] G. Pinkas, "Reasoning, nonmonotonicity and learning in connectionist networks that capture propositional knowledge," *Artificial Intelligence*, vol. 77, no. 2, pp. 203 – 247, 1995.

[33] A. Argyriou, T. Evgeniou, and M. Pontil, "Multi-task feature learning," in *Advances in Neural Information Processing Systems 19*. MIT Press, 2007.

[34] G. G. Towell and J. W. Shavlik, "Knowledge-based artificial neural networks," *Artificial Intelligence*, vol. 70, no. 1-2, pp. 119–165, 1994.

[35] A. S. Avila Garcez and G. Zaverucha, "The connectionist inductive learning and logic programming system," *Applied Intelligence*, vol. 11, no. 1, p. 5977, Jul. 1999.

[36] M. Richardson and P. Domingos, "Markov logic networks," *Machine Learning*, vol. 62, no. 1-2, p. 107136, feb 2006. [Online]. Available: http://dx.doi.org/10.1007/s10994-006-5833-1

[37] V. Gogate, K. Kersting, S. Natarajan, and D. Poole, "Statistical relational artificial intelligence, papers from the 2013 aaai workshop, bellevue, washington, usa, july 15, 2013," in *AAAI Workshop: Statistical Relational Artificial Intelligence*, ser. AAAI Workshops, vol. WS-13-16. AAAI, 2013.

[38] J. Shawe-Taylor and N. Cristianini, *Kernel Methods for Pattern Analysis*. New York, NY, USA: Cambridge University Press, 2004.

[39] Y. Yao, L. Rosasco, and A. Caponnetto, "On early stopping in gradient descent learning," *Constructive Approximation*, vol. 26, no. 2, pp. 289–315, 2007. [Online]. Available: http://dx.doi.org/10.1007/s00365-006-0663-2

[40] W. Liu, T. Mei, Y. Zhang, C. Che, and J. Luo, "Multi-task deep visual-semantic embedding for video thumbnail selection," in *The IEEE Conference on Computer Vision and Pattern Recognition (CVPR)*, June 2015.

[41] A. Forechi, A. F. D. Souza, J. de Oliveira Neto, E. de Aguiar, C. Badue, A. S. d'Avila Garcez, and T. Oliveira-Santos, "Fat-fast VG-RAM WNN: A high performance approach," *Neurocomputing*, vol. 183, pp. 56–69, 2016. [Online]. Available: http://dx.doi.org/10.1016/j.neucom.2015.06.104

[42] C. C. Yan, Y. Zhang, J. Xu, F. Dai, J. Zhang, Q. Dai, and F. Wu, "Efficient parallel framework for HEVC motion estimation on many-core processors," *IEEE Trans. Circuits Syst. Video Techn.*, vol. 24, no. 12, pp. 2077–2089, 2014.

[43] C. Yan, Y. Zhang, J. Xu, F. Dai, L. Li, Q. Dai, and F. Wu, "A highly parallel framework for HEVC coding unit partitioning tree decision on many-core processors," *IEEE Signal Process. Lett.*, vol. 21, no. 5, pp. 573–576, 2014.