Neural Disjunctive Normal Form: Vertically Integrating Logic With Deep Learning For Classification

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Abstract

We present Neural Disjunctive Normal Form (Neural DNF), a hybrid neuro-symbolic classifier that *vertically* integrates propositional logic with a deep neural network. Here, we aim at a *vertical* integration of logic and deep learning: we utilize the ability of deep neural networks as feature extractors to extract intermediate representation from data, and then a Disjunctive Normal Form (DNF) module to perform logical rule-based classification; we also seek this integration to be *tight* that these two normally-incompatible modules can be learned in an end-to-end manner, for which we propose the *BOAT* algorithm.

Compared with standard deep classifiers which use a linear model or variants of additive model as the classification head, Neural DNF provides a new choice of model based on logic rules. It offers interpretability via an explicit symbolic representation, strong model expressity, and a different type of model inductive bias. Neural DNF is particularly suited for certain tasks that require some logical composition and provides extra interpretability.

1 Introduction

In the recent years, the emphasis of machine learning, particularly deep learning, has been to increase the capacity to accurately model complex patterns, but typically such flexibility results in *blackboxes* that are too complex for humans to understand. While the ability of deep learning on feature extraction and pattern recognition is widely recognized, the blackbox nature makes it hard for human to interpret the underlying mechanism; furthermore, this lack of interpretability leads to difficulties for human to interact with or manipulate the model, when trying to debug undesired behaviors or to improve model by incorporating human knowledge.

A possible solution to this limitation of deep learning, as discussed and promoted by many researchers [Marcus, 2020, Bengio, 2019, Yi et al., 2019, Mao et al., 2019, Hudson and Manning, 2019, Penkov, 2019] , is to develop hybird neuro-symbolic models. While there are many different approaches on integrating neural and symbolic models, one of these approaches called **Vertical Integration**[1], aims at exploiting the best of both worlds in a straight-forward way: it utilizes deep learning to learn high-level features from raw sensory data (which deep learning are good at), and utilizes symbolic models to reason about the high-level features (which symbolic models are good at). More formally, the vertical integration approach can be represented as a two stage model $f = g \circ \phi$ whose prediction on a sample x is given by $\hat{y} = f(x) = g(\phi(x))$ where the first-stage ϕ is a neural network feature extractor and the second-stage g is the symbolic model processing the extracted features into final prediction. Vertical integration has its biological inspiration: we know that

[1]The term vertical integration is categorized in a recent survey [Garcez et al., 2019] on neuro-symbolic models. The neuro-symbolic literatute [Besold et al., 2017] offers a multilitude of approaches covering different settings, making it hard to discuss in brief due to space. We provide a more discussion in appendix.

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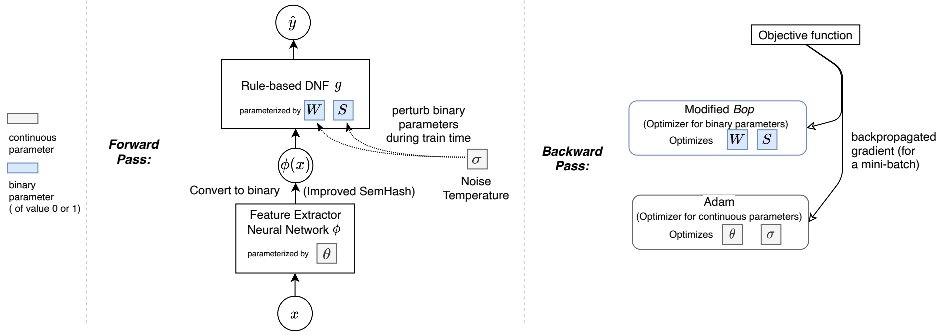
certain areas in the brain are used to process input signals [Grill-Spector and Malach, 2004] while others are responsible for logical reasoning [Shokri-Kojori et al., 2012]. But from a more practical perspective, vertical integration promises a solution to demystify the blackbox by decomposing the prediction task into two stages, handled by different models; and a better-demystified *interpretable* model can enable easier human interactions and manipulations on the model.

The choice of symbolic model to integrate naturally depends on the task. SAT-Net [Wang et al., 2019a] utilizes a symbolic SAT solver layer on top of a convolutional neural network (CNN) for solving a satisfiability-based task of *visual Sudoku*; Donadello et al. [2017] utilizes first-order fuzzy logic on top of a Fast-RCNN to extract structured semantic descriptions from images; DeepProbLog [Manhaeve et al., 2018] builds a probabilistic logic program on top of a CNN within a domain-specified grammar template for tasks like visual digit addition and sorting. In this paper, since we deal with the most basic task of binary classification, we choose propositional logic in Disjunctive Normal Form (DNF), also known as 'decision rules' or 'rule set'. As a well-studied symbolic model, DNF has been established as being general and interpretable. DNF performs a simple and transparent 'OR-of-ANDs' prediction: if at least one AND clause (a conjunction of conditions) is satisfied, it predicts the positive class; otherwise negative. DNF is interpretable not only because its symbolic structure is intuitive to follow, but also that each conjunctive clause of DNF can be viewed as a separate IF-THEN rule, providing 'smaller-than-global' interpretations [Rudin, 2019]. DNF is a general rule format, as any propositional logic formula has an equivalent DNF formula, and thus any rule-based binary classifier including decision set/list/tree can be expressed by a DNF.

We seek Neural DNF's vertical integration to be tight, i.e. we wish to optimize the deep feature extractor and the DNF end-to-end. However, the main technical challenge here is that the learning algorithms for rule-based models and deep learning models are generally incompatible, making end-to-end learning not directly possible. In order to address this challenge, we propose BOAT (Bi-Optimizer learning with Adaptively-Temperatured noise) to train ϕ and g jointly (see fig. 1): we use standard continuous-parameter optimizer Adam [Kingma and Ba, 2014] to optimize the first-stage neural network ϕ and modify a binary-parameter optimizer from Helwegen et al. [2019] to optimize the parameters of the second-stage rule-based g. As the novel key ingredient of BOAT, we propose adaptively-temperatured noise to perform weight perturbation which enables the learning of the rule-based g. Our experiments demonstrate that learning constantly fails without such noise. Compared with standard deep learning classifiers which has a fully-connected linear layer as g, Neural DNF offers (1) a logic-based inductive bias and (2) better interpretability at competitive accuracy.



continuous parameter
binary parameter (of value 0 or 1)
Forward Pass:
$\hat{y}$
Rule-based DNF g
parameterized by W S
perturb binary parameters during train time
σ
Noise Temperature
$\phi(x)$
Convert to binary
(Improved SemHash)
Feature Extractor Neural Network ϕ
parameterized by θ
x
Backward Pass:
Objective function
Modified *Bop* (Optimizer for binary parameters)
Optimizes W S
backpropagated gradient (for a mini-batch)
Adam (Optimizer for continuous parameters)
Optimizes θ σ

Figure 1: *Overview of Neural DNF and the proposed BOAT Algorithm*

The rule-based Neural DNF is particularly suited for classification tasks that require the logical compositions of certain concepts. We demonstrate that with experiments on a toy dataset called 2D-XOR, an extension of the XOR problem which has received special interest in the literature [Minsky and Papert, 1969]. We consider 2D-XOR as a minimal example to show the benefits of Neural DNF's vertical integration, because 2D-XOR requires a model to both learn the right high-level features (concepts) from the raw data and the right XOR function. We further apply Neural DNF to image datasets in two scenarios: In the first scenario, we use a regular deep network as feature extractor with no further constraints. We show that Neural DNF can successfully learn both the feature extractor and the logical rules for classification, and achieve competitive accuracy. Note that in this case there is no guarantee that the extracted features are meaningful to human. In the second scenario, we constrain the feature extractor to produce human-aligned interpretable features by enforcing an auxiliary concept loss based on human concept annotations. In this scenario, Neural DNF becomes highly interpretable that the interpretability enables human to easily interact with and manipulate the learned model, such as performing human-intervention on the extracted features to improve accuracy, or slightly tweaking the model to recognize an imaginary class that does not exist in the dataset. In conclusion, our experiments show that Neural DNF achieves accuracy comparable that of blackbox deep learning models while offering an interpretable symbolic DNF representation, that makes human easier to interact with or manipulate the model.

2 Neural Disjunctive Normal Form

We consider a standard supervised learning setting of classification: given a dataset of $D = \{(x,y)\}_1^{|D|}$, we wish to learn a classification function f. For simplicity, we now assume y to be binary labels ($y \in \{0,1\}$) and will extend to multi-class later. We use the two-stage formulation : the classifier function $f = g \circ \phi$ is a composition of two functions ϕ and g, where ϕ is a neural network feature extractor, taking raw data x as input and returning a set of intermediate representations $\{c_1, c_2, \ldots, c_K\} \in \{0,1\}^K$ where K is a predefined number. We use 0 and 1 to represent False and True. We call each c a concept *predicate* to emphasize that c has a Boolean interpretation: it indicates the presence or the absence of a concept. A Disjunctive Normal Form module g is used for the actual classification. The overall classification is given by $\hat{y} = f(x) = g(\phi(x))$.

The logical rule-based g is formulated as a Disjunctive Normal Form (DNF). g takes a set of Boolean predicates as input feature and makes binary prediction. g can be more intuitively interpreted as a decision set, consisting of a set of if-then rules: g predicts the positive class if at least one of the rules is satisfied and predicts the negative class otherwise. We define a rule r_i to be a conjunction of one or more conditions (literals): $r_i = b_{i1} \wedge b_{i2} \wedge \ldots$ where b_j for $j \in \{1, 2, \cdots 2K\}$ can be a predicate c or its negation $\neg c$. A DNF is a disjunction of one or more rules: $r_1 \vee r_2 \vee \ldots \vee r_n$.

Rule learning algorithm for DNF can be viewed as a subset selection problem: first, a pool of all candidate rules is constructed and then 'learning' corresponds to finding a good subset of rules as the learned DNF. Let N to be the size of pool of rules and K the number of predicates, we formulate using a binary matrix $\boldsymbol{W}_{2K\times N}$ and a binary vector $\boldsymbol{S}_N$. $\boldsymbol{W}_{2K\times N}$ represents the pool of candidate rules: each column represents a rule and the non-zero elements of a column indicate the conditions of that rule. $\boldsymbol{S}_N$ can be viewed as a membership vector that determines which rules are selected as the learned DNF. Given input concept predicates $\boldsymbol{c} = \{c\}_1^K$, g computes the Boolean function as:

$$\hat{y} = g(\boldsymbol{c}) = \bigvee_{\boldsymbol{S}_j=1}^{N} \bigwedge_{\boldsymbol{W}_{i,j}=1} b_i \qquad \text{where } \{b\}_i^{2K} = \{c_1, \neg c_1, c_2, \neg c_2, \ldots, c_k, \neg c_k\} \tag{1}$$

Note that eq. (1) is used during training; after training, $\boldsymbol{W}_{2K\times N}$ is discarded and only the selected rules are stored. Conventional methods of rule learning [Lakkaraju et al., 2016, Wang et al., 2017] usually construct a fixed $\boldsymbol{W}$ by rule pre-mining; and then 'learning' corresponds to the discrete optimization of the membership vector $\boldsymbol{S}$. However, this is not compatible if we wish to jointly optimize g with the neural network ϕ end-to-end. In order to do so, we make two essential modifications: (I) we make both $\boldsymbol{W}_{2K\times N}$ and $\boldsymbol{S}_N$ learnable parameters; (II) we introduce a differentiable replacement[2] of the logical operation of eq. (1) so that gradients can be properly backpropagated:

$$r_j = \bigwedge_{\boldsymbol{W}_{i,j}=1} b_i \quad \xrightarrow{\text{replaced by}} \quad r_j = \prod_i^{2k} \boldsymbol{F}_{\text{conj}}(b_i, \boldsymbol{W}_{i,j}), \text{ where } \boldsymbol{F}_{\text{conj}}(b,w) = 1 - w(1-b) \tag{2}$$

$$\hat{y} = \bigvee_{\boldsymbol{S}_j=1} r_j \quad \xrightarrow{\text{replaced by}} \quad \hat{y} = 1 - \prod_j^{N}(1 - \boldsymbol{F}_{\text{disj}}(r_j, \boldsymbol{S}_j)), \text{ where } \boldsymbol{F}_{\text{disj}}(r,s) = r \cdot s \tag{3}$$

eqs. (2) and (3) computes the DNF function exactly as eq. (1), but note that since $\boldsymbol{W}$ and $\boldsymbol{S}$ are binary, optimizing $\{\boldsymbol{W}, \boldsymbol{S}\}$ with mini-batch gradient descent is non-trivial. The above formulation can be easily extended to multi-class settings by using a different $\boldsymbol{W}$ and $\boldsymbol{S}$ for each class (thus we have a different DNF 'tower' for each class) while the concept predicates being shared across classes; in test time when more than one classes are predicted as positive, some tie-breaking procedure can be employed. In this paper, we simply use lazy tie-breaking by selecting the first encountered positive class in ascending order (e.g. when class 1, 4, 7 are all predicted as positive, we select class 1).

[2]Obtaining eqs. (2) and (3) is not new, similar formulation can be found in the literature such as the logical activation functions [Payani and Fekri, 2019, Wang et al., 2019b] or soft NAND gate [Sajjadi et al., 2016].

The neural network feature extractor ϕ processes the raw input x into a set of intermediate representations $\{c_1, c_2, \ldots, c_k\}$ called concept predicates. The neural network ϕ's output $\tilde{c_i}$ is real-valued. To ensure the extracted c can be processed by the DNF g, c needs to be binary. We use a binary step function to discretize $\tilde{c_i}$ into Boolean predicates: c_i = 1 if $\tilde{c_i} > 0$ and c_i = 0 otherwise. However, since gradient through this step function is zero almost anywhere and thus prevents training, we utilize the *Improved SemHash* [Kaiser and Bengio, 2018]. It does not need any manual annealing of temperature [Bulat et al., 2019, Hansen et al., 2019] or additional loss functions and has been demonstrated to be a robust discretization technique in various domains [Kaiser and Bengio, 2018, Chen et al., 2019b, Kaiser et al., 2019]. Ideally, the intermediate output $\boldsymbol{c}$ should be the high-level 'natural' features that are aligned with human-comprehensible concepts. Quoted from Melis and Jaakkola [2018], for medical image processing, the concept predicate $\boldsymbol{c}$ should indicate tissue ruggedness, irregularity, elongation, etc, and are 'the first aspects that doctors look for when diagnosing'. However, this is ill-defined and indeed a very much more challenging task. We explore two options of ϕ on some image datasets: in section 4.3. we choose to use a convolutional neural network and do not put any extra constraints; in section 4.4, we enforce the feature extractor to produce interpretable representations by enforcing an auxiliary concept loss based on human annotations.

Objective function of Neural DNF is given as $\boldsymbol{L} = \mathbb{L}_{loss} + \lambda_g \mathbb{R}_g(\boldsymbol{W}, \boldsymbol{S})$ where $\mathbb{L}_{loss} = \frac{1}{|D|}\sum_{(x,y)\in D} L(y, g_{\boldsymbol{W}}(\phi_\theta(x)))$ is the classification loss (using MSE or BCE) and $\mathbb{R}_g$ is the regularization for g. For a simple regularization of g, we want the number of rules and the length of rules to be small. Note that as only rules selected by $\boldsymbol{S}$ are actually used, we can use a grouped L1-norm by $\mathbb{R}_g(\boldsymbol{W}, \boldsymbol{S}) = \lambda_g \sum_j^N |\boldsymbol{S}_j|_1 |\boldsymbol{W}_{\cdot,j}|_1$. Note that in the multi-class setting, our extension of Neural DNF is simply treating a multi-class classification as multiple one-versus-all binary classifications. In this case, the objective function sums up the classification loss for all the classes.

3 The *BOAT* algorithm for learning Neural DNF

In this section, we introduce Bi-Optimizer learning with Adaptively-Temperatured noise(BOAT), the learning algorithm for Neural DNF. BOAT utilizes two optimizers: a standard deep learning optimizer Adam [Kingma and Ba, 2014] that optimizes the continuous parameters θ of the neural network ϕ and a binary-parameter optimizer adopted from [Helwegen et al., 2019] that optimizes the binary parameters $\{\boldsymbol{W}, \boldsymbol{S}\}$ of the DNF g. As the key ingredient of BOAT, during training the binary parameters $\boldsymbol{W}$ and $\boldsymbol{S}$ are perturbed by noise whose magnitude is controlled by the noise temperature σ (eq. (4)). We emphasize that (1) the introduced noise is necessary as otherwise learning of $\{\boldsymbol{W}, \boldsymbol{S}\}$ constantly fails even in very simple cases (section 4.1) and (2) the noise temperature σ is also a learnable continuous parameter, which can be optimized together with other continuous parameters by Adam. Making the temperature learnable avoids the tedious tuning of temperature schedules.

Joint optimization of $g_{\boldsymbol{W},\boldsymbol{S}}$ and ϕ_θ is non-trivial, because although the overall model is differentiable, $\{\boldsymbol{W}, \boldsymbol{S}\}$ consists of binary values ($\{0, 1\}$) and thus standard deep learning optimizers designed for continuous parameters cannot be directly applied. One alternative, denoted as DNF-Real [Payani and Fekri, 2019, Wang et al., 2019b], is to simply use real-valued weight $\{\tilde{\boldsymbol{W}}, \tilde{\boldsymbol{S}}\}$ transformed using sigmoid/tanh functions as a surrogate and then use Adam as the optimizer. After training, real-valued weights are thresholded to binary values, and performance drop can occur. In practice, we find DNF-Real to be optimization-friendly just like any other real-valued DNNs but it is not guaranteed to result in binary-valued parameters. Another alternative, which we denote as DNF-STE, is adopted from binary neural network research [Courbariaux et al., 2016, Darabi et al., 2018]. It maintains real-valued *latent* parameters which are binarized in forward pass computation. In backward computation the gradients are updated to the latent real-valued parameters using the straight-through estimator (STE) [Bengio et al., 2013]. This technique is widely used and works quite well for large-scale binary neural networks. However, for a small-sized DNF g, DNF-STE is very sensitive to initialization and hyperparameters and can easily be stuck in local minima.

The introduced BOAT combines the best of both approaches: (1) It is optimization-friendly and not very sensitive to initialization and hyperparameters. This is especially important as g is not overparameterized; (2) It naturally optimizes binary parameters.

Modified Bop: BOAT uses a modified version of the *Bop* optimizer [Helwegen et al., 2019] to optimize the binary-valued parameter $\{\boldsymbol{W}, \boldsymbol{S}\}$ given gradient as learning signals. We make minor modifications to suit *Bop* (originally for $\{-1, 1\}$) into the case of $\{0, 1\}$. The Modified *Bop* optimizer introduced in this paper uses gradient as the learning signal and flips the value of $w \in$

Algorithm 1 The BOAT algorithm for learning Neural DNF

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Hyperparameters: Accepting threshold $\tau > 0$; Exponential decay rate $\gamma \in [0, 1)$ ; Initial noise temperature $\sigma_0 \in [0, 0.5]$ ; Size of rule pool $N$. (Default:$\tau$=$10^{-6}$, $\gamma$=1-$10^{-5}$, $\sigma_0$=0.2, $N$=64.)
Input: Dataset $\boldsymbol{D}$; Output: The DNF $g(\{\boldsymbol{W}, \boldsymbol{S}\})$; The neural network $\phi(\theta)$.
 1: Initialize $\theta$ randomly.
 2: For every $w$ in $\{\boldsymbol{W}, \boldsymbol{S}\}$: initialize $w \in \{0, 1\}$ randomly, $m_w \leftarrow 0, \sigma_w \leftarrow \sigma_0$.
 3: while stopping criterion not met do
 4:     Sample mini-batch $\{(x_i, y_i)\}^{\text{batch size}}$ from the training set $\boldsymbol{D}$.
 5:     Compute the perturbed $\{\tilde{\boldsymbol{W}}, \tilde{\boldsymbol{S}}\}$ where each entry $\tilde{w}$ is perturbed according to $\sigma_w$ (eq. (4)).
 6:     Use $\theta$ and perturbed $\tilde{\boldsymbol{W}}, \tilde{\boldsymbol{S}}$ to compute the objective function $\sum_{x_i, y_i} \boldsymbol{L}(g_{\tilde{\boldsymbol{W}}, \tilde{\boldsymbol{S}}}(\phi_\theta(x_i)), y_i)$
 7:     for every binary parameter $w$ in $\{\boldsymbol{W}, \boldsymbol{S}\}$ do
 8:         Compute gradient $\nabla_w$ w.r.t the objective function computed at line 4.
 9:         Update exponential moving average of gradient: $m_w \leftarrow \gamma m_w + (1 - \gamma)\nabla_w$.
10:         if $|m_w| > \tau$ and ($m_w < 0$ and $w = 0$ or $m_w > 0$ and $w = 1$) then
11:             $w \leftarrow 1 - w$                ▷ Line 7-11: update binary parameters using Modified Bop
12:     Update $\theta$ by Adam given the objective function computed at line 6.
13:     for every $\sigma_w$ do
14:         Update $\sigma_w$ by Adam given the objective function computed at line 6.
15:         Clip $\sigma_w = min(0.5, max(\sigma_w, 0))$
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$\{0, 1\}$ only if the gradient signal m exceeds a predefined *accepting threshold* τ:

$$w = \begin{cases} 1 - w, & \text{if } |m| > \tau \text{ and } (w = 1 \text{ and } m > 0 \text{ or } w = 0 \text{ and } m < 0) \\ w, & \text{otherwise.} \end{cases}$$

where m is the gradient-based learning signal computed in the backward pass. A non-zero τ is introduced to avoid rapid back-and-forth flips of the binary parameter and we find it helpful to stabilize the learning because m is of high variance. To obtain consistent learning signals, instead of using vanilla gradient ∇ as m, the exponential moving average of gradients is used:

$$m = \gamma m + (1 - \gamma)\nabla$$

where γ is the exponential decay rate and ∇ is the mini-batch gradient. We use $\gamma = 1 - 10^{-5}$ and $\tau = 10^{-6}$ as default value while the trick for tuning γ and τ can be found in original *Bop* paper.

Key ingredient of BOAT: Adaptively-temperatured Noise: The reason we introduce adaptively-temperatured noise is that simply using the introduced Modified *Bop* shares the same drawback as using DNF-STE: optimization is very sensitive to initialization and hyperparameters and can be stuck in local minima very easily. When stuck in local minima, the gradients w.r.t $\boldsymbol{W}$ and $\boldsymbol{S}$ effectively become zero, and thus any further updates for $\boldsymbol{W}$ and $\boldsymbol{S}$ are disabled. We suspect the reason is that even the DNF function eqs. (2) and (3) is well defined on $[0, 1]$, since the choice of values of $\boldsymbol{W}$ and $\boldsymbol{S}$ can only take $\{0, 1\}$, the loss surface is non-smooth and thus the optimization becomes hard. To overcome this, we propose to perturb the binary weights w during training by adding noise in the forward pass such that the perturbed $\tilde{w}$ lies in $[0, 1]$. We believe the introduced noise smoothes the loss surface and helps the optimization. Specifically, for every entry w in $\boldsymbol{W}$ and $\boldsymbol{S}$, we utilize a noise temperature parameter $\sigma_w \in [0, 0.5]$ to perturb w with noise as follows:

$$\tilde{w} = \begin{cases} 1 - \sigma_w \cdot \epsilon & \text{if } w = 1 \\ 0 + \sigma_w \cdot \epsilon & \text{if } w = 0 \end{cases}, \text{ where } \epsilon \sim \text{Uniform}(0, 1) \tag{4}$$

During training the perturbed weight $\tilde{w}$ is used in the forward pass computation of the objective function; in test time, we simply disable this perturbation. To force σ_w lies in range $[0, 0.5]$, we clip σ_w by σ_w = $min(0.5, max(\sigma_w, 0))$ after evey mini-batch update. Note that σ_w is not globally shared: we have a σ_w for every w in $\boldsymbol{W}$ and $\boldsymbol{S}$ (so in total $2K * N + N$). We make σ_w also a learnable parameter. We initialize σ_w = σ_0 and optimize σ_w by Adam as well. The choice of initial value σ_0 requires heuristic: with a too large σ_0 optimization becomes slower (fig. 2c) , and σ cannot be too small: in the extreme case with zero noise the optimization of $\boldsymbol{W}, \boldsymbol{S}$ will constantly fail (fig. 2b) . We find values in $[0.1, 0.3]$ all work fine and we use $\sigma_0 = 0.2$ as the default initial value. **Remark**:

We can also apply same noise for DNF-STE, but it converges slower (fig. 3) . We conjecture the reason to be the acceptance threshold τ which effectively filters out noisy learning signals so that rapid flipping is prevented, suggested as main advantage of *Bop*.

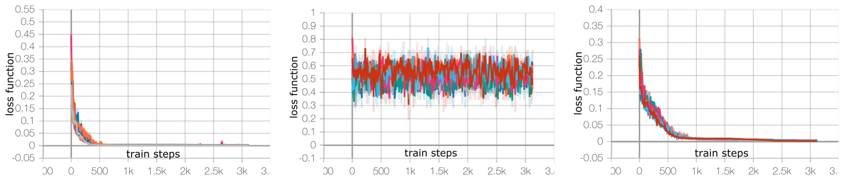
4 Experiments

4.1 Evaluation of the BOAT Optimizer with the second stage alone

What comes first is to evaluate BOAT , the optimization algorithm with its alternatives. Here we evaluate BOAT on datasets with Boolean features so that we learn only the DNF g. We use a synthetic dataset adopted from Payani and Fekri [2019] which consists of 10-bit Boolean strings and a randomly-generated DNF as ground-truth.

First, to show the proposed noise is indeed necessary and helps the optimization, we learn the DNF with/without the noise on multiple datasets generated with different random seeds (so the ground-truth DNF is different) and plot the loss curves. From fig. 2a we observe that multiple runs of BOAT give very similar and stable convergence, while in fig. 2b, surprisingly, runs consistently fail to converge without the noise. We view this as strong evidence for the necessity of the proposed noise. On the other hand, if noise temperature is initialized larger, the convergence is slower (fig. 2b).

There are some other issues with a large noise rate: (1) The slower learning of a larger noise rate can also be explained from the multiplicity nature of the DNF function we use (eq 2 and 3 in the main paper). This becomes more severe in high dimensional inputs. And finding a small noise rate initialization value will help. (2) when the noise rate intialized too high (and the hyperparameter of adaptivity rate not set right), it is also possible that the binary parameters cannot get huge gradient enough to flip, while it is only the continuous parameters including the noise rate are getting updated. This is an undesired result. In this case, find a smaller initilization rate.



(a) with noise (σ_0=0.2) (b) with NO noise (c) with noise (σ_0=0.4)

Figure 2: Loss curve with 10 differently-generated synthetic dataset

Next, we apply BOAT and compared the convergence speed with the following baselines: (1) DNF-Real [Payani and Fekri, 2019, Wang et al., 2019b] and (2) DNF-STE which are discussed in section 3. (3) A Linear Model. (4) A multi-layer perceptron. Note that we also use the adaptive noise for DNF-STE since otherwise optimization will fail. As shown in fig. 3, BOAT gives the fastest convergence, while MLP, DNF-STE and DNF-Real converge much more slowly. The linear model does not converge. As for the reason of DNF-STE's slower and less stable convergence, we believe it is because that unlike the modified *Bop*, DNF-STE does not have the mechanism to prevent rapid flipping and thus optimization becomes more unstable. As for performance, all above methods except linear model achieve 100% F1 score on test set and BOAT can always find the ground truth DNF on different synthetic datasets generated with different random seeds. **Remark:** Note that since we use random initialization for $\boldsymbol{W}, \boldsymbol{S}$, a natural suspicion is that the ground truth DNF happens to be discovered by the random initialization, not learned. To refute it, we can use zero initialization and find that BOAT converges similarly to random initialization. We report it in the appendix together with the performance results on some UCI datasets.

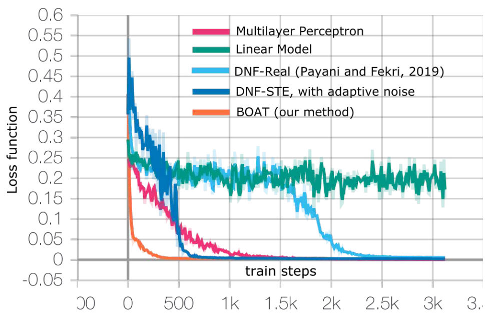


Figure 3: Loss Curve on the synthetic dataset

4.2 On a 2D toy dataset.

Here we first apply Neural DNF on a 2D toy dataset 2D-XOR (fig. 4). 2D-XOR is generated by first drawing four isotropic 2D Gaussian clusters and mark them as red square, blue square, blue circle and red circle (in clockwise order). We use a XOR-like label assigningment, labeling red squares and blue circles as positive and the rest two clusters as negative. We consider 2D-XOR as an extension of the historically important XOR problem, and its difficulty is that the feature of being 'red'/'non-red' and 'square'/'non-square' is not provided as input directly but needs to be learned in a 2-d input space. This makes the learning harder since it requires to learn both the correct intermediate feature and the correct logical decision function. We use a one fully-connected layer network as ϕ to produce two concept predicates c_1, c_2 and can visualize in as two lines in the 2-d space. We expect the learned Neural DNF to find the two correct concept predicates that represent shape and color, respectively, and the correct classification function ('color is red and shape is square or color is not red and shape is not square'). As shown in fig. 4, we visualize the decision boundary of c_1 and c_2 by two lines and we find c_1, c_2 do separate red-against-blue and square-against-circle as expected. We view fig. 4 as a minimal working example of Neural DNF demonstrating that it is useful when (1) the feature used for logic-based function are not provided but needs to be learned and (2) the underlying classification process consists of subtypes (each described as one rule) and requires some logical compositions.

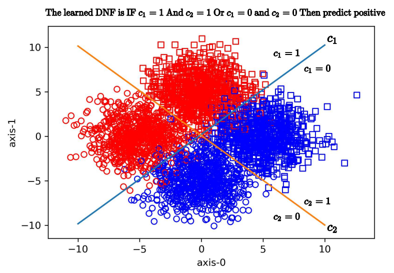


Figure 4: Neural DNF on 2D-XOR

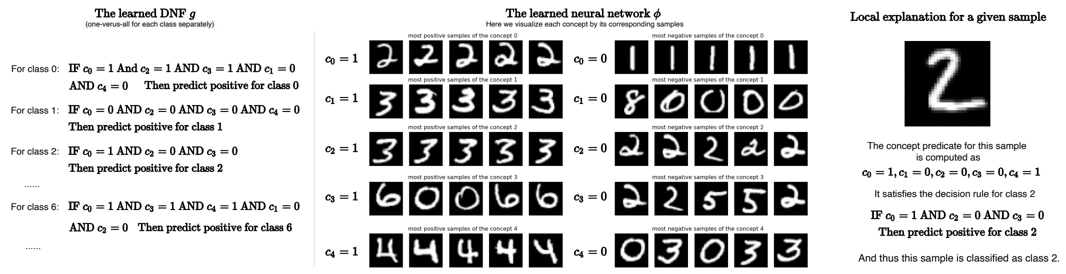
4.3 On image datasets. Scenario 1

In this section we apply Neural DNF with a CNN as feature extractor without any further contraints. and then demonstrate empirically that given the same first-stage feature extractor architecture, Neural DNF sacrifices slight loss of accuracy (table 1) while gaining more faithful interpretations (fig. 6). We first evaluate the accuracy of Neural DNF on several image datasets table 1. Using the same architecture for ϕ, the models we compare are (1) Neural DNF (2) a standard DNN (i.e. a linear model as g) and (3) self-explaining neural network (SENN) [Melis and Jaakkola, 2018], which uses a neural network to generate the coefficients of a linear model conditioned on the input and claims to have better interpretability. Since binarization is not required for DNN or SENN, we also evaluate DNN and SENN with/without it. We observe that all models perform similarly well in terms of test accuracy across datasets, while Neural DNF loses accuracy only slightly. Comparing DNN and SENN with/without binarization, we can see that both DNN and SENN loses accuracy slightly because of the binarization. So the loss of Neural DNF 's accuracy can be explained from two sources: (1) the binarization (Improved SemHash) and (2) the use of rules as the classifier instead of the more well-studied linear (additive) models. We suspect this is also partially because Neural DNF treats multi-class settomg as multiple one-versus-all classifications and does not produce probabilistic outputs like DNN and SENN. However, this should not be viewed as a weakness as long as the accuracy loss is slight. We believe that this issue can be alleviated that given a sufficiently flexible ϕ, the accuracy loss of Neural DNF can be negligible like the case of simple dataset MNIST.

Table 1: Test Accuracy on some image datasets

	MNIST	KMNIST	SVHN	CIFAR10
Neural DNF	99.08%	95.43%	90.13%	67.91%
standard DNN	99.12%	95.86%	90.74%	70.43%
standard DNN (without Binarization)	99.11%	96.02%	91.45%	71.45%
SENN	98.48%	92.64%	90.79%	71.09%
SENN (without Binarization)	98.50%	91.46%	92.15%	72.32%

We provide an anecdotal example on the explanations Neural DNF can derive in (fig. 5) as a direct comparison to the explanations provided by linear models (e.g., the MNIST example from the self-explaining network [Melis and Jaakkola, 2018]). We show the learned rules of DNF as well as maximum/minimum activated sampele for each concept predicates.


The learned DNF g
(one-verus-all for each class separately)
For class 0: IF $c_0 = 1$ And $c_2 = 1$ AND $c_3 = 1$ AND $c_1 = 0$ AND $c_4 = 0$ Then predict positive for class 0
For class 1: IF $c_0 = 0$ AND $c_2 = 0$ AND $c_3 = 0$ AND $c_4 = 0$ Then predict positive for class 1
For class 2: IF $c_0 = 1$ AND $c_2 = 0$ AND $c_3 = 0$ Then predict positive for class 2
......
For class 6: IF $c_0 = 1$ AND $c_3 = 1$ AND $c_4 = 1$ AND $c_1 = 0$ AND $c_2 = 0$ Then predict positive for class 6
......
The learned neural network ϕ
Here we visualize each concept by its corresponding samples
most positive samples of the concept 0
most negative samples of the concept 0
$c_0 = 1$
$c_0 = 0$
$c_1 = 1$
$c_1 = 0$
$c_2 = 1$
$c_2 = 0$
$c_3 = 1$
$c_3 = 0$
$c_4 = 1$
$c_4 = 0$
Local explanation for a given sample
The concept predicate for this sample is computed as
$c_0 = 1, c_1 = 0, c_2 = 0, c_3 = 0, c_4 = 1$
It satisfies the decision rule for class 2
IF $c_0 = 1$ AND $c_2 = 0$ AND $c_3 = 0$
Then predict positive for class 2
And thus this sample is classified as class 2.

(a) Global explanation for the overall Neural DNF Model (b) Local explanation

Figure 5: Explanations provided by Neural DNF on MNIST

Now regarding the interpretability, the problem here is, we can in principle inspect the meaning of concept and rules of Neural DNF, but since we have no constraints on ϕ, the extracted features are only highly discriminative and is not guaranteed to be aligned with human perceptible concepts. A symbolic DNF that operates on non-interpretable representations is still non-interpretable. We will revisit this interpretable representation problem in next section; but despite tje first-stage, here we can still compare the interpretability of the second-stage model. Despite many qualitive arguments for favouring the interpretability of the symbolic DNF (appendix B.3), we can further quantitively evaluate the faithfulness of models' interpretability, a critical critera that measures how faithful the explanation for a particular prediction are to the underlying computation of prediction. We adopt the *faithfulness metric* proposed by [Melis and Jaakkola, 2018] which measures the correlation of the change of the prediction (class probabilities) and the change of the explanation (relevance scores of features) upon perturbation of test examples.[3] We report the faithfulness metric on test set for DNN, SENN and Neural DNF in fig. 6. For DNN, we use the coefficients of final linear layer as rele-

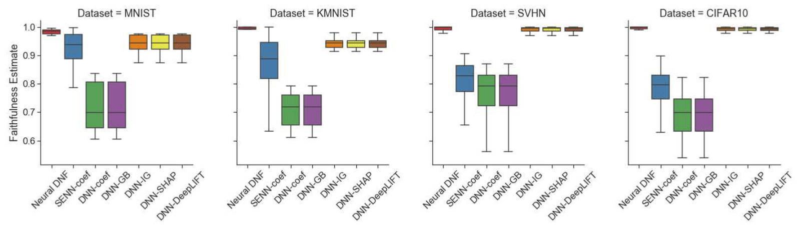


Figure 6: Evaluating the faithfulness of explanations on test set

vance scores. Alternatively, for DNN we can also utilize some representitive post-hoc interpretation methods (also known as attribution methods): Guided Backprop (GB) [Springenberg et al., 2014], gradient SHAP [Lundberg and Lee, 2017], Integrated Gradient (IG) [Sundararajan et al., 2017] and DeepLIFT [Shrikumar et al., 2017]. SENN can use its self-generated coefficients as relevance scores [Melis and Jaakkola, 2018]. For Neural DNF, we use the difference analysis [Robnik-Šikonja and Kononenko, 2008], a model-agnostic relevance score assignment method to assign scores. As shown in fig. 6, Neural DNF consistently achieves the highest faithfulness estimates for all datasets and its faithfulness has the smallest variance. This means Neural DNF's explanations are highly faithful in a robust way across different test samples. SENN is more faithful than DNN; and for the post-hoc methods while GB performs very similarly with DNN-coef, IG/SHAP/DeepLIFT drastically improves the faithfulness. This is because the latter three methods compute the relevance w.r.t to a baseline reference, a concept that is now considered very essential [Sturmfels et al., 2020]. However, we emphasize that even these sophisticated post-hoc methods do not reach the same level of faithfulness as Neural DNF, in particular not on MNIST and KMNIST. We believe that Neural DNF's extremely high faithfulness is the direct result of the symbolic nature of DNF.

4.4 On image datasets, scenario 2

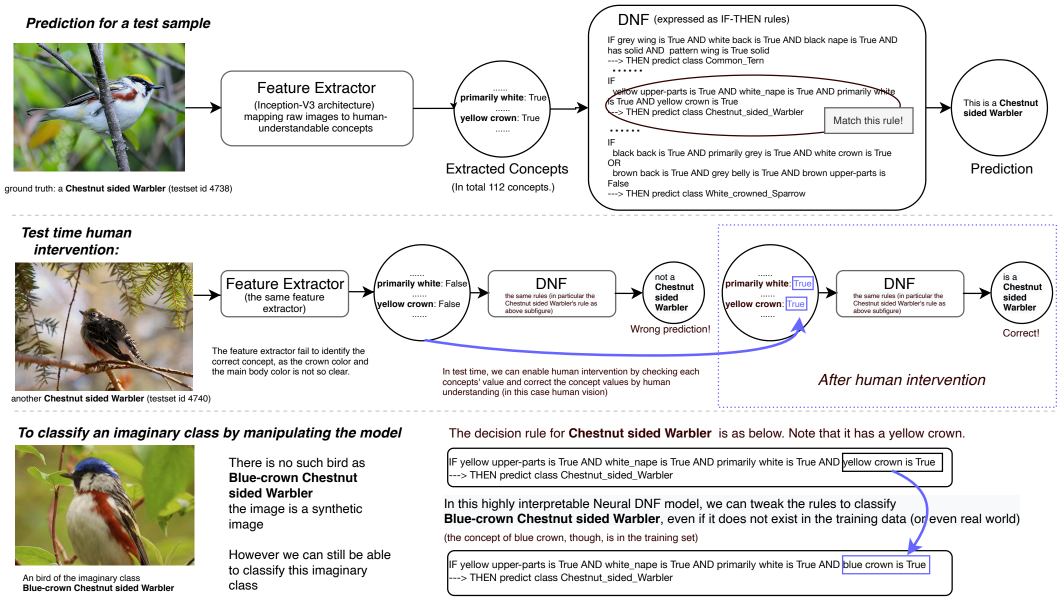
Here we test a new scenario where we have concept annotations so we can train the feature extractor to produce human-aligned interpretable representations. Our goal is that if we can align the extracted

[3]As in [Melis and Jaakkola, 2018], the relevance score assignment and feature perturbation is done for the extracted feature $\phi(x)$, not at the level of the raw data x.

features with human understanding, then we can achieve a highly interpretable model which human can easily interact with and manipulate. We use the CUB dataset [Wah et al., 2011] which has 200 class and 112 binary annotataed concepts (preprocessed by Koh et al. [2020]). In Koh et al. [2020] the authors propose the concept bottleneck model, a similar two-stage model using a Inception-V3 based feature extractor ϕ and a linear layer g. Given concepts the annotations, a concept prediction loss can be applied so that the extracted faetures are constrained to align with annotated values. Koh et al. [2020] also propose the *test-time human intervention*: since the extracted concepts can be wrong, human can check and correct extracted concepts so that test accuracy can be improved significantly through this interaction. We follow Koh et al. [2020] and replace the second-stage g with a DNF. Koh et al. [2020] evaluate several strategies for training the two-stage model. Here we use the independent training strategy: we train ϕ to predict concepts and train g to predict class label using concepts; only in test time we stack ϕ and g together. The reason of choosing independent training instead of joint training is counterintuive, however, this is because we find that the extracted concepts after joint training are less well-aligned with human annotations, and it then makes the human intervention less effective than independent trained models. In other words, based on non-interpretable features, any human interaction/manipulation will be unreliable. This phenomenon is consistent with Koh et al. [2020], and we think novel architectures that extracts interpretable features without the need of annotations can solve it, in that case joint training should give better results. In table 2 we report the accuracy of Neural DNF, the concept bottleneck model and blackbox DNN. Neural DNF achieves less test accuracy compared with the concept bottleneck model by a large margin, we suspect it might because Neural DNF is dealing with too many (200-class) one-versus-all prediction and does not produce probabilistic outputs like other models do. But after intervention both Neural DNF and the concept bottleneck model achiveve perfect accuracy. This indicates that (1) the accuracy by applying human intervention can be improved significantly which is the benefits of having an highly interpretable model; (2) the bottleneck of accuracy is the feature extractor: the classification of CUB can be effectively solved given a perfect feature extractor.

Table 2: Test Accuracy on CUB dataset

	test acc	test acc with human intervention
Neural DNF	61.94%	100.00%
Concept bottleneck model	72.38%	100.00%
Blackbox DNN	74.69%	N/A



Prediction for a test sample
ground truth: a Chestnut sided Warbler (testset id 4738)
Feature Extractor
(Inception-V3 architecture) mapping raw images to human-understandable concepts
primarily white: True
yellow crown: True
Extracted Concepts
(In total 112 concepts.)
DNF (expressed as IF-THEN rules)
IF grey wing is True AND white back is True AND black nape is True AND has solid AND pattern wing is True solid ---> THEN predict class Common_Tern
IF yellow upper-parts is True AND white_nape is True AND primarily white is True AND yellow crown is True ---> THEN predict class Chestnut_sided_Warbler
Match this rule!
IF black back is True AND primarily grey is True AND white crown is True OR brown back is True AND grey belly is True AND brown upper-parts is False ---> THEN predict class White_crowned_Sparrow
This is a Chestnut sided Warbler
Prediction
Test time human intervention:
another Chestnut sided Warbler (testset id 4740)
Feature Extractor
(the same feature extractor)
primarily white: False
yellow crown: False
DNF
the same rules (in particular the Chestnut sided Warbler's rule as above subfigure)
not a Chestnut sided Warbler
Wrong prediction!
The feature extractor fail to identify the correct concept, as the crown color and the main body color is not so clear.
In test time, we can enable human intervention by checking each concepts' value and correct the concept values by human understanding (in this case human vision)
primarily white: True
yellow crown: True
DNF
the same rules (in particular the Chestnut sided Warbler's rule as above subfigure)
is a Chestnut sided Warbler
Correct!
After human intervention
To classify an imaginary class by manipulating the model
An bird of the imaginary class Blue-crown Chestnut sided Warbler
There is no such bird as Blue-crown Chestnut sided Warbler the image is a synthetic image
However we can still be able to classify this imaginary class
The decision rule for Chestnut sided Warbler is as below. Note that it has a yellow crown.
IF yellow upper-parts is True AND white_nape is True AND primarily white is True AND yellow crown is True ---> THEN predict class Chestnut_sided_Warbler
In this highly interpretable Neural DNF model, we can tweak the rules to classify Blue-crown Chestnut sided Warbler, even if it does not exist in the training data (or even real world)
(the concept of blue crown, though, is in the training set)
IF yellow upper-parts is True AND white_nape is True AND primarily white is True AND blue crown is True ---> THEN predict class Chestnut_sided_Warbler

Figure 7: (top) illustration of a correct prediction of Neural DNF for class 'Chestnut sided Warbler'; (middle) illustration of human interaction: an incorrect prediction of Neural DNF for class 'Chestnut sided Warbler' can be corrected by human intervention; (bottom) illustration of manipulating a learned Neural DNF to classify an imaginary class 'Blue-crown Chestnut sided Warbler'.

While losing quite much in accuracy, the symbolic nature enables the Neural DNF to do the things the concept bottleneck model cannot. We show in fig. 7 (top) a correctly predicted sample for the class of ‘Chestnut sided Warbler’ and in fig. 7 (middle) an incorretly predicted sample and how human intervention can correct the prediction. DNF rules are a very human-readable format, that the rules are very sparse involving only a few concepts and the logical operation is intuitive to understand. The DNF rules also alleviate the burden of human intervention compared to the concept bottleneck, as only a few concepts are used in the decision rule, a human user can only check and correct these concepts indicated in the rules and does not have to go through every concepts which the concept bottleneck model requires. Also, the symbolic nature of DNF enables us to incorporate knowledge and manipulate the models easily in a way that the concept bottleneck model (with a linear g) cannot offer. In in fig. 7 (bottom), we provide an illustration on how we can tweak the Neural DNF to predict an imaginary class ”blue-crown Chestnut sided Warbler” that does not exist in the training dataset (not even in real world). Taking the rule for ‘Chestnut sided Warbler’, we can simply replacing the condition of ‘yellow crown is True’ with ‘blue crown is True’. Note that ’blue crown’ is already in the training set and one of the concepts ϕ can extract. Of course we can go further that we can train and append new feature extractors for new concepts and then play with new concepts. There are, however, limitations because of the expressity of prositional logic.

5 Conclusion and future work

In this paper, we have presented Neural DNF, a vertically integrated neuro-symbolic classifier. Neural DNF takes a step towards the fundamental problem of integrating continuous perception and logical reasoning. Neural DNF adopts a two-stage model that utlizes a DNN to extract features, called concept predicates, and a propositional logic DNF module to make classification based on the concepts. We propose the BOAT algorithm for joint learning of the DNF module and the feature extractor DNN. In order to avoid laborious manual tuning, we employ an Improved SemHash method to binarize the extracted features, to obtain concept predicates, because it does not need to manually tune any extra parameters or add further losses. We also introduce adaptive temperatured-noise, which is a minimal modification of the binary-parameter optimizer *Bop* that enables the effective optimization of the parameters of the second-stage rule-based model.

This paper suggests several directions for future research. In our experiments in Neural DNF , we have used concept annotations and the concept-bottleneck DNN architecture to extract interpretable features. However, in practice there is often no prior knowledge of ‘concept annotations’ available. Therefore, novel deep learning architectures that can extract human-understandable concepts from data without the need of concept annotations should be investigated. This may require domain-specific knowledge representations and loss functions [Melis and Jaakkola, 2018, Chen et al., 2019a, Biffi et al., 2018, Kim and Canny, 2017, Johnson et al., 2016]. Another future direction is the use of more powerful languages than propositional logic, for example, the more general inductive logic programming. Since BOAT requires only minimal changes of the standard deep learning optimization, we believe it can be potentially applied to models with a more powerful second-stage rule-based module, or to other models with mixed binary-continuous parameters.

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Supplementary Material

The appendix mainly consists of 5 parts.

- Appendix A: We present details about the key ideas and techniques used in the paper but is not discussed in details due to page limitsm, including details of the model Neural DNF and the learning algorithm BOAT.
- Appendix B: We discuss related works on interpretability research. we first answer why we prefer inherently interpretable models, we only mention briefly in the main paper, here we discuss more. We then talk about recent works on interpretable deep learning. We end with a discussion of a comparision of interpretability of rule-based models and linear model.
- Appendix C: We discuss more about Disjunctive Normal Form (DNF). for classification, previous works on learning DNF and more closely, some recent works to learn DNF by gradient descent using a differentiable DNF function.
- Appendix D: We relatin Neural DNF to the literature of neuro-symbolic integration.
- Appendix E: We present details of experiment setup and experimental results not covered in the main paper.

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B Related Works on Interpretability **4**

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A Algorithm Details

we introduce some key ideas and techniques and the details of algorithm

A.1 The modified *Bop*

Helwegen et al. [2019] proposes the *Bop* optimizer in the context of binarized neural networks of value $\{-1, 1\}$. As suggested by Helwegen et al. [2019], the Bop can be viewed as a basic (gradient-based) binary optimizer, in the same sense that SGD is a basic (gradient-based) continuous-valued optimizer. The update rule for the original Bop is

$$w = \begin{cases} -w, & \text{if } |m| > \tau \text{ and } \operatorname{sign}(w) = \operatorname{sign}(m) \\ w, & \text{otherwise.} \end{cases}$$

And the modified bop for $\{0, 1\}$ used in this paper is

$$w = \begin{cases} 1 - w, & \text{if } |m| > \tau \text{ and } (w = 1 \text{ and } m > 0 \text{ or } w = 0 \text{ and } m < 0) \\ w, & \text{otherwise.} \end{cases}$$

The modification of suiting the case of $\{-1, 1\}$ to $\{0, 1\}$ is minor.

Also, in the implementation we add a bias correction procedure. Let $\hat{m}_t$ be the non-corrected gradient momentum that is updated as $\hat{m}_t = \gamma \hat{m}_{t-1} + (1 - \gamma)\nabla$, The bias correction is given by

$$m_t = \hat{m}_t / (1 - \gamma^t)$$

We need this correction because in the original Bop paper Helwegen et al. [2019] uses random initialization for m but in our implementation we make specific that m is zero-initialized. So we will need this bias correction.

A.2 BOAT

Basically, BOAT consists of the modified bop and the proposed temperatured noise. We differ from the Helwegen et al. [2019] as follows: (1) First, we fit into the case of $\{0, 1\}$ instead of $\{-1, 1\}$, which is trivial; (2) we introduces the adaptively-temperatured noise controlled by the learnable temperature parameter. (3) we add a bias-correction procedure.

We mentioned in the main paper that we suspect the noise smoothes the loss surfaces so to help the optimization. But it is far from a rigorous statement and we do lack some theoretical understanding of why and how this noise helps learning.

We refer interested readers to the original Bop paper Helwegen et al. [2019] or a more recent paper by Meng et al. [2020] who discusses the connection of Bop and STE-Binary network and also provides a bayesian perspective on binary network learning. We believe that the our method BOAT can in principle be linked to approximate variational inference [Khan et al., 2018, Kingma et al., 2015, Potapczynski et al., 2019]. In particular, the variational Adam [Khan et al., 2018] is very like ours, except they works for continuous values and we add noise for binary parameters. We leave further theoretical investigation of BOAT for future works.

A.3 Improved SemHash

Since the feature extractor ϕ processes the raw input x into a set of intermediate representations $\{c_1, c_2, \ldots, c_k\}$ called concept predicates. As ϕ is parameterized by a neural network θ, ϕ's output $\tilde{c_i}$ is real-valued. We use a binary step function to discretize $\tilde{c_i}$ into Boolean predicates:

$$c_i = \begin{cases} 1, & \text{if } \tilde{c_i} > 0 \\ 0, & \text{otherwise.} \end{cases}$$

However, since gradient through this step function is zero almost anywhere and thus prevents training, we utilize the *Improved SemHash*[Kaiser and Bengio, 2018] as one way to make the overall model differentiable.

During training, Improved SemHash first draw Gaussian noise ϵ with mean 0 and standard deviation 1. The noise ϵ is added to $\tilde{c}$, two vectors c and c' are then computed.

$$c = \mathbf{1}(\tilde{c} + \epsilon)$$

Algorithm 1 The BOAT algorithm for learning Neural DNF

```
Hyperparameters: Accepting threshold $\tau > 0$; Exponential decay rate $\gamma \in [0, 1)$ ; Initial noise temperature $\sigma_0 \in [0, 0.5]$ ; Size of rule pool $N$. (Default:$\tau$=$10^{-6}$, $\gamma$=1-$10^{-5}$, $\sigma_0$=0.2, $N$=64.)
Input: Dataset $\boldsymbol{D}$; Output: The DNF $g$ ($\{\boldsymbol{W}, \boldsymbol{S}\}$); The neural network $\phi$ ($\theta$).
1:  Initialize $\theta$ randomly.
2:  For every $w$ in $\{\boldsymbol{W}, \boldsymbol{S}\}$: initialize $w \in \{0, 1\}$ randomly, $m_w \leftarrow 0, \sigma_w \leftarrow \sigma_0$.
3:  while stopping criterion not met do
4:      Sample mini-batch $\{(x_i, y_i)\}^{\text{batch size}}$ from the training set $\boldsymbol{D}$.
5:      Compute the perturbed $\{\tilde{\boldsymbol{W}}, \tilde{\boldsymbol{S}}\}$ where each entry $\tilde{w}$ is perturbed according to $\sigma_w$ (??).
6:      Use $\theta$ and perturbed $\tilde{\boldsymbol{W}}, \tilde{\boldsymbol{S}}$ to compute the objective function $\sum_{x_i, y_i} \boldsymbol{L}(g_{\tilde{\boldsymbol{W}}, \tilde{\boldsymbol{S}}}(\phi_\theta(x_i)), y_i)$
7:      for every binary parameter $w$ in $\{\boldsymbol{W}, \boldsymbol{S}\}$ do
8:          Compute gradient $\nabla_w$ w.r.t the objective function computed at line 4.
9:          Update exponential moving average of gradient: $m_w \leftarrow \gamma m_w + (1 - \gamma)\nabla_w$.
10:         if $|m_w| > \tau$ and ($m_w < 0$ and $w = 0$ or $m_w > 0$ and $w = 1$) then
11:             $w \leftarrow 1 - w$                 ▷ Line 7-11: update binary parameters using Modified Bop
12:     Update $\theta$ by Adam given the objective function computed at line 6.
13:     for every $\sigma_w$ do
14:         Update $\sigma_w$ by Adam given the objective function computed at line 6.
15:         Clip $\sigma_w = min(0.5, max(\sigma_w, 0))$
```

c is the result after applying the binary step function and

$$c' = max(0, min(1, 1.2 * sigmoid(\tilde{c} + \epsilon) - 0.1))$$

c' is computed by the above function called saturating sigmoid function [Kaiser and Sutskever, 2015, Kaiser and Bengio, 2016]. During training, c is used half of the time and and c' is used for the other half of the time in the forward pass; for the backward pass we define the gradient of c to $\tilde{c}$ the same as c' to $\tilde{c}$. During testing, the noise is disabled and c is used as output.

It is not clear according to the description of [Kaiser and Bengio, 2018] what 'half of time' for c and c' means, that is, whether we use c for one mini-batch and c' for the next mini-batch, or we use c and c' for half of the samples for each mini-batch. In our implementation, we choose the latter option: we use c for half of the samples in the mini-batch, and use c' for the other half of samples in the mini-batch, determined randomly.

The use of saturating sigmoid function, instead of just sigmoid function, is introduced first by Kaiser and Sutskever [2015] who claims to have slight improvement. But we do not observe such improvement in Neural DNF so in our implementation we simply computed

$$c' = sigmoid(\tilde{c} + \epsilon)$$

We use the simple sigmoid function instead of the saturating sigmoid function.

We name two reason of using Improved SemHash: (1) Improved SemHash does not need any manual annealing of temperature [Bulat et al., 2019, Hansen et al., 2019] or additional loss functions. There are some serveral alternative that need tuning of annealing, including the annealed sigmoid/tanh [Bulat et al., 2019] and gumbel-softmax trick [Maddison et al., 2016], but we believe tuning this annealing schedule is difficult. (2) Improved SemHash achieves good results compared with many alternative solutions. Comparisons with other discretized latent representation learning can be found at [Kaiser et al., 2018], semHash performs great despite being very simple. It also has been demonstrated to be a robust discretization technique in various domains [Kaiser and Bengio, 2018, Chen et al., 2019b, Kaiser et al., 2019]. But of course, we note that Improved SemHash is not the only option for binarizing the extracted features.

A.4 Initialization of $\tilde{W}$

We will initializes $\boldsymbol{W}$ and $\boldsymbol{S}$ randomly, each entry is drawn from a Bernoulli disctribution where $p_{\text{Bernoulli}} < 0.1$. This is because we want $\boldsymbol{W}$ and $\boldsymbol{S}$ to be sparse.

Remark: note that if we are really careful about the initialization, there is a small issue for initialization of $\boldsymbol{W}$, because some w can the value of c or the negation value. In principle, a condition and the negation of it cannot be set to 1 at the same time; but we do not consider it in our implementation. It seems that it does not matter in our optimization using BOAT .

A.5 Regularization of DNF: R_g and possible Alternatives

The simplest choice of $\mathbb{R}_g(W)$ is to use a L2 regularization. However, this is not what we really want. Recall that we wish to obtain a DNF, a set of rules where the number of total rules is small and the length of each rule is small. So more technically we want a small number of columns of $\boldsymbol{W}$ that have non-zero elements and small number of non-zero elements for each column (that is indicated by the membership vector $\boldsymbol{S}$). This can be realized by penalizing the number of rules as the L1-norm of $\boldsymbol{S}$ and the length of selected rules also by the L1-norm (note that as only rules selected by $\boldsymbol{S}$ are actually used), we use a grouped L1-norm by

$$\mathbb{R}_g(\boldsymbol{W}, \boldsymbol{S}) = \lambda_g \sum_{j}^{N} |\boldsymbol{S}_j|_1 |\boldsymbol{W}_{\cdot,j}|_1$$

which is very like group lasso.

The reason we use this the grouped L1-norm is that does variable selection at the group level and in our case can effectively eliminate a group of weights by columns(rules). We support the use of grouped L1-norm (like group lasso) instead of L2 norm by an empirical study on the cognitive preference of rules Fürnkranz et al. which shows that there is no strong preference on shorter rules but instead even a slight preference on longer rules. In other words, a small number of long rules is preferred over many short rules.

We leave more sophisticated metrics like feature overlaps [Lakkaraju et al., 2016] as future work. There are, indeed, many metrics but it remains hard to apply them for Neural DNF because some of them is not differentiable. If we use a discrete optimization algorithm this is not a problem, but in the case of our Neural DNF , we need the objective function to be end-to-end differentiable, so we need the regularization terms to be differentiable as well.

A.6 Possible direction of improvement

In the main paper we only discuss the regularization for the second stage DNF g, so the overall objective is given as

$$\boldsymbol{L} = \mathbb{L}_{loss} + \lambda_g \mathbb{R}_g(\boldsymbol{W}, \boldsymbol{S})$$

This is because we do not focus or design anything for the first stage neural network feature extractor. If we consider this (for future works), we can extend the objective to

$$\boldsymbol{L} = \mathbb{L}_{loss} + \lambda_g \mathbb{R}_g(\boldsymbol{W}, \boldsymbol{S}) + \lambda_\phi \mathbb{R}_\phi(\theta)$$

by considering a regularization term for the feature extractor that somehow defines some interpretability constraints.

B Related Works on Interpretability

The interest for interpretability is not new. It appears with the development of rule-based expert systems in the mid-1980's Amel [2019]. Of course the current situation is different because recently we have seen an increasing trend of interpretability research in machine learning [Lipton, 2018], in particular interpretable deep learning[Xie et al., 2020, Fan et al., 2020].

There are many definitions on interpretability, we use Lipton [2018]'s Simulatability definition of interpretability: for a prediction to be fully understood, the human should be able to re-calculate and reach the same prediction given resonable time.

B.1 Inherent interpretability, not Post-hoc interpretation

We summarize two main tracks of approaches for interpretability research, namely *post-hoc interpretation* and *building inherently interpretable models*, and we favor the latter. Post-hoc interpretation builds a secondary model to explain the given pre-trained deep learning model. Representative works include saliency maps [Simonyan et al., 2013], LIME [Ribeiro et al., 2016], Concept Activation Vectors [Kim et al., 2017]; some aim at giving counterfactual explanation [Dhurandhar et al., 2018, Zhang et al., 2018, Grath et al., 2018]. However, the provided explanation is in fact provided by a secondary model, not the original one, so it might not correspond faithfully to how the original blackbox model actually computes its prediction. Recent works further suggest that post-hoc interpretations are not robust [Adebayo et al., 2018, Fen et al., 2019, Alvarez-Melis and Jaakkola, 2018] and can even be misleading [Lakkaraju and Bastani, 2019, Rudin, 2019], and more specifically, the counterfactual explanations have the ‘unjustify’ issue [Laugel et al., 2019].

The second track, on the contrary, is to build an inherently interpretable deep learning model, so that the explanation it provided is exactly how it calculates the prediction. Inherently interpretale models are more preferred to examine and use when deployed in real world applications for various advantages (See [Khandani et al., 2010, Florez-Lopez and Ramon-Jeronimo, 2015]): it derives explanations to justify decision (legal issue), so people are less likely to refuse to use, easier to be combined with experts. An inherently interpretable classifier uses a interpretable prediction process to compute the prediction, and provides such computation process itself as the explanation for prediction.

B.2 Related works on Interpretable Deep Learning

For tabular datasets where each feature is already-meaningful, linear model or rule-based model are well-established choices of interpretable models[Amel, 2019], but for other data types such as image where each feature dimension itself is not meaningful, interpretable model is harder to construct.

A reasonable approach, which we call the two-stage paradigm, is to first construct intermediate representations $\phi(x)$ that is interpretable, and on top of that a simple interpretable classifier g is applied as the second stage such that the prediction is given by $\hat{y} = f(x) = g(\phi(x))$.

Most works on interpretable deep learning [Melis and Jaakkola, 2018, Chen et al., 2019a, Vaughan et al., 2018] choose linear model as the second-stage model g. Indeed, any neural network can be intuively viewed as a two-stage model where the second-stage is a linear model, as long we treat the network up to the last hidden layer as a generic feature extractor ϕ. But the notion of interpretability means we wish to make certain heuristics to make $\phi(x)$ interpretable.

Vaughan et al. [2018] formularize g as a linear model that $g(\phi(x)) = \sum_i w_i \phi_i(x)$ where $\phi(x)$ is a set of ridge functions, each of which are produced by a neural network. It claims to be more interpretable than general networks, because such a function has simpler partial derivatives that can simplify saliency analysis, statistical analysis and so on.

Chen et al. [2019a] also uses a linear model g and proposes a prototype-based design for $\phi(x)$. It learns interpretable $\phi(x)$ in the sense that each dimension of $\phi(x)$ is the similarity score to an image patch. It provides extra interpretability tailed for vision tasks as the similarity scores $\phi(x)$ can be visualized with the corresponding ‘prototype’ image patches. Melis and Jaakkola [2018] takes a step further that they use neural networks to produce not only $\phi(x)$ but also the coefficient of the linear model, such that prediction function is given by $g(\phi(x)) = \sum_i w_i(x)\phi_i(x)$ where $\phi(x)$ (called ‘concepts’) are regularized by auto-encoding reconstruction loss and $w_i(x)$ can be intuitively understood as an input-dependent relevance score for a concept $\phi_i(x)$. Here we can see that the implementation of $\phi(x)$ is domain-specific and customizable.

Theses works extend standard deep neural networks to interpretable ones by improving the design of the feature extractor ϕ and use a linear model for g. This is because a linear model, or its general form of general additive model, can be integrated into the automatic differentiation very easily.

Taking an opposite direction, we differ with previous works by considering to a rule-based classifier for g and do not put our focus on ϕ. However, because of the discrete struture, integrating a rule-based model g remains an hard and unexplored direction. But in terms of interpretability we favor rule-based models over linear models, not only because the discrete structure is more intutive for human to follow, but also that it can provide only the satisfied rules for explanation, unlike that for linear model for which we need to present the full model coefficients.

B.3 why favouring the symbolic DNF for interpretability

we argue that there are two major reasons for preferring rules over linear models as the second-stage classifier: (1) **Rules as combinations of conditions are more interpretable than feature importance** (at least for classification). It is widely acknowledged that the rule-based models are interpretable [Freitas, 2014, Huysmans et al., 2011, Wachter et al., 2018] because the rules give explanations by explicitly describing the decision boundary as logical combinations of conditions. Therefore, rules can more naturally provide counterfactual explanations in the form of *‘Would changing a certain factor have changed the decision?’* which is often considered to be the most important property of explanation [Doshi-Velez et al., 2017, Wachter et al., 2018, Grath et al., 2018, Miller, 2019].

On the other hand, coefficients as feature importances are arguably 'harder to use and to understand for a non-expert user' [Wachter et al., 2018]. We conjecture that rules are probably closer to human's mental model for classification, which can be corroborated by the fact that rules have been the most intuitive choice of model for human categorization learning [Bruner et al., 1956]. (2) **Using rules as a second-stage classifier g requires the feature extractor ϕ to produce Boolean output**($\{0, 1\}$), which is less complex than continuous ones. Compared with continuous values, Boolean output is simpler as it has only two states, making it easier for human to probe its meaning or to potentially align it with human knowledge. as future works

Rules can derive counterfactual explanations while linear models cannot (at least, not easy for linear models). The explicit decision boundary of rules not only can give factual explanations, namely giving the conjunctive conditions of the satisfied rule, but also give counterfactual explanations, by simply presenting that could have changed the prediction. Unlike weighted feature importance, rules explicitly presents all the sufficient conditions for prediction and thus can naturally handles counterfactual explanations in the form of *'Would changing a certain factor have changed the decision?'*. Indeed, the counterfactual explanation is often considered to be the most important property of explanation, confirmed not only from a more practical perspective [Doshi-Velez et al., 2017, Wachter et al., 2018, Grath et al., 2018] and also from cognitive/psychological research [Miller, 2019].

C DNF

Here we first explain the reason of choosing DNF as the rule module.

We choose DNF, one of the most powerful and historically significant symbolic methods, for its interpretability and its generality. It has a simple and transparent '*OR-of-ANDs*' prediction process: if at least one *AND* clause (a conjunction of Boolean predicates) is satisfied, it predicts positive; otherwise it predicts negavtive. DNF is interpretable not only that the discrete structure is intuitive to follow, each conjunctive clauses (AND) of DNF can be viewed as subtype for explanation, i.e. the DNF can be decomposed into individual local patterns. We also appreciate the generality of DNF, as any propositional logic formula has a equivalent DNF and thus any rule-based binary classifier including decison set/list/tree can be expressed as a DNF.

DNF have a long history but learning DNF is still a very hard problem, not to mention that we need to add interpretability contraints. Theoretical results on learning DNF in the PAC (probably approximately correct) setting are often unrealistic in practice and are hard to incorporate extra interpretability contraints. On the other hand, the practical use of rule learning of a DNF form attracts more attention from data mining community, namely, desciptive pattern discovery [Novak et al., 2009]. Seminal algorithms include CN2 and RIPPER (constrained for binary classification). More recent state of the art machine learning algorthms for learning DNF can work quite well on small tabular datasets, but not very scalable on high dimensional datasets, we name few representative recent works using greedy heuristics [Obermann and Waack, 2015, 2016]. Bayesian approximation [Wang et al., 2015], linear programming [Su et al., 2015]. We name the interpretable decision set by Lakkaraju et al. [2016] and Bayesian rule set by Wang et al. [2017] as two recent work as representative.

However, we note that these approach is not compatible here if we wish to jointly optimize g with the neural network feature extractor ϕ in an end-to-end way. It is because that first, constructing $\boldsymbol{W}$ by rule mining becomes non-sense if the neural module is currently being trained; second, discrete optimization methods for learning $\boldsymbol{S}$ is not compatible with gradient-based optimization.

C.1 Differentiable replacement of the DNF function g

The differentiable replacement of the DNF function we use in the paper is adopted from Payani and Fekri [2019], Wang et al. [2019b]. However, as we mentioned in the footnote in the main paper, we believe that this relaxation is not new but rather re-invented. Simialr formulations on differentiable operations see [Sajjadi et al., 2016, Arabshahi et al., Nomura et al., 1992]. It is also likely that we miss critical references on neuro-fuzzy system research in the 90s.

Basically, we construct differentiable g following the approaches of [Payani and Fekri, 2019, Wang et al., 2019b], where neural networks that execute differentiable logical operations are learned for inductive logic programming [Payani and Fekri, 2019] and multiple DNF layers are stacked to classify on tabular datasets [Wang et al., 2019b].

We here introduce some works that also uses a similar differentiable replacement of the DNF function below. Sajjadi et al. [2016] learns a DNF in the context of tackling the *moving target* problem (herd-effect) [Fahlman and Lebiere, 1990]. For each rule there is no selection of conditions, but rather, all conditions are taking as conjection. One thing worth mentioning is that Sajjadi et al. [2016] do not actually train the parameters of the disjunctive function but only gives a good initialization.

Payani and Fekri [2019] propose the *neural logical networks* to solve inductive logic programming, optimized in a gradient-based way. It does not add any extra regularizations to push the parameters to binary values, in the other hand it carefully discusses the problem of initialization to solve the problem.

Wang et al. [2019b] proposes to stack many DNF layers to make accurate and interpretable predictions (at least the authors claim that the resulted networks is interpretable), although we doubt it as the stacked DNF may in fact corresponding to a rule set that is so complicated for human too understand. Wang et al. [2019b] also propose the randomized binarzation to make the parameters of the matrix $\hat{\boldsymbol{W}}$ to be close to binary values. We view this as a binarization version of dropout, at each round, some parameters in $\hat{\boldsymbol{W}}$ are thresholded to 0 or 1 and get fixed, and other parameters are optimized as usual by backprop. However, it seems in the experiment of [Wang et al., 2019b] that the rate of binarization plays an important role, often the rate need to set in a very high value (for example, 80 90%) We also think that, it is not very efficient in terms of learning, by fixing such a high percentage of parameters to thresholded values. Because there binarized parameters are not getting updated at all (no gradient).

Optimization issues. The presense of both discrete and continuous parameters in Neural DNF introduces a hard optimization problem. A straightforward solution is to use a EM-like approach, by applying well-studied optimization techniques for neural and rule-based module separately. But we argue such separate training scheme might not be as efficient as joint end-to-end training. Another solution is to end-to-endly optimizing the overall model, which is challenging. We discuss in the main paper of two straightforward alternatives for joint learning: DNF-Real and DNF-STE and we also propose BOAT , the key algorithm in our paper.

Possible future directions. We consider possible directions about moving from DNF (propositional logic) to more flexible and powerful rule languages, And we are hoping that the proposed BOAT can possibly help.

For example, there is an inductive program synthesis project called 'TerpreT' [Gaunt et al., 2016], where the authors design a special language TerpreT for inductive program synthesis. It is designed to separate the program specificaion and the inference algorithm so that it can be optimized by different backends such as SGD, relaxed linear programming and non-machine-learning solvers so that compare all these optimization backends. Its key surprising finding is that in terms of empirical performance, SGD is dominated by more traditional constraint solvers. It also gives a very simple case where SGD can fail consistently with a exponential number of local minima, yet constraint solvers can work it out very easily. Note that in [Gaunt et al., 2016], the binary parameters is not in fact binary but only transformed by sigmoid/tanh/etc, so it is like the DNF-Real [Payani and Fekri, 2019] we mentioned in the main paper.

D Connections to Neural-symbolic Integration

It turns out that interpretable deep learning is very close to neuro-symbolic integration, just slightly different focus. Neural DNF can also be seen as achieving an interpretable model by neuro-symbolic integration. In fact, this 'explainability or interpretability through neuro-symbolic integration' approach is recently gaining attention (for example, see David Cox's AAAI/IAAI 2020 invited talk).

Neuro-symbolic integration [Besold et al., 2017], which aims at combining neural methods with symbolic-logic methods, learning and reasoning, seems to be very related to our Neural DNF . However, the literature on this topic is vast and offers a multitude of approaches covering different settings, making it difficult to discuss related works completely. We follow a most recent survey [Garcez et al., 2019], which divides neuro-symbolic integarion into the two categories: Horizontal and Vertical.

Horizontal integration contains most of the research, aims at integrating neural and symbolic techniques into one inseparable model: either by making neural model behaves more like a symbolic model (also known as deep learning with logical contraints), which using logical knowledge to improve neural network learning, or the making symbolic method neural, using a neural network as interpreter to execute symbolic programs. Some approaches for Horizontal integration are

- Put logic as constraints on a DNN: a deep net is extended with an extra regularization term derived from some logical property or from extra heavy annotations. But it is not guaranteed that such a DNN can make consistent symbolic prediction, as suggested by Xu et al. [2017] that deep nets trained with additional logical regularizations cannot consistently make predicions that is from the logic they were trained on.
- Enable a DNN to execute logical programs Cohen et al. [2017]. We can make a logic program differentiable by using differentiable functions and let a neural network to execute the logical program, such as querying a database. These approaches predicts a transparent struture as output, but its prediction process is not transparent or following logical property at all.

Vertical integration, the category to which our Neural DNF belong, assembles a deep learning model and a symbolic model in a sequential manner. It intends to use deep learning for pattern recognition (perception), and the symbolic model for high-level reasoning. However vertical integration but does not recieve much attention even it has a strong neuroscience inspiration.

- SATNet by Wang et al. [2019a] opens a framework to design flexible combinatorial function in a smoothed differentiable way and the combinatorial relationship is learned instead of hard-coded grammar. But still, we do not have a control or a sense of understanding to interpret the prediction.
- Manhaeve et al. [2018] use DNN for perception and symbolic reasoning given a defined grammar . They use a DNN to handle perception and outputs a classification as a neural predicate, and then use this predicates to do reasoning. It learn a Probabilistic ProgLog program by gradient descent enabled by compiling a Sentential Decision Diagram. But the relationship of these predicates are hard-coded by the used grammar, not learned; and the symbols (that is, the extracted feature $\phi(x)$) is not learned from scratch.

Learning neural predicates that represent the abstract features/symbols ('cat's mouth', etc) and learning the relationship among these variables are a novel thing! And this is also very important if we wish to do symbolic prediction on raw unstrutured data. It is genrally true that most of the methods will need pre-training or heavy annotations of the symbols extracted by a DNN.

But note that for our Neural DNF both the features $\phi(x)$ and the rules g are learned from scratch. This is in fact quite non-trivial if we consider Neural DNF in the context of neuro-symbolic integration.

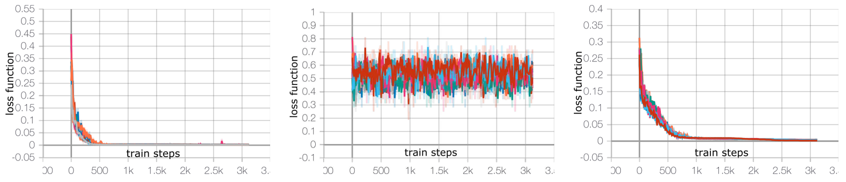
E Experiment

E.1 Evaluation of the BOAT Optimizer

Here we evaluate BOAT on datasets with Boolean features so that we learn only the DNF g. We use a synthetic dataset adopted from Payani and Fekri [2019] which consists of 10-bit Boolean strings and a randomly-generated DNF as ground-truth.

First, to show the proposed noise is indeed necessary and helps the optimization, we learn the DNF with/without the noise on multiple datasets generated with different random seeds (so the ground-truth DNF is different) and plot the loss curves. From fig. 1a we observe that multiple runs of BOAT give very similar and stable convergence, while in fig. 1b, surprisingly, runs consistently fail to converge without the noise. We view this as strong evidence for the necessity of the proposed noise. On the other hand, if noise temperature is initialized larger, the convergence is slower (fig. 1b).

There are some other issues with a large noise rate: (1) The slower learning of a larger noise rate can also be explained from the multiplicity nature of the DNF function we use (eq 2 and 3 in the main paper). This becomes more severe in high dimensional inputs. And finding a small noise rate initialization value will help. (2) when the noise rate intialized too high (and the hyperparameter of adaptivity rate not set right), it is also possible that the binary parameters cannot get huge gradient enough to flip, while it is only the continuous parameters including the noise rate are getting updated. This is an undesired result. In this case, find a smaller initilization rate.



(a) with noise (σ_0=0.2) (b) with NO noise (c) with noise (σ_0=0.4)

Figure 1: Loss curve with 10 differently-generated synthetic dataset

Next, we apply BOAT and compared the convergence speed with the following baselines: (1) DNF-Real [Payani and Fekri, 2019, Wang et al., 2019b] and (2) DNF-STE which are discussed in **??**. (3) A Linear Model. (4) A multi-layer perceptron. Note that we also use the adaptive noise for DNF-STE since otherwise optimization will fail. As shown in fig. 2, BOAT gives the fastest convergence, while MLP, DNF-STE and DNF-Real converge much more slowly. The linear model does not converge. As for the reason of DNF-STE's slower and less stable convergence, we believe it is because that unlike the modified *Bop*, DNF-STE does not have the mechanism to prevent rapid flipping and thus optimization becomes more unstable. As for performance, all above methods except linear model achieve 100% F1 score on test set and BOAT can always find the ground truth DNF on different synthetic datasets generated with different random seeds. **Remark:** Note that since we use random initialization for $\boldsymbol{W}$, $\boldsymbol{S}$, a natural suspicion is that the ground truth DNF happens to be discovered by the random initialization, not learned. To refute it, we can use zero initialization and find that BOAT converges similarly to random initialization. We report it in the appendix together with the performance results on some UCI datasets.

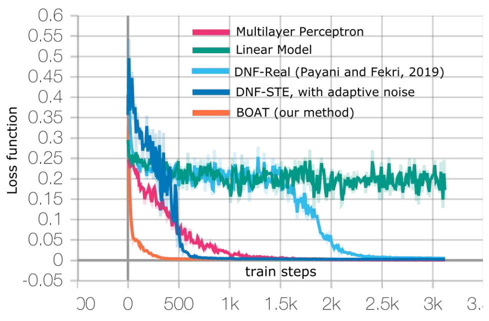


Figure 2: Loss Curve on the synthetic dataset

Here we evaluate only the second stage of our model, i.e., we use some datasets that the input features are already Boolean attributes, so we can use an identity function for the first stage neural module ϕ.

By removing ϕ, we focus on the evaluation of the learning algorithm, i.e., the proposed BOAT . We decide to use the synthetic Boolean bit-string dataset introduced by [Payani and Fekri, 2019] where this dataset is used for comparing the convergence of learning of the introduced DNF layer.

We randomly draw 5000 bit-strings where each bit is 0 or 1 (uniformly drawed). We then also randomly generate a ground-truth DNF and use this ground-truth DNF to assign labels to the bit-strings. Hopefully this ground-truth DNF should be recovered and indeed it is recovered. The ground-truth DNF consists of 5 clauses (rules) and each clause (rule) has 3 conditions. The conditions include negations. We random choose 4000 strings as the training set.

The generation of this synthetic Boolean bit-string dataset can be found at dataloaders.py. Note that in [Payani and Fekri, 2019], the bit is drawn with prob 0.75 to be zero and 0.25 to be one, and in our case we just use prob 0.5 to be zero and 0.5 to be one. This is because we also use negation in the generation of ground-truth DNF.

The DNF structure is 2K$\to$N$\to$1. We set $N = 64$ for the DNF as the default value for our method as well as DNF-Real and DNF-STE. For MLP and Linear model, we concatenate the input with its negation, and use a three-layer architecture (2K$\to$N$\to$1) for MLP, and the linear model is in essential a two-layer perceptron (2K$\to$1). As the DNF layer uses negations, we will also do the same for the linear model and multi-layer perceptron(MLP). We simple concanate the input feature with its negations so that the linear model is of structure (2K$\to$1) and the MLP (2K$\to$N$\to$1) For our method and all baselines we compare, we use Adam with initial learning rate 0.001. We use $\lambda_g = 0.0001$ as the default value.

Note that for compared baselines, if we use a larger learning rate such as 0.01 and since the synthetic Boolean bit-string dataset is not very difficult, the learning of DNF will be quicker (thus the covergence figure will looks different). However for our method, if we also set the initial learning rate for the noise from 0.001 to 0.01, the learning of BOAT will also be quicker (and a similar convergence figure should be able to be reproduced).

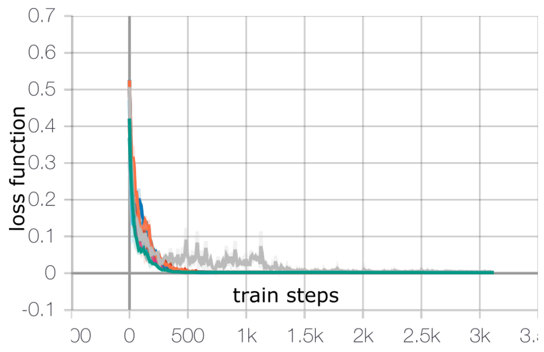


Figure 3: *Loss curve with 10 differently-generated synthetic dataset using zero-initialization*

random initialization and zero initialization. As we've mentioned in the main paper, one might suspect that the ground-truth DNF is not learned by our algorithm BOAT , but is only happened to be discovered by the random initialization. So here we also run our method with 10 different random seeds (differently-generated dataset) but with all-zero-initialization for $\boldsymbol{W}$ and $\boldsymbol{S}$. We can observe that the learning is still successful.

On real-world tabular datasets. In order to further investigate the performance, we also applied our method (learning the DNF g only) on several real-world datasets (table 1). We discretize the input features as preprocessing. Since these datasets are more complicated than the above synthetic dataset, we set N to 128; we set λ_g to 1e-4 as the default value. We find that our method perform competitively well and does not have performance decrease when the noise is removed. DNF-Real's performance slightly decreases after parameters are thresholded for Banknote dataset. One point worth noting is that learned DNF can achieve 100% F1-score on the tic-tac-toe dataset while weighted-sum-style models (linear Model/MLP/SENN[1]) can only approach to 100%. We think it is because the tic-tac-toe data is gathered from the status of a combinatorial game and thus may be more easily learned by rule-based models.

	DNF-BOAT With / Without noise	DNF-REAL Before / After thresholding	DNF-STE With / Without noise	Linear Model	MLP	SENN
Banknote	92.11%/92.11%	92.56%/91.05%	91.49%/91.49%	92.56%	92.11%	92.11%
tic-tac-toe	100%/100%	100%/100%	93.59%/93.59%	98.79%	99.59%	99.59%
Blogger	81.81%/81.81%	81.81%/81.81%	78.78%/78.78%	71.42%	86.95%	86.95%

Table 1: Test F1 score of learned DNF

Note that learning rule-based models using neural networks is already a challenging task, which we will not further investigate here.

E.2 The 2d-XOR

Four gaussians are drawn using scikit's 'make_blob' function with cluster mean (0,5), (5,0), (10,5) and (5,10).

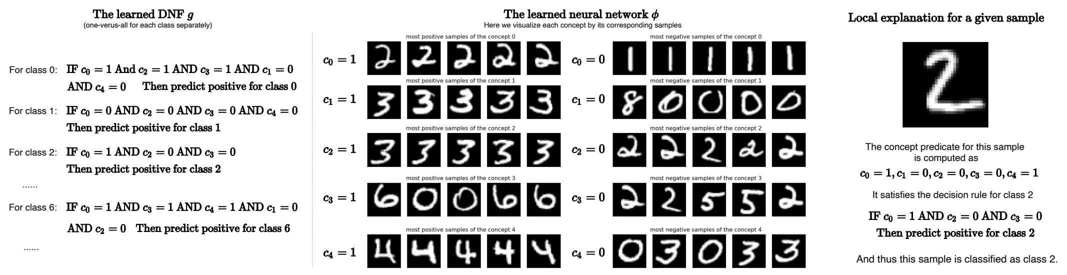
E.3 MNIST

We use the standard train-test split for MNIST (in total 10000 test samples.)

We use a randomly-initialized LeNet-like convolutional network as the feature extractor ϕ to produce 5 concept predicates. Since MNIST has 10 class, we use a separate $\boldsymbol{W}, \boldsymbol{S}$ for each class. After

[1]Note that SENN here is the second stage module of [Melis and Jaakkola, 2018] which is a MLP that takes input and generate the coefficients of a linear model.

training Neural DNF finds one or two rules for each class and can achieve over 99% test accuracy. In order to give an example of Neural DNF 's explanation, we first apply Neural DNF on MNIST as a direct comparison to the explanations provided by linear models (e.g., the MNIST example from [Melis and Jaakkola, 2018]).



The learned DNF g
(one-verus-all for each class separately)
The learned neural network ϕ
Here we visualize each concept by its corresponding samples
most positive samples of the concept 0
most negative samples of the concept 0
$c_0 = 1$
$c_0 = 0$
most positive samples of the concept 1
most negative samples of the concept 1
$c_1 = 1$
$c_1 = 0$
most positive samples of the concept 2
most negative samples of the concept 2
$c_2 = 1$
$c_2 = 0$
most positive samples of the concept 3
most negative samples of the concept 3
$c_3 = 1$
$c_3 = 0$
most positive samples of the concept 4
most negative samples of the concept 4
$c_4 = 1$
$c_4 = 0$
Local explanation for a given sample

For class 0: IF $c_0 = 1$ And $c_2 = 1$ AND $c_3 = 1$ AND $c_1 = 0$ AND $c_4 = 0$ Then predict positive for class 0

For class 1: IF $c_0 = 0$ AND $c_2 = 0$ AND $c_3 = 0$ AND $c_4 = 0$ Then predict positive for class 1

For class 2: IF $c_0 = 1$ AND $c_2 = 0$ AND $c_3 = 0$ Then predict positive for class 2

......

For class 6: IF $c_0 = 1$ AND $c_3 = 1$ AND $c_4 = 1$ AND $c_1 = 0$ AND $c_2 = 0$ Then predict positive for class 6

......

The concept predicate for this sample is computed as $c_0 = 1, c_1 = 0, c_2 = 0, c_3 = 0, c_4 = 1$

It satisfies the decision rule for class 2

IF $c_0 = 1$ AND $c_2 = 0$ AND $c_3 = 0$ Then predict positive for class 2

And thus this sample is classified as class 2.

(a) Global explanation for the overall Neural DNF Model (b) Local explanation

Figure 4: Explanations provided by Neural DNF on MNIST

Here we provide the explanations that Neural DNF derives: (1) In fig. 4a, we provide a *global* explanation for Neural DNF that explains the working of the overall model, by presenting the rules for each class as well as the image samples that triggers each concept predicate ($c = 1$) or not ($c = 0$). As it is necessary to understand what each each concept c means, we provide representative samples for $c = 1$ and $c = 0$ by retrieving samples that maximize or minimize the pre-binarization value $\tilde{c}$. (2) In fig. 4b, Neural DNF is also able to derive *local* explanations which explain the classification for a particular sample. Given a test sample, we present the value of its concept predicate (computed by ϕ) as well as the satisfied rule by which prediction is computed. Note in particular that the satisfied rules are not only the explanation but also how the predication is exactly computed, thus *inherently* interpretable.

Unlike explaining by feature importance that can only indicate some of $\phi(x)$ contributes more significantly to the final prediction, Neural DNF's explanation describes the decision boundary explicitly as combinations of conditions. For example, in fig. 4b as the decision rule for class 2 is 'If c_0=1 and c_2=0 and c_3=0 Then class 2', it becomes clear that only c_0, c_2, c_3 are essential for predicting class 2 while c_1, c_4 are not. In other words, for this test sample, we know precisely that if we change any of c_1 or c_4, the prediction will remain but changing of any of c_0, c_2, c_3 will give a different prediction.

The detailed decision rule for each class is:

Decision rule for class 0 is IF c-0,c-2,c-3 = 1 AND c-1, c-4 = 0 THEN predict class 0

Decision rule for class 1 is IF = 1 AND c-0, c-2, c-3, c-4 = 0 THEN predict class 1

Decision rule for class 2 is IF c-0 = 1 AND c-2, c-3 = 0 THEN predict class 2

Decision rule for class 3 is IF c-0,c-1,c-2 = 1 AND c-3, c-4 = 0 THEN predict class 3

Decision rule for class 4 is IF c-3,c-4 = 1 AND c-0, c-2 = 0 THEN predict class 4

Decision rule for class 5 is IF c-1,c-2 = 1 AND c-0, c-3 = 0 OR c-0,c-1,c-2 = 1 AND c-0, c-1, c-2, c-4 = 0 THEN predict class 5

Decision rule for class 6 is IF c-0,c-3,c-4 = 1 AND c-1, c-2 = 0 THEN predict class 6

Decision rule for class 7 is IF c-0,c-1,c-3 = 1 AND = 0 THEN predict class 7

Decision rule for class 8 is IF c-0,c-2,c-4 = 1 AND c-3 = 0 OR c-2,c-4 = 1 AND c-1, c-3 = 0 THEN predict class 8

Decision rule for class 9 is IF c-1,c-2,c-3 = 1 AND c-0 = 0 THEN predict class 9

E.4 Other datasets in Section 4.2

We evaluate our method on datasets as follows: MNIST, KMNIST, SVHN, CIFAR10. These are not new but very standard image datasets and we just use standard train-test split comes with the pytorch backend. Note that the four datasets are image datasets so use an convolutional neural network.

We use a fixed adam learning rate and fixed γ for the modified *Bop* optimizer. So there is no learning rate decay or other scheduling. For MNIST and KMNIST we use 5 concept predicate and run for 100 epoch. For SVHN and CIFAR10 we use 32 concept predicate and run for 200 epoch as these two datasets are more challenging.

Note that we present results of Neural DNF using lazy tie-breaking: by selecting the first encountered positive class in ascending order (e.g., when class 1, 4, 7 are all predicted as positive, we select class 1.). We can also use a random tie-breaking: when multiple classes are predicted as positive, we randomly pick one. We run 10 times on test set and report mean and standard deviation

Table 2: Test Accuracy of Neural DNF on some image datasets with two different tie-breaking

	MNIST	KMNIST	SVHN	CIFAR10
lazy tie-breaking	99.08%	95.43%	90.13%	67.91%
random tie-breaking	99.08% $\pm$ 0.02%	95.43% $\pm$ 0.03%	90.29% $\pm$ 0.04%	68.26% $\pm$ 0.12%

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