Neuro-Symbolic Entropy Regularization

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Abstract

In structured prediction, the goal is to jointly predict many output variables that together encode a structured object – a path in a graph, an entity-relation triple, or an ordering of objects. Such a large output space makes learning hard and requires vast amounts of labeled data. Different approaches leverage alternate sources of supervision. One approach – entropy regularization – posits that decision boundaries should lie in low-probability regions. It extracts supervision from unlabeled examples, but remains agnostic to the structure of the output space. Conversely, neuro-symbolic approaches exploit the knowledge that not every prediction corresponds to a valid structure in the output space. Yet, they do not further restrict the learned output distribution. This paper introduces a framework that unifies both approaches. We propose a loss, neuro-symbolic entropy regularization, that encourages the model to confidently predict a valid object. It is obtained by restricting entropy regularization to the distribution over only valid structures. This loss is efficiently computed when the output constraint is expressed as a tractable logic circuit. Moreover, it seamlessly integrates with other neuro-symbolic losses that eliminate invalid predictions. We demonstrate the efficacy of our approach on a series of semi-supervised and fully-supervised structured-prediction experiments, where we find that it leads to models whose predictions are more accurate and more likely to be valid.

1 Introduction

Neural networks have achieved breakthroughs across a wide range of domains. Such breakthroughs are often only possible in the presence of large labeled datasets, which can be hard to obtain. Increasing efforts are therefore being devoted to approaches that utilize alternate sources of supervision in lieu of more labeled data. Entropy regularization constitutes one such approach [Grandvalet and Bengio, 2005; Chapelle et al., 2010]. It posits that data belonging to the same class tend to form discrete clusters. Minimizing the entropy of the predictive distribution can thus be regarded as minimizing a measure of class overlap under the learned representation. Intuitively, a classifier guessing uniformly at random has maximum entropy, and has not learned features informative of the underlying class. Consequently, we prefer a minimum entropy classifier that learns features maximally informative of the underlying class, even on unlabeled data.

The need for labeled data is only exacerbated in structured prediction, where the objective is to predict multiple interdependent output variables representing a discrete object. Viewed as traditional classification, the number of classes in structured prediction is exponential in the number of output variables – all possible output configurations. Neuro-symbolic methods can provide additional supervision leveraging symbolic knowledge regarding the structure of the output space [De Raedt et al., 2020]. This knowledge, typically expressed in logic, characterizes the set of valid structures; for instance, not every selection of edges in a graph is a path.

In this paper we take a principled approach to unifying the aforementioned forms of supervision. Naively, we might consider simply optimizing both losses simultaneously. However, computed in that manner, the entropy does not account for the output-space structure, and is therefore likely to push the network towards invalid structures. Instead, we restrict the entropy loss to the network’s distribution over the valid structures, as characterized by the constraint, as opposed to the entire predictive distribution, proposing a new loss neuro-symbolic entropy regularization. That is, we require that the network’s output distribution be maximally informative subject to the constraint. Intuitively, the network should “know” the right structure among the valid structures. Computing the entropy of a distribution subject to a constraint is, in general, computationally hard. We provide an algorithm leveraging structural properties of tractable logical circuits to efficiently compute this quantity. Our framework integrates seamlessly with other neuro-symbolic approaches that maximize the constraint probability, in effect “eliminating” invalid structures.

Empirically, we evaluate our loss on four structured prediction tasks, in both semi-supervised and fully-supervised settings. We observe it leads to models whose predictions are more accurate, as well as more likely to satisfy the constraint.

2 Neuro-Symbolic Entropy Loss

We first introduce background on logical constraints and probability distributions over output structures. Afterwards,
we motivate and define our neuro-symbolic entropy loss.

2.1 Background

We write uppercase letters (X, Y) for Boolean variables and lowercase letters (x, y) for their instantiation (Y = 0 or Y = 1). Sets of variables are written in bold uppercase (X, Y), and their joint instantiation in bold lowercase (x, y). A literal is a variable (Y) or its negation (¬Y). A logical sentence (α or β) is constructed from variables and logical connectives (∧, ∨, etc.), and is also called a (logical) formula or constraint. A state or world y is an instantiation to all variables Y. A state y satisfies a sentence α, denoted y = α, if the sentence evaluates to true in that world. A state y that satisfies a sentence α is also said to be a model of α. We denote by m(α) the set of all models of α. The notation for states y is used to refer to an assignment, the logical sentence enforcing the assignment, or the binary output vector capturing the assignment, as these are all equivalent notions. A sentence α entails another sentence β, denoted α |= β, if all worlds that satisfy α also satisfy β.

A Probability Distribution over Possible Structures Let α be a logical sentence defined over Boolean variables Y = {Y₁, ..., Yᵣ}. Let p be a vector of probabilities for the same variables Y, where pᵢ denotes the predicted probability of variable Yᵢ and corresponds to a single output of the neural network. The neural network’s outputs induce a probability distribution Pr(·) over all possible states y of α

\[
Pr(y) = \prod_{i : y = Yᵢ} pᵢ \prod_{i : y = ¬Yᵢ} (1 - pᵢ). \tag{1}
\]

Semantic Loss The semantic loss is a function of α and p. It quantifies how close the neural network comes to satisfying the constraint by computing the probability of the constraint under the distribution Pr(·). It does so by reducing the problem of probability computation to the weighted model counting (WMC): summing up the models of α, each weighted by its likelihood under Pr(·). It, therefore, maximizes the probability mass allocated by the network to the models of α

\[
E_{y \sim Pr} [| \{ y = α \}] = \sum_{y \models α} Pr(y). \tag{2}
\]

Taking the negative logarithm recovers semantic loss. We use semantic loss in experiments to “eliminate” invalid structures.

2.2 Motivation and Definition

Consider the plots in Figure 1. A neural network can be fairly uncertain regarding the target class accommodating both valid and invalid predictions under its learned distribution.

A common underlying assumption in many machine learning methods is that data belonging to the same class tend to form discrete clusters [Chapelle et al., 2010] — an assumption deemed justified on the sheer basis of the existence of classes. Consequently, a classifier is expected to favor decision boundaries lying in regions of low data density, separating the clusters. Entropy-regularization [Grandvalet and Bengio, 2005] directly implements the above assumption, requiring the classifier output confident — low-entropy — predictive distributions, pushing the decision boundary away from unlabeled points, thereby supplementing scarce labeled data with abundant unlabeled data. Through that lens, minimizing the entropy of the predictive distribution can be seen as minimizing a measure of class overlap under the learned features.

Entropy regularization, however, fails to exploit situations where we have knowledge characterizing valid predictions in the domain. It can often be detrimental to the model’s performance by guiding it towards confident yet invalid predictions.

Conversely, neuro-symbolic approaches steer the network towards distributions disallowing invalid predictions, by maximizing the constraint probability, but do little by way of ensuring the network learn features conducive to classification.

Clearly then, there is a benefit to combining the merits of both approaches. We restrict the entropy computation to the distribution over models of the logical formula, ensuring the network only grow confident in valid predictions. Complemented with maximizing the constraint probability, the network learns to allocate all of its mass to models of the constraint, while being maximally informative of the target.

Defining the Loss More precisely, let Y be a random variable distributed according to eqn. (1), Y ~ Pr(·). We are interested in minimizing the entropy of Y conditioned on α

\[ H(Y|α) = −\sum_{yᵢ=α} Pr(y|α) \log Pr(y|α) \]

\[ = −E_{y|α} [\log Pr(Y|α)]. \tag{3} \]

3 Computing the Loss

The above loss is, in general, hard to compute. To see this, consider the uniform distribution over models of a constraint α. That is, let Pr(y|α) = 1/m(α) for all y = α. Then,
Algorithm 1 \(\text{ENT}(\alpha, \Pr, c)\)

**Input:** a smooth, deterministic and decomposable logical circuit \(\alpha\), a fully-factorized probability distribution \(\Pr(\cdot)\) over states of \(\alpha\), and a cache \(c\) for memoization

**Output:** \(H_{\Pr}(Y|\alpha)\), where \(Y \sim \Pr(\cdot)\)

1. **if** \(\alpha \in c\) **then** return \(c(\alpha)\)
2. **if** \(\alpha\) is a literal **then**
   
   \(e \leftarrow 0\)
3. **else if** \(\alpha\) is an AND gate **then**
4. \(e \leftarrow \text{ENT}(\beta, \Pr, c) + \text{ENT}(\gamma, \Pr, c)\)
5. **else if** \(\alpha\) is an OR gate **then**
6. \(e \leftarrow \sum_{i=1}^{m(\alpha)} \Pr(\beta_i) \log \Pr(\beta_i) + \Pr(\beta_i) \text{ENT}(\beta_i, \Pr, c)\)
7. **end if**
8. \(c(\alpha) \leftarrow e\)
9. return \(e\)

\(H(Y|\alpha) = -\sum_{\alpha \in \alpha} \frac{1}{m(\alpha)} \log \frac{1}{m(\alpha)} = \log |m(\alpha)|\). This tells us how many models of \(\alpha\) there are, which is a well-known \#P-hard problem [Valiant, 1979a; Valiant, 1979b]. We will show that, through compilation into tractable circuits, we can compute eqn. (3) in time linear in the size of the circuit.

### 3.1 Computation through Compilation

**Tractable Circuit Compilation** We resort to knowledge compilation techniques – a class of methods that transform, or *compile*, a logical theory into a target form with certain properties that allow certain probabilistic queries to be answered efficiently. More precisely, we know of circuit languages that compute the probability of constraints [Darwiche, 2003], and that are amenable to backpropagation. We use the circuit compilation techniques in Darwiche [2011] to build a logical circuit representing our constraint. Due to the structural properties of this circuit form, we can use it to compute both the probability of the constraint as well as its gradients with respect to the network’s weights, in time linear in the size of the circuit [Darwiche and Marquis, 2002]. This does not, in general, escape the complexity of the computation: worst case, the compiled circuit can be exponential in the size of the constraint. In practice, however, constraints often exhibit enough structure (repeated sub-problems) to make compilation feasible. We refer to the literature for details of this compilation.

**Logical Circuits** More formally, a logical circuit is a directed, acyclic computational graph representing a logical formula. Each node \(n\) in the DAG encodes a logical sub-formula, denoted \([n]\). Each inner node in the graph is either an AND or an OR gate, and each leaf node encodes a Boolean literal \((Y\text{ or } \neg Y)\). We denote by \(in(n)\) the set of \(n\)'s children.

**Structural Properties** As already alluded to, circuits enable the tractable computation of certain classes of queries over encoded functions granted that a set of structural properties are enforced. We explicate such properties down below.

A circuit is decomposable if the inputs of every AND gate depend on disjoint sets of variables i.e. for \(\alpha = \beta \land \gamma\), \(\text{vars}(\beta) \cap \text{vars}(\gamma) = \emptyset\). Intuitively, decomposable AND nodes encode local factorizations of the function. For simplicity, we assume decomposable AND gates to have two inputs, a condition enforceable on any circuit for a polynomial increase in its size [Vergari et al., 2015; Peharz et al., 2020].

A second useful property is smoothness. A circuit is smooth if the children of every OR gate depend on the same set of variables i.e. for \(\alpha = \bigvee_i \beta_i\), \(\text{vars}(\beta_i) = \text{vars}(\beta_j) \forall i, j\). Decomposability and smoothness are a sufficient and necessary condition for tractable integration over arbitrary sets of variables in a single pass, as they allow larger integrals to decompose into smaller ones [Choi et al., 2020].

Lastly, a circuit is said to be deterministic if, for any input, at most one child of every OR node has a non-zero output i.e. for \(\alpha = \bigvee_i \beta_i\), for every \(i\) \(\beta_i \land \beta_j = \bot\) for \(i \neq j\). Figure 2 shows an example of smooth, decomposable and deterministic circuit.

### 3.2 Algorithm

Let \(\alpha\) be a smooth, deterministic and decomposable logical circuit encoding our constraint, defined over Boolean variables \(Y = \{Y_1, \ldots, Y_\alpha\}\). We now show that we can compute the constrained entropy in eqn (3) in time linear in the size \(\alpha\). The key insight is, using circuits, we’re able to efficiently decompose an expectation with respect to a distribution by alternatingly splitting the query variables and the support of the distribution till we reach the leaves of the circuit – literals – when we proceed by combining solutions to our subproblems.

**Base Case:** \(\alpha\) is a literal

When \(\alpha\) is a literal, \(l = y_i\) or \(l = \neg y_i\), we have that

\[
\Pr(y_i|\alpha) = 1 \{y_i = |\alpha|\}, \quad \text{and} \quad H(y_i|\alpha) = -\Pr(y_i|\alpha) \log \Pr(y_i|\alpha) = 0.
\]

Intuitively, a literal has no uncertainty associated with it.

**Recursive Case:** \(\alpha\) is a conjunction

When \(\alpha\) is a conjunction, decomposability enables us to write

\[
\Pr(y|\alpha) = \Pr(Y_1|\beta) \Pr(Y_2|\gamma),
\]

where \(\text{vars}(\beta) \cap \text{vars}(\gamma) = \emptyset\) as it decomposes \(\alpha\) into two independent constraints \(\beta\) and \(\gamma\), and \(y\) into two independent assignments \(y_1\) and \(y_2\). The neuro-symbolic entropy \(-E_{Y|\alpha} \log \Pr(Y|\alpha)\) thus becomes

\[
-\mathbb{E}_{Y_1, Y_2|\alpha} \left[ \log \Pr(Y_1|\beta) + \log \Pr(Y_2|\gamma) \right] = -\mathbb{E}_{Y_1|\beta} \left[ \log \Pr(Y_1|\beta) \right] + \mathbb{E}_{Y_2|\gamma} \left[ \log \Pr(Y_2|\gamma) \right].
\]

That is, the entropy given a decomposable conjunction \(\alpha\) is the sum of entropies given the conjuncts of \(\alpha\).

**Recursive Case:** \(\alpha\) is a disjunction

When \(\alpha\) is a smoothness and deterministic disjunction, we have that \(\alpha = \bigvee_i \beta_i\), where the \(\beta_i\)s are mutually exclusive, and therefore partition \(\alpha\). Consequently, we have that

\[
\Pr(y|\alpha) = \sum_i \Pr(\beta_i) \cdot \Pr(y|\beta_i).
\]

The neuro-symbolic entropy decomposes as well:

\[
-\mathbb{E}_{Y|\alpha} \log \Pr(Y|\alpha) = -\sum_{y|\alpha} \Pr(y|\alpha) \log \Pr(y|\alpha) = \sum_i \Pr(\beta_i) \log \left[ \sum_j \Pr(\beta_j) \cdot \Pr(y|\beta_j) \right]
\]
where by determinism, we have that, for any y such that y \models \alpha, y \models \beta_i \implies y \not\models \beta_j \text{ for all } i \neq j. In other words, any state that satisfies the constraint \alpha satisfies one and only one of its terms, and therefore, the above expression is equal to

\[ -\sum_{y\models\alpha} \sum_i \Pr(\beta_i) \Pr(y|\beta_i) \log \left[ \sum_j \Pr(\beta_j) \Pr(y|\beta_j) \right] \text{,} \]

Further simplifying the above expression, expanding the logarithm, and using the fact conditional probability sums to 1

\[ = -\sum_i \Pr(\beta_i) \log \Pr(\beta_i) \sum_{y\models\beta_i} \Pr(y|\beta_i) \]

\[ + \Pr(\beta_i) \sum_{y\models\beta_i} \Pr(y|\beta_i) \log \Pr(y|\beta_i) \]

\[ = -\sum_i \Pr(\beta_i) \log \Pr(\beta_i) + \Pr(\beta_i) \text{E}_{Y|\beta_i} \log \Pr(Y|\beta_i) \]

That is, the entropy of the random variable Y conditioned on a disjunction \alpha is the sum of the entropy of the distributions induced on the children of \alpha, and the average entropy of its children. The full algorithm is illustrated in Algorithm 1.

4 Experimental Evaluation

In this section we set out to empirically test our neuro-symbolic entropy loss. To that end, we devise a series of semi-supervised and fully-supervised structured prediction experiments. Such are settings where, contrary to their dominant use, classifiers are expected to predict structured objects rather than scalar, discrete or real values. Such objects are defined in terms of constraints: a set of rules characterizing the set of solutions. We aim to answer the following:

1. Does entropy regularization, in general, lead to predictive models with improved generalization capabilities?
2. If the answer to the above question is in the positive, it is our expectation that restricting the distribution acted upon by entropy regularization to that over just the models of the constraint might seem more sensible as compared to entropy-regularizing the entire predictive distribution—including non-models of the constraint. Do experiments corroborate such a hypothesis?
3. Finally, entropy regularization can be interpreted as clustering the different classes, and has intimate connections to transductive Support Vector Machines [Chapelle et al., 2010]. Does such an interpretation carry over to models and non-models of the constraint? Put differently, can we expect entropy-regularized predictive models to better conform to our constraints, measured by the percentage of predictions satisfying the constraint regardless of their correctness.

4.1 Semi-Supervised: Entity-Relation Extraction

We begin by testing our research questions in the semi-supervised setting. Here the model is presented with only a portion of the labeled training set, with the rest used exclusively in an unsupervised manner by the respective approach.

We make use of the natural ontology of entity types and their relations present when dealing with relational data. This defines a set of relations and their permissible argument types. As is with all of our constraints, we express the aforementioned ontology in the language of Boolean logic.

Our approach to recognizing the named entities and their pairwise relations is most similar to Zhong and Chen [2020]. Contextual embeddings are first procured for every token in the sentence. These are then fed into a named entity recognition module that outputs a vector of per-class probability for every entity. A classifier then classifies the concatenated contextual embeddings and entity predictions into a relation.

We employ two entity-relation extraction datasets, the Automatic Content Extraction (ACE) 2005 [Walker et al., 2006] and SciERC datasets [Luan et al., 2018]. ACE05 defines an ontology over 7 entities and 18 relations from mixed-genre text, whereas SciERC defines 6 entity types with 7 possible relation between them and includes annotations for scientific entities and there relations, assimilated from 12 AI conference/workshop proceedings. We report the percentage of coherent predictions: data points for which the predicted entity
Table 1: Experimental results for joint entity-relation extraction on ACE05 and SciERC. #Labels indicates the number of labeled data points made available to the network per relation. The remaining training set is stripped of labels and is utilized in an unsupervised manner.

| # Labels | 3   | 5   | 10  | 15  | 25  | 50  | 75  |
|----------|-----|-----|-----|-----|-----|-----|-----|
| ACE05    |     |     |     |     |     |     |     |
| Baseline | 4.92 ± 1.12 | 7.24 ± 1.75 | 13.66 ± 0.18 | 15.07 ± 1.79 | 21.65 ± 3.41 | 28.96 ± 0.98 | 33.02 ± 1.17 |
| Self-training | 7.72 ± 1.21 | 12.83 ± 2.97 | 16.22 ± 3.08 | 17.55 ± 1.41 | 27.00 ± 3.66 | 32.90 ± 1.71 | 37.15 ± 1.42 |
| Product t-norm | 8.89 ± 5.09 | 14.52 ± 2.13 | 19.22 ± 5.81 | 21.80 ± 7.67 | 30.15 ± 1.01 | 34.12 ± 2.75 | 37.35 ± 2.53 |
| Semantic Loss | 12.00 ± 3.81 | 14.92 ± 3.14 | 22.23 ± 3.64 | 27.35 ± 3.10 | 30.78 ± 0.68 | 36.76 ± 1.40 | 38.49 ± 1.74 |
| + Full Entropy | 14.80 ± 3.70 | 15.78 ± 1.90 | 23.34 ± 4.07 | 28.09 ± 1.46 | 31.13 ± 2.26 | 36.05 ± 1.00 | 39.39 ± 1.21 |
| + NeSy Entropy | 14.72 ± 1.57 | 18.38 ± 2.50 | 26.41 ± 0.49 | 31.17 ± 1.68 | 35.85 ± 0.75 | 37.62 ± 2.17 | 41.28 ± 0.46 |
| SciERC    |     |     |     |     |     |     |     |
| Baseline | 2.71 ± 1.1 | 2.94 ± 1.0 | 3.49 ± 1.8 | 3.56 ± 1.1 | 8.83 ± 1.0 | 12.32 ± 3.0 | 12.49 ± 2.6 |
| Self-training | 3.56 ± 1.4 | 3.04 ± 0.9 | 4.14 ± 2.6 | 3.73 ± 1.1 | 9.44 ± 3.8 | 14.82 ± 1.2 | 13.79 ± 3.9 |
| Product t-norm | 6.50 ± 2.0 | 8.86 ± 1.2 | 10.92 ± 1.6 | 13.38 ± 0.7 | 13.83 ± 2.9 | 19.20 ± 1.7 | 19.54 ± 1.7 |
| Semantic Loss | 6.47 ± 1.02 | 9.31 ± 0.76 | 11.50 ± 1.53 | 12.97 ± 2.86 | 14.07 ± 2.33 | 20.47 ± 2.50 | 23.72 ± 0.38 |
| + Full Entropy | 6.26 ± 1.21 | 8.49 ± 0.85 | 11.12 ± 1.22 | 14.10 ± 2.79 | 17.25 ± 2.75 | 22.42 ± 0.43 | 24.37 ± 1.62 |
| + NeSy Entropy | 6.19 ± 2.40 | 8.11 ± 3.66 | 13.17 ± 1.08 | 15.47 ± 2.19 | 17.45 ± 1.52 | 22.14 ± 1.46 | 25.11 ± 1.03 |

4.2 Fully-Supervised Learning

We now turn our attention to testing our hypotheses in a fully supervised setting, where our aim is to examine the effect of constraints enforced on the training set. We note that this is a seemingly harder setting in the following sense: In a semi-supervised setting we might make the argument that, despite its abundance, imposing an auxiliary loss on unlabeled data provides the predictive model with an unfair advantage as compared to the baseline. We concern ourselves with two tasks: predicting paths in a grid and preference learning.

Table 2: Test results for grids, preference learning, and warcraft

|            | Test accuracy % | Coherent Incoherent Constraint |
|------------|-----------------|-------------------------------|
| Grid       |                 |                               |
| 5-layer MLP| 5.6             | 85.9                          | 7.0                          |
| Semantic loss | 28.5            | 83.1                          | 69.9                         |
| + Full Entropy | 29.0            | 83.8                          | 75.2                         |
| + NeSy Entropy | 30.1            | 83.0                          | 91.6                         |
| Preference |                 |                               |
| 3-layer MLP| 1.0             | 75.8                          | 2.7                          |
| Semantic loss | 15.0            | 72.4                          | 69.8                         |
| + Full Entropy | 17.5            | 71.8                          | 80.2                         |
| + NeSy Entropy | 18.2            | 71.5                          | 96.0                         |
| Warcraft   |                 |                               |
| ResNet-18  | 44.8            | 97.7                          | 56.9                         |
| Semantic loss | 50.9            | 97.7                          | 67.4                         |
| + Full Entropy | 51.5            | 97.6                          | 67.7                         |
| + NeSy Entropy | 55.0            | 97.9                          | 69.8                         |

Predicting Simple Paths For this task, our aim is to find the shortest path in a graph, or more specifically a 4-by-4 grid, $G = (V, E)$ with uniform edge weights. Our input is a binary vector of length $|V| + |E|$, with the first $|V|$ variables indicating the source and destination, and the next $|E|$ variables encoding a subgraph $G' \subseteq G$. Each label is a binary vector of length $|E|$ encoding the shortest simple path in $G'$, a requirement that we enforce through our constraint. We follow the algorithm proposed by Nishino et al. [2017] to generate a constraint for each simple path in the grid, conjoined with indicators specifying the corresponding source-destination pair. Our constraint is then the disjunction of all such conjunctions.

To generate the data, we begin by randomly removing one third of the edges in the graph $G$, resulting in a subgraph, $G'$. Subsequently, we filter out connected components in $G'$ with fewer than 5 nodes to reduce degenerate cases. We then sample a source and destination node uniformly at random. The latter constitutes a single data point. We generate a dataset of 1600 examples, with a 60/20/20 train/validation/test split.

Preference Learning We also consider the task of preference learning. Given the user’s ranking of a subset of elements, we wish to predict the user’s preferences over the re-
Incorporating constraints into learning improves the coherent \( \text{constitute valid paths}. \) Our results are shown in Table 2.

The percentage of individual vertices matching the groundtruth, “Incoherent” denotes the path. We report three metrics: “Coherent” denotes the percentage indicating the vertices that constitute the minimum cost neural network – following Poganˇcic et al. [2020], our training set consists of 10,000 terrain maps curated using Warcraft II tileset. Each map encodes an underlying grid of dimension 12 \( \times \) 12, where each vertex is assigned a cost depending on the type of terrain it represents (e.g., earth has lower cost than water). The shortest (minimum cost) path between the top left and bottom right vertices is encoded as an indicator matrix, and serves as label.

Table 2 compares the baseline to the same MLP augmented with semantic loss, semantic loss with entropy regularization over the entire predictive distribution, dubbed “Full Entropy” as well as entropy regularization over the distribution under the constraint’s models, dubbed “NeSy Entropy”. Similar to Xu et al. [2018], we observe that the semantic loss has a marginal effect on incoherent accuracy, but significantly improves the network’s ability to output coherent predictions. Furthermore, we observe that, similar to our semi-supervised learning settings, entropy-regularization leads to more coherent predictions using both “Full Entropy” and “NeSy Entropy”, with “NeSy Entropy” leading to the best performing predicting models. Remarkably, we also observe that “NeSy Entropy” leads to predictive models whose predictions almost always satisfy the constraint, as captured by “Constraint”.

Warcraft Shortest Path

Lastly, we consider a more real-world variant of the task of predicting simple paths. Following Poganˇcic et al. [2020], our training set consists of 10,000 terrain maps curated using Warcraft II tileset. Each map encodes an underlying grid of dimension 12 \( \times \) 12, where each vertex is assigned a cost depending on the type of terrain it represents (e.g., earth has lower cost than water). The shortest (minimum cost) path between the top left and bottom right vertices is encoded as an indicator matrix, and serves as label. Fig. 3 shows an example input presented to the network, the groundtruth, and the input with the annotated shortest path.

Presented with an image of a terrain map, a convolutional neural network – following Poganˇcic et al. [2020], we use ResNet18 [He et al., 2016] – outputs a 12 \( \times \) 12 binary matrix indicating the vertices that constitute the minimum cost path. We report three metrics: “Coherent” denotes the percentage of optimal-cost predictions, “Incoherent” denotes the percentage of individual vertices matching the groundtruth, and “Constraint” indicates the percentage of predictions that constitute valid paths. Our results are shown in Table 2.

In line with our previous experiments, we observe that incorporating constraints into learning improves the coherent accuracy from 44.8% to 50.9%, and of valid predictions from 56.9% to 67.4%. Further augmenting semantic loss with the entropy over the network’s predictive distribution, “Full Entropy”, we attain a modest improvement from 50.9% to 51.5% and 67.4% to 67.7% for the “Coherent” and “Constraint” metrics respectively. Restricting the entropy minimization to models of the constraint, “NeSy Entropy”, we observe that we attain a large improvement to 55.0% and 69.8% for the “Coherent” and “Constraint” metrics respectively.

5 Related Work and Conclusion

In an acknowledgment to the need for both symbolic as well as sub-symbolic reasoning, there has been a plethora of recent works studying how to best combine neural networks and logical reasoning, dubbed neuro-symbolic reasoning. The focus of such approaches is typically making probabilistic reasoning tractable through first-order approximations, and differentiable, through reducing logical formulas into arithmetic objectives, replacing logical operators with their fuzzy t-norms, and logical implications with simple inequalities [Rocktäschel et al., 2015; Fischer et al., 2019].

Diligenti et al. [2017] and Donadello et al. [2017] use first-order logic to specify constraints on the outputs of a neural network. They employ fuzzy logic to reduce logical formulas into differential, arithmetic objective functions denoting the extent to which neural network outputs violate the constraints, thereby supporting end-to-end learning under constraints. More recently, Xu et al. [2018] introduced semantic loss, which circumvents the shortcomings of fuzzy approaches, while still supporting end-to-end learning under constraints. More precisely, fuzzy reasoning is replaced with exact probabilistic reasoning, made possible through compiling logical formulae into data structures that support efficient probabilistic queries.

Another class of neuro-symbolic approaches have their roots in logic programming. DeepProbLog [Manhaeve et al., 2018] extends ProbLog, a probabilistic logic programming language, with the capacity to process neural predicates, whereby the network’s outputs are construed as the probabilities of the corresponding predicates. This simple idea retains all essential components of ProbLog: the semantics, inference mechanism, and the implementation. In a similar vein, Dai et al. [2018] combine domain knowledge specified as purely logical Prolog rules with the output of neural networks, dealing with the network’s uncertainty through revising the hypothesis by iteratively replacing the output of the neural network with anonymous variables until a consistent hypothesis can be formed. Bošnjak et al. [2017] present a framework combining prior procedural knowledge, as a Forth program, with neural functions learned through data. The resulting neural programs are consistent with the specified prior knowledge and optimized with respect to the data.

In conclusion, we proposed neuro-symbolic entropy regularization, a principled approach to unifying neuro-symbolic learning and entropy regularization. It encourages the network to output distributions that are peaked over models of the logical formula. We are able to compute our loss due to structural properties of circuit languages. We validate our hypothesis on four different tasks under semi-supervised and fully-supervised settings and observed an increase in accuracy as well as the validity of the predictions across the board.
References

[Bošnjak et al., 2017] Matko Bošnjak, Tim Rocktäschel, Jason Naradowsky, and Sebastian Riedel. Programming with a differentiable forth interpreter. In Proceedings of the 34th ICML, 2017.

[Chang et al., 2007] Ming-Wei Chang, Lev Ratinov, and Dan Roth. Guiding semi-supervision with constraint-driven learning. In Proceedings of the 45th ACL, 2007.

[Chapelle et al., 2010] Olivier Chapelle, Bernhard Schlkopf, and Alexander Zien. Semi-Supervised Learning. The MIT Press, 1st edition, 2010.

[Choi et al., 2020] YooJung Choi, Antonio Vergari, and Guy Van den Broeck. Probabilistic circuits: A unifying framework for tractable probabilistic modeling. 2020.

[Dai et al., 2018] Wang-Zhou Dai, Qiu-Ling Xu, Yang Yu, and Zhi-Hua Zhou. Tunneling neural perception and logic reasoning through abductive learning, 2018.

[Darwiche and Marquis, 2002] Adnan Darwiche and Pierre Marquis. A knowledge compilation map. JAIR, 2002.

[Darwiche, 2003] Adnan Darwiche. A differential approach to inference in bayesian networks. UAI, 2003.

[De Raedt et al., 2020] Luc De Raedt, Sebastijan Dumančić, Robin Manhaeve, and Giuseppe Marra. From statistical relational to neuro-symbolic artificial intelligence. In IJCAI, 2020.

[Diligenti et al., 2017] Michelangelo Diligenti, Marco Gori, and Claudio Saccà. Semantic-based regularization for learning and inference. Artificial Intelligence, 2017.

[Donadello et al., 2017] Ivan Donadello, Luciano Serafini, and Artur d’Avila Garcez. Logic tensor networks for semantic image interpretation. In IJCAI, 2017.

[Fischer et al., 2019] Marc Fischer, Mislav Balunovic, Dana Drachsler-Cohen, Timon Gehr, Ce Zhang, and Martin Vechev. DL2: Training and querying neural networks with logic. In ICML, 2019.

[Grandvalet and Bengio, 2005] Yves Grandvalet and Yoshua Bengio. Semi-supervised learning by entropy minimization. In NeurIPS, 2005.

[He et al., 2016] Kaiming He, Xiangyu Zhang, Shaoqing Ren, and Jian Sun. Deep residual learning for image recognition. In CVPR, June 2016.

[Luan et al., 2018] Yi Luan, Luheng He, Mari Ostendorf, and Hannaneh Hajishirzi. Multi-task identification of entities, relations, and coreference for scientific knowledge graph construction. In EMNLP, 2018.

[Manhaeve et al., 2018] Robin Manhaeve, Sebastijan Dumančić, Angelika Kimmig, Thomas Demeester, and Luc De Raedt. Deephproblog: Neural probabilistic logic programming. In NeurIPS, 2018.

[Mattei and Walsh, 2013] Nicholas Mattei and Toby Walsh. Preflib: A library of preference data \url{HTTP://PREFLIB.ORG}. In ADT, 2013.

[Nishino et al., 2017] Masaaki Nishino, Norihito Yasuda, Shin ichi Minato, and Masaaki Nagata. Compiling graph substructures into sentential decision diagrams. In AAAI, 2017.

[Peharz et al., 2020] Robert Peharz, Steven Lang, Antonio Vergari, Karl Stelzner, Alejando Molina, Martin Trapp, Guy Van den Broeck, Kristian Kersting, and Zoubin Ghahramani. Einsum networks: Fast and scalable learning of tractable probabilistic circuits. In International Conference of Machine Learning, 2020.

[Pogančić et al., 2020] Marin Vlastelica Pogančić, Anselm Paulus, Vit Musil, Georg Martius, and Michal Rolinek. Differentiation of blackbox combinatorial solvers. In ICLR, 2020.

[Rocktäschel et al., 2015] Tim Rocktäschel, Sameer Singh, and Sebastian Riedel. Injecting logical background knowledge into embeddings for relation extraction. In Proceedings of the 2015 Conference of the NAACL, 2015.

[Valiant, 1979a] Leslie G. Valiant. The complexity of enumeration and reliability problems. SIAM Journal on Computing, 1979.

[Valiant, 1979b] L.G. Valiant. The complexity of computing the permanent. Theoretical Computer Science, 1979.

[Vergari et al., 2015] Antonio Vergari, Nicola Di Mauro, and Floriana Esposito. Simplifying, regularizing and strengthening sum-product network structure learning. In Joint European Conference on Machine Learning and Knowledge Discovery in Databases, 2015.

[Walker et al., 2006] Christopher Walker, Stephanie Strassel, Julie Medero, and Kazuaki Maeda. Ace 2005 multilingual training corpus. LDC, 2006.

[Xu et al., 2018] Jingyi Xu, Zilu Zhang, Tal Friedman, Yitao Liang, and Guy Van den Broeck. A semantic loss function for deep learning with symbolic knowledge. In Proceedings of the 35th ICML 2018, 2018.

[Zhong and Chen, 2020] Zexuan Zhong and Danqi Chen. A frustratingly easy approach for joint entity and relation extraction. CoRR, 2020.