Self-supervised self-supervision by combining deep learning and probabilistic logic

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Abstract

Labeling training examples at scale is a perennial challenge in machine learning. Self-supervision methods compensate for the lack of direct supervision by leveraging prior knowledge to automatically generate noisy labeled examples. Deep probabilistic logic (DPL) is a unifying framework for self-supervised learning that represents unknown labels as latent variables and incorporates diverse self-supervision using probabilistic logic to train a deep neural network end-to-end using variational EM. While DPL is successful at combining pre-specified self-supervision, manually crafting self-supervision to attain high accuracy may still be tedious and challenging. In this paper, we propose Self-Supervised Self-Supervision (S4), which adds to DPL the capability to learn new self-supervision automatically. Starting from an initial “seed,” S4 iteratively uses the deep neural network to propose new self-supervision. These are either added directly (a form of structured self-training) or verified by a human expert (as in feature-based active learning). Experiments show that S4 is able to automatically propose accurate self-supervision and can often nearly match the accuracy of supervised methods with a tiny fraction of the human effort.

1 Introduction

Machine learning has made great strides in enhancing model sophistication and learning efficacy, as exemplified by recent advances in deep learning (LeCun et al., 2015). However, contemporary supervised learning techniques require a large amount of labeled data, which is expensive and time-consuming to produce. This problem is particularly acute in specialized domains like biomedicine, where crowdsourcing is difficult to apply. Self-supervision has emerged as a promising paradigm to overcome the annotation bottleneck by automatically generating noisy training examples from unlabeled data. In particular, task-specific self-supervision converts prior knowledge into self-supervision templates for label generation, as in distant supervision (Mintz et al., 2009), data programming (Ratner et al., 2016), and joint inference (Poon and Domingos, 2008).

Deep probabilistic logic (DPL) is a unifying framework for self-supervision that combines deep learning with probabilistic logic (Wang and Poon, 2018). It represents unknown labels as latent variables, and incorporates prior beliefs over labels and their dependencies as virtual evidence in a graphical model. The marginal beliefs over the latent variables are used as probabilistic labels to train a deep neural network for the end prediction task. The trained neural network in turn provides belief updates to refine the graphical model parameters, and the process continues, using variational EM.

Wang and Poon (2018) show that DPL can effectively combine diverse sources of self-supervision in a coherent probabilistic framework and subsume supervised and semi-supervised learning as special cases. While promising, DPL and related approaches still require human experts to manually specify self-supervision. This is particularly challenging for self-supervision techniques such as data programming and joint inference, which require domain expertise and extensive effort to identify the many relevant virtual evidences for attaining high accuracy in the end task.

In this paper, we propose self-supervised self-supervision (S4) as a general framework for learning to add new self-supervision. In particular, we extend deep probabilistic logic (DPL) with structure learning and active learning capabilities (see Figure 1). After running DPL using the pre-specified seed self-supervision, S4 iteratively proposes new virtual evidence using the trained deep neural network and graphical model, and determines whether to add this evidence directly to the graphical model or ask a human expert to vet it. The former can be viewed as structured self-training, which generalizes...
Figure 1: Self-supervised self-supervision (S4): S4 builds on deep probabilistic logic and uses probabilistic logic to represent self-supervision for learning a deep neural network for the end prediction task. Starting from pre-specified self-supervision, S4 interleaves structure learning and active learning steps to introduce new self-supervision for training the neural network and refining the graphical model parameters. Self-supervision factors from initialization, structure learning, and active learning are shown in blue, red, and black, respectively.

self-training (e.g., McClosky et al., 2006) by adding not only individual labels but also arbitrary probabilistic factors over them. The latter subsumes feature-based active learning Druck et al. (2009) with arbitrary features expressible using probabilistic logic. By combining the two in a unified framework, S4 can leverage both paradigms for generating new self-supervision and subsume many related approaches as special cases.

We use transformer-based models for the deep neural network in DPL and explore various self-supervision proposal mechanisms based on neural attention and label entropy. Our method can learn to propose both unary potential factors over individual labels and joint-inference factors over multiple labels. We conducted experiments on various natural language processing (NLP) tasks to explore the potential of our method. We held out gold labels for evaluation only, and used them to simulate oracle self-supervision for initial self-supervision and active learning. We find that S4 can substantially improve over the seed self-supervision by proposing new virtual evidence, and can match the accuracy of fully supervised systems with a fraction of human effort.

2 Deep probabilistic logic

Given a prediction task, let \( \mathcal{X} \) and \( \mathcal{Y} \) denote the sets of possible inputs and outputs, respectively. The goal is to train a prediction module \( \Psi(x, y) \) that scores output \( y \) given input \( x \). We assume that \( \Psi(x, y) \) represents the conditional probability \( P(y|x) \). Let \( X = (X_1, \cdots, X_N) \) denote a sequence of inputs and \( Y = (Y_1, \cdots, Y_N) \) the corresponding outputs. If \( Y \) is observed, \( \Psi(x, y) \) can be learned using standard supervised learning. In this paper, we consider the setting where \( Y \) is unobserved, and \( \Psi(x, y) \) is learned using self-supervision.

The key idea of deep probabilistic logic (DPL) is to represent self-supervision as prior belief over the latent label variables \( Y \) and their interdependencies by combining probabilistic logic and deep learning (Wang and Poon, 2018). Pearl (1988) first introduced virtual evidence to represent prior belief on the value of a random variable. Specifically, the prior belief on \( Y \) can be represented by introducing a binary variable \( v \) as a dependent of \( Y \) such that \( P(v = 1|Y = y) \) is proportional to the belief of \( Y = y \). The virtual evidence \( v = 1 \) can be viewed as a reified variable representing the unary potential function \( \Phi(y) \propto P(v = 1|y) \). More generally, this can represent arbitrary potential functions \( \Phi(X, Y) \) over the inputs and outputs, so as to model prior beliefs over arbitrary high-order factors. DPL uses Markov logic Richardson and Domingos (2006) to represent virtual evidences and uses a deep neural network as the prediction module \( \Psi(x, y) \). Let \( V = \{v_1, \cdots, v_k\} \) be a set of pre-specified virtual evidences, with the corresponding potential functions being \( (\Phi_1, \cdots, \Phi_k) \). We will use \( K \) as shorthand for...
the event $V = 1$ (i.e., $v_1 = 1, \ldots, v_k = 1$). DPL defines a probability distribution over $K, X, Y$ by combining a factor graph with potentials $\Phi$ representing $P(K|Y, X)$ and the prediction module $P(Y|X)$:

$$P(K, Y|X) \propto \prod_v \Phi_v(X, Y) \cdot \prod_i \Psi_i(X_i, Y_i)$$  

(1)

Here, the potential functions $\Phi_v(X, Y)$ are represented by weighted first-order logic formulas (i.e., $\Phi_v(X, Y) = \exp(w_v f_v(X, Y))$, with $f_v(X, Y)$ being a binary feature represented by a first-order logical formula). DPL considers a Bayesian setting where each $w_v$ is drawn from a prespecified prior distribution $P(w_v|\alpha_v)$. Fixed $w_v$ amounts to the special case when the prior is concentrated on the preset value. For uncertain $w_v$’s, DPL computes their maximum a posteriori (MAP) estimates.

Parameter learning in DPL maximizes the conditional log likelihood of virtual evidences $\log P(K|X)$, which can be done using variational EM. In the E-step, DPL computes a variational approximation $q(Y)$ for $P(Y|K, X)$, using loopy belief propagation (Murphy et al., 1999) with current parameters $\Phi, \Psi$, by conducting message passing in $P(K, Y|X)$ iteratively. In the M-step, DPL treats $q(Y)$ as the probabilistic label distribution to train $\Phi$ and $\Psi$ via standard supervised learning. For the prediction module $\Psi$, this reduces to standard deep learning, with the marginals $q_i(Y_i) = \mathbb{E}_{q(Y)}(Y_i)$ serving as probabilistic labels for $X_i$. For the supervision module, this reduces to standard parameter learning for log-linear models (i.e., learning non-fixed $w_v$’s), and can be solved using gradient descent, with the partial derivative for $w_v$ being $\mathbb{E}_{q(Y,X)} [f_v(X, Y)] - \mathbb{E}_{q(Y)} [f_v(X, Y)]$. The second expectation can be done by simple counting. The first expectation, on the other hand, requires probabilistic inference in the graphical model. But it can be computed using belief propagation, similar to the E-step, except that the messages are limited to factors in the supervision module (i.e., messages from $\Psi$ are not included).

### Algorithm 1 Self-Supervised Self-Supervision (S4)

**Input:** Seed virtual evidences $I$, deep neural network $\Psi$, inputs $X = (X_1, \ldots, X_N)$, unobserved outputs $Y = (Y_1, \ldots, Y_N)$, human query budget $T$.

**Output:** Learned prediction module $\Psi$ and virtual evidences $K = \{(f_v(X, Y), w_v) : v\}$.

**Initialize:** $K = I; Q = \emptyset; i = 0$.

for $i = 1 \ldots M$ do

while Structured Self-Training not converged do

$v = \text{PropSST}(K, \Psi, X, Y)$;

$K \leftarrow K \cup v$;

end while

if $|Q| < T$ then

$v = \text{PropFAL}(K, \Psi, X, Y, Q)$;

$Q \leftarrow Q \cup v$;

if Human–Accept($v$) then $K \leftarrow K \cup v$;

end if

end for

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**3 Self-supervised self supervision**

In this section, we present the self-supervised self supervision (S4) framework, which extends deep probabilistic logic (DPL) with the capability to learn new self-supervision. Let $V = \{(f_v, w_v, \alpha_v) : v\}$ be the set of all candidate virtual evidences, where $f_v(X, Y)$ is a first-order logical formula, $w_v$ is the weight, and $\alpha_v$ is the weight prior (for non-fixed $w_v$). Let $K$ be the set of virtual evidences maintained by the algorithm, initialized by the seed $I$. The key idea of S4 is to interleave structure learning and active learning to iteratively propose new virtual evidence $v \in V$ to augment $K$ (Figure 1). Self-training is a special case where candidate virtual evidences are individual label assignments (i.e., $f_v = I|y_v = l_v$). S4 can thus be viewed as conducting structured self-training (SST) by generalizing self-training to admit arbitrary Markov logic formulas as virtual evidence.

S4 can also be viewed as conducting structure learning in the factor graph that specifies the virtual evidence. Structure learning has been studied intensively in the graphical model literature (Friedman and Koller, 2003). It is also known as feature selection or feature induction in general machine learning literature (Hall, 1999). Here, we are introducing structured factors for self-supervision, rather than as feature templates to be used during training. Another key difference from standard structure learning is the deep neural network, which provides an alternative view from the virtual evidence space and enables multi-view learning in DPL. The neural network can also help identify candidate virtual evidences, e.g., via neural attention.

In data programming and many other prior methods, human experts need to pre-specify all self-supervision upfront. While it is easy to generate a small seed by identifying the most salient self-supervision, this effort can quickly become tedious and more challenging as the experts are required to enumerate the less salient templates. On the other hand, given a candidate, it’s generally much easier for experts to validate it. This suggests that for the best utilization of human bandwidth, we should focus on leveraging them to produce the initial self-supervision and verify candidate self-supervision. Consequently, in
addition to structured self-training (SST), S4 incorporates feature-based active learning (FAL) (i.e., active learning of self-supervision). When SST converges, S4 will switch to the active learning mode by proposing a candidate virtual evidence for human verification (i.e., labeling a feature rather than an instance in standard active learning). Intuitively, in FAL we are proposing virtual evidences for which the labels of the corresponding instances are still uncertain. If the human expert can provide definitive supervision on the label, the information gain will be large. By contrast, in SST, we favor virtual evidences with skewed posterior label assignments for their corresponding instances, as they can potentially amplify the signal.

Algorithm 1 describes the S4 algorithm. S4 first conducts DPL using the initial self-supervision \(I\), then interleaves structured self-training (SST) with feature-based active learning (FAL). SST steps are repeated until there is little change in the probabilistic labels (less than 1% in our experiments). DPL learning updates the deep neural network and the graphical model parameters with warm start (i.e., the parameters are initialized with the previous parameters). All proposed queries are stored and won’t be proposed again. The total amount of human effort consists of generating the seed \(I\) and validating \(T\) queries in active learning.

S4 is a general algorithm framework that can combine various strategies for designing \(V\), PropSST, and PropFAL. In standard structure learning, PropSST would attempt to maximize the learning objective (e.g., conditional likelihood of seed virtual evidences) by iteratively conducting greedy structure changes. However, this is very expensive to compute, since it requires a full DPL run just to score each candidate. Instead, we take inspiration from the feature-induction and relational learning literature and use heuristic approximations that are much faster to evaluate. In the most general setting, \(V\) contains all possible potential functions. In practice, we can restrict it to a tractable subset to obtain a good trade-off between expressiveness and computation for the problem domain. Interestingly, as we will see in the experiment section, even with relatively simple classes of self-supervision, S4 can dramatically improve over DPL through structure learning and active learning.

We use text classification from natural language processing (NLP) as a running example to illustrate how to apply S4 in practice. Here, the input \(X_i = (t_1, \ldots, t_n)\) is a sequence of tokens and the output \(Y_i\) is the classification label (e.g., pos or neg in sentiment analysis).

### 3.1 Candidate self-supervision

For \(V\), the simplest choice is to use tokens. Namely, \(f_{t,l}(X_i, Y_i) = \mathbb{I}[t \in X_i \land Y_i = l]\). For simplicity, we can use a fixed weight and prior for all initial virtual evidence, i.e., \(V = \{(f_{t,l}, w, \alpha) : t, l\}\). Take sentiment analysis as an example. \(X_i\) may represent a movie review and \(Y_i \in \{0, 1\}\) the sentiment. A virtual evidence for self-supervision may stipulate that if the review contains the word “good”, the sentiment is more likely to be positive. This can be represented by the formula \(f_{\text{good},1}(X_i, Y_i) = \mathbb{I}[^{\text{"good"}}] \in X_i \land Y_i = 1\) with a positive weight. A more advanced choice for \(V\) may include high-order factors, such as \(f_{ij}(Y_i, Y_j) = \mathbb{I}[Y_i = Y_j]\). If we add this factor for similar pairs \(X_i, X_j\), it stipulates that instances with similar input are likely to share the same label. Here we define similar pairs with a similarity function \(\text{Sim}(X_i, X_j)\) between \(X_i\) and \(X_j\), such as the cosine similarity between the sentence (or document) embeddings of \(X_i\) and \(X_j\), based on the current deep neural network. Note that this is different from graph-based semi-supervised learning or other kernel-based methods in that the similarity metric is not pre-specified and fixed, but rather evolving along with the deep neural network for the end task.

### 3.2 Structured self-training (PropSST)

From DPL learning, we obtain the current marginal estimate of the latent label variables \(q_l(Y_i)\), which we would treat as probabilistic labels in assessing candidate virtual evidence. There are many sensible strategies for proposing candidates in structured self-training (i.e., PropSST). For token-based self-supervision, a common technique from the feature-selection literature is to choose a token highly correlated with a label. For example, we can choose the token \(t\) that occurs much more frequently in instances for a given label \(l\) than others using our noisy label estimates. We find that this often leads to very noisy proposals and semantic drift. A simple refinement is to restrict our scoring to instances containing some initial self-supervised tokens. However, this still has the drawback that a word may occur more often in instances of a class for reasons other than contributing to the label classification. We therefore consider a more sophisticated strategy based on neural attention. Namely, we will credit occurrences using the normalized attention weight for the given token in each instance.

Formally, let \(A_{\Phi}(X_i, j)\) represent the normalized attention weight the neural network \(\Sigma\) assigns to the \(j\)-th token in \(X_i\) for the final classification. We define average weighted attention for token \(t\) and label \(l\) as \(\text{Attn}(t, l) = \frac{1}{C_t} \sum_{i : X_{i,j} = t} q_l(Y_i = l) \cdot A_{\Phi}(X_i, j)\), where \(C_t\) is the number of occurrences of \(t\) in \(X\). Then PropSST would simply score token-based self-supervision \(f_{t,l}\) using relative average weighted attention: \(S_{\text{token}}(t, l) = \text{Attn}(t, l) - \sum_{t' \neq t} \text{Attn}(t', l)\). In each iteration, PropSST picks the top scoring \(f_{t,l}\) that has not been proposed yet as the new virtual evidence to add to \(K\).

We also consider an entropy-based score function that
works for arbitrary input-based features. It treats the prediction module $\Psi$ as a black box, and only uses the posterior label assignments $q_i(Y_i)$. Consider candidate virtual evidence $f_k(X_i, Y_i) = \|b(X_i) \land Y_i = l\|$, where $b$ is a binary function over input $X_i$. This clearly generalizes token-based virtual evidence. Define $\text{Ent}(b) = H\left(\frac{1}{C_b} \sum_{i:b(X_i)=1} q_i(Y_i)\right)$, where $H$ is the Shannon entropy and $C_b$ is the number of instances for which the feature $b$ holds true. This function represents the entropy of the average posterior among all instances with $b(X_i) = 1$. PropSST will then use $S_{\text{entropy}}(b) = 1 / \text{Ent}(b)$ to choose the $b^*$ with the lowest average entropy and then pick label $l^*$ with the highest average posterior probability for $b^*$. In our experiments, this performs similarly to attention-based scores.

For joint-inference self-supervision, we consider the similarity-based factors defined earlier, and leave the exploration of more complex factors to future work. To distinguish task-specific similarity from pretrained similarity, we use the difference between the similarity computed using the current fine-tuned BERT model and that using the pretrained one.

Formally, let $\text{Sim}_{\text{pretrained}}(X_i, X_j)$ be the cosine similarity between the embeddings of $X_i$ and $X_j$ generated by the pretrained BERT model, and $\text{Sim}_{\Psi}(X_i, X_j)$ be that between the embeddings using the current learned network $\Psi$. PropSST would score the joint-inference factor using the relative similarity and choose the top scoring pairs to add to self-supervision: $S_{\text{joint}}(X_i, X_j) = \text{Sim}_{\Psi}(X_i, X_j) - \text{Sim}_{\text{pretrained}}(X_i, X_j)$.

### 3.3 Feature-based active learning (PropFAL)

For active learning, a common strategy is to pick the instance with highest entropy in the label distribution based on the current marginal estimate. In feature-based active learning, we can similarly pick the feature $b$ with the highest average entropy $\text{Ent}(b)$. Note that this is opposite to how we use the entropy-based score function in PropSST, where we choose the feature with the lowest average entropy. In PropFAL, we will identify $b^* = \arg\max(\text{Ent}(b))$, present $f_{b^*, l}(X, Y) = \|b^*(X) \land Y = l\|$ for all possible labels $l$, and ask the human expert to choose a label $l^*$ to accept or reject them all.

### 4 Experiments

We use the natural language processing (NLP) task of text classification to explore the potential for S4 to improve over DPL using structure learning and active learning. We used three standard text classification datasets: IMDb (Maas et al., 2011), Stanford Sentiment Treebank (Socher et al., 2013), and Yahoo! Answers (Zhang et al., 2015). IMDb contains movie reviews with polarity labels (positive/negative). There are 25,000 training instances with equal numbers of positive and negative labels, and the same numbers for test. Stanford Sentiment Treebank (StanSent) also contains movie reviews, but was annotated with five labels ranging from very negative to very positive. We used the binarized version of StanSent, which collapses the polarized categories and discards the neutral sentences. It contains 6,920 training instances and 1,821 test instances, with roughly equal split. Overall, the StanSent reviews are shorter than IMDb’s, and they often exhibit more challenging linguistic phenomena (e.g., nested negations or sarcasm). The Yahoo dataset contains 1.4 million training questions and 60,000 test questions from Yahoo! Answers; these are equally split into 10 classes. The Yahoo results are contained in the appendix.

In all our experiments with S4, we withheld gold labels from the system, used the training instances as unlabeled data, and evaluated on the test set. We reported test accuracy, as all of the datasets are class-balanced. For our neural network prediction module $\Psi(X_i, Y_i)$, we used the standard BERT-base model pretrained using Wikipedia (Devlin et al., 2018), along with a global-context attention layer as in Yang et al. (2016), which we also used for attention-based scoring. We truncated the input text to 512 tokens, the maximum allowed by the standard BERT model. All of our baselines (except supervised bag-of-words) use the same BERT model. For all virtual evidence, we used initial weight $w = 2.2$ (the log-odds of 90% probability) and used an $\alpha$ corresponding to an $L2$ penalty of $5 \times 10^{-8}$ on $w$. Our results are not sensitive to these values. In all experiments, we use the Adam optimizer with an initial learning rate tuned over $[0.1, 0.01, 0.001]$. The optimizer’s history is reset after each EM iteration to remove old gradient information. We always performed 3 EM iterations and trained $\Psi$ for 5 epochs per iteration.

For virtual evidence, we focus on token-based unary factors and similarity-based joint factors, as discussed in the previous section, and leave the exploration of more complex factors to future work. Even with these factors, our self-supervised $\Psi$ models often nearly match the accuracy of the best supervised models. We also compare with Snorkel, a popular self-supervision system (Ratner et al., 2016). We use the latest Snorkel version (Ratner et al., 2019), which models correlations among same-instance factors. Snorkel cannot incorporate joint-inference factors across different instances.

To simulate human supervision for unary factors, we trained a unigram model using the training data with $L1$ regularization and selected the 100 tokens with the highest weights for each class as the oracle self-supervision. By default, we used the top tokens for each class in the initial self-supervision $I$. We also experimented with using ran-
dom tokens from the oracle in \( I \) to simulate lower-quality initial supervision and to quantify the variance of S4. For the set of oracle joint factors, we fine-tuned the standard BERT model on the training set, used the CLS embedding BERT produces to compute input similarity, and picked the 100 input pairs whose similarity changed the most between the fine-tuned model and the initial model.

We first investigate whether structure learning can help in S4 by running without feature-based active learning. We set the query budget \( T = 0 \) in Algorithm 1. Because we only take structured self-training steps when \( T = 0 \), we denote this version of S4 as S4-SST. Table 1 shows the results on IMDb. With just six self-supervised tokens (three per class), S4-SST already attained 86% test accuracy, which outperforms self-training with 100 labeled examples by 16 absolute points, and is only slightly worse than self-training with 1000 labeled examples or supervised training with 25,000 labeled examples. By conducting structure learning, S4-SST substantially outperformed DPL, gaining about 5 absolute points in accuracy (a 25% relative reduction in error), and also outperformed the Snorkel baseline by 8.9 points. Interestingly, with more self-supervision at 20 tokens, DPL’s performance drops slightly, which might stem from more noise in the initial self-supervision. By contrast, S4-SST capitalized on the larger seed self-supervision and attained steady improvement. On average across different initial amounts of supervision \(| I |\), S4-SST outperforms DPL by 5.6 points and Snorkel by 5.3 points.

Next, we consider the full S4 algorithm with a budget of up to \( T = 20 \) human queries (S4 \((T = 20)\)). Overall, by automatically generating self-supervision from structure learning, S4-SST already attained very high accuracy on this dataset. However, active learning can still produce some additional gain. The only randomness in Table 1 is the initialization of the deep network \( \Psi \), which has a negligible effect.

Figure 2 (leftmost) shows how S4-SST iterations improve the test accuracy of the learned neural network with different amounts of initial virtual evidence. Not surprisingly, with more initial self-supervision, the gain is less pronounced, but still significant. Figure 2 (center left) compares the learning curves of S4-SST with those of self-training. Remarkably, with just six self-supervised tokens, S4-SST not only attained substantial gain over the iterations, but also easily outperformed self-training despite the latter using an order of magnitude more label information (up to 200 labeled examples). This shows that S4 is much more effective in leveraging bounded human effort for supervision.

Figure 2 (center right) shows 10 runs of S4-SST when it was initialized with 20 random oracle tokens (10 per class), rather than the top 20 tokens from the oracle. As expected, DPL’s initial performance is worse than with

| Algorithm | Sup. size | \(| I |\) | Test acc (%) |
|-----------|-----------|---------|-------------|
| BoW       | 25k       | 6       | 87.1        |
| DNN       | 25k       | 6       | 91.0        |
| Self-training | 100   | 6       | 69.9        |
| Self-training | 1k   | 6       | 88.5        |
| Snorkel   | 6         | 6       | 76.6        |
| DPL       | 6         | 6       | 80.7        |
| S4-SST    | 6         | 6       | 85.5        |
| S4 \((T = 20)\) | 6   | 6       | 85.6        |
| Snorkel   | 20        | 6       | 82.4        |
| DPL       | 20        | 6       | 78.9        |
| S4-SST    | 20        | 6       | 86.4        |
| S4 \((T = 20)\) | 20  | 6       | 86.9        |

Table 2: System comparison on Stanford

| \(| I |\)       | 6       | 10      | 20      | 40      |
|-------------|---------|---------|---------|---------|
| \(T = 5\)   | 79.0    | 83.8    | 84.0    | 85.9    |
| \(T = 10\)  | 79.5    | 83.7    | 85.0    | 86.0    |
| \(T = 20\)  | 82.7    | 84.5    | 85.8    | 86.4    |

Table 3: S4-FAL results on IMDb (no SST steps)
The Stanford results also demonstrated that active learning could play a bigger role in more challenging scenarios. With limited initial self-supervision ($|I| = 6$), the full S4 system (S4+J (T=20)) gained 8 absolute points over S4-SST and 5 absolute points over S4-SST+J. With sufficient initial self-supervision and joint-inference, however, active learning was actually slightly detrimental ($|I| = 20, 40$).

Finally, we evaluate S4-FAL, which conducts active learning but not structure learning. See Tables 3 and 4. As expected, performance improved with larger initial self-supervision ($I$) and human query budget ($T$). Active learning helps the most when initial self-supervision is limited. Compared to S4 with structure learning, however, active learning alone is less effective. For example, without requiring any human queries, S4-SST outperformed S4-FAL on both IMDB and Stanford even when the latter was allowed up to $T = 20$ human queries.

## 5 Related work

Techniques to compensate for the lack of direct supervision come in many names and forms (Mintz et al., 2009; Ratner et al., 2016; Bach et al., 2017; Roth, 2017; Wang and Poon, 2018). Self-supervision has emerged as an encompassing paradigm that views these as instances of using self-specified templates to generate noisy labeled examples on unlabeled data. The name self-supervision is closely related to self-training McClosky et al. (2006), which bootstraps from a supervised classifier, uses it to annotate unlabeled instances, and iteratively uses the confident labels to retrain the classifier. Task-agnostic self
supervision generalizes word embedding and language modeling by learning to predict self-specified masked tokens, as exemplified by recent pretraining methods such as BERT (Devlin et al., 2018). In this paper, we focus on task-specific self-supervision and use pretrained models as a building block for task-specific learning.

Existing self-supervision paradigms are typically special cases of deep probabilistic logic (DPL). E.g., the popular data programming methods (Ratner et al., 2016; Bach et al., 2017; Varma et al., 2017) admit only virtual evidences for individual instances (labeling functions or their correlations). Anchor learning (Halpern et al., 2016) is an earlier form of data programming that, while more restricted, allows for stronger theoretical learning guarantees. Prototype learning is an even earlier special case with labeling functions provided by “prototypes” (Haghighi and Klein, 2006; Poon, 2013). Using Markov logic to model self-supervision, DPL can incorporate arbitrary prior beliefs on both individual labels and their interdependencies, thereby unleashing the full power of joint inference (Chang et al., 2007; Druck et al., 2008; Poon and Domingos, 2008; Ganchev et al., 2010) to amplify and propagate self-supervision signals.

Self-supervised self-supervision (S4) further extends DPL with structure learning capability. Most structure learning techniques are developed for the supervised setting, where structure search is guided by labeled examples (Friedman and Koller, 2003; Kok and Domingos, 2005). Moreover, traditional relational learning induces deterministic rules and is susceptible to noise and uncertainty. Bootstrapping learning is one of the earliest and simplest self-supervision methods with some rule-learning capability, by alternating between inducing characteristic contextual patterns and classifying instances Hearst (1992); Carlson et al. (2010). The pattern classes are limited and only applicable to special problems (e.g., “A such as B” to find ISA relations). Most importantly, they lack a coherent probabilistic formulation and may suffer catastrophic semantic drift due to ambiguous patterns (e.g., “cookie” as food or compute use). Yarowsky (1995) and Collins and Singer (1999) designed a more sophisticated rule induction approach, but their method uses deterministic rules and may be sensitive to noise and ambiguity. Recently, Snuba (Varma and Ré, 2018) extends the data programming framework by automatically adding new labeling functions, but like prior data programming methods, their self-supervision framework is limited to modeling prior beliefs on individual instances. Their method also requires access to a small number of labeled examples to score new labeling functions.

Another significant advance in S4 is by extending DPL with the capability to conduct structured active learning, where human experts are asked to verify arbitrary virtual evidences, rather than a label decision. Note that by admitting joint inference factors, this is more general than prior use of feature-based active learning, which focuses on per-instance features (Druck et al., 2009). As our experiments show, interleaving structured self-training learning and structured active learning results in substantial gains, and provides the best use of precious human bandwidth. Tong and Koller (2001) previously considered active structure learning in the context of Bayesian networks. Anchor learning (Halpern et al., 2016) can also suggest new self-supervision for human review. Darwin (Galhotra et al., 2020) incorporates active learning for verifying proposed rules, but it doesn’t conduct structure learning, and like Snuba and other data programming methods, it only models individual instances.

Neural-symbolic learning and reasoning has received increasing attention Besold et al. (2017). In particular, combining deep learning with probabilistic models can leverage their complementary strengths in modeling complex patterns and infusing rich prior knowledge. Prior work tends to focus on deep generative models that aim to uncover latent factors for generative modeling and semi-supervised learning (Kingma and Welling, 2013; Kingma et al., 2014). They admit limited forms of self-supervision (e.g., latent structures such as Markov chains (Johnson et al., 2016)). S4 and DPL instead combine a discriminative neural network predictor with a generative self-supervision model based on Markov logic, and can fully leverage their respective capabilities to advance co-learning (Blum and Mitchell, 1998; Grechkin et al., 2017). Deep neural networks also provide a powerful feature-induction engine to support structure learning and active learning.

6 Conclusion

We present Self-Supervised Self-Supervision (S4), a general self-supervision framework that can automatically induce new self-supervision by extending deep probabilistic logic (DPL) with structure learning and active learning capabilities. Our experiments on various natural language processing (NLP) tasks show that compared to prior systems for task-specific self-supervision, such as Snorkel and DPL, S4 can obtain gain up to 20 absolute accuracy points with the same amount of supervision. S4 only relies on humans to identify the most salient self-supervision for initialization and to verify proposed self-supervision, which tends to be the most effective use of human bandwidth. While we focus on NLP tasks in this paper, our methods are general and can potentially be applied to other domains. Future directions include: further investigation in combining structure learning and active learning; exploring more sophisticated self-supervision classes and proposal algorithms; applications to other domains.
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8 Supplementary material

8.1 Structured self-training convergence

In Algorithm 1, structured self-training (SST) iterations are repeated until convergence in the while loop. Here we elaborate on the convergence criterion described in the main text (Self-Supervised Self-Supervision Section). Intuitively, convergence occurs when the expected latent labels change little despite the addition of new self-supervision from SST.

Formally, consider the set \( \Delta = \{ i | \arg \max_{y_{it}} E_{\Phi_{t-1}(X,Y)}[y_i] \neq \arg \max_{y_{it}} E_{\Phi_{t}(X,Y)}[y_i] \} \). This is the set of instances for which the labels based on self-supervision alone (excluding the neural network prediction module \( \Psi \)) have changed between subsequent iterations. We stop the SST iterations once \( |\Delta|/N < \alpha \) for some small \( \alpha \), as we don’t expect there will be much change afterwards. We used \( \alpha = 1\% \), which worked well in preliminary experiments, and performed no further tuning.

8.2 Count normalization in score functions

All the score functions in PropSST and PropFAL normalize the score using the feature count (e.g., \( C_t, C_b \)). In practice, if we apply this to all features, we may inadvertently promote rare features. Thus Druck et al. (2009) additionally multiplied by the logarithm of the count (i.e., they normalize using \( \log C_t \)). By contrast, we found it preferable to use standard count normalization, but simply skip the rare features. In all of our experiments, we only consider the top 2.5% most frequent features. We found that this worked well in preliminary experiments on the held-out data in IMDb, and our results are not sensitive to this value.

8.3 Additional experimental details and results

8.3.1 Yahoo.

We provide additional results for S4-SST on Yahoo using token-based factors and attention scoring. See Table 5. We focused our experiments on a fixed 10% of the training set due to its very large size (1.4 million examples). There are 10 classes, so initial self-supervision size of 50 (100) represents 5 (10) initial tokens per class (for S4, DPL, and Snorkel), or 5 (10) labeled examples per class (for self-training). Compared to binary sentiment analysis in IMDb and Stanford, Yahoo represents a much more challenging dataset, with ten classes and larger input text for each instance. The linguistic phenomena are much more diverse, and therefore neither Snorkel or DPL performed much better than self-training, as a token-based self-supervision confers not much more information than a labeled example. However, S4-SST is still able to attain substantial improvement over the initial self-supervision. E.g., with initial supervision size of 100, S4-SST gained about 11 absolute accuracy points over DPL, and 16 absolute points over Snorkel. Additionally, S4-SST is able to better utilize the new factors than Snorkel. If we run Snorkel using the same initial factors as S4-SST and also add the new factors proposed by S4-SST in each iteration, the accuracy improved from 36.5 to 44.2, but still trailed S4-SST (52.3) by 8 absolute points. Interestingly, both DPL and Snorkel perform better on Yahoo with fewer initial factors, at 5 per class, suggesting they are sensitive to noise in the less reliable initial self-supervision. By contrast, S4-SST is more noise-tolerant and benefits from additional initial supervision.

8.3.2 Entropy-based scoring.

As stated in the main text, entropy-based scoring \( S_{\text{entropy}} \) is a more general scoring function that works for arbitrary features in self-supervision. Tables 6a and 6b show the results comparing S4-SST test accuracy using entropy-based scoring \( S_{\text{entropy}} \) and attention-based scoring \( S_{\text{token}} \). Entropy-based scoring slightly outperforms attention-based scoring on Stanford Sentiment and slightly trails on IMDb. Overall, the two perform comparably but entropy-based scoring is more generally applicable.

8.3.3 Hyperparameters

In all of our experiments, we used three variational EM iterations and trained the deep neural network for 5 epochs per EM iteration. For the global-context attention layer, we used a context dimension of 5. The model is warm-started across EM iterations (in DPL), but not across the outer iterations in S4 (the for loop). In all experiments, we used
| Algorithm      | Sup. size | Test acc (%) |
|---------------|-----------|--------------|
| BoW           | 140k      | 71.2         |
| DNN           | 140k      | 79.8         |
| Self-training | 50        | 38.4         |
| Snorkel       | 50        | 37.2         |
| DPL           | 50        | 41.8         |
| S4-SST        | 50        | 49.1         |
| Self-training | 100       | 38.2         |
| Snorkel       | 100       | 36.5         |
| DPL           | 100       | 41.7         |
| S4-SST        | 100       | 52.3         |

Table 5: Comparison of test accuracy on Yahoo.

| $|I|$ | Entropy-based | Attention-based |
|----|----------------|-----------------|
| 6  | 82.1           | 85.5            |
| 20 | 84.9           | 86.4            |
| 40 | 85.5           | 86.6            |

(a) IMDb

| $|I|$ | Entropy-based | Attention-based |
|----|----------------|-----------------|
| 6  | 77.2           | 73.0            |
| 20 | 85.1           | 83.3            |
| 40 | 85.7           | 84.9            |

(b) Stanford

Table 6: Comparison of test accuracy on IMDb and Stanford. Entropy-based scoring ($S_{\text{entropy}}$) perform comparably as attention-based scoring ($S_{\text{token}}$).

the Adam optimizer with an initial learning rate tuned over $[0.1, 0.01, 0.001]$. The optimizer’s history is reset after each EM iteration to remove old gradient information. In all of our Snorkel baselines, we separately tuned the initial learning rate over the same set, and trained the deep neural network for the same number of total epochs that DPL uses to ensure a fair comparison.