A Probabilistic Model for Discriminative and Neuro-Symbolic Semi-Supervised Learning

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Abstract

Much progress has been made in semi-supervised learning (SSL) by combining methods that exploit different aspects of the data distribution, e.g. consistency regularisation relies on properties of $p(x)$, whereas entropy minimisation pertains to the label distribution $p(y|x)$. Focusing on the latter, we present a probabilistic model for discriminative SSL, that mirrors its classical generative counterpart. Under the assumption $y|x$ is deterministic, the prior over latent variables becomes discrete. We show that several well-known SSL methods can be interpreted as approximating this prior, and can be improved upon. We extend the discriminative model to neuro-symbolic SSL, where label features satisfy logical rules, by showing such rules relate directly to the above prior, thus justifying a family of methods that link statistical learning and logical reasoning, and unifying them with regular SSL.

1 Introduction

Semi-supervised learning (SSL) learns to predict a label $y$ for each data point $x$ from labelled data $\{(x^i, y^i)\}$ and a set of, often more abundant, unlabelled data $\{x^j\}$. For unlabelled data to help predict labels, the distribution $p(x)$ must contain information relevant to that prediction [4, 35]. State-of-the-art SSL algorithms [e.g. 3, 2] combine several underlying methods, some of which directly leverage properties of $p(x)$, such as data augmentation and consistency regularisation [25, 13, 28, 19]. Others utilise properties of the conditional label distributions $p(y|x)$ by adding a bespoke function of the model’s predictions for unlabelled data to a standard supervised loss function, e.g. entropy minimisation [11], mutual exclusivity [24, 33] and pseudo-labelling [15]. We refer to such methods as discriminative semi-supervised learning (DSSL) and show that they can be justified and unified under a probabilistic model, comparable to the classical generative model for SSL [4, 35, 30].

In some tasks, vector labels indicate the presence/absence of a set of attributes that obey logical rules, e.g. legs $\Rightarrow \neg$ fins. A neural network-based SSL algorithm that takes such rules into account combines statistical machine learning with logical reasoning, a paradigm known as neuro-symbolic learning (NSL). Several methods for neuro-symbolic SSL [e.g. 34, 31] add a term based on logical constraints to a supervised loss function. We show that such methods, although often disjoint from ‘regular’ SSL in the literature, are also theoretically justified under the proposed probabilistic model for discriminative SSL. Thus, within the scope considered, the DSSL model provides a principled basis for integrating logical reasoning and statistical learning.

The proposed DSSL model is a hierarchical latent variable model in which each data point $x \in \mathcal{X}$ has an associated label distribution $p(y|x)$ with parameter $\theta \in \Theta$. Parameters $\theta$ are treated as latent random variables sampled from a distribution $p(\theta)$. A parametric function $f_\omega : \mathcal{X} \rightarrow \Theta$ (e.g. a neural network) is assumed to learn $\theta$ as a function of $x$, $f_\omega(x) = \hat{\theta} \approx \theta$; e.g. in $K$-class classification, $f_\omega(x)$ maps to a particular multinomial parameter on the simplex $\Delta^K \subset \mathbb{R}^K$. It follows that the empirical

While we focus on classification as a common SSL use-case, the DSSL model generalises to other tasks.
distribution of model outputs \( \theta \) is expected to follow \( p(\theta) \). In particular, the distribution of outputs for unlabelled data should accord with \( p(\theta) \), and \( f_w \) can be updated if not – providing a learning signal from unlabelled data. In general, the form of \( p(\theta) \) may be unknown or aligning the empirical distribution of unlabelled predictions to it may be non-trivial. However, in classification tasks where \( y|x \) is deterministic, i.e. each \( x \in \mathcal{X} \) has a unique label, \( p(\theta) \) simplifies to a discrete distribution and aligning the distribution of unlabelled predictions to it can be achieved by standard gradient-based optimisation methods by approximating the discrete \( p(\theta) \) with a suitable continuous relaxation \( q(\theta) \).

Stepping back, it may seem counter-intuitive to tackle SSL with discriminative methods that rely on \( p(y|x) \), rather than those pertaining to \( p(x) \), when fewer labels are available by its definition. However, the latter methods require additional knowledge of \( p(x) \), e.g. domain-specific invariance, which may not always be available; and, where it is, the two approaches can be successfully combined, as in recent state-of-the-art methods \([3,2]\), making it relevant to understand discriminative approaches.

The key contributions of this work are:

• to propose a probabilistic model for discriminative SSL (DSSL), comparable to the classical generative model, contributing to the theoretical understanding of semi-supervised learning \([13]\);

• to justify several previous SSL methods, e.g. entropy minimisation, as DSSL under the assumption \( y|x \) is deterministic, and to propose a new deterministic prior loss that improves upon them; and

• to show that the DSSL model extends also to a family of (often distinct) neuro-symbolic SSL methods, to rigorously justify and unify them with ‘regular’ SSL \([15]\), contributing to bridging the gap between connectionist and symbolic approaches.

2 Background and related work

Notation: \( X = \{x^i\}_{i=1}^n, Y = \{y^i\}_{i=1}^n \) are labelled data, treated as samples of random variables \( x, y \), with domains \( \mathcal{X}, \mathcal{Y} \), \( X' = \{x'^i\}_{i=1}^m, Y' = \{y'^i\}_{i=1}^m \) are unlabelled data and their unobserved labels. Each \( \theta \) parameterises a distribution \( p(y|x) \) and is treated as a realisation of random variable \( \Theta \). \( \theta_k \) denotes component \( k \) of \( \theta \). (Subscripts are dropped where possible to lighten notation.)

Semi-supervised learning (SSL) is a well-established field, covered by several surveys and taxonomies \([26,35,4,30]\). Methods can be categorised by how they adapt supervised learning algorithms \([30]\), or their assumptions \([4]\), such as that the data of each class form a cluster/manifold, or that different classes are separated by low density regions. It has been suggested that all such assumptions are variations of clustering \([30]\). Although clustering is not well defined \([8]\), from a probabilistic perspective this suggests that SSL methods assume \( p(x) \) to be a mixture of class-conditional distributions that are distinguishable by some property, satisfying the condition that for unlabelled \( x \) to help in learning to predict \( y \) from \( x \), the distribution of \( x \) must contain information relevant to the prediction \([4,35]\). We categorise SSL methods according to the properties of \( p(x) \) they leverage.

A canonical SSL method that relies on explicit assumptions of \( p(x) \) is the classical generative model:

\[
p(X,Y,X') = \int_{\psi,\pi} p(\psi, \pi)p(X|Y, \psi)p(Y|\pi) \sum_{Y'} p(X'|Y', \psi)p(Y'|\pi)
\]  

Parameters \( \psi, \pi \) of \( p(x|y) \) and \( p(y) \) are learned from labelled and unlabelled data (e.g. via the EM algorithm), and predictions \( p(y|x) = p(x|y)p(y)/p(x) \) follow by Bayes’ rule. Fig. 1 (left) shows the corresponding graphical model. Whilst generative SSL has an appealing probabilistic rationale, it is rarely used in practice, similarly to its supervised counterpart, because \( p(x|y) \) is often complex yet must be accurately modelled \([11,35,14]\). That said, domain-specific invariances may be known without knowing \( p(x|y) \) in full, e.g. translation-invariance in images, allowing data augmentation and consistency regularisation methods \([25,13,28,19]\) that adapt real \( x \) samples into artificial samples.
The SSL methods on which we focus take a particular discriminative approach: a parametric function $f_\omega: \mathcal{X} \rightarrow \Theta$ (typically a neural network) predicts $\theta$ as a function of $x$. $f_\omega(x) \approx \theta \approx \theta$; and a function of unlabelled predictions $\ell^n = \sum_{i \in \mathcal{I}} l(\theta^i)$ is added to a negative log-likelihood loss function. Such methods are often applied to $K$-class classification where $\theta$ is a vector on the simplex $\Delta^K \subset \mathbb{R}^K$ and $p(y|x)$ is multinomial. Entropy minimisation \cite{11} assumes classes are “well separated” and uses entropy of $p(y|x)$ as a proxy for class overlap. Mutual exclusivity \cite{24, 33} assumes no class overlap whereby predictions form one-hot vectors that, seen as logical variables $z$, satisfy the formula $\bigvee_k (z_k \land \neg \bigwedge_{j \neq k} z^j)$, from which $\ell^n$ is derived. Pseudo-labelling \cite{15} treats currently predicted class labels $k^* = \arg \max_k \theta_k$ for unlabelled data as though true labels. Table \ref{tab:loss} (col. 1) shows the loss component $l(\theta)$ each method applies to unsupervised data. Although intuitive, these methods lack theoretical justification comparable to generative SSL (Eq. \ref{eq:gen_ssl}). In this respect, \cite{14} notes that summing $\Delta K$ is of no use: 

$$p(Y|X, \phi) = \int_\Theta p(\theta) p(Y|X, \phi) \sum_{Y'} p(Y'|X', \phi) = \int_\phi p(\theta) p(Y|X, \phi). \quad (2)$$

Indeed, parameters $\phi$ of $p(Y|X, \phi)$ are provably independent of $X'$ \cite{26}. To break the independence, previous works introduce additional variables \cite{14}, or assume that parameters of $p(y|x)$ are dependent on those of $p(x)$ \cite{26}. We extend this line of research to propose a hierarchical latent variable model for discriminative SSL (DSSL), analogous to that for generative SSL (Eq. \ref{eq:gen_ssl}).

**Neuro-symbolic learning (NSL)** combines statistical machine learning, often using neural networks, and logical reasoning [e.g. see \cite{9}]. Approaches often introduce statistical methods into a logical framework [e.g. \cite{22, 16}]; or inject logical rules into statistical learning methods \cite{23, 7, 17, 31}. Figure \ref{fig:nsl} shows a conceptual framework for NSL \cite{29, 9} that places statistical methods within a low-level perceptual component that processes raw data (e.g. performing pattern recognition), which feeds a reasoning module, e.g. performing logical inference. This template can be seen in many NSL works [e.g. \cite{32, 5}]: those closest to our own propose a 2-layer graphical model comprising a neural network and a “semantic layer” \cite{17} (Fig. 1), and a graphical model for SSL comprising a neural network component and a logic-based prior \cite{31} (Fig. 1). By comparison, where \cite{17} introduces logical constraints as a design choice (their Eq. 2), in our DSSL model, logical rules innately define the support of a probability distribution. In \cite{31}, knowledge base rules directly influence labels of only unlabelled data, whereas under the DSSL model such rules affect parameters of all label distributions $p(y|x, \theta)$. At an intuitive level, where \cite{31} treats probabilities as “continuous relaxations” of logical rules, the DSSL model treats logical rules akin to limiting (discrete) cases of continuous probability distributions. We note that many other works consider comparable latent variable models (e.g. treating logical rules as constraints in a quasi-variational Bayesian approach \cite{18}) or structured label spaces [e.g. see \cite{55}], but we restrict attention to neuro-symbolic approaches for SSL.

### 3 Probabilistic model for discriminative semi-supervised learning

Here we present the probabilistic model for discriminative semi-supervised learning methods (DSSL) in which a parametric function $f_\omega$ (with weights $\omega$) learns to map each data point $x \in \mathcal{X}$ to parameter $\theta \in \Theta$ of the respective distribution $p(y|x)$. Our running example is $K$-class classification, where $\theta$ is
We briefly highlight the symmetry between the two probabilistic models for SSL, slightly restating $y$ where $(\cdot)$ shows the corresponding graphical model with brevity and letting $\theta = \{\theta^X, \theta^\psi\}$, $\theta^X = \{\theta^i\}_{i=1}^n$, $\theta^\psi = \{\theta^j\}_{j=1}^m$, the conditional likelihood is given by:

$$p(Y|X,X') = \int_\theta \prod_i p(y^i|x^i,\theta^i) p(\theta^i) \prod_j p(\theta^j) \quad \approx \prod_j p(y^j|x^j,\theta^{i*}) p(\theta^{i*}) \int_\theta \prod_i p(\theta^i) \quad (3)$$

The approximation (1) assumes that parameters of $\text{labelled}$ data $\theta^i$ are learned with sufficient certainty that posterior distributions $p(\theta^i|x^i, y^i) \propto p(y^i|x^i, \theta^i) p(\theta^i)$ are well approximated by delta functions $\delta_{y^i-\theta^i}$ (discussed further in [4]). Rather than considering all possible parameter values, $\theta$ is substituted by $\hat{\theta} = f_\omega(x)$ and a maximum a posteriori approach taken by maximising (w.r.t. $\omega$):

$$l_{\text{DSSL}}(\omega) = \sum_{\omega} \sum_{k} y^i_k \log \theta^i_k + \sum_{i} \log p(\hat{\theta}^i|\alpha) + \sum_{j} \log p(\hat{\theta}^j|\alpha) \quad (4)$$

Here, the first term encourages $\hat{\theta}^i \approx \theta^{i*}$, so that the model learns the parameter for labelled data, as in supervised learning. In principle, the middle term allows parameters $\alpha$ of $p(\theta)$ to be learned from the labelled data. In the last term, parameter predictions for unlabelled data $\theta^j$, as influenced by the predictions of nearby labelled data (due to continuity of $f_\omega$), are encouraged towards a local mode of $p(\theta)$. In general, the analytic form of $p(\theta)$ required in Eq. 4 may not be known, or encouraging predictions to the modes of $p(\theta)$ could be undesirable, however, in the cases we are interested in where $y|x$ is deterministic, we see in [4] that both concerns are satisfied.

We briefly highlight the symmetry between the two probabilistic models for SSL, slightly restating Eq. 1 for clearer comparison (e.g. omitting $\pi$ for brevity) together with the joint equivalent of Eq. 3:

$$p(X,Y,X') = \int_\psi \prod_i p(\psi)p(X|\psi,Y)p(Y) \sum_{X'} \int p(X'|Y',\psi)p(Y') \quad (G)$$

$$= \int_\theta p(\theta)p(Y|X,\theta^X)p(X) \sum_{X'} \int p(X'|Y',\theta^X)p(Y') \quad (D)$$

Under the generative model, a conditional distribution parameter $\psi$ is sampled and assigned to (or indexed by) each value in the domain $Y$ (i.e. each label); as $y$ are then sampled, their corresponding parameter $\psi$ (a latent variable) defines a distribution from which $x$ is sampled. Parameters $\psi$ are learned for each class $k$, equivalent to an implicit mapping $f(k) = \psi_k$. The discriminative model follows analogously: parameters $\theta$ are notionally sampled and assigned to every value in $X'$; as $x$ are sampled, their corresponding parameter $\theta$ defines the distribution from which a label $y$ is drawn. Here, the mapping $f(x) = \theta$ is learned explicitly. Both models can be seen to leverage a distribution across data samples to enable SSL: $p(x)$ in the generative case, $p(\theta)$ in the discriminative case.

To put this another way, note that applying $f_\omega$ to $x \sim p(x)$ induces an empirical distribution over predictions $p_\omega(\hat{\theta})$, dependent on $\omega$. The last term effectively minimises the KL divergence $D_{KL}[p_\omega(\hat{\theta})||p(\hat{\theta}|\alpha)] \approx \int_\theta p_\omega(\hat{\theta}) \log \frac{p_\omega(\hat{\theta})}{p(\hat{\theta}|\alpha)}$, but ignoring the entropy of $p_\omega(\hat{\theta})$ that would prevent $p_\omega(\hat{\theta})$ ‘collapsing’ to modes of $p(\theta)$.
We now consider implementations of the DSSL model. Our main interest is in classification where \( p \) with class probabilities \( q \), practice, \( q \) to a supervised loss function, as seen in entropy minimisation [11], mutual exclusivity [24, 33] and the final term gives a probabilistic rationale for adding a function \( \ell \) is common (e.g. 

larising a supervised learning model, but note it is a function of model 

means of updating them (via \( \omega \)) is suitable not precisely one-hot and provides no gradient to update \( \omega \) p to substitute into Eq. 4. However, this discrete 

p since each parameter \( \theta \) is fully determined by a single observation 

assumption. We distinguish between whether labels represent distinct classes or sets of binary features. 

For semi-supervised, this means that assumption (†) in Eq. 5 is immediately more plausible since each parameter \( \theta \) is fully determined by a single observation \((x, y)\), rather than requiring multiple samples and being subject to sampling error. Also, the analytic form of \( p(\theta) \) is available to substitute into Eq. 4. However, this discrete \( p(\theta) \) has zero support for any prediction \( \theta \) that is not precisely one-hot and provides no gradient to update \( \omega \). As such, \( p(\theta) \) can be substituted by a suitable relaxation \( q(\theta) \). Lastly, since parameters for labelled data are accurately learned from the data, applying the prior is largely redundant and the middle term in Eq. 4 can be dropped, to give:

\[
\ell_{\text{det-DSSL}}(\omega) = \sum_k \sum_i y_i^k \log \hat{\theta}_i^k + \sum_j \log q(\hat{\theta}^j),
\]

a general loss function for deterministic discriminative SSL. The last term may be viewed as regularising a supervised learning model, but note it is a function of model outputs \( \theta \) not weights \( \omega \), as is common (e.g. \( \xi_1, \xi_2 \)). \( q(\theta) \) can also be considered a critic of unlabelled predictions, providing a means of updating them (via \( \omega \)) to be more plausible. Comparing Eq. 5 to existing methods (2), the final term gives a probabilistic rationale for adding a function \( \ell^u \) of the unlabelled predictions to a supervised loss function, as seen in entropy minimisation [11], mutual exclusivity [24, 33] and pseudo-labelling [15]. Accordingly, those methods are probabilistically justified and unified as instances of Eq. 5 (for choices of \( q(\theta) \) (up to proportionality) shown in Table 1 and plotted in Fig. 3). (In practice, \( q(\theta) \) need not be normalised since optimisation depends on relative gradients of \( q(\theta) \).)
Deterministic prior (DP): We propose a new relaxation to $p(\theta)$ by replacing each $\delta_{\theta-e_k}$ term by $\theta^T_k$, a ‘spike’ at $e_k$ parameterised by $T$, similar to temperature [10] (see Table 1, Fig. 3). Note, $q_{\text{DP}}(\theta) \rightarrow p(\theta)$ as $T \rightarrow \infty$. Our aim is not to find an optimal $q(\theta)$, but to test the hypothesis that previous $q(\theta)$ are not justified beyond approximating $p(\theta)$, by better approximating $p(\theta)$. We compare performance of each $q(\theta)$ using architecture (Wide ResNet “WRN-28-2” [34]), image datasets (MNIST, SVHN, CIFAR-10) and methodology of previous SSL studies [20, 3] (see Appendix B for implementation details). Results in Table 2 show that $DP$ loss matches or slightly outperforms prior DSSL methods across all datasets considered. (We note that the performance of $DP$ loss is broadly insensitive to $T$ across a range of values. $T=10$ is used for all datasets.)

To analyse whether the choice of $q(\theta)$ has the effect intuited above, Fig. 5 shows histograms of the prediction $\hat{\theta}^k$ assigned to each true class $k^*$, which should always be 1, for all SVHN data, split by training (labelled and unlabelled) and test set. As expected, all models do well on the labelled training data (top row) and the distribution of learned parameters suggests that $y|x$ is indeed deterministic. All models make errors on unlabelled and test data (low predictions), but the DSSL methods encourage predictions towards simplex vertices (0 or 1), making fewer in between (see overlay, bottom right). Fewer intermediate predictions can be seen to correlate with performance (Table 2) and the extent to which unlabelled predictions are encouraged to align with the true prediction (i.e. the nearer to a simplex vertex) the more it influences the update of $f$. (The higher $q(\theta)$). Conversely, ‘uncertain’ proto-predictions far from simplex vertices should have little effect.

Choosing $q(\theta)$: The DSSL model does not justify one choice of $q(\theta)$ over another, beyond a need to approximate $p(\theta)$. However, some prior methods may appear to have other theoretical justification, e.g. minimising entropy [11] or satisfying various axioms [33]. Fig. 3 shows that the $q(\theta)$ of prior methods are locally maximal at simplex vertices, but do not otherwise closely approximate $p(\theta)$.

Intuitively, the general DSSL approach can be seen to leverage what methods are locally maximal at simplex vertices, but do not otherwise closely approximate $p(\theta)$. For example, minimum entropy [11] or satisfying various axioms [33]. Fig. 3 shows that the $q(\theta)$ of prior methods are locally maximal at simplex vertices, but do not otherwise closely approximate $p(\theta)$.

### Table 2: Test set accuracy (mean ± std err over 10 runs) for DSSL methods. (#) = num labels (n).

| Model                     | MNIST (100) | SVHN (1000) | CIFAR-10 (4000) |
|---------------------------|-------------|-------------|-----------------|
| Fully supervised (all data: $X \cup X'$) | 99.50 ±0.01  | 97.02 ±0.12  | 94.63 ±0.06     |
| Deterministic Prior, DP ($T=10$) | **97.07** ±0.19  | **91.32** ±0.12  | **84.86** ±0.14  |
| Minimum entropy [11]      | 97.06 ±0.19  | 90.63 ±0.15  | 84.57 ±0.08     |
| Mutual Exclusivity [24, 33]| 96.58 ±0.18  | 90.36 ±0.21  | 84.37 ±0.09     |

### Notes:
- **Deterministic classification (binary features):** In some classification tasks, label vectors $y \in \{0,1\}^K$ represent $K$ binary attributes of the data, e.g. the presence/absence of features in an image, the configuration of a chessboard or the semantic relations that hold between two knowledge graph entities. As previously, $p(y|x)$ may be deterministic (as those examples demonstrate): whenever a

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Figure 5: Histograms of predictions $\hat{\theta}^k$ assigned to the true class $k^*$ ($\hat{\theta}^k = 1 \Rightarrow$ correct) for all (SVHN) data, split by training (labelled $X$, unlabelled $X'$) and test ($X'$) set. y-axes on log scale.
particular \( x \) is observed, the same set of attributes occur without stochasticity, and each \( x \) has exactly one label \( y \). Considering a multinomial distribution over all \( 2^K \) possible attribute combinations is typically prohibitive and a classifier learns to predict a vector \( \theta \in [0, 1]^K \), where each \( \theta_k \) parameterises a conditional feature distribution \( p(y_k | x) \). Analogously to the case of distinct classes, the deterministic assumption restricts each component \( \theta_k \) to \( \{0, 1\} \) and so \( \theta \) to \( \{0, 1\}^K \), the vertices of the unit hypercube (equivalent to one-hot vectors). Parameters can be seen to uniquely define labels, and vice versa, under a one-to-one (identity) correspondence between labels and \( \theta \) in the support of \( p(\theta) \).

Accordingly, \( p(\theta | y) = \delta_{\theta = y} \); and \( p(\theta) \), as required for DSSL (Eq. 4), is again a discrete distribution \( p(\theta) = \sum_y \pi_y \delta_{\theta = y} \) with marginal label probabilities \( \pi_y = p(y) \). As before, a suitable relaxation \( q(\theta) \), e.g. DP loss, enables gradient-based SSL by optimising Eq. 5.

[Note, the identity mapping between each label \( y \) and its corresponding \( \theta \) suggests that \( p(\theta) \) could be learned from unpaired labels \( y \sim p(y) \), an alternative SSL scenario that we leave to future work.]

5 Neuro-symbolic semi-supervised learning

When classifying multiple binary features (see §4), certain feature combinations may be impossible, e.g. an animal having legs and fins, three kings on a chessboard, or knowledge graph entities being related by capital_of but not city_in. Here, valid attribute combinations form a subset \( \mathcal{V} \) of all feasible labels \( \mathcal{F} \subseteq \{0, 1\}^K \), defined by constraints such as attributes being mutually exclusive, the rules of the game, or relationships between relations. Such constraints can often be expressed as a set of logical rules and incorporating them in statistical learning is appealing: they often apply globally, in contrast to the uncertain generalisation in statistical models; and they may allow a large set \( \mathcal{V} \) to be defined succinctly. Fig. 6 (left, centre) gives a simple illustration of \( \mathcal{V} \) and \( \mathcal{F} \) for a set of logical rules \( \mathcal{R} \).

Where \( p(y | x) \) is deterministic, the one-to-one correspondence between labels \( y \in \{0, 1\}^K \) and parameters in the support of \( p(\theta) \) (see §4), means that valid labels correspond to valid parameters (we thus let \( \mathcal{V} / \mathcal{F} \) denote valid/feasible labels or parameters). It follows that \( p(\theta) \) is given by:

\[
p(\theta) = \sum_{y \in \mathcal{V}} p(y) p(\theta | y) = \sum_{y \in \mathcal{V}} \pi_y \delta_{\theta = y},
\]

where \( \pi_y = p(y) \) and \( \theta \in \Theta = [0, 1]^K \). Eq. 6 shows that if labels are subject to logical rules, those rules define the support of \( p(\theta) \), the distribution required for DSSL (Eq. 4). (Note: Eq. 6 also holds for any ‘larger’ set \( \mathcal{V} \), where \( \mathcal{V} \subseteq \mathcal{V}' \subseteq \mathcal{F} \).) Thus, logical rules can be integrated into semi-supervised learning if they can be mapped into the mathematical form of Eq. 6. By dropping \( \pi_y \) terms in Eq. 6, the support of \( p(\theta) \) can be defined explicitly as \( s: \Theta \rightarrow \{0, \infty\} \), which factorises:

\[
s(\theta) = \sum_{y \in \mathcal{V}} \delta_{\theta = y} = \sum_{y \in \mathcal{V}} \prod_{y_k = 1} \delta_{\theta_k = 1} \prod_{y_k = 0} \delta_{\theta_k = 0}.
\]

Each term in the summation of Eq. 7 effectively tests whether the argument \( \theta \) matches a valid label \( y \in \mathcal{V} \): \( s(\theta) = \infty \) if \( \theta \in \mathcal{V} \), \( s(\theta) = 0 \) otherwise. When restricted to feasible \( \theta \in \mathcal{F} \) (i.e. binary vectors), Eq. 7 mirrors a logical formula in propositional logic over logical variables \( z_k \in \{True, False\} \):

\[
t(z) = \bigvee_{y \in \mathcal{V}} \bigwedge_{k: y_k = 1} z_k \bigwedge_{k: y_k = 0} \neg z_k,
\]

Here, \( t(z) \) evaluates to True if and only if \( z \) corresponds to a valid label \( y \in \mathcal{V} \), in the sense that \( z_k = True \iff y_k = 1 \), for all \( k \); hence \( t \) and \( s \) perform analogous tests of validity.

The relationship between Eqs. 7 and 8 reflects a correspondence between logical and algebraic formulae familiar in fuzzy logic and neuro-symbolic learning [e.g. 12731]. Under specific mappings of variables and operators, satisfiability (SAT) problems, defined by a set of logical rules over logical variables (e.g. Eq. 9), can be transformed into algebraic functions of binary variables that evaluate to a particular value (often 1) if the constraint is satisfied and 0 otherwise.

Rather than mapping truth values of logical variables to values of binary variables, the transformation of Eq. 8 to Eq. 7 requires an analogous mapping from \( z_k \) to \( \delta \)-functions over \( \theta_k \in [0, 1] \), indicating whether \( \theta_k \) is 0 or 1. Specifically, \( z_k \rightarrow \delta_{\theta_k = 1}, \neg z_k \rightarrow \delta_{\theta_k = 0} \) (\( z_k \) is not defined for \( \theta_k \notin \{0, 1\} \)). An evaluation to True (resp. False) in the logic domain corresponds to \( \infty \) (resp. 0) in the numeric. Under this mapping, logical operators \( \wedge \) (AND) and \( \vee \) (OR) are equivalent to ‘\&’ and ‘\+’, respectively, e.g. \( z_k \wedge z_l \) evaluates to True iff \( \delta_{\theta_k = 1} \times \delta_{\theta_l = 1} = \infty \). This gives a well-defined mapping between Eqs. 7 and 8: any set of logical rules in the form of Eq. 8 can be transformed to a sum of delta functions, each corresponding to a valid variable combination (Eq. 7); similarly, any function in the form of Eq. 4 possibly learned from the data, can be converted to a set of logical rules (Fig. 6 left centre).
Where labels represent the presence/absence of multiple attributes, logical relationships between attributes may rule out certain combinations. We show that a function representing such rules, familiar in fuzzy logic and NSL, corresponds to the support of $p(\theta)$. Thus a family of neuro-symbolic SSL methods that employ functions representing logical rules are justified under the DSSL model and unified with ‘regular’ SSL. This establishes a principled way to combine statistical machine learning and logical reasoning for semi-supervised learning, fitting a conceptual framework for neuro-symbolic computation \cite{29, 9}. Possible extensions of this work may combine logical rules with fully supervised learning (Eq. 3), or consider SSL with extra labels $y$ rather than $x$ \cite{34}.

6 Conclusion

We present a probabilistic model for discriminative semi-supervised learning, analogous to the classical model for generative semi-supervised learning. Central to the DSSL model are parameters $\theta$ of distributions $p(y|x)$, e.g. as predicted by a typical classifier. Treating those parameters as latent random variables, their distribution $p(\theta)$ serves as a prior over model outputs for unlabelled data. Where $y|x$ is deterministic, the analytical form of $p(\theta)$ is known and discrete, enabling the DSSL model to be used. We show that the SSL methods entropy minimisation, mutual exclusivity and pseudo-labelling are explained by the DSSL model for different choices of $q(\theta)$, a relaxation of $p(\theta)$; and that a simple alternative, deterministic prior, better reflecting $p(\theta)$ outperforms them.

Where labels represent the presence/absence of multiple attributes, logical relationships between those attributes may rule out certain combinations. We show that a function representing such rules, familiar in fuzzy logic and NSL, corresponds to the support of $p(\theta)$. Thus a family of neuro-symbolic SSL methods that employ functions representing logical rules are justified under the DSSL model and unified with ‘regular’ SSL. This establishes a principled way to combine statistical machine learning and logical reasoning for semi-supervised learning, fitting a conceptual framework for neuro-symbolic computation \cite{29, 9}. Possible extensions of this work may combine logical rules with fully supervised learning (Eq. 3), or consider SSL with extra labels $y$ rather than $x$ \cite{34}.
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A Derivation of \( p(\theta) \) for Classification of Gaussians

For a general mixture distribution:

\[
\theta_k = p(y=k|x) = \sigma \left( \log \frac{p(x|y=k)p_k}{\sum_{k' \neq k} p(x|y=k')p_{k'}} \right);
\]

\[
\frac{d\theta_k}{dx} = \theta_k (1-\theta_k) \left( \frac{d}{dx} \log p(x|y=k) - \sum_{k' \neq k} \frac{p(x|y=k')\pi_{k'}}{\sum_{k' \neq k} p(x|y=k')\pi_{k'}} \frac{d}{dx} \log p(x|y=k') \right)
\]

For a mixture of 2 equivariate Gaussians, these become:

\[
\theta_1 = \sigma \left( \log \frac{\pi_1}{\pi_0} + \frac{\mu_1-\mu_0}{\sigma^2} x - \frac{1}{2} \left( \frac{\sigma^2}{\sigma^2} - \frac{\mu_0^2}{\sigma^2} \right) \right), \quad \frac{d\theta_k}{dx} = \theta_k (1-\theta_k) \left( \frac{\sigma^2}{\sigma^2} - \frac{\mu_0^2}{\sigma^2} \right).
\]

Rearranging the former gives \( x \) in terms of \( \theta \):

\[
x = \frac{\sigma^2}{\mu_1-\mu_0} \left( \log \frac{\theta_1}{1-\theta_1} - \log \frac{\pi_1}{\pi_0} + \frac{1}{2} \left( \frac{\mu_0^2}{\sigma^2} - \frac{\mu_1^2}{\sigma^2} \right) \right).
\]

Substituting into \( p(\theta) = |\frac{dx}{d\theta}| p(x) \) gives:

\[
p(\theta) = \sqrt{\frac{\sigma^2}{2\pi}} \frac{1}{|\mu_1-\mu_0|\theta_1} \sum_{k=0}^{1} \pi_k \exp \{ a(\log \frac{\theta_k}{\theta_1})^2 + b_k (\log \frac{\theta_k}{\theta_1}) + c_k \}
\]

where:

\[
a = \frac{\sigma^2}{2 \sigma^2 (\mu_1-\mu_0)^2}, \quad b_k = \frac{\mu_k}{\mu_1-\mu_0} + \frac{\sigma^2}{(\mu_1-\mu_0)^2} \left( \frac{\mu_1^2-\mu_0^2}{\sigma^2} - \log \frac{\pi_1}{\pi_0} \right), \quad c_k = -\frac{(\mu_1-\mu_0)^2 b_k^2}{2 \sigma^2}.
\]

B Experiment Implementation Details

Our experiments follow the methodology, including hyperparameter choice, of [20, 3] and use code provided by [34]. We run all models over 10 random seeds and report mean and standard error.

C Omission of mixture probabilities in the relaxation of \( p(\theta) \)

In [5] we consider relaxations of \( p(\theta) \) that restrict attention to the support of \( p(\theta) \), i.e. the discrete locations \( \Theta \) where \( p(\theta) \) may be non-zero, and ignore the relative probabilities at each support, given by class probabilities \( p(y) = \pi_y \). We note that previous discriminative SSL methods ignore class weights also (see Table 1). Practical reasons for this are (i) that \( \pi_y \) may be unknown, and (ii) that unless attributes are independent, i.e. \( p(y) = \prod_k p(y_k) \), class probabilities cannot be factorised equivalently to the support, as in Eq. [7]. This is not a theoretical justification for omitting \( \pi_y \) terms, hence we consider the validity and possible (non-rigorous) rationale for doing so.

Validity: Considering only the support of \( p(\theta) \) is equivalent to assuming a uniform label distribution over that support. Where classes are well-balanced, omitting \( \pi_y \) is clearly justified, elsewhere to do so might be seen as using a “partially-uninformative” prior.

Rationale: If predictions for unlabelled data were chosen simply to maximise \( p(\theta) \), the most commonly occurring label (i.e. the global mode of \( p(\theta) \)) would be assigned to all unlabelled data. However, \( p(\theta) \) acts on predictions \( \theta \) given by a model that learns to take class weighting into account. Thus, where \( f(\omega) \) predicts a less frequent class for a particular unlabelled data point, intuitively, that signal should be taken into account and not blindly over-ridden by a class weighting in \( p(\theta) \). In short, omitting class weights may be appropriate under DSSL since \( p(\theta) \) acts as a prior over unlabelled predictions that, to some extent, already take class weights into account. We hope to provide a more rigorous argument in future work.

[https://github.com/szagoruyko/wide-residual-networks/tree/master/pytorch](https://github.com/szagoruyko/wide-residual-networks/tree/master/pytorch)