Robust Semi-Supervised Learning when Labels are Missing at Random

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Abstract

Semi-supervised learning methods are motivated by the relative paucity of labeled data and aim to utilize large sources of unlabeled data to improve predictive tasks. It has been noted, however, such improvements are not guaranteed in general in some cases the unlabeled data impairs the performance. A fundamental source of error comes from restrictive assumptions about the unlabeled features. In this paper, we develop a semi-supervised learning approach that relaxes such assumptions and is robust with respect to labels missing at random. The approach ensures that uncertainty about the classes is propagated to the unlabeled features in a robust manner. It is applicable using any generative model with associated learning algorithm. We illustrate the approach using both standard synthetic data examples and the MNIST data with unlabeled adversarial examples.

1 Introduction

In statistical machine learning, the size and quality of training data sets has a notable impact on the performance. The labeled data is often considered to be expensive to obtain, and therefore typically limited size. By contrast, unlabeled data are often available or can be collected with reasonable costs. Therefore, there is a strong motivation to improve the performance by utilizing both labeled or unlabeled data, which is known as semi-supervised learning.

Semi-supervised learning is readily achieved using generative models, cf. Zhu & Goldberg (2009); Kingma et al. (2014); Gordon & Hernandez-Lobato (2017). However, several studies have reported that improved performance of learning methods is not guaranteed by incorporating the unlabeled data (cf. (Cozman et al., 2003; Krijthe & Loog, 2016; Oliver et al., 2018)), especially for those unlabeled data with features which are rarely observed in the labeled data.

Let the pair \( (x, y) \) denote features and an associated class. For unlabeled data, \( y \) is missing and we only observe \( x \). The appropriate utilization of unlabeled data depends critically on assumptions made about the data-generating distributions underlying labeled and unlabeled pairs, respectively (see Chawla et al. (2005)).

- Missing completely at random (MCAR): The labeled and unlabeled data-generating processes match exactly, i.e.,

\[
p(x, y \mid \text{unlabeled}) \equiv p(x, y \mid \text{labeled})
\]

MCAR is a common assumption but also highly restrictive and requires careful considerations when collecting unlabeled data. In a medical diagnosis scenario, this means that the features from an unscreened population must match the population of screened patients. When this assumption fails, the performance of a semi-supervised learning method can degrade drastically. For an illustration of this limitation, consider Figure 1a.

- Missing at random (MAR): The feature distributions may not match each other, i.e.,

\[
p(x \mid \text{unlabeled}) \neq p(x \mid \text{labeled}),
\]

\[
p(y \mid x, \text{unlabeled}) \equiv p(y \mid x, \text{labeled})
\]

The features by which it is possible to discriminate between classes in the labeled data are the same as those for the unlabeled data, which therefore can potentially be used in semi-supervised learning. In the medical diagnosis case this means that unscreened population data can be used in conjunction with screened patient data.
Figure 1: Example of semi-supervised learning problem with labels missing at random (MAR), cf. Example 3.7 in Zhu & Goldberg (2009). The learned probabilities of a semi-supervised learning approach based on the MCAR assumption produces a decision boundary that is orthogonal to the optimal boundary obtained if all data were labeled.

- Missing not at random (MNAR): Neither features nor conditional class distributions may match each other, i.e.,
  \[ p(x, \mid \text{labeled}) \neq p(x \mid \text{unlabeled}), \quad p(y \mid x, \text{labeled}) \neq p(y \mid x, \text{unlabeled}) \]

MNAR is a very conservative assumption since there is no necessary relation between labeled and unlabeled data. The features by which it is possible to discriminate between classes in the labeled data may therefore be different from those for the unlabeled data. This effectively means that the unlabeled data cannot be used to improve a classifier and thus not considered here.

In this paper, we consider the use of generative models for semi-supervised learning under MAR. We develop an approach that utilizes part of the unlabeled data to refine the models obtained from the labeled data, while the remaining unlabeled data is used to robustify the learned class probabilities of rarely observed features.

The method is applicable using any generative model and associated learning algorithm, cf. Hastie et al. (2016); Bishop (2016); Murphy & Bach (2012).

2 Problem Formulation

The observed datasets are denoted
\[ D_{\text{labeled}} = \{(x_i, y_i)\} \quad \text{and} \quad D_{\text{unlabeled}} = \{x_i\}, \]
where the features belong to a \(d\)-dimensional space \(X\) and we consider a set of class labels \(Y\). The samples are obtained as i.i.d. from unknown distributions \(p(x, y | \ell = 1)\) and \(p(x | \ell = 0)\), respectively, where \(\ell\) indicates whether the data is labeled or unlabeled.

Using \(D_{\text{labeled}}\) and \(D_{\text{unlabeled}}\), the goal is to develop a classifier that provides both class predictions \(\hat{y}(x_*)\) for test points \(x_*\), as well as a robust estimate of the class probability. The semi-supervised learning problem is motivated by the fact that typically \(|D_{\text{unlabeled}}| \gg |D_{\text{labeled}}|\).

2.1 Optimal Classifier under MAR

For a test sample \(x_*\), we pursue the optimal classification rule \(\hat{y}(x_*) \in Y\) which minimizes an expected loss function. The most common loss function for classification problems is the zero-one loss function (Hastie et al., 2016),
\[ L(\hat{y}(x_*), y_*) = \begin{cases} 0 & \text{if } \hat{y}(x_*) = y_* \\ 1 & \text{if } \hat{y}(x_*) \neq y_* \end{cases} \]
The expected loss function is
\[ \mathbb{E}[L(y(x_*), y_*)] = \int_X \sum_{y \in Y} L(\hat{y}(x_*), y_* ) p(y \mid x_*) p(x) dx \]
and the optimal classifier is given by
\[ \hat{y}(x_*) = \arg \min_{y \in Y} [1 - p(y \mid x_*)] \]
where \(p(x_* \mid y)\) is the likelihood of observing \(x_*\), and \(p(y)\) is the prior class probabilities. The error probability of the optimal classifier evaluated at the test
sample \( x_s \), is given by
\[
\begin{align*}
\hat{p}_e(x_s) &= p(y \neq \hat{y} \mid x_s) \\
&= 1 - \frac{p(x_s \mid \hat{y})p(\hat{y})}{\sum_y p(x_s \mid y)p(y)}.
\end{align*}
\]
Note that the above distributions marginalize over the labeling process, i.e.,
\[
\begin{align*}
p(y) &= \sum_{\ell=0,1} p(\ell) p(y \mid \ell) \\
p(x \mid y) &= \sum_{\ell=0,1} p(\ell) p(x \mid y, \ell).
\end{align*}
\]

### 2.2 Learning model of \( p(x \mid y) \) and \( p(y) \)

Our aim is to learn models of (9) so as to approximate the optimal classifier (7) as well as providing estimates of the error probability (8) in a robust manner under MAR.

The labeled data \( D_{\text{labeled}} \) provides information about \( p(x \mid y, \ell = 1) \) and \( p(y \mid \ell = 1) \). Together with \( D_{\text{unlabeled}} \), it also provides information about the prior probability of obtaining samples from the labeled population \( p(\ell) \). However, under MAR, the unlabeled data \( D_{\text{unlabeled}} \) does not necessarily provide information about \( p(x \mid y, \ell = 0) \) or \( p(y \mid \ell = 0) \). Learning models of (9) using both \( D_{\text{labeled}} \) and \( D_{\text{unlabeled}} \) is therefore an open question.

In supervised learning, \( p(x \mid y) \) and \( p(y) \) are replaced by \( p(x \mid y, \ell = 1) \) and \( p(y \mid \ell = 1) \) and thus \( D_{\text{unlabeled}} \) is discarded. This approach, however, can lead to serious misclassifications and highly inaccurate error probabilities in regions of the feature space where we observe unlabeled data, see Figure 1a for an illustration. Since only samples from the top-right and bottom-right regions of the feature space are labeled, the labeling process is obviously selective in the feature space.

Most semi-supervised learning algorithms are based on the MCAR assumption in which
\[
\begin{align*}
p(y \mid \ell = 0) &\equiv p(y \mid \ell = 1) \\
p(x \mid y, \ell = 0) &\equiv p(x \mid y, \ell = 1)
\end{align*}
\]

These methods are therefore not robust to MAR data (Chawla et al., 2005). As exemplified by a generative models in Figure 1a, the MCAR assumption may lead to serious performance degradation, cf. the discussion in Zhu & Goldberg (2009).

Considering Figure 1a, we draw two conclusions about \( D_{\text{unlabeled}} \): In the top-left and bottom-right regions of the feature space, the unlabeled data is not informative about the classes. By contrast, the top-right and bottom-left regions represent features that are shared with the labeled population.

Next, we generalize these observation to a robust learning approach.

### 3 Learning Approach under MAR

We now develop a semi-supervised approach for learning (9) that is robust to MAR data. The approach is applicable to any generative model of the data using any supervised method of choice.

Under MAR, feature regions represented in \( D_{\text{unlabeled}} \) that are

- not shared with \( D_{\text{labeled}} \) provide no information about \( y \),
- shared with \( D_{\text{labeled}} \) may provide information about \( y \).

For unlabeled features in the first case, the principle of insufficient reason dictates a robust model of the prior class probability \( p(y \mid \ell = 0) \) as uniform, i.e.,
\[
q(y \mid \ell = 0) \equiv \frac{1}{|\mathcal{Y}|}.
\]

For the same reason, the class will not provide any information about these features so that a robust model of \( p(x \mid y, \ell = 0) \) should be class independent, i.e.,
\[
q(x \mid y, \ell = 0) \equiv q(x \mid \ell = 0)
\]

The unlabeled features in the second case are, however, statistically indistinguishable from the labeled features and thus informative of class under (3). Such unlabeled data used to provide high-quality estimates of \( p(x \mid y, \ell = 1) \) as we show below.

Next, we partition the feature space \( \mathcal{X} \) using the likelihood ratio and use this partitioning to utilize \( D_{\text{unlabeled}} \) in a robust manner.

### 3.1 Regions of Statistically Similar Features

Consider learning initial generative models

- \( q'(x \mid y, \ell = 1) \) and \( q'(y \mid \ell = 1) \) from \( D_{\text{labeled}} \)
- \( q'(x \mid \ell = 0) \) from \( D_{\text{unlabeled}} \),

using any method of choice, see for instance Hastie et al. (2016); Bishop (2016); Murphy & Bach (2012).

From the labeled models we construct the marginal
\[
q'(x \mid \ell = 1) = \sum_{y \in \mathcal{Y}} q'(x \mid y, \ell = 1) q'(y \mid \ell = 1)
\]
with which we partition of the feature space using the likelihood ratio:

$$
\mathcal{X}_\ell = \left\{ \mathbf{x} \in \mathcal{X} : \frac{q'(\mathbf{x} | \ell = 0)}{q'(\mathbf{x} | \ell = 1)} < 1 \right\}.
$$

(12)

Thus all features \(\mathbf{x}\) in \(\mathcal{X}_\ell\) are statistically indistinguishable from features of the labeled population. These \(\mathbf{x}\) contain information about \(y\).

Testing whether a feature \(\mathbf{x} \in \mathcal{D}_{\text{unlabeled}}\) belongs to \(\mathcal{X}_\ell\) corresponds to a likelihood ratio test. When an unlabeled feature belongs to \(\mathcal{X}_\ell\), we assign it a class with the appropriate uncertainty under MAR. That is, if \(\mathbf{x} \in \mathcal{D}_{\text{unlabeled}} \cap \mathcal{X}_\ell\), we assign class \(y\) with probability

$$
q'(\mathbf{x}|\ell = 0) = q'(\mathbf{x}|\ell = 1)
\propto q'(\mathbf{x}|y, \ell = 1)q'(\mathbf{y}|\ell = 1).
$$

All unlabeled features in that are statistically indistinguishable from labeled samples, i.e.,

$$
\mathcal{D}_{\text{unlabeled}} \cap \mathcal{X}_\ell
$$

are assigned a class in a manner that propagates their uncertainty consistent with MAR. The resulting pair \((\mathbf{x}, y)\) is augmented with the labeled data to form a dataset \(\mathcal{D}'\), while the remaining unlabeled samples \(\mathcal{D}_{\text{unlabeled}} \cap \mathcal{X}_\ell\) form the set \(\mathcal{D}''\).

3.2 Robust Classifier

Using \(\mathcal{D}'\) and \(\mathcal{D}''\) together with (10) and (11), we can learn robust models of (9) denoted \(q(y)\) and \(q(\mathbf{x}|y)\). The procedure is summarized in Algorithm 1 and can be implemented using any generative model and learning algorithm of choice. This general applicability is similar to the self-training approach (Zhu & Goldberg (2009)), but unlike that approach it achieves robustness by cautiously assigning labels to parts of the unlabeled data under the MAR assumption while preserving the uncertainty with respect to \(y\).

For a test sample \(\mathbf{x}_*\), the resulting classifier is given by

$$
\hat{y}(\mathbf{x}_*) = \arg\max_{y \in \mathcal{Y}} q(\mathbf{x}_* | y)q(y)
$$

and the error probability is

$$
q_e(\mathbf{x}_*) = \frac{q(\mathbf{x}_* | \hat{y})q(\hat{y})}{\sum_y q(\mathbf{x}_* | y)q(y)}.
$$

Using the learned model, we may also introduce a reject option if \(q_e(\mathbf{x}_*) \geq \alpha\) for additional robustness, see Bishop (2016). An illustration of the learned model under MAR is shown in Figure 1b, where uncertainty about class \(y\) is preserved in regions where there is only unlabeled data.

Algorithm 1: Robust Semi-Supervised Method

**Input:** \(\mathcal{D}_{\text{labeled}}\) and \(\mathcal{D}_{\text{unlabeled}}\)

1. Learn \(q(\mathbf{x}|y, \ell = 1)\) and \(q(y|\ell = 1)\) using \(\mathcal{D}_{\text{labeled}}\);
2. Learn \(q(\mathbf{x}|\ell = 0)\) using \(\mathcal{D}_{\text{unlabeled}}\);
3. Set \(\mathcal{D}' := \mathcal{D}_{\text{labeled}}\) and \(\mathcal{D}'' := \mathcal{D}_{\text{unlabeled}} \cap \mathcal{X}^c\);
4. For \(\mathbf{x} \in \mathcal{D}_{\text{unlabeled}} \cap \mathcal{X}_\ell\) do
   1. Draw \(y \sim q'(\mathbf{x}|\ell = 0)\);
   2. \(\mathcal{D}' := \mathcal{D}' \cup \{(\mathbf{x}, y)\}\);
5. End
6. Learn \(q(\mathbf{x}|y, \ell = 1)\) and \(q(y|\ell = 1)\) using \(\mathcal{D}'\);
7. Learn \(q(\mathbf{x}|\ell = 0)\) using \(\mathcal{D}''\);
8. Let \(w = |\mathcal{D}'| / (|\mathcal{D}'| + |\mathcal{D}''|)\);
9. Output: \(q(\mathbf{x}|y) = wq(\mathbf{x}|y, \ell = 1) + (1 - w)q(\mathbf{x}|\ell = 0)\)

### 4 Experimental Results

4.1 Two-moons dataset

Two illustrate our approach using more complex generative models we consider the popular two-moons type dataset, see Gordon & Hernandez-Lobato (2017); Oliver et al. (2018). Here we use a Gaussian mixture model that is learned using variational approximation. Each class conditional distribution is estimated using 8 components with full covariance matrices and a Dirichlet process prior with weight concentration prior set to 1e-2. The mean precision prior was set to 1 and the covariance prior to the identity matrix. In The self-training method, only one label was added at each iteration.

We contrast the case when MCAR assumption holds and when it fails in Figures 2a and 2b, respectively. If we compare the self-training method in both cases, we clearly see that the resulting model \(q(y|x)\) is very accurate under MCAR in Fig. 3a but it is grossly inaccurate for about half of the data region under MAR in Fig. 3b. By contrast, our proposed method is conservative when MAR data is given in Fig. 4a, leaving \(q(y|x)\) near 0.50 for large portions of the unlabeled data. However, under MAR this corresponds to robustness, cf. Fig. 4b and 2b.

4.2 MNIST dataset with adversarial features

To illustrate the robustness our approach in a more realistic scenario, we consider training a classifier for hand-written digits using MNIST with unlabeled data. For each class, we introduce a certain proportion of adversarial features \(\mathbf{x}_*\), see Fig. 5. Since some hand-written digits are invariant to the rotation,
Figure 2: Dataset used in the two-moons example. Each class contains 8 labeled points and a total of 500 labeled and unlabeled points is used.

Figure 3: Class probability for all data points together with decision boundary for the self-train algorithm.

ideally these features $x_\star$, such as those representing ‘0’, should be correctly classified while others should, representing, say, ‘4’, should have a low probability $q(y \mid x_\star)$ and thus rejected.

Here we use the generative model considered in Bishop (2016). Each conditional distribution $q(x \mid y), y \in \mathcal{Y}$, is approximated with a mixture of Bernoulli models with 784 dimensions and 3 components. The parameters in the mixture models are optimized with the expectation maximization (EM) algorithm.

We compare the supervised case, which discards the unlabeled data, the self-training method and the proposed approach all using an option to reject test points for which $q_e(x_\star) \geq 0.50$. The results are summarized in Table 1. Neither the supervised or self-trained models reject any adversarial examples and consequently make significant errors for certain classes that are not invariant to flipping (such as class ‘7’). By contrast, the robust approach rejects many more adversarial examples, or erroneously classifies them to a lesser degree, than the standard approaches.

### Table 1: Error + reject rates % on adversarial testing samples

| Class | Supervised | Self-training | Robust  |
|-------|------------|---------------|---------|
| 0     | 62.5       | 45            | 17.5 + 57.5 |
| 1     | 42.5       | 42.5          | 7.5 + 37.5  |
| 2     | 92.5       | 97.5          | 52.5 + 47.5 |
| 3     | 100        | 95.0          | 40.0 + 60.0 |
| 4     | 95.0       | 97.5          | 10.0 + 90.0 |
| 5     | 85.0       | 80.0          | 22.5 + 75.0 |
| 6     | 100        | 100           | 72.5 + 27.5 |
| 7     | 100        | 100           | 32.5 + 67.5 |
| 8     | 90         | 95.0          | 35.0 + 60.0 |
| 9     | 100        | 100           | 35.0 + 65.0 |

5 Conclusion

We have developed a semi-supervised learning approach that is robust to cases in which labels are
missing at random. Unlike methods based on labels missing completely at random, this approach does not make the restrictive assumption that labeled and unlabeled features have matching distributions. The proposed ensures that uncertainty about the classes is propagated to the unlabeled features in a robust manner. Moreover, it is widely applicable using any generative model with an associated learning algorithm. Finally, we demonstrated the robustness of the method in both synthetic datasets and real datasets with adversarial examples.

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