Estimation of Squared-Loss Mutual Information from Positive and Unlabeled Data

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Abstract

Capturing input-output dependency is an important task in statistical data analysis. Mutual information (MI) is a vital tool for this purpose, but it is known to be sensitive to outliers. To cope with this problem, a squared-loss variant of MI (SMI) was proposed, and its supervised estimator has been developed. On the other hand, in real-world classification problems, it is conceivable that only positive and unlabeled (PU) data are available. In this paper, we propose a novel estimator of SMI only from PU data, and prove its optimal convergence to true SMI. Based on the PU-SMI estimator, we further propose a dimension reduction method which can be executed \textit{without} estimating the class-prior probabilities of unlabeled data. Such PU class-prior estimation is often required in PU classification algorithms, but it is unreliable particularly in high-dimensional problems, yielding a biased classifier. Our dimension reduction method significantly boosts the accuracy of PU class-prior estimation, as demonstrated through experiments. We also develop a method of independent testing based on our PU-SMI estimator and experimentally show its superiority.

1 Introduction

Capturing input-output dependency is an important task in statistical data analysis. Mutual information (MI) (Cover and Thomas, 2006) is a vital tool for this purpose. Indeed, based on the information-maximization principle (Linsker, 1988), empirical estimators of MI have been employed for solving various machine learning tasks (Torkkola, 2003; Krause et al., 2010). However, since such MI estimators are sensitive to outliers (Basu et al., 1998), their usefulness is limited in practice.

To cope with this problem, a squared-loss variant of MI called squared-loss MI (SMI) and its empirical estimator have been proposed (Suzuki et al., 2009). Compared with MI, the SMI estimator is robust to noise and outliers, and having superior numerical properties (Kanamori et al., 2012). So far, the SMI estimator has been successfully applied to various machine learning tasks such as independent testing, dimension reduction, object matching, and clustering (Sugiyama, 2013).

On the other hand, in real-world classification problems, it is conceivable that only positive and unlabeled (PU) data are available (Letouzey et al., 2000). Thus, it is
practically desirable to have statistical data analysis tools that can be executed by using
only PU data. For PU data analysis, attention has mostly been paid to classification so
far (Elkan and Noto, 2008; du Plessis et al., 2015), and there are few studies on statistical
dependency analysis. Recently, Sechidis et al. (2014) proposed a PU-based method of
independent testing based on the G-test (Sokal and Rohl, 1981). However, this method
can handle only one-dimensional categorical input variable, and therefore its range of
applications is limited. Furthermore, there seem no dimension reduction method that
can be executed only from PU data, which prohibits the analysis of high-dimensional
data.

In this paper, we propose a novel estimator of SMI only from PU data, and prove
its optimal convergence to true SMI. Based on the PU-SMI estimator, we propose a
dimension reduction method which can be executed without estimating the class-prior
probabilities of unlabeled data. Such PU class-prior estimation is often required in PU
classification algorithms, e.g., in du Plessis et al. (2015), but estimation of the class-prior
only from PU data is still highly challenging particularly in high-dimensional problems
(du Plessis and Sugiyama, 2014; Ramaswamy et al., 2016; Jain et al., 2016; du Plessis
et al., 2017). Through experiments, we demonstrate that our PU dimensionality reduc-
tion method helps improve the accuracy of PU class-prior estimation, leading to better
classification accuracy.

Additionally, we also develop a method of independent testing based on our PU-SMI
estimator and experimentally show its superiority.

2 SMI Estimation from Positive-Negative Data

In this section, we first define MI and SMI, and then review how SMI can be estimated
from positive and negative data.

2.1 MI and SMI

Let $x \in \mathbb{R}^d$ be an input pattern, $y \in \{\pm 1\}$ be a corresponding class label, and $p(x, y)$
be the underlying joint density, where $d$ is a positive integer.

Mutual information (MI) (Cover and Thomas, 2006) is a statistical dependency
measure defined as

$$
MI := \sum_{y=\pm 1} \int p(x, y) \log \left( \frac{p(x, y)}{p(x)p(y)} \right) dx,
$$

where $p(x)$ and $p(y)$ are the marginal densities of $x$ and $y$, respectively.\(^1\) MI can be
regarded as the Kullback-Leibler divergence from $p(x, y)$ to $p(x)p(y)$, and therefore,
MI is non-negative and takes zero if and only if $p(x, y) = p(x)p(y)$, i.e., $x$ and $y$ are
statistically independent. This property allows us to evaluate the dependency between
$x$ and $y$, but MI is known to be sensitive to outliers (Basu et al., 1998).

To cope with this problem, squared-loss MI (SMI) has been proposed (Suzuki et al.,
2009), which is a squared-loss variant of MI defined as

$$
SMI := \sum_{y=\pm 1} \frac{p(y)}{2} \int \left( \frac{p(x, y)}{p(x)p(y)} - 1 \right)^2 p(x) dx.
$$

\(^1\) Although $p(y)$ is a probability mass, we refer to it as a probability density with abuse of terminology
for simplicity.
SMI can be regarded as the *Pearson divergence* (Pearson, 1990) from \( p(x, y) \) to \( p(x)p(y) \). SMI is also non-negative and takes zero if and only if \( x \) and \( y \) are independent. So far, various SMI-based machine learning algorithms have been proposed and demonstrated their effectiveness (Suzuki et al., 2009; Niu et al., 2013; Yamada et al., 2015).

### 2.2 SMI Estimation

Since \( p(x, y) \) is unknown, SMI cannot be directly computed. Here, we suppose that we are given a set of *independent and identically distributed* (i.i.d.) paired samples from the underlying joint density:

\[
\{(x_i, y_i)\}_{i=1}^n \sim p(x, y).
\]

A naive approach to estimate SMI is that densities \( p(x, y), p(x), \) and \( p(y) \) are first estimated from the samples, and then the estimated densities \( \hat{p}(x, y), \hat{p}(x), \) and \( \hat{p}(y) \) are plugged into the definition of SMI. However, such a two-step approach is not reliable since estimation error of densities can be magnified, e.g., when division by estimated densities is performed in \( \frac{\hat{p}(x, y)}{\hat{p}(x)\hat{p}(y)} \).

To cope with this problem, Suzuki et al. (2009) proposed to directly estimate the density-ratio function:

\[
r(x, y) := \frac{p(x, y)}{p(x)p(y)}.
\]

More specifically, let \( g(x, y) \) be a model of the density-ratio. The model is learned so that it minimizes the squared error defined as

\[
J(g) = \frac{1}{2} \sum_{y \in Y} \int (g(x, y) - r(x, y))^2 p(x)p(y)dx - C
\]

where we used \( r(x, y)p(x)p(y) = p(x, y) \) to obtain the second term and \( C = \frac{1}{2} \sum_{y \in Y} \int r^2(x, y)p(x)p(y)dx \). By replacing the expectations with corresponding sample averages, we obtain the empirical squared error as

\[
\hat{J}(g) = \frac{1}{2} \sum_{y \in Y} \frac{n_y}{n} \sum_{i=1}^{n} g^2(x_i, y) - \frac{1}{n} \sum_{i=1}^{n} g(x_i, y),
\]

where \( n_y \) is the number of samples for each class in \( \{(x_i, y_i)\}_{i=1}^{n} \). The learned model \( \hat{g} \) can be obtained by minimizing the regularized empirical squared loss:

\[
\hat{g} := \arg\min_g \hat{J}(g) + \lambda R(g),
\]

where \( R(g) \) is a regularizational functional and \( \lambda \geq 0 \) is the regularization parameter. Since SMI can be expressed as

\[
\text{SMI} = \sum_{y \in Y} \int r(x, y)p(x, y)dx - \frac{1}{2} \sum_{y \in Y} \int r^2(x, y)p(x)p(y)dx - \frac{1}{2},
\]

\[\text{See the derivation in, e.g., Sugiyama (2013).}\]
an SMI approximator can be obtained by

\[
\hat{\text{SMI}} := -\sum_{y \in Y} \frac{n_y}{2n^2} \sum_{i=1}^{n} \hat{g}^2(x_i, y) + \frac{1}{n} \sum_{i=1}^{n} \hat{g}(x_i, y_i) - \frac{1}{2}.
\]

In practice, the model \( g \) can be either parametric or non-parametric. A simple choice is to use a linear-in-parameter model:

\[
g(x, y) := \sum_{\ell=1}^{b} \alpha_\ell \psi_\ell(x, y) = \alpha^\top \psi(x, y),
\]

where \( \alpha := (\alpha_1, \ldots, \alpha_b)^\top \) is the parameter vector, \( \psi(x, y) := (\psi_1(x, y), \ldots, \psi_b(x, y)) \) is the basis function vector, \( b \) is the number of basis functions, and \( \top \) denotes the transpose of vectors and matrices. Then, with the \( \ell_2 \)-regularizer \( R(g) = \alpha^\top \alpha / 2 \), the optimization problem yields

\[
\hat{\alpha} := \text{argmin}_{\alpha \in \mathbb{R}^b} \frac{1}{2} \alpha^\top \hat{H} \alpha - \alpha^\top \hat{h} + \frac{\lambda}{2} \alpha^\top \alpha,
\]

where

\[
\hat{H}_{\ell,\ell'} := \sum_{y \in Y} \frac{n_y}{n^2} \sum_{i=1}^{n} \psi_\ell(x_i, y) \phi_{\ell'}(x_i, y)^\top,
\]

\[
\hat{h}_\ell := \frac{1}{n} \sum_{i=1}^{n} \psi_\ell(x_i, y_i).
\]

The solution can be obtained analytically by differentiating the objective function with respect to \( \alpha \) and set it to zero:

\[
\hat{\alpha} = (\hat{H} + \lambda I_b)^{-1} \hat{h},
\]

where \( I_b \) is the \( b \times b \) identity matrix. Then, the density-ratio can be estimated by

\[
\hat{g}(x, y) = \hat{\alpha}^\top \psi(x, y).
\]

With the estimated density-ratio, the SMI approximator can be expressed as

\[
\hat{\text{SMI}} = \hat{\alpha}^\top \hat{h} - \frac{1}{2} \hat{\alpha}^\top \hat{H} \hat{\alpha} - \frac{1}{2}.
\]

## 3 SMI Estimation from Positive-Unlabeled Data

In this section, we first reformulate SMI with only positive and unlabeled data, which is equivalent to SMI with positive and negative data, and then propose an SMI estimation method.

### 3.1 SMI with Positive-Unlabeled Data

In PU learning, we do not have negative data, but we alternatively have unlabeled data. Let us define positive (P) and unlabeled (U) data as

\[
\{x_i^P\}_{i=1}^{n_P} \overset{\text{i.i.d.}}{\sim} p(x \mid y = +1),
\]

\[
\{x_k^U\}_{k=1}^{n_U} \overset{\text{i.i.d.}}{\sim} p(x) = \theta_P p(x \mid y = +1) + \theta_N p(x \mid y = -1),
\]
where $\theta_P := p(y = +1)$ and $\theta_N := p(y = -1)$ are the class-prior probabilities. Our goal is to estimate SMI from PU data.

Let us express SMI in Eq. (1) as

$$\text{SMI} = \frac{\theta_P}{2} \int \left( \frac{p(x | y = +1)}{p(x)} - 1 \right)^2 dx + \frac{\theta_N}{2} \int \left( \frac{p(x | y = -1)}{p(x)} - 1 \right)^2 dx. \quad (2)$$

From the marginal density $p(x)$, we have

$$\theta_N \frac{p(x | y = -1)}{p(x)} = 1 - \theta_P \frac{p(x | y = +1)}{p(x)},$$

$$\theta_N \left( \frac{p(x | y = -1)}{p(x)} - 1 \right) = \theta_P \left( 1 - \frac{p(x | y = +1)}{p(x)} \right),$$

$$\left( \frac{p(x | y = -1)}{p(x)} - 1 \right)^2 = \frac{\theta_P^2}{\theta_N^2} \left( \frac{p(x | y = +1)}{p(x)} - 1 \right)^2,$$

where the equality between the first and second equations can be confirmed by using $\theta_P + \theta_N = 1$. Plugging the last equation into the second term of Eq. (2), we then obtain an expression of SMI only with positive and unlabeled data (PU-SMI) as

$$\text{SMI} = \frac{\theta_P}{2 \theta_N} \int \left( \frac{p(x | y = +1)}{p(x)} - 1 \right)^2 p(x) dx := \text{PU-SMI}.$$

### 3.2 PU-SMI Estimation

In this section, we propose an SMI estimation method from only positive and unlabeled data.

Let us define another density ratio function as

$$s(x) := \frac{p(x | y = +1)}{p(x)}.$$

Let $w$ be a model of $s$, and we learn $s$ so that the squared error between model $w$ and true ratio $s$ is minimized:

$$J_{PU}(w) := \frac{1}{2} \int \left( w(x) - \frac{p(x | y = +1)}{p(x)} \right)^2 p(x) dx - C'$$

$$= \frac{1}{2} \int w^2(x) p(x) dx - \int w(x)p(x | y = +1) dx,$$

where $C' := \frac{1}{2} \int \frac{p^2(x | y = +1)}{p(x)} dx$. An empirical squared error can be obtained by

$$\hat{J}_{PU}(w) := \frac{1}{2n_U} \sum_{k=1}^{n_U} w^2(x_k^U) - \frac{1}{n_P} \sum_{i=1}^{n_P} w(x_i^P). \quad (3)$$

Similarly to the existing SMI estimation method, we formulate our optimization problem as

$$\hat{w} := \arg \min_w \hat{J}_{PU}(w) + \lambda_{PU} R(w),$$

where $\lambda_{PU} \geq 0$ is the regularization parameter.
Expanding PU-SMI by using \( s(x)p(x) = p(x | y = +1) \), we can express SMI as

\[
\text{PU-SMI} = \frac{\theta_P}{\theta_N} \left( \frac{1}{2} \int s(x)p(x | y = +1)dx - \frac{1}{2} \right)
\]

where the equality of the first and second equations can be confirmed by plugging \( s(x)p(x) = p(x | y = +1) \) into the second term of the second equation. Finally, with the obtained density-ratio estimator, we can compute an approximator of PU-SMI as

\[
\hat{\text{PU-SMI}} = \frac{\theta_P}{\theta_N} \left( \frac{1}{n_P} \sum_{i=1}^{n_P} \hat{w}(x_i^P) - \frac{1}{2n_U} \sum_{k=1}^{n_U} \hat{w}^2(x_k^U) - \frac{1}{2} \right).
\]

Similarly to Suzuki and Sugiyama (2013), the minimization of the squared error \( \hat{J}_{PU} \) corresponds to the maximization of \(-\hat{J}_{PU}\) that is a lower-bound of PU-SMI as in the \( f \)-divergence estimation (Keziou, 2003; Nguyen et al., 2007). That is, the PU-SMI approximator can also be obtained by maximizing the lower-bound:

\[
\hat{\text{PU-SMI}} = \max_w -\theta_P \hat{J}_{PU}(w) = -\frac{\theta_P}{\theta_N} \hat{J}_{PU}(\hat{w}).
\]

Based on this fact, we derive convergence results of the estimated density ratio and the PU-SMI approximator in Section 3.4.

The estimation procedure for density-ratio model \( w \) does not involve class-prior \( \theta_P \) (and \( \theta_N \)), and PU-SMI is proportional to class-prior ratio \( \theta_P/\theta_N \). Therefore, an estimate of the class-prior is not needed when our purpose is just maximizing/minimizing PU-SMI. For example, in SMI-based dimensionality reduction discussed in Section 4.1, we can safely ignore the ratio of the class-prior \( \theta_P/\theta_N \) from the PU-SMI maximization. Since class-prior estimation only from PU data is known to be challenging (du Plessis and Sugiyama, 2014; Ramaswamy et al., 2016; Jain et al., 2016; du Plessis et al., 2017), being able to avoid class-prior estimation is a significant advantage of the proposed method in practice.

### 3.3 Implementation

Here, we explain a practical implementation of the proposed method.

When we use a neural network model, a solution can be typically obtained by back-propagation. To this end, various deep learning implementations may be used for obtaining a learned model.

Another candidate of the model is a linear-in-parameter model:

\[
w(x) = \sum_{\ell=1}^{b} \beta_{\ell}\phi_{\ell}(x) = \beta^\top \phi(x),
\]

where \( \beta := (\beta_1, \ldots, \beta_b)^\top \) is a vector of parameters, and \( \phi(x) := (\phi_1(x), \ldots, \phi_b(x))^\top \) is a vector of basis functions. This model allows us to obtain an analytic-form solution and a PU-SMI estimator, similarly to the existing SMI estimation method. Furthermore, the optimal convergence is theoretically guaranteed as shown in Section 3.4.
With the $\ell_2$-regularizer, the optimization problem is given by

$$\hat{\beta} := \arg\min_\beta \frac{1}{2} \beta^T \hat{H}^U \beta - \beta^T \hat{h}^P + \frac{\lambda_{PU}}{2} \beta^T \beta,$$

where $\lambda_{PU} \geq 0$ is the regularization parameter and

$$\hat{H}_{\ell,\ell'}^U := \frac{1}{n_U} \sum_{k=1}^{n_U} \phi_\ell(x_k^U)\phi_{\ell'}(x_k^U),$$

$$\hat{h}_\ell^P := \frac{1}{n_P} \sum_{i=1}^{n_P} \phi_\ell(x_i^P).$$

The solution can be obtained analytically by differentiating the objective function with respect to $\beta$ and set it to zero:

$$\hat{\beta} = (\hat{H}^U + \lambda_{PU} I_b)^{-1} \hat{h}^P.$$

Finally, with the obtained estimator, we can compute an SMI approximator only from positive and unlabeled data:

$$\text{PU-SMI} = \frac{\theta_P}{\theta_N} \left( \beta^T \hat{h}^P - \frac{1}{2} \beta^T \hat{H}^U \beta - \frac{1}{2} \right).$$

### 3.4 Theoretical Analysis

In this section, we derive the convergence rate of the parameter of the density-ratio model and the PU-SMI approximator based on the perturbation analysis of optimization problems (Bonnans and Cominetti, 1996; Bonnans and Shapiro, 1998).

Assume the linear-in-parameter model in Eq.(5) for the density-ratio $\frac{p(x|y=+1)}{p(x)}$. Without loss of generality, we assume that the basis function satisfies $0 \leq \phi_\ell(x) \leq 1$ for all $\ell = 1, \ldots, b$ and $x \in \mathbb{R}^d$, and there exists a constant $M$ such that $\|\beta\|_2 \leq M$ for the estimated solution $\beta$, i.e., $\beta$ is regularized. Moreover, assume that the basis functions $\{\phi_\ell(x)\}_{\ell=1}^b$ are linearly independent over the marginal density $p(x)$.

Let

$$\beta^* := \arg\min_\beta J_{PU}(\beta)$$

be the ideal estimate of the density-ratio model. Let $O_p$ denote the order in probability. Then we have the following convergence results (its proof is given in Appendix A):

**Theorem 1.** As $n_P, n_U \to \infty$, we have

$$\|\hat{\beta} - \beta^*\|_2 = O_p(1/\sqrt{n_P} + 1/\sqrt{n_U}),$$

$$|\text{PU-SMI} - \text{PU-SMI}| = O_p(1/\sqrt{n_P} + 1/\sqrt{n_U}),$$

provided that $\lambda_{PU} = O_p(1/\sqrt{\min(n_P, n_U)}).$

---

$^3$ It means that the convergence rate of $\lambda_{PU}$ is dominated by the smaller size of positive or unlabeled data.
Theorem 1 guarantees that the convergence of the density-ratio estimator and the PU-SMI approximator. In our setting, since \( n_P \) and \( n_U \) can increase independently, this is the optimal convergence rate without any additional assumption (Kanamori et al., 2009, 2012).

Note that Theorem 1 shows that both positive and unlabeled data contribute to convergence, implying that unlabeled data is directly used in the estimation rather than extracting the information of a data structure, such as the cluster structure frequently assumed in semi-supervised learning (Chapelle et al., 2006).

### 3.5 Model Selection

In practice, the performance of the proposed PU-SMI approximator depends on hyperparameters such as the regularization parameter and the number of epochs for backpropagation.

One way is to prepare a validation dataset and tune hyperparameters based on it. With positive and unlabeled samples for validation, we compute the squared error in Eq. (3) and choose the best model that minimizes the squared error from all model candidates.

Another way is to use cross-validation. For cross-validation, we first split the positive and unlabeled samples, \( S^P \) and \( S^U \), into \( K \) disjoint subsets, \( \{S^p_k\}_{k=1}^K \) and \( \{S^u_k\}_{k=1}^K \) of almost the same size. Based on them, we construct \( K \) disjoint subsets \( \{S_k := S^p_k \cup S^u_k\}_{k=1}^K \). Then, we estimate the model \( \hat{w}_{S_k} \) by using \( S \setminus S_k \) training samples. The approximation error is computed by the hold-out samples \( S_k \). We repeat this procedure for \( k = 1, \ldots, K \), and compute its mean:

\[
\hat{J}^\text{CV} := \frac{1}{K} \sum_{k=1}^K \left( \frac{1}{2} \sum_{x^u \in S^u_k} \hat{w}_{S_k}^2(x^u) - \sum_{x^p \in S^p_k} \hat{w}_{S_k}(x^p) \right).
\]

Finally, we choose the model that minimizes \( \hat{J}^\text{CV} \).

### 4 Application based on PU-SMI

In this section, we propose two applications of PU-SMI, along the line of existing SMI-based applications.

#### 4.1 Dimensionality Reduction

Here, we extend the existing SMI-based dimension reduction (Suzuki and Sugiyama, 2013), called least-squares dimension reduction (LSDR), to the PU learning setting.

**Algorithm:** Let \( v: \mathbb{R}^d \to \mathbb{R}^m \), where \( m < d \), be a mapping function from an input vector to its low-dimensional representation. Following the information-maximization principle (Linsker, 1988), we maximize PU-SMI with respect to the mapping function to find low-dimensional representation that maximally preserves dependency between inputs and outputs.
Algorithm 1 PUDR

Require: \( \{x_i^P\}_{i=1}^{n^P}, \{x_k^U\}_{k=1}^{n^U} \), \( w \), and \( v \)

1: Initialize \( w \) and \( v \)
2: repeat
3: \( \hat{w} \leftarrow \hat{w} - \varepsilon_w \nabla_w \hat{J}_{PU}(w \circ \hat{v}) \)
4: \( \hat{v} \leftarrow \hat{v} - \varepsilon_v \nabla_v \hat{J}_{PU}(\hat{w} \circ v) \)
5: until stopping conditions meet

To obtain such a mapping function, we propose an alternating optimization procedure to maximize SMI.\(^4\)—First, we estimate PU-SMI, and then we maximize the estimated PU-SMI with respect to the mapping function. More specifically, we solve the objective function in Eq. (3) to approximate PU-SMI while fixing the mapping function \( \hat{v} \):

\[
\min_w \hat{J}_{PU}(w \circ \hat{v}),
\]

where \( \hat{w} \) is a current estimate of the mapping function and “\( \circ \)” denotes the function composition, i.e., \( (w \circ v)(x) = w(v(x)) \).\(^5\) Then, we maximize the estimated PU-SMI with respect to \( v \) while fixing \( \hat{w} \):

\[
\max_v \text{PU-SMI}(\hat{w} \circ v),
\]

where \( \hat{w} \) is a current estimate of the density ratio.

As discussed in Section 3.2, an advantage of our dimension reduction method is that the whole procedure can be executed without estimating the class-prior, unlike existing PU learning methods (Elkan and Noto, 2008; du Plessis et al., 2015). This can be easily confirmed by Eq. (4):

\[
\argmax_v \text{PU-SMI}(\hat{w} \circ v) = \argmax_v -\hat{J}_{PU}(\hat{w} \circ v).
\]

Since minimization of the squared error does not require an estimate of the class-prior, our dimension reduction method does not require a class-prior estimation in advance.

We refer to the dimension reduction method for PU data as \textit{PUDR}. A pseudo-code of PUDR is summarized in Algorithm 1.

Linear Transformation: A choice of a mapping function is to use a linear transformation similarly to the existing SMI-based dimension reduction method (Suzuki and Sugiyama, 2013). As in the existing method, we search a projection matrix \( W \in \mathbb{R}^{d \times m} \) that satisfies \( W^\top W = I_m \) to avoid degenerated solutions.

Non-Linear Transformation: Another choice is to utilize non-linear transformation for capturing complex structures of the data. To obtain low-dimensional representation from a non-linear mapping, we adopt a neural network because we can use several useful techniques proposed recently. Specifically, we regard \( w \circ v \) as a neural network. We set

\(^4\) Unlike the existing SMI-based dimension reduction method, we do not restrict the mapping function to be a linear transformation. When a linear transformation is used, the maximization of SMI corresponds to \textit{sufficient dimension reduction} (Li, 1991)

\(^5\) Accordingly, the input dimension of \( w \) is redefined as \( m \), i.e., \( w : \mathbb{R}^m \to \mathbb{R} \).
the top layer as a fully-connected layer, which corresponds to \( w \) and the parameter \( \beta \) of the linear-in-parameter model. Layers below the top layer can be regarded as the basis function \( \phi \) and it can be anything; we could choose, for example, a convolution layer or a pretrained network.

### 4.2 Independence Test

Here, we extend the existing SMI-based independence test, called the least-squares independence test (LSIT), to the PU learning setting.

In the independence test, we test whether two random variables are independent or not. Since SMI takes zero if and only if two random variables are independent, we utilize the property to detect independence of variables. Similarly to Sugiyama and Suzuki (2011), we employ a permutation test (Efron and Tibshirani, 1994) for computing a \( p \)-value for the test.

In the original SMI-based test, we first estimate SMI from paired samples; then we repeatedly compute SMI with samples whose labels are randomly shuffled to construct a distribution of the SMI approximator when two random variables are independent. However, unlike the fully supervised case, we do not have labels to be shuffled in our setting. To conduct the permutation test, we propose the following procedure. We assign random labels \( \{\tilde{y}_k\}_{k=1}^{n_U} \) to unlabeled data \( \{x^U_k\}_{k=1}^{n_U} \) and compute SMI from the randomly labeled data \( \{(x^U_k, \tilde{y}_k)\}_{k=1}^{n_U} \). We compute SMI many times and then construct a distribution of SMI. Then, we approximate a \( p \)-value from the constructed distribution by comparing the estimate of \( \hat{\text{PU-SMI}} \) obtained from the obtained data. Finally, we test a hypothesis with the obtained \( p \)-value. We refer to the above independence test for PU data as PUIT.

Note that the class proportion of random labels \( \{\tilde{y}_k\}_{k=1}^{n_U} \) is determined by the estimated class-prior from PU data so that the class-prior of randomly paired samples \( \{(x^U_k, \tilde{y}_k)\}_{k=1}^{n_U} \) is the same as that of the marginal distribution \( p(x) \), i.e., \( p(x \mid y)p(y) = p(x)p(y) \).

### 5 Experiments

In this section, we experimentally investigate the behavior of the proposed PU-SMI estimator and evaluate the performance of the proposed dimension reduction and independence testing methods on various benchmark datasets.

#### 5.1 Accuracy of PU-SMI

First, we investigate the estimation accuracy of the proposed PU-SMI estimator on datasets obtained from the LIBSVM webpage (Chang and Lin, 2011).

We use the linear-in-parameter model with the Gaussian basis functions \( \phi_\ell(x) := \exp(-\|x - x_\ell\|^2/(2\sigma^2)) \), where \( \sigma \) is the bandwidth and \( \{x_\ell\}_{\ell=1}^b \) are the centers of the Gaussian functions randomly sampled from \( \{x^U_k\}_{k=1}^{n_U} \). The bandwidth and regularization parameter are determined by five-fold cross-validation. We vary the number of positive/unlabeled samples from 10 to 200, with the number of unlabeled/positive samples fixed. The class-prior was assumed to be known in this illustrative experiment and set at \( \theta_p = 0.5 \).
Figure 1 summarizes the average and standard error of the squared error of PU-SMI over 50 trials. This shows that, the mean squared error decreases both when the number of positive samples is increased and the number of unlabeled samples is increased. Therefore, both positive and unlabeled data contribute to improving the estimation accuracy of SMI, which well agrees with our theoretical analysis in Section 3.4.

5.2 Dimension Reduction

Next, we evaluate the performance of the proposed dimension reduction method, PUDR.

Illustration: We first illustrate how our proposed method works on an artificial data set. As a reference, we also show the result of the existing SMI-based dimension reduction method (LSDR) (Suzuki and Sugiyama, 2013) that uses both positive and negative data. For this illustrative experiment, we use a linear transformation as a projection matrix (i.e., linear dimension reduction).

We generate samples from the following densities:

\[
p(x \mid y = +1) = \mathcal{N}(x; \begin{pmatrix} -3 \\ 0 \\ 0 \\ 2 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix}),
\]

\[
p(x \mid y = -1) = \mathcal{N}(x; \begin{pmatrix} 3 \\ 0 \\ 0 \\ 2 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix}),
\]

where \( \mathcal{N}(x; \mu, \Sigma) \) is the normal density with the mean vector \( \mu \) and the covariance matrix \( \Sigma \). From the densities, we draw \( n_P = 200 \) positive and \( n_U = 400 \) unlabeled samples for PUDR, and \( n_P = 200 \) positive and \( n_N = 200 \) negative samples for LSDR. Other experimental settings are the same as those in Section 5.1.

We plot the estimated subspaces obtained by the PUDR and LSDR methods in Figure 2, showing that from only PU samples, the proposed PUDR obtained a subspace similar to that obtained by LSDR.

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6 True SMI was computed by a supervised SMI estimator (Suzuki et al., 2009) with a sufficiently large number of positive and negative samples.
Figure 2: Illustration of linear dimension reduction. (a) Estimated subspace obtained by PUDR, where positive “●” and unlabeled samples “□” are used. (b) Estimated subspace obtained by LSDR, where positive “●” and negative samples “×” are used. The results show that the proposed PUDR from only PU data gives a subspace similar to that obtained by its supervised counterpart.

Table 1: Mean absolute error (with standard error) between the estimated class-prior and the true value over 20 trials. KM means the class-prior estimation method based on kernel mean embedding, PCA is the principal component analysis. The boldface denotes the best and comparable approach in terms of the average absolute error according to the t-test at the significance level 5%.

| Dataset  | \( \theta_p \) | KM   | PCA+KM [d/4] | PCA+KM [d/2] | PCA+KM [3d/4] | PUDR+KM |
|----------|----------------|------|--------------|--------------|--------------|----------|
| mushrooms| 0.3 0.05 (0.00)| 0.03 (0.00) 0.05 (0.00) 0.05 (0.00) | 0.03 (0.00) |
| a9a      | 0.5 0.04 (0.01)| 0.04 (0.00) 0.04 (0.01) 0.04 (0.01) | 0.04 (0.01) |
| MNIST    | 0.3 0.10 (0.01)| 0.10 (0.01) 0.10 (0.01) 0.10 (0.01) | 0.04 (0.01) |
| CIFAR10  | 0.7 0.30 (0.02)| 0.30 (0.02) 0.30 (0.01) 0.30 (0.01) | 0.30 (0.01) |
| SVHN     | 0.3 0.08 (0.03)| 0.08 (0.03) 0.08 (0.01) 0.08 (0.01) | 0.08 (0.01) |

**Benchmark Data:** Next we apply the PUDR method to benchmark datasets. To obtain low-dimensional representation, we use a fully-connected neural network with four layers \((d=60–20–1)\), the sigmoid function is used as the activation function, and batch normalization (Ioffe and Szegedy, 2015) is applied to all hidden layers. Stochastic gradient descent is used for optimization with learning rate 0.01. Also, weight decay with 0.0005 and gradient noise with 0.01 are applied. We iteratively update \(w\) with four minibatches and \(v\) with one minibatch.

We compare the accuracy of class-prior estimation with and without dimension re-
duction. For comparison, we also consider principal component analysis (PCA) with different numbers of components: \( \lfloor d/4 \rfloor, \lfloor d/2 \rfloor, \) and \( \lfloor 3d/4 \rfloor \), where \( \lfloor \cdot \rfloor \) is the floor function. As a class-prior estimation method, we use the method based on the \textit{kernel mean embedding} (KMM) method proposed by Ramaswamy et al. (2016). We use the mushrooms (Lichman, 2013), the a9a (Lichman, 2013), the MNIST (LeCun et al., 1998), the CIFAR10 (Torralba et al., 2008), and the SVHN (Netzer et al., 2011) datasets. For multi-class classification datasets, we divide the whole classes into 2 groups to make binary classification tasks. From the datasets, we draw \( n_P = 1000 \) positive and \( n_U = 2000 \) unlabeled samples. For model selection, we use validation samples of size \( n_P = 50 \) and \( n_U = 200 \).

Table 1 lists the mean absolute error (with standard error) between an estimated class-prior and the true value. Overall, our proposed dimension reduction method tends to outperform other methods, meaning that our method provides useful low-dimensional representation except the SVHN dataset when \( \theta_P = 0.3, 0.5 \). For the mushrooms, a9a, and MNIST datasets, applying the unsupervised dimension reduction method, PCA, does not improve the estimation accuracy. In fact, PCA performs poorly on the CIFAR10 and SVHN datasets, in particular, when \( \theta_P = 0.3 \).

5.3 Independence Test

Finally, we evaluate the performance of our proposed independence test, PUIT.

We compute the frequency of the \textit{type-II} error, i.e., the number of times the null hypothesis (two random variables are independent) is accepted when the alternative hypothesis is true. Similarly to Section 5.1, we use classification datasets. Thus, the two random variables (pattern \( x \) and class label \( y \)) are highly dependent, i.e., the frequency of the type-II error is expected to be low. Other experimental settings are the same as those in Section 5.1.

Figure 3 summarizes the frequency of the type-II error by the proposed PU-based independence testing method at the significance level 5%. In both cases, the frequency decreases as the number of positive and unlabeled samples increases, showing that our
method can well detect statistical dependency only from PU data.

6 Conclusions

In this paper, we proposed a novel estimation method of SMI only from positive and unlabeled (PU) data. We theoretically proved the optimal convergence of our proposed SMI approximator to the true SMI. We then applied the proposed SMI estimator to develop PU-based dimension reduction and independence testing methods. Our dimensionality reduction method does not involve class-prior estimation, which is a significant advantage in practice. We also proposed a PU-based independence testing method. Experimental results demonstrated that our proposed methods work well on various benchmark datasets.

Since an SMI estimator is applicable not only to dimension reduction and independence testing, but also to other tasks including feature selection (Suzuki et al., 2009), clustering (Sugiyama et al., 2014), and object matching (Yamada et al., 2015). In our future work, we will apply our PU-based SMI estimator to those problems and evaluate the performance.

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A Proof of Theorem 1

The idea of the proof is to view the approximated squared error as perturbed optimization of expected one. Recall the linear-in-parameter model  \( f(x) = \sum_{\ell=1}^{b} \beta_{\ell} \phi_{\ell}(x) = \beta^{T} \phi(x) \). We assume that 0 \( \leq \phi_{\ell} \leq 1 \) for all  \( \ell = 1, \ldots, b \) and  \( x \in \mathbb{R}^{d} \), and there exists a constant such that  \( \| \beta \|_{2} \leq M \). Moreover, we assume that the basis functions  \( \{ \phi_{\ell}(x) \}_{\ell=1}^{b} \) are linearly independent over the marginal density  \( p(x) \).

Let

\[
J_{PU}(\beta) := \frac{1}{2} \beta^{T} H^{U} \beta^{T} - \beta^{T} h^{P},
\]

\[
\hat{J}_{PU}(\beta) := \frac{1}{2} \beta^{T} \hat{H}^{U} \beta^{T} - \beta^{T} \hat{h}^{P} + \frac{\lambda_{PU}}{2} \beta^{T} \beta
\]

be the expected squared error and the  \( \ell_{2} \)-regularized empirical squared error, respectively.

Firstly, we have the following second order growth condition.

**Lemma 2.** Let  \( \epsilon \) be the smallest eigenvalue of  \( H^{U} \). The second order growth condition holds

\[
J_{PU}(\beta) \geq J_{PU}(\beta^{*}) + \epsilon \| \beta - \beta^{*} \|_{2}^{2}.
\]
Proof. Since $H^U$ is positive definite given the linearly independent basis functions over $p(x)$, $J_{PU}(\beta)$ is strongly convex with parameter at least $\epsilon$. Then, we have

$$J_{PU}(\beta) \geq J_{PU}(\beta^*) + \nabla J_{PU}(\beta^*)^\top (\beta - \beta^*) + \epsilon \|\beta - \beta^*\|_2^2$$

where the optimality condition $\nabla J_{PU}(\beta^*) = \mathbf{0}$ is used.

Then, let us define a set of perturbation parameters as

$$u := \{U^U, u^P, u^\lambda \mid U^U \in \mathbb{S}^b_+, u^P \in \mathbb{R}^b, u^\lambda \in \mathbb{R}\},$$

where $\mathbb{S}^b_+ \subset \mathbb{R}^{b \times b}$ is the cone of $b \times b$ positive semi-definite matrices. Our perturbed objective function and the solution are given by

$$J_{PU}(\beta, u) := \frac{1}{2} \beta^\top (H^U + U^U) \beta - \beta^\top (h^P + u^P) + \frac{u^\lambda}{2} \beta^\top \beta,$$

$$\beta(u) := \arg\min_{\beta} J_{PU}(\beta, u),$$

where

$$H^U := \int \phi(x)\phi(x)^\top p(x)dx,$$

$$h^P := \int \phi(x)p(x \mid y = +1)dx.$$

Apparently, $J_{PU}(\beta) = J_{PU}(\beta, 0)$. We then have the following Lemma:

**Lemma 3.** $J_{PU}(\cdot, u) - J_{PU}(\cdot)$ is Lipschitz continuous modulus $\omega(u) = \mathcal{O}(\|U^U\|_{\text{Fro}} + \|u^P\|_2 + |u^\lambda|)$ on a sufficiently small neighborhood of $\beta^*$, where $\|\cdot\|_{\text{Fro}}$ is the Frobenius norm.

Proof. Firstly, we have

$$J_{PU}(\beta, u) - J_{PU}(\beta) = \frac{1}{2} \beta^\top U^U \beta - \beta^\top u^P + \frac{u^\lambda}{2} \beta^\top \beta.$$

The partial gradient is given by

$$\frac{\partial}{\partial \beta} (J_{PU}(\beta, u) - J_{PU}(\beta)) = U^U \beta - u^P + u^\lambda \beta.$$

Let us define the $\delta$-ball of $\beta^*$ as $B_\delta(\beta^*) := \{\beta \mid \|\beta - \beta^*\|_2 \leq \delta\}$. For any $\beta \in B_\delta(\beta^*)$, we can easily show

$$\|\beta\|_2 \leq \|\beta - \beta^*\|_2 + \|\beta^*\|_2 \leq \delta + M.$$

Thus,

$$\left\| \frac{\partial}{\partial \beta} (J_{PU}(\beta, u) - J_{PU}(\beta)) \right\|_2 \leq (\delta + M)(\|U^U\|_{\text{Fro}} + |u^\lambda|) + \|u^P\|_2.$$

This means that $J_{PU}(\cdot, u) - J_{PU}(\cdot)$ is Lipschitz continuous on $B_\delta(\beta^*)$ with a Lipschitz constant of order $\mathcal{O}(\|U^U\|_{\text{Fro}} + \|u^P\|_2 + |u^\lambda|)$. 

\[ \square \]
Finally, we prove Theorem 1.

\textit{Proof.} According to the central limit theorem and our assumption about \(\lambda_{PU}\), we have

\[\|U^U\|_{\text{Fro}} = O_p(1/\sqrt{n_P}), \quad \|u^P\|_2 = O_p(1/\sqrt{n_U}), \quad |u^\lambda| = O_p(1/\sqrt{\min(n_P, n_U)})\]

as \(n_P, n_U \to \infty\). Thus, by using Lemma 2, Lemma 3, and Proposition 6.1 in Bonnans and Shapiro (1998), we have the first half of Theorem 1:

\[
\|\hat{\beta} - \beta^*\|_2 \leq \epsilon^{-1}\omega(u) = O(\|U^U\|_{\text{Fro}} + \|u^P\|_2 + |u^\lambda|) = O_p(1/\sqrt{n_P} + 1/\sqrt{n_U}).
\]

Next, we prove the latter half of Theorem 1. For the squared errors, we have

\[
|\hat{J}_{PU}(\hat{\beta}) - J_{PU}(\beta^*)| \leq |\hat{J}_{PU}(\hat{\beta}) - \hat{J}_{PU}(\beta^*)| + |\hat{J}_{PU}(\beta^*) - J_{PU}(\beta^*)|.
\]

Here, we have

\[
\hat{J}_{PU}(\hat{\beta}) - \hat{J}_{PU}(\beta^*) = \frac{1}{2}(\hat{\beta} + \beta^*)^\top \hat{H}^U(\hat{\beta} - \beta^*) - (\hat{\beta} - \beta^*)^\top \hat{h}^P,
\]

\[
\hat{J}_{PU}(\beta^*) - J_{PU}(\beta^*) = \frac{1}{2}\beta^*^\top U^U \beta^* - u^P \beta^* + \frac{\lambda_{PU}}{2}\beta^*^\top \beta^*.
\]

Since \(0 \leq \phi_\ell(x) \leq 1, \|\beta^*\|_2 \leq M\), and \(\lambda_{PU} = O_p(1/\sqrt{\min(n_P, n_U)})\), it leads to

\[
|\hat{J}_{PU}(\hat{\beta}) - J_{PU}(\beta^*)| \leq |\hat{J}_{PU}(\hat{\beta}) - \hat{J}_{PU}(\beta^*)| + |\hat{J}_{PU}(\beta^*) - J_{PU}(\beta^*)| \\
\leq O_p(\|\hat{\beta} - \beta^*\|_2) + O_p(\|U^U\|_{\text{Fro}} + \|u^P\|_2 + \lambda_{PU}) \\
= O_p(1/\sqrt{n_P} + 1/\sqrt{n_U}).
\]

Recall

\[
\text{PU-SMI} = -\frac{\theta_P}{\theta_N} J_{PU}(\beta^*), \quad \text{PU-SMI} = -\frac{\theta_P}{\theta_N} \hat{J}_{PU}(\hat{\beta}).
\]

as discussed in Section 3.2. The final result means

\[
|\text{PU-SMI} - \text{PU-SMI}| = O_p(1/\sqrt{n_P} + 1/\sqrt{n_U}).
\]

\[\square\]

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