Efficient Cross-Validation for Semi-Supervised Learning

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Abstract

Manifold regularization, such as laplacian regularized least squares (LapRLS) and laplacian support vector machine (LapSVM), has been widely used in semi-supervised learning, and its performance greatly depends on the choice of some hyper-parameters. Cross-validation (CV) is the most popular approach for selecting the optimal hyper-parameters, but it has high complexity due to multiple times of learner training. In this paper, we provide a method to approximate the CV for manifold regularization based on a notion of robust statistics, called Bouligand influence function (BIF). We first provide a strategy for approximating the CV via the Taylor expansion of BIF. Then, we show how to calculate the BIF for general loss function, and further give the approximate CV criteria for model selection in manifold regularization. The proposed approximate CV for manifold regularization requires training only once, hence can significantly improve the efficiency of traditional CV. Experimental results show that our approximate CV has no statistical discrepancy with the original one, but much smaller time cost.

1 Introduction

Semi-supervised learning (SSL), which exploits the prior knowledge from the unlabeled data to improve performance, has attracted considerable attention in recent years. Manifold regularization, such as laplacian regularized least squares (LapRLS) [Belkin et al., 2006], laplacian support vector machine (LapSVM) [Sindhwani et al., 2005; Belkin et al., 2006], has been widely used and very successful under the circumstance of a few of labeled examples and amount of unlabeled examples. The performance of these algorithms greatly depends on the choice of some hyper-parameters (such as kernel parameters, regularization parameters and graph Laplacian parameters), hence model selection is foundational to manifold regularization and is also a challenging problem in manifold regularization.

Cross-validation (CV) is a tried and tested approach for selecting the optimal model [Josse and Husson, 2012]. In t-fold CV, data set is split into t disjoint subset of (approximately) equal size and the learner machine is trained t times, each time leaving out one of subsets from training, but using the omitted subset to compute the validation error. The t-fold CV estimate is then simply the average of the validation errors observed in each of the t iterations, or folds. Although t-fold CV is a commonly used approach for selecting the hyper-parameters, it requires training t times, making it disabled for large-scale model selection.

To address this problem, in this paper, we present a novel approximate approach to CV for model selection of manifold regularization based on a theoretical notion of Bouligand influence function (BIF) [Christmann and Messe, 2008], which requires training on the full data only once. Specifically, we first introduce the notion of BIF, and verify that it is the first derivative of an operator. Then, we provide a strategy to approximate the CV via the first order approximation of Taylor expansion of BIF. Finally, we propose a novel method to calculate the BIF for general loss function, and further give two approximate CV criteria for LapRLS and LapSVM, respectively. Experimental results on lots of datasets show that our approximate CV has no statistical discrepancy with the original one, but can significantly improve the efficiency. This is the first attempt to use the notion of robust statistics to approximate the general t-CV for model selection in SSL community.

Related Work

In this subsection, we will introduce the related work about approximate CV. For kernel-based algorithms in supervised learning, such as SVM, least square SVM (LSSVM), kernel ridge regression (KRR), much work has been done to reduce the time complexity of leave-one-out CV, see [Chapelle et al., 2002; Vapnik and Chapelle, 2000; Opper and Winther, 1999; Keerthi, 2002; Liu et al., 2018] for SVM, [Cawley and Talbot, 2007; Cawley, 2006] for LSSVM, [Cawley and Talbot, 2004] for sparse LSSVM, [Debruyne et al., 2008; Debruyne, 2007] for KRR, etc. [Debruyne et al., 2008] proposed an approach to approximating the leave-one-out CV based on the notion of influence function [Hampel et al., 1986] for kernel-based regression.


Although there is much work on improving the efficiency of the leave-one-out CV for kernel-based algorithms in supervised learning, but little work focuses on the general t-CV. [Liu et al., 2014] presented a strategy for approximating the general CV based on the notion of Bouligand influence function (BIF) [Christmann and Mepsem, 2008; Robinson, 1991] for LSSVM and quadratic $\epsilon$-insensitive support vector regression algorithms. [Liu et al., 2019] extended the above method to various kernel-based algorithms, and established an approximation theory of CV. [Liu et al., 2018] further improved the efficiency of the computation of the BIF matrix for large scale problem. However, as far as we know, how to approximate the general t-CV in semi-supervised learning community is still unknown. In this paper, we will fill this gap.

The rest of the paper is organized as follows. We introduce some notations and preliminaries in Section 2. In Section 3, we present an approximate CV method via BIF. In Section 4, we give the final model section criteria for LapRLS and LapSVM. In Section 5, we empirically analyze the performance of our proposed approximate CV. We end in Section 6 with a conclusion. The proof is given in the last part.

2 Notations and Preliminaries

In semi-supervised learning, we are given a small number of labeled examples $L = \{(x_i, y_i), i = 1, \ldots, l\}$, and a large number of unlabeled examples $U = \{x_i, i = l + 1, \ldots, l + u\}$, $l$ and $u$ denote the number of labeled and unlabeled points respectively. Typically, $l \ll u$. Let $S = L \cup U$ be a set of $l + u$ examples, and $T = L \backslash U = \{x_i, i = 1, \ldots, l + u\}$. Labeled examples are generated according to the distribution $P$ on $X \times Y$, whereas unlabeled examples are drawn according to the marginal distribution $P_X$ of $P$. Labels are obtained from the conditional probability distribution $P(y|x)$. For classification, $Y = \{+1, -1\}$, for regression, $Y \in \mathbb{R}$.

Given a Mercer kernel $\kappa$ and its associated reproduce kernel Hilbert space (RKHS) $H_\kappa$, the manifold regularization can be written as

$$f_{\text{MR}}^\epsilon = \arg\min_{f \in H_\kappa} E_{(x,y) \sim P_S}[\ell(y, f(x)) + \gamma_A \|f\|_P^2 + \gamma_I \|f\|_P^2],$$

where $P_S$ is the empirical distribution, that is, $P_S(z) = \frac{1}{l}$ when $z \in L$, $P_S(z) = \frac{1}{u}$ when $z \in T$, $P_S(z) = 0$, otherwise. $\ell: X \times Y \rightarrow \mathbb{R}^+$ $\ell$ is a loss function, $\|\cdot\|_P$ is the norm in RKHS, $\gamma_A$ is the weight of the norm of the function in the RKHS, $\gamma_I$ is the weight of the norm of the function in the low dimensional manifold, $f = [f(x_1), \ldots, f(x_{l+u})]^T$, $L_S = D - W$ is the graph Laplacian matrix associated with $S$, where $W$ is the affinity matrix defining the similarity between any pair of samples of $S$, and $D$ is the diagonal matrix with diagonal elements $D_{ii} = \sum_j W_{ij}$. Laplacian Regularized Least Squares (LapRLS) and Laplacian Support Vector Machine (LapSVM) are two special cases of manifold regularized with different loss functions. For LapRLS, $\ell$ is the square loss: $\ell(y, f(x)) = (f(x) - y)^2$; For LapSVM, $\ell$ is the hinge loss: $\ell(y, f(x)) = \max(0, 1 - y f(x))$.

For the graph construction, a $k$NN graph is commonly used due to its simplicity and effectiveness [Melacci and Belkin, 2011]. In a $k$NN graph, the affinity matrix $W$ is calculated as $W_{ij} = \exp(-\frac{|x_i - x_j|^2}{2\sigma_w^2})$, if $x_i$ is the $k$ nearest neighbors of $x_j$, and 0 otherwise.

Let $\{L_i\}_{i=1}^t$ and $\{U_i\}_{i=1}^t$ be a random equipartition of $L$ and $U$ into $t$ parts, and $S_i = L_i \cup U_i, T_i = L_i \cup U_i, i = 1, \ldots, t$. For simplicity, assume that $l$ and $u$ both mod $t$, and hence, $|L_i| = \frac{1}{t} = m$, $|U_i| = \frac{1}{t} = n, i = 1, \ldots, t$. Let $P_{S_i \backslash S_i}$ be the empirical distribution of $S$ without the observations $S_i$, that is,

$$P_{S_i \backslash S_i}(z) = \begin{cases} 1/(t-1)m, & z \in L \setminus L_i, \\ 1/(t-1)(m+n), & z \in T \setminus T_i, \\ 0, & \text{otherwise}. \end{cases}$$

Let $f_{\text{MR}}^{\epsilon, S_i}$ be the hypothesis learned on all of the data excluding $S_i$. Then, the t-fold CV can be written as

$$t-CV := \sum_{i=1}^t \sum_{(x_j, y_j) \in L_i} V(y_j, f_{\text{MR}}^{\epsilon, S_i}(x_j)).$$

From the above definition of t-CV, one can see that we need train the learning algorithm $t$ times to obtain t-CV. Thus, the time complexity of t-CV is $O((t-1)^3(t+u)^3)$, which is computationally expensive.

**Remark 1.** The loss function $V$ adopted in the t-CV of (2) is not should be the same as the learning machine. In this paper, $V$ is the 0-1 loss for classification, $V$ is the square loss for regression.

3 Approximate CV with BIF

In this section, we will first introduce the notion of Bouligand influence function (BIF), and further show how to use BIF to approximate t-CV in manifold regularization.

3.1 Bouligand Influence Function

**Definition 1.** [Christmann and Mepsem, 2008] Let $P$ be a distribution and $f_{\text{MR}}^{\epsilon}$ be an operator $f_{\text{MR}}^{\epsilon} : P \rightarrow f_{\text{MR}}^{\epsilon}$, then the Bouligand influence function (BIF) of $f_{\text{MR}}^{\epsilon}$ at $P$ in the direction of a distribution $Q \neq P$ is defined as

$$\text{BIF}(Q, f_{\text{MR}}^{\epsilon}, P) = \lim_{\epsilon \to 0} \frac{f_{\text{MR}}^{\epsilon}((1-\epsilon)P+\epsilon Q) - f_{\text{MR}}^{\epsilon}(P)}{\epsilon}.$$
Denote $P_{\epsilon,Q} = (1 - \epsilon)P + \epsilon Q$. Note that the derivative of $f_{MR}^{\text{BIF}}$ at $\epsilon$ can be written as $\lim_{\Delta \epsilon \to 0} \frac{f_{MR}^{\text{BIF}}(P_{\epsilon',Q}) - f_{MR}^{\text{BIF}}(P_{\epsilon,Q})}{\Delta \epsilon}$. If setting $\epsilon = 0$, one can see that $\lim_{\Delta \epsilon \to 0} \frac{f_{MR}^{\text{BIF}}(P_{\epsilon',Q}) - f_{MR}^{\text{BIF}}(P_{\epsilon,Q})}{\Delta \epsilon} = \text{BIF}(Q; f_{MR}^{\text{BIF}}, P)$. So, BIF($Q; f_{MR}^{\text{BIF}}, P$) is the first order derivative of $f_{MR}^{\text{BIF}}$ at $\epsilon = 0$. Thus, if BIF exists, the following Taylor expansion holds:

$$f_{MR}^{\text{BIF}}(P_{\epsilon,Q}) = f_{MR}^{\text{BIF}}(Q; f_{MR}^{\text{BIF}}, P) + \epsilon \cdot \text{BIF}(Q; f_{MR}^{\text{BIF}}, P).$$

(3)

Note that

$$P_{S \setminus S_i} = \left(1 - \frac{1}{l-1}\right)P_S + \frac{1}{l-1}P_{S_i},$$

where $P_{S \setminus S_i}$ is the empirical distribution of $S$ without the observations $S_i$ defined in (1), $P_S$ is the sample distribution corresponding to $S_i$,

$$P_{S_i}(z) = \begin{cases} \frac{1}{m}, & z \in L_i, \\ \frac{1}{m+n}, & z \in T_i, \\ 0, & \text{otherwise}. \end{cases}$$

Thus, if taking $Q = P_{S_i}$, $\epsilon = \frac{1}{l-1}$, $P_{\epsilon,Q} = P_{S \setminus S_i}$, $P = P_S$, Equation (3) gives

$$f_{MR}^{\text{BIF}}(P_{S \setminus S_i}) = f_{MR}^{\text{BIF}}(P_S) + \frac{1}{1 - \epsilon} \cdot \text{BIF}(P_S; f_{MR}^{\text{BIF}}, P_S).$$

(4)

Thus, the approximation of t-CV can be written as $\text{t-BIF} := \sum_{i=1}^{t} \sum_{(x_i,y_i) \in L_i} V(y_i, f_{MR}^{\text{BIF}}(x_i) + \frac{\text{BIF}(P_S; f_{MR}^{\text{BIF}}, P_S)(x_i)}{1 - \epsilon}).$

Note that t-BIF only depends on the calculation of $f_{MR}^{\text{BIF}}$ and $\text{BIF}(P_S; f_{MR}^{\text{BIF}}, P_S)$. Thus, if given the BIF($P_S; f_{MR}^{\text{BIF}}, P_S$), we need to train the algorithm only once on the full data set $S$ to obtain $f_{MR}^{\text{BIF}}$ for approximating the $f_{MR}^{\text{BIF}}$, $i = 1, \ldots, t$.

3.2 The Computation of BIF

Let $K_{SS}$ be the $(l+u) \times (l+u)$ kernel matrix with $[K_{SS}]_{jk} = \kappa(x_j, x_k)$, $K_{SS}$, the $(l+u) \times (m+n)$ kernel matrix with $[K_{SS}]_{jk} = \kappa(x_j, x_k)$, $x_j \in T$, $x_k \in T_i$, $\ell'(\cdot)$ and $\ell''(\cdot)$ be the first and second derivative of $\ell(\cdot)$ with respect to the second variable respectively.

Theorem 1. Let $B$ be the $(l+u) \times t$ BIF matrix with $[B]_{ij} = \text{BIF}(P_S; f_{MR}^{\text{BIF}}, P_S)(x_j)$, and

$$H = \frac{1}{l}J_S K_{SS} F_S + 2\gamma A I + \frac{2\gamma}{(l+u)^2} K_{SS} L_S,$$

then the $i$th column of $B$ can be written as

$$B_{i} = H^{-1} \left[ -\frac{K_{SS} \mu_S}{m} - 2\gamma A f_{MR}^{\text{BIF}} S - \frac{2\gamma I K_{SS} L_S f_{MR}^{\text{BIF}}}{(m+n)^2} \right],$$

where $F_S$ is an $(l+u) \times (l+u)$ diagonal matrix with the first $l$ diagonal entries as $\ell''(y_i, f_{MR}^{\text{BIF}}(x_i))$ and the rest 0, $\mu_S$ is an $m+n$ vector with the first $m$ entries as $

\ell'(y_i, f_{MR}^{\text{BIF}}(x_i)), (x_i, y_i) \in L_i$, and the rest 0, $L_S$ is the graph Laplacian associated to $S_i$, $J_S$ is an $(l+u) \times (l+u)$ diagonal matrix with the first $l$ diagonal entries as 1 and the rest 0, $f_{MR}^{\text{BIF}}(x_i), \ldots, f_{MR}^{\text{BIF}}(x_i+u)^T$, $f_{MR}^{\text{BIF}}(x_i), \ldots, f_{MR}^{\text{BIF}}(x_i+u)^T$, $x_i \in T_i$.

The above theorem shows that if the first and second derivative of loss function $\ell$ exists, the BIF can be obtained. In the following, we will show how to calculate the BIF matrix for LapRLS and LapSVR, respectively.

Laplacian Regularized Least Squares (LapRLS)

Note that the loss function of LapRLS is the least square loss, according to the definitions of $F_S$ and $\mu_S$, in Theorem 1, it is easy to verify that $F_S$ is the diagonal matrix with the first $l$ entries as 2 and the rest 0, $\mu_S$, is an $m+n$ vector with the first $m$ entries as $2(f_{MR}^{\text{BIF}}(x_i) - y_i)$, $(x_i, y_i) \in L_i$, and the rest 0. Thus, from Theorem 1, the BIF matrix of LapRLS can be written as:

$$B_{i} = H^{-1} \left[ -\frac{K_{SS} \mu_S}{m} - 2\gamma A f_{MR}^{\text{BIF}} S - \frac{2\gamma I K_{SS} L_S f_{MR}^{\text{BIF}}}{(m+n)^2} \right],$$

where $H = 2J_S K_{SS} F_S + 2\gamma A I + \frac{2\gamma I K_{SS} L_S}{(l+u)^2}$.

Laplacian Support Vector Machine (LapSVR)

Since the hinge loss $\ell(y, t) = \max(0, 1 - yt)$ is not differentiable, but according to Theorem 1, to obtain the BIF matrix, loss function should be differentiable. Thus, we propose to use a differentiable approximation of it, inspired by the Huber loss:

$$\ell(y, t) = \begin{cases} \frac{1}{4h} (1 + h - yt)^2 & \text{if } yt > 1 + h, \\ \frac{1}{4h} (1 - yt)^2 & \text{if } |yt| \leq h, \\ 1 - yt & \text{if } yt < 1 - h. \end{cases}$$

Note that if $h \to 0$, the Huber loss converges to the hinge loss. From the Huber loss, we know that:

$$\ell'(y, t) = \begin{cases} 0 & \text{if } yt > 1 + h, \\ \frac{-y(1 + h - yt)}{2h} & \text{if } |yt| \leq h, \\ -y & \text{if } yt < 1 - h, \end{cases}$$

$$\ell''(y, t) = \begin{cases} 0 & \text{if } yt > 1 + h, \\ \frac{1}{2h} & \text{if } |yt| \leq h, \\ 0 & \text{if } yt < 1 - h. \end{cases}$$

We say that $x_i$ is a support vector if $|y_i(f_{MR}^{\text{BIF}}(x_i)) - 1| < h$. Let us reorder the training points such that the first labeled lsv points are support vectors. From the definition of $F_S$, one can see that $F_S = \frac{1}{m+n}I_{lsv}$, where $I_{lsv}$ is the $(l+u) \times (l+u)$ diagonal matrix with the first $lsv$ entries being 1 and the others 0, $\mu_S$, is an $m+n$ vector with the first $m$ entries as $\ell''(y_i, f_{MR}^{\text{BIF}}(x_i))$, $(x_i, y_i) \in L_i$, and the rest 0. Thus, according to Theorem 1, the BIF matrix of LapSVR can be written as:

$$B_{i} = H^{-1} \left[ -\frac{K_{SS} \mu_S}{m} - 2\gamma A f_{MR}^{\text{BIF}} S - \frac{2\gamma I K_{SS} L_S f_{MR}^{\text{BIF}}}{(m+n)^2} \right],$$
we randomly sample columns, without replacement. Let $P$ be the matrix formed by the selected columns, $\tilde{S}$ the Moore-Penrose generalized inverse of $P$, and $C$ the $c \times c$ matrix consisting of the intersection of these $c$ columns with the corresponding $c$ rows of $K_{SS}$. Without loss of generality, we can rearrange the columns and rows of $K_{SS}$ based on this sampling such that:

$$K_{SS} = \begin{pmatrix} P & K_{S,S}^c \end{pmatrix} \begin{pmatrix} K_{S,S} \end{pmatrix}_{(S \times S)} \begin{pmatrix} P \end{pmatrix}_{(c \times S)}.$$

The Nyström method uses $P$ and $C$ to construct an approximation $\tilde{K}$ of $K$ defined by:

$$\tilde{K}_{SS} = CP^+C^T \approx K_{SS},$$

where $P^+$ is the Moore-Penrose generalized inverse of $P$.

### Remark 2
In this paper, we only consider the use of square hinge loss functions, such as square hinge loss $\max(0, 1 - yt)^2$, logistic loss $\ln(1 + \exp(-yt))$, and so on.

### 4 Model Selection

According to the above discussion, we know that $t$-BIF is an efficient approximation of CV for manifold regularization, which only need to training once. However, to obtain $t$-BIF, we need $O((l + u)^3)$ to calculate $H^{-1}$ to obtain the BIF matrix $B$.

To accelerate the computation of the inversion of $H$, we consider the use of the popular Nyström method. Suppose we randomly sample $c$ columns of the matrix $K_{SS}$ uniformly without replacement. Let $C$ be the $n \times c$ matrix formed by these columns, $P$ the $c \times c$ matrix consisting of the intersection of these $c$ columns with the corresponding $c$ rows of $K_{SS}$. Without loss of generality, we can rearrange the columns and rows of $K_{SS}$ based on this sampling such that:

$$K_{SS} = \begin{pmatrix} P & K_{S,S}^c \end{pmatrix} \begin{pmatrix} K_{S,S} \end{pmatrix}_{(S \times S)} \begin{pmatrix} P \end{pmatrix}_{(c \times S)}.$$

Denote $T$ as

$$T = \begin{cases} 2J_{SS}K_{SS}J_S + 2\gamma_A I, \quad \text{for LapRLS} \\ J_{SS}K_{SS}I_{SS} + 2\gamma_A I, \quad \text{for LapSVM}, \end{cases}$$

so $H$ can be approximated by $\tilde{H} = T + \frac{2\gamma}{(l + u)^2}CP^+TT^{-1}C$. According to the Woodbury formula:

$$(A + XYZ)^{-1} = A^{-1} - A^{-1}X(Y^{-1} + ZA^{-1}X)^{-1}ZA,$$

it is easy to verify that $H^{-1} = T^{-1} = \frac{2\gamma}{(l + u)^2}C + \frac{2\gamma}{(l + u)^2}C^{-1}C^{-1}TT^{-1}C^{-1}$, where

$$T^{-1} = \begin{pmatrix} \frac{K_{LL}}{2l} + 2\gamma_A I \end{pmatrix}^{-1} \begin{pmatrix} 0 \end{pmatrix}, \quad \text{LapRLS}$$

$$T^{-1} = \begin{pmatrix} \frac{K_{LL}}{2l} + 2\gamma_A I \end{pmatrix}^{-1} \begin{pmatrix} 0 \end{pmatrix}, \quad \text{LapSVM}$$

Note that $P + \frac{2\gamma^2}{(l + u)^2}C^{-1}C^{-1}C \in \mathbb{R}^{c \times c}$, and the time complexity of $T^{-1}$ is $O(l^3)$ for LapRLS and $O(l^3)$ for LapSVM, so we only need $O(l^3 + c^3 + (l + u)c^3)$ and $O(l^3 + c^3 + (l + u)c^3)$ to compute the $H^{-1}$ for LapRLS and LapSVM, respectively.

Therefore, in this paper, we finally consider the use of the following fast $t$-fold CV for model selection:

$$t\text{-BIF} := \sum_{t=1}^{t} \sum_{i \in \mathcal{L}_i} V(y_j, y_j^m + \frac{B_{SVM}^i j_i}{1 - t}),$$
where $\tilde{B}$ is the approximation of $B$ with $\tilde{H}$ replace of $H$.

4.1 Time Complexity

To compute $t$-BIF, we need $O(l^3 + (l + u)c^2 + c^3)$ and $O(l^3 + c^3 + (l + u)c^2)$ to compute the $\tilde{H}^{-1}$ for LapRLS and LapSVM, and $O((l(l+u)+(l+u)c+u)(l+u)c)$ to compute $B$. Since $f_{LS}^*$ has been obtained in the training process, thus the overall time complexity of $t$-BIF for LapRLS is $O(l^3 + (l + u)c^2 + c^3 + t(l + u)c + (l + u)c + l(l + u)c + l + u))$, which is much faster than the traditional $t$-CV of time complexity $O\left(\frac{l-1}{l-1}l^3(l + u)^3\right)$, $l \ll u, c \ll u$.

5 Experiment

In this section, we will compare our proposed approximate $t$-CV ($t$-BIF) with the original $t$-CV ($t$-CV), $t = 5, 10, 20$. The data sets are 18 publicly available data sets from LIBSVM Data\textsuperscript{1}: 11 data sets for classification and 7 data sets for regression. All data sets are normalized to zero-mean and unit-variance on every attribute to avoid numerical problems. Experiments are performed on a single machine with two cores (Intel Xeon E5-2630@2.40GHz) and 64 GB memory. We use the Gaussian kernel $\kappa(x, x') = \exp\left(\frac{-\|x-x'\|^2}{2\sigma}\right)$ as our candidate kernel $\sigma \in \{2^i, i = -10, -8, \ldots, 10\}$. The candidate regularization parameters $\gamma_A \in \{10^i, i = -6, -5, \ldots, 2\}$, $\gamma_I \in \{10^i, i = -6, -5, \ldots, 2\}$. The candidate graph Laplacian parameters $k \in \{2, 4, 8\}$ and $\sigma_w \in \{2^i, i = -4, -2, \ldots, 4\}$.

The learning algorithm used in our experiments for regression is LapRLS and for classification is LapSVM. For each data set, we run all methods 30 times with randomly selected 70% of all data for training and the other 30% for testing. Meanwhile, from each train data, we randomly select 10% examples as labeled data. The use of multiple training/test partitions allows an estimate of the statistical significance of differences in performance between methods. Let $A_i$ and $B_i$ be the test errors of methods A and B in partition $i$, and $d_i = B_i - A_i$, $i = 1, \ldots, 30$. Let $\bar{d}$ and $S_d$ be the mean and standard error of $d_i$. Then under $t$-test, with confidence level 95%, we claim that A is significantly better than B (or equivalently B significantly worse than A) if the statistic $\frac{\bar{d}}{S_d/\sqrt{30}} > 1.699$. All statements of statistical significance in the remainder refer to a 95% level of significance.

5.1 Accuracy

The test errors for classification and test mean square errors for regression are reported in Table 1. For our $t$-BIF, we set $c = \sqrt{l + u}$ (in fact, we have tried many other setting of $c$ on some small datasets in advance, we find that if $c \geq \sqrt{l + u}$, the accuracy of our approximate CV is good, so in this paper, we set $c = \sqrt{l + u}$ on all dataset for simplicity) and set $h = 0.01$ for LapSVM (note that if $h$ is small, the Huber loss is a good approximation of Hinge loss, thus we set $h = 0.01$). The elements are obtained as follows: For each training set, we select the kernel parameter $\sigma$, the regularization parameters $\gamma_A$ and $\gamma_I$, the graph Laplacian parameters $k$ and $\sigma_w$, by each criterion on the training set, and evaluate the test error for the chosen parameters on the test set. The results in Table 1 can be summarized as follows: (1) Neither of $t$-CV and $t$-BIF for classification and regression is statistically superior at the 95% level of significance, $t=5, 10, 20$. (2) For regression, $t$-BIF gives almost the same testing errors as the traditional $t$-CV, $t=5, 10, 20$. In particular, on abalone, bodyfat, cpu small, mg. space-ga, $t$-BIF gives the same testing errors as $t$-CV. On the remaining data sets, both $t$-BIF and $t$-CV give the similar results.

The above results implicate that the quality of our approximation based on the BIF is quite good.

5.2 Efficiency

The run time of $t$-BIF and $t$-CV is reported in Table 2. We can find that $t$-BIF is much faster than $t$-CV. In particular, $t$-BIF is nearly $t$ (or more) times faster than $t$-CV on most data sets. For large datasets, such as a3a, w1a, w2a, cpusmall, 20-BIF is nearly 40 times faster than 20-CV. Thus, $t$-BIF significantly improves the efficiency of $t$-CV for model selection of manifold regularization.

6 Conclusion

In this paper, we present an approximate CV method based on the theoretical notion of BIF for manifold regularization in semi-supervised learning. The proposed approximate CV requires training on the full data only once, hence can significantly improve the efficiency. Experimental results on 18 data sets show that our approximate CV much more efficiency and has no statistical discrepancy when compared to the original one. This is an interesting attempt to apply the theoretical notion of BIF for practical model selection in semi-supervised learning.

Future work includes extending our results to other manifold regularization algorithms, such as square laplacian support vector machine and laplacian logistic regression.

Appendix: Proof of Theorem 1

Proof. The derivative of the objective function vanishes at the

$$-2\gamma_A f_{S}^{MR} = \frac{(J_{S} \phi_{S})^{T} \mu_{S}}{l} + \frac{2\gamma_I \phi_{S}^{T} L_{S} f_{S}^{S}}{(l + u)^{2}},$$

where $\phi_{S} = (\kappa(x_1), \ldots, \kappa(x_{l+u}))^{T}$, $\mu_{S}$ is an $l + u$ vector with the first $l$ entries as $e^{T}(y_j, f_{S}^{MR}(x_j))$, $(x_j, y_j) \in \mathcal{L}$ and the rest 0.

Denote $F_{S, s, l} = (1 - \epsilon)F_{S} + \epsilon F_{S, s}$, we can obtain that

$$-2\gamma_{M} f_{S_{s, l}} = \frac{(1 - \epsilon)(J_{S} \phi_{S})^{T} \mu_{S, l}}{l} + 2\gamma_I \phi_{S}^{T} L_{S} f_{S_{s, l}} + \frac{(1 - \epsilon)\gamma_{I} \phi_{S}^{T} L_{S} f_{S_{s, l}}}{(l + u)^{2}},$$

$$+ \frac{2\gamma_I \phi_{S}^{T} L_{S} f_{S_{s, l}}}{(m + n)^{2}}.$$
Table 2: The run time. Our methods: $t$-FBIF, compared methods: $t$-CV ($t$-CV), $t$=5,10,20.

| Classification | 5-CV  | 5-FBIF | 10-CV  | 10-FBIF | 20-CV  | 20-FBIF |
|---------------|-------|--------|--------|---------|--------|---------|
| a1a           | 36.80 | 8.55   | 87.50  | 9.16    | 251.46 | 15.23   |
| a2a           | 86.21 | 16.11  | 215.45 | 20.46   | 887.99 | 30.82   |
| a3a           | 155.01| 43.90  | 254.52 | 22.24   | 1161.33| 30.12   |
| fourclass     | 10.92 | 3.14   | 24.30  | 3.01    | 57.13  | 4.01    |
| german        | 10.47 | 2.77   | 22.69  | 3.05    | 48.57  | 4.21    |
| madelon       | 64.72 | 14.57  | 117.15 | 14.13   | 276.64 | 15.31   |
| svmguide3     | 15.82 | 4.43   | 25.93  | 5.89    | 56.29  | 7.02    |
| splice        | 11.43 | 4.33   | 30.92  | 4.78    | 64.53  | 5.62    |
| w1a           | 144.02| 22.69  | 382.56 | 23.47   | 1188.36| 37.31   |
| w2a           | 181.91| 26.04  | 595.33 | 30.89   | 1147.22| 29.14   |
| w3a           | 209.87| 29.40  | 458.01 | 23.88   | 721.27 | 17.75   |

Regression

| Classification | 5-CV  | 5-FBIF | 10-CV  | 10-FBIF | 20-CV  | 20-FBIF |
|---------------|-------|--------|--------|---------|--------|---------|
| abalone       | 101.09| 17.08  | 195.75 | 15.09   | 217.93 | 20.01   |
| bodfat        | 1.10  | 0.17   | 2.50   | 0.13    | 5.59   | 0.15    |
| cupsmall      | 212.43| 22.58  | 481.85 | 25.88   | 1706.09| 37.61   |
| mg            | 17.10 | 5.74   | 70.40  | 6.46    | 91.86  | 11.27   |
| mpg           | 1.58  | 0.20   | 4.20   | 0.18    | 9.20   | 0.19    |
| housing       | 1.29  | 0.17   | 3.18   | 0.15    | 7.25   | 0.16    |
| space-ga      | 70.68 | 20.58  | 151.87 | 18.58   | 443.62 | 16.68   |

where $\mu_{l+u}$ is an $l + u$ vector with the first $l$ entries as $\ell'(y_j, f_{j,F_{S,s_i}}(x_j))$, $(x_j, y_j) \in L$, and the rest 0, $\nabla f_{S,s_i}^F = (f_{S,s_i}^{MR}(x_1), \ldots, f_{S,s_i}^{MR}(x_{l+u}))^T$, $f_{S,s_i}^S = (f_{S,s_i}^{MR}(x_1), \ldots, f_{S,s_i}^{MR}(x_{m+n}))^T$, where $x_j \in T_i, \ S_i$ is an $(m+n) \times (m+n)$ diagonal matrix with the first $m$ diagonal entries as $\ell'(y_j, f_{j,F_{S,s_i}}(x_j))$, $(x_j, y_j) \in L_i$, and the rest 0, $\mu_{l+u}$ is an $(m+n)$ vector with the first $m$ entries as $\ell'(y_j, f_{j,F_{S,s_i}}(x_j))$, $(x_j, y_j) \in L_i$, and the rest 0.

Setting $\epsilon = 0$ on (9), we have $-2\gamma_A \frac{\partial f_{S,s_i}^F}{\partial \epsilon} \bigg|_{\epsilon=0} = -2\gamma_A \frac{\partial f_{S,s_i}^F}{\partial \epsilon} \bigg|_{\epsilon=0} = -2\gamma_A \nu_{l+u}^T \nu_{l+u} + \nu_{m+n}^T \nu_{m+n}$.

where $\frac{\partial f_{S,s_i}^F}{\partial \epsilon} = \frac{\partial f_{S,s_i}^{MR}}{\partial \epsilon}(x_1), \ldots, \frac{\partial f_{S,s_i}^{MR}}{\partial \epsilon}(x_{l+u})$, $\frac{\partial f_{S,s_i}^S}{\partial \epsilon} = \frac{\partial f_{S,s_i}^{MR}}{\partial \epsilon}(x_1), \ldots, \frac{\partial f_{S,s_i}^{MR}}{\partial \epsilon}(x_{m+n})$.

From equation (11), it is easy to verify that

$$-2\gamma_A \frac{\partial f_{S,s_i}^F}{\partial \epsilon} \bigg|_{\epsilon=0} = -2\gamma_A \nu_{l+u}^T \nu_{l+u} + \nu_{m+n}^T \nu_{m+n}$$
Since $\text{BIF}(\mathbb{P}_S; f^{\text{MR}}, \mathbb{P}_S)$ is the first order derivative of $f^{\text{MR}}_{P_S, S}$ at $\epsilon = 0$, we have $\mathbf{B}_{-i} = \left( \frac{\partial}{\partial \epsilon} f^S_{P_S, S} \bigg|_{\epsilon=0} \right)$. Substituting the above Equation into (12), which finishes the proof. 

\section*{References}

[Belkin et al., 2006] Mikhail Belkin, Partha Niyogi, and Vikas Sindhwani. Manifold regularization: A geometric framework for learning from labeled and unlabeled examples. \textit{Journal of machine learning research}, 7(Nov):2399–2434, 2006.

[Cawley and Talbot, 2004] Gavin C. Cawley and Nicola LC Talbot. Fast leave-one-out cross-validation of sparse least-squares support vector machines. \textit{Neural Networks}, 17(10):1467–1475, 2004.

[Cawley and Talbot, 2007] Gavin C. Cawley and Nicola L. C. Talbot. Preventing over-fitting during model selection via Bayesian regularisation of the hyper-parameters. \textit{Journal of Machine Learning Research}, 8:841–861, 2007.

[Cawley, 2006] Gavin C. Cawley. Leave-one-out cross-validation based model selection criteria for weighted LS-SVMs. In \textit{Proceeding of the International Joint Conference on Neural Networks (IJCNN 2006)}, pages 1661–1668, 2006.

[Chapelle et al., 2002] Olivier Chapelle, Vladimir Vapnik, Olivier Bousquet, and Sayan Mukherjee. Choosing multiple parameters for support vector machines. \textit{Machine Learning}, 46(1-3):131–159, 2002.

[Christmann and Messem, 2008] Andreas Christmann and Arnout Van Messem. Bouligand derivatives and robustness of support vector machines for regression. \textit{Journal of Machine Learning Research}, 9:915–936, 2008.

[Debruyne et al., 2008] Michiel Debruyne, Mia Hubert, and Johan A.K. Suykens. Model selection in kernel based regression using the influence function. \textit{Journal of Machine Learning Research}, 9:2377–2400, 2008.

[Debruyne, 2007] Michiel Debruyne. \textit{Robustness of censored depth quantiles, PCA and kernel based regression, with new tools for model selection}. PhD thesis, Katholieke Universiteit Leuven, 2007.

[Hampel et al., 1986] Frank R Hampel, Elvezio M Ronchetti, Peter J Rousseeuw, and Werner A Stahel. \textit{Robust statistics: The approach based on influence functions}. Wiley, New York, 1986.

[Josse and Husson, 2012] Julie Josse and François Husson. Selecting the number of components in principal component analysis using cross-validation approximations. \textit{Computational Statistics and Data Analysis}, 56(6):1869–1879, 2012.

[Keerthi, 2002] Sathiya Keerthi. Efficient tuning of svm hyperparameters using radius/margin bound and iterative algorithms. \textit{IEEE Transactions on Neural Networks}, 13(5):1225–1229, 2002.

[Liu et al., 2014] Yong Liu, Shali Jiang, and Shizhong Liao. Efficient approximation of cross-validation for kernel methods using Bouligand influence function. In \textit{Proceedings of The 31st International Conference on Machine Learning (ICML 2014 (1))}, pages 324–332, 2014.

[Liu et al., 2018] Yong Liu, Hailun Lin, Li-Zhong Ding, Weiping Wan, and Shizhong Liao. Fast cross-validation. In \textit{Proceedings of the 27th International Joint Conference on Artificial Intelligence (IJCAI)}, pages 2497–2503, 2018.

[Liu et al., 2019] Yong Liu, Shizhong Liao, Shali Jiang, Lizhong Ding, Hailun Lin, and Weiping Wang. Fast cross-validation for kernel-based algorithms. \textit{IEEE Transactions on Pattern Analysis and Machine Intelligence}, 2019.

[Melacci and Belkin, 2011] Stefano Melacci and Mikhail Belkin. Laplacian support vector machines trained in the primal. \textit{Journal of Machine Learning Research}, 12:1149–1184, 2011.

[Opper and Winther, 1999] Manfred Opper and Ole Winther. Gaussian processes and SVM: Mean field and leave-one-out. In \textit{Advances in Large Margin Classifiers}, pages 311–326, 1999.

[Robinson, 1991] Stephen M Robinson. An implicit-function theorem for a class of nonsmooth functions. \textit{Mathematics of Operations Research}, 16:292–309, 1991.

[Sindhwani et al., 2005] Vikas Sindhwani, Partha Niyogi, Mikhail Belkin, and Sathiya Keerthi. Linear manifold regularization for large scale semi-supervised learning. In \textit{Proceedings of the 22nd ICML Workshop on Learning with Partially Classified Training Data}, volume 28, 2005.

[Vapnik and Chapelle, 2000] Vladimir Vapnik and Olivier Chapelle. Bounds on error expectation for support vector machines. \textit{Neural Computation}, 12(9):2013–2036, 2000.