
Multi-Class Learning: From Theory to Algorithm

Jian Li^{1,2}, Yong Liu^{1*}, Rong Yin^{1,2}, Hua Zhang¹, Lizhong Ding⁵, Weiping Wang^{1,3,4}

¹Institute of Information Engineering, Chinese Academy of Sciences

²School of Cyber Security, University of Chinese Academy of Sciences

³National Engineering Research Center for Information Security

⁴National Engineering Laboratory for Information Security Technology

⁵Inception Institute of Artificial Intelligence (IIAI), Abu Dhabi, UAE

{lijian9026, liuyong, yinrong, wangweiping}@iie.ac.cn

lizhong.ding@inceptioniai.org

Abstract

In this paper, we study the generalization performance of multi-class classification and obtain a sharper data-dependent generalization error bound with fast convergence rate, substantially improving the state-of-art bounds in the existing data-dependent generalization analysis. The theoretical analysis motivates us to devise two effective multi-class kernel learning algorithms with statistical guarantees. Experimental results show that our proposed methods can significantly outperform the existing multi-class classification methods.

1 Introduction

Multi-class classification is an important problem in various applications, such as natural language processing, information retrieval, computer vision, web advertising, etc. The statistical learning theory of binary classification is by now relatively well developed [19, 20, 21, 23, 27, 34], but there are still numerous statistical challenges to its multi-class extensions [25].

To understand the existing multi-class classification algorithms and guide the development of new ones, people have investigated the generalization ability of multi-class classification algorithms. In recent years, some generalization bounds have been proposed to estimate the ability of multi-class classification algorithms based on different measures, such as VC-dimension [1], Natarajan dimension [7], covering Number [9, 11, 37], Rademacher Complexity [5, 14, 27], Stability [10], PAC-Bayesian [26], etc. Although there have been several recent advances in the studying of generalization bounds of multi-class classification algorithms, convergence rates of the existing generalization bounds are usually $\mathcal{O}(K^2/\sqrt{n})$, where K and n are the number of classes and size of the sample, respectively.

In this paper, we derive a novel data-dependent generalization bound for multi-class classification via the notion of local Rademacher complexity and further devise two effective multi-class kernel learning algorithms based on the above theoretical analysis. The rate of this bound is $\mathcal{O}((\log K)^{2+1/\log K}/n)$, which substantially improves on the existing data-dependent generalization bounds. Moreover, the proposed multi-class kernel learning algorithms have statistical guarantees and fast convergence rates. Experimental results on lots of benchmark datasets show that our proposed methods can significantly outperform the existing multi-class classification methods. The major contributions of this paper include: 1) A new local Rademacher complexity based bound with fast convergence rate for multi-class classification is established. Existing works [16, 27] for multi-class classifiers with Rademacher complexity does not take into account couplings among different classes. To obtain sharper bound, we introduce a new structural complexity result on function classes induced by general classes via the maximum operator, while allowing to preserve the correlations among

*Corresponding author

different components meanwhile. Thus, our result in this paper is a non-trivial extension of the binary classification of local Rademacher complexity to multi-classification; 2) Two novel multi-class classification algorithms are proposed with statistical guarantees: a) Conv-MKL. Using precomputed kernel matrices regularized by local Rademacher complexity, this method can be implemented by any ℓ_p -norm multi-class MKL solvers; b) SMSD-MKL. This method puts local Rademacher complexity in penalized ERM with $\ell_{2,p}$ -norm regularizer, implemented by stochastic sub-gradient descent with updating dual weights.

2 Related Work

2.1 Multi-Class Classification Bounds

Rademacher Complexities Bounds. Koltchinskii and Panchenko [14] and Koltchinskii, Panchenko, and Lozano [15] first introduced a margin-based bound for multi-class classification in terms of Rademacher complexity. This bound was slightly improved in [27, 5]. Maximov and Reshetova [25] gave a new Rademacher complexity based bound that is linear in the number of classes. Based on the ℓ_p -norm regularization, Lei, Binder, and Kloe [18] introduced a bound with a logarithmic dependence on the number of class size. Instead of global Rademacher complexity, in this paper, we use local Rademacher complexity to obtain a sharper bound, which substantially improves generalization performance upon existing global Rademacher complexity methods.

VC-dimension Bounds. Allwein, Schapire, and Singer [1] used the notion of VC-dimension for multi-class learning problems, and derived a VC-dimension based bound. Natarajan dimension was introduced in [28] in order to characterize multi-class PAC learnability, which exactly matches the notion of Vapnik-Chervonenkis dimension in the case of binary classification. Daniely and Shalev-Shwartz [7] derived a risk bound with Natarajan dimension for multi-class classification. VC dimension and Natarajan dimension are important tools to derive generalization bounds, however, these bounds are usually dimension dependent, which makes them hardly applicable to practical large-scale problems (such as typical computer vision problems).

Covering Number Bounds. Based on the ℓ_∞ -norm covering number bound of linear operators, Guermur [9] obtained a generalization bound exhibiting a linear dependence on the class size, which was improved by [37] to a radical dependence. Hill and Doucet [11] derived a class-size independent risk guarantee. However, their bound is based on a delicate definition of margin, which is not commonly used in mainstream multi-class literature.

Stability Bounds and PAC-Bayesian Bounds. Stability [10] and PAC-Bayesian [26] are two popular tools to analyze generalization performance on neural networks for multi-class setting. Hardt, Recht and Singer [10] generated generalization bounds for models learned with stochastic gradient descent. McAllester [26] proposed a dropout bound for neural networks with PAC-Bayesian. However, the convergence rate based on stability and PAC-Bayesian is usually at most $\mathcal{O}(1/\sqrt{n})$.

2.2 Local Rademacher Complexity

In recent years, several authors have applied *local* Rademacher complexity to obtain better generalization error bounds for traditional binary classification [2, 13, 22, 24], similar analysis has been explored in multi-label learning [35] and multi-task learning [36] as well. However, numerous statistical challenges remain in the multi-class case, and it is still unclear how to use this tool to derive a tighter bound for multi-class. In this paper, we bridge this gap by deriving a sharper generalization bound using local Rademacher complexity.

2.3 Multi-Class Kernel Learning Algorithms

As one of the success stories in multiple kernel learning, improvements in multi-class MKL have emerged [38], in which a one-stage multi-class MKL algorithm was presented as a generalization of multi-class loss function [6, 33]. And Orabona designed stochastic gradient methods, named OBSCURE [30] and UFO-MKL [29], which optimize primal versions of equivalent problems. In this paper, we consider the use of the local Rademacher complexity to devise the novel multi-class classification algorithms, which have statistical guarantees and fast convergence rates.

3 Notations and Preliminaries

We consider multi-class classification problems with $K \geq 2$ classes in this paper. Let \mathcal{X} be the input space and $\mathcal{Y} = \{1, 2, \dots, K\}$ the output space. Assume that we are given a sample $\mathcal{S} = \{z_1 = (\mathbf{x}_1, y_1), \dots, z_n = (\mathbf{x}_n, y_n)\}$ of size n drawn i.i.d. from a fixed, but unknown probability distribution μ on $\mathcal{Z} = \mathcal{X} \times \mathcal{Y}$. Based on the training examples \mathcal{S} , we wish to learn a scoring rule h from a space \mathcal{H} mapping from \mathcal{Z} to \mathbb{R} and use the mapping $\mathbf{x} \rightarrow \arg \max_{y \in \mathcal{Y}} h(\mathbf{x}, y)$ to predict. For any hypothesis $h \in \mathcal{H}$, the margin of a labeled example $z = (\mathbf{x}, y)$ is defined as

$$\rho_h(z) := h(\mathbf{x}, y) - \max_{y' \neq y} h(\mathbf{x}, y').$$

The h misclassifies the labeled example $z = (\mathbf{x}, y)$ if $\rho_h(z) \leq 0$ and thus the expected risk incurred from using h for prediction is $L(h) := \mathbb{E}_\mu[1_{\rho_h(z) \leq 0}]$, where $1_{t \leq 0}$ is the 0-1 loss, $1_{t \leq 0} = 1$ if $t \leq 0$, otherwise 0. Since 0-1 loss is hard to handle in learning machines, one usually considers the proxy loss: such as the square hinge $\ell(t) = (1 - t)_+^2$ and the square margin loss $\ell^s(t) = (1_{t \leq 0} + (1 - ts^{-1})1_{0 < t \leq s})^2$, $s > 0$. In the following, we assume that: 1) $\ell(t)$ bounds the 0-1 loss: $1_{t \leq 0} \leq \ell(t)$; 2) ℓ is decreasing and it has a zero point c_ℓ , i.e., $\ell(c_\ell) = 0$; 3) ℓ is ζ -smooth, that is $|\ell'(t) - \ell'(s)| \leq \zeta|t - s|$. Note that both square hinge loss and margin loss satisfy the above assumptions.

Any function $h : \mathcal{X} \times \mathcal{Y} \rightarrow \mathbb{R}$ can be equivalently represented by the vector-valued function (h_1, \dots, h_K) with $h_j(\mathbf{x}) = h(\mathbf{x}, j)$, $\forall j = 1, \dots, K$. Let $\kappa : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ be a Mercer kernel with ϕ being the associated feature map, i.e., $\kappa(\mathbf{x}, \mathbf{x}') = \langle \phi(\mathbf{x}), \phi(\mathbf{x}') \rangle$. The ℓ_p -norm hypothesis space associated with the kernel κ is denoted by:

$$\mathcal{H}_{p,\kappa} = \left\{ h_{\mathbf{w}} = (\langle \mathbf{w}_1, \phi(\mathbf{x}) \rangle, \dots, \langle \mathbf{w}_K, \phi(\mathbf{x}) \rangle) : \|\mathbf{w}\|_{2,p} \leq 1, 1 \leq p \leq 2 \right\}, \quad (1)$$

where $\mathbf{w} = (\mathbf{w}_1, \dots, \mathbf{w}_K)$ and $\|\mathbf{w}\|_{2,p} = \left[\sum_{i=1}^K \|\mathbf{w}_i\|_2^p \right]^{\frac{1}{p}}$ is the $\ell_{2,p}$ -norm. For any $p \geq 1$, let q be the dual exponent of p satisfying $1/p + 1/q = 1$.

The space of loss function associated with $\mathcal{H}_{p,\kappa}$ is denoted by

$$\mathcal{L} = \{\ell_h := \ell(\rho_h(z)) : h \in \mathcal{H}_{p,\kappa}\}. \quad (2)$$

Let $L(\ell_h)$ and $\hat{L}(\ell_h)$ be expected generalization error and empirical error with respect to ℓ_h :

$$L(\ell_h) := \mathbb{E}_\mu[\ell(\rho_h(z))] \text{ and } \hat{L}(\ell_h) = \frac{1}{n} \sum_{i=1}^n \ell(\rho_h(z_i)).$$

Definition 1 (Rademacher complexity). Assume \mathcal{L} is a space of loss functions as defined in Equation (2). Then the empirical Rademacher complexity of \mathcal{L} is:

$$\hat{\mathcal{R}}(\mathcal{L}) := \mathbb{E}_\sigma \left[\sup_{\ell_h \in \mathcal{L}} \frac{1}{n} \sum_{i=1}^n \sigma_i \ell_h(z_i) \right],$$

where $\sigma_1, \sigma_2, \dots, \sigma_n$ is an i.i.d. family of Rademacher variables taking values -1 and 1 with equal probability independent of the sample $\mathcal{S} = (z_1, \dots, z_n)$. The Rademacher complexity of \mathcal{L} is $\mathcal{R}(\mathcal{L}) = \mathbb{E}_\mu \hat{\mathcal{R}}(\mathcal{L})$.

Generalization bounds based on the notion of Rademacher complexity for multi-class classification are standard [14, 15, 27]: with probability $1 - \delta$, $L(h) \leq \inf_{0 < \gamma < 1} (\hat{L}(h_\gamma) + \mathcal{O}(\mathcal{R}(\mathcal{L})/\gamma + \log(1/\delta)/\sqrt{n}))$, where $\hat{L}(h_\gamma) = \frac{1}{n} \sum_{i=1}^n [1_{\rho_h(z_i) \leq \gamma}]$. Since $\mathcal{R}(\mathcal{L})$ is in the order of $\mathcal{O}(K^2/\sqrt{n})$ for various kernel multi-class in practice, so the standard Rademacher complexity bounds converge at rate $\mathcal{O}(K^2/\sqrt{n})$, usually.

Although Rademacher complexity is widely used in bound generalization analysis, it does not take into consideration the fact that, typically, the hypotheses selected by a learning algorithm have a better performance than in the worst case and belong to a more favorable sub-family of the set of all hypotheses [4]. Therefore, to derive sharper generalization bound, we consider the use of the local Rademacher complexity in this paper.

Definition 2 (Local Rademacher Complexity). *For any $r > 0$, the local Rademacher complexity of \mathcal{L} is defined as*

$$\mathcal{R}(\mathcal{L}^r) := \mathcal{R} \left\{ a\ell_h \mid a \in [0, 1], \ell_h \in \mathcal{L}, L[(a\ell_h)^2] \leq r \right\},$$

where $L(\ell_h^2) = \mathbb{E}_\mu [\ell^2(\rho_h(z))]$.

The key idea to obtain sharper generalization error bound is to choose a much smaller class $\mathcal{L}^r \subseteq \mathcal{L}$ with as small a variance as possible, while requiring that the solution is still in $\{h \mid h \in \mathcal{H}_{p,\kappa}, \ell_h \in \mathcal{L}^r\}$.

In the following, we assume that $\vartheta = \sup_{\mathbf{x} \in \mathcal{X}} \kappa(\mathbf{x}, \mathbf{x}) < \infty$, and $\ell_h : \mathcal{Z} \rightarrow [0, d]$, $d > 0$ is a constant. The above two assumptions are two common restrictions on kernel function and loss functions, which are satisfied by the popular Gaussian kernels and the bounded hypothesis, respectively.

4 Sharper Generalization Bounds

In this section, we first estimate the local Rademacher complexity, and further derive a sharper generalization bound.

4.1 Local Rademacher Complexity

The estimate the local Rademacher complexity of multi-class classification is given as follows.

Theorem 1. *With probability at least $1 - \delta$,*

$$\mathcal{R}(\mathcal{L}^r) \leq \frac{c_{d,\vartheta} \xi(K) \sqrt{\zeta r} \log^{\frac{3}{2}}(n)}{\sqrt{n}} + \frac{4 \log(1/\delta)}{n},$$

where

$$\xi(K) = \begin{cases} \sqrt{e} (4 \log K)^{1 + \frac{1}{2 \log K}}, & \text{if } q \geq 2 \log K, \\ (2q)^{1 + \frac{1}{q}} K^{\frac{1}{q}}, & \text{otherwise,} \end{cases}$$

$c_{d,\vartheta}$ is a constant depends on d and ϑ .

Note that the order of the (global) Rademacher complexity over \mathcal{L} is usually $\mathcal{O}(K^2/\sqrt{n})$ for various kernel multi-classes. From Theorem 1, one can see that the order of the local Rademacher complexity is $\mathcal{R}(\mathcal{L}^r) = \mathcal{O}(\sqrt{r} \xi(K)/\sqrt{n} + 1/n)$. Note that $\xi(K)$ is logarithmic dependence on K when $q \geq 2 \log K$. For $2 \leq q < 2 \log K$, $\xi(K) = \mathcal{O}(K^{\frac{2}{q}})$ which is also substantially milder than the quadratic dependence for Rademacher complexity. If we choose a suitable value of r , the order can even reach $\mathcal{O}((\log K)^{2+1/\log K}/n)$ (see in the next subsection), which substantially improves the Rademacher complexity bounds.

4.2 A Sharper Generalization Bound

A sharper bound for multi-class classification based on the notion of local Rademacher complexity is derived as follows.

Theorem 2. $\forall h \in \mathcal{H}_{p,\kappa}$ and $\forall k > \max(1, \frac{\sqrt{2}}{2d})$, with probability at least $1 - \delta$, we have

$$L(h) \leq \max \left\{ \frac{k}{k-1} \hat{L}(\ell_h), \hat{L}(\ell_h) + \frac{c_{d,\vartheta,\zeta,k} \xi^2(K) \log^3 n}{n} + \frac{c_\delta}{n} \right\},$$

where

$$\xi(K) = \begin{cases} \sqrt{e} (4 \log K)^{1 + \frac{1}{2 \log K}}, & \text{if } q \geq 2 \log K, \\ (2q)^{1 + \frac{1}{q}} K^{\frac{1}{q}}, & \text{otherwise,} \end{cases}$$

$c_{d,\vartheta}$ is a constant depending on d, ϑ, ζ, k , and c_δ is a constant depending on δ .

The order of the generalization bound in Theorem 2 is $\mathcal{O}(\xi^2(K)/n)$. From the definition of $\xi(K)$, we can obtain that

$$\mathcal{O}\left(\frac{\xi^2(K)}{n}\right) = \begin{cases} \mathcal{O}\left((\log K)^{2+1/\log K}/n\right), & \text{if } q \geq 2 \log K, \\ \mathcal{O}\left(K^{2/q}/n\right), & \text{if } 2 \leq q < 2 \log K. \end{cases}$$

Note that our bounds is linear dependence on the reciprocal of sample size n , while for the existing data-dependent bounds are all radical dependence. Furthermore, our bounds enjoy a mild dependence on the number of classes. The dependence is polynomial with degree $2/q$ for $2 \leq q < 2 \log K$ and becomes logarithmic if $q \geq 2 \log K$, which is substantially milder than the quadratic dependence established in [14, 15, 27, 5].

4.3 Comparison with the Related Work

Rademacher Complexity Bounds Koltchinskii and Panchenko [14] and Koltchinskii, Panchenko, and Lozano [15] introduce a margin-based bound for multi-class classification in terms of Rademacher complexities: $L(h) \leq \inf_{0 < \gamma < 1} \hat{L}(h_\gamma) + \mathcal{O}\left(\frac{K^2}{\gamma\sqrt{n}} + \frac{\log 1/\delta}{\sqrt{n}}\right)$. The order is $\mathcal{O}\left(\frac{K^2}{\sqrt{n}}\right)$, which is slightly improved (by a constant factor prior to the Rademacher complexity term) by [27, 5]. Maximov and Reshetova [25] give a new Rademacher complexity bound: $L(h) \leq \inf_{0 < \gamma < 1} \hat{L}(h_\gamma) + \mathcal{O}\left(K/(\gamma\sqrt{n}) + \log(1/\delta)/\sqrt{n}\right)$, which has the form of $\mathcal{O}(K/\sqrt{n})$. Based on the ℓ_p -norm regularization, Lei, Binder, and Klof [18] derive a new bound: $L(h) \leq \hat{L}(\ell_h) + \mathcal{O}(\log^2 K/\sqrt{n})$. The existing bounds based on Rademacher complexity are all radical dependence on the reciprocal of sample size.

In this paper, we derive a sharper bound based on the local Rademacher complexity with order $\mathcal{O}((\log K)^{2+\frac{1}{\log K}}/n)$, substantially sharper than the existing bounds of Rademacher complexity.

Covering Number Bounds Based on the ℓ_∞ -norm covering number bound of linear operators, Guermur [9] obtains a generalization of form $\mathcal{O}(K/\sqrt{n})$, which is improved by [37] to a radical dependence: $L(h) \leq \hat{L}(\ell_h) + \mathcal{O}(\sqrt{K/n})$. Hill and Doucet [11] derive a class-size independent risk guarantee of form $\mathcal{O}(\sqrt{1/n})$. However, their bound is based on a delicate definition of margin, which is not commonly used in mainstream multi-class literature.

VC-dimension Bounds VC-dimension is an important tool to derive the generalization bound for binary classification. Allwein, Schapire, and Singer [1] show how to use it for multi-class learning problems, and derive a VC-dimension based bounds: $L(h) \leq \hat{L}(h_\gamma) + \mathcal{O}(\sqrt{V \log K}/\sqrt{n})$, where V is the VC-dimension. Natarajan dimension is introduced in [28] in order to characterize multi-class PAC learnability. Daniely and Shalev-Shwartz [7] derive a generalization bound with Natarajan dimension: $L(h) \leq \hat{L}(h_\gamma) + \mathcal{O}(d_{Nat}/n)$, where d_{Nat} is the Natarajan dimension. Note that VC dimension bounds, as well as Natarajan dimension bounds, are usually dimension dependent, which makes them hardly applicable for practical large scale problems (such as typical computer vision problems).

Stability and PAC-Bayesian Bounds Stability [10] and PAC-Bayesian [26] are two useful tools to analyze generalization performance on neural networks for a multi-class setting. Hardt, Recht and Singer [10] generated generalization bounds for models learned with stochastic gradient descent using stability: $L(h) \leq \hat{L}(h_\gamma) + \mathcal{O}(1/\sqrt{n})$. McAllester [26] used the PAC-Bayesian theory to derive generalization bound: $L(h) \leq \hat{L}(h_\gamma) + \mathcal{O}(\sqrt{\hat{L}(h_\gamma)/n})$.

5 Multi-Class Multiple Kernel Learning

Motivated by the above analysis of generalization bound, we will exploit the properties of the local Rademacher complexity to devise two algorithms for multi-class multiple kernel learning (MC-MKL).

In this paper, we consider the use of multiple kernels, $\kappa_\mu = \sum_{m=1}^M \mu_m \kappa_m$. A common approach to multi-class classification is the use of joint feature maps $\phi(\mathbf{x}) : \mathcal{X} \rightarrow \mathcal{H}$ [33]. For multiple kernel learning, we have M feature mappings ϕ_m , $m = 1, \dots, M$ and $\kappa_m(\mathbf{x}, \mathbf{x}') = \langle \phi_m(\mathbf{x}), \phi_m(\mathbf{x}') \rangle$, where $m = 1, \dots, M$. Let $\phi_\mu(\mathbf{x}) = [\phi_1(\mathbf{x}), \dots, \phi_M(\mathbf{x})]$. Using Theorem 2, to obtain a shaper

generalization bound, we confine $q \geq 2 \log K$, thus $1 < p \leq \frac{2 \log K}{2 \log K - 1}$. The ℓ_p hypothesis space of multiple kernels can be written as:

$$\mathcal{H}_{mkl} = \left\{ h_{\mathbf{w}, \kappa_{\mu}} = (\langle \mathbf{w}_1, \phi_{\mu}(\mathbf{x}) \rangle, \dots, \langle \mathbf{w}_K, \phi_{\mu}(\mathbf{x}) \rangle), \|\mathbf{w}\|_{2,p} \leq 1, 1 < p \leq \frac{2 \log K}{2 \log K - 1} \right\}.$$

5.1 Conv-MKL

The global Rademacher complexity of \mathcal{H}_{mkl} can be bounded by the trace of kernel matrix $\mathbf{K}_{\mu} = \sum_{m=1}^M \mathbf{K}_m$. Existing works on [17, 32] use the following constraint to \mathcal{H}_{mkl} : $\text{Tr}(\mathbf{K}_{\mu}) \leq 1$. According to the above theoretical analysis, the local Rademacher complexity (the tail sum of the eigenvalues of the kernel) leads to tighter generalization bounds than the global Rademacher complexity (the trace). Thus, we add the local Rademacher complexity to restrict \mathcal{H}_{mkl} :

$$\mathcal{H}_1 = \left\{ h_{\mathbf{w}, \kappa_{\mu}} \in \mathcal{H}_{mkl} : \sum_{j > \zeta} \lambda_j(\mathbf{K}_{\mu}) \leq 1 \right\},$$

where $\lambda_j(\mathbf{K}_{\mu})$ is the j -th eigenvalues of \mathbf{K}_{μ} and ζ is free parameter removing the ζ largest eigenvalues to control the tail sum. Note that the tail sum is the difference between the trace and the ζ largest eigenvalues: $\sum_{j > \zeta} \lambda_j(\mathbf{K}_{\mu}) = \text{Tr}(\mathbf{K}_{\mu}) - \sum_{j=1}^{\zeta} \lambda_j(\mathbf{K}_{\mu})$, thus the tail sum can be calculated in $O(n^2 \zeta)$ for each kernel.

One can see that \mathcal{H}_1 is not convex, and we know that: $\sum_{m=1}^M \mu_m \sum_{j > \zeta} \lambda_j(\mathbf{K}_m) = \sum_{m=1}^M \mu_m / \|\mu\|_1 \sum_{j > \zeta} \lambda_j(\|\mu\|_1 \mathbf{K}_m) \leq \sum_{j > \zeta} \lambda_j(\mathbf{K}_{\mu})$. Thus, we consider the use of the convex \mathcal{H}_2 :

$$\mathcal{H}_2 = \left\{ h_{\mathbf{w}, \kappa_{\mu}} \in \mathcal{H}_{mkl} : \sum_{m=1}^M \mu_m \sum_{j > \zeta} \lambda_j(\mathbf{K}_m) \leq 1 \right\}.$$

According to normalized kernels $\tilde{\kappa}_m = \left(\sum_{j > \zeta} \lambda_j(\mathbf{K}_m) \right)^{-1} \kappa_m$ and $\tilde{\kappa}_{\mu} = \sum_{m=1}^M \mu_m \tilde{\kappa}_m$, we can simply rewrite \mathcal{H}_2 as $\left\{ h_{\mathbf{w}, \tilde{\kappa}_{\mu}} = (\langle \mathbf{w}_1, \tilde{\phi}_{\mu}(\mathbf{x}) \rangle, \dots, \langle \mathbf{w}_K, \tilde{\phi}_{\mu}(\mathbf{x}) \rangle), \|\mathbf{w}\|_{2,p} \leq 1, 1 < p \leq \frac{2 \log K}{2 \log K - 1}, \mu \succeq 0, \|\mu\|_1 \leq 1 \right\}$, which is a commonly studied hypothesis class in multi-class multiple kernel learning. A simple process with precomputed kernel matrices regularized by local Rademacher complexity can be seen in Algorithm 1:

Algorithm 1 Conv-MKL

Input: precomputed kernel matrices $\mathbf{K}_1, \dots, \mathbf{K}_M$ and ζ
for $i = 1$ **to** M **do**
 Compute tail sum: $r_m = \sum_{j > \zeta} \lambda_j(\mathbf{K}_m)$
 Normalize precomputed kernel matrix: $\tilde{\mathbf{K}}_m = \mathbf{K}_m / r_m$
end for
Use $\tilde{\mathbf{K}}_m, m = 1, \dots, M$, as the basic kernels in any ℓ_p -norm MKL solver

5.2 SMSD-MKL

Considering a more challenging case, we perform penalized ERM over the class \mathcal{H}_1 , aiming to solve a convex optimization problem with an additional term representing local Rademacher complexity:

$$\min_{\mathbf{w}, \mu} \underbrace{\frac{1}{n} \sum_{i=1}^n \ell(\mathbf{w}, \phi_{\mu}(\mathbf{x}_i), y_i)}_{C(\mathbf{w})} + \underbrace{\frac{\alpha}{2} \|\mathbf{w}\|_{2,p}^2 + \beta \sum_{m=1}^M \mu_m r_m}_{\Omega(\mathbf{w})}, \quad (3)$$

where $\ell(\mathbf{w}, \phi_{\mu}(\mathbf{x}_i), y_i) = \left| 1 - \left(\langle \mathbf{w}_{y_i}, \phi_{\mu}(\mathbf{x}_i) \rangle - \max_{y \neq y_i} \langle \mathbf{w}_y, \phi_{\mu}(\mathbf{x}_i) \rangle \right) \right|_+$ and $r_m = \sum_{j > \zeta} \lambda_j(\mathbf{K}_m)$ is the tail sum of the eigenvalues of the m -th kernel matrix, $m = 1, \dots, M$.

Algorithm 2 SMSD-MKL

Input: α, β, r, T
Initialize: $\mathbf{w}^1 = \mathbf{0}, \boldsymbol{\theta}^1 = \mathbf{0}, \boldsymbol{\mu}^1 = \mathbf{1}, q = 2 \log K$
for $t = 1$ **to** T **do**
 Sample at random (\mathbf{x}^t, y^t)
 Compute the dual weight: $\boldsymbol{\theta}^{t+1} = \boldsymbol{\theta}^t - \partial C(\mathbf{w}^t)$
 $\nu_m^{t+1} = \|\boldsymbol{\theta}_m^{t+1}\| - t\beta r_m, \forall m = 1, \dots, M$
 $\mu_m^{t+1} = \frac{\text{sgn}(\nu_m^{t+1})|\nu_m^{t+1}|^{q-1}}{\alpha\|\boldsymbol{\theta}_m^{t+1}\|\|\nu_m^{t+1}\|_q^{q-2}}, \forall m = 1, \dots, M$
end for

Based on the stochastic mirror descent framework for minimization problems in [31, 29], we design a stochastic mirror and sub-gradient descent algorithm, called SMSD-MKL, to minimize (3), seen in Algorithm 2.

As shown in the mirror descent algorithm, it maintains two weight vectors: the primal vector \mathbf{w} and the dual vector $\boldsymbol{\theta}$. Meanwhile, the optimization formulation can be divided into two parts: $C(\mathbf{w})$ to update $\boldsymbol{\theta}$ and $\Omega(\mathbf{w})$ to update \mathbf{w} by the gradient of the Fenchel dual of Ω . Actually, the algorithm puts the kernel weight $\boldsymbol{\mu}$ aside when updating $\boldsymbol{\theta}$, but $\boldsymbol{\mu}$ is updated together with \mathbf{w} according to a tricky link function given in Theorem 3.

- For $C(\mathbf{w})$, the algorithm updates the dual vector with the gradient of $C(\mathbf{w})$. Since hinge loss used in $C(\mathbf{w})$ is not differentiable, the algorithm uses sub-gradient of $z^t = \partial \ell(\mathbf{w}^t, \phi_{\boldsymbol{\mu}}(\mathbf{x}^t), y^t)$, where $\partial \ell(\mathbf{w}^t, \phi_{\boldsymbol{\mu}}(\mathbf{x}^t), y^t)$ is the sub-gradient w.r.t \mathbf{w}^t .
- For $\Omega(\mathbf{w})$, as in the UFO-MKL [29], the algorithm uses $\mathbf{w} = \nabla \Omega^*(\boldsymbol{\theta})$ to update the primal vector \mathbf{w} , of which the calculation has been given in Theorem 3.

The algorithm starts with $\mathbf{w}^1 = \mathbf{0}, \boldsymbol{\theta}^1 = \mathbf{0}$ and $\boldsymbol{\mu}^1 = \mathbf{1}$. Especially, the algorithm initializes $q = 2 \log K$ to make the order of generalization reach $\mathcal{O}\left(\frac{(\log K)^{2+1/\log K}}{n}\right)$, according to Theorem 2. In each iteration, the algorithm randomly samples a training example from the train set.

Actually, the algorithm updates real numbers $\|\boldsymbol{\theta}_m^{t+1}\|, \nu_m^{t+1}$ and μ_m^{t+1} in scalar products instead of high-dimensional variables \mathbf{w}^{t+1} and $\boldsymbol{\theta}_m^{t+1}$. The $\|\boldsymbol{\theta}_m^{t+1}\|$ can be calculated in an efficient incremental way by scalar values as following:

$$\|\boldsymbol{\theta}_m^{t+1}\|_2^2 = \|\boldsymbol{\theta}_m^t - z_m^t\|_2^2 = \|\boldsymbol{\theta}_m^t\|_2^2 - 2\boldsymbol{\theta}_m^t \cdot z_m^t + \|z_m^t\|_2^2$$

where $z^t = \partial \ell(\mathbf{w}^t, \phi_{\boldsymbol{\mu}}(\mathbf{x}^t), y^t)$.

Theorem 3. Let $\boldsymbol{\nu} = [\|\boldsymbol{\theta}_1\| - \beta r_1, \dots, \|\boldsymbol{\theta}_M\| - \beta r_M]$, then the component m -th of $\nabla \Omega^*(\boldsymbol{\theta})$ is

$$\frac{\text{sgn}(\nu_m)\boldsymbol{\theta}_m |\nu_m|^{q-1}}{\alpha\|\boldsymbol{\theta}_m\| \|\boldsymbol{\nu}\|_q^{q-2}},$$

where $\text{sgn}(x)$ is defined as $\text{sgn}(x) = 1$ if $x > 0$, $\text{sgn}(x) = -1$ if $x < 0$ and $\text{sgn}(x) \in [-1, +1]$, if $x = 0$.

6 Experiments

In this section, we compare our proposed Conv-MKL (Algorithm 1) and SMSD-MKL (Algorithm 2) with 7 popular multi-class classification methods: One-against-One [12], One-against-the-Rest [3], ℓ_1 -norm linear multi-class SVM (LMC) [6], generalized minimal norm problem solver (GMNP) [8], the Multiclass MKL (MC-MKL) with ℓ_1 -norm and ℓ_2 -norm [38] and mixed-norm MKL solved by stochastic gradient descent (UFO-MKL) [29]. Actually, we complete comparison tests via implements in LIBSVM (One-against-One and One-against-the-Rest), the DOGMA library² (LMC, GMNP, ℓ_1 -norm and ℓ_2 -norm MC-MKL) and the SHOGUN-6.1.3³ (UFO-MKL). We implement our proposed Conv-MKL and SMSD-MKL algorithms based on UFO-MKL.

²Available at <http://dogma.sourceforge.net>

³Available at <http://www.shogun-toolbox.org/>

Table 1: Comparison of average test accuracies of our Conv-MKL and SMSD-MKL with the others. We bold the numbers of the best method and underline the numbers of the other methods which are not significantly worse than the best one.

	Conv-MKL	SMSD-MKL	LMC	One vs. One	One vs. Rest	GMNP	ℓ_1 MC-MKL	ℓ_2 MC-MKL	UFO-MKL
plant	77.14±2.25	78.01±2.17	70.12±2.96	75.83±2.69	75.17±2.68	75.42±3.64	77.60±2.63	75.49±2.48	76.77±2.42
psortPos	74.41±3.35	76.23±3.39	63.85±3.94	73.33±4.21	71.70±4.89	73.55±4.22	71.87±4.87	70.70±4.89	74.56±4.04
psortNeg	74.07±2.16	74.66±1.90	57.85±2.49	73.74±2.87	71.94±2.50	74.27±2.51	72.83±2.20	72.42±2.65	73.80±2.26
nonpl	79.15±1.51	78.69±1.58	75.16±1.48	77.78±1.52	77.49±1.53	78.35±1.46	77.89±1.79	77.95±1.64	78.07±1.56
sector	92.83±2.62	93.39±0.70	93.16±0.66	90.61±0.69	91.34±0.61	\	\	92.15±2.57	92.60±0.47
segment	96.79±0.91	97.62±0.83	95.07±1.11	97.08±0.61	97.02±0.80	96.87±0.80	96.98±0.64	97.58±0.68	97.20±0.82
vehicle	79.35±2.27	77.28±2.78	75.61±3.56	78.72±1.92	79.11±1.94	81.57±2.24	74.96±2.93	76.27±3.15	76.92±2.83
vowel	98.82±1.19	98.83±5.57	62.32±4.97	98.12±1.76	98.22±1.83	97.04±1.85	98.27±1.22	97.86±1.75	98.22±1.62
wine	99.63±0.96	99.63±0.96	97.87±2.80	97.24±3.05	98.14±3.04	97.69±2.43	98.61±1.75	98.52±1.89	99.44±1.13
dna	96.08±0.83	96.30±0.79	92.02±1.50	95.89±0.56	95.61±0.73	94.60±0.94	96.27±0.68	95.06±0.92	95.84±0.61
glass	75.19±5.05	73.72±5.80	63.95±6.04	71.98±5.75	70.00±5.75	71.24±8.14	69.07±8.08	74.03±6.41	72.46±6.12
iris	96.67±2.94	97.00±2.63	88.00±7.82	95.93±3.25	95.87±3.20	95.40±7.34	95.40±6.46	94.00±7.82	95.93±2.88
svmguid2	82.69±5.65	85.17±3.83	81.10±4.15	84.79±3.45	84.27±3.03	81.77±3.45	83.16±3.63	83.84±4.21	82.91±3.09
satimage	91.64±0.88	<u>91.78±0.82</u>	84.95±1.15	90.67±0.91	89.29±0.96	89.97±0.81	<u>91.86±0.62</u>	90.43±1.27	91.92±0.83

We experiment on 14 publicly available datasets: four of them evaluated in [38] (plant, nonpl, psortPos, and psortNeg) and others from LIBSVM Data. For each dataset, we use the Gaussian kernel $K(\mathbf{x}, \mathbf{x}') = \exp(-\|\mathbf{x} - \mathbf{x}'\|_2^2 / 2\tau)$ as our basic kernels, where $\tau \in 2^i, i = -10, -9, \dots, 9, 10$. For single kernel methods (One vs. One, One vs. Rest and GMNP), we choose the kernel which have the highest performance among basic kernels estimated by 10-folds cross-validation. Meanwhile, we use all basic kernels in MKL methods (Conv-MKL, SMSD-MKL, ℓ_1 MC-MKL, ℓ_2 MC-MKL and UFO-MKL). The regularization parameterized $\alpha \in 2^i, i = -2, \dots, 12$ in all algorithms and $\zeta \in 2^i, i = 1, 2, \dots, 4, \beta \in 10^i, i = -4, \dots, 1$ in SMSD-MKL are determined by 10-folds cross-validation on training data. Other parameters in compared algorithms follow the same experimental setting in their papers. For each dataset, we run all methods 50 times with randomly selected 80% for training and 20% for testing, offering an estimate of the statistical significance of differences in performance between methods. All statement of statistical significance in the remainder refer to a 95% level of significance under t -test.

The average test accuracies are reported in Table 1. The results show: 1) Our methods Conv-MKL and SMSD-MKL give best results on nearly all datasets except *vehicle* and *satimage*; 2) SMSD-MKL is better than Conv-MKL because it wins on 2/3 datasets; 3) Compared with typical MKL methods, our methods get better results over almost all datasets except that only UFO-MKL works slightly better than ours on *satige*; 4) The MKL methods usually work better than the compared single kernel methods (One vs. One, One vs. Rest and GMNP); 5) The kernel classification methods have better performance than the linear classification machine (LMC) on all datasets.

The above results show that the use of the local Rademacher complexity can significantly improve the performance of multi-class multiple kernel learning algorithms, which conforms to our theoretical analysis.

7 Conclusion

In this paper, we studied the generalization performance of multi-class classification, and derived a sharper data dependent generalization error bound using the local Rademacher complexity, which is much sharper than existing data-dependent generalization bounds of multi-class classification. Then, we designed two algorithms with statistical guarantees and fast convergence rates: Conv-MKL and SMSD-MKL. Based on local Rademacher complexity, our analysis can be used as a solid basis for the design of new multi-class kernel learning algorithms.

Acknowledgments

This work is supported in part by the National Natural Science Foundation of China (No.61703396, No.61673293, No.61602467), the National Key Research and Development Program of China (No.2016YFB1000604), the Science and Technology Project of Beijing (No.Z181100002718004) and the Excellent Talent Introduction of Institute of Information Engineering of CAS (Y7Z0111107).

References

- [1] E. L. Allwein, R. E. Schapire, and Y. Singer. Reducing multiclass to binary: A unifying approach for margin classifiers. *Journal of machine learning research*, 1:113–141, 2000.
- [2] P. L. Bartlett, O. Bousquet, and S. Mendelson. Local Rademacher complexities. *The Annals of Statistics*, 33(4):1497–1537, 2005.
- [3] L. Bottou, C. Cortes, J. S. Denker, H. Drucker, I. Guyon, L. D. Jackel, Y. LeCun, U. A. Muller, E. Sackinger, P. Simard, et al. Comparison of classifier methods: a case study in handwritten digit recognition. In *Proceedings of the 12th IAPR International Conference on Pattern Recognition*, pages 77–82, 1994.
- [4] C. Cortes, M. Kloft, and M. Mohri. Learning kernels using local Rademacher complexity. In *Advances in Neural Information Processing Systems 25 (NIPS)*, pages 2760–2768, 2013.
- [5] C. Cortes, M. Mohri, and A. Rostamizadeh. Multi-class classification with maximum margin multiple kernel. In *Proceedings of the 30th International Conference on Machine Learning (ICML)*, pages 46–54, 2013.
- [6] K. Crammer and Y. Singer. On the algorithmic implementation of multiclass kernel-based vector machines. *Journal of Machine Learning Research*, 2:265–292, 2002.
- [7] A. Daniely and S. Shalev-Shwartz. Optimal learners for multiclass problems. In *Proceedings of the 27th Conference on Learning Theory (COLT)*, pages 287–316, 2014.
- [8] V. Franc. Optimization algorithms for kernel methods. *Prague: A PhD dissertation. Czech Technical University*, 2005.
- [9] Y. Guermeur. Combining discriminant models with new multi-class SVMs. *Pattern Analysis & Applications*, 5(2):168–179, 2002.
- [10] M. Hardt, B. Recht, and Y. Singer. Train faster, generalize better: Stability of stochastic gradient descent. In *Proceedings of the 33rd International Conference on Machine Learning (ICML)*, pages 1225–1234, 2016.
- [11] S. I. Hill and A. Doucet. A framework for kernel-based multi-category classification. *Journal of Artificial Intelligence Research*, 30:525–564, 2007.
- [12] S. Knerr, L. Personnaz, and G. Dreyfus. Single-layer learning revisited: a stepwise procedure for building and training a neural network. In *Neurocomputing*, pages 41–50. Springer, 1990.
- [13] V. Koltchinskii. Local Rademacher complexities and oracle inequalities in risk minimization. *The Annals of Statistics*, 34(6):2593–2656, 2006.
- [14] V. Koltchinskii and D. Panchenko. Empirical margin distributions and bounding the generalization error of combined classifiers. *The Annals of Statistics*, 30:1–50, 2002.
- [15] V. Koltchinskii, D. Panchenko, and F. Lozano. Some new bounds on the generalization error of combined classifiers. In *Advances in Neural Information Processing Systems 14 (NIPS)*, pages 245–251, 2001.
- [16] V. Kuznetsov, M. Mohri, and U. Syed. Multi-class deep boosting. In *Advances in Neural Information Processing Systems 27 (NIPS)*, pages 2501–2509, 2014.
- [17] G. R. G. Lanckriet, N. Cristianini, P. L. Bartlett, L. E. Ghaoui, and M. I. Jordan. Learning the kernel matrix with semidefinite programming. *Journal of Machine Learning Research*, 5:27–72, 2004.
- [18] Y. Lei, U. D. A. Binder, and M. Kloft. Multi-class SVMs: From tighter data-dependent generalization bounds to novel algorithms. In *Advances in Neural Information Processing Systems 27 (NIPS)*, pages 2035–2043, 2015.
- [19] Y. Liu, S. Jiang, and S. Liao. Eigenvalues perturbation of integral operator for kernel selection. In *Proceedings of the 22nd ACM International Conference on Information and Knowledge Management (CIKM)*, pages 2189–2198, 2013.

- [20] Y. Liu, S. Jiang, and S. Liao. Efficient approximation of cross-validation for kernel methods using Bouligand influence function. In *Proceedings of the 31st International Conference on Machine Learning (ICML)*, pages 324–332, 2014.
- [21] Y. Liu and S. Liao. Preventing over-fitting of cross-validation with kernel stability. In *Proceedings of the European Conference on Machine Learning and Principles and Practice of Knowledge Discovery in Databases (ECML)*, pages 290–305, 2014.
- [22] Y. Liu and S. Liao. Eigenvalues ratio for kernel selection of kernel methods. In *Proceedings of the 29th AAAI Conference on Artificial Intelligence (AAAI)*, pages 2814–2820, 2015.
- [23] Y. Liu, S. Liao, and Y. Hou. Learning kernels with upper bounds of leave-one-out error. In *Proceedings of the 20th ACM International Conference on Information and Knowledge Management (CIKM)*, pages 2205–2208, 2011.
- [24] Y. Liu, S. Liao, H. Lin, Y. Yue, and W. Wang. Infinite kernel learning: generalization bounds and algorithms. In *Proceedings of the 21st AAAI Conference on Artificial Intelligence (AAAI)*, pages 2280–2286, 2017.
- [25] Y. Maximov and D. Reshetova. Tight risk bounds for multi-class margin classifiers. *Pattern Recognition and Image Analysis*, 26(4):673–680, 2016.
- [26] D. McAllester. A pac-bayesian tutorial with a dropout bound. *Arxiv’13*, 2013.
- [27] M. Moh, A. Rostamizadeh, and A. Talwalkar. *Foundations of machine learning*. MIT press, 2012.
- [28] B. K. Natarajan. On learning sets and functions. *Machine Learning*, 4(1):67–97, 1989.
- [29] F. Orabona and J. Luo. Ultra-fast optimization algorithm for sparse multi kernel learning. In *Proceedings of the 28th International Conference on Machine Learning (ICML)*, pages 249–256, 2011.
- [30] F. Orabona, J. Luo, and B. Caputo. Online-batch strongly convex multi kernel learning. In *The 23rd IEEE Conference on Computer Vision and Pattern Recognition (CVPR)*, pages 787–794, 2010.
- [31] S. Shalev-Shwartz and A. Tewari. Stochastic methods for l_1 -regularized loss minimization. *Journal of Machine Learning Research*, 12:1865–1892, 2011.
- [32] S. Sonnenburg, G. Rätsch, C. Schäfer, and B. Schölkopf. Large scale multiple kernel learning. *Journal of Machine Learning Research*, 7:1531–1565, 2006.
- [33] I. Tsochantaris, T. Hofmann, T. Joachims, and Y. Altun. Support vector machine learning for interdependent and structured output spaces. In *Proceedings of the 21st International Conference on Machine Learning (ICML)*, page 104, 2004.
- [34] V. Vapnik. *The nature of statistical learning theory*. Springer Verlag, 2000.
- [35] C. Xu, T. Liu, D. Tao, and C. Xu. Local rademacher complexity for multi-label learning. *IEEE Transactions on Image Processing*, 25(3):1495–1507, 2016.
- [36] N. Yousefi, Y. Lei, M. Kloft, M. Mollaghasemi, and G. Anagnostopoulos. Local rademacher complexity-based learning guarantees for multi-task learning. *arXiv preprint arXiv:1602.05916*, 2016.
- [37] T. Zhang. Statistical analysis of some multi-category large margin classification methods. *Journal of Machine Learning Research*, 5:1225–1251, 2004.
- [38] A. Zien and C. S. Ong. Multiclass multiple kernel learning. In *Proceedings of the 24th International Conference on Machine Learning (ICML)*, pages 1191–1198, 2007.