

Experiential Study of Kernel Functions to Design an Optimized Multi-class SVM

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ABSTRACT- Support Vector Machine is a powerful classification technique based on the idea of Structural risk minimization. Use of a kernel function enables the curse of dimensionality to be addressed. However, a proper kernel function for a certain problem is dependent on the specific dataset and till now there is no good method on how to choose a kernel function. In this paper, the choice of the kernel function was studied empirically and optimal results were achieved for multi-class SVM by combining several binary classifiers. The performance of the multi-class SVM is illustrated by extensive experimental results which indicate that with suitable kernel and parameters better classification accuracy can be achieved as compared to other methods. The experimental results of three datasets show that Gaussian kernel is not always the best choice to achieve high generalization of classifier although it often the default choice.

I. INTRODUCTION

In the past two decades valuable work has been carried out in the area of text categorization [10],[11], optical character recognition [13], intrusion detection [14], speech recognition [18], handwritten digit recognition [20] etc. All such real-world applications are essentially multi-class classification problems. Multi-class classification is intrinsically harder than binary classification problem because the classification has to learn to construct a greater number of separation boundaries or relations. Classification error rate is greater in multi-class problem than that of binary as there can be error in determination of any one of the decision boundaries or relations.

There are basically two types of multi-class classification algorithms. The first type deals directly with multiple values in the target field *i.e.* K- Nearest Neighbor, Naive Bayes, classification trees in the class etc... Intuitively, these methods can be interpreted as trying to construct a conditional probability density for each class, then classifying by selecting the class with maximum a posteriori probability. For data with high dimensional input space and very few samples per class, it is very difficult to construct accurate densities. While the other approaches decompose the multi -class problem into a set of binary problems and then combining them to make a final multi-class classifier. This group contains support vector machines, boosting and more generally, any binary classifier. In certain settings the later approach results in better performance than the multiple target approaches.

Support Vector Machines (SVMs) originally designed for binary classification are based on statistical learning theory developed by Vapnik [5][19]. Larger and more complex classification problems have subsequently been solved with SVMs. How to effectively extend it for multi-class classification is still an ongoing research issue [16]. The most common way to build a k - class SVM is by constructing and combining several binary classifiers [9]. In designing machine learning algorithms, it is often easier to first devise algorithms to distinguish between two classes.

SVMs are learning machines that transform the training vectors into a high-dimensional feature space, labeling each vector by its class. It classifies data by determining a set of support vectors, which are members of the set of training inputs that outline a hyperplane in feature space [19]. It is based on the idea of Structural risk minimization, which minimizes the generalization error. The number of free parameters used in the SVM depends on the margin that separates the data points and not on the number of input features. SVM provides a generic technique to fit the surface of the hyperplane to the data through the use of an appropriate kernel function. Use of a kernel function enables the curse of dimensionality to be addressed, and the solution implicitly contains support vectors that provide a description of the significant data for classification [17]. The most commonly kernel functions are polynomial, gaussian and sigmoidal functions. Although in literature, the default choice of kernel function for most of the applications is gaussian. In training a support vector machine we need to select kernel function and its parameters, and value of margin parameter C . The choice of kernel function and parameters to map dataset well in high dimension may depend on specific datasets. There is no method to determine how to choose a appropriate kernel function and its parameters for a given dataset to achieve high generalization of classifier. The main modeling freedom consists in the choice of the kernel function and the corresponding kernel parameters, which influences the speed of convergence and the quality of results. Furthermore, the choice of the regularization parameter C is vital to obtain good classification results.

In this paper, we have studied the choice of the kernel function empirically and optimal results were achieved for multi-class SVM using three benchmark datasets of UCI repository of Machine Learning Databases [1]. This paper is organized as follows. Section 2 briefly reviews the basic theory of SVM. In section 3, we demonstrates the experiments of multi-class SVM (one against all) using different kernel functions on few datasets of UCI repository and provides the comparative result of classifier accuracy of multi-class SVM for different kernel functions. We also

compare the accuracy with the available results for different datasets. We conclude and discuss scope of future work in section 4.

1. SUPPORT VECTOR MACHINES

A. Theory of Support Vector Machines

This section briefly introduces the theory of SVM. Let $\{(x_1, y_1), \dots, (x_m, y_m)\} \in \mathbb{R}^n \times \{+1, -1\}$ be a training set. The SVM classifier finds a canonical hyperplane $\{x \in \mathbb{R}^n : w^T x + b = 0, w \in \mathbb{R}^n, b \in \mathbb{R}\}$, which maximally separates given two classes of training samples in \mathbb{R}^n . The corresponding decision function $f : \mathbb{R}^n \rightarrow \{+1, -1\}$ is then given by $f(x) = \text{sgn}(w^T x + b)$. For many practical applications, the training set may not be linearly separable. In such cases, the optimal decision function is found by solving the following quadratic optimization problem:

$$\begin{aligned} \text{Minimize:} \quad & J(w, \xi) = \frac{1}{2} w^T w + C \sum_{i=1}^l \xi_i \\ \text{Subject to} \quad & y_i (w^T x_i + b) \geq 1 - \xi_i, \\ & \xi_i \geq 0, i = 1, 2, \dots, m \end{aligned} \quad (1)$$

where ξ_i is a slack variable introduced to relax the hard-margin constraints and the regularization constant $C > 0$ determines the trade-off between the empirical error and the complexity term. The generalized optimization is based on a theorem about the VC dimension of canonical hyperplanes. It was shown that if the hyperplane is constructed under the constraint $\|w\| \leq A$ then the VC- dimension of the class H is bounded by $h \leq \min(R^2 A^2, n) + 1$ [19], where R is the radius of the smallest sphere around the data. Thus, if we bound the margin of a function class from below, say by $2/A$, we can control its VC dimension and hence apply the SRM principle.

Applying the Karush-Kuhn Tucker complimentary condition [7] which gives optimal solution of a non-linear programming problem, we can write $w = \sum_{i=1}^m y_i \alpha_i x_i$ after minimizing (1). This is called the dual representation of w . A x_i with nonzero α_i is called a support vector. The coefficients α_i can be found by solving the dual problem of (1):

$$\begin{aligned} \text{Maximize:} \quad & L(\alpha) = \sum_{i=1}^l \alpha_i - \frac{1}{2} \sum_{i,j=1}^l \alpha_i \alpha_j y_i y_j x_i x_j \\ \text{Subject to} \quad & 0 \leq \alpha_i \leq C, i = 1, 2, \dots, l \\ \text{and} \quad & \sum_{i=1}^m \alpha_i y_i = 0 \end{aligned} \quad (2)$$

Let S be the index set of support vectors, then the optimal decision function becomes

$$f(x) = \text{sgn} \left(\sum_{i \in S} y_i \alpha_i x_i^T x + b \right) \quad (3)$$

The above equation gives an optimal hyperplane in \mathbb{R}^n . However, more complex decision surfaces can be generated by employing a nonlinear mapping $\Phi : \mathbb{R}^n \rightarrow F$ while at the same time controlling their complexity and solving the same optimization problem in F. It can be seen from (2) that x_i always appears in the form of inner product $x_i^T x_j$. This implies that there is no need to evaluate the nonlinear mapping Φ as long as we know the inner product in F for a given $x_i, x_j \in \mathbb{R}^n$. So, instead of defining $\Phi : \mathbb{R}^n \rightarrow F$ explicitly, a function $K : \mathbb{R}^n \times \mathbb{R}^n \rightarrow \mathbb{R}$ is introduced to define an inner product in F. The only requirement on the kernel $K(x, y)$ is to satisfy Mercer's condition, which states: There exists a mapping Φ and an expansion

$$K(x, y) = \sum_i \Phi(x)_i \cdot \Phi(y)_i$$

if and only if, for any $g(x)$ such that

$$\int g(x)^2 dx \text{ is finite}$$

then

$$\int K(x, y) g(x) g(y) dx dy \geq 0.$$

Substituting $K(x_i, x_j)$ for $x_i^T x_j$ in (3) produces a new optimization problem:

$$\begin{aligned} \text{Maximize} \quad & L(\alpha) = \sum_{i=1}^m \alpha_i - \frac{1}{2} \sum_{i,j=1}^m \alpha_i \alpha_j y_i y_j K(x_i, x_j) \\ \text{Subject to} \quad & 0 \leq \alpha_i \leq C, i = 1, \dots, m \\ \text{and} \quad & \sum_{i=1}^m \alpha_i y_i = 0 \end{aligned} \quad (4)$$

Solving it for α gives a decision function of the form

$$f(x) = \text{sgn} \left(\sum_{i=1}^m y_i \alpha_i K(x_i, x) + b \right) \quad (5)$$

Whose decision boundary is a hyperplane in F, and translates to nonlinear boundaries in the original space.

B. Multi-class Support Vector Machines

All real world classification problems often involve more than two classes. Therefore, binary SVMs' are usually not enough to solve the whole problem. The most common way to build a k-class SVM is by constructing and combining several binary classifiers. To solve multi-class classification problems, we divide the whole pattern into a number of binary classification problems. The two representative ensemble schemes are One against All (1-vs-many) and One

against One (1-vs-1) [12]. One against All is also known as “one against others.” It trains k binary classifiers, each of which separates one class from the other $(k-1)$ classes. Given a point X to classify, the binary classifier with the largest output determines the class of X . One against One constructs $k(k-1)/2$ binary classifiers. The outputs of the classifiers are aggregated to make the final decision. Decision tree formulation is a variant of One against All formulation based on decision tree. Error Correcting output code is general representation of One against All or One Vs One formulation, which uses error correcting codes for encoding outputs [dieterich]. The One against All approach,

provides better classification accuracy in comparison to others [16]. Consequently, we have applied One against All approach in our experiments.

Commonly used kernels for decision functions of a binary SVM classifier such as polynomial, Gaussian and sigmoid may not be suitable for binary classification to map every dataset well in high dimensional space. There can be other functions, which satisfy Mercer’s condition and can enhance classifier accuracy by appropriate transformation in high dimensional space. Few kernel functions [2] used in our experiment are shown in Table I.

Table I: Kernel Functions

Kernel Function	$K(x, x_i)$ for $\gamma > 0$
Cauchy	$1 / (1 + \gamma x - x_i ^2)$
Gaussian	$e^{-\gamma x - x_i ^2}$
Hyperbolic Secant	$2 / (\exp(\gamma x - x_i) + \exp(-\gamma x - x_i))$
Laplace	$\exp(-\gamma x - x_i)$
Squared Sinc	$\sin^2(\gamma x - x_i) / (\gamma x - x_i)^2$
Symmetric Triangle	$\max(1 - \gamma x - x_i , 0)$
Gaussian_polynomial	$e^{-\gamma x - x_i ^2} * (1 + x * x_i)^2$
Polynomial	$(1 + x * x_i)^2$

II. EXPERIMENTAL RESULTS

1. Dataset

In this section, we evaluated the performance of multi-class SVM using different kernel functions on datasets of UCI repository of Machine Learning [1], Statlog collection[.]. From the UCI Repository we choose the following datasets: iris, wine, glass and vowel. From Statlog collection we choose all multiclass datasets: vehicle, segment, satimage, letter, shuttle. The *iris* dataset records the physical dimensions of three different classes of Iris flowers. There are four attributes in the *Iris* dataset. The class Setosa is linearly separable from the other two classes, whereas the latter two are not linearly separable from each other. The *Wine* dataset was obtained from chemical analysis of wines produced in the same regions of Italy but

derived from three different cultivars. There are 13 attributes and 178 patterns in this *wine* dataset. There are three classes corresponding to the three different cultivars. The collections of the *Glass* dataset were for the study of different types of glass, which was motivated by criminological investigations. At the scene of crime, the glass left can be used as evidence if it is correctly identified. The *Glass* dataset contains 214 cases. There are nine attributes and six classes in the *Glass* Dataset. The Vehicle dataset contains 846 cases. There are eighteen attributes and four classes. Segment dataset has total 2310 samples with seven class labels and total 19 attributes. Vowel dataset contains 528 cases with 10 attributes and 11 classes. We give problem Statistics in table II

Table II
Problem Statistics

Problem	#training data	#testing data	#class	#attributes	Statlog rate
Iris	150	0	3	4	
Wine	178	0	3	13	
Glass	214	0	6	9	
Vowel	528	0	11	10	
Vehicle	846	0	4	18	
Segment	2310	0	7	19	
Satimage	4435	2000	6	36	90.6
Letter	15000	5000	26	16	93.6
Shuttle	43500	14500	7	9	99.99

III. Experimental Setup

The generalization performance is evaluated via a ten-fold cross-validation for each dataset. We have considered *One against All* method for designing a multi-class SVM using SVM Light.

Results

For a k -class problem, we have developed multi-class SVM by combining k -binary SVM with the same value of C and γ and tested the performance for different choices of kernel functions on predefined datasets. The most important criterion for evaluating the performance of multi-class. The experiments were performed on different datasets using other kernel functions. We observed that multi-class SVM with genetic programming demonstrates better accuracy for certain value of C and γ .

The best and average cross-validation accuracy are shown in Table III with their optimal parameters C and γ . For comparison with multi-class SVM, we have also applied decision tree construction algorithm C4.5 [15] on the same datasets for determining the best and average cross-validation accuracy. It can be observed that the best and average cross-validation accuracy using multi-class SVM is same or better than obtained by C4.5 for all datasets. Similarly, Table IV compares the accuracy of multi-class SVM classifier with results obtained by C4.5 and available results [9] [20]. The best results in each category are indicated in bold. From Table IV, It can be observed that our results are better in each category.

Table III

A comparison of classifier accuracy using different kernel functions

Dataset	Kernel	Gauss	Cauchy	Laplace	Hyper Secant	Squared Sinc	Symmetric Triangle	Polynomial	Guass_poly	C4.5
	→									
Iris	Best	100 ($2^4, 2^{-5}$)	100 ($2^8, 2^{-10}$)	100 ($2^3, 2^{-5}$)	100 ($2^6, 2^{-3}$)	100 ($2^2, 2^{-1}$)	100 ($2^8, 2^{-1}$)	100 (all values of C & γ)	100 ($2^3, 2^{-2}$)	100
	Average	98 ($2^4, 2^{-5}$)	96.667 ($2^8, 2^{-10}$)	96.667 ($2^3, 2^{-5}$)	98 ($2^6, 2^{-3}$)	97.333 ($2^2, 2^{-1}$)	96.667 ($2^8, 2^{-10}$)	100		94
Wine	Best	94.444 ($2^5, 2^{-10}$)	94.444 ($2^9, 2^{-10}$)	100 ($2^9, 2^{-10}$)	100 ($2^{12}, 2^{-9}$)	100 ($2^{12}, 2^{-8}$)	100 ($2^{12}, 2^{-10}$)	100 (all values of C & γ)	89.47 (all values of $C, 2^{-11}$)	100
	Average	82.778 ($2^5, 2^{-10}$)	81.111 ($2^9, 2^{-10}$)	81.667 ($2^9, 2^{-10}$)	94.444 ($2^{12}, 2^{-9}$)	96.111 ($2^{12}, 2^{-9}$)	82.222 ($2^{12}, 2^{-10}$)	100 (all values of C & γ)		92.222
Glass	Best	86.364 ($2^{-1}, 2^{-4}$)	77.2727 ($2^4, 2^1$)	81.818 ($2^2, 2^1$)	86.364 ($2^0, 2^0$)	86.364 ($2^0, 2^0$)	81.818 ($2^0, 2^{-1}$)			81.818
	Average	69.091 ($2^0, 2^1$)	71.818 ($2^1, 2^2$)	70.909 ($2^0, 2^0$)	70.909 ($2^{-1}, 2^1$)	70.455 ($2^{-1}, 2^1$)	69.546 ($2^0, 2^0$)			71.818
Vowel	Best					100 (all values of C & γ)				

	Average					100 (all values of C & γ)				
Vehicle	Best					100 (all C & γ values)				
	Average					100 (all C & γ values)				
Segment	Best	100	(all values of C & γ)							
	Average									
Satimage	Best	91.95	92.8	92.65	92.75	100 (all values of C & γ)	92.5	-----	91.6	
	Average	50.458	87.296	77.406	75.197	100 (all values of C & γ)	59.307	-----	48.458	
Letter	Best	97.84	97.9	97.84	97.82	100 (all values of C & γ)	97.62	----	97.64	
	Average	92.39333	95.14976	92.2252	78.20952	100	79.29786	-----	81.764 27	
Shuttle	Best	99.85	99.88	99.9	99.91	100	99.93		84.46	
	Average	97.95143	99.73214	98.83688	98.419	100 (all values of C & γ)	96.96186		38.662 57	

Table IV
 A comparison of classifier accuracy using different methods for multi-class

Dataset	Different Methods	One against one	DAG	One against all	C & S	[20]	Ours
		[9]					
Iris	Accuracy (C, γ)	97.333 ($2^{12}, 2^{-9}$)	96.667 ($2^{12}, 2^{-8}$)	96.667 ($2^9, 2^{-3}$)	97.333 ($2^{10}, 2^{-7}$)	97.333 ($2^{12}, 2^{-8}$)	100 (Gauss, $2^8, 2^{-3}$)
Wine	Accuracy (C, γ)	99.438 ($2^7, 2^{-10}$)	98.876 ($2^6, 2^{-9}$)	98.876 ($2^7, 2^{-6}$)	98.876 ($2^1, 2^{-3}$)	98.876 ($2^9, 2^{-2}$)	100 (poly, all values of C & γ)
Glass	Accuracy (C, γ)	71.495 ($2^{11}, 2^{-2}$)	73.832 ($2^{12}, 2^{-3}$)	71.963 ($2^{11}, 2^{-2}$)	71.963 ($2^4, 2^1$)	71.028 ($2^9, 2^{-4}$)	86.364 (HyperSec, $2^9, 2^0$)
Vowel	Accuracy (C, γ)	99.053 ($2^4, 2^0$)	98.674 ($2^2, 2^2$)	98.485 ($2^4, 2^1$)	98.674 ($2^1, 2^2$)	98.485 ($2^3, 2^0$)	100 (sq. sinc, all values of C & γ)
Vehicle	Accuracy (C, γ)	86.643 ($2^9, 2^{-3}$)	86.052 ($2^{11}, 2^{-3}$)	87.470 ($2^{11}, 2^{-4}$)	86.761 ($2^8, 2^{-4}$)	86.998 ($2^{10}, 2^{-4}$)	100 (sq. sinc, all values of C & γ)
Segment	Accuracy (C, γ)	97.403 ($2^6, 2^0$)	97.359 ($2^{11}, 2^{-3}$)	97.532 ($2^7, 2^0$)	97.316 ($2^9, 2^3$)	97.576 ($2^5, 2^0$)	100 (sq. sinc, all values of C & γ)
Dna	Accuracy (C, γ)	95.447 ($2^3, 2^{-6}$)	95.447 ($2^3, 2^{-6}$)	95.784 ($2^2, 2^{-6}$)	95.869 ($2^1, 2^{-6}$)	95.616 ($2^4, 2^{-6}$)	100 (sq. sinc, all values of C & γ)
Satimage	Accuracy (C, γ)	91.3 ($2^4, 2^0$)	91.25 ($2^4, 2^0$)	91.7 ($2^2, 2^1$)	92.35 ($2^2, 2^2$)	91.25 ($2^3, 2^0$)	100 (sq. sinc, all values of C & γ)

Letter	Accuracy (C, γ)	97.98 ($2^4, 2^3$)	97.98 ($2^4, 2^3$)	97.88 ($2^2, 2^3$)	97.68 ($2^3, 2^3$)	97.76 ($2^1, 2^2$)	97.9
Shuttle	Accuracy (C, γ)	99.924 ($2^{11}, 2^3$)	99.924 ($2^{11}, 2^3$)	99.910 ($2^9, 2^4$)	99.938 ($2^{12}, 2^4$)	99.910 ($2^9, 2^4$)	100 (sq. sinc. all values of C & γ)

IV. CONCLUSION

The experimental results of three datasets show that Gaussian kernel is not always the best choice to achieve high generalization of classifier although it often the default choice. We exhibit the dependency of classifier accuracy on the different kernel functions of the multi-class SVM using different dataset. With the choice of kernel function and optimal values of parameters C and γ , it is possible to achieve maximum classification accuracy for all datasets. It will be interesting and practically more useful to determine some method for determining the kernel function and its parameters based on statistical properties of the given data. Then the proposed method in conjunction with multi-class SVM can be tested on application domains such as image processing, text classification, intrusion detection etc. We are also examining the possibility of integrating fuzzy approach in the multi-class SVM classifier.

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