Probability Estimates for Multi-class Classification by Pairwise Coupling

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Abstract

Pairwise coupling is a popular multi-class classification method that combines together all pairwise comparisons for each pair of classes. This paper presents two approaches for obtaining class probabilities. Both methods can be reduced to linear systems and are easy to implement. We show conceptually and experimentally that the proposed approaches are more stable than two existing popular methods: voting and [3].

1 Introduction

The multi-class classification problem refers to assigning each of the observations into one of k classes. As two-class problems are much easier to solve, many authors propose to use two-class classifiers for multi-class classification. In this paper we focus on techniques that provide a multi-class classification solution by combining all pairwise comparisons.

A common way to combine pairwise comparisons is by voting [6, 2]. It constructs a rule for discriminating between every pair of classes and then selecting the class with the most winning two-class decisions. Though the voting procedure requires just pairwise decisions, it only predicts a class label. In many scenarios, however, probability estimates are desired. As numerous (pairwise) classifiers do provide class probabilities, several authors [12, 11, 3] have proposed probability estimates by combining the pairwise class probabilities.

Given the observation $\mathbf{x}$ and the class label y, we assume that the estimated pairwise class probabilities r_{ij} of $\mu_{ij} = p(y = i \mid y = i \text{ or } j, \mathbf{x})$ are available. Here r_{ij} are obtained by some binary classifiers. Then, the goal is to estimate $\{p_i\}_{i=1}^k$, where $p_i = p(y = i \mid \mathbf{x}), i = 1, \ldots, k$. We propose to obtain an approximate solution to an identity, and then select the label with the highest estimated class probability. The existence of the solution is guaranteed by theory in finite Markov Chains. Motivated by the optimization formulation of this method, we propose a second approach. Interestingly, it can also be regarded as an improved version of the coupling approach given by [12]. Both of the proposed methods can be reduced to solving linear systems and are simple in practical implementation. Furthermore, from conceptual and experimental points of view, we show that the two proposed methods are more stable than voting and the method in [3].

We organize the paper as follows. In Section 2, we review two existing methods. Sections 3 and 4 detail the two proposed approaches. Section 5 presents the relationship among the four methods through their corresponding optimization formulas. In Section 6, we compare these methods using simulated and real data. The classifiers considered are support vector machines. Section 7 concludes the paper. Due to space limit, we omit all detailed proofs. A complete version of this work is available at `http://www.csie.ntu.edu.tw/~cjlin/papers/svmprob/svmprob.pdf`.

2 Review of Two Methods

Let r_{ij} be the estimates of $\mu_{ij} = p_i/(p_i + p_j)$. The voting rule [6, 2] is

$$\delta_V = \text{argmax}_i [\sum_{j:j \neq i} I_{\{r_{ij} > r_{ji}\}}]. \tag{1}$$

A simple estimate of probabilities can be derived as $p_i^v = 2\sum_{j:j\neq i} I_{\{r_{ij}>r_{ji}\}}/(k(k-1))$. The authors of [3] suggest another method to estimate class probabilities, and they claim that the resulting classification rule can outperform δ_V in some situations. Their approach is based on the minimization of the Kullback-Leibler (KL) distance between r_{ij} and μ_{ij}:

$$l(\mathbf{p}) = \sum_{i \neq j} n_{ij} r_{ij} \log(r_{ij}/\mu_{ij}), \tag{2}$$

where $\sum_{i=1}^k p_i = 1, p_i > 0, i = 1, \ldots, k$, and n_{ij} is the number of instances in class i or j. By letting $\nabla l(\mathbf{p}) = 0$, a nonlinear system has to be solved. [3] proposes an iterative procedure to find the minimum of (2). If $r_{ij} > 0, \forall i \neq j$, the existence of a unique global minimal solution to (2) has been proved in [5] and references therein. Let $\mathbf{p}^*$ denote this point. Then the resulting classification rule is

$$\delta_{HT}(x) = \text{argmax}_i [p_i^*].$$

It is shown in Theorem 1 of [3] that

$$p_i^* > p_j^* \text{ if and only if } \tilde{p}_i > \tilde{p}_j, \text{ where } \tilde{p}_j = \frac{2\sum_{s:s\neq j} r_{js}}{k(k-1)}; \tag{3}$$

that is, the $\tilde{p}_i$ are in the same order as the p_i^*. Therefore, $\tilde{\mathbf{p}}$ are sufficient if one only requires the classification rule. In fact, as pointed out by [3], $\tilde{\mathbf{p}}$ can be derived as an approximation to the identity by replacing $p_i + p_j$ with $2/k$, and μ_{ij} with r_{ij}.

$$p_i = \sum_{j:j\neq i} (\frac{p_i + p_j}{k-1})(\frac{p_i}{p_i + p_j}) = \sum_{j:j \neq i} (\frac{p_i + p_j}{k-1}) \mu_{ij} \tag{4}$$

3 Our First Approach

Note that δ_{HT} is essentially $\text{argmax}_i[\tilde{p}_i]$, and $\tilde{\mathbf{p}}$ is an approximate solution to (4). Instead of replacing $p_i + p_j$ by $2/k$, in this section we propose to solve the system:

$$p_i = \sum_{j:j\neq i} (\frac{p_i + p_j}{k-1}) r_{ij}, \forall i, \qquad \text{subject to } \sum_{i=1}^k p_i = 1, p_i \geq 0, \forall i. \tag{5}$$

Let $\bar{\mathbf{p}}$ denote the solution to (5). Then the resulting decision rule is

$$\delta_1 = \text{argmax}_i [\bar{p}_i].$$

As δ_{HT} relies on $p_i + p_j \approx k/2$, in Section 6.1 we use two examples to illustrate possible problems with this rule.

To solve (5), we rewrite it as

$$Q\mathbf{p} = \mathbf{p}, \quad \sum_{i=1}^{k} p_i = 1, \quad p_i \geq 0, \forall i, \text{ where } Q_{ij} = \begin{cases} r_{ij}/(k-1) & \text{if } i \neq j, \\ \sum_{s:s\neq i} r_{is}/(k-1) & \text{if } i = j. \end{cases} \tag{6}$$

Observe that $\sum_{j=1}^{k} Q_{ij} = 1$ for $i = 1, \ldots, k$ and $0 \leq Q_{ij} \leq 1$ for $i, j = 1, \ldots, k$, so there exists a finite Markov Chain whose transition matrix is Q. Moreover, if $r_{ij} > 0$ for all $i \neq j$, then $Q_{ij} > 0$, which implies this Markov Chain is irreducible and aperiodic. These conditions guarantee the existence of a unique stationary probability and all states being positive recurrent. Hence, we have the following theorem:

Theorem 1 *If $r_{ij} > 0$, $i \neq j$, then (6) has a unique solution $\mathbf{p}$ with $0 < p_i < 1, \forall i$.*

With Theorem 1 and some further analyses, if we remove the constraint $p_i \geq 0, \forall i$, the linear system with $k+1$ equations still has the same unique solution. Furthermore, if any one of the k equalities $Q\mathbf{p} = \mathbf{p}$ is removed, we have a system with k variables and k equalities, which, again, has the same single solution. Thus, (6) can be solved by Gaussian elimination. On the other hand, as the stationary solution of a Markov Chain can be derived by the limit of the n-step transition probability matrix Q^n, we can solve $\mathbf{p}$ by repeatedly multiplying Q^T with any initial vector.

Now we reexamine this method to gain more insight. The following arguments show that the solution to (5) is a global minimum of a meaningful optimization problem. To begin, we express (5) as $\sum_{j:j\neq i} r_{ji}p_i - \sum_{j:j\neq i} r_{ij}p_j = 0, i = 1, \ldots, k$, using the property that $r_{ij} + r_{ji} = 1$, $\forall i \neq j$. Then the solution to (5) is in fact the global minimum of the following problem:

$$\min_{\mathbf{p}} \sum_{i=1}^{k} (\sum_{j:j\neq i} r_{ji}p_i - \sum_{j:j\neq i} r_{ij}p_j)^2 \qquad \text{subject to } \sum_{i=1}^{k} p_i = 1, p_i \geq 0, \forall i. \tag{7}$$

Since the object function is always nonnegative, and it attains zero under (5) and (6).

4 Our Second Approach

Note that both approaches in Sections 2 and 3 involve solving optimization problems using the relations like $p_i/(p_i + p_j) \approx r_{ij}$ or $\sum_{j:j\neq i} r_{ji}p_i \approx \sum_{j:j\neq i} r_{ij}p_j$. Motivated by (7), we suggest another optimization formulation as follows:

$$\min_{\mathbf{p}} \frac{1}{2} \sum_{i=1}^{k} \sum_{j:j\neq i} (r_{ji}p_i - r_{ij}p_j)^2 \qquad \text{subject to } \sum_{i=1}^{k} p_i = 1, p_i \geq 0, \forall i. \tag{8}$$

In related work, [12] proposes to solve a linear system consisting of $\sum_{i=1}^{k} p_i = 1$ and *any* $k-1$ equations of the form $r_{ji}p_i = r_{ij}p_j$. However, pointed out in [11], the results of [12] strongly depends on the selection of $k-1$ equations. In fact, as (8) considers all $r_{ij}p_j - r_{ji}p_i$, not just $k-1$ of them, it can be viewed as an improved version of [12].

Let $\mathbf{p}^\dagger$ denote the corresponding solution. We then define the classification rule as

$$\delta_2 = \text{argmax}_i [p_i^\dagger].$$

Since (7) has a unique solution, which can be obtained by solving a simple linear system, it is desired to see whether the minimization problem (8) has these nice properties. In the rest of the section, we show that this is true. The following theorem shows that the nonnegative constraints in (8) are redundant.

Theorem 2 *Problem* (8) *is equivalent to a simplification without conditions* $p_i \geq 0, \forall i$.

Note that we can rewrite the objective function of (8) as

$$\min_{\mathbf{p}} = \frac{1}{2}\mathbf{p}^T Q\mathbf{p}, \qquad \text{where } Q_{ij} = \begin{cases} \sum_{s:s\neq i} r_{si}^2 & \text{if } i = j, \\ r_{ji}r_{ij} & \text{if } i \neq j. \end{cases} \tag{9}$$

From here we can show that Q is positive semi-definite. Therefore, without constraints $p_i \geq 0, \forall i$, (9) is a linear-constrained convex quadratic programming problem. Consequently, a point $\mathbf{p}$ is a global minimum if and only if it satisfies the KKT optimality condition: There is a scalar b such that

$$\begin{bmatrix} Q & \mathbf{e} \\ \mathbf{e}^T & 0 \end{bmatrix} \begin{bmatrix} \mathbf{p} \\ b \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}. \tag{10}$$

Here $\mathbf{e}$ is the vector of all ones and b is the Lagrangian multiplier of the equality constraint $\sum_{i=1}^k p_i = 1$. Thus, the solution of (8) can be obtained by solving the simple linear system (10). The existence of a unique solution is guaranteed by the invertibility of the matrix of (10). Moreover, if Q is positive definite(PD), this matrix is invertible. The following theorem shows that Q is PD under quite general conditions.

Theorem 3 *If for any* $i = 1, \ldots, k$*, there are* $s \neq i$ *and* $j \neq i$ *such that* $\frac{r_{si}r_{sj}}{r_{is}} \neq \frac{r_{ji}r_{js}}{r_{ij}}$*, then* Q *is positive definite.*

In addition to direct methods, next we propose a simple iterative method for solving (10):

Algorithm 1

1. *Start with some initial* $p_i \geq 0, \forall i$ *and* $\sum_{i=1}^k p_i = 1$.
2. *Repeat* $(t = 1, \ldots, k, 1, \ldots)$

$$p_t \leftarrow \frac{1}{Q_{tt}}[-\sum_{j:j\neq t} Q_{tj}p_j + \mathbf{p}^T Q\mathbf{p}] \tag{11}$$

$$normalize\ \mathbf{p} \tag{12}$$

until (10) is satisfied.

Theorem 4 *If* $r_{sj} > 0, \forall s \neq j$*, and* $\{\mathbf{p}^i\}_{i=1}^{\infty}$ *is the sequence generated by Algorithm 1, any convergent sub-sequence goes to a global minimum of (8).*

As Theorem 3 indicates that in general Q is positive definite, the sequence $\{\mathbf{p}^i\}_{i=1}^{\infty}$ from Algorithm 1 usually globally converges to the unique minimum of (8).

5 Relations Among Four Methods

The four decision rules δ_{HT}, δ_1, δ_2, and δ_V can be written as $\text{argmax}_i[p_i]$, where $\mathbf{p}$ is derived by the following four optimization formulations under the constants $\sum_{i=1}^k p_i = 1$

and $p_i \geq 0, \forall i$:

$$\delta_{HT}: \min_{\mathbf{p}} \sum_{i=1}^{k} [\sum_{j:j\neq i}^{k} (r_{ij}\frac{1}{k} - \frac{1}{2}p_i)]^2, \tag{13}$$

$$\delta_1: \quad \min_{\mathbf{p}} \sum_{i=1}^{k} [\sum_{j:j\neq i}^{k} (r_{ij}p_j - r_{ji}p_i)]^2, \tag{14}$$

$$\delta_2: \quad \min_{\mathbf{p}} \sum_{i=1}^{k} \sum_{j:j\neq i}^{k} (r_{ij}p_j - r_{ji}p_i)^2, \tag{15}$$

$$\delta_V: \quad \min_{\mathbf{p}} \sum_{i=1}^{k} \sum_{j:j\neq i}^{k} (I_{\{r_{ij}>r_{ji}\}}p_j - I_{\{r_{ji}>r_{ij}\}}p_i)^2. \tag{16}$$

Note that (13) can be easily verified, and that (14) and (15) have been explained in Sections 3 and 4. For (16), its solution is

$$p_i = \frac{c}{\sum_{j:j\neq i} I_{\{r_{ji}>r_{ij}\}}},$$

where c is the normalizing constant;* and therefore, $\text{argmax}_i[p_i]$ is the same as (1). Clearly, (13) can be obtained from (14) by letting $p_j \approx 1/k, \forall j$ and $r_{ji} \approx 1/2, \forall i, j$. Such approximations ignore the differences between p_i. Similarly, (16) is from (15) by taking the extreme values of r_{ij}: 0 or 1. As a result, (16) may enlarge the differences between p_i. Next, compared with (15), (14) may tend to underestimate the differences between the p_i's. The reason is that (14) allows the difference between $r_{ij}p_j$ and $r_{ji}p_i$ to get canceled first. Thus, conceptually, (13) and (16) are more extreme – the former tends to underestimate the differences between p_i's, while the latter overestimate them. These arguments will be supported by simulated and real data in the next section.

6 Experiments

6.1 Simple Simulated Examples

[3] designs a simple experiment in which all p_i's are fairly close and their method δ_{HT} outperforms the voting strategy δ_V. We conduct this experiment first to assess the performance of our proposed methods. As in [3], we define class probabilities $p_1 = 1.5/k$, $p_j = (1 - p_1)/(k - 1)$, $j = 2, \ldots, k$, and then set

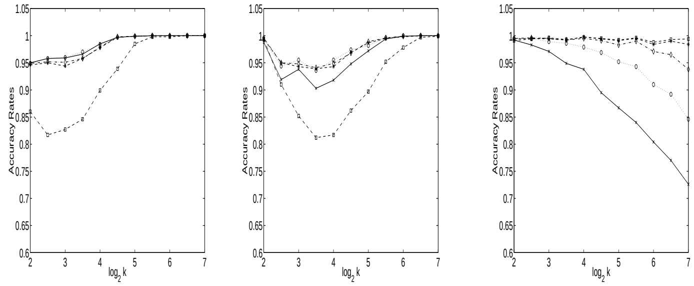
$$r_{ij} = \frac{p_i}{p_i + p_j} + 0.1z_{ij} \text{ if } i > j, \tag{17}$$

$$r_{ji} = 1 - r_{ij} \qquad\qquad \text{if } j > i, \tag{18}$$

where z_{ij} are standard normal variates. Since r_{ij} are required to be within (0,1), we truncate r_{ij} at ϵ below and $1 - \epsilon$ above, with $\epsilon = 0.00001$. In this example, class 1 has the highest probability and hence is the correct class.

Figure 1 shows accuracy rates for each of the four methods when $k = 3, 5, 8, 10, 12, 15, 20$. The accuracy rates are averaged over 1,000 replicates. Note that in this experiment all classes are quite competitive, so, when using δ_V, sometimes the highest vote occurs at two

*For I to be well defined, we consider $r_{ij} \neq r_{ji}$, which is generally true. In addition, if there is an i for which $\sum_{j:j\neq i} I_{\{r_{ji}>r_{ij}\}} = 0$, an optimal solution of (16) is $p_i = 1$, and $p_j = 0, \forall j \neq i$. The resulting decision is the same as that of (1).



(a) balanced p_i (b) unbalanced p_i (c) highly unbalanced p_i

Figure 1: Accuracy of predicting the true class by the methods δ_{HT} (solid line, cross marked), δ_V (dash line, square marked), δ_1 (dotted line, circle marked), and δ_2 (dashed line, asterisk marked) from simulated class probability $p_i, i = 1, 2 \cdots k$.

or more different classes. We handle this problem by randomly selecting one class from the ties. This partly explains why δ_V performs poor. Another explanation is that the r_{ij} here are all close to 1/2, but (16) uses 1 or 0 instead; therefore, the solution may be severely biased. Besides δ_V, the other three rules have done very well in this example.

Since δ_{HT} relies on the approximation $p_i + p_j \approx k/2$, this rule may suffer some losses if the class probabilities are not highly balanced. To examine this point, we consider the following two sets of class probabilities:

(1) We let $k_1 = k/2$ if k is even, and $(k+1)/2$ if k is odd; then we define $p_1 = 0.95 \times 1.5/k_1$, $p_i = (0.95 - p_1)/(k_1 - 1)$ for $i = 2, \ldots, k_1$, and $p_i = 0.05/(k - k_1)$ for $i = k_1 + 1, \ldots, k$.

(2) If $k = 3$, we define $p_1 = 0.95 \times 1.5/2$, $p_2 = 0.95 - p_1$, and $p_3 = 0.05$. If $k > 3$, we define $p_1 = 0.475$, $p_2 = p_3 = 0.475/2$, and $p_i = 0.05/(k-3)$ for $i = 4, \ldots, k$.

After setting p_i, we define the pairwise comparisons r_{ij} as in (17)-(18). Both experiments are repeated for 1,000 times. The accuracy rates are shown in Figures 1(b) and 1(c). In both scenarios, p_i are not balanced. As expected, δ_{HT} is quite sensitive to the imbalance of p_i. The situation is much worse in Figure 1(c) because the approximation $p_i + p_j \approx k/2$ is more seriously violated, especially when k is large.

In summary, δ_1 and δ_2 are less sensitive to p_i, and their overall performance are fairly stable. All features observed here agree with our analysis in Section 5.

6.2 Real Data

In this section we present experimental results on several multi-class problems: segment, satimage, and letter from the Statlog collection [9], USPS [4], and MNIST [7]. All data sets are available at `http://www.csie.ntu.edu.tw/~cjlin/libsvmtools/t`. Their numbers of classes are 7, 6, 26, 10, and 10, respectively. From thousands of instances in each data, we select 300 and 500 as our training and testing sets.

We consider support vector machines (SVM) with RBF kernel $e^{-\gamma\|x_i - x_j\|^2}$ as the binary classifier. The regularization parameter C and the kernel parameter γ are selected by cross-validation. To begin, for each training set, a five-fold cross-validation is conducted on the following points of (C, γ): $[2^{-5}, 2^{-3}, \ldots, 2^{15}] \times [2^{-5}, 2^{-3}, \ldots, 2^{15}]$. This is done by modifying LIBSVM [1], a library for SVM. At each (C, γ), sequentially four folds are

Table 1: Testing errors (in percentage) by four methods: Each row reports the testing errors based on a pair of the training and testing sets. The mean and std (standard deviation) are from five 5-fold cross-validation procedures to select the best (C, γ).

Dataset	k	δ_{HT}		δ_1		δ_2		δ_V	
		mean	std	mean	std	mean	std	mean	std
satimage	6	14.080	1.306	14.600	0.938	14.760	0.784	15.400	0.219
		12.960	0.320	13.400	0.400	13.400	0.400	13.360	0.080
		14.520	0.968	14.760	1.637	13.880	0.392	14.080	0.240
		12.400	0.000	12.200	0.000	12.640	0.294	12.680	1.114
		16.160	0.294	16.400	0.379	16.120	0.299	16.160	0.344
segment	7	9.960	0.480	9.480	0.240	9.000	0.400	8.880	0.271
		6.040	0.528	6.280	0.299	6.200	0.456	6.760	0.445
		6.600	0.000	6.680	0.349	6.920	0.271	7.160	0.196
		5.520	0.466	5.200	0.420	5.400	0.580	5.480	0.588
		7.440	0.625	8.160	0.637	8.040	0.408	7.840	0.344
USPS	10	14.840	0.388	13.520	0.560	12.760	0.233	12.520	0.160
		12.080	0.560	11.440	0.625	11.600	1.081	11.440	0.991
		10.640	0.933	10.000	0.657	9.920	0.483	10.320	0.744
		12.320	0.845	11.960	1.031	11.560	0.784	11.840	1.248
		13.400	0.310	12.640	0.080	12.920	0.299	12.520	0.917
MNIST	10	17.400	0.000	16.560	0.080	15.760	0.196	15.960	0.463
		15.200	0.400	14.600	0.000	13.720	0.588	12.360	0.196
		17.320	1.608	14.280	0.560	13.400	0.657	13.760	0.794
		14.720	0.449	14.160	0.196	13.360	0.686	13.520	0.325
		12.560	0.294	12.600	0.000	13.080	0.560	12.440	0.233
letter	26	39.880	1.412	37.160	1.106	34.560	2.144	33.480	0.325
		41.640	0.463	39.400	0.769	35.920	1.389	33.440	1.061
		41.320	1.700	38.920	0.854	35.800	1.453	35.000	1.066
		35.240	1.439	32.920	1.121	29.240	1.335	27.400	1.117
		43.240	0.637	40.360	1.472	36.960	1.741	34.520	1.001

used as the training set while one fold as the validation set. The training of the four folds consists of $k(k-1)/2$ binary SVMs. For the binary SVM of the ith and the jth classes, using decision values $\hat{f}$ of training data, we employ an improved implementation [8] of Platt's posterior probabilities [10] to estimate r_{ij}:

$$r_{ij} = P(i \mid i \text{ or } j, x) = \frac{1}{1 + e^{A\hat{f}+B}}, \tag{19}$$

where A and B are estimated by minimizing the negative log-likelihood function.†

Then, for each validation instance , we apply the four methods to obtain classification decisions. The error of the five validation sets is thus the cross-validation error at (C, γ).

After the cross-validation is done, each rule obtains its best (C, γ).‡ Using these parameters, we train the whole training set to obtain the final model. Next, the same as (19), the decision values from the training data are employed to find r_{ij}. Then, testing data are tested using each of the four rules.

Due to the randomness of separating training data into five folds for finding the best (C, γ), we repeat the five-fold cross-validation five times and obtain the mean and standard deviation of the testing error. Moreover, as the selection of 300 and 500 training and testing instances from a larger dataset is also random, we generate five of such pairs. In Table 1, each row reports the testing error based on a pair of the training and testing sets. The results show that when the number of classes k is small, the four methods perform similarly; however, for problems with larger k, δ_{HT} is less competitive. In particular, for problem letter which has 26 classes, δ_2 or δ_V outperforms δ_{HT} by at least 5%. It seems that for

†[10] suggests to use $\hat{f}$ from the validation instead of the training. However, this requires a further cross-validation on the four-fold data. For simplicity, we directly use $\hat{f}$ from the training.

‡If more than one parameter sets return the smallest cross-validation error, we simply choose one with the smallest C.

problems here, their characteristics are closer to the setting of Figure 1(c), rather than that of Figure 1(a). All these results agree with the previous findings in Sections 5 and 6.1. Note that in Table 1, some standard deviations are zero. That means the best (C, γ) by different cross-validations are all the same. Overall, the variation on parameter selection due to the randomness of cross-validation is not large.

7 Discussions and Conclusions

As the minimization of the KL distance is a well known criterion, some may wonder why the performance of δ_{HT} is not quite satisfactory in some of the examples. One possible explanation is that here KL distance is derived under the assumptions that $n_{ij}r_{ij} \sim \text{Bin}(n_{ij}, \mu_{ij})$ and r_{ij} are independent; however, as pointed out in [3], neither of the assumptions holds in the classification problem.

In conclusion, we have provided two methods which are shown to be more stable than both δ_{HT} and δ_V. In addition, the two proposed approaches require only solutions of linear systems instead of a nonlinear one in [3].

The authors thank S. Sathiya Keerthi for helpful comments.

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