An Improved Conjugate Gradient Scheme to the Solution of Least Squares SVM

Wei Chu, Chong Jin Ong, and S. Sathiya Keerthi

Abstract— **The Least Square Support Vector Machines (LS-SVM) formulation corresponds to the solution of a linear system of equations. Several approaches to its numerical solutions have been proposed in the literature. In this paper, we propose an improved method to the numerical solution of LS-SVM and show that the problem can be solved using one reduced system of linear equations. Compared with the existing algorithm [1] for LS-SVM, our approach is about twice as efficient. Numerical results using the proposed method are provided for comparisons with other existing algorithms.**

Index Terms— **Least Square Support Vector Machines, Conjugate Gradient, Sequential Minimal Optimization**

I. Introduction

As an interesting variant of the standard support vector machines [2], least squares support vector machines (LS-SVM) have been proposed by Suykens and Vandewalle [3] for solving pattern recognition and nonlinear function estimation problems. The links between LS-SVM classifiers and kernel Fisher discriminant analysis have also been established by Van Gestel et al. [4]. The LS-SVM formulation has been further extended to kernel principal component analysis, recurrent networks and optimal control [5]. As for the training of the LS-SVM, Suykens et al. [1] proposed an iterative algorithm based on the conjugate gradient algorithm. Keerthi and Shevade [6] adapted the Sequential Minimal Optimization (SMO) algorithm for SVM [7] for the solution of LS-SVM.

In this paper, we propose an improved algorithm with conjugate gradient methods for LS-SVM. We first show the optimality conditions of LS-SVM, and establish its equivalence to a reduced linear system. Conjugate gradient methods can then be employed for its solution. Compared with the algorithm proposed by Suykens et al. [1], our algorithm is equally robust and is at least twice as efficient.

We adopt the following notations. $x \in R^d, D \in R^{n\times m}$ are d-dimensional column vector and $n \times m$ matrix of real entries respectively; x^T is the transpose of x; $\mathbf{1_n}$ and $\mathbf{0_n}$ are $n-$column vectors of entries 1 and 0 respectively. This paper is organized as follows. In section II, we review the optimization formulation of LS-SVM, and then show the simplification of the optimality conditions to a reduced linear system. In section III, we present the results of numerical experiments using our proposed algorithm on some benchmark data sets of different sizes, and compare with the results obtained using the conjugate method by Suykens et al. [1] and the SMO algorithm by Keerthi and Shevade [6]. We conclude in section IV.

Manuscript received September 21, 2003; revised March 7, 2004. This work was supported by the research scholarship of National University of Singapore.

W. Chu is with Gatsby Computational Neuroscience Unit, University College London. C. J. Ong is with Department of Mechanical Engineering, National University of Singapore. S. S. Keerthi is with Yahoo! Research Labs.

II. LS-SVM and its Solution

Suppose that we are given a training data set of n data points $\{x_i, y_i\}_{i=1}^n$, where $x_i \in R^d$ is the i-th input vector and y_i is the corresponding i-th target. For binary classification problems y_i takes only two possible values $\{-1, +1\}$, whereas y_i takes any real value, i.e. $y_i \in R$, for regression problems. We employ the idea to transform the input patterns into the reproducing kernel Hilbert space (RKHS) by a set of mapping functions $\boldsymbol{\phi}(x)$ [5]. The reproducing kernel $K(x, x')$ in the RKHS is the dot product of the mapping functions at x and x', i.e.

$$K(x, x') = \langle \boldsymbol{\phi}(x) \cdot \boldsymbol{\phi}(x') \rangle \tag{1}$$

In the RKHS, a linear classification/regression is performed. The discriminant function takes the form $f(x) = \sum_{i=1}^n \langle \boldsymbol{w} \cdot \boldsymbol{\phi}(x) \rangle + b$, where $\boldsymbol{w}$ is the weight vector in the RKHS, and $b \in R$ is called the bias term. The discriminant function of LS-SVM classifier [3] is constructed by solving the following minimization problem:

$$\min_{\boldsymbol{w},b,\boldsymbol{\xi}} P(\boldsymbol{w}, b, \boldsymbol{\xi}) = \frac{1}{2}\langle \boldsymbol{w} \cdot \boldsymbol{w} \rangle + \frac{C}{2}\sum_{i=1}^n \xi_i^2 \tag{2}$$

$$\text{s.t. } y_i - (\langle \boldsymbol{w} \cdot \boldsymbol{\phi}(x_i) \rangle + b) = \xi_i \quad i = 1, \cdots, n \tag{3}$$

where $C > 0$ is the regularization factor and ξ_i is the difference between the output y_i and $f(x_i)$. Using standard techniques [8], the Lagrangian for (2)-(3) is:

$$\begin{aligned} L(\boldsymbol{w}, b, \boldsymbol{\xi}; \boldsymbol{\alpha}) \quad = \quad & \frac{1}{2}\langle \boldsymbol{w} \cdot \boldsymbol{w} \rangle + \frac{C}{2}\sum_{i=1}^n \xi_i^2 \\ & + \sum_{i=1}^n \alpha_i \left(y_i - (\langle \boldsymbol{w} \cdot \boldsymbol{\phi}(x_i) \rangle + b) - \xi_i \right) \end{aligned} \tag{4}$$

where $\alpha_i, i = 1, \cdots, n$ are the Lagrangian multipliers corresponding to (3). The Karush-Kuhn-Tucker (KKT) conditions (2) are:

$$\begin{cases} \frac{\partial L}{\partial \boldsymbol{w}} = 0 & \rightarrow \quad \boldsymbol{w} = \sum_{i=1}^n \alpha_i \boldsymbol{\phi}(x_i) \\ \frac{\partial L}{\partial b} = 0 & \rightarrow \quad \sum_{i=1}^n \alpha_i = 0 \\ \frac{\partial L}{\partial \xi_i} = 0 & \rightarrow \quad \alpha_i = C\xi_i \qquad \forall i \\ \frac{\partial L}{\partial \alpha_i} = 0 & \rightarrow \quad \xi_i = y_i - (\langle \boldsymbol{w} \cdot \boldsymbol{\phi}(x_i) \rangle + b) \qquad \forall i \end{cases} \tag{5}$$

In the numerical solution proposed by Suykens et al. [1], the KKT conditions of (5) are reduced to a linear system by eliminating $\boldsymbol{w}$ and $\boldsymbol{\xi}$, resulting in

$$\begin{bmatrix} \boldsymbol{Q} & \mathbf{1_n} \\ \mathbf{1_n}^T & 0 \end{bmatrix} \cdot \begin{bmatrix} \boldsymbol{\alpha} \\ b \end{bmatrix} = \begin{bmatrix} \boldsymbol{y} \\ 0 \end{bmatrix} \tag{6}$$

where $\boldsymbol{Q} \in R^{n\times n}$ with ij-th entry $\boldsymbol{Q}_{ij} = K(x_i, x_j) + \frac{1}{C}\delta_{ij}$,[1] $\boldsymbol{y} = [y_1, y_2, \ldots, y_n]^T$ and $\boldsymbol{\alpha} = [\alpha_1, \alpha_2, \ldots, \alpha_n]^T$. Note that $\boldsymbol{Q}$ is symmetric and positive definite since the matrix $\boldsymbol{K} \in R^{n\times n}$ with $\boldsymbol{K}_{ij} = K(x_i, x_j)$ is semi-positive definite and the diagonal term $\frac{1}{C}$ is positive. Solving (6) for $\boldsymbol{\alpha}$ and b, the discriminant function can be obtained from $f(x) = \sum_{i=1}^{n} \alpha_i K(x_i, x) + b$.

Suykens et al. [1] suggested the use of the conjugate gradient method for the solution of (6). In addition, they reformulated (6) so as to exploit the positive definiteness of $\boldsymbol{Q}$ and proposed to solve two systems of linear equations for $\boldsymbol{\alpha}$. More exactly, their algorithm can be described as

1) Solve the intermediate variables $\boldsymbol{\eta}$ and $\boldsymbol{\nu}$ from $\boldsymbol{Q}\cdot\boldsymbol{\eta} = \boldsymbol{y}$ and $\boldsymbol{Q}\cdot\boldsymbol{\nu} = \mathbf{1_n}$ using conjugate gradient methods.
2) Find solution $b = (\mathbf{1_n}^T\cdot\boldsymbol{\eta})/(\mathbf{1_n}^T\cdot\boldsymbol{\nu})$, and $\boldsymbol{\alpha} = \boldsymbol{\eta} - b\cdot\boldsymbol{\nu}$.

In step 1, the n^{th}-order linear equations are solved twice, using conjugate gradient method, for the solutions of $\boldsymbol{\eta}$ and $\boldsymbol{\nu}$. In the following, we propose a single step approach that solves the linear system having $n-1$ order. We begin by stating some known results.

Lemma 1: Consider the partition of the symmetric and positive definite matrix $\boldsymbol{Q} := \begin{bmatrix} \bar{\boldsymbol{Q}} & \boldsymbol{q} \\ \boldsymbol{q}^T & \boldsymbol{Q}_{nn} \end{bmatrix}$, where $\bar{\boldsymbol{Q}} \in R^{(n-1)\times(n-1)}$, $\boldsymbol{q} \in R^{n-1}$ and $\boldsymbol{Q}_{nn} \in R$. Then

$$\tilde{\boldsymbol{Q}} := \bar{\boldsymbol{Q}} - \mathbf{1}_{n-1}\cdot\boldsymbol{q}^T - \boldsymbol{q}\cdot\mathbf{1}_{n-1}^T + \boldsymbol{Q}_{nn}\cdot\mathbf{1}_{n-1}\cdot\mathbf{1}_{n-1}^T \tag{7}$$

is positive definite.

Proof : Let $\boldsymbol{M} = \begin{bmatrix} \mathbf{I}_{n-1} & \mathbf{0}_{n-1} \\ -\mathbf{1}_{n-1}^T & 1 \end{bmatrix}$ and note that

$$\begin{aligned} & \boldsymbol{M}^T\cdot\boldsymbol{Q}\cdot\boldsymbol{M} \\ = & \begin{bmatrix} \mathbf{I}_{n-1} & -\mathbf{1}_{n-1} \\ \mathbf{0}_{n-1}^T & 1 \end{bmatrix} \begin{bmatrix} \bar{\boldsymbol{Q}} & \boldsymbol{q} \\ \boldsymbol{q}^T & \boldsymbol{Q}_{nn} \end{bmatrix} \begin{bmatrix} \mathbf{I}_{n-1} & \mathbf{0}_{n-1} \\ -\mathbf{1}_{n-1}^T & 1 \end{bmatrix} \\ = & \begin{bmatrix} \tilde{\boldsymbol{Q}} & \tilde{\boldsymbol{q}} \\ \tilde{\boldsymbol{q}}^T & \boldsymbol{Q}_{nn} \end{bmatrix} \end{aligned} \tag{8}$$

where $\tilde{\boldsymbol{Q}}$ is as given by (7). Since $\boldsymbol{Q}$ is positive definite, so is the matrix at the right-hand side of (8). As $\tilde{\boldsymbol{Q}}$ is a sub-matrix of a positive definite matrix, the result follows.

Lemma 2: Let $\tilde{\boldsymbol{\alpha}}^*$ be the solution of $\tilde{\boldsymbol{Q}}\cdot\tilde{\boldsymbol{\alpha}} = \tilde{\boldsymbol{y}} - y_n\cdot\mathbf{1}_{n-1}$ with $\tilde{\boldsymbol{y}} = [y_1, y_2, \ldots, y_{n-1}]^T$ and $\tilde{\boldsymbol{Q}}$ as given by (7). Then the vector $\boldsymbol{\alpha}^* = \begin{bmatrix} \tilde{\boldsymbol{\alpha}}^* \\ -\mathbf{1}_{n-1}^T\cdot\tilde{\boldsymbol{\alpha}}^* \end{bmatrix}$ and $b^* = y_n + \boldsymbol{Q}_{nn}\cdot(\mathbf{1}_{n-1}^T\cdot\tilde{\boldsymbol{\alpha}}^*) - \boldsymbol{q}^T\cdot\tilde{\boldsymbol{\alpha}}^*$ are the solution of the optimization problem (2).

Proof : Since $\tilde{\boldsymbol{Q}}$ is positive definite, $\tilde{\boldsymbol{\alpha}}^*$ is unique. Using $\tilde{\boldsymbol{Q}}$ from (7) and $\tilde{\boldsymbol{Q}}\cdot\tilde{\boldsymbol{\alpha}}^* = \tilde{\boldsymbol{y}} - y_n\cdot\mathbf{1}_{n-1}$, we have

$$\begin{aligned} & \bar{\boldsymbol{Q}}\cdot\tilde{\boldsymbol{\alpha}}^* - \boldsymbol{q}\cdot\mathbf{1}_{n-1}^T\cdot\tilde{\boldsymbol{\alpha}}^* - \tilde{\boldsymbol{y}} \\ = & (\boldsymbol{q}^T\cdot\tilde{\boldsymbol{\alpha}}^* - \boldsymbol{Q}_{nn}\cdot(\mathbf{1}_{n-1}^T\cdot\tilde{\boldsymbol{\alpha}}^*) - y_n)\cdot\mathbf{1}_{n-1} \\ = & -b^*\cdot\mathbf{1}_{n-1} \end{aligned} \tag{9}$$

where we have used

$$b^* = y_n + \boldsymbol{Q}_{nn}\cdot(\mathbf{1}_{n-1}^T\cdot\tilde{\boldsymbol{\alpha}}^*) - \boldsymbol{q}^T\cdot\tilde{\boldsymbol{\alpha}}^* \tag{10}$$

Rewriting (9) and (10) into matrix form, we have

$$\boldsymbol{Q}\cdot\boldsymbol{\alpha}^* + b^*\cdot\mathbf{1_n} = \boldsymbol{y} \tag{11}$$

From (11) and the fact that $\mathbf{1}_n^T\cdot\boldsymbol{\alpha}^* = 0$, it follows that $\boldsymbol{\alpha}^*$ and b^* are the solution of (6) and hence satisfy the optimization problem (2)-(3).

Following Lemma 2, we can use the standard conjugate gradient algorithm [8] for the solution of the reduced linear system $\tilde{\boldsymbol{Q}}\cdot\tilde{\boldsymbol{\alpha}} = \tilde{\boldsymbol{y}} - y_n\cdot\mathbf{1}_{n-1}$. Clearly, compared with the scheme proposed by Suykens et al. [1], our algorithm can save at least 50% of the computational effort. In addition, $\tilde{\boldsymbol{Q}}$ is positive definite and the numerical stability of our approach is the similar to that proposed by Suykens et al. [1].

III. Numerical Experiments

For comparison purpose, we implemented our proposed algorithm with standard conjugate gradient methods (CG), the algorithm proposed by Suykens et al. [1], and the SMO algorithm given by Keerthi and Shevade [6]. The stopping conditions used in all three algorithms are the same, and is based on the value of the duality gap, i.e., $P(\boldsymbol{w}, b, \boldsymbol{\xi}) - D(\boldsymbol{\alpha}) \le \epsilon D(\boldsymbol{\alpha})$, where $P(\boldsymbol{w}, b, \boldsymbol{\xi})$ is defined as in (2), $D(\boldsymbol{\alpha})$ is the dual functional given by $D(\boldsymbol{\alpha}) = \frac{1}{2}\cdot\boldsymbol{\alpha}^T\cdot\boldsymbol{Q}\cdot\boldsymbol{\alpha} - \boldsymbol{\alpha}^T\cdot\boldsymbol{y}$, and $\epsilon = 10^{-6}$. Note that this is not the traditional stopping condition for conjugate gradient algorithm. We have discounted the extra cost caused by computing the stopping condition in CG for a fair comparison. In the implementations, the diagonal entries of $\boldsymbol{Q}$ were cached for efficiency, and we also cached the vector $\boldsymbol{q}$ for our improved CG scheme. The programs used in the experiments were written in ANSI C and executed on a Pentium III 866 PC running on Windows 2000 platform.[2] Six benchmark data sets were used in these experiments: Banana, Waveform, Image, Splice, MNIST and Computer Activity.[3] The Gaussian kernel $K(x, x') = \exp\left(-\frac{\|x-x'\|^2}{2\sigma^2}\right)$ was used as the kernel function. The values of σ^2 used are based on the suggested values given in Duan et al. [9].

We carried out the numerical experiments on the six data sets with several different regularization factor C, and recorded their results in Table I and Table II respectively. All the algorithms are stable and closely reach the same dual functional $D(\boldsymbol{\alpha})$. The computational cost of our approach is about half of that used by the algorithm in [1]. The increase in computational cost of the SMO algorithm at large C values (greater than 10^3) is sharp as seen from the results on Banana and Image data sets.[4] For small to medium data sets, the CG algorithm is more efficient than SMO. Experimentally, SMO scales better than the CG methods based on the two large data sets that we have solved. Consequently, there is no

[1] δ_{ij} is 1 only when $i = j$, otherwise 0.

[2] The programs and their source code can be accessed at http://guppy.mpe.nus.edu.sg/∼chuwei/code/lssvm.zip.

[3] Image and Splice datasets can be accessed at http://ida.first.gmd.de/∼raetsch/data/benchmarks.htm. We used the first partition in the twenty partitions. MNIST is available at http://yann.lecun.com/exdb/mnist/, and we selected the samples of the digit 0 and 8 only to set up the binary classification problem. Computer Activity dataset is available in DELVE at http://www.cs.toronto.edu/∼delve/, and it corresponds to a regression problem.

[4] Keerthi and Shevade [6] argued that too large C values might actually be out of our interest since the optimal C is seldom greater than 10^3 in practice.

TABLE I

COMPUTATIONAL COSTS FOR SMO AND CG ALGORITHMS ($\boldsymbol{\alpha} = 0$ INITIALIZATION) ON SMALL-SIZE AND MEDIUM-SIZE DATA SETS. KERNEL DENOTES THE NUMBER OF KERNEL EVALUATIONS, IN WHICH EACH UNIT DENOTES 10^6 EVALUATIONS. CPU DENOTES THE CPU TIME IN SECONDS CONSUMED BY THE OPTIMIZATION. $D(\boldsymbol{\alpha})$ DENOTES THE DUAL FUNCTIONAL AT THE OPTIMAL SOLUTION. σ^2 IS THE PARAMETER IN GAUSSIAN KERNEL, WHICH IS CHOSEN AS IN [9]. C IS THE REGULARIZATION FACTOR IN (2).

	Banana Dataset, 400 samples with 2-dimensional inputs, $\sigma^2 = 1.8221$,								
	Suyken et al.'s CG			Our CG Approach			SMO		
$\log_{10} C$	Kernel	CPU	$D(\boldsymbol{\alpha})$	Kernel	CPU	$D(\boldsymbol{\alpha})$	Kernel	CPU	$D(\boldsymbol{\alpha})$
-4	0.320	0.080	0.0198	0.239	0.070	0.0198	0.902	0.290	0.0198
-3	0.479	0.120	0.197	0.239	0.070	0.197	0.825	0.260	0.197
-2	0.639	0.160	1.881	0.398	0.111	1.881	0.530	0.171	1.881
-1	1.277	0.380	15.544	0.715	0.221	15.546	0.509	0.160	15.546
0	2.235	0.641	97.214	1.192	0.320	97.232	0.710	0.200	97.232
+1	3.990	1.153	665.313	1.986	0.592	665.397	3.496	1.122	665.396
+2	7.821	2.294	5668.911	3.733	1.013	5669.293	31.350	10.054	5669.291
+3	15.641	4.444	52684.905	7.067	2.104	52687.397	319.759	103.199	52687.378
+4	32.718	9.484	494210.847	15.563	4.616	494245.928	3306.155	1070.269	494245.799
	Waveform Dataset, 400 samples with 21-dimensional inputs, $\sigma^2 = 24.5325$								
	Suyken et al.'s CG			Our CG Approach			SMO		
$\log_{10} C$	Kernel	CPU	$D(\boldsymbol{\alpha})$	Kernel	CPU	$D(\boldsymbol{\alpha})$	Kernel	CPU	$D(\boldsymbol{\alpha})$
-4	0.320	0.150	0.0176	0.239	0.110	0.0176	0.929	0.450	0.0176
-3	0.479	0.210	0.173	0.239	0.090	0.173	0.910	0.441	0.173
-2	0.639	0.331	1.477	0.318	0.140	1.477	0.517	0.251	1.477
-1	1.118	0.501	9.398	0.636	0.291	9.398	0.413	0.200	9.398
0	2.394	1.112	55.415	1.192	0.560	55.415	0.557	0.250	55.415
+1	6.225	3.025	304.430	2.939	1.485	304.431	2.355	1.141	304.430
+2	14.684	6.541	972.925	7.147	3.183	972.925	10.600	5.138	972.925
+3	23.462	10.447	1428.193	11.514	5.327	1428.192	21.774	10.575	1428.193
+4	27.611	12.316	1510.109	13.340	6.101	1510.110	28.214	14.040	1510.110
	Image Dataset, 1300 samples with 18-dimensional inputs, $\sigma^2 = 2.7183$								
	Suyken et al.'s CG			Our CG Approach			SMO		
$\log_{10} C$	Kernel	CPU	$D(\boldsymbol{\alpha})$	Kernel	CPU	$D(\boldsymbol{\alpha})$	Kernel	CPU	$D(\boldsymbol{\alpha})$
-4	3.379	1.983	0.0635	2.532	1.642	0.0635	9.301	6.830	0.0635
-3	5.067	2.654	0.618	2.532	1.572	0.618	7.444	5.367	0.618
-2	8.445	4.897	5.050	4.218	2.364	5.050	5.166	3.776	5.050
-1	20.266	11.466	28.671	10.962	6.350	28.671	4.833	3.505	28.671
0	48.974	28.452	133.878	26.980	16.873	133.878	7.036	4.997	133.878
+1	135.097	78.922	574.150	70.819	39.212	574.150	33.935	24.225	574.150
+2	417.110	243.238	2554.951	216.667	137.470	2554.951	253.361	187.459	2554.950
+3	1269.904	740.442	11554.667	705.636	450.154	11554.666	1910.307	2802.560	11554.662
+4	4186.289	2446.655	39458.945	2256.850	1436.888	39458.946	11806.379	17331.135	39458.943
	Splice Dataset, 1000 samples with 60-dimensional inputs, $\sigma^2 = 29.9641$								
	Suyken et al.'s CG			Our CG Approach			SMO		
$\log_{10} C$	Kernel	CPU	$D(\boldsymbol{\alpha})$	Kernel	CPU	$D(\boldsymbol{\alpha})$	Kernel	CPU	$D(\boldsymbol{\alpha})$
-4	1.000	2.113	0.0499	0.999	2.143	0.0499	4.726	8.262	0.0499
-3	1.999	4.216	0.497	1.498	3.215	0.497	4.364	7.551	0.497
-2	2.998	6.319	4.775	1.996	4.325	4.775	2.925	5.088	4.775
-1	5.995	12.628	36.459	3.492	7.531	36.459	3.120	5.408	36.459
0	12.988	27.350	159.990	6.483	14.001	159.990	3.120	5.348	159.990
+1	29.971	63.261	309.340	16.951	36.816	309.340	5.391	9.464	309.340
+2	65.935	138.911	348.659	35.396	77.757	348.659	10.767	18.697	348.659
+3	89.911	189.836	353.380	55.834	120.547	353.380	32.722	56.892	353.380
+4	111.889	232.535	353.866	62.813	134.298	353.865	119.222	207.278	353.866

clear overall superiority in the performance for either of the methods. We suggest that CG algorithm is suitable for small to moderate data sets i.e., the number of samples is less than two thousands, while SMO is suitable for large data sets.

TABLE II

COMPUTATIONAL COSTS FOR SMO AND CG ALGORITHMS ($\boldsymbol{\alpha} = 0$ INITIALIZATION) ON LARGE-SIZE DATA SETS. COMPUTER ACTIVITY IS A REGRESSION PROBLEM. KERNEL DENOTES THE NUMBER OF KERNEL EVALUATIONS, IN WHICH EACH UNIT DENOTES 10^6 EVALUATIONS. CPU DENOTES THE CPU TIME IN SECONDS CONSUMED BY THE OPTIMIZATION. $D(\boldsymbol{\alpha})$ DENOTES THE DUAL FUNCTIONAL AT THE OPTIMAL SOLUTION. σ^2 IS THE PARAMETER IN GAUSSIAN KERNEL, WHICH IS SET TO AN APPROPRIATE VALUE. C IS THE REGULARIZATION FACTOR IN (2).

	MNIST Dataset, 11739 samples with 400-dimensional inputs, $\sigma^2 = 0.0025$					
	Our CG Approach			SMO		
$\log_{10} C$	Kernel	CPU	$D(\boldsymbol{\alpha})$	Kernel	CPU	$D(\boldsymbol{\alpha})$
-2	413.302	5611.010	56.136	401.397	3515.685	56.136
-1	757.752	10284.239	493.689	403.956	3540.721	493.689
0	1722.135	23495.622	2685.667	420.814	3688.304	2685.668
+1	4064.206	56682.010	4965.833	669.879	5872.334	4965.836
+2	9643.847	134222.101	5558.749	1257.794	11027.597	5558.752

	Computer Activity, 8192 samples with 21-dimensional inputs, $\sigma^2 = 20$					
	Our CG Approach			SMO		
$\log_{10} C$	Kernel	CPU	$D(\boldsymbol{\alpha})$	Kernel	CPU	$D(\boldsymbol{\alpha})$
-2	335.438	423.450	19.510	158.590	149.785	19.510
-1	805.028	1021.007	80.608	159.148	150.226	80.608
0	1710.666	2185.105	275.971	220.706	207.939	275.971
+1	4662.375	5880.373	1002.054	845.302	798.177	1002.054
+2	14221.886	17926.644	5453.505	6382.203	6028.509	5453.501

IV. CONCLUSION

In this paper, we proposed a new scheme for the numerical solution of LS-SVM using conjugate gradient methods. The new scheme is simple and efficient and involves the solution of the linear system of equations of $n-1$ order. Numerical results provided shows that the proposed scheme is at least twice as efficient when compared with the algorithm proposed by Suykens et al. [1]. It also has a comparable performance when compared with the SMO approach by Keerthi and Shevade [6].

ACKNOWLEDGMENTS

Wei Chu gratefully acknowledges the financial support provided by the National University of Singapore through Research Scholarship. A part of the revision work was done at Gatsby Computational Neuroscience Unit of University College London supported by the National Institutes of Health (NIH) and its National Institute of General Medical Sciences (NIGMS) division under Grant Number 1 P01 GM63208 (NIH/NIGMS grant title: Tools and Data Resources in Support of Structural Genomics).

REFERENCES

[1] J. A. K. Suykens, L. Lukas, P. Van Dooren, B. De Moor, and J. Vandewalle, “Least squares support vector machine classifiers: a large scale algorithm,” in *Proc. of the European Conference on Circuit Theory and Design (ECCTD’99)*, 1999, pp. 839–842.

[2] V. N. Vapnik, *The Nature of Statistical Learning Theory*. New York: Springer-Verlag, 1995.

[3] J. A. K. Suykens and J. Vandewalle, “Least squares support vector machine classifiers,” *Neural Processing Letters*, vol. 9, no. 3, pp. 293–300, 1999.

[4] T. Van Gestel, J. A. K. Suykens, G. Lanckriet, A. Lambrechts, B. De Moor, and J. Vandewalle, “A Bayesian framework for least squares support vector machine classifiers, Gaussian processes and kernel fisher discriminant analysis,” *Neural Computation*, vol. 14, pp. 1115–1147, 2002.

[5] J. A. K. Suykens, T. Van Gestel, J. De Brabanter, B. De Moor, and J. Vanthienen, *Least Squares Support Vector Machines*. World Scientific, 2002.

[6] S. S. Keerthi and S. K. Shevade, “SMO algorithm for least squares SVM formulations,” *Neural Computation*, vol. 15, no. 2, Feb. 2003.

[7] J. C. Platt, “Fast training of support vector machines using sequential minimal optimization,” in *Advances in Kernel Methods - Support Vector Learning*, B. Schölkopf, C. J. C. Burges, and A. J. Smola, Eds. MIT Press, 1999, pp. 185–208.

[8] R. Fletcher, *Practical methods of optimization*. John Wiley and Sons, 1987.

[9] K. Duan, S. S. Keerthi, and A. N. Poo, “Evaluation of simple performance measures for tuning svm hyperparameters,” *Neurocomputing*, vol. 51, pp. 41–59, 2003.