

UNIVERSITY OF TARTU  
FACULTY OF MATHEMATICS AND COMPUTER SCIENCE

Institute of Computer Science  
Computer Science speciality

Olga Agen

# Parallelization of Support Vector Machines

Master Thesis (30 EAP)

Supervisor: Oleg Batrashev, MSc

Co-Supervisor: Artjom Lind, MSc

Author: ..... “.....” May 2013

Supervisor: ..... “.....” May 2013

Co-Supervisor: ..... “.....” May 2013

Allowed to defence

Professor: ..... “.....” May 2013

TARTU 2013

# Contents

<b>1</b>	<b>Introduction</b>	<b>5</b>
<b>2</b>	<b>Support Vector Machine</b>	<b>8</b>
2.1	Perceptron . . . . .	8
2.2	Support vector machine . . . . .	10
2.2.1	Linearly separable case . . . . .	10
2.2.2	Linearly non-separable case . . . . .	12
<b>3</b>	<b>Optimization</b>	<b>14</b>
3.1	Sequential minimal optimization . . . . .	14
3.2	Interior point method . . . . .	16
3.3	Gradient methods . . . . .	18
<b>4</b>	<b>Parallelization</b>	<b>20</b>
4.1	Parallel SMO . . . . .	20
4.2	Cascade SVM . . . . .	21
4.3	PSVM . . . . .	21
4.4	P-packSVM . . . . .	23
<b>5</b>	<b>Performance tests</b>	<b>25</b>
5.1	Setup . . . . .	25
5.2	Results . . . . .	25
<b>6</b>	<b>Support Vector Clustering</b>	<b>27</b>
6.1	Support Vector Clustering . . . . .	27
6.2	Improved support vector clustering (iSVC) . . . . .	29
6.2.1	Optimization piece of iSVC . . . . .	29
6.2.2	The labeling piece of iSVC . . . . .	30
6.3	Parallel SVC . . . . .	31
<b>7</b>	<b>Summary</b>	<b>32</b>

# Notations

$\alpha, \beta, \mu, \lambda$	Lagrange multipliers
$b$	bias or threshold parameter
$y = \{1, -1\}$	set of classes of the training set
$x_i$	$i^{th}$ input feature vector of the training set
$w$	normal to separating hyperplane
$\Phi(x)$	objective function
$\xi$	slack variable, defines allowed errors
$K(x, x)$	kernel function
$\Psi : X \rightarrow H$	transformation function

# Abbreviations

SVM	support vector machine
SV	support vector
BSV	bounded support vector
SVC	support vector clustering
QP	quadratic programming
SMO	sequential minimal optimization
ICF	Incomplete Cholesky Factorization
IPM	interior point method
KKT	Karush-Kuhn-Tucker conditions
SGD	stochastic gradient descent

# Chapter 1

## Introduction

For many decades, computer scientists have been dealing with the idea of making a machine that is capable of learning just like the ordinary human being. Machine learning, a branch of artificial intelligence, researches the algorithms and techniques for teaching a machine or software using a large set of data. One of the main problems machine learning tries to solve is the problem of data classification, i.e separating instances of the data into several classes or groups. The first attempt to create a device capable of classifying data was perceptron, created by Frank Rosenblatt in 1957. It was based on the structure of humans neurons, and used a simple to comprehend model of penalties for incorrectly classified objects. Rosenblatt's perceptron left a huge impact on machine learning society and led to further researches in the field of data classification.

One of the techniques used for data classification is support vector machine (SVM), proposed by Vladimir Vapnik in 1990s. SVM takes binary classification as the fundamental problem and follows the geometrically intuitive approach to find a hyperplane that divides objects into two separate classes. The training part of the SVM aims to both maximize the width of the margin that surrounds the separating hyperplane and minimize the occurrence of classification errors.

Training of SVM involves solving of a convex quadratic problem, which becomes computationally expensive as the size of the training data grows. The quadratic form of optimization problem that SVM has to solve involves a matrix that has a number of elements equal to the square of the number of training examples, which means that with a large set of data, the matrix simply will not fit into memory and will be stored at the hard drive of the computer, making computation even slower.

The above problem has led to the understanding that a new approach to the SVM algorithm is required. Several suggestions regarding matrix size were made:

- Using the fact that the value of the quadratic form is the same if you remove the rows and columns of the matrix that corresponds to zero Lagrange multipliers, a chunking method to solve SVM was proposed[18]. The large quadratic programming problem is broken down into a series of smaller problems, that discard all of the zero Lagrange multipliers. Chunking seriously reduces the size of the matrix to the number of non-zero Lagrange multipliers squared, however, even reduced matrix may not fit into memory.
- John Platt suggested that it is possible to get rid of the matrix calculations entirely and proposed an analytical approach for solving SVM, called sequential

minimal optimization (SMO). SMO decomposes the overall quadratic programming problem into sub-problems, at every step, two Lagrange multipliers are chosen for optimization, which is done analytically, allowing to avoid the numerical quadratic programming optimization[12].

However, there was still room and need for the improvement. In the advent of parallel computers, with new computer architectures and the huge computational power available, it was only natural that a parallel approach to SVM's quadratic programming problem was considered. Despite the fact that parallelizing the linear algebra kernels of optimization algorithms is not trivial, several attempts were made to improve the performance of the SVM by running it in the distributed mode, using the following approaches:

- Distributed storage of data. Kernel matrix is distributed on several machines.
- Sub-problems are solved in parallel. The training set is divided into smaller subsets, and QP problem is solved for each subset in parallel.

Growth of datasets size also led to the necessity for the new clustering algorithms to deal with such large databases. In 2001, a novel clustering algorithm - support vector clustering, based on the SVM approach - was developed. Support vector clustering algorithm data points are mapped from data space to a high dimensional feature space using a Gaussian kernel. The sphere is then mapped back to data space, where it forms a set of contours that enclose the data points and can be interpreted as cluster boundaries. SVC has a unique advantage compared to the known clustering algorithms as it can generate cluster boundaries of arbitrary shape and is capable of dealing with noise and outliers[1]. Still, SVC also lacks the good performance results, and despite the proposed improvements, there is room for further development.

The goal of given thesis is to research efficiency in performance gained by using parallel approach to solve SVM and compare proposed techniques for parallelization in accuracy and computation speed. Also, since SVC also boils down to solving a quadratic programming problem, it is our interest to see, how well the parallel solutions proposed for SVM will work with SVC, and develop a method for SVC that would be suitable for parallel and multi-core environment.

The structure of this thesis is as follows:

- Chapter 2 describes the binary classification problem, introducing one of the first attempts for solving it - Rosenblatt's perceptron and a mathematical model behind it. Main idea behind SVM for both linearly separable and non-separable cases is introduced.
- Chapter 3 outlines some of the optimization approaches to SVM training, such as interior point methods, sequential minimal optimization and gradient methods.
- At chapter 4, an overview of the parallel implementations of SVM is given, showing both their advantages and disadvantages.
- Chapter 5 describes the experimental results obtained while measuring performance of the methods, described in chapter 4.
- Chapter 6 describes the support vector clustering and proposed improvements, including the attempts to apply parallelization techniques used for SVM solving on SVC.

- Finally, chapter 7 provides our conclusion and ideas about the possibility of further research.

# Chapter 2

## Support Vector Machine

Machine learning deals with several problems, one of them is image recognition and the attempts to create computer vision. One of the first attempts to create a machine capable of learning just like the human being was the perceptron model created by Rosenblatt in the 1950s. His model influenced further developments and research in machine learning.

In 1990s Vapnik came up with a new classification technique called support vector machines. Support vector machines is used for data classification as it finds a optimal separating hyperplane between objects that belong to different classes. The SVM algorithm implements many of the ideas used in the perceptron model.

### 2.1 Perceptron

In 1958 an American psychologist Frank Rosenblatt proposed the perceptron model based on McCulloch-Pitts units. It introduced numerical weights and a special connection pattern. In the original Rosenblatt model the computing units are threshold elements and their connectivity is determined stochastically. Learning is committed by adapting the weights of the network with a numerical algorithm.

The structure of perceptron can be observed in Figure 2.1. The connections from the retina to the projection units are deterministic and non-adaptive, while the connections to and from the second layer are stochastically selected.

The idea behind perceptron is to train the system to recognize certain input patterns in the connection region, which in turn leads to the appropriate path through the connections to the association layer. The learning algorithm must derive suitable weights for the connections[14]. The learning rule has been proven to converge on a solution in finite time if a solution exists. The learning rule can be summarized in the

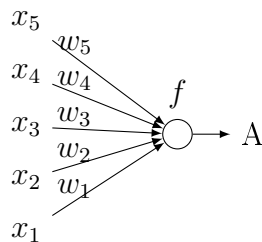


Figure 2.1: The structure of the perceptron



following two equations:

$$\begin{aligned} w(i) &= w(i) + (T - A) \cdot x(i) \\ b &= b + (T - A) \quad \text{for } \forall i, \end{aligned} \tag{2.1}$$

where  $w$  is the vector of weights,  $x$  is the input vector,  $T$  is the correct result that the neuron should have shown,  $A$  is the actual output of the neuron, and  $b$  is the bias.

Perceptron could work in two modes: the learning mode and the operation mode. In the learning mode, perceptron would adjust the weight vector based on the learning rule (2.1). In the operation mode, perceptron would classify an input to the corresponding class.

The mathematical model of perceptron could be described as following[17]:

1. Input vector  $x$  is depicted as a binary vector with only two possible values  $\{0, 1\}$ .
2. At the second layer the input  $x$  is transformed into a new binary vector  $y$ . The transformation  $y = f(x)$  follows the rules:
  - (a) transformation is conducted by threshold elements
  - (b) connection from and to the threshold elements are random
3. Perceptron classifies an input as an element of class  $P$  if for an input vector  $y = (y_1, \dots, y_n)$  the following holds true:

$$\sum_{i=1}^n \alpha_i^p y_i \geq 0, \quad \sum_{i=1}^n \alpha_i^t y_i < 0 \quad \text{for each } t \neq p$$

The idea of the training part of perceptron is to find the weight vectors for each elements in the input data  $X$ . Let's assume that we already have  $\alpha_1^p, \dots, \alpha_n^p$  denoting weights for  $x_p \in X$ . A new input vector  $x_i$  enters perceptron. There are two possible situations:

1. Input vector  $x_i$  belongs to class  $p$ . In this case, the the following must must hold:

$$\sum_{i=1}^n \alpha_i^p y_i \geq 0$$

If actual output and expected results match, then the weight vector does not change. In the other case, each weight vector is changed according to the next rule:

$$\alpha_i^{new} = \alpha_i^{old} + y_i \quad \text{where } i \in [1, n]$$

2. Input vector  $x_i$  does not belong to the class  $p$ , which means that  $\sum_{i=1}^n \alpha_i^p y_i < 0$  must hold. If the output of perceptron is correct, then weight vector remains unchanged. In other case, they are replaced by new coefficients:

$$\begin{aligned} \alpha_i^{new} &= \alpha_i^{old} - y_i \\ \text{where } i &\in [1, n] \end{aligned}$$

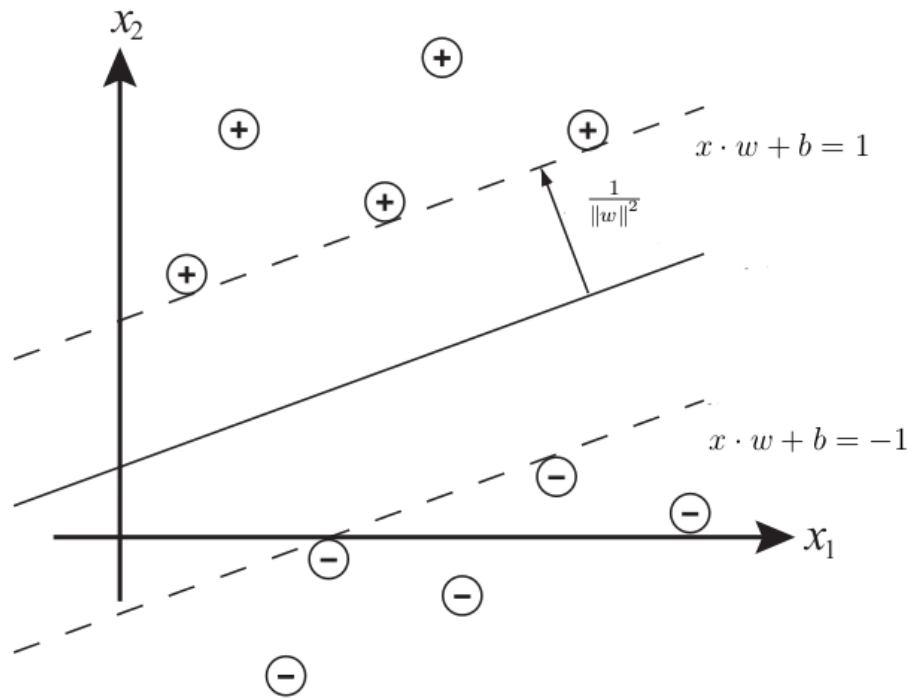


Figure 2.2: Linearly separable data, showing the hyperplane decision boundary and the separating margin

## 2.2 Support vector machine

Support vector machine (SVM) is a machine learning technique for data classification. A classification task usually involves separating data into training and testing sets. Each object in the training set contains one class label and several features. The goal of SVM is to produce a model that is capable of predicting the class labels of the test data given only the test data features.

The input for SVM is provided as a set of training samples  $x_i \in \mathbb{R}^n$  and corresponding classes  $y_i \in \{1, -1\}^n$ , where  $n$  is the size of the training set. The input space is divided into decision regions, and the boundaries that separate regions are called decision boundaries.

### 2.2.1 Linearly separable case

Let's assume that the data is linearly separable, meaning that we can draw a hyperplane between points belonging to different classes. This hyperplane can be described by  $w \cdot x + b = 0$  where  $w$  is normal to the hyperplane,  $\frac{b}{\|w\|}$  is the perpendicular distance from the hyperplane to the origin.

Points located closest to the separating hyperplane are called support vectors. The perpendicular distance between a point and the hyperplane is called margin:

- The functional margin uses the measure  $y_i(x_i \cdot w + b)$  and is always positive for a correctly classified point.
- The geometric margin measures the Euclidean distance from the point to the

hyperplane.

The margin of the hyperplane is the minimum geometric margin of all correctly classified points. The aim of SVM is to orientate the separating hyperplane as far as possible from the closest members of both classes or, in other words, to maximize the margin.

SVM introduces a fixed functional half-margin of 1, so the points from the training set can be described by the following equations:

$$x_i \cdot w + b \geq 1 \quad \text{for } y_i = 1$$

$$x_i \cdot w + b \leq -1 \quad \text{for } y_i = -1$$

These equations can be combined into:

$$y_i(x_i \cdot w + b) - 1 \geq 0 \quad \forall i$$

Planes, where support vectors lie, are called decision boundaries and can be described by:

$$x \cdot w + b = 1$$

$$x \cdot w + b = -1$$

The idea of finding the maximal margin hyperplane, while keeping the points classified correctly, can be formalized in the following way:

$$\begin{aligned} & \min_{w,b} \frac{1}{2} \|w\|^2 \\ & \text{subject to } y_i(w \cdot x_i + b) \geq 1. \end{aligned} \tag{2.2}$$

This problem is referred to as a primal problem. A Lagrangian function associated with 2.2 can be formulated as following:

$$L = \frac{1}{2} \|w\|^2 + \sum_{i=1}^N \alpha_i (1 - y_i(w \cdot x_i + b)) \tag{2.3}$$

Optimization problem 2.2 can be converted into the dual form, which is a convex quadratic problem where the objective function  $\Phi$  depends solely on Lagrangian multipliers  $\alpha_i$ :

$$\min_{\alpha} \Phi(\alpha) = \min_{\alpha} \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N y_i y_j (x_i \cdot x_j) \alpha_i \alpha_j - \sum_{i=1}^N \alpha_i$$

$$\text{subject to } \alpha_i \geq 0$$

$$\sum_{i=1}^N y_i \alpha_i = 0$$

The dual form represents the minimum bound of the Lagrangian 2.3, in case of the strong duality, the optimal values of the primal problem and dual problem are equal.

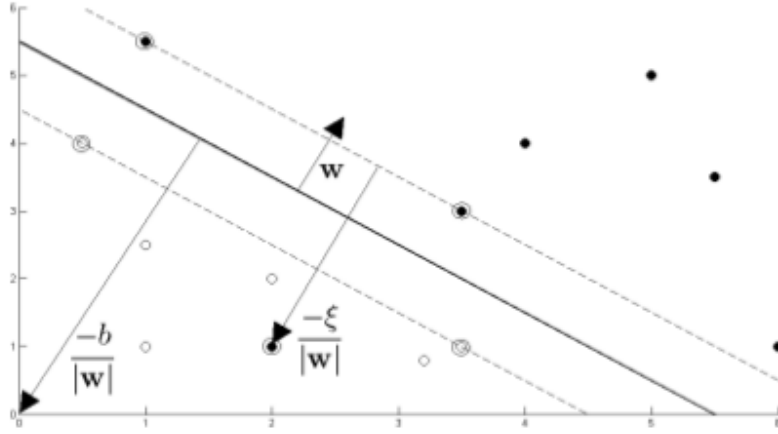


Figure 2.3: Non-separable data showing misclassification error  $\xi$

## 2.2.2 Linearly non-separable case

Since not all data sets are linearly separable, a modification to original statement 2.2 was introduced[5], which allows, but penalizes, error classifications, i.e inability of the elements to reach the correct margin. Modification is done by adding slack variables  $\xi$  that permit margin failure:

$$\min_{w,b,\xi} \frac{1}{2} \|w\|^2 + C \sum_{i=1}^N \xi_i$$

$$\text{subject to } y_i(w \cdot x_i + b) \geq 1 - \xi_i.$$

Here,  $C$  is a parameter allowing to balance between margin maximization and minimization of classification error.

Using the Lagrangian, optimization problem can be presented in dual form as following:

$$\min_{\alpha} \Phi(\alpha) = \min_{\alpha} \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N y_i y_j (x_i \cdot x_j) \alpha_i \alpha_j - \sum_{i=1}^N \alpha_i$$

$$\text{subject to } 0 \leq \alpha_i \leq C$$

$$\sum_{i=1}^N y_i \alpha_i = 0$$

Lagrange multipliers extend the unconstrained first-order condition to the case of equality constraints. To add inequality constraints, Karush-Kuhn-Tucker (KKT) conditions must be applied. KKT conditions are necessary conditions for the local minimum solutions. If point  $x_i$  is an optimal point, then the following KKT conditions are satisfied:

$$\alpha_i = 0 \implies y_i(x_i \cdot w + b) \geq 1$$

$$0 < \alpha_i < C \implies y_i(x_i \cdot w + b) = 1$$

$$\alpha_i = C \implies y_i(x_i \cdot w + b) \leq 1$$

In the case when decision function is not the linear function, the input data has to be mapped to some other space (possibly, with infinite dimensions), using a mapping  $\Psi : X \rightarrow H$ . Since the data appears in the training problem only in the form of dot products  $x_i \cdot x_j$ , explicit knowledge of  $\Psi$  is not required, all we need is a function that would represent the dot product of the mapped input points  $\Psi(x_i) \cdot \Psi(x_j)$ . Such function is called a kernel function:

$$K(x_i, x_j) = \langle \Psi(x_i) \cdot \Psi(x_j) \rangle$$

Replacing the dot product by kernel function, we obtain the output of a non-linear SVM:

$$\sum_{j=1}^N y_j \alpha_j K(x_j, x_i) + b$$

It is possible to extend SVM binary classification to the more general case of  $n$  classes, by repeatedly applying binary classifications. Binary classifiers are trained for each pair of classes. Majority voting of the classifiers is used to determine the class of the test sample.

# Chapter 3

## Optimization

Optimization deals with finding the optimum point, where the objective function reaches its minimum or maximum value. Optimization problem can be of two types - constrained and unconstrained. If the unconstrained optimization problem requires to find an optimum point, then with constrained optimization several additional conditions have to be satisfied.

Optimization approaches have been widely used in machine learning due to their attractive theoretical properties[16]. Since the mid-1990s, there has been extensive research on algorithms for SVMs, and a variety of techniques have been proposed.

The optimization techniques for SVM can be divided into three main groups:

- decomposition methods – the idea behind this method is to chunk the variables from the QP into subsets and then solve the QP on each of the subset.
- interior point methods – reformulates the problem with logarithmic barrier functions instead of inequalities
- gradient-based methods – use the properties of the gradient to find the location of optimal point

The following chapter gives overview of some of these techniques.

### 3.1 Sequential minimal optimization

Sequential minimal optimization (SMO) is an algorithm for solving SVM optimization problem analytically and uses Osuna's theorem[9] to ensure convergence. It was proposed by John C. Platt in 1998. SMO is one of the decomposition methods, that takes the smallest possible subset of two Lagrange multipliers and optimizes them analytically. Its runtime is linear in the number of training examples, in the worst case being  $\Omega(n^2d)$ , which is a big improvement over older methods that scale like  $n^3$ , but is obviously infeasible on large datasets.

Platt changes the definition of the hyperplane, denoting is as following:

$$u = w \cdot x - b \tag{3.1}$$

SMO algorithm solves the following quadratic programming problem:

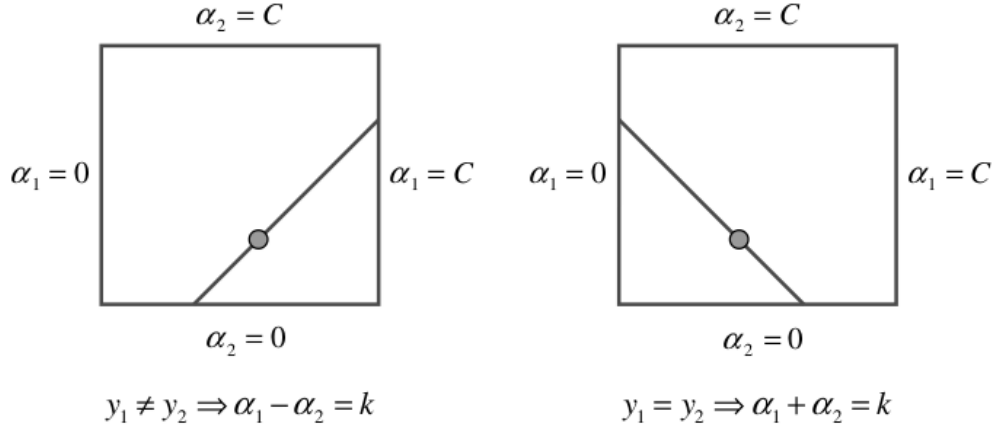


Figure 3.1: The two Lagrange multipliers must fulfill all of the constraints of the full problem. The inequality constraints cause the Lagrange multipliers to lie in the box. The linear equality constraint causes them to lie on a diagonal line[12].

$$\min_{\alpha} \Phi(\alpha) = \min_{\alpha} \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N y_i y_j K(x_i \cdot x_j) \alpha_i \alpha_j - \sum_{i=1}^N \alpha_i$$

subject to  $0 \leq \alpha_i \leq C$

$$\sum_{i=1}^N y_i \alpha_i = 0$$

To ensure that the kernel is actually a dot product in the feature space, the kernel function  $K$  must obey Mercer's conditions:

$$\int \int K(x, y) g(x) g(y) dx dy \geq 0 \quad (3.2)$$

At every step, SMO takes the smallest possible set of Lagrange multipliers (in standard case, two), finds an optimal value for them and updates SVM to reflect this optimization. The numerical QP optimization is avoided since optimization of multipliers is done analytically. Additional advantage of SMO lies in a little resource usage, since no matrix storage is required[12].

In order to optimize two Lagrange multipliers, SMO computes the constraints on chosen multipliers and then solves the constrained minimum. Because only two multipliers are used, the constraints can be displayed in two dimensions 3.1.

The algorithm first computes the second Lagrange multiplier  $\alpha_2$  and finds the ends of the corresponding diagonal segment. If the classes  $y_1$  and  $y_2$  are not equal, then the following bounds apply to  $\alpha_2$ :

$$L = \max(0, \alpha_2 - \alpha_1)$$

$$H = \min(C, C + \alpha_2 - \alpha_1)$$

If the classes  $y_1$  and  $y_2$  are the same, the bounds are following:

$$L = \max(0, \alpha_2 + \alpha_1 - C)$$

$$H = \min(C, \alpha_2 + \alpha_1)$$

The second derivative along the diagonal line is:

$$\eta = K(x_1, x_1) + K(x_2, x_2) - 2K(x_1, x_2)$$

Due to limitation 3.2 derivative of the objective function will always be positive definite and  $\eta$  will always be positive, and minimum along the diagonal line can be computed:

$$\alpha_2^{new} = \alpha_2 + \frac{y_2(E_1 - E_2)}{\eta},$$

where  $E_i = u_i - y_i$  is the error on the  $i^{th}$  training entry.

At the next step, the constrained minimum is computed by clipping the constrained minimum to the ends of the diagonal segment:

$$\alpha_2^{clipped} = \begin{cases} H & \text{if } \alpha_2^{new} \geq H \\ \alpha_2^{new} & \text{if } L < \alpha_2^{new} < H \\ L & \text{if } \alpha_2^{new} \leq L \end{cases}$$

The value of the first Lagrange multiplier  $\alpha_1$  is computed from the obtained  $\alpha_2$ :

$$\alpha_1^{new} = \alpha_1 + y_1 y_2 (\alpha_2 - \alpha_2^{clipped})$$

To ensure that KKT conditions are fulfilled for both optimized multipliers, a threshold is recomputed at each step:

$$\begin{aligned} b_1 &= E_1 + y_1(\alpha_1^{new} - \alpha_1)K(x_1, x_1) + y_2(\alpha_2^{clipped} - \alpha_2)K(x_1, x_2) + b \\ b_2 &= E_2 + y_1(\alpha_1^{new} - \alpha_1)K(x_1, x_2) + y_2(\alpha_2^{clipped} - \alpha_2)K(x_2, x_2) + b \end{aligned}$$

SMO chooses the threshold to be halfway in between  $b_1$  and  $b_2$ .

In order to speed convergence, SMO uses heuristics to choose which two Lagrange multipliers should be optimized at the current iteration. There are two separate heuristics for each of the two Lagrange multipliers.

The first Lagrange multiplier is chosen by iterating over the entire training data to find the element that violates the KKT conditions. The second multiplier is chosen among the non-bound examples that also violate KKT conditions. The SMO algorithm terminates if the entire training set obeys the KKT conditions.

## 3.2 Interior point method

The early attempts to apply IPMs in the support vector machine training context were successful enough to generate further interest towards new developments. IPM is capable to reduce the cost of linear algebra operations due to the problem's special structure.

IPM solves the convex quadratic programming (QP) problem, which can be represented in the primal and dual forms in the following way:



$$\begin{aligned} & \text{Primal} \\ \min & c^T x + \frac{1}{2} x^T Q x \\ \text{subject to} & Ax = b \\ & x \geq 0 \end{aligned}$$

$$\begin{aligned} & \text{Dual} \\ \max & b^T y - \frac{1}{2} x^T Q x \\ \text{subject to} & A^T y + s - Qx = c \\ & s \geq 0 \end{aligned}$$

where  $A \in \mathbb{R}^{m \times n}$  has full row rank  $m \leq n$ ,  $Q \in \mathbb{R}^{n \times n}$  is a positive semidefinite matrix,  $x, s, c \in \mathbb{R}^n$  and  $y, b \in \mathbb{R}^m$ .

Using Lagrangian duality theory, the first-order optimality conditions can be written as:

$$\begin{aligned} Ax &= b \\ A^T y + s - Qx &= c \\ XSe &= 0 \\ (x, s) &\geq 0, \end{aligned}$$

where  $X$  and  $S$  are diagonal matrices in  $\mathbb{R}^{n \times n}$  with elements of vector  $x$  and  $s$  spread across the diagonal, respectively, and  $e \in \mathbb{R}^n$  is the vector of ones. The third equation,  $XSe = 0$ , is called the complementarity condition and is often a source of difficulty when solving optimization problems.

Interior-point methods replace  $XSe = 0$  with  $XSe = \mu$ , where the parameter  $\mu$  is driven to zero. This operation removes the need to partition inequality constraints into active and inactive: the algorithm gradually reduces  $\mu$ , and the partition of vectors  $x$  and  $s$  into zero and nonzero elements is gradually revealed as the algorithm progresses[16].

The best IPM algorithm known to date finds the  $\varepsilon$ -accurate solution of an LP or convex QP problem in  $O(\sqrt{n} \log(\frac{1}{\varepsilon}))$  iterations [13]. However, one iteration of an IPM may be costly. IPM involves the complete matrix to compute the Newton direction based on first-order optimality conditions, and this operation may be expensive due to nontrivial sparsity patterns in the matrix.

The derivation of an interior-point method for optimization relies on three basic ideas:

1. Inequality constraints are replaced by logarithmic barrier functions
2. Duality theory is applied to barrier subproblems to derive the first-order optimality conditions which take the form of a system of nonlinear equations
3. The system of nonlinear equations is solved by Newton's method

Implementation of IPMs deals with reducing the barrier term from a large initial value to small values needed to weaken the barrier and to allow the algorithm to approach an optimal solution[16]. In the linear programming case, the optimal solution lies on the boundary of the feasible region and many components of vector  $x$  are zero (3.2).

Interior-point methods have proved effective on convex quadratic programs. However, the density and the size of the kernel matrix make it difficult to achieve efficiency. To get around this difficulty a method to replace the Hessian with a low-rank approximation (of the form  $VV^T$ , where  $V \in \mathbb{R}^{m \times r}$  for  $r \ll m$ ) is proposed. This approach works well on problems of moderate scale, but may be too expensive for larger problems[16].

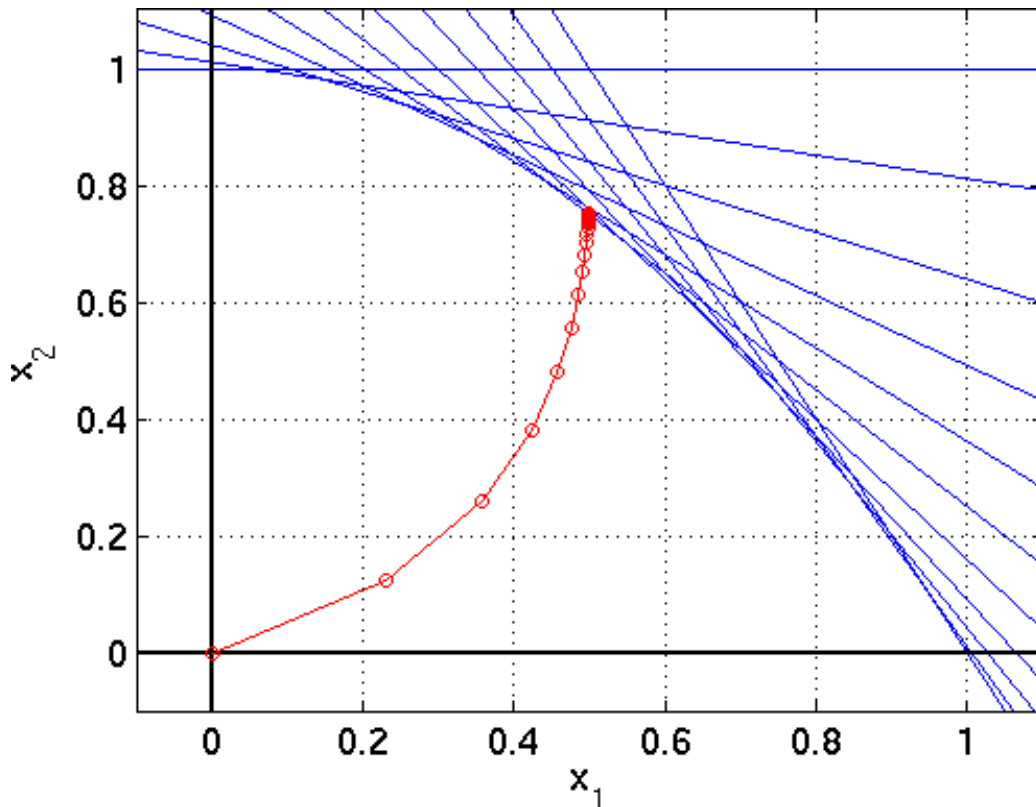


Figure 3.2: Trajectory of optimality conditions as  $\mu$  ranges from infinity down to zero

### 3.3 Gradient methods

Gradient methods are based on gradient information. They can be grouped into two classes, first-order and second-order methods. First-order methods are based on the linear approximation of the Taylor series, and entail the gradient  $g$ . Second-order methods, or Newton methods, are based on the quadratic approximation of the Taylor series. They entail the gradient  $g$  as well as the Hessian  $H$ . The drawback of a second-order method is that the Hessian for a training set with  $n$  features is a  $n \times n$  matrix. When  $n$  is large, computing or storing this matrix can be impossible.

One of the first-order methods is a gradient descent, also known as steepest descent method (algorithm 3.1). This method uses the fact that the gradient  $\nabla f$  of a function points in the direction of greatest increase, meaning that  $-\nabla f$  points in the direction

---

**Algorithm 3.1** Gradient descent

---

1. Input  $x_o$  and initialize the tolerance  $\varepsilon$ . Set  $k = 0$
  2. Calculate gradient  $g_k$  and set  $d_k = -g_k$
  3. Using line search, find  $\alpha_k$ , the value of  $\alpha$  that minimizes  $f(x_k + \alpha d_k)$
  4. Set  $x_{k+1} = x_k + \alpha_k d_k$  and calculate  $f_{k+1} = f(x_{k+1})$
  5. If  $\|\alpha_k d_k\| < \varepsilon$ , then output  $x^* = x_{k+1}$  and  $f(x^*) = f_{k+1}$ , and stop. Otherwise, set  $k = k + 1$  and repeat from 2.
-

of greatest decrease.

In gradient descent, the gradient is computed using the entire training set. A simple alteration of this is to find the gradient with respect to a single randomly chosen example. This technique is called stochastic gradient descent (SGD). By using only a single example an approximation to the true gradient is obtained, therefore, there is no guarantee of movement in the direction of the greatest descent. Still, there are at least two important reasons why stochastic gradient descent is used for SVM training:

- it is significantly quicker than gradient descent when data set is large
- stochastic gradient descent minimizes the generalization error quicker than gradient descent

While gradient based methods are known to exhibit slow convergence rates, the computational demands imposed by large scale classification and regression problems of high dimension feature space, renewed the interest in gradient methods[16].

# Chapter 4

## Parallelization

One of SVM algorithm's disadvantages is the large memory requirement and computation time required to deal with large datasets. The reason is the core problem of an SVM - a quadratic programming problem (QP) that separates support vectors from the rest of the training data. General-purposed QP solvers tend to scale with the cube of the number of training vectors  $O(n^3)$ [10]. To speed up the process of training SVM, parallel methods have been proposed and have proved to be efficient.

### 4.1 Parallel SMO

Sequential minimal optimization algorithm has proved to be inefficient due to usage of a single threshold value. A modification of SMO was proposed introducing two threshold variables  $b_{low}$  and  $b_{up}$  that are used to check the solution for optimality[8]. To speed up optimality verification, indexes of Lagrange multipliers  $i \in 1...n$  are divided into four subsets based on the value of Lagrange multiplier and corresponding class label. At each step the worst pair of multipliers is chosen for optimization. These modified algorithms perform significantly faster than the original SMO[15].

It was noted that the most time consuming operation of SMO is the update of  $u_i$  array (see equation 3.1), that holds the output of SVM for the  $i^{th}$  training sample. To decrease the computation time, a parallel implementation of SMO was proposed[2] that would calculate  $u$  in parallel.

In the parallel implementation of SMO, the input data is divided into a number of subsets, based on the amount of nodes in use. Each node gets its own set of the Lagrange multipliers to optimize.

The program terminates, when duality gap gets close to zero. Duality gap is a variable, holding the difference between the primal and dual forms of the objective function. If it reduces to zero, the optimum is reached.

$$DualityGap = \sum_{i=0}^N \alpha_i y_i \xi_i + \sum_{i=0}^n \varepsilon_i, \text{ where}$$
$$\varepsilon_i = \begin{cases} C \cdot \max(0, b - \xi_i) & y_i = 1 \\ C \cdot \max(0, -b + \xi_i) & y_i = -1 \end{cases}$$

The global instance of the duality gap is introduced, shared by all nodes, and equal to the sum of the  $DualityGap$  of the all processors.

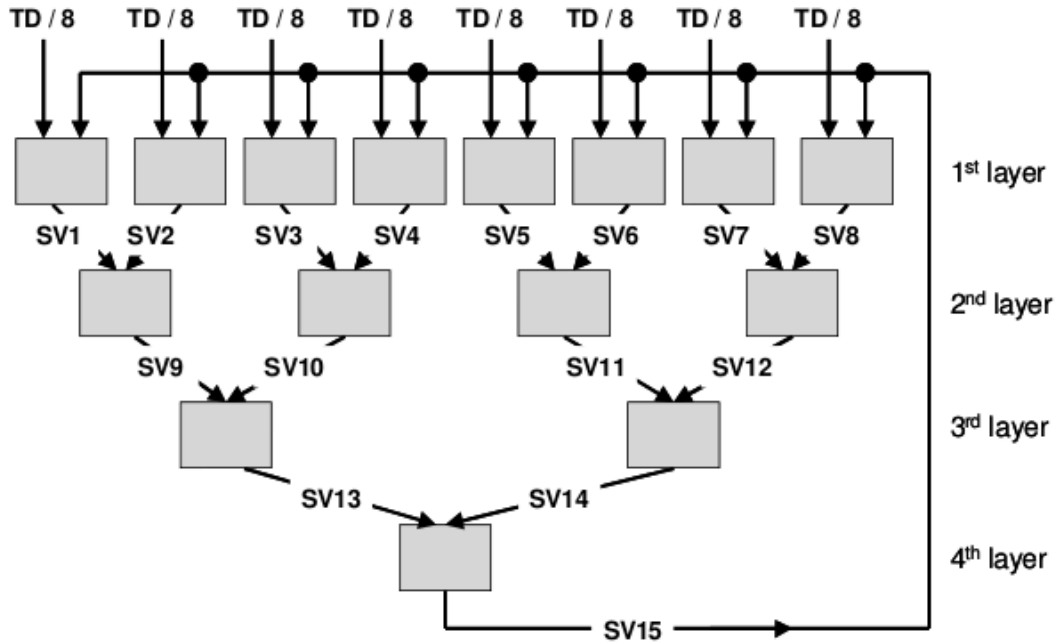


Figure 4.1: Schematic of a binary Cascade architecture. TD: Training data,  $SV_i$ : Support vectors produced by optimization i.[7]

## 4.2 Cascade SVM

Another approach to parallelization of SVM has been proposed by splitting the problem into smaller subsets and training a network to assign samples to different subsets.

It has been proved that eliminating non-support vectors early from the optimization can speed-up SVM efficiently[7]. A filtering process for the elimination can be done in parallel.

The problem is initialized with a number of independent, smaller optimizations. Then, the partial results are combined in a hierarchical fashion. In the architecture, shown on Figure 4.2, sets of support vectors from two SVMs are combined and the optimization process continues with search for the support vectors in each of the combined subsets. The process ends when only one set of the vectors is left. Often it is enough to pass the cascade only once to get satisfactory accuracy, but if the global optimum has to be reached, the result of the last layer is sent back to the first layer. Each of the SVMs in the first layer receives all the support vectors of the last layer as inputs and then tests if any of them have to be incorporated into the optimization. If this is not the case for all SVMs of the input layer, then the global optimum is reached, otherwise another pass through the network is made.

One of the main advantages of the Cascade architecture is that it requires far less memory than a single SVM, because the size of the kernel matrix scales with the square of the active set.

## 4.3 PSVM

PSVM is a parallel approximate implementation of SVM that aims to reduce both loading and computation time. Training set is loaded into several machines in a cyclic

fashion, and a parallel row-based Incomplete Cholesky Factorization (ICF) is then applied on the data. At the end of ICF, each machine stores only a part of factorized matrix. PSVM then performs parallel IPM to solve quadratic optimization problem.

PSVM devises parallel row-based ICF (PICF) at its initial step, which loads training instances onto parallel machines and performs factorization simultaneously on these machines. The size of kernel matrix is reduced through factorization, which helps to reduce used space to  $O(np/m)$ , where  $p/m$  is much smaller than  $n$ .

ICF can approximate  $Q \in \mathbb{R}^{n \times n}$  by smaller matrix  $H \in \mathbb{R}^{n \times p}$ ,  $p \ll n$ , i.e  $Q \approx HH^T$ . Row-based parallel ICF (PICF) works as follows. Let vector  $v$  be the diagonal of  $Q$  and suppose the pivots (the largest diagonal values) are  $\{i_1, \dots, i_k\}$ , the  $k^{th}$  iteration of ICF computes three equations:

$$H(i_k, k) = \sqrt{v(i_k)}$$

$$H(J_k, k) = \frac{Q(J_k, k) - \sum_{j=1}^{k-1} H(J_k, j)H(i_k, j)}{H(i_k, k)}$$

$$v(J_k) = v(J_k) - H(J_k, k)^2,$$

where  $J_k$  denotes the complement of  $\{i_1, \dots, i_k\}$ . The algorithm iterates until the approximation of  $Q$  by  $H_k H_k^T$  is satisfactory, or the predicted maximum of iterations (or, the desired rank of the ICF matrix)  $p$  is reached.

Row-based approach starts by initializing variables and loading training data to  $m$  machines in a cyclic way. In each iteration  $k$ , five tasks are performed:

1. A pivot, which is the largest value in the diagonal  $v$  of matrix  $Q$ , is found in parallel
2. Machines that hold the pivot are marked as master
3. On the master, PICF calculates  $H(i_j, k)$  according to  $H(i_k, k) = \sqrt{v(i_k)}$
4. The pivot instance  $x_{i_k}$  and the pivot row  $H(i_k, :)$  are broadcasted by the master node
5.  $H(J_k, k) = \frac{Q(J_k, k) - \sum_{j=1}^{k-1} H(J_k, j)H(i_k, j)}{H(i_k, k)}$  and  $v(J_k) = v(J_k) - H(J_k, k)^2$  are computed in parallel manner

At the end of the algorithm,  $H$  is distributed on  $m$  machines, and the system is ready for parallel IPM to be applied.

PICF has three advantages: parallel memory use, parallel computations and low communication overhead.[4]

Parallel IPM minimizes both storage and communication cost by distributing the data:

1. Distributed matrix data. At the end of PICF matrix  $H$  is divided between the nodes.
2. Distribute  $n \times 1$  vector data. All  $n \times 1$  vectors are distributed in a round-robin fashion on  $m$  machines. These vectors are  $\alpha, \lambda, \xi, z, \Delta z, \Delta \alpha, \Delta \xi, \Delta \lambda$ .

3. Replicated global scalar data. Every machine caches a copy of global data including  $v, t, n$  and  $\Delta v$ . Whenever scalar is changed, a broadcast is required to maintain global consistency.

When the IPM iteration stops, we have the value of  $\alpha$  and the classification function:

$$f(x) = \sum_{i=1}^N \alpha_i y_i k(s_i, x) + b$$

Here  $N$  is the number of support vectors and  $s_i$  are support vectors.

In order to complete classification function,  $b$  must be computed. An average value of  $b$  can be computed in parallel using mapReduce[6].

## 4.4 P-packSVM

P-packSVM is based on simple stochastic gradient descent (SGD) based algorithm that directly optimizes primal objective  $f(w) = \frac{\sigma}{2} \|w\|_2^2 + \frac{1}{m} \sum_{i=1}^m \max\{0.1 - y_i \langle w, \phi(x_i) \rangle\}$ . At each iteration, a single sample from the training set is picked at random to approximate  $l(w) = \frac{1}{m} \sum_{i=1}^m \max\{0.1 - y_i \langle w, \phi(x_i) \rangle\}$ , and then the gradient is calculated and the predictor  $w$  is updated accordingly. Parallelized is done with the help of a distributed hash table and a special packing strategy. SGD algorithms have huge communication cost, which is non-trivially reduced by packing strategy that also allows a sub-linear speed-up.

At each iteration  $t \in \{1, \dots, T\}$ , a random example  $(x_i(t), y_i(t)) \in \psi$  is picked and the empirical loss  $l(w) = \frac{1}{m} \sum_{i=1}^m \max\{0.1 - y_i \langle w, \phi(x_i) \rangle\}$  and the objective  $f(w) = \frac{\sigma}{2} \|w\|_2^2 + \frac{1}{m} \sum_{i=1}^m \max\{0.1 - y_i \langle w, \phi(x_i) \rangle\}$  are approximated in a following manner:

$$l(w) \approx l_t(w) := \max\{0.1 - y_{i(t)} \cdot \langle w, \phi(x_{i(t)}) \rangle\}$$

$$f(w) \approx f_t(w) := \frac{\sigma}{2} \|w\|_2^2 + l_t(w)$$

In iteration  $t$  the predictor is modified:

$$w \leftarrow w - \frac{1}{\sigma t} \nabla f_t(w)$$

The sub-gradient can be written down explicitly:

$$\nabla f_t = \begin{cases} \sigma w & y_{i(t)} \cdot \langle w, \phi(x_{i(t)}) \rangle \geq 1 \\ \sigma w - y_{i(t)} \phi(x_{i(t)}) & y_{i(t)} \cdot \langle w, \phi(x_{i(t)}) \rangle < 1 \end{cases}$$

At each update of  $w$ , a projection is applied to make  $w$  closer to the optimum:

$$w \leftarrow \min\left\{1, \frac{1/\sqrt{\sigma}}{\|w\|_2}\right\} w$$

There are two main characteristics that have to be considered when applying parallel paradigm:

- Merit. A single iteration can be parallelized. The calculation of  $\langle v, \phi(x) \rangle$  can be parallelized by storing of the entries  $(x_i, \beta_i)$  in  $H$  in the distributed mode.

- Defect. The mass communication will slow down the parallel program.

Taking these characteristics into consideration, a distributed hash table to develop merit is proposed, and a packaging strategy is used to overcome the defect.

### Distributed hash table

Entries in  $H$  are averagely divided to all the processors. Suppose the  $i^{th}$  processor saves a subset

$$H_i = \{(x_{i,j}, \beta_{i,j})\}_{j=1}^{|H_i|} \subset H \text{ to represent } v_i = \sum_j \beta_{i,j} \phi(x_{i,j})$$

The calculation of inner product  $\langle v, \phi(x) \rangle$  can be distributed to all the processors, by each calculation  $\langle v_i, \phi(x) \rangle = \sum_j \beta_{i,j} K(x_{i,j}, x)$  and sum-up via inter-processor communications.

All the processors check whether the given key  $x$  exists in the local hash table  $H_i$ . If any of the processors finds the key, it simply updates the value and informs other processors of the existence of the key.

### Packing strategy

Several iterations  $r \in \mathbb{N}$  are packed into a single one, and thus the number of communications is reduced by a factor of  $O(r)$ [20]. The total bits in communication will not be reduced.

Let  $w_t, x_t, y_t$  denote the predictor  $w$  and the random sample  $(x_t, y_t)$  in the  $t^{th}$  iteration.

Packing algorithm for  $r$  consecutive iterations  $t, \dots, t+r-1$  is summarized as follows:

1. Calculate  $y'_i = \langle w_t, \phi(x_t) \rangle$  for  $i = t \dots t + r - 1$
2. Calculate  $K(x_i, x_j)$  for  $t \leq i < j \leq t + r - 1$
3. Iterate  $i$  through  $t$  to  $t + r - 1$  and process the  $i^{th}$  iteration as before. Whenever iteration  $i$  is finished  $a_i, b_i$  can be calculated and  $y'_{i+1}, \dots, y'_{t+r-1}$  are updated offline (without communication):
4.  $y'_{i+j} \leftarrow \alpha_i y'_{i+j} + b_i K(x_{i+j}, x_i)$
5. The distributed hash table  $H$  is updated after all  $r$  iterations finish, by communicating to confirm the existing entries, and then add new entries to the least occupied processor.



# Chapter 5

## Performance tests

To make sure that parallelization does increase the performance speed, it is required to conduct some experiments on the data of different size and density. It must be noted, that performance is not the only parameter that should be taken into consideration - the accuracy of class prediction should not decrease. To test the algorithms, described above, we used several datasets[3] that vary by data size and the number of features of the input vectors.

### 5.1 Setup

For the experiments, we chose the following algorithms:

- LIBSVM
- PSVM
- SVM<sup>Light</sup>

The algorithms chosen use different type of solvers for the optimization problem, which makes it possible to compare the methods described in chapter 3. All algorithms were fed the same training data, characteristics of which can be observed in Table 5.1.

### 5.2 Results

The results obtained during the experiments, can be observed in tables 5.2 and 5.3. The dataset name is specified in the column, and the row denotes SVM implementation. Each cell contains training time in seconds.

As we can see from the table 5.2, LIBSVM runs even faster than PSVM on the data sets with a relatively small amount of features. PSVM, however, proves to be the

	a2a	a3a	a4a	a5a	a6a	a7a	gisette
Features	123	123	123	123	123	123	5000
Classes	2	2	2	2	2	2	2
Training size	2265	3185	4781	6414	11200	16100	6000
Testing size	30296	29376	27780	26147	21341	16461	1000

Table 5.1: Parameters of used datasets

	a2a	a3a	a4a	a5a	a6a	a7a	gisette
libSVM	0.283	0.422	1.287	1.987	6.4	13.071	279.406
SVMLight	0.530	0.972	2.367	4.267	13.645	28.714	408.214
PSVM nodes							
1	2.039	6.029	21.250	55.337	401.784	1924.519	105.108
2	1.205	3.583	12.361	31.548	499.043	823.182	64.907
4	1.125	3.557	12.145	29.676	234.812	499.208	63.774
8	0.823	1.8	7.863	17.296	131.847	429.786	49.002
16	0.906	1.699	4.792	11.729	83.428	282.933	30.782
32		2.518	4.503	10.142	65.650	200.362	24.298
64			4.802	10.543	50.296	159.619	20.617

Table 5.2: Training Performance SVM implementations on different datasets.

	a2a	a3a	a4a	a5a	a6a
libSVM	0.839748	0.838644	0.840857	0.842468	0.842463
SVMLight	0.760100	0.759400	0.789600	0.816500	0.829500
PSVM nodes					
1	0.841233	0.841231	0.841685	0.841014	0.843915
2	0.841101	0.841401	0.841541	0.841205	0.843915
4	0.841332	0.841061	0.841829	0.841014	0.843915
8	0.841134	0.841027	0.841937	0.841167	0.843587
16	0.8412	0.841095	0.841793	0.841282	0.843915
32		0.841027	0.841685	0.841014	0.843728
64			0.841865	0.84197	0.843494

Table 5.3: Prediction accuracy

most efficient when the input vector has a large number of features, since it stores the feature vectors in parallel. That can be easily explain by the nature of the QP problem solvers used in both implementations. LIBSVM uses SMO and does not store the kernel function values, so they have to be calculated on demand, while PSVM stores the kernel matrix in parallel, and kernel function for each point has to be calculated only once. As the number of features grows, the calculation of kernel function becomes more and more time and resource consuming.

The accuracy of the class prediction for all tested implementations does not vary significantly, and is not dependent on the size of the dataset. It can be easily explained by the fact that all the SVM solvers look for the global optimal point of the same objective function and the result should not depend on the way optimization problem is solved.

# Chapter 6

## Support Vector Clustering

Support vector clustering (SVC) is a non-parametric clustering algorithm based on the support vector approach. Support vector clustering algorithm data points are mapped from data space to a high dimensional feature space using a Gaussian kernel. The sphere is then mapped back to data space, where it forms a set of contours that enclose the data points and can be interpreted as cluster boundaries. Points enclosed by each separate contour belong to the same cluster.

SVC algorithm is known to have two main bottlenecks - expensive computation and poor labeling performance. To overcome these disadvantages, an improved version of algorithm was proposed. Parallel algorithms, used for training SVM to improve the performance of SVC, are applied to SVC for performance improvement.

### 6.1 Support Vector Clustering

Support vector clustering is a non-parametric clustering algorithm based on the support vector approach. The mathematical formulation of the SVC algorithm can be summarized as follows: assume a dataset containing  $N$  points  $\{x_1, x_2, \dots, x_N\}, x_i \in \mathbb{R}^d$ , where  $d$  is the dimension of the data space. A nonlinear mapping function  $\Psi$  is used to map the data set into a high-dimensional feature space such that the radius of the sphere,  $R$ , enclosing all the data points is as small as possible. Such an objective can be formulated by the following optimization problem:

$$\begin{aligned} \min R^2 + C \sum_j \xi_j \\ \text{subject to } \|\Psi(x_j) - a\|^2 \leq R^2 + \xi_j \quad \forall j, \end{aligned} \quad (6.1)$$

where  $\|\cdot\|$  is the Euclidean norm,  $a$  is the center of the sphere,  $\xi_j$  are slack variables that loosen the constraints to allow some data points to lie outside the sphere,  $C$  is a constant, and  $C \sum \xi_j$  is a penalty term. To solve the optimization problem in 6.1, it is convenient to introduce the Lagrangian function:

$$L(R, a, \xi_j, \alpha_j, \mu_j) = R^2 - \sum_j (R^2 + \xi_j - \|\Psi(x_j) - a\|^2) \alpha_j - \sum \xi_j \mu_j + C \sum \xi_j, \quad (6.2)$$

where  $\alpha_j \geq 0$  and  $\mu_j \geq 0$  are the Lagrange multipliers. With 6.2, we can derive the following conditions by the Lagrange theorem and the Karush-Kuhn-Tucker (KKT) complementarity[5]:

$$\xi_j \mu_j = 0, \quad (6.3)$$

$$(R^2 + \xi_j - \|\Psi(x_j) - a\|^2) \alpha_j = 0 \quad (6.4)$$

According to 6.3 and 6.4, we can classify each data point into

1. an internal point
2. an external point
3. a boundary point in the feature space

Point  $x_j$  is classified as an internal point if  $\alpha_j = 0$ . When  $0 < \alpha_j < C$ , the data point  $x_j$ , is denoted as a support vector. Support vectors lying on the surface of the feature-space sphere are called boundary points. These support vectors are used to describe the cluster contour in the input space. When  $\alpha_j = C$ , the data points located outside the feature space are defined as the external points or bounded support vectors.

Using the above conditions, 6.1 can be turned into the Wolfe dual optimization problem with only variables  $\alpha_j$ :

$$\begin{aligned} & \max \sum_j \Psi(x_j)^2 \alpha_j - \sum_{i,j} \alpha_i \alpha_j \Psi(x_i) \cdot \Psi(x_j) \\ & \text{subject to } 0 \leq \alpha_j \leq C \\ & \sum_j \alpha_j = 1 \quad \forall j, \end{aligned} \quad (6.5)$$

where the dot product of  $(\Psi(x_i) \cdot \Psi(x_j))$  represents the Mercer kernel  $K(x_i, x_j)$ . Gaussian functions are selected as kernels, i.e.,  $K(x_i, x_j) = \exp(-q\|x_i - x_j\|^2)$ . For any point  $x$  in the data space, the distance of its image in the feature space from the center of the sphere is described by

$$R^2(x) = \|\Psi(x) - a\|^2 = K(x, x) - 2 \sum_j \alpha_j K(x_j, x) + \sum_{i,j} \alpha_i \alpha_j K(x_i, x_j) \quad (6.6)$$

The radius  $R$  of the sphere can be obtained by

$$R = \{R(x_i) | x_i \text{ is a support vector}\}. \quad (6.7)$$

The average of the above set is used as the radius  $R$ . The support vectors, bounded support vectors, and the other points are located on the cluster boundaries, the outside of the boundaries, and the inside of the boundaries, respectively.

There are two important parameters in SVC algorithm:  $q$  and  $C$ . The value of  $q$  governs the number of clusters and the tightness of the cluster boundaries, while the value of  $C$  determines the existence of outliers during the clustering process.

The cluster description does not differentiate points that belong to different clusters. If there are two data points,  $x_i$  and  $x_j$ , that belong to the same cluster in the input space, one can check if the line segment between them always lies within the high dimensional sphere. Checking the line segment is implemented by sampling a number of points on the segment. Two data points,  $x_i$  and  $x_j$ , satisfying the above condition

are defined as the components of the same cluster. An adjacency matrix  $A$  is defined to identify the components of a cluster. The components of  $A$ ,  $a_{ij}$ , between pairs of points  $x_i$  and  $x_j$ , are defined as follows:

$$a_{ij} = \begin{cases} 1, & \text{if all } y \text{ on the line segment connecting } x_i \text{ and } x_j, R(y) \leq R \\ 0, & \text{otherwise} \end{cases} \quad (6.8)$$

The values of  $a_{ij}$  can be obtained by sampling a number of points from the line segment connecting  $x_i$  and  $x_j$ . In the matrix  $A$ , if  $a_{ij} = 1$  that means  $x_i$  and  $x_j$  belong to the same cluster; otherwise, they are in different clusters. A positive decision function guarantees that  $x_i$  and  $x_j$  are part of the same cluster. In case of the negative decision function, it is still possible that points belong to the same cluster, but are recognized as the points from different contours, which is likely to occur in the case of complex contours. In general, the cluster labeling step that checks the connectivity for each pair of samples is more time-consuming than the SVC training step. The time complexity of this procedure is  $O(lN^2)$ , where  $l$  is the number of samples on the line segment[19].

## 6.2 Improved support vector clustering (iSVC)

An improved SVC algorithm, iSVC, address two known bottlenecks of SVC (costly computation and labeling) simultaneously[11]. iSVC includes a reduction strategy that can help to develop clustering model on a qualified subset. Reduction strategy aims to increase efficiency. It is based on the Schrödinger equation and extracts a desired subset based on which the clustering model is formulated.

iSVC labels data according to the geometric properties of the feature space. Firstly it handles arbitrary-shaped clusters through its boundary-based clustering model. Secondly it deals with structured data by employing Kernel function.

### 6.2.1 Optimization piece of iSVC

In iSVC's optimization piece, reduction strategy is performed on the whole dataset, and then the modified objective is optimized on the subset.

Reduction strategy is based on the Schrödinger equation that describes the law of energy conservation of a particle, written as follows:

$$H\psi(x) \equiv \left(-\frac{\sigma^2}{2}\nabla^2 + P(x)\right)\psi(x) = e\psi(x),$$

where  $e$  is the energy,  $P(x)$  the Schrödinger potential,  $r$  the Laplacian, and  $s$  the variance parameter.  $c(x)$  expresses the state of a quantum system, so  $c(x)$  can be explained as the wave function of particle. When applied in machine learning,  $c(x)$  can be considered a data probability distribution function, and its maxima is associated with cluster centers[11]. For the given  $\psi(x)$ ,  $P(x)$  is solved as follows:

$$P(x) = e + \frac{\sigma^2}{2\psi(x)}\nabla^2\psi(x)$$

From geometry meaning, minima of  $P(x)$  tells cluster centers, so  $P(x)$ 's maximum indicate the boundary information of clusters.

iSVC develops clustering model from a subset. Points located around cluster contours should be included in the subset. The subset should cover all clusters. Qualified subset is found by employing the Schrödinger equation to explore data position information.

$P(x)$  values reveal data location: points with top  $P(x)$  values tend to be around cluster boundaries, while points with small  $P(x)$  values are usually located in cluster central zones. The reduction strategy has the following steps:

1. Sort  $\{P(x_i)\}$  values in the descending order:  $\{P_{(i)}\}$ , with  $P_{(i)} \geq P_{(i+1)}$ , where  $P_{(i)} = P(x_i), i = 1, \dots, N$
2. Specify the interval length  $G$  of  $\{P_{(i)}\}$  list to separate the list into  $L$  intervals  $L = N/G$ :

$$\{P_{(1)} \dots P_{(G)}\}, \{P_{(G+1)} \dots P_{(2G)}\}, \dots, \{P_{((L-1)G)} \dots P_{(LG)}\}$$

1. In each interval, some data are sampled randomly at a certain ratio. For  $J^{th}$  interval,  $\{P_{((J-1)G)} \dots P_{(JG)}\}$  its sampling ratio is as follows:

$$\eta_J = \max\left\{\frac{1}{J}, \frac{1}{G}\right\}$$

$G$  balances the clustering quality and the cost. The higher the  $G$ , the bigger the subset size.

The reduction strategy reduces the optimization from the whole set to the subset.

## 6.2.2 The labeling piece of iSVC

iSVC introduces the new labeling approach, whose idea is to cluster support vectors first, then construct a classifier based on labeled support vectors. Finally, other data is labeled using the classifier.

1. Create affinity matrix  $H$  with respect to support vectors according to Gaussian Kernel:  $H_{ij} = k(v_i, v_j)$  with  $v_i$  and  $v_j$  being support vectors.
2. Normalize  $H$  into  $H'$ :  $H' = \Lambda^{-1/2} H \Lambda^{-1/2}$ , where  $\Lambda = \text{diag}(\sum_j H_{ij})$
3. Do eigenvalue decomposition on  $H'$ , and take top  $g$  eigenvectors as columns to form matrix  $H''$ .
4. Perform K-means on rows of  $H''$ ; the cluster number is initialized as  $g$ .  $g$  is specified by the number of eigenvalues that are larger than 1.
5. Label  $v_i$  as the  $i^{th}$  row's cluster membership.
6. Label other data in terms of its nearest SV's label.

---

**Algorithm 6.1** Parallel SVC pseudocode

---

```
p := number of processors
subProblems := divideIntoSubproblems(trainingSet, p)
while(not optimumIsReached()){
    subProblems[i].eliminateNonSV()
    merge(subProblems[i], subProblems[i+1])
}
R := calculateRadius()

each(subProblems){
    calculateAdjacencyMatrix()
}
```

---

### 6.3 Parallel SVC

The experiments conducted on parallel implementations of SVM showed that parallelization can efficiently increase the performance of the algorithm without losing the accuracy of class prediction. It was proposed that it is possible to apply the parallelization techniques to SVC algorithm and a parallel SVC was proposed (Algorithm 6.1).

First of all, we are seeking to reduce the size of the original training data. Since only support vectors are required to calculate the radius of the enclosing sphere, it was decided to apply the filtering technique used in CascadeSVM, which would eliminate non-support vectors in parallel.

Calculation of adjacency matrix, which is the most time-consuming part of SVC algorithm, can also be done in parallel. Input vectors are divided into subsets and then are evenly distributed among the nodes. The accuracy of cluster prediction does not change and remains the same as the one in the non-parallel implementation, since calculation of the adjacency matrix in parallel does not change its contents.

# Chapter 7

## Summary

Support vector machine is a powerful machine learning technique used for binary classification of data. The algorithm of SVM separates objects of one class from another by solving the quadratic programming problem. For that reason, SVM's training takes a lot of computation time and consumes a large amount of memory.

To speed up the SVM algorithm, several parallel implementations were proposed, using different optimization techniques and approaches to parallelization. We looked at some parallel algorithms for SVM, such as PSVM, pPackSVM and CascadeSVM. Techniques for distributed computing proposed in these algorithms can be summarized as follows:

- Distributed storage of data. Kernel matrix and training data are divided into subsets and each subset is stored on the separate machine.
- Sub-problems are solved in parallel. QP problem is solved for each of the training data subset in the separate node.
- Training data is reduced by parallel preprocessing. Training data is filtered and non-support vectors are eliminated.
- Reduced number of communications between nodes. Each node is sending results of several iterations at once, which reduces the time required for network communication.

Experimental results obtained has shown, that parallelization of SVM can considerably decrease the computation time and the amount of memory used by each machine. The prediction accuracy of the parallel algorithms is as high as the accuracy of the iterative implementations.

The given thesis also provided a description of SVC, a clustering algorithm based on SVM, and proposed several ways to increase its performance and calculation speed of the adjacency matrix. We proposed a parallel algorithm for SV that significantly reduces the computation time, while the assignation of points into the clusters remains the same.

The parallel approach to solving the optimization problem and assigning the data points to clusters reduces the computation speed and makes the SVC algorithm applicable for large datasets. In the future, a parallel SVC might be applied to real life problems and might prove to be both efficient and accurate clustering algorithm, which will increase the popularity of SVC in the scientific community.



# Resüme

## Vektormasinate paralleelseerimine

Magistritöö

Olga Agen

Tugivektormasin (Support Vector Machine) on masinõppe meetod, mida kasutakse andmete klassifitseerimiseks. Binaarse klassifikatsiooni probleem seisneb sellise funktsiooni või mudel leidmisel, mis oskaks ennustada, mis klassi etteantud punkt  $x_i$  kuulub. Mudeli treenimiseks kasutatakse treeningandmeid.

Treeningandmed on esitatud hulgast  $\{(x_i, y_i) | x_i \in X, y_i \in \{1, -1\}, i = 1, \dots, n\}$ , kus  $X$  on punktide hulk ning  $y_i$  on klass, millesse antud punkt  $x_i$  kuulub.

Sisendpunktid  $x_i$  tavaliselt teisendatakse omaduste ruumi  $H$  kasutades tuuma funktsiooni  $\varphi : X \rightarrow H$ , ning mudel õpitakse teisendatud andmete peal. Õppimisprotsessis leitakse optimaalset hüpertasandit, mis eraldab erinevasse klassidesse kuuluvaid punkte. Leitud hüpertasand on optimaalne siis, kui mõlema klassi punktide kaugus tasandist on maksimaalne. Kauguse maksimiseerimist on võimalik väljendada järgmise optimeerimisprobleemi kaudu:

$$\min_{w,b} \frac{1}{2} \|w\|^2 \text{ tingimusel, et } y_i(w \cdot x_i - b) \geq 1, \forall i$$

Optimeerimisprobleemi lahendamiseks on mitu algoritmi. Meie vaatame nendest ainult mõnda, seal hulgas:

- Järjestikune minimaalne optimeerimine (Sequential Minimal Optimization)
- Sisepunkti meetod (Interior point method)

Tugivektormasinal põhineb klasterdamisalgoritm, mis otsib omaduste ruumis minimaalse raadiusega sfääri, mis ümbritsed teisendatud sisendpunkte. Seda sfääri kirjeldab järgmine võrrand:

$$\|\varphi(x_i) - a\|^2 \leq R^2 \quad \forall j,$$

kus  $a$  on sfääri keskpunkt.

Selleks, et jaotada punkte erinevate klasterite vahel, kasutatakse punktide vahelist kaugust  $d(x)$ . Punktid kuuluvad samasse klassi kui nende vaheline lõik on täielikult sfääri sees, ehk iga lõigu punkti  $y$  puhul kehtib  $d(y) > R$ , kus  $R$  on sfääri raadius.

Oma töös võrdlesime iteratiivsed ja paralleelseid tugivektormasina algoritmide implementatsioone. Uurimise käigus avastasime et paralleelsed algoritmid, nagu oligi oodatud, töötavad palju kiiremini kui iteratiivsed, seejuures valesti klassifitseeritud punktide arv ei suurene.

Lisaks implementeersime klasterdamisalgoritmi kasutades paralleelseerimise viise, mida kasutatakse klassifitseerimisprobleemi lahendamiseks. Paralleelne imelementat-

sioon näitas, et klasterdamisalgoritmi jaoks on võimalik kasutada samu paralleliseerimismeetodeid, mida on kasutatud vektormasinate puhul.

# Bibliography

- [1] Asa Ben-Hur, David Horn, Hava T. Siegelmann, and Vladimir Vapnik. Support vector clustering. *JOURNAL OF MACHINE LEARNING RESEARCH*, 2:125–137, 2001.
- [2] L. J. Cao, S. S. Keerthi, Chong-Jin J. Ong, J. Q. Zhang, Uvaraj Periyathamby, Xiu Ju J. Fu, and H. P. Lee. Parallel sequential minimal optimization for the training of support vector machines. *IEEE transactions on neural networks / a publication of the IEEE Neural Networks Council*, 17(4):1039–1049, July 2006.
- [3] Chih-Chung Chang and Chih-Jen Lin. Libsvm: A library for support vector machines. *ACM Trans. Intell. Syst. Technol.*, 2(3):27:1–27:27, May 2011.
- [4] Edward Y. Chang, Kaihua Zhu, Hao Wang, Hongjie Bai, Jian Li, Zhihuan Qiu, and Hang Cui. Psvm: Parallelizing support vector machines on distributed computers.
- [5] Corinna Cortes and Vladimir Vapnik. Support-vector networks. In *Machine Learning*, pages 273–297, 1995.
- [6] Jeffrey Dean and Sanjay Ghemawat. Mapreduce: simplified data processing on large clusters. *Commun. ACM*, 51(1):107–113, January 2008.
- [7] Hans Peter Graf, Eric Cosatto, Leon Bottou, Igor Durdanovic, and Vladimir Vapnik. Parallel support vector machines: The cascade svm. In *In Advances in Neural Information Processing Systems*, pages 521–528. MIT Press, 2005.
- [8] S. S. Keerthi, S. K. Shevade, C. Bhattacharyya, and K. R. K. Murthy. Improvements to platt’s smo algorithm for svm classifier design. *Neural Comput.*, 13(3):637–649, March 2001.
- [9] Edgar Osuna, Robert Freund, and Federico Girosi. An improved training algorithm for support vector machines. pages 276–285. IEEE, 1997.
- [10] Jian pei Zhang, Zhong-Wei Li, and Jing Yang. A parallel svm training algorithm on large-scale classification problems. In *Machine Learning and Cybernetics, 2005. Proceedings of 2005 International Conference on*, volume 3, pages 1637–1641 Vol. 3, 2005.
- [11] Ling Ping, Zhou Chun-Guang, and Zhou Xu. Improved support vector clustering. *Eng. Appl. Artif. Intell.*, 23(4):552–559, June 2010.
- [12] John C. Platt. Advances in kernel methods. chapter Fast training of support vector machines using sequential minimal optimization, pages 185–208. MIT Press, Cambridge, MA, USA, 1999.

- [13] James Renegar. A polynomial-time algorithm, based on newton’s method, for linear programming. *Mathematical Programming*, 40(1-3):59–93, 1988.
- [14] Raul Rojas. *Neural Networks - A Systematic Introduction*. Springer-Verlag, Berlin, 1996.
- [15] S. K. Shevade, S. S. Keerthi, C. Bhattacharyya, K. R. K. Murthy, and In Smola. Improvements to the smo algorithm for svm regression. *IEEE Trans. Neural Netw*, pages 1188–1193, 2000.
- [16] Sebastian Nowozin Suvrit Sra and Stephen J. Wright. *Optimization for Machine Learning*. The MIT Press, 2012.
- [17] V. N. Vapnik and A. Ya. Chervonenkis. *Theory of Pattern Recognition [in Russian]*. Nauka, USSR, 1974.
- [18] Vladimir Vapnik. *Estimation of Dependences Based on Empirical Data: Springer Series in Statistics (Springer Series in Statistics)*. Springer-Verlag New York, Inc., Secaucus, NJ, USA, 1982.
- [19] Jeen-Shing Wang and Jen-Chieh Chiang. An efficient data preprocessing procedure for support vector clustering. *j-jucs*, 15(4):705–721, feb 2009.
- [20] Zeyuan A. Zhu, Weizhu Chen, Gang Wang, Chenguang Zhu, and Zheng Chen. P-packSVM: Parallel primal gradient descent kernel SVM. In *ICDM*, 2009.

# License

## **Non-exclusive licence to reproduce thesis and make thesis public**

I, Olga Agen (14.09.1989),

1. herewith grant the University of Tartu a free permit (non-exclusive licence) to:
  - (a) reproduce, for the purpose of preservation and making available to the public, including for addition to the DSpace digital archives until expiry of the term of validity of the copyright, and
  - (b) make available to the public via the web environment of the University of Tartu, including via the DSpace digital archives until expiry of the term of validity of the copyright,

“Parallelization of Support Vector Machines” supervised by Oleg Batrashev and Artjom Lind,

2. I am aware of the fact that the author retains these rights.
3. I certify that granting the non-exclusive licence does not infringe the intellectual property rights or rights arising from the Personal Data Protection Act.

Tartu, 20.05.2013