Scaling up Machine Learning techniques via parallelization for large data

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Abstract

Support Vector Regression suffers from known scalability issues with respect to both memory usage as well as computational time, which makes it unusable with larger datasets. To alleviate these bottlenecks, Parallel Support Vector Regression (PSVR) has been proposed and implemented, which utilizes multi-core processors and computing clusters to distributedly compute the regression model as well as use matrix factorization techniques to reduce the overall computation required to be performed. If the number of training instances is n, the rank of the factorized matrix is p and the number of available machines is m, PSVR successfully reduces the memory requirement from $O(n^2)$ to $O(np/m)$ where $p << n$; and the computational complexity from $O(n^3)$ to $O(np^2/m)$. Experiments performed examine the effectiveness of PSVR from both an accuracy and scalability standpoint. The implementation of PSVR is available at:

`https://github.com/akshayv/psvr`

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Contents

1 Introduction

This research project focuses on developing a parallel implementation of the Support Vector Regression(SVR) algorithm which allows usage of SVR for analysis of large datasets by exploiting multi-core processors and computing clusters.

1.1 Motivation

Regression analysis is a Machine Learning task which aims to establish relationships among variables, and has several applications including prediction and forecasting of variables. With the increasing ease of data collection over the recent years, the dependence on regression analysis to model this data has risen as well. One instance of a learning model which can be effectively used for regression analysis is Support Vector Regression.

Support Vector Regression (SVR), a variation of Support Vector Machines, is a supervised learning algorithm which produces a regression model using a relevant subset of the training data. Although several different approaches exist for regression analysis, SVR boasts many advantages over the conventional regression methods, which make it suitable for several regression applications. These advantages include:

- **Mapping data to higher dimensional spaces.** For a regression technique to be effective, it must be robust in being able to determine non-linear regression models from the input data. SVR achieves this but utilizing the Kernel Trick, which efficiently maps data instances to higher dimensional spaces without explicitly mapping each of the data instances. The Kernel function operates on the inner product of two data instances to map them to a suitable higher dimension space, wherein the regression model is determined.

- **Allowance for maximum deviation.** The commonly used SVR variation, $\epsilon-$SVR utilizes a $\epsilon-$ insensitive loss function to determine a regression model where each data instance has at most ϵ deviation from the predicted value. This loss function allows

SVR to modify the regression model depending on the requirements, for example if you are performing a currency exchange and do not want a deviation greater than ϵ.

- **Robust Regression Model.** Soft-Margin SVR, similar to Soft-Margin SVM, has an allowance for corrupt data instances. This is important for real data since incorrect data instances may be present due to a variety of factors. The hyper parameter C eliminates usage of most incorrect data instances and ensures a robust regression model, thereby avoiding overfitting.

- **Complexity Independent of Input Attributes size.** The complexity of the SVR with regard to both computational cost and memory are negligibly affected by the number of attributes for each data instance, meaning that several supporting attributes can be added to the training instances with negligible difference to the cost.

With increase in data availability and ease of data collection, the number of data instances available for every real-world situation such as Stock Market data, Traffic Speed data, and Electricity Load data have increased significantly, requiring the algorithms used for regression analysis to scale with larger datasets.

Ideally, SVR would scale comfortably with the increase in data instances to produces a regression model, but this is not the case. SVR suffers from some well documented limitations concerning usage with large datasets, including:

- **Large initial memory requirement.** As detailed in section 2.1, one of the initial steps in using the SVR algorithm is to build a matrix $K(x_i, x_j)$, known as the Kernel Matrix, which is the inner product of every data instance with every other data instance, the entirety of which is required to be built as an initial step of the training. The memory requirement to build and maintain this matrix is $O(n^2)$, it is quadratic in the number of training instances. As the number of training instances increases, not only does the computational cost to build this matrix increase, it becomes increasingly difficult to maintain this entire matrix in memory without running out of hardware

resources.

- **Large computational cost.** In all Quadratic Programming solvers of the SVR convex optimization problem, an inverse of the Kernel Matrix is required to be performed at several separate instances, the computational cost of which is $O(n^3)$, cubic in the number of training instances. Again, as the number of training instances increases, the computational cost of performing this inverse increases significantly creating a bottleneck in the SVR process, thereby making it unusable with large datasets.

These limitations make it increasingly impossible to use the standard SVR algorithm for use with larger datasets; The larger datasets correspond to real-world requirements and situations and an algorithm which is unable to cater to these requirements would be highly ineffective.

1.2 Objective

In this report a parallel SVR algorithm (PSVR) is proposed which utilizes computing clusters to allow SVR to effectively scale with larger datasets. Specifically, the following questions will be addressed:

How can we ensure that the initial memory requirements of of $O(n^2)$ for SVR are satisfied for increasingly large datasets in a scalable manner?

How can we manage the computational cost of $O(n^3)$ for the SVR training process for increasingly large datasets in a scalable manner?

To improve scalability of the SVR algorithm with respect to both memory requirement and computational time, a Parallel Support Vector Regression(PSVR) algorithm has been proposed which uses a low-rank matrix approximation of the Kernel Matrix while simultaneously distributing the computational load amongst parallel machines to achieve improved scalability by decreasing the time complexity from $O(n^3)$ to $O(np^2/m)$ and decreasing the

memory requirement from $O(n^2)$ to $O(np/m)$ where n is the number of training examples, p is the rank of the reduced matrix after approximation and m is the number of processing cores available.

The successful implementation of the PSVR algorithm would mean:

- **Highly efficient SVR algorithm** Subject to the availability of a computing cluster, PSVR would be able substantially increase the efficiency of the SVR training procss by utilizing a low-rank matrix approximation and parallel computing.
- **Usability with large datasets** By utilizing more machines in parallel the bottlenecks of SVR can be alleviated and this would mean that even for larger datasets, which correspond to real-word scenarios, PSVR can be utilized increasing the number of machines used.
- **Real Time Predictions using distributed model** A by-product of the data distribution across machines is that the support vectors for each subset only reside on that corresponding machine. This would mean that predictions for a data instance can be done distributedly to potentially achieve real time predictions.

Formulation and successful implementation of this algorithm would mean that the bottlenecks of SVR would be effectively alleviated and speedup would be achieved by increasing hardware usage.

1.3 Contributions

The specific contributions of this project are:

- A comprehensive Literature Review of existing SVR implementations which leverage on parallel machines is presented and the differences in the approaches are analysed (Section 2.3).

- A novel Parallel SVR formulation is proposed, which leverages on the availability of multiple processing cores and matrix approximation[1]to effectively scale with increasingly large data. The computational time and space complexity of the PSVR formulation (Section 3) is simultaneously determined .

- This PSVR formulation is implemented using the Message Parsing Interface (MPI) and its functioning and correctness is verified on a computing cluster.

- The predictive performance of PSVR is verified to be approximately equivalent to existing state-of-the-art SVR implementation (Section 4.1).

- The scalability and computational time of PSVR is verified to significantly outperform the state-of-the-art SVR implementation (Section 4.2).

[1]The rank of the approximated matrix is controlled by a parameter and the value of this parameter can varied to achieve the required trade off between accuracy and scalability.

2 Literature Review

The literature review section of this report consists of two subsections, one corresponding to the established background for SVR and the other corresponding to related works in improving the efficiency of SVR.

2.1 Background

In this section, the details of Support Vector Regression will briefly be explained. For a more detailed explanation, the reader can refer to Elements of Statistical Learning[1] and A Tutorial on Support Vector Regression[2].

Given training data: $\{(x_1, y_1) \ldots (x_l, y_l)\} \subset \chi \times R$, where χ denotes the space of input patterns, in ϵ-SVR our goal is to estimate a function $f(x)$ that has at most ϵ deviation from each of the targets y_i obtained from the training instances while at the same time is as flat as possible. The required function is described as:

$$f(x) = \langle w, x \rangle + b \; with \; w \; \epsilon \; \chi, \; b \; \epsilon \; R$$

where $\langle \; . \; , \; . \; \rangle$ denotes the dot product in χ. The flatness of this function can be ensure by minimizing $||w||^2$ leading to the convex minimization:

$$minimize \quad \frac{1}{2}||w||^2$$

$$\begin{aligned} subject \; to \; y_i - \langle w, x_i \rangle - b \; &\leq \; \epsilon \\ \langle w, x_i \rangle + b \; - y_i &\leq \; \epsilon \end{aligned}$$

where each of the above two inequality constraints correspond to the case where the corresponding data instance lie above and below the hyperplane described by the target function.

As with (soft-margin) SVMs, SVR has an allowance for some degree of error in the training instances, to deal with "corrupt" instances which otherwise lead to an infeasible formulation as per the above constraints. This allowance is represented by the variables ζ, ζ^* which correspond to slack variables for data instances above and below the regression hyperplane respectively.

In order to minimize both the flatness of the hyperplane as well as the error margin for the model, the formulation can be modified to:

$$\begin{aligned} \textit{minimize} \quad & \frac{1}{2}||w||^2 + C\sum_{i=1}^{l}(\zeta_i + \zeta_i^*) \\ \textit{subject to } y_i - \langle w, x_i\rangle - b \ &\leq \ \epsilon + \zeta_i \\ \langle w, x_i\rangle + b \ - y_i &\leq \ \epsilon + \zeta_i^* \\ \zeta_i, \zeta_i^* &\geq 0 \end{aligned}$$

where the parameter $C > 0$ determines the trade-off between flatness of f and the extent upto which deviations from $f(x)$ greater than ϵ are tolerated.

The above convex optimization can be solved more easily in its dual form, so the method of Lagrangian multipliers is employed to convert the optimization problem to its dual form:

$$\begin{aligned} L \ := \ \frac{1}{2}||w||^2 + C\sum_{i=1}^{l}(\zeta_i + \zeta_i^*) - \sum_{i=1}^{l}(\eta_i\zeta_i + \eta_i^*\zeta_i^*) \\ - \sum_{i=1}^{l}\alpha_i(\epsilon + \zeta_i - y_i + \langle w, x_i\rangle + b) \\ - \sum_{i=1}^{l}\alpha_i^*(\epsilon + \zeta_i^* + y_i - \langle w, x_i\rangle - b) \end{aligned}$$

Here $\eta_i, \eta_i^*, \alpha_i, \alpha_i^*$ are Lagrange multipliers and satisfy the constraints

$$\eta_i^{(*)}, \alpha_i^{(*)} \geq 0$$

After some tedious partial differentials and substitutions, we arrive at the dual optimization problem:

$$max\ \frac{-1}{2}\sum_{i,j=0}^{n}(\alpha_i-\alpha_i^*)(\alpha_j-\alpha_j^*)K(x_i,x_j)-\epsilon\sum_{i=0}^{n}(\alpha_i+\alpha_i^*)+\sum_{i=0}^{n}y_i(\alpha_i-\alpha_i^*)$$

$$Subject\ to:\sum_{i=0}^{n}(\alpha_i-\alpha_i^*)=0,\ 0\leq\alpha,\alpha^*\leq C$$

and

$$w=\sum_{i=1}^{l}(\alpha_i-\alpha_i^*)x_i, which\ implies \tag{1}$$

$$f(x)=\sum_{i=1}^{l}(\alpha_i-\alpha_i^*)\langle x_i,x\rangle+b \tag{2}$$

Similar to SVMs, after optimization, only a subset of the $(\alpha_i-\alpha_i^*)$ values are non-zero and these constitute the Support Vectors for the Regression model. The parameter b in the regression model can be computed as a by-product of the convex optimization process as described later.

The $K(x_i,x_j)$ component of the above formulation is an inner product matrix between each of the training instances in the datasets[2]. Similar to SVMs the Kernel Trick can be used during the construction of the above matrix to map the training instances in the matrix to a higher dimensional space if required. This component of the formulation will further be represented as Q in the rest of the report.

2.2 Related Work

Support Vector Machines, proposed by Vapnik et al. in 1963 is a Supervised Machine Learning algorithm used for classification by constructing a hyperplane to achieve maximum

[2]The construction and maintenance of this matrix in memory is one of the key bottlenecks of the SVR process since the size of the matrix is quadratic in the number of training instances.

separation from the training instances. The regression version of SVM, SVR, was proposed by Smola et al. in 1996 and utilized a different loss function from the traditional SVM while retaining several of the useful properties of SVMs.

Currently, two variations of SVR exist, ϵ-SVR, ν-SVR (Schölkopf et al.), both of which require solving the same convex optimization problem. Since its inception, the SVR algorithm has remained fairly standard with several works exploring the validity and usefulness of SVR through experiments.

With the increase in data availability over the recent years, the idea of scaling up traditionally unscalable and computationally expensive machine learning techniques has received considerable amount of interest.

These attempts at optimization or scaling the algorithms can be classified into two categories:

(a) **Distributing the computational load across machines**

Several groups have concentrated on different approaches to scaling machine learning algorithms by using distributed computing techniques as using MapReduce frameworks, offloading the computation to high performance GPUs or FGPA boards, exploring a P2P architecture relying on TCP and exploiting multicore processors using Multi Threading and/or Message Parsing Interface (MPI)(Bekkerman et al.).

Under the sub category of using MPI, there have been works to parallelize other algorithms similar to PSVR: Parallel Gaussian Process Regression(Chen et al.) utilizes computing clusters to achieve scalable performance for Gaussian Process Regression. Similarly, Parallel Support Vector Machines(PSVM) (Chang et al.) utilizes parallel computing to ensure scalability in the process of Support Vector Machines for classification. Specific to SVR, three techniques that utilize computing clusters have been

analyzed in Section 2.3.

(b) **Optimizing the underlying algorithm using heuristic methods.**
Various attempts have also been made improve the performance of the Quadratic Programming solver to speed up the process of solving the SVR convex optimization problem. These attempts include using heuristic techniques such as chunking (Osuna et al.), kernel caching (Joachims et al.), shrinking (Chang et al.) etc and although they significantly improve the performance for the regression analysis for a given dataset, they do not scale with larger datasets. In some cases, these techniques have been used in conjunction with distributed computing to achieve improved performance and scalability (Section 2.3.1).

PSVR attempts to produce a scalable SVR algorithm for use with large data, which relies on using distributed computing techniques in conjuction with the Kernel Matrix approximation.

2.3 Other Parallel SVR approaches

This section analyses the different approaches to parallelize SVR and compares these approaches to PSVR.

2.3.1 PiSvM and MRPsvm

PiSvM and MRPsvm follow a similar approach to solving the Convex Optimization problem; Both use matrix decomposition techniques to decompose the original Kernel Matrix into several smaller matrices and optimize (using a Sequential Minimal Optimization solver) each portion in parallel using parallel processors, before merging the Support Vectors from each of these parallel machines to a *master* machine.
There exist minor differences between the two implementations:

- PiSvM utilizes MPI and hence relies on a distributed memory system while MRPsvm uses a Map-Reduce framework with a shared-memory system.

- Due to the distributed nature of the implementation as a consequence of using MPI, PiSvM requires each processor to locally cache a piece of the Kernel Matrix and the task of updating gradients is assigned to the corresponding processors, according to cache locality. MRPsvm maintains a single shared copy of the matrix and each processor accesses the cache equally.

- PiSvM requires each processor to maintain a copy of all data instances and MRPsvm maintains a shared copy of all instances.

Both these approaches boast many advantages and some disadvantages with respect to accuracy and scalability. One clear advantage is the high accuracy of the regression model due to usage of the full-rank Kernel Matrix. Both these algorithms also use heuristic methods such as Kernel Caching to speed up the Convex Optimization problem.
Unfortunately, due to the usage of a full-rank Kernel Matrix, these methods will be ineffective when run on smaller computing clusters while attempting to train large datasets due to limited memory and processsing power. Also, due to the distributed nature of the Kernel Matrix and high dependence on data residing on other processors, the communication overhead for PiSvM will drastically increase for large datasets.

Table 2.1 compares these approaches to other parallel implementations of SVR.

2.3.2 Parallel Cascade SVM

Parallel Cascade SVM takes a significantly different approach to solving the Convex Optimization problem. The idea behind Cascade SVM is that the training instances that are not Support Vectors can be eliminated early in the process and do not contribute to the regression model. In Parallel Cascade SVM, each parallel machine optimizes a subset of the training instances, filtering out the instances that do not correspond to Support Vectors. The filtering takes place hierarchically and the instances from the previous layer are merged at subsequent layers. To obtain global minimum for the optimization, the result of the last layer is fed back to the first layer. The entire training set is (almost) never dealt with at

each instance and the last layer has to deal with only a subset of the training instances, depending on the quality of filtering.

The advantages and disadvantages of Parallel Cascade SVM are very similar to those of MRPsvm: Due to the usage of a full-rank Kernel Matrix, the generated regression model will be highly accurate. For datasets whose regression models contain fewer number of Support Vectors, this model will be very effective for usage with large datasets.
Unfortunately - similar to MRPsvm - due to usage of full-rank Kernel Matrix, this method will not be applicable to smaller computing clusters while using larger datasets. A significant disadvantage, specific to Parallel Cascade SVM, is the fact that its effectiveness is dependent on the nature of the data; If the dataset to be modeled contains a large number of Support Vectors, the top-level processor will be required to optimize all these Support Vectors independently, causing Parallel Cascade SVM to be highly ineffective.

Table 2.1 compares the Parallel Cascade SVM approach to other parallel SVR approaches.

2.3.3 Comparison between approaches

The salient features of the different approaches to parallelize SVR have been compared in Table 2.1. Through this comparison, the weaknesses of the prior attempts to parallelize SVR will be established, along with the efforts made by PSVR to overcome these weaknesses.

The following terminology is used in Table 2.1:

- m corresponds to number of processing cores used, n is the number of training instances and p isis the reduced rank of the Kernel Matrix used in PSVR with $p << n$.
- With regard to the Quadratic Programming(QP) solvers for the Convex Optimization problem, IPM corresponds to Interior Point Method while SMO corresponds to Sequential Minimal Optimization.

	PSVR	PiSvM	MRPsvm	P-Cascade SVM
Worst Case Time Complexity	$O(np^2/m)$	$O(n^3/m)$	$O(n^3/m)$	$O(n^3)$
Worst Case Space Complexity	$O(np/m)$	$O(n^2/m)$	$O(n^2/m)$	$O(n^2)$
QP Solver	IPM	SMO	SMO	SMO
Framework used	MPI	Map-Reduce	MPI	Map-Reduce
Matrix Decomposition	Yes	Yes	Yes	No
Data Distribution	Yes	Yes	Yes	No
Local Optimization	No	Yes	Yes	Yes
Kernel Matrix Approximation	Yes	No	No	No
Effective with Small Clusters	Yes	No	No	No

Table 2.1. Comparison of attempts to parallelize SVR.

It is evident from the rows corresponding to 'Worst Case Time Complexity' and 'Worst Case Space Complexity' in Table 2.1 that while the PSVR model is only linearly affected by the increase in size of a dataset, the other models are cubically affected with regards to time and quadratically affected with respect to space. This would mean that for PiSvM, MRPsvm and Parallel Cascade SVM, the increase in size of a dataset causes the resource requirements (memory and processing speed) to handle this larger dataset to rise sharply, which is undesirable.

The advantage that PSVR boasts over other approaches to parallelize SVR is that it gracefully and effectively scales with large datasets, which is not the case for the other approaches, whose requirements rise abruptly with the increase in size of datasets.

The question now is, how should PSVR be formulated and implemented to effectively scale with large datasets?

3 Technical Approach

This section explains, in detail, the steps taken by PSVR to ensure scalability with large datasets.

The approach that PSVR takes is to leverage on both the availability of parallel machines as well as approximation the Kernel Matrix with a low-rank matrix.

A high-level overview of the PSVR process is as follows:

1. PSVR begins by distributing the data instances among the available machines in an i *modulo* m manner for each data instance i on machine m. (Section 3.1)
2. The Kernel Matrix is then approximated using the parallel machines and maintained distributedly. (Section 3.2)
3. The parallel machines perform the convex optimization for the instances stored on their respective machines. (Section 3.3)
4. The results after optimization are reduced and stored distributedly on the respective machines. (Section 3.4, 3.1)

The remainder of this section will explain each of these steps in detail and specify the steps taken to ensure PSVR effectively scales with large data.

3.1 Distributed Data Loading and Storage

Through distributed data loading and storage we ensure that in both the training and prediction phase, all data instance never stored on the same machine hence scalable with respect to memory requirement.

Each of the n training instances are distributedly loaded onto the m machines in a round

robin manner so that instance i is loaded onto machine $i\%m$. The variables computed corresponded to these data instances are stored locally on each machine, while the global variables in the process are replicated on all machines as required. The instances that correspond to Support Vectors after the optimization are also retained locally during the prediction phase, there by reducing the overall computational memory requirement during the entire process.

3.2 Parallel Incomplete Cholesky factorization

Parallel Incomplete Cholesky factorization approximates the original Kernel Matrix without constructing the matrix completely. The process occurs in a parallel manner with the resulting matrix stored distributedly. The large memory requirements of SVR are scaled in this phase, while minimizing communication overhead.

A key step in PSVR is the Parallel Incomplete Cholesky Factorization (PICF). While Choleskly Factorization factorizes a symmetric positive-definite matrix of order $n \times n$ into two identical symmetric matrices each of order $n \times n$, Incomplete Cholesky Factorization factorizes the same matrix into two identical symmetric matrices of order $n \times p$, where $p << n$. In both cases, the original matrix G can be computed as $G \approx HH^T$ where H is the result of the factorization.

Application of ICF therefore allows the original Kernel matrix of order $n \times n$ to be approximated by a smaller matrix of order $n \times p$. This matrix can be distributed on m machines to reduce the memory requirement to $O(np/m)$ per machine.

G. Golub proposed a parallel ICF algorithm which obtains the matrix H by constraining the Cholesky Factorization to be performed at most p times. This algorithm (named Column-Based Cholesky Factorization) distributes the matrix H in a column-based manner across m machines. The column-based approach is suitable when the order of n is small and

when only a few parallel machines are available. It is not optimal for usage with large n and high availability of machines for the following reasons:

- The memory requirement after Column-Based ICF is $O(np)$ on each machine which is impractical for large values of n.
- The parallelizability of the algorithm is limited. The sequential portions of the algorithm incur a high communication overhead and hence is impractical, especially for matrices with larger ranks.

To overcome these limitations, PSVR performs ICF in a row-based manner(Row-Based ICF), which both maximizes the portions of the algorithm that can be parallelized while allowing a scalable memory requirement of $O(np/m)$ (the rows of the matrix H are distributed across m machines rather than the columns).

At the end of ICF, a low-rank approximation of the Kernel Matrix is distributed across m machines while benefiting from:

- **A scalable memory requirement of $\boldsymbol{O(np/m)}$.**
- **A scalable computational cost $\boldsymbol{O(np^2/m)}$.**
- A low communication overhead of $O(p^2 log(m))$.

The details of Row-Based PICF algorithm have been described in Appendix A.

3.3 Interior Point Method

The Interior Point Method is utilized in a parallel manner to solve the convex optimization problem. The computation for each data instance is performed on the corresponding machine and global values are communicated when required.

The computational bottlenecks of SVRs exist primarily in solving the Convex Optimization problem. Although there exist many approaches to solving the Convex Optimization

problem, Primal Dual Interior Point Methods(PD-IPM) is utilized to solve it as it is highly effective in efficiently traversing the interior of the feasible region and also enables solutions of linear programming problems (something that several other solvers do not support). Currently, the most effective IPM algorithm is the Primal Dual Interior Point Method which utilizes barrier functions to eliminate the inequalities following which uses the iterative Newton's method to reach the optimal solution.
This is adapted for PSVR in the following equations.

From Section 2.1, the dual to be maximized is of the form:

$$max\ \frac{-1}{2}\sum_{i,j=0}^{n}(\alpha_i-\alpha_i^*)(\alpha_j-\alpha_j^*)K(x_i,x_j)-\epsilon\sum_{i=0}^{n}(\alpha_i+\alpha_i^*)+\sum_{i=0}^{n}y_i(\alpha_i-\alpha_i^*)$$
$$Subject\ to:\sum_{i=0}^{n}(\alpha_i-\alpha_i^*)=0,\ 0\le\alpha,\alpha^*\le C$$

To optimize this dual equation, consider its Lagrangian dual:

$$min\ \frac{1}{2}\sum_{i,j=0}^{n}(\alpha_i-\alpha_i^*)(\alpha_j-\alpha_j^*)Q+\epsilon\sum_{i=0}^{n}(\alpha_i+\alpha_i^*)-\sum_{i=0}^{n}y_i(\alpha_i-\alpha_i^*)-\sum_{i=0}^{n}\lambda_i(C-\alpha_i)$$
$$-\sum_{i=0}^{n}\xi_i(C-\alpha_i^*)-\sum_{i=0}^{n}\theta_i\alpha_i-\sum_{i=0}^{n}\phi_i\alpha_i^*+\nu\sum_{i=0}^{n}(\alpha_i-\alpha_i^*)$$
$$Subject\ to:\ \lambda_i,\ \xi_i,\ \theta_i,\ \phi_i\ge 0$$

Applying the modified Karush-Kuhn-Tucker(KKT) conditions to the dual and the constraints, we get:

$$\frac{dL}{d\alpha} = Q(\alpha - \alpha^*) + 1_n.\epsilon - y + \lambda - \theta + 1_n.\nu = 0$$
$$\frac{dL}{d\alpha^*} = -Q(\alpha - \alpha^*) + 1_n.\epsilon + y + \xi - \phi - 1_n.\nu = 0$$
$$\lambda_i(C - \alpha_i) = \frac{1}{t} \qquad \theta_i\alpha_i = \frac{1}{t}$$
$$\xi_i(C - \alpha_i^*) = \frac{1}{t} \qquad \phi_i\alpha_i^* = \frac{1}{t}$$
$$\sum_{i=0}^{n} \alpha_i - \alpha_i^* = 0$$
$$where\ Q = K(x_i, x_j)$$

Solving the Convex Optimization problem then resolves to computing the Newton increments for the variables until a feasible solution is achieved. Adapting the literature in Convex Optimization (Boyd et al.), these increments in the Newton's iterations can be described as:

$$\begin{pmatrix} Q_{nn} & -Q_{nn} & I_{nn} & 0_{nn} & -I_{nn} & 0_{nn} & 1_n \\ -Q_{nn} & Q_{nn} & 0_{nn} & I_{nn} & 0_{nn} & -I_{nn} & -1_n \\ -diag(\lambda)_{nn} & 0_{nn} & diag(C-\alpha)_{nn} & 0_{nn} & 0_{nn} & 0_{nn} & 0_n \\ 0_{nn} & -diag(\xi)_{nn} & 0_{nn} & diag(C-\alpha^*)_{nn} & 0_{nn} & 0_{nn} & 0_n \\ diag(\theta)_{nn} & 0_{nn} & 0_{nn} & 0_{nn} & diag(\alpha)_{nn} & 0_{nn} & 0_n \\ 0_{nn} & diag(\phi)_{nn} & 0_{nn} & 0_{nn} & 0_{nn} & diag(\alpha^*)_{nn} & 0_{nn} \\ 1_n^T & -1_n^T & 0_n^T & 0_n^T & 0_n^T & 0_n^T & 0 \end{pmatrix}$$

$$\begin{pmatrix} \Delta\alpha \\ \Delta\alpha^* \\ \Delta\lambda \\ \Delta\xi \\ \Delta\theta \\ \Delta\phi \\ \Delta\nu \end{pmatrix} = - \begin{pmatrix} Q(\alpha-\alpha^*) + 1_n.\epsilon - y + \lambda - \theta + 1_n.\nu \\ -Q(\alpha-\alpha^*) + 1_n.\epsilon + y + \xi - \phi - 1_n.\nu \\ vec(\lambda(C-\alpha) - \frac{1}{t}) \\ vec(\xi(C-\alpha^*) - \frac{1}{t}) \\ vec(\theta\alpha - \frac{1}{t}) \\ vec(\phi\alpha^* - \frac{1}{t}) \\ \sum_{i=0}^{n}(\alpha_i - \alpha_i^*) \end{pmatrix}$$

From this matrix we get:

$$\Delta\lambda_i = -\lambda_i + diag(\frac{\lambda_i}{(C-\alpha_i)})\Delta\alpha_i + vec(\frac{1}{t(C-\alpha_i)})$$

$$\Delta\theta_i = -\theta_i - diag(\frac{\theta_i}{\alpha_i})\Delta\alpha_i + vec(\frac{1}{t\alpha_i})$$

$$\Delta\xi_i = -\xi_i + diag(\frac{\xi}{(C-\alpha_i^*)})\Delta\alpha_i^* + vec(\frac{1}{t(C-\alpha_i^*)})$$

$$\Delta\phi_i = -\phi_i - diag(\frac{\phi_i}{\alpha_i^*})\Delta\alpha_i^* + vec(\frac{1}{t\alpha_i^*})$$

$$Q\Delta\alpha - Q\Delta\alpha^* + \Delta\lambda - \Delta\theta + 1_n\Delta\nu = -Q(\alpha-\alpha^*) - 1_n.\epsilon + y - \lambda + \theta - 1_n.\nu$$

$$-Q\Delta\alpha + Q\Delta\alpha^* + \Delta\xi - \Delta\phi - 1_n\Delta\nu = Q(\alpha-\alpha^*) - 1_n.\epsilon - y - \xi + \phi + 1_n.\nu$$

After substitutions, we get

$$Q\Delta\alpha - Q\Delta\alpha^* + \frac{1}{t(C-\alpha)} - \lambda + diag(\frac{\lambda}{(C-\alpha)})\Delta\alpha - \frac{1}{t\alpha} + \theta + diag(\frac{\theta}{\alpha})\Delta\alpha + \Delta\nu$$
$$= -Q(\alpha - \alpha^*) - 1_n.\epsilon + y - \lambda + \theta - 1_n.\nu$$
$$-Q\Delta\alpha + Q\Delta\alpha^* + \frac{1}{t(C-\alpha^*)} - \xi + diag(\frac{\xi}{(C-\alpha^*)})\Delta\alpha^* - \frac{1}{t\alpha^*} + \phi + diag(\frac{\phi}{\alpha^*})\Delta\alpha^* - \Delta\nu$$
$$= Q(\alpha - \alpha^*) - 1_n.\epsilon - y - \xi + \phi + 1_n.\nu$$

Simplifying the above, we get

$$(Q + diag(\frac{\lambda}{C-\alpha} + \frac{\theta}{\alpha}))\Delta\alpha - Q\Delta\alpha^* + \Delta\nu = -Q(\alpha - \alpha^*) - 1_n.\epsilon + y + \frac{1}{t}(\frac{1}{\alpha} - \frac{1}{(C-\alpha)}) - 1_n.\nu$$
$$-Q\Delta\alpha + (Q + diag(\frac{\xi}{C-\alpha^*} + \frac{\phi}{\alpha^*}))\Delta\alpha^* - \Delta\nu = Q(\alpha - \alpha^*) - 1_n.\epsilon - y + \frac{1}{t}(\frac{1}{\alpha^*} - \frac{1}{(C-\alpha^*)}) + 1_n.\nu$$

$$Setting: \ \delta = diag(\frac{\lambda}{C-\alpha} + \frac{\theta}{\alpha}); \ \delta^* = diag(\frac{\xi}{C-\alpha^*} + \frac{\phi}{\alpha^*})$$
$$\rho = -Q(\alpha - \alpha^*) - 1_n.\epsilon + y + \frac{1}{t}(\frac{1}{\alpha} - \frac{1}{(C-\alpha)}) - 1_n.\nu \ and$$
$$\rho^* = Q(\alpha - \alpha^*) - 1_n.\epsilon - y + \frac{1}{t}(\frac{1}{\alpha^*} - \frac{1}{(C-\alpha^*)}) + 1_n.\nu$$

Giving us:

$$\begin{pmatrix} Q+\delta & -Q_{nn} & 1_n \\ -Q_{nn} & Q_{nn}+\delta^* & -1_n \\ 1_n & -1_n & 0 \end{pmatrix} \begin{pmatrix} \Delta\alpha \\ \Delta\alpha^* \\ \Delta\nu \end{pmatrix} = \begin{pmatrix} \rho \\ \rho^* \\ -\sum_{i=0}^{n}(\alpha_i - \alpha_i^*) \end{pmatrix}$$

From this matrix, we get:

$$\Delta\alpha^* = (\delta^*)^{-1}(\rho + \rho^*) - (\delta^*)^{-1}\delta\Delta\alpha \tag{3}$$
$$\Delta\alpha = \Sigma^{-1}(z - \Delta\nu) \tag{4}$$
$$\Delta\nu = \frac{\sum_{i=0}^{n}(I + (\delta^*)^{-1}\delta)\Sigma^{-1}z + \sum_{i=0}^{n}(\alpha_i - \alpha_i^*) - \sum_{i=0}^{n}(\delta^*)^{-1}(\rho + \rho^*)}{\sum_{i=0}^{n}(I + (\delta^*)^{-1}\delta)\Sigma^{-1}1_n} \tag{5}$$

$$where\ z = \rho + Q((\delta^*)^{-1}(\rho + \rho^*))$$

$$and\ \Sigma = Q(I + (\delta^*)^{-1}\delta) + \delta \tag{6}$$

After each iteration, t is updated as $t = \dfrac{4n}{\lambda(C-\alpha) + \xi(C-\alpha^*) + \theta\alpha + \phi\alpha^*}$

Iterations are performed until certain conditions described by the IPM are satisfied, namely:

$$1^T(\alpha_i - \alpha_i^*) \leq s \approx 0,$$
$$1^T(Q(\alpha - \alpha^*) + 1_n.\epsilon - y + \lambda - \theta + 1_n.\nu) \leq s \approx 0\ and$$
$$1^T(-Q(\alpha - \alpha^*) + 1_n.\epsilon + y + \xi - \phi - 1_n.\nu) \leq s \approx 0$$

The computational bottleneck of complexity $O(n^3)$ in this process is of determining the inverse of the Kernel Matrix Q, which occurs during each iteration in solving for both $\Delta\nu$ and $\Delta\alpha$.

The matrix Q that is to be inverted, has already been approximated by the low-rank matrix H as HH^T and is distributedly stored, so **the bottleneck of the Newton iterations can be sped up from $O(n^3)$ to $O(p^2n)$, and can be parallelized to $O(p^2n/m)$** using the Sherman-Morrison-Woodbury formula (Section 3.3.1).

3.3.1 Morrison-Woodbury formula

Incomplete Cholesky Factorization in conjunction with Morrison-Woodbury formula, both applied in a parallel manner, reduce the computational complexity to $O(np^2/m)$, ensuring scalability with large data.

From equation (6), we have

$$\Sigma = Q(I + (\delta^*)^{-1}\delta) + \delta$$

$$where$$

$$\delta = diag(\frac{\lambda}{C-\alpha} + \frac{\theta}{\alpha});\ \delta^* = diag(\frac{\xi}{C-\alpha^*} + \frac{\phi}{\alpha^*})$$

$$where\ \delta\ and\ \delta^*\ are\ diagonal\ matrices$$

As part of the IPM process, it can be observed that Σ^{-1} needs to be calculated in the computation of both $\Delta\alpha$ and $\Delta\nu$ (Equations (4) and (5)). Computation of Σ^{-1} involves computing the inverse of the matrix Q, which is the bottleneck of the SVR process. In the standard SVR implementation, this operation incurs a $O(n^3)$ cost.

Through the application on Incomplete Cholesky Factorization and Morrison-Woodbury formula, the time complexity can be reduced to $O(np^2)$ and can be parallelized to $O(np^2/m)$.

Parallelizing the computation of $\Sigma^{-1}(z - \Delta\nu)$ (or $\Sigma^{-1}.1_n$) is simpler than parallelizing the computation Σ^{-1} by applying the Morrison-Woodbury formula. The following section describes how parallelization of the computation of $\Sigma^{-1}(z-\Delta\nu)$ through the usage of Morrison-Woodbury formula works.

For convenience, $(z - \Delta\nu)$ will be referred to as the vector u, and $(I + (\delta^*)^{-1}\delta)$ will be referred to as the diagonal matrix E.

The SMW (the Sherman-Morrison-Woodbury formula) is not directly applicable to our case, it needs to be modified to account for the additional matrix factor, E, which is fortunately

a diagonal matrix. So, $\Sigma^{-1}u$ can be equated to:

$$\Sigma^{-1}u = (\delta + QE)^{-1}u \approx (\delta + HEH^T)^{-1}u \tag{7}$$

$$= \delta^{-1}u - \delta^{-1}H(I + H^T\delta^{-1}EH)^{-1}EH^T\delta^{-1}u \tag{8}$$

$$= \delta^{-1}u - \delta^{-1}H(GG^T)^{-1}EH^T\delta^{-1}u \tag{9}$$

$\Sigma^{-1}u$ can be computed in four steps:

1. Compute $\delta^{-1}u$. δ can be derived from locally stored vectors, as part of IPM. $\delta^{-1}u$ is a $n \times 1$ vector, and can be computed locally on each of the m machines.

2. Compute $t_1 = EH^T\delta^{-1}u$. Every machine stores some rows of H and their corresponding part of $\delta^{-1}u$ as well as E. This step can be computed locally on each machine. The results are sent to the master (which can be a randomly picked machine for all PIPM iterations) to aggregate into t_1 for the next step.

3. Compute $(GG^T)^{-1}t_1$. This step is completed on the master, since it has all the required data. G can be obtained from H by performing a Cholesky Factorization (Section 3.3.2). Computing $t_2 = (GG^T)^{-1}t_1$ is equivalent to solving the linear equation system $t_1 = (GG^T)t_2$. PIPM first solves $t_1 = Gy_0$, then $y_0 = G^Tt_2$. Once it has obtained y_0, PIPM can solve $G^Tt_2 = y_0$ to obtain t_2. The master then broadcasts t_2 to all machines.

4. Compute $\delta^{-1}Ht_2$ All machines have a copy of t_2, and can compute $\delta^{-1}Ht_2$ locally to solve for $\Sigma^{-1}u$.

Similarly, $\Sigma^{-1}.1_n$ can be computed with a minor modification to the above formulation. Once both $\Sigma^{-1}.1_n$ and $\Sigma^{-1}.(z - \Delta\nu)$ have been obtained, values of $\Delta\nu$ and $\Delta\alpha$ can be determined by substituting the values.

3.3.2 Cholesky Factorization

Cholesky Factorization is needed to reduce a positive symmetric matrix, H to a form GG^T. This process is sequential and not parallelizable since parallelization

requires each of the entries of the matrix H to be broadcast independently incurring extremely high communication cost between machines.

As per the SMW formula above (Equations (8) and (9)), the matrix $(I + H^T\delta^{-1}EH)$ needs to be reduced to a form GG^T for it to be functional. This is achieved through performing a Cholesky Factorization.

Cholesky Factorization decomposes a symmetric positive semi-definite matrix into into the product of a lower triangular matrix and its conjugate transpose, ie $A = LL^T$

The decomposition boils down to solving the following equations for each element:

$$L_{j,j} = \sqrt{A_{j,j} - \sum_{k=1}^{j-1} L_{j,k}^2}$$

$$L_{i,j} = \frac{1}{L_{j,j}}(A_{i,j} - \sum_{k=1}^{j-1} L_{i,j}L_{j,k}^T)$$

From these equations, it can be observed that every element in the matrix depends on the elements in the rows and columns upto the current row and column. If this computation is to be done in parallel, after the computation of every element, the element must be broadcast to all the other processors so that they can maintain a copy of the entire matrix for subsequent computations. Experiments conducted on the computational time for both a parallel model and a sequential model of the Cholesky factorization showed that the time taken for the sequential model << time taken for parallel model.

In favour of these results, the Cholesky Factorization of the matrix is implemented sequentially and is the only purely sequential portion of the implementation. The time complexity for this portion is $O(p^2)$.

Depending on the nature of the training instances, only a subset of instances will correspond to a non-zero $(\alpha - \alpha^*)$ value and since the SVR model depends on a non-zero value of $(\alpha - \alpha^*)$, only the corresponding subset will be considered relevant for the model and used in the prediction phase the remaining instances

are discarded. These instances are the support vectors of the model.

3.4 Computing b

The final step of the PSVR process, the support vectors from the different machines distributedly compute the value of b of the regression model and the mean of these results is selected as the final value.

By the end of the IPM process, the Support Vectors for the model are identifiable by a non-zero $(\alpha - \alpha^*)$ value. Since most of the training instances have $(\alpha - \alpha^*) = 0$, from equation (2), computation of the target regression model only requires summation over all Support Vectors which can be equated to:

$$f(x) = \sum_{i=1}^{N_{sv}} (\alpha_i - \alpha_i^*)\langle sv_i, x\rangle + b$$

where N_{sv} is the number of Support Vectors and sv_i corresponds to each Support Vector. Every training instance provided can be utilized to compute the value of b by substituting the corresponding value of x_i and y_i.

For practical reasons, a maximum of 1000 training instances are considered to determine the value of b and the average of the computed values for all these instances is selected as the final value of b.

4 Experiments

This section of the report examines the performance of PSVR with respect to 2 metrics,

- **Prediction Accuracy**: Root Mean Square Error to determine accuracy of regression model
- **Speedup**: Relative performance increase by usage of parallel machines

The various overheads associated with PSVR, which impact the Scalability and Speedup of PSVR are also analyzed.

For these experiments, 4 datasets are considered. For each dataset, experimentation and cross validation is used to determine the optimal parameters and Kernel Function to use to model that dataset. These datasets correspond to :

(a) AIMPEAK dataset (Chen et al., 2012) of size $|D| = 41790$ which corresponds to traffic speeds (km/h) along 775 road segments of an urban road network during morning peak hours on April 20, 2011. Each input (i.e., road segment) comprises of 5 dimension input space: length, number of lanes, speed limit, direction, and time. The time dimension comprises 54 five-minute time slots. The outputs correspond to the traffic speeds. The regression model for this dataset was configured to use a Lapacian Kernel function ($f(x) = e^{\gamma|a-b|}$) with $\gamma = 0.1$, $\epsilon = 1$ and hyper parameter $C = 1$;

(b) SARCOS dataset (Vijayakumar et al., 2005) of size $|D| = 48933$ which relates to an inverse dynamics problem for a seven degrees-of-freedom SARCOS anthropomorphic robot arm. The task is to map from a 21-dimensional input space (7 joint positions, 7 joint velocities, 7 joint accelerations) to the corresponding 7 joint torques. The output corresponds to one of the seven joint torques.The regression model for this dataset was configured to use a Polynomial Kernel function ($f(x) = (c_0 + p(a^T b))^d$) with degree(d) = 3, coefficient sum(c_0) = 1003, coefficient product(p) = 2, $\epsilon = 0.01$ and hyper parameter $C = 13$;

(c) HADSST dataset of size $|D| = 168147$ corresponds to the Met Office Hadley Centre's sea surface temperature data set. More information is available at: http://www.metoffice.gov.uk/hadobs/. The regression model for this dataset was configured to use a Radial Basis Kernel function ($f(x) = e^{\gamma||a-b||^2}$)with $\gamma = 0.1$, $\epsilon = 0.01$ and hyper parameter $C = 1$;

(d) Housing dataset of size $|D| = 606507$ which tracks the residential property sales in England and Wales that are lodged with Land Registry for registration with each data instance containing two input features. More information is available at: http://data.gov.uk/dataset/land-registry-monthly-price-paid-data/. The regression model for this dataset was configured to use a Radial Basis Kernel function ($f(x) = e^{\gamma||a-b||^2}$) with $\gamma = 10$, $\epsilon = 0.01$ and hyper parameter $C = 25$;

For each dataset, 10% of the training instances were randomly selected as test data for prediction and the remaining data was used to generate the regression model.

The experiments were conducted on the NUS Tembusu Computing cluster using 1-50 processing cores, each of which had a nearly identical configuration of Intel(R) Xeon(R) CPU E5620 @ 2.40GHz, across 10 physical machines each of which had 20 GB memory, running Linux CentOS 6.5. The experiments were conducted by varying the number of processing cores (m) = 1, 2, 5, 10, 20, 40 and 50.

4.1 Prediction Accuracy

One of the distinguishing factors of PSVR, which allows it to be scalable and time-efficient is the usage of ICF (Section 3.2) to approximate the Kernel matrix with dimensions $n \times n$ using a matrix with dimensions $n \times p$ with $p << n$. One concern with the usage of this matrix approximation technique is the accuracy of the Regression model. To address this issue, in this section, **the prediction accuracy of PSVR will be compared to that of a state-of-the-art SVR implementation (which uses the full-rank matrix).**

LIBSVM has has been selected for this comparison as it is arguably the most efficient open-source SVR implementation in terms of both speed and accuracy (Lin et al.). Specifically, LIBSVM-3.2 has been used and the parameters for training remain uniform for both implementations.

The accuracy for each implementation along with the corresponding rank ratios of the approximated matrices have been tabulated below. The accuracy measure selected in this case is the Root Mean Square Error (RMSE) = $\sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - f(x_i))^2}$, where n corresponds to the number of testing instances.

Dataset	Size	p/n	PSVR Accuracy (RMSE)	LIBSVM Accuracy (RMSE)
SARCOS	40k	0.02	5.21	4.84
AIMPEAK	40k	0.03	8.93	8.88
HADSST	170k	0.01	0.673	0.646
HOUSING	600k	0.002	0.820	0.804

Table 4.1. Predictive accuracy of PSVR. (p is set to the optimal value after experimentation)

From Table 4.1, it can be seen that **for the larger datasets, the accuracy for PSVR when $p << n$ is nearly equal to that of LIBSVM.** For the smaller datasets, the required value of p to achieve similar accuracy is relatively larger.

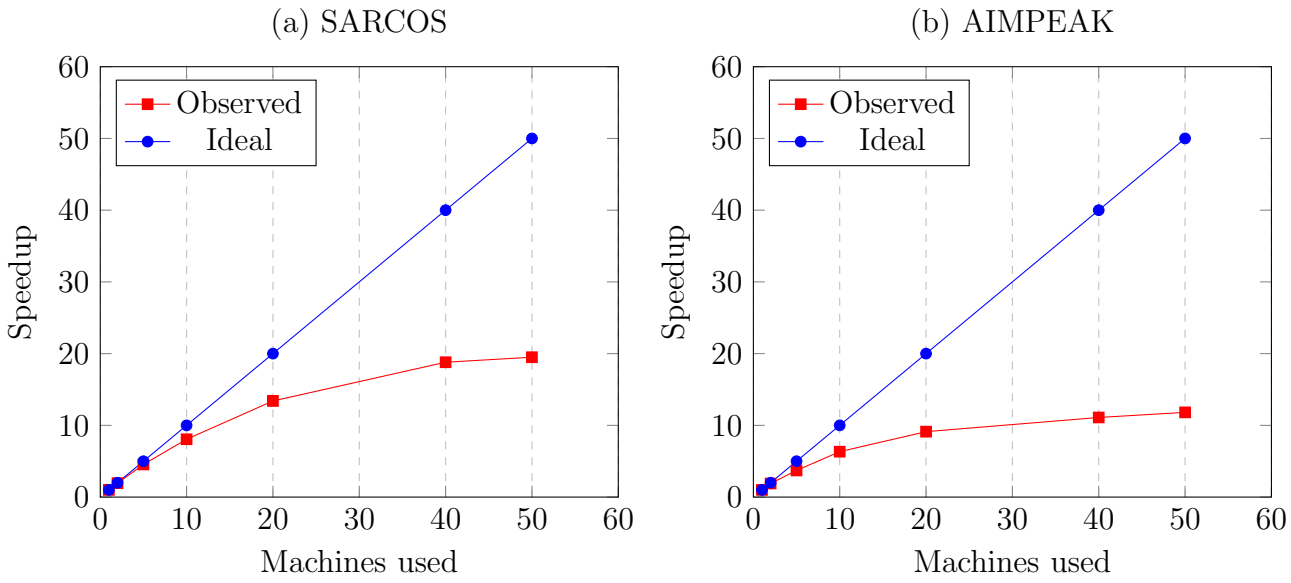
4.2 Scalability/Speedup

To determine the scalability of PSVR, the same 4 datasets have been considered and the time taken to determine the regression model (over 3 separate readings, considering the average) for each dataset while using a varying number of processing cores have been tabulated. Using these timings, **the speedup relative to the number of processing cores used will be determined will be used to judge the scalability of PSVR**. For comparison, the time taken to train the regression model using the state-of-the-art SVR implementation (LIBSVM) for each dataset with the same parameters as PSVR and same processor configuration have also been included.

	SARCOS (40K)		AIMPEAK (40K)		HADSST (170K)		HOUSING (600K)	
Machines	Time (s)	Speedup	Time (s)	Speedup	Time (s)	Speedup	Time (s)	Speedup
1	1072	1	5185	1	10451	1	17146	1
2	550	1.94	2733	1.89	5564	1.87	8938	1.91
5	237	4.55	1396	3.71	2254	4.63	3407	5.03
10	141	8.06	818	6.33	1208	8.65	1965	8.72
20	80	13.4	568	9.12	718	14.55	909	18.86
40	57	18.8	467	11.10	423	24.70	559	30.67
50	55	19.5	439	11.81	367	28.47	476	36.02
LIBSVM	449	NA	638	NA	12875	NA	186056	NA

Table 4.2. Speedup of process using PSVR. (p is set to the corresponding value in Table 4.1 and the predictive accuracy remains constant for each dataset)

The observed speedup from Table 4.2 have been plotted in the following graphs.



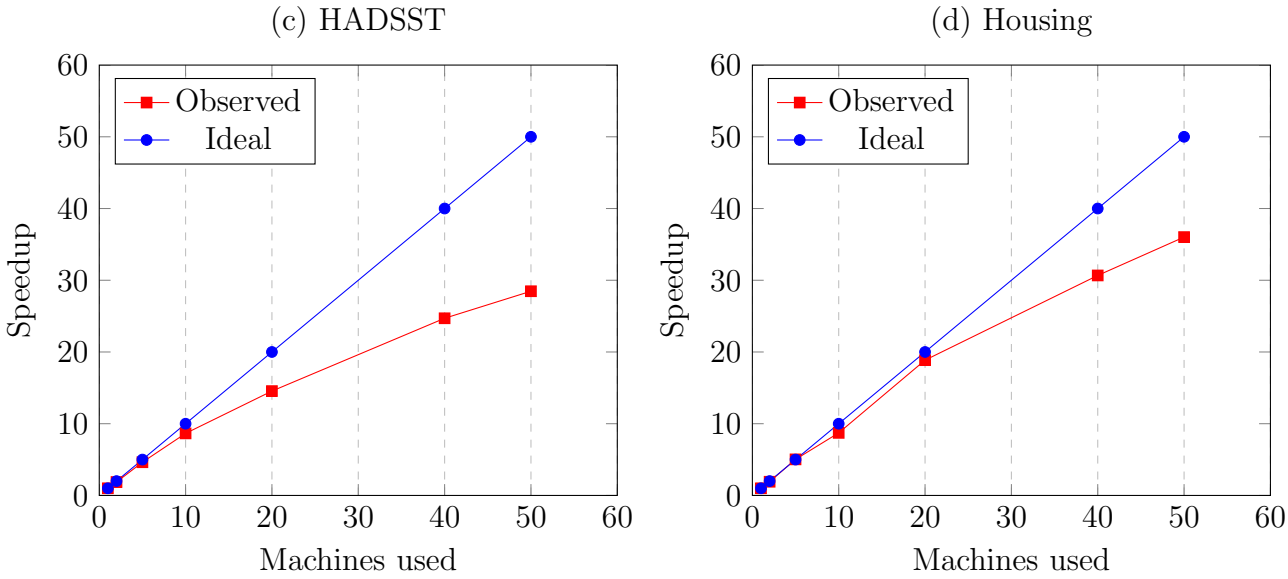


Figure 4.1. Speedup for various datasets

The following observations can be made from the tabulation and graphs,

(a) Larger the size of the dataset, larger is the speedup as the number of machines used increases.

(b) For all datasets, the speedup begins to decreases after a threshold number of machines are used.

(c) For datasets of the same size, the speedup obtained depends on the time for the sequential run (time taken for a single processor to train the dataset).

Points (a) and (b) are analyzed in detail in the following section.
The reasoning behind point (c) is intuitive: depending on the nature of the dataset, the number of iterations required for the convergence of the solution varies, and larger number of iterations implies increased training time. Increase in the number of iterations would also mean that the total communication overhead incurred and executions of the sequential portion of the code (see Section 3.3.2) increases leading to decrease in speedup.

From Figure 4.1 and Table 4.2, it can be observed that although the speedup

is not ideal, PSVR is able to parallelize the SVR algorithm and scales with increased number of machines used, more effectively so for larger datasets.

4.3 Overhead

From the graphs in Figure 4.1, it can be observed that for each of the datasets, the speedups are not ideal, and that the individual speedups vary between datasets. **The following section attempts to explain the overheads incurred by PSVR which affect the overall speedup of the training process.**

Usage of parallel computing in PSVR incurs two types of overheads, Communication overhead and Synchronization overhead.

- Communication overhead corresponds to the overhead incurred due to broadcast and transmission of messages over the network as part of MPI.
  As the number of machines used increases, the communication over the network at each step increases as well, implying more Communication overhead with increase number of machines. The increase in overhead could be minimal[3]or substantial depending on the underlying architecture of the computing cluster.

- Synchronization overhead occurs due to non-identical configuration of the machines used. Various machines are capable of executing the program at various speeds and after each step in PSVR, a synchronization occurs (using MPIBarrier) which ensures that every machine has reached the same point of execution (to prevent the situation that one of the machines fails but the other machines aren't notified).

The graphs below plot the Communication and Synchrnoization overhead for each of the datasets using varying number of machines.

[3]In Figure 4.2, we notice that the Communication overhead rises significantly until m = 5 and then the increase is minor; The collective operations using MPI3 are substantially faster for processors on the same physical machine (since network traffic is minimized) and after m $\geq$ 5, while the number of processors per physical machines used increases, the number of physical machines used remains the same, causing the overhead to increase minimally for subsequent values of m(since inter-processor communication does not rely on the network).

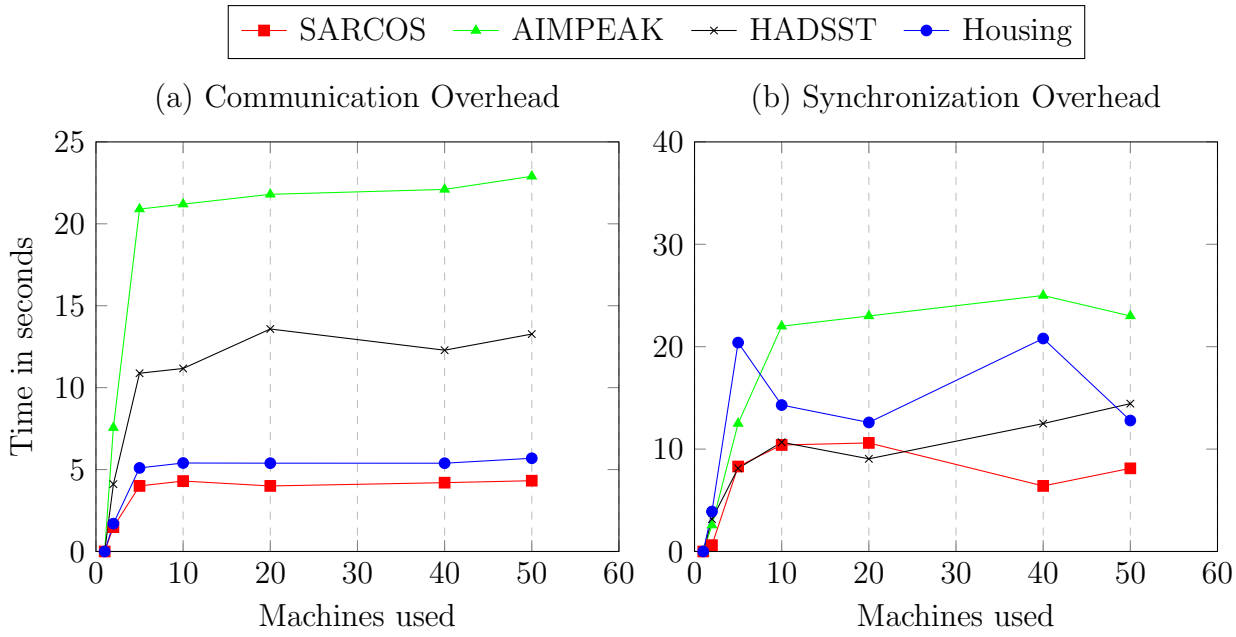


Figure 4.2. Overheads incurred for datasets

Certain observations can be made from these graphs.

(a) For the larger datasets, although both the overheads are comparable to that of the smaller datasets, the speedup is affected less due to the fact that the computational time for the program is much more than the time for the overheads.

(b) For the SARCOS and AIMPEAK datasets (which have approximately the same number of training instances,), there is significant difference in the overhead, and therefore the speedups. This is due to the nature if the datasets; The SARCOS dataset converges to a solution in much fewer iterations than the AIMPEAK dataset, causing the AIMPEAK dataset to incur much more overhead due to increased number of iterations.

4.3.1 Sequential Cost

A cost not considered until now is the cost for the sequential part of the program i.e Cholesky Factorization(Section 3.3.2). As mentioned above, the cost for Cholesky Factorization is incurred for every IPM iteration and is dependent only on the square of the reduced rank of

the Kernel Matrix, p^2. Since the process is non-parallelizable, the overhead will be constant for the PSVR process for a particular dataset, independent of the number of machines used. The graphs below plot the observed speedup, speedup without the Cholesky Factorization(CF) and the ideal speedup.

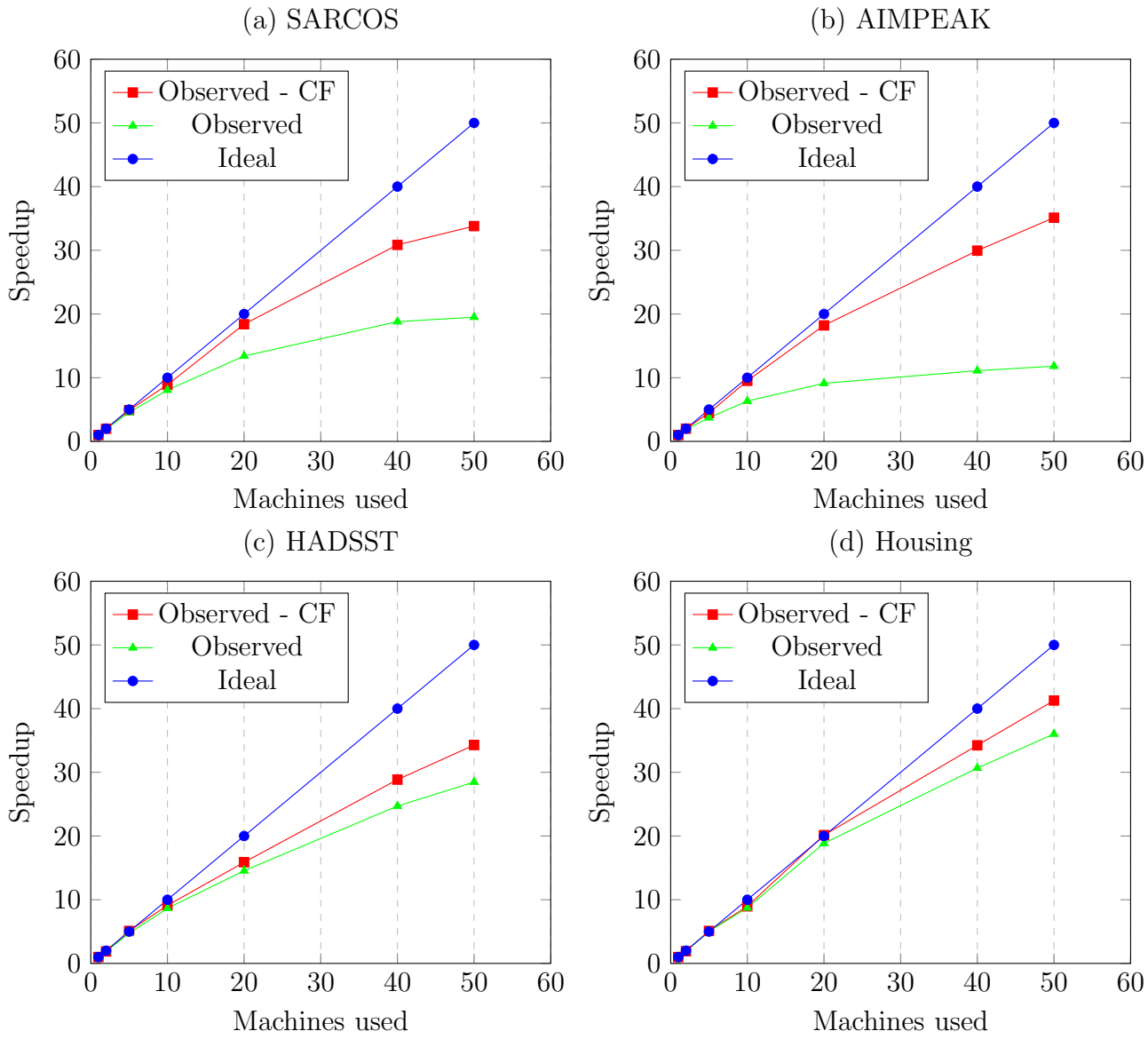


Figure 4.3. Speedup for various datasets excluding sequential component.

From the graphs in Figure 4.3, the following observations can be made regarding the nature of the speedup curve:

(a) If the time taken for Cholesky Factorization is disregarded for all datasets, the speedup curve obtained by varying number of machines used is similar (not identical) across datasets, establishing the effect of the Sequential portion of the program on the speedup. The deviation of the speedup curves obtained after disregarding the time for Cholesky Factorization from the ideal speedup in these graphs is due to the Synchronization and Communication overheads explained in Section 4.3.

(b) With fewer machines, the effect of the Cholesky Factorization portion of the program on the speedup is not observable, as the time taken for this computation is insignificant when compared to the time taken for the overall computation. As the number of machines used increases, the time taken for computation of other portions decreases (nearly linearly) while the time for executing the Cholesky Factorization remains the same, making the cost of executing the sequential portion significant.

(c) For smaller datasets, the speedup deteriorates at a much faster rate as compared to the larger ones when the Cholesky Factorization is considered. The same reasoning as for (b) can be applied here. The time taken for execution of the program for larger datasets is much more than for the smaller datasets. So for smaller datasets, fewer machines are needed to make the time taken for the execution of the sequential portion to be significant when compared to the larger datasets.

(d) The effect of Choleskly Factorization on datasets of similar size but requiring different number of iterations required for convergence(SARCOS and AIMPEAK) is significant. The speedup curves obtained after disregarding the time for Cholesky Factorization are similar for both datasets, but if the Choleskly Factorization is included, the speedup for the SARCOS dataset is much more than for the AIMPEAK dataset. This is because for the AIMPEAK dataset, more iterations are required for the convergence of a solution implying more executions of the sequential portion of the program, which negatively

affects the speedup at each iteration.

From Amdahl's law, the speedup that can be achieved is capped by the un-parallelizable portions of the program. From the results and observations above, this means that for a larger speedup, the time taken for the un-parallelizable portion of the program needs to be insignificant compared to the rest of the program, which is the case for larger datasets. So, **larger the dataset, greater is the speedup we can achieve by increasing the machines used.** For smaller datasets, since the time taken for the un-parallelizable portion of the program is significant, the speedup that can be achieved will be limited.

4.4 Summary of Results

From the observations in the previous subsections, the following observations can be made:

(a) **PSVR successfully parallelizes SVR algorithm**

The following observation can be made from Table 4.2; For a given dataset, PSVR can effectively parallelize the SVR algorithm to provide increased speedup with increasing number of machines used. The speedup achieved with increasing number of machines is nearly linear, except for the overheads detailed in Section 4.3. This would mean that the PSVR algorithm can be scaled almost linearly (by using more machines) to be used with larger datasets which correspond to real-world data.

(b) **Predictive performance of PSVR nearly equivalent to existing state-of-the-art**

In Table 4.1, the predictive performance of PSVR was compared to that of the state-of-the-art SVR implementation (LIBSVM) and it was observes that for each of the datasets, the predictive performance of PSVR is nearly equivalent to that of LIBSVM even with the Kernel Matrix approximation.

The rank-ratio(p/n) of the approximated Kernel Matrix, utilized to achieve a nearly equivalent predictive performance, is dependent on the size of the dataset. As the size of the dataset increases, the rank-ratio of the approximated matrix used decreases.

This means for larger datasets, the size of the matrix to actually be considered will be smaller.

(c) **PSVR outperforms existing state-of-the-art with respect to computational time**

In Table 4.2, the time taken for the state-of-the-art (LIBSVM) SVR implementation to produce a the regression is tabulated along with the time for PSVR to do the same and it can be observed that the time taken for PSVR to compute the solution, in most cases, is much less than that for LIBSVM. For larger datasets, the computational time is significantly less for each setting of machines used.

For smaller datasets, this is not always the case; LIBSVM outperforms PSVR when run on only one machine, but with parallelization PSVR converges to a solution much faster than LIBSVM. The reason for LIBSVM initially outperforming PSVR is that LIBSVM is better equipped to handle smaller datasets and can perform several optimizations (Kernel Caching) to speed up performance. These optimizations do not scale well with larger datasets. When parallel machines are used, the PSVR process speeds up nearly linearly to decrease the time taken for computation.

5 Conclusion

Through the course of this paper, the salient features of Support Vector Regression have been highlighted and the need for a SVR implementation that allows usage of large datasets have been identified. Following this, a novel Parallel Support Vector Regression(PSVR) algorithm was proposed which allowed the SVR convex optimization problem to be efficiently solved by reducing the initial memory requirement from $O(n^2)$ to $O(np/m)$ and the computational complexity from $O(n^3)$ to $O(np^2/m)$, where m is the number of machines available, n is the number of training instance and p is the reduced matrix dimension with $p << n$. PSVR achieves this through a combination of distributing the computational load among parallel machines and performing a matrix approximation of the Kernel Matrix.

The proposed PSVR algorithm was implemented in C++ using the Message Parsing Interface and through experiments it was verified that PSVR outperformed the state-of-the-art SVR implementation with respect to computational complexity in almost all cases. It was also verified that PSVR had nearly equivalent predictive accuracy as the state-of-the-art implementation. The overheads associated with the PSVR algorithm and implementation were also explained and supported by the results of the experiments.

Through the course of these experiments, it can be firmly establish that Parallel Support Vector Regression effectively solves the scalability issues associated with Support Vector Regression for usage with larger datasets.

This being said, although PSVR is effective and can be used for smaller datasets, LIBSVM and other SVR implementations which have been specifically optimized for smaller datasets may be a better option, if an insufficient number of parallel machines are available. For larger datasets, PSVR outperforms LIBSVM even if only a single machine is used and is the clear choice for usage.

The PSVR implementation is available at `https://github.com/akshayv/psvr`.

5.1 Future Improvements

The PSVR project still has potential for improvements, the most salient of which being:

- A pre-processing step could be introduced to determine the optimal parameter values for the SVR training process, possibly through maximum likelihood estimates. The importance of this feature stems from the fact that the tuning of parameters in the SVR process makes a significant difference in the predictive accuracy and re-training the entire model to find the optimal parameter values would significantly increase the computational time.

- One of the requirements for both the Incomplete Cholesky Factorization and Cholesky Factorization processes is that the matrix to be factorized be a symmetric, positive, semi-definite matrix and the matrices generated by using the standard Kernel Functions satisfy this criteria. There exists an extension of the standard Radial Basis Kernel Function which allows varying the hyperparameters for each of the input features to provide a more accurate regression model. Unfortunately, the Kernel matrix that is constructed from this modified function does not satisfy the conditions of a positive semi-definite matrix. Using a smaller rank ratio to approximate this matrix provides worse results compared to matrix generated by the standard Kernel Functions with the same rank ratio. This issue can be alleviated by using a large rank ratio for the approximated matrix, but this would incur a larger computational cost in the process of performing a Cholesky factorization, so is currently sub-optimal. Resolving this issue would improve predictive performance of PSVR (although not significantly).

6 Appendix

6.1 A: Parallel Incomplete Cholesky factorization

ICF can approximate $Q(Q \in R^{n \times n})$ by a smaller matrix $H(H \in R^{n \times p}, p \ll n)$, i.e., $Q \approx HH^T$. Our 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 $\{i_1, i_2, ..., i_k\}$, the k^{th} iteration of ICF computes three equations:

$$H(i_k, k) = \sqrt{v(i_k)} \tag{10}$$

$$H(J_k, k) = \frac{(Q(J_k, k) - \sum_{j=1}^{k-1} H(J_k, j)(H(i_k, j))}{H(i_k, k)} \tag{11}$$

$$v(J_k) = v(J_k) - H(J_k, k)^2, \tag{12}$$

where J_k denotes the complement of $\{i_1, i_2, ..., i_k\}$. The algorithm iterates until the approximation of Q by $H_k H_k^T$ (measured by $trace(QH_kH_k^T)$) is satisfactory, or the predefined maximum iterations (or say, the desired rank of the ICF matrix) p is reached.

The details of computing the pivots and updating the vectors in each iteration have been explained in Algorithm 1.

At the end of the algorithm, H is stored distributedly on m machines, ready for parallel IPM. PICF enjoys three advantages: parallel memory use ($O(np/m)$), parallel computation ($O(p^2n/m)$), and low communication overhead ($O(p^2log(m))$).

Algorithm 1 Row-based PICF

Input n training instances; p: rank of ICF matrix H; m: number of machines
Output H distributed on m machines
Variables:
v: fraction of the diagonal vector of Q that resides in local machine
k: iteration number;
x_i: the ith training instance
M: machine index set, $M = 0, 1, ..., m-1$
I_c: row-index set on machine c ($c \in M$), $I_c = c, c+m, c+2m, ...$

1: **for** $i = 0$ to $n-1$ **do**
2: Load x_i into machine $imodulom$.
3: **end for**
4: $k \leftarrow 0; H \leftarrow 0; v \leftarrow$ the fraction of the diagonal vector of Q that resides in local machine.($v(i)(i \in I_m)$ can be obtained from x_i).
5: Initialize *master* to be machine 0.
6: **while** $k < p$ **do**
7: Each machine $c \in M$ selects its local pivot value, which is the largest element in v:

$$\boldsymbol{lpv_{k,c}} = max\ \boldsymbol{v(i)}, i \in I_c.$$

and records the local pivot index, the row index corresponds to $\boldsymbol{lpv_{k,c}}$:

$$\boldsymbol{lpi_{k,c}} = arg\ max\ \boldsymbol{v(i)}, i \in I_c.$$

8: Gather $\boldsymbol{lpv_{k,c}}$s and $\boldsymbol{lpi_{k,c}}$s ($c \in M$) to *master*.
9: The *master* selects the largest local pivot value as global pivot value $\boldsymbol{gpv_k}$ and records in i_k, row index corresponding to the global pivot value.

$$\boldsymbol{gpv_k} = max\ \boldsymbol{lpv_{k,c}}, c \in M$$

10: The master broadcasts $\boldsymbol{gpv_k}$ and i_k.
11: Change *master* to machine $i_k \% m$.
12: Calculate $H(i_k, k)$ according to (10) on master.
13: The *master* broadcasts the pivot instance x_{i_k} and the pivot row $H(i_k, :)$. (Only the first $k+1$ values of the pivot row need to be broadcast, since the remainder are zeros.)
14: Each machine $c \in M$ calculates its part of the kth column of H according to (11).
15: Each machine $c \in M$ updates v according to (12).
16: $k \leftarrow k+1$
17: **end while**

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