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Accurate On-line Support Vector Regression

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Batch implementations of support vector regression (SVR) are inefficient when used in an on-line setting because they must be retrained from scratch every time the training set is modified. Following an incremental support vector classification algorithm introduced by Cauwenberghs and Poggio (2001), we have developed an accurate on-line support vector regression (AOSVR) that efficiently updates a trained SVR function whenever a sample is added to or removed from the training set. The updated SVR function is identical to that produced by a batch algorithm. Applications of AOSVR in both on-line and cross-validation scenarios are presented. In both scenarios, numerical experiments indicate that AOSVR is faster than batch SVR algorithms with both cold and warm start.

1 Introduction

Support vector regression (SVR) fits a continuous-valued function to data in a way that shares many of the advantages of support vector machine (SVM) classification. Most algorithms for SVR (Smola & Schölkopf, 1998; Chang & Lin, 2002) require that training samples be delivered in a single batch. For applications such as on-line time-series prediction or leave-one-out cross-validation, a new model is desired each time a new sample is added to (or removed from) the training set. Retraining from scratch for each new data point can be very expensive. Approximate on-line training algorithms have previously been proposed for SVMs (Syed, Liu, & Sung, 1999; Csato & Opper, 2001; Gentile, 2001; Graepel, Herbrich, & Williamson, 2001; Herbster, 2001; Li & Long, 1999; Kivinen, Smola, & Williamson, 2002; Ralaivola & d'Alche-Buc, 2001). We propose an accurate on-line support vector regression (AOSVR) algorithm that follows the approach of Cauwenberghs and Poggio (2001) for incremental SVM classification.

This article is organized as follows. The formulation of the SVR problem and the development of the Karush-Kuhn- Tucker (KKT) conditions that its solution must satisfy are presented in section 2. The incremental SVR algorithm is derived in section 3, and a decremental version is described in section 4. Two applications of the AOSVR algorithm are presented in section 5, along with a comparison to batch algorithms uing both cold start and warm start.

2 Support Vector Regression and the Karush-Kuhn Tucker Conditions

A more detailed version of the following presentation of SVR theory can be found in Smola and Schölkopf (1998).

Given a training set $T = \{(\mathbf{x}_i, y_i), i = 1 \cdots l\}$, where $\mathbf{x}_i \epsilon \boldsymbol{R}^N$, and $y_i \epsilon \boldsymbol{R}$, we construct a linear regression function,

$$f(\mathbf{x}) = \mathbf{W}^T \Phi(\mathbf{x}) + b, \tag{2.1}$$

on a feature space $\boldsymbol{F}$. Here, $\boldsymbol{W}$ is a vector in $\boldsymbol{F}$, and $\Phi(\mathbf{x})$ maps the input $\mathbf{x}$ to a vector in $\boldsymbol{F}$. The $\mathbf{W}$ and b in equation 2.1 are obtained by solving an optimization problem:

$$\begin{aligned} \min_{\mathbf{W},b} \quad & P = \frac{1}{2}\mathbf{W}^T\mathbf{W} + C\sum_{i=1}^{l}(\xi_i + \xi_i^*) \\ s.t. \quad & y_i - (\mathbf{W}^T\Phi(\mathbf{x}) + b) \le \varepsilon + \xi_i \\ & (\mathbf{W}^T\Phi(\mathbf{x}) + b) - y_i \le \varepsilon + \xi_i^* \\ & \xi_i, \xi_i^* \ge 0, \ i = 1 \cdots l. \end{aligned} \tag{2.2}$$

The optimization criterion penalizes data points whose y-values differ from $f(\mathbf{x})$ by more than ε. The slack variables, ξ and ξ^*, correspond to the size of this excess deviation for positive and negative deviations, respectively, as shown in Figure 1.

Introducing Lagrange multipliers α, α^*, η, and η^*, we can write the corresponding Lagrangian as

$$\begin{aligned} L_P = & \frac{1}{2}\mathbf{W}^T\mathbf{W} + C\sum_{i=1}^{l}(\xi_i + \xi_i^*) - \sum_{i=1}^{l}(\eta_i\xi_i + \eta_i^*\xi_i^*) \\ & - \sum_{i=1}^{l}\alpha_i(\varepsilon + \xi_i + y_i - \mathbf{W}^T\Phi(\mathbf{x}_i) - b) \\ & - \sum_{i=1}^{l}\alpha_i^*(\varepsilon + \xi_i^* - y_i + \mathbf{W}^T\Phi(\mathbf{x}_i) + b) \\ s.t. \quad & \alpha_i, \alpha_i^*, \eta_i, \eta_i^* \ge 0. \end{aligned}$$

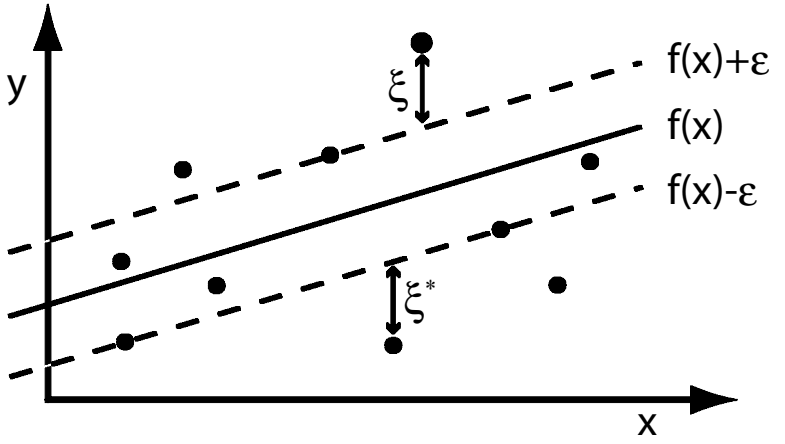

Figure 1: The ε-insensitive loss function and the role of the slack variables ξ and ξ^*.

This in turn leads to the dual optimization problem:

$$\begin{aligned} \min_{\alpha,\alpha^*} \quad & D = \frac{1}{2}\sum_{i=1}^{l}\sum_{j=1}^{l} Q_{ij}(\alpha_i - \alpha_i^*)(\alpha_j - \alpha_j^*) + \varepsilon\sum_{i=1}^{l}(\alpha_i + \alpha_i^*) \\ & - \sum_{i=1}^{l} y_i(\alpha_i - \alpha_i^*) \\ s.t. \quad & 0 \le \alpha_i, \alpha_i^* \le C \quad i = 1, \ldots, l, \\ & \sum_{i=1}^{l}(\alpha_i - \alpha_i^*) = 0, \end{aligned} \tag{2.3}$$

where $Q_{ij} = \mathbf{\Phi}(\mathbf{x}_i)^T\mathbf{\Phi}(\mathbf{x}_j) = K(\mathbf{x}_i, \mathbf{x}_j)$. Here $K(\mathbf{x}_i, \mathbf{x}_j)$ is a kernel function (Smola & Schölkopf, 1998). Given the solution of equation 2.3, the regression function (2.1) can be written as

$$f(\mathbf{x}) = \sum_{i=1}^{l}(\alpha_i - \alpha_i^*)K(\mathbf{x}_i, \mathbf{x}) + b. \tag{2.4}$$

The Lagrange formulation of equation 2.3 can be represented as

$$\begin{aligned} L_D = & \frac{1}{2}\sum_{i=1}^{l}(\alpha_i - \alpha_i^*)(\alpha_j - \alpha_j^*) + \varepsilon\sum_{i=1}^{l}(\alpha_i + \alpha_i^*) - \sum_{i=1}^{l} y_i(\alpha_i - \alpha_i^*) \\ & - \sum_{i=1}^{l}(\delta_i\alpha_i + \delta_i^*\alpha_i^*) + \sum_{i=1}^{l}[u_i(\alpha_i - C) + u_i^*(\alpha_i^* - C)] \\ & + \zeta\sum_{i=1}^{l}(\alpha_i - \alpha_i^*), \end{aligned} \tag{2.5}$$

where $\delta_i^{(*)}$, $u_i^{(*)}$, and ζ are the Lagrange multipliers. Optimizing this Lagrangian leads to the Karush-Kuhn-Tucker (KKT) conditions:

$$\begin{aligned} & \frac{\partial L_D}{\partial \alpha_i} = \sum_{j=1}^{l} Q_{ij}(\alpha_j - \alpha_j^*) + \varepsilon - y_i + \zeta - \delta_i + u_i = 0 \\ & \frac{\partial L_D}{\partial \alpha_i^*} = -\sum_{j=1}^{l} Q_{ij}(\alpha_j - \alpha_j^*) + \varepsilon + y_i - \zeta - \delta_i^* + u_i^* = 0 \\ & \delta_i^{(*)} \geq 0, \quad \delta_i^{(*)}\alpha_i^{(*)} = 0 \\ & u_i^{(*)} \geq 0, \quad u_i^{(*)}(\alpha_i^{(*)} - C) = 0. \end{aligned} \tag{2.6}$$

Note that ζ in equation 2.6 is equal to b in equations 2.1 and 2.4 at optimality (Chang & Lin, 2002).

According to the KKT conditions 2.6, at most one of α_i and α_i^* will be nonzero, and both are nonnegative. Therefore, we can define a coefficient difference θ_i as

$$\theta_i = \alpha_i - \alpha_i^*, \tag{2.7}$$

and note that θ_i determines both α_i and α_i^*.

Define a margin function $h(\mathbf{x}_i)$ for the ith sample $\mathbf{x}_i$ as

$$h(x_i) \equiv f(x_i) - y_i = \sum_{j=1}^{l} Q_{ij}\theta_j - y_i + b. \tag{2.8}$$

Combining equations 2.6, 2.7, and 2.8, we can obtain:

$$\begin{cases} h(\mathbf{x}_i) \geq \varepsilon, & \theta_i = -C \\ h(\mathbf{x}_i) = \varepsilon, & -C < \theta_i < 0 \\ -\varepsilon \leq h(\mathbf{x}_i) \leq \varepsilon & \theta_i = 0 \\ h(\mathbf{x}_i) = -\varepsilon, & 0 < \theta_i < C \\ h(\mathbf{x}_i) \leq -\varepsilon, & \theta_i = C \end{cases} \tag{2.9}$$

There are five conditions in equation 2.9, compared to the three conditions in support vector classification (see equation 2 in Cauwenberghs & Poggio, 2001), but like the conditions in support vector classification, they can be identified with three subsets into which the samples in training set T can be classified. The difference is that two of the subsets (E and S) are themselves composed of two disconnected components, depending on the sign of the error $f(x_i) - y_i$.

$$\text{The } E \text{ Set: Error support vectors: } E = \{i \mid |\theta_i| = C\} \tag{2.10}$$

$$\text{The } S \text{ Set: Margin support vectors: } S = \{i \mid 0 < |\theta_i| < C\} \tag{2.11}$$

$$\text{The } R \text{ Set: Remaining samples: } R = \{i \mid \theta_i = 0\}. \tag{2.12}$$

3 Incremental Algorithm

The incremental algorithm updates the trained SVR function whenever a new sample $\mathbf{x}_c$ is added to the training set T. The basic idea is to change the coefficient θ_c corresponding to the new sample $\mathbf{x}_c$ in a finite number of discrete steps until it meets the KKT conditions, while ensuring that the existing samples in T continue to satisfy the KKT conditions at each step. In this section, we first derive the relation between the change of θ_c, or $\Delta\theta_c$, and the change of other coefficients under the KKT conditions, and then propose a method to determine the largest allowed $\Delta\theta_c$ for each step. A pseudocode description of this algorithm is provided in the appendix.

3.1 Derivation of the Incremental Relations. Let $\mathbf{x}_c$ be a new training sample that is added to T. We initially set $\theta_c = 0$ and then gradually change (increase or decrease) the value of θ_c under the KKT conditions, equation 2.9.

According to equations 2.6, 2.7, and 2.9, the incremental relation between $\Delta h(\mathbf{x}_i)$, $\Delta\theta_i$, and Δb is given by:

$$\Delta h(\mathbf{x}_i) = Q_{ic}\Delta\theta_c + \sum_{i=1}^{l} Q_{ij}\Delta\theta_j + \Delta b. \tag{3.1}$$

From the equality condition in equation 2.3, we have

$$\theta_c + \sum_{i=1}^{l} \theta_i = 0. \tag{3.2}$$

Combining equations 2.9 through 2.12 and 3.1 and 3.2, we obtain:

$$\sum_{j\in S} Q_{ij}\Delta\theta_j + \Delta b = -Q_{ic}\Delta\theta_c \quad \text{where } i \in S$$

$$\sum_{j\in S} \Delta\theta_j = -\Delta\theta_c. \tag{3.3}$$

If we define the index of the samples in the S set as

$$S = \{s_1, s_2, \ldots, s_{l_s}\}, \tag{3.4}$$

equation 3.3 can be represented in matrix form as

$$\begin{bmatrix} 0 & 1 & \cdots & 1 \\ 1 & Q_{s_1 s_1} & \cdots & Q_{s_1 s_{l_s}} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & Q_{s_{l_s} s_1} & \cdots & Q_{s_{l_s} s_{l_s}} \end{bmatrix} \begin{bmatrix} \Delta b \\ \Delta\theta_{s_1} \\ \vdots \\ \Delta\theta_{s_{l_s}} \end{bmatrix} = - \begin{bmatrix} 1 \\ Q_{s_1 c} \\ \vdots \\ Q_{s_{l_s} c} \end{bmatrix} \Delta\theta_c, \tag{3.5}$$

that is,

$$\begin{bmatrix} \Delta b \\ \Delta\theta_{s_1} \\ \vdots \\ \Delta\theta_{s_{l_s}} \end{bmatrix} = \beta \Delta\theta_c \tag{3.6}$$

where

$$\beta = \begin{bmatrix} \beta \\ \beta_{s_1} \\ \vdots \\ \beta_{s_{l_s}} \end{bmatrix} = -\mathbf{R} \begin{bmatrix} 1 \\ Q_{s_1 c} \\ \vdots \\ Q_{s_{l_s} c} \end{bmatrix},$$

$$\text{where} \quad \mathbf{R} = \begin{bmatrix} 0 & 1 & \cdots & 1 \\ 1 & Q_{s_1 s_1} & \cdots & Q_{s_1 s_{l_s}} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & Q_{s_{l_s} s_1} & \cdots & Q_{s_{l_s} s_{l_s}} \end{bmatrix}^{-1} \tag{3.7}$$

Define a non-S, or N, set as $N = E \cup R = \{n_1, n_2, \ldots, n_{l_n}\}$. Combining equations 2.9 through 2.12, 3.1, and 3.6, we obtain

$$\begin{bmatrix} \Delta h(\mathbf{x}_{n_1}) \\ \Delta h(\mathbf{x}_{n_2}) \\ \vdots \\ \Delta h(\mathbf{x}_{n_{l_n}}) \end{bmatrix} = \gamma \Delta\theta_c \tag{3.8}$$

where,

$$\gamma = \begin{bmatrix} Q_{n_1 c} \\ Q_{n_2 c} \\ \vdots \\ Q_{n_{l_n} c} \end{bmatrix} + \begin{bmatrix} 1 & Q_{n_1 s_1} & \cdots & Q_{n_1 s_{l_s}} \\ 1 & Q_{n_2 s_1} & \cdots & Q_{n_2 s_{l_s}} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & Q_{n_{l_n} s_1} & \cdots & Q_{n_{l_n} s_{l_s}} \end{bmatrix} \beta. \tag{3.9}$$

In the special case when S set is empty, according to equations 3.1 and 3.2, equation 3.9 simplifies to $\Delta h(\mathbf{x}_n) = \Delta b$, for all $n \in E \cup R$.

Given $\Delta\theta_c$, we can update $\theta_i, i \in S$ and b according to equation 3.6 and update $h(\mathbf{x}_i), i \in N$ according to equation 3.8. Moreover, equation 2.9 suggests that $\theta_i, i \in N$, and $h(\mathbf{x}_i), i \in S$ are constant if the S set stays unchanged. Therefore, the results presented in this section enable us to update all the θ_i and $h(\mathbf{x}_i)$ given $\Delta\theta_c$. In the next section, we address the question of how to find an appropriate $\Delta\theta_c$.

3.2 AOSVR Bookkeeping Procedure. Equations 3.6 and 3.8 hold only when the samples in the S set do not change membership. Therefore, $\Delta\theta_c$ is chosen to be the largest value that either can maintain the S set unchanged or lead to the termination of the incremental algorithm.

The first step is to determine whether the change $\Delta\theta_c$ should be positive or negative. According to equation 2.9,

$$sign(\Delta\theta_c) = sign(y_c - f(\mathbf{x}_c)) = sign(-h(\mathbf{x}_c)). \tag{3.10}$$

The next step is to determine a bound on $\Delta\theta_c$ imposed by each sample in the training set. To simplify exposition, we consider only the case $\Delta\theta_c > 0$ and remark that the case $\Delta\theta_c < 0$ is similar.
For the new sample $\mathbf{x}_c$, there are two cases:

> Case 1: $h(x_c)$ changes from $h(\mathbf{x}_c) < -\varepsilon$ to $h(\mathbf{x}_c) = -\varepsilon$, and the new sample $\mathbf{x}_c$ is added to the S set, and the algorithm terminates.
>
> Case 2: If θ_c increases from $\theta_c < C$ to $\theta_c = C$, the new sample $\mathbf{x}_c$ is added to the E set, and the algorithml terminates.

For each sample $\mathbf{x}_i$ in the set S,

> Case 3: If θ_i changes from $0 < |\theta_i| < C$ to $|\theta_i| = C$, sample $\mathbf{x}_i$ changes from the S set to the E set. If θ_i changes to $\theta_i = 0$, sample $\mathbf{x}_i$ changes from the S set to the R set.

For each sample $\mathbf{x}_i$ in the set E,

> Case 4: If $h(\mathbf{x}_i)$ changes from $|h(\mathbf{x}_i)| > \varepsilon$ to $|h(x_i)| = \varepsilon$, $\mathbf{x}_i$ is moved from the E set to the S set.

For each sample $\mathbf{x}_i$ in the set R,

> Case 5: If $h(\mathbf{x}_i)$ changes from $|h(\mathbf{x}_i)| < \varepsilon$ to $|h(\mathbf{x}_i)| = \varepsilon$, $\mathbf{x}_i$ is moved from the R set to the S set.

The bookkeeping procedure is to trace each sample in the training set T against these five cases and determine the allowed $\Delta\theta_c$ for each sample according to equation 3.6 or 3.8. The final $\Delta\theta_c$ is defined as the one with minimum absolute value among all the possible $\Delta\theta_c$.

3.3 Efficiently Updating the R Matrix. The matrix $\mathbf{R}$ that is used in equation 3.7,

$$\mathbf{R} = \begin{bmatrix} 0 & 1 & \cdots & 1 \\ 1 & Q_{s_1 s_1} & \cdots & Q_{s_1 s_{l_s}} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & Q_{s_{l_s} s_1} & \cdots & Q_{s_{l_s} s_{l_s}} \end{bmatrix}^{-1}, \tag{3.11}$$

must be updated whenever the S set is changed. Following Cauwenberghs and Poggio (2001), we can efficiently update $\mathbf{R}$ without explicitly computing the matrix inverse. When the kth sample $\mathbf{x}_{s_k}$ in the S set is removed from the S set, the new $\mathbf{R}$ can be obtained as follows:

$$\begin{aligned} \mathbf{R}^{new} &= \mathbf{R}_{\mathbf{I},\mathbf{I}} - \frac{\mathbf{R}_{\mathbf{I},k}\mathbf{R}_{k,\mathbf{I}}}{R_{k,k}}, \text{ where} \\ \mathbf{I} &= [1 \quad \cdots \quad k \quad k+2 \quad \cdots \quad S_{l_s}+1]. \end{aligned} \tag{3.12}$$

When a new sample is added to S set, the new $\mathbf{R}$ can be updated as follows:

$$\mathbf{R}^{new} = \begin{bmatrix} & & & 0 \\ & \mathbf{R} & & \vdots \\ & & & 0 \\ 0 & \cdots & 0 & 0 \end{bmatrix} + \frac{1}{\gamma_i} \begin{bmatrix} \boldsymbol{\beta} \\ 1 \end{bmatrix} \begin{bmatrix} \boldsymbol{\beta}^T & 1 \end{bmatrix}, \tag{3.13}$$

where β is defined as

$$\boldsymbol{\beta} = -\mathbf{R} \begin{bmatrix} 1 \\ Q_{s_1 i} \\ \vdots \\ Q_{s_{l_s} i} \end{bmatrix},$$

and γ_i is defined as

$$\gamma_i = Q_{ii} + \begin{bmatrix} 1 \\ Q_{s_1 i} \\ \vdots \\ Q_{s_{l_s} i} \end{bmatrix} \boldsymbol{\beta}$$

when the sample $\mathbf{x}_i$ was moved from E set to R set. In contrast, when the sample $\mathbf{x}_c$ is the sample added to S set, $\boldsymbol{\beta}$ is can be obtained according to equation 3.7, and γ_i is the last element of γ defined in equation 3.9.

3.4 Initialization of the Incremental Algorithm. An initial SVR solution can be obtained from a batch SVR solution, and in most cases that is the most efficient approach. But it is sometimes convenient to use AOSVR to

produce a full solution from scratch. An efficient starting point is the two-sample solution. Given a training set $T = \{(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2)\}$, with $y_1 \geq y_2$, the solution of equation 2.3 is

$$\begin{aligned} \theta_1 &= \max\left(0, \min\left(C, \frac{y_1 - y_2 - 2\varepsilon}{2(K_{11} - K_{12})}\right)\right) \\ \theta_2 &= -\theta_1 \\ b &= (y_1 = y_2)/2. \end{aligned} \tag{3.14}$$

The sets E, S, and R are initialized from these two points based on equations 2.10 through 2.12. If the set S is nonempty, the matrix $\mathbf{R}$ can be initialized from equation 3.11. As long as S is empty, the matrix $\mathbf{R}$ will not be used.

4 Decremental Algorithm

The decremental (or "unlearning") algorithm is employed when an existing sample is removed from the training set. If a sample $\mathbf{x}_c$ is in the R set, then it does not contribute to the SVR solution, and removing it from the training set is trivial; no adjustments are needed. If, on the other hand, $\mathbf{x}_c$ has a nonzero coefficient, then the idea is to gradually reduce the value of the coefficient to zero, while ensuring all the other samples in the training set continue to satisfy the KKT conditions.

The decremental algorithm follows the incremental algorithm with a few small adjustments:

- The direction of the change of θ_c is:

$$sign(\Delta\theta_c) = sign(f(\mathbf{x}_c) - y_c) = sign(h(\mathbf{x}_c)). \tag{4.1}$$

- There is no case 1 because the removed $\mathbf{x}_c$ need not satisfy KKT conditions.
- The condition in case 2 becomes: θ_c changing from $|\theta_c| > 0$ to $\theta_c = 0$.

5 Applications and Comparison with Batch Algorithms

The accurate on-line SVR (AOSVR) learning algorithm produces exactly the same SVR as the conventional batch SVR learning algorithm and can be applied in all scenarios where batch SVR is currently employed. But for on-line time-series prediction and leave-one-out cross-validation (LOOCV), the AOSVR algorithm is particularly well suited. In this section, we demonstrate AOSVR for both of these applications and compare its performance to existing batch SVR algorithms. These comparisons are based on direct timing of runs using Matlab implementations; such timings should be treated with some caution, as they can be sensitive to details of implementation.

5.1 AOSVR versus Batch SVR Algorithms with Warm Start. Most batch algorithms for SVR are implemented as "cold start." This is appropriate when a fit is desired to a batch of data that has not been seen before. However, in recent years, there has been a growing interest in "warm-start" algorithms that can save time by starting from an appropriate solution, and quite a few articles have addressed this issue in the generic context of numeric programming (Gondzio, 1998; Gondzio & Grothey, 2001; Yildirim & Wright, 2002; Fliege & Heseler, 2002). The warm-start algorithms are useful for incremental (or decremental) learning, because the solution with $N-1$ (or $N+1$) data points provides a natural starting point for finding the solution with N data points. In this sense, AOSVR is a kind of warm-start algorithm for the QP problem, equation 2.3, which is specially designed for the incremental or decremental scenario. This specialty allows AOSVR to achieve more efficiency when handling SVR incremental or decremental learning, as demonstrated in our subsequent experiments.

In the machine learning community, three algorithms for batch SVR training are widely recognized: Gunn (1998) solved SVR training as a generic QP optimization; we call this implementation QPSVMR; Shevade, Keerthi, Bhattacharyya, and Murthy (1999) proposed an algorithm specially designed for SVR training, and it is an improved version of the sequential minimal optimization for SVM regression (SMOR); and Chang and Lin (2001) proposed another algorithm specially designed for SVR training, which we call LibSVMR since it is implemented as part of the LibSVM software package. We implemented all these algorithms so that they can run in both a cold-start and a warm-start mode. SMOR and LibSVMR are implemented in Matlab, and both algorithms allow a straightforward warm-start realization. Because QPSVMR is based on a generic QP algorithm, it is much less efficient than SMOR or LibSVMR. To make our subsequent experiments feasible, we had to implement the QPSVMR core in C (Smola, 1998). Smola essentially employs the interior point QP code of LOQO (Vanderbei, 1999). The warm start of QPSVMR directly adopts the warm-start method embedded in Smola's (1998) implementation.

5.2 On-line Time-Series Prediction. In recent years, the use of SVR for time-series prediction has attracted increased attention (Müller et al., 1997; Fernández, 1999; Tay & Cao, 2001). In an on-line scenario, one updates a model from incoming data and at the same time makes predictions based on that model. This arises, for instance, in market forecasting scenarios. Another potential application is the (near) real-time prediction of electron density around a satellite in the magnetosphere; high charge densities can damage satellite equipment (Friedel, Reeves, and Obara, 2002), and if times of high charge can be predicted, the most sensitive components can be turned off before they are damaged.

In time-series prediction, the prediction origin, denoted O, is the time from which the prediction is generated. The time between the prediction

origin and the predicted data point is the prediction horizon, which for simplicity we take as one time step.

A typical on-line time-series prediction scenario can be represented as follows (Tashman, 2000):

1. Given a time series $\{x(t), \quad t = 1, 2, 3, \ldots\}$ and prediction origin O, construct a set of training samples, $\mathbf{A}_{O,B}$, from the segment of time series $\{x(t), \quad t = 1, \ldots, O\}$ as $\mathbf{A}_{O,B} = \{(\mathbf{X}(t), y(t)), t = B, \ldots, 0 - 1\}$, where $\mathbf{X}(t) = [x(t), \ldots, x(t - B + 1)]^T$, $y(t) = x(t + 1)$, and B is the embedding dimension of the training set $\mathbf{A}_{O,B}$.
2. Train a predictor $P(\mathbf{A}_{O,B}; \mathbf{X})$ from the training set $\mathbf{A}_{O,B}$.
3. Predict $x(O + 1)$ using $\hat{x}(O + 1) = P(\mathbf{A}_{O,B}; \mathbf{X}(O))$.
4. When $x(0 + 1)$ becomes available, update the prediction origin: $O = O + 1$. Then go to step 1 and repeat the procedure.

Note that the training set $\mathbf{A}_{O,B}$ keeps growing as O increases, so the training of the predictor in step 2 becomes increasingly expensive. Therefore, many SVR-based time-series predictions are implemented in a compromised way (Tay & Cao, 2001). After the predictor is obtained, it stays fixed and is not updated as new data arrive. In contrast, an on-line prediction algorithm can take advantage of the fact that the training set is augmented one sample at a time and continues to update and improve the model as more data arrive.

5.2.1 Experiments. Two experiments were performed to compare the AOSVR algorithm with the batch SVR algorithm. We were careful to use the same algorithm parameters for on-line and batch SVR, but since our purpose is to compare computational performance, we did not attempt to optimize these parameters for each data set. In these experiments, the kernel function is a gaussian radial basis function, $\exp(-\gamma \|\mathbf{X}_i - \mathbf{X}_j\|^2)$, where $\gamma = 1$; the regularization coefficient C and the insensitivity parameter ε in equation 2.1 are set to 10 and 0.1, respectively; the embedding dimension, B, of the training $\mathbf{A}_{O,B}$, is 5. Also, we scale all the time-series to $[-1,1]$.

Three widely used benchmark time series are employed in both experiments: (1) the Santa Fe Institute Competition time series A (Weigend & Gershenfeld,1994), (2) the Mackey-Glass equation with $\tau = 17$ (Mackey & Glass, 1977), and (3) the yearly average sunspot numbers recorded from 1700 to 1995. Some basic information about these time series is listed in Table 1. The SV ratio is the number of support vectors divided by the number of training samples. This is based on a prediction of the last data point using all previous data for training. In general, a higher SV ratio suggests that the underlying problem is harder (Vapnik, 1998).

The first experiment demonstrates that using a fixed predictor produces less accurate predictions than using a predictor that is updated as new data

Table 1: Information Regarding Experimental Time Series.

	Number of Data Points	SV Ratio
Santa Fe Institute	1000	4.52%
Mackey-Glass	1500	1.54
Yearly Sunspot	292	41.81

become available. Two measurements are used to quantify the prediction performance: mean squared error (MSE) and mean absolute error (MAE). The predictors are initially trained on the first half of the data in the time series. In the fixed case, the same predictor is used to predict the second half of the time series. In the on-line case, the predictor is updated whenever a new data point is available. The performance measurements for both cases are calculated from the predicted and actual values of the second half of the data in the time series. As shown in Table 2, the on-line predictor outperforms the fixed predictor in every case. We also note that the errors for the three time series in Table 2 coincide with the estimated prediction difficulty in Table 1 based on the SV ratio.

The second experiment compares AOSVR with batch implementations using both cold start and warm start in the on-line prediction scenario. For each benchmark time series, an initial SVR predictor is trained on the first two data points using the batch SVR algorithms. For AOSVR, we used equation 3.14. Afterward, both AOSVR and batch SVR algorithms are employed in the on-line prediction mode for the remaining data points in the time series. AOSVR and the batch SVR algorithms produce exactly the same prediction errors in this experiment, so the comparison is only of prediction speed. All six batch SVR algorithms are compared with AOSVR on the sunspot time series, and the experimental results are plotted in Figure 2. The x-axis of this plot is the number of data points to which the on-line prediction model is applied. Note that the core of QPSVMR is implemented in C. Because the cold start and warm start of LibSVMR clearly outperform those of both SMOR and QPSVMR, only the comparison between LibSVMR and AOSVR is carried out in our subsequent experiments. The experimental re-

Table 2: Performance Comparison for On-line and Fixed Predictors.

		On-line	Fixed
Santa Fe Institute	**MSE**	0.0072	0.0097
	MAE	0.0588	0.0665
Mackey-Glass	**MSE**	0.0034	0.0036
	MAE	0.0506	0.0522
Yearly Sunspot	**MSE**	0.0263	0.0369
	MAE	0.1204	0.1365

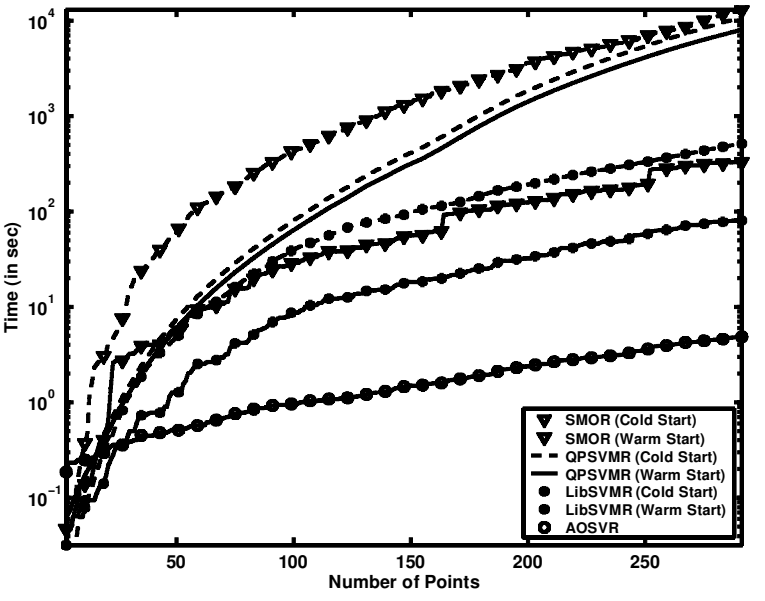

Figure 2: Real-time prediction time of yearly sunspot time series.

sults of both Santa Fe Institute and Mackey-Glass time series are presented in Figures 3 and 4, respectively.

These experimental results demonstrate that AOSVR algorithm is generally much faster than the batch SVR algorithms when applied to on-line prediction. Comparison of Figures 2 and 4 furthermore suggests that more speed improvement is achieved on the sunspot data than on the Mackey-Glass. We speculate that this is because the sunspot problem is "harder" than the Mackey-Glass (it has a higher support vector ratio) and that the performance of the AOSVR algorithm is less sensitive to problem difficulty.

To test this hypothesis, we compared the performance of AOSVR to LibSVMR on a single data set (the sunspots) whose difficulty was adjusted by changing the value of ε. A smaller ε leads to a higher support vector ratio and a more difficult problem. Both the AOSVR and LibSVMR algorithms were employed for on line prediction of the full time series. The overall prediction times are plotted against ε in Figure 5. Where AOSVR performance varied by a factor of less than 10 over the range of ε, the LibSVMR performance varied by a factor of about 100.

5.2.2 Limited-Memory Version of the On-line Time-Series Prediction Scenario. One problem with on-line time-series prediction in general is that the longer the prediction goes on, the bigger the training set $\mathbf{A}_{O,B}$ will become, and the

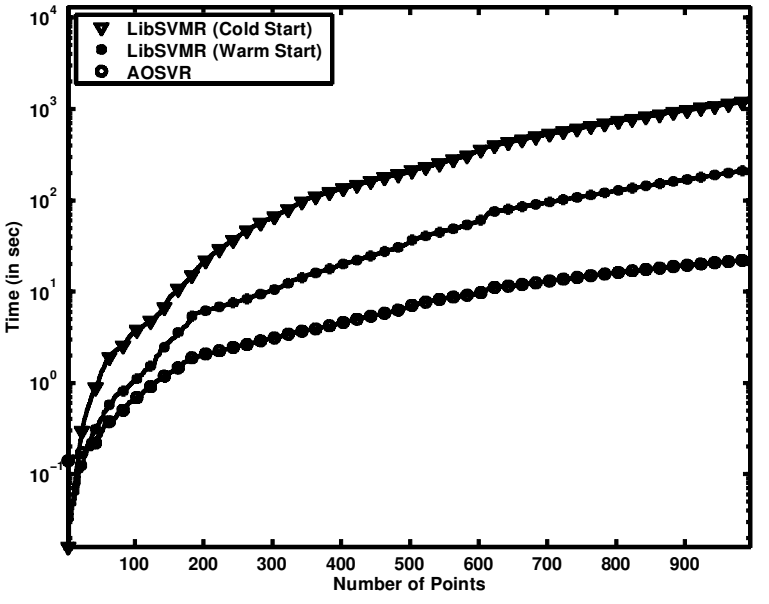

Figure 3: Real-time prediction time of Santa Fe Institute time series.

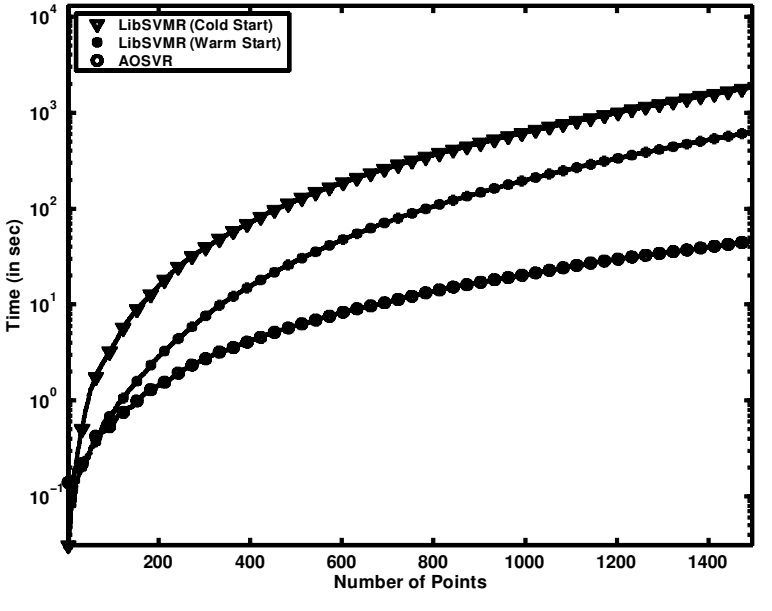

Figure 4: Real-time prediction time of Mackey-Glass time series.

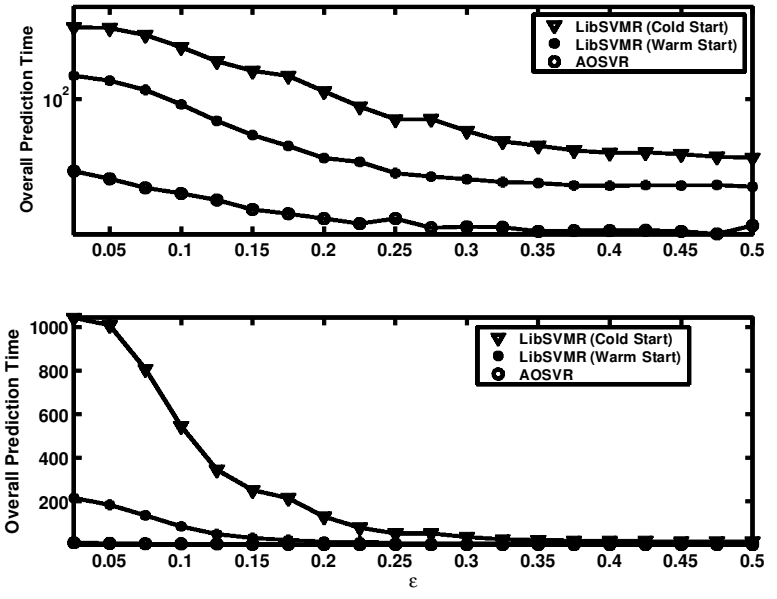

Figure 5: Semilog and linear plots of prediction time of yearly sunspot time series.

more SVs will be involved in SVR predictor. A complicated SVR predictor imposes both memory and computation stress on the prediction system. One way to deal with this problem is to impose a "forgetting" time W. When training set $\mathbf{A}_{O,B}$ grows to this maximum W, then the decremental algorithm is used to remove the oldest sample before the next new sample is added to the training set.

We note that this variant of the on-line prediction scenario is also potentially suitable for nonstationary time series, as it can be updated in real time to fit the most recent behavior of the time series. More rigorous investigation in this direction will be a future effort.

5.3 Leave-One-Out Cross-Validation. Cross-validation is a useful tool for assessing the generalization ability of a machine learning algorithm. The idea is to train on one subset of the data and then to test the accuracy of the predictor on a separate disjoint subset. In leave-one-out cross-validation (LOOCV), only a single sample is used for testing, and all the rest are used for training. Generally, this is repeated for every sample in the data set. When the batch SVR is employed, LOOCV can be very expensive, since a full retraining is done for each sample. One compromise approach is to estimate LOOCV with related but less expensive approximations, such as the xi-

alpha bound (Joachims, 2000), and approximate span bound (Vapnik & Chapelle, 1999). Although Lee and Lin (2001) proposed a numerical solution to reduce the computation for directly implementing LOOCV, the amount of computation required is still considerable. Also, the accuracy of the LOOCV result obtained using this method can be potentially compromised because a different parameter set is employed in LOOCV and in the final training.

The decremental algorithm of AOSVR provides an efficient implementation of LOOCV for SVR:

1. Given a data set $\mathbf{D}$, construct the SVR function $f(\mathbf{x})$ from the whole data set $\mathbf{D}$ using batch SVR learning algorithm.
2. For each nonsupport vector $\mathbf{x}_i$ in the data set $\mathbf{D}$, calculate error e_i corresponding to $\mathbf{x}_i$ as: $e_i = y_i - f(\mathbf{x}_i)$, where y_i is the target value corresponding to $\mathbf{x}_i$.
3. For each support vector $\mathbf{x}_i$ involved in the SVR function $f(\mathbf{x})$,
   (a) Unlearn $\mathbf{x}_i$ from the SVR function $f(\mathbf{x})$ using the decremental algorithm to obtain the SVR function $f_i(\mathbf{x})$, which would be constructed from the data set $\mathbf{D}_i = \mathbf{D}/\{\mathbf{x}_i\}$.
   (b) Calculate error e_i corresponding to support vector $\mathbf{x}_i$ as: $e_i = y_i - f_i(\mathbf{x}_i)$, where y_i is the target value corresponding to $\mathbf{x}_i$.
4. Knowing the error for each sample $\mathbf{x}_i$ in $\mathbf{D}$, it is possible to construct a variety of overall measures; a simple choice is the MSE,

$$MSE_{LOOCV}(\mathbf{D}) = \frac{1}{N}\sum_{i}^{N} e_i^2, \tag{5.1}$$

   where N is the number of samples in data set $\mathbf{D}$. Other choices of error metric, such as MAE, can be obtained by altering equation 5.1 appropriately.

5.3.1 Experiment. The algorithm parameters in this experiment are set the same as those in the experiments in section 5.1.1. Two famous regression data sets, the Auto-MPG and Boston Housing data sets, are chosen from the UCI Machine-Learning Repository. Some basic information on these data sets is listed in Table 3.

Table 3: Information Regarding Experimental Regression Data Sets.

	Number of Attributes	Number of Samples	SV Ratio
Auto-MPG	7	392	41.07%
Boston Housing	13	506	36.36%

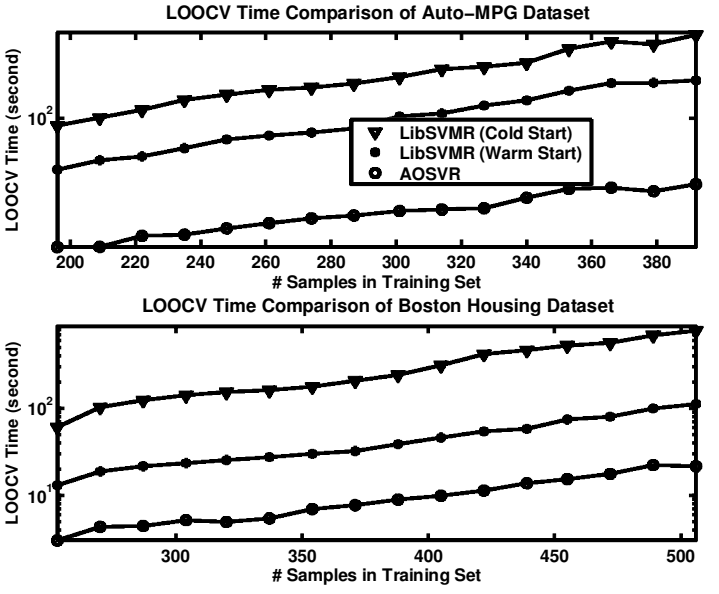

Figure 6: Semilog plots of LOOCV time of Auto-MPG and Boston Housing data set.

The experimental results of both data sets are presented in Figure 6. The x-axis is the size of the training set, upon which the LOOCV is implemented. These plots show that AOSVR-based LOOCV is much faster than its LibSVMR counterpart.

6 Conclusion

We have developed and implemented an accurate on-line support vector regression (AOSVR) algorithm that permits efficient retraining when a new sample is added to, or an existing sample is removed from, the training set. AOSVR is applied to on-line time-series prediction and to leave-one-out cross-validation, and the experimental results demonstrate that the AOSVR algorithm is more efficient than conventional batch SVR in these scenarios. Moreover, AOSVR appears less sensitive than batch SVR to the difficulty of the underlying problem.

After this manuscript was prepared, we were made aware of a similar on-line SVR algorithm, which was independently presented in Martin (2002).

Appendix: Pseudocode for Incrementing AOSVR with a New Data Sample

Inputs

- Training set $T = \{\mathbf{x}_i, y_i), i = 1, \ldots, l\}$
- Coefficients $\{\theta_i, i = 1, \ldots, l\}$, and bias $\boldsymbol{b}$
- Partition of samples into sets S, E, and R
- Matrix $\mathbf{R}$ defined in equation 3.11
- New sample $(\mathbf{x}_c, y_c)$

Outputs

- Updated coefficients $\{\theta_i, i = 1, \ldots, l+1\}$ and bias $\boldsymbol{b}$.
- Updated Matrix $\mathbf{R}$
- Updated partition of samples into sets S, E, and R

AOSVR Incremental Algorithm

- Initialize $\theta_c = 0$
- Compute $f(\mathbf{x}_c) = \sum_{i \in E \cup S} \theta_i Q_{ic} + b$
- Compute $h(\mathbf{x}_c) = f(\mathbf{x}_c) - y_c$
- I $|h(\mathbf{x}_c)| \leq \varepsilon$, then assign $\mathbf{x}_c$ to R, and terminate.
- Let $q = sign(-h(\mathbf{x}_c))$ be the sign that $\Delta\theta_c$ will take
- Do until the new sample $\mathbf{x}_c$ meets the KKT condition
  - — Update β, γ according to equations 3.7 and 3.9
  - — Start bookkeeping procedure:

    Check the new sample $\mathbf{x}_c$,
    —$L_{c1} = (-h(\mathbf{x}_c) - q\varepsilon)/\gamma_c$ (Case 1)
    —$L_{c2} = qC - \theta_c$ (Case 2)
    Check each sample $\mathbf{x}_i$ in the set S (Case 3)
    —If $q\beta_i > 0$ and $C > \theta_i \geq 0$, $L_i^S = (C - \theta_i)/\beta_i$
    —If $q\beta_i > 0$ and $0 > \theta_i \geq -C$, $L_i^S = -\theta_i/\beta_i$
    —If $q\beta_i < 0$ and $C \geq \theta_i > 0$, $L_i^S = -\theta_i/\beta_i$
    —If $q\beta_i < 0$ and $0 \geq \theta_i > -C$, $L_i^S = (-C - \theta_i)/\beta_i$
    Check each sample $\mathbf{x}_i$ in the set E (Case 4)
    —$L_i^E = (-h(\mathbf{x}_i) - sign(q\beta_i)\varepsilon)/\beta_i$
    Check each sample $\mathbf{x}_i$ in the set R (Case 5)
    —$L_i^R = (-h(\mathbf{x}_i) - sign(q\beta_i)\varepsilon)/\beta_i$

Set $\Delta\theta_c = q\min(|L_{c1}|, \quad |L_{c2}|, \quad |\mathbf{L}^S|, \quad |\mathbf{L}^E| \quad |\mathbf{L}^R|)$, where $\mathbf{L}^S = \{L_i^S, i \in S\}$, $\mathbf{L}^E = \{L_i^E, i \in E\}$, and $\mathbf{L}^R = \{L_i^R, i \in R\}$.

Let ***Flag*** be the case number that determines $\Delta\theta$.

Let $\mathbf{x}_l$ be the particular sample in T that determines $\Delta\theta_c$.

— End Bookkeeping Procedure.

— Update θ_c, b, and θ_i, $i \in S$ according to equation 3.6

— Update $h(\mathbf{x}_i)$, $i \in E \cup R$ according to equation 3.8

— Switch ***Flag***

(***Flag***=1):

Add new sample $\mathbf{x}_c$ to set S; update matrix $\mathbf{R}$ according to equation 3.13

(***Flag***=2):

Add new sample $\mathbf{x}_c$ to set E

(***Flag***=3):

If $\theta_l = 0$, move $\mathbf{x}_l$ to set R; update $\mathbf{R}$ according to equation 3.12

If $|\theta_l| = C$, move $\mathbf{x}_l$ to set E; update $\mathbf{R}$ according to equation 3.12

(***Flag***=4):

Move $\mathbf{x}_l$ to set S; update $\mathbf{R}$ according to equation 3.13

(***Flag***=5):

Move $\mathbf{x}_l$ to set S; update $\mathbf{R}$ according to equation 3.13

— End Switch ***Flag***

— If ***Flag***≤ 2, terminate; otherwise continue the Do-Loop.

- Terminate incremental algorithm; ready for the next sample.

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