

LIBSVM: a Library for Support Vector Machines

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Abstract

LIBSVM is a library for support vector machines (SVM). Its goal is to help users to easily use SVM as a tool. In this document, we present all its implementation details. For the use of LIBSVM, the README file included in the package and the LIBSVM FAQ provide the information.

1 Introduction

LIBSVM is a library for support vector classification (SVM) and regression. Its goal is to let users can easily use SVM as a tool. In this document, we present all its implementation details. For the use of LIBSVM, the README file included in the package provides the information.

In Section 2, we show formulations used in LIBSVM: C -support vector classification (C -SVC), ν -support vector classification (ν -SVC), distribution estimation (one-class SVM), ϵ -support vector regression (ϵ -SVR), and ν -support vector regression (ν -SVR). We discuss the implementation of solving quadratic problems in Section 3. Section 4 describes two implementation techniques: shrinking and caching. Then in Section 6 we discuss the implementation of multi-class classification. We now also support different penalty parameters for unbalanced data. Details are in Section 5. Model selection is very important for obtaining the best generalization. LIBSVM provides simple and useful tools which are discussed in 7.

2 Formulations

2.1 C -Support Vector Classification (Binary Case)

Given training vectors $\mathbf{x}_i \in R^n, i = 1, \dots, l$, in two classes, and a vector $\mathbf{y} \in R^l$ such that $y_i \in \{1, -1\}$, C -SVC (Cortes and Vapnik, 1995; Vapnik, 1998) solves the following primal problem:

$$\begin{aligned} \min_{\mathbf{w}, b, \xi} \quad & \frac{1}{2} \mathbf{w}^T \mathbf{w} + C \sum_{i=1}^l \xi_i \\ \text{subject to} \quad & y_i (\mathbf{w}^T \phi(\mathbf{x}_i) + b) \geq 1 - \xi_i, \\ & \xi_i \geq 0, i = 1, \dots, l. \end{aligned} \tag{2.1}$$

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Its dual is

$$\begin{aligned}
\min_{\boldsymbol{\alpha}} \quad & \frac{1}{2} \boldsymbol{\alpha}^T Q \boldsymbol{\alpha} - \mathbf{e}^T \boldsymbol{\alpha} \\
& 0 \leq \alpha_i \leq C, \quad i = 1, \dots, l, \\
\text{subject to} \quad & \mathbf{y}^T \boldsymbol{\alpha} = 0,
\end{aligned} \tag{2.2}$$

where \mathbf{e} is the vector of all ones, $C > 0$ is the upper bound, Q is an l by l positive semidefinite matrix, $Q_{ij} \equiv y_i y_j K(\mathbf{x}_i, \mathbf{x}_j)$, and $K(\mathbf{x}_i, \mathbf{x}_j) \equiv \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j)$ is the kernel. Here training vectors \mathbf{x}_i are mapped into a higher (maybe infinite) dimensional space by the function ϕ .

The decision function is

$$\text{sgn}\left(\sum_{i=1}^l y_i \alpha_i K(\mathbf{x}_i, \mathbf{x}) + b\right).$$

2.2 ν -Support Vector Classification (Binary Case)

The ν -support vector classification (Schölkopf et al., 2000) uses a new parameter ν which let one control the number of support vectors and errors. The parameter $\nu \in (0, 1]$ is an upper bound on the fraction of training errors and a lower bound of the fraction of support vectors.

Given training vectors $\mathbf{x}_i \in R^n, i = 1, \dots, l$, in two classes, and a vector $\mathbf{y} \in R^l$ such that $y_i \in \{1, -1\}$, the primal form considered is:

$$\begin{aligned}
\min_{\mathbf{w}, b, \boldsymbol{\xi}, \rho} \quad & \frac{1}{2} \mathbf{w}^T \mathbf{w} - \nu \rho + \frac{1}{l} \sum_{i=1}^l \xi_i \\
\text{subject to} \quad & y_i (\mathbf{w}^T \phi(\mathbf{x}_i) + b) \geq \rho - \xi_i, \\
& \xi_i \geq 0, i = 1, \dots, l, \rho \geq 0.
\end{aligned}$$

The dual is:

$$\begin{aligned}
\min_{\boldsymbol{\alpha}} \quad & \frac{1}{2} \boldsymbol{\alpha}^T Q \boldsymbol{\alpha} \\
\text{subject to} \quad & 0 \leq \alpha_i \leq 1/l, \quad i = 1, \dots, l, \\
& \mathbf{e}^T \boldsymbol{\alpha} \geq \nu, \\
& \mathbf{y}^T \boldsymbol{\alpha} = 0.
\end{aligned} \tag{2.3}$$

where $Q_{ij} \equiv y_i y_j K(\mathbf{x}_i, \mathbf{x}_j)$.

The decision function is:

$$\text{sgn}\left(\sum_{i=1}^l y_i \alpha_i (K(\mathbf{x}_i, \mathbf{x}) + b)\right).$$

In (Crisp and Burges, 2000; Chang and Lin, 2001), it has been shown that $\mathbf{e}^T \boldsymbol{\alpha} \geq \nu$ can be replaced by $\mathbf{e}^T \boldsymbol{\alpha} = \nu$. With this property, in LIBSVM, we solve a scaled version of (2.3):

$$\begin{aligned} \min_{\boldsymbol{\alpha}} \quad & \frac{1}{2} \boldsymbol{\alpha}^T Q \boldsymbol{\alpha} \\ \text{subject to} \quad & 0 \leq \alpha_i \leq 1, \quad i = 1, \dots, l, \\ & \mathbf{e}^T \boldsymbol{\alpha} = \nu l, \\ & \mathbf{y}^T \boldsymbol{\alpha} = 0. \end{aligned}$$

We output $\boldsymbol{\alpha}/\rho$ so the computed decision function is:

$$\text{sgn}\left(\sum_{i=1}^l y_i (\alpha_i / \rho) (K(\mathbf{x}_i, \mathbf{x}) + b)\right)$$

and then two margins are

$$y_i (\mathbf{w}^T \phi(\mathbf{x}_i) + b) = \pm 1$$

which are the same as those of C -SVC.

2.3 Distribution Estimation (One-class SVM)

One-class SVM was proposed by (Schölkopf et al., 2001) for estimating the support of a high-dimensional distribution. Given training vectors $\mathbf{x}_i \in R^n, i = 1, \dots, l$ without any class information, the primal form in (Schölkopf et al., 2001) is:

$$\begin{aligned} \min_{\mathbf{w}, b, \boldsymbol{\xi}, \rho} \quad & \frac{1}{2} \mathbf{w}^T \mathbf{w} - \rho + \frac{1}{\nu l} \sum_{i=1}^l \xi_i \\ \text{subject to} \quad & \mathbf{w}^T \phi(\mathbf{x}_i) \geq \rho - \xi_i, \\ & \xi_i \geq 0, i = 1, \dots, l. \end{aligned}$$

The dual is:

$$\begin{aligned} \min_{\boldsymbol{\alpha}} \quad & \frac{1}{2} \boldsymbol{\alpha}^T Q \boldsymbol{\alpha} \\ \text{subject to} \quad & 0 \leq \alpha_i \leq 1/(\nu l), i = 1, \dots, l, \\ & \mathbf{e}^T \boldsymbol{\alpha} = 1, \end{aligned} \tag{2.4}$$

where $Q_{ij} = K(\mathbf{x}_i, \mathbf{x}_j) \equiv \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j)$.

In LIBSVM we solve a scaled version of (2.4):

$$\begin{aligned} \min_{\boldsymbol{\alpha}} \quad & \frac{1}{2} \boldsymbol{\alpha}^T Q \boldsymbol{\alpha} \\ \text{subject to} \quad & 0 \leq \alpha_i \leq 1, \quad i = 1, \dots, l, \\ & \mathbf{e}^T \boldsymbol{\alpha} = \nu l. \end{aligned}$$

The decision function is

$$\text{sgn}\left(\sum_{i=1}^l \alpha_i K(\mathbf{x}_i, \mathbf{x}) - \rho\right).$$

2.4 ϵ -Support Vector Regression (ϵ -SVR)

Given a set of data points, $\{(\mathbf{x}_1, z_1), \dots, (\mathbf{x}_l, z_l)\}$, such that $\mathbf{x}_i \in R^n$ is an input and $z_i \in R^1$ is a target output, the standard form of support vector regression (Vapnik, 1998) is:

$$\begin{aligned} \min_{\mathbf{w}, b, \xi, \xi^*} \quad & \frac{1}{2} \mathbf{w}^T \mathbf{w} + C \sum_{i=1}^l \xi_i + C \sum_{i=1}^l \xi_i^* \\ \text{subject to} \quad & \mathbf{w}^T \phi(\mathbf{x}_i) + b - z_i \leq \epsilon + \xi_i, \\ & z_i - \mathbf{w}^T \phi(\mathbf{x}_i) - b \leq \epsilon + \xi_i^*, \\ & \xi_i, \xi_i^* \geq 0, i = 1, \dots, l. \end{aligned}$$

The dual is:

$$\begin{aligned} \min_{\alpha, \alpha^*} \quad & \frac{1}{2} (\alpha - \alpha^*)^T Q (\alpha - \alpha^*) + \epsilon \sum_{i=1}^l (\alpha_i + \alpha_i^*) + \sum_{i=1}^l z_i (\alpha_i - \alpha_i^*) \\ \text{subject to} \quad & \sum_{i=1}^l (\alpha_i - \alpha_i^*) = 0, 0 \leq \alpha_i, \alpha_i^* \leq C, i = 1, \dots, l, \end{aligned} \quad (2.5)$$

where $Q_{ij} = K(\mathbf{x}_i, \mathbf{x}_j) \equiv \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j)$.

The approximate function is:

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

2.5 ν -Support Vector Regression (ν -SVR)

Similar to ν -SVC, for regression, (Schölkopf et al., 2000) use a parameter ν to control the number of support vectors. However, unlike ν -SVC where C is replaced by ν here ν replaces the parameter ϵ of ϵ -SVR. The primal form is

$$\begin{aligned} \min_{\mathbf{w}, b, \xi, \xi^*, \epsilon} \quad & \frac{1}{2} \mathbf{w}^T \mathbf{w} + C(\nu \epsilon + \frac{1}{l} \sum_{i=1}^l (\xi_i + \xi_i^*)) \\ \text{subject to} \quad & (\mathbf{w}^T \phi(\mathbf{x}_i) + b) - z_i \leq \epsilon + \xi_i, \\ & z_i - (\mathbf{w}^T \phi(\mathbf{x}_i) + b) \leq \epsilon + \xi_i^*, \\ & \xi_i, \xi_i^* \geq 0, i = 1, \dots, l, \epsilon \geq 0. \end{aligned} \quad (2.6)$$

and the dual is

$$\begin{aligned}
& \min_{\boldsymbol{\alpha}, \boldsymbol{\alpha}^*} && \frac{1}{2}(\boldsymbol{\alpha} - \boldsymbol{\alpha}^*)^T Q(\boldsymbol{\alpha} - \boldsymbol{\alpha}^*) + \mathbf{z}^T(\boldsymbol{\alpha} - \boldsymbol{\alpha}^*) \\
& \text{subject to} && \mathbf{e}^T(\boldsymbol{\alpha} - \boldsymbol{\alpha}^*) = 0, \mathbf{e}^T(\boldsymbol{\alpha} + \boldsymbol{\alpha}^*) \leq C\nu, \\
& && 0 \leq \alpha_i, \alpha_i^* \leq C/l, \quad i = 1, \dots, l,
\end{aligned} \tag{2.7}$$

Similarly, the inequality $\mathbf{e}^T(\boldsymbol{\alpha} + \boldsymbol{\alpha}^*) \leq C\nu$ can be replaced by an equality. In LIBSVM, we consider $C \leftarrow C/l$ so the dual problem solved is:

$$\begin{aligned}
& \min_{\boldsymbol{\alpha}, \boldsymbol{\alpha}^*} && \frac{1}{2}(\boldsymbol{\alpha} - \boldsymbol{\alpha}^*)^T Q(\boldsymbol{\alpha} - \boldsymbol{\alpha}^*) + \mathbf{z}^T(\boldsymbol{\alpha} - \boldsymbol{\alpha}^*) \\
& \text{subject to} && \mathbf{e}^T(\boldsymbol{\alpha} - \boldsymbol{\alpha}^*) = 0, \mathbf{e}^T(\boldsymbol{\alpha} + \boldsymbol{\alpha}^*) = Cl\nu, \\
& && 0 \leq \alpha_i, \alpha_i^* \leq C, \quad i = 1, \dots, l.
\end{aligned} \tag{2.8}$$

Then the decision function is

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

the same as that of ϵ -SVR.

3 Solving the Quadratic Problems

3.1 The Decomposition Method for C -SVC, ϵ -SVR, and One-class SVM

We consider the following general form of C -SVC, ϵ -SVR, and one-class SVM:

$$\begin{aligned}
& \min_{\boldsymbol{\alpha}} && \frac{1}{2} \boldsymbol{\alpha}^T Q \boldsymbol{\alpha} + \mathbf{p}^T \boldsymbol{\alpha} \\
& \text{subject to} && \mathbf{y}^T \boldsymbol{\alpha} = \Delta, \\
& && 0 \leq \alpha_t \leq C, t = 1, \dots, l,
\end{aligned} \tag{3.1}$$

where $y_t = \pm 1, t = 1, \dots, l$. It can be clearly seen that C -SVC and one-class SVM are already in the form of (3.1). For ϵ -SVR, we consider the following reformulation of (2.5):

$$\begin{aligned}
& \min_{\boldsymbol{\alpha}, \boldsymbol{\alpha}^*} && \frac{1}{2} [\boldsymbol{\alpha}^T, (\boldsymbol{\alpha}^*)^T] \begin{bmatrix} Q & -Q \\ -Q & Q \end{bmatrix} \begin{bmatrix} \boldsymbol{\alpha} \\ \boldsymbol{\alpha}^* \end{bmatrix} + [\epsilon \mathbf{e}^T + \mathbf{z}^T, \epsilon \mathbf{e}^T - \mathbf{z}^T] \begin{bmatrix} \boldsymbol{\alpha} \\ \boldsymbol{\alpha}^* \end{bmatrix} \\
& \text{subject to} && \mathbf{y}^T \begin{bmatrix} \boldsymbol{\alpha} \\ \boldsymbol{\alpha}^* \end{bmatrix} = 0, 0 \leq \alpha_t, \alpha_t^* \leq C, t = 1, \dots, l,
\end{aligned} \tag{3.2}$$

where \mathbf{y} is a $2l$ by 1 vector with $y_t = 1, t = 1, \dots, l$ and $y_t = -1, t = l+1, \dots, 2l$.

The difficulty of solving (3.1) is the density of Q because Q_{ij} is in general not zero. In LIBSVM, we consider the decomposition method to conquer this difficulty. Some work

on this method are, for example, (Osuna et al., 1997a; Joachims, 1998; Platt, 1998). This method modifies only a subset of α per iteration. This subset, denoted as the working set B , leads to a small sub-problem to be minimized in each iteration. An extreme case is the Sequential Minimal Optimization (SMO) (Platt, 1998), which restricts B to have only two elements. Then in each iteration one solves a simple two-variable problem without needing optimization software. Here we consider an SMO-type decomposition method proposed in (Fan et al., 2005).

Algorithm 1 (An SMO-type Decomposition method in (Fan et al., 2005))

1. Find α^1 as the initial feasible solution. Set $k = 1$.
2. If α^k is a stationary point of (2.2), stop. Otherwise, find a *two-element* working set $B = \{i, j\}$ by WSS 1 (described in Section 3.2). Define $N \equiv \{1, \dots, l\} \setminus B$ and α_B^k and α_N^k to be sub-vectors of α^k corresponding to B and N , respectively.
3. If $a_{ij} \equiv K_{ii} + K_{jj} - 2K_{ij} > 0$

Solve the following sub-problem with the variable α_B :

$$\begin{aligned} \min_{\alpha_i, \alpha_j} \quad & \frac{1}{2} [\alpha_i \quad \alpha_j] \begin{bmatrix} Q_{ii} & Q_{ij} \\ Q_{ij} & Q_{jj} \end{bmatrix} \begin{bmatrix} \alpha_i \\ \alpha_j \end{bmatrix} + (\mathbf{p}_B + Q_{BN} \alpha_N^k)^T \begin{bmatrix} \alpha_i \\ \alpha_j \end{bmatrix} \\ \text{subject to} \quad & 0 \leq \alpha_i, \alpha_j \leq C, \\ & y_i \alpha_i + y_j \alpha_j = \Delta - \mathbf{y}_N^T \alpha_N^k, \end{aligned} \tag{3.3}$$

else

Solve

$$\begin{aligned} \min_{\alpha_i, \alpha_j} \quad & \frac{1}{2} [\alpha_i \quad \alpha_j] \begin{bmatrix} Q_{ii} & Q_{ij} \\ Q_{ij} & Q_{jj} \end{bmatrix} \begin{bmatrix} \alpha_i \\ \alpha_j \end{bmatrix} + (\mathbf{p}_B + Q_{BN} \alpha_N^k)^T \begin{bmatrix} \alpha_i \\ \alpha_j \end{bmatrix} \\ & + \frac{\tau - a_{ij}}{4} ((\alpha_i - \alpha_i^k)^2 + (\alpha_j - \alpha_j^k)^2) \\ \text{subject to} \quad & \text{constraints of (3.3)}. \end{aligned} \tag{3.4}$$

4. Set α_B^{k+1} to be the optimal solution of (3.3) and $\alpha_N^{k+1} \equiv \alpha_N^k$. Set $k \leftarrow k + 1$ and goto Step 2.

Note that B is updated in each iteration. To simplify the notation, we simply use B instead of B^k . If $a_{ij} \leq 0$, (3.3) is a concave problem. Hence we use a convex modification in (3.4).

3.2 Stopping Criteria and Working Set Selection for C -SVC, ϵ -SVR, and One-class SVM

The Karush-Kuhn-Tucker (KKT) optimality condition of (3.1) shows that a vector α is a stationary point of (3.1) if and only if there is a number b and two nonnegative vectors λ and μ such that

$$\nabla f(\alpha) + b\mathbf{y} = \lambda - \mu,$$

$$\lambda_i \alpha_i = 0, \mu_i (C - \alpha_i) = 0, \lambda_i \geq 0, \mu_i \geq 0, i = 1, \dots, l,$$

where $\nabla f(\alpha) \equiv Q\alpha + \mathbf{p}$ is the gradient of $f(\alpha)$. This condition can be rewritten as

$$\nabla f(\alpha)_i + by_i \geq 0 \quad \text{if } \alpha_i < C, \quad (3.5)$$

$$\nabla f(\alpha)_i + by_i \leq 0 \quad \text{if } \alpha_i > 0. \quad (3.6)$$

Since $y_i = \pm 1$, by defining

$$I_{\text{up}}(\alpha) \equiv \{t \mid \alpha_t < C, y_t = 1 \text{ or } \alpha_t > 0, y_t = -1\}, \text{ and} \quad (3.7)$$

$$I_{\text{low}}(\alpha) \equiv \{t \mid \alpha_t < C, y_t = -1 \text{ or } \alpha_t > 0, y_t = 1\},$$

a feasible α is a stationary point of (3.1) if and only if

$$m(\alpha) \leq M(\alpha), \quad (3.8)$$

where

$$m(\alpha) \equiv \max_{i \in I_{\text{up}}(\alpha)} -y_i \nabla f(\alpha)_i, \text{ and } M(\alpha) \equiv \min_{i \in I_{\text{low}}(\alpha)} -y_i \nabla f(\alpha)_i.$$

From this we have the following stopping condition:

$$m(\alpha^k) - M(\alpha^k) \leq \epsilon. \quad (3.9)$$

About the selection of the working set set B , we consider the following procedure:

WSS 1

1. For all t, s , define

$$a_{ts} \equiv K_{tt} + K_{ss} - 2K_{ts} > 0, b_{ts} \equiv -y_t \nabla f(\alpha^k)_t + y_s \nabla f(\alpha^k)_s > 0 \quad (3.10)$$

and

$$\bar{a}_{ts} \equiv \begin{cases} a_{ts} & \text{if } a_{ts} > 0, \\ \tau & \text{otherwise.} \end{cases} \quad (3.11)$$

Select

$$\begin{aligned} i &\in \arg \max_t \{-y_t \nabla f(\alpha^k)_t \mid t \in I_{\text{up}}(\alpha^k)\}, \\ j &\in \arg \min_t \left\{ -\frac{b_{it}^2}{\bar{a}_{it}} \mid t \in I_{\text{low}}(\alpha^k), -y_t \nabla f(\alpha^k)_t < -y_i \nabla f(\alpha^k)_i \right\}. \end{aligned} \quad (3.12)$$

2. Return $B = \{i, j\}$.

Details of how we choose this working set is in (Fan et al., 2005, Section II).

3.3 Convergence of the Decomposition Method

See (Fan et al., 2005, Section III) or (Chen et al., 2006) for detailed discussion of the convergence of Algorithm 1.

3.4 The Decomposition Method for ν -SVC and ν -SVR

Both ν -SVC and ν -SVR can be considered as the following general form:

$$\begin{aligned} \min_{\boldsymbol{\alpha}} \quad & \frac{1}{2} \boldsymbol{\alpha}^T Q \boldsymbol{\alpha} + \mathbf{p}^T \boldsymbol{\alpha} \\ \text{subject to} \quad & \mathbf{y}^T \boldsymbol{\alpha} = \Delta_1, \\ & \mathbf{e}^T \boldsymbol{\alpha} = \Delta_2, \\ & 0 \leq \alpha_t \leq C, t = 1, \dots, l. \end{aligned} \tag{3.13}$$

The KKT condition of (3.13) shows

$$\begin{aligned} \nabla f(\boldsymbol{\alpha})_i - \rho + by_i &= 0 \text{ if } 0 < \alpha_i < C, \\ &\geq 0 \text{ if } \alpha_i = 0, \\ &\leq 0 \text{ if } \alpha_i = C. \end{aligned}$$

Define

$$r_1 \equiv \rho - b, \quad r_2 \equiv \rho + b.$$

If $y_i = 1$ the KKT condition becomes

$$\begin{aligned} \nabla f(\boldsymbol{\alpha})_i - r_1 &\geq 0 \text{ if } \alpha_i < C, \\ &\leq 0 \text{ if } \alpha_i > 0. \end{aligned} \tag{3.14}$$

On the other hand, if $y_i = -1$, it is

$$\begin{aligned} \nabla f(\boldsymbol{\alpha})_i - r_2 &\geq 0 \text{ if } \alpha_i < C, \\ &\leq 0 \text{ if } \alpha_i > 0. \end{aligned} \tag{3.15}$$

Hence given a tolerance $\epsilon > 0$, the stopping condition is:

$$\begin{aligned} \max(& - \min_{\alpha_i < C, y_i = 1} \nabla f(\boldsymbol{\alpha})_i + \max_{\alpha_i > 0, y_i = 1} \nabla f(\boldsymbol{\alpha})_i, \\ & - \min_{\alpha_i < C, y_i = -1} \nabla f(\boldsymbol{\alpha})_i + \max_{\alpha_i > 0, y_i = -1} \nabla f(\boldsymbol{\alpha})_i) < \epsilon. \end{aligned}$$

The working set selection is by extending WSS 1 to the following

WSS 2 (Extending WSS 1 to ν -SVM)

1. Find

$$i_p \in \arg m_p(\boldsymbol{\alpha}^k),$$

$$j_p \in \arg \min_t \left\{ -\frac{b_{i_p t}^2}{\bar{a}_{i_p t}} \mid y_t = 1, \boldsymbol{\alpha}_t \in I_{\text{low}}(\boldsymbol{\alpha}^k), -y_t \nabla f(\boldsymbol{\alpha}^k)_t < -y_{i_p} \nabla f(\boldsymbol{\alpha}^k)_{i_p} \right\}.$$

2. Find

$$i_n \in \arg m_n(\boldsymbol{\alpha}^k),$$

$$j_n \in \arg \min_t \left\{ -\frac{b_{i_n t}^2}{\bar{a}_{i_n t}} \mid y_t = -1, \boldsymbol{\alpha}_t \in I_{\text{low}}(\boldsymbol{\alpha}^k), -y_t \nabla f(\boldsymbol{\alpha}^k)_t < -y_{i_n} \nabla f(\boldsymbol{\alpha}^k)_{i_n} \right\}.$$

3. Return $\{i_p, j_p\}$ or $\{i_n, j_n\}$ depending on which one gives smaller $-b_{ij}^2/\bar{a}_{ij}$.

3.5 Analytical Solutions

Details are described in Section 5 in which we discuss the solution of a more general sub-problem.

3.6 The Calculation of b or ρ

After the solution $\boldsymbol{\alpha}$ of the dual optimization problem is obtained, the variables b or ρ must be calculated as they are used in the decision function. Here we simply describe the case of ν -SVC and ν -SVR where b and ρ both appear. Other formulations are simplified cases of them.

The KKT condition of (3.13) has been shown in (3.14) and (3.15). Now we consider the case of $y_i = 1$. If there are α_i which satisfy $0 < \alpha_i < C$, then $r_1 = \nabla f(\boldsymbol{\alpha})_i$. Practically to avoid numerical errors, we average them:

$$r_1 = \frac{\sum_{0 < \alpha_i < C, y_i = 1} \nabla f(\boldsymbol{\alpha})_i}{\sum_{0 < \alpha_i < C, y_i = 1} 1}.$$

On the other hand, if there is no such α_i , as r_1 must satisfy

$$\max_{\alpha_i = C, y_i = 1} \nabla f(\boldsymbol{\alpha})_i \leq r_1 \leq \min_{\alpha_i = 0, y_i = 1} \nabla f(\boldsymbol{\alpha})_i,$$

we take r_1 the midpoint of the range.

For $y_i = -1$, we can calculate r_2 in a similar way.

After r_1 and r_2 are obtained,

$$\rho = \frac{r_1 + r_2}{2} \text{ and } -b = \frac{r_1 - r_2}{2}.$$

4 Shrinking and Caching

4.1 Shrinking

Since for many problems the number of free support vectors (i.e. $0 < \alpha_i < C$) is small, the shrinking technique reduces the size of the working problem without considering some bounded variables (Joachims, 1998). Near the end of the iterative process, the decomposition method identifies a possible set A where all final free α_i may reside in. Indeed we can have the following theorem which shows that at the final iterations of the decomposition proposed in Section 3.2 only variables corresponding to a small set are still allowed to move:

Theorem 4.1 (Theorem IV in (Fan et al., 2005)) *Assume Q is positive semi-definite.*

1. *The following set is independent of any optimal solution $\bar{\alpha}$:*

$$I \equiv \{i \mid -y_i \nabla f(\bar{\alpha})_i > M(\bar{\alpha}) \text{ or } -y_i \nabla f(\bar{\alpha})_i < m(\bar{\alpha})\}. \quad (4.1)$$

Problem (2.2) has unique and bounded optimal solutions at $\alpha_i, i \in I$.

2. *Assume Algorithm 1 generates an infinite sequence $\{\alpha^k\}$. There is \bar{k} such that after $k \geq \bar{k}$, every $\alpha_i^k, i \in I$ has reached the unique and bounded optimal solution. It remains the same in all subsequent iterations and $\forall k \geq \bar{k}$:*

$$i \notin \{t \mid M(\alpha^k) \leq -y_t \nabla f(\alpha^k)_t \leq m(\alpha^k)\}. \quad (4.2)$$

Hence instead of solving the whole problem (2.2), the decomposition method works on a smaller problem:

$$\begin{aligned} \min_{\alpha_A} \quad & \frac{1}{2} \alpha_A^T Q_{AA} \alpha_A - (\mathbf{p}_A - Q_{AN} \alpha_N^k)^T \alpha_A \\ \text{subject to} \quad & 0 \leq (\alpha_A)_t \leq C, t = 1, \dots, q, \\ & \mathbf{y}_A^T \alpha_A = \Delta - \mathbf{y}_N^T \alpha_N^k, \end{aligned} \quad (4.3)$$

where $N = \{1, \dots, l\} \setminus A$ is the set of shrunken variables.

Of course this heuristic may fail if the optimal solution of (4.3) is not the corresponding part of that of (2.2). When that happens, the whole problem (2.2) is reoptimized starting from a point α where α_A is an optimal solution of (4.3) and α_N are bounded variables identified before the shrinking process. Note that while solving the shrunken problem (4.3), we only know the gradient $Q_{AA} \alpha_A + Q_{AN} \alpha_N + \mathbf{p}_A$ of (4.3). Hence when problem (2.2) is reoptimized we also have to reconstruct the whole gradient $\nabla f(\alpha)$, which is quite expensive.

Many implementations began the shrinking procedure near the end of the iterative process, in LIBSVM however, we start the shrinking process from the beginning. The procedure is as follows:

1. After every $\min(l, 1000)$ iterations, we try to shrink some variables. Note that during the iterative process

$$m(\boldsymbol{\alpha}^k) > M(\boldsymbol{\alpha}^k) \quad (4.4)$$

as (3.9) is not satisfied yet. Following Theorem 4.1, we conjecture that variables in the following set can be shrunk:

$$\begin{aligned} & \{t \mid t > m(\boldsymbol{\alpha}^k), t \in I_{low}(\boldsymbol{\alpha}^k), \alpha_t^k \text{ is bounded}\} \cup \\ & \{t \mid t < M(\boldsymbol{\alpha}^k), t \in I_{up}(\boldsymbol{\alpha}^k), \alpha_t^k \text{ is bounded}\} \\ = & \{t \mid t > m(\boldsymbol{\alpha}^k), \alpha_t^k = C, y_t = 1 \text{ or } \alpha_t^k = 0, y_t = -1\} \cup \\ & \{t \mid t < M(\boldsymbol{\alpha}^k), \alpha_t^k = 0, y_t = 1 \text{ or } \alpha_t^k = C, y_t = -1\}. \end{aligned} \quad (4.5)$$

Thus the set A of activated variables is dynamically reduced in every $\min(l, 1000)$ iterations.

2. Of course the above shrinking strategy may be too aggressive. Since the decomposition method has a very slow convergence and a large portion of iterations are spent for achieving the final digit of the required accuracy, we would not like those iterations are wasted because of a wrongly shrunk problem (4.3). Hence when the decomposition method first achieves the tolerance

$$m(\boldsymbol{\alpha}^k) \leq M(\boldsymbol{\alpha}^k) + 10\epsilon,$$

where ϵ is the specified stopping criteria, we reconstruct the whole gradient. Then we inactive some variables based on the current set (4.5). and the decomposition method continues.

Therefore, in LIBSVM, the size of the set A of (4.3) is dynamically reduced. To decrease the cost of reconstructing the gradient $\nabla f(\boldsymbol{\alpha})$, during the iterations we always keep

$$\bar{G}_i = C \sum_{\alpha_j=C} Q_{ij}, i = 1, \dots, l.$$

Then for the gradient $\nabla f(\boldsymbol{\alpha})_i, i \notin A$, we have

$$\nabla f(\boldsymbol{\alpha})_i = \sum_{j=1}^l Q_{ij} \alpha_j + p_i = \bar{G}_i + \sum_{0 < \alpha_j < C} Q_{ij} \alpha_j + p_i.$$

For ν -SVC and ν -SVR, as the stopping condition (3.16) is different from (3.9), the set (4.5) must be modified. For $y_t = 1$, we shrink elements in the following set

$$\{t \mid t > m(\boldsymbol{\alpha}^k), \alpha_t = 0, y_t = 1\} \cup \{t \mid t < M(\boldsymbol{\alpha}^k), \alpha_t = C, y_t = 1\}.$$

The set for $y_t = -1$ is similar.

4.2 Caching

Another technique for reducing the computational time is caching. Since Q is fully dense and may not be stored in the computer memory, elements Q_{ij} are calculated as needed. Then usually a special storage using the idea of a cache is used to store recently used Q_{ij} (Joachims, 1998). Hence the computational cost of later iterations can be reduced.

Theorem 4.1 also supports the use of the cache as in final iterations only some columns of the matrix Q are still needed. Thus if the cache can contain these columns, we can avoid most kernel evaluations in final iterations.

In LIBSVM, we implement a simple least-recent-use strategy for the cache. We dynamically cache only recently used columns of Q_{AA} of (4.3).

4.3 Computational Complexity

The discussion in Section 3.3 is about the asymptotic convergence of the decomposition method. Here, we discuss the computational complexity.

The main operations are on finding $Q_{BN}\boldsymbol{\alpha}_N^k + \mathbf{p}_B$ of (3.3) and the update of $\nabla f(\boldsymbol{\alpha}^k)$ to $\nabla f(\boldsymbol{\alpha}^{k+1})$. Note that $\nabla f(\boldsymbol{\alpha})$ is used in the working set selection as well as the stopping condition. They can be considered together as

$$Q_{BN}\boldsymbol{\alpha}_N^k + \mathbf{p}_B = \nabla f(\boldsymbol{\alpha}^k) - Q_{BB}\boldsymbol{\alpha}_B^k, \quad (4.6)$$

and

$$\nabla f(\boldsymbol{\alpha}^{k+1}) = \nabla f(\boldsymbol{\alpha}^k) + Q_{:,B}(\boldsymbol{\alpha}_B^{k+1} - \boldsymbol{\alpha}_B^k), \quad (4.7)$$

where $Q_{:,B}$ is the sub-matrix of Q with column in B . That is, at the k th iteration, as we already have $\nabla f(\boldsymbol{\alpha}^k)$, the right-hand-side of (4.6) is used to construct the sub-problem. After the sub-problem is solved, (4.7) is employed to have the next $\nabla f(\boldsymbol{\alpha}^{k+1})$. As B has only two elements and solving the sub-problem is easy, the main cost is $Q_{:,B}(\boldsymbol{\alpha}_B^{k+1} - \boldsymbol{\alpha}_B^k)$ of (4.7). The operation itself takes $O(2l)$ but if $Q_{:,B}$ is not available in the cache and each kernel evaluation costs $O(n)$, one column indexes of $Q_{:,B}$ already needs $O(ln)$. Therefore, the complexity is:

1. #Iterations $\times O(l)$ if most columns of Q are cached during iterations.

2. $\# \text{Iterations} \times O(nl)$ if most columns of Q are cached during iterations and each kernel evaluation is $O(n)$.

Note that if shrinking is incorporated, l will gradually decrease during iterations.

5 Unbalanced Data

For some classification problems, numbers of data in different classes are unbalanced. Hence some researchers (e.g. (Osuna et al., 1997b)) have proposed to use different penalty parameters in the SVM formulation: For example, C -SVM becomes

$$\begin{aligned} \min_{\mathbf{w}, b, \xi} \quad & \frac{1}{2} \mathbf{w}^T \mathbf{w} + C_+ \sum_{y_i=1} \xi_i + C_- \sum_{y_i=-1} \xi_i \\ \text{subject to} \quad & y_i (\mathbf{w}^T \phi(\mathbf{x}_i) + b) \geq 1 - \xi_i, \\ & \xi_i \geq 0, i = 1, \dots, l. \end{aligned}$$

Its dual is

$$\begin{aligned} \min_{\boldsymbol{\alpha}} \quad & \frac{1}{2} \boldsymbol{\alpha}^T Q \boldsymbol{\alpha} - \mathbf{e}^T \boldsymbol{\alpha} \\ \text{subject to} \quad & 0 \leq \alpha_i \leq C_+, \text{ if } y_i = 1, \end{aligned} \tag{5.1}$$

$$0 \leq \alpha_i \leq C_-, \text{ if } y_i = -1, \tag{5.2}$$

$$\mathbf{y}^T \boldsymbol{\alpha} = 0.$$

Note that by replacing C with different $C_i, i = 1, \dots, l$, most of the analysis earlier are still correct. Now using C_+ and C_- is just a special case of it. Therefore, the implementation is almost the same. A main difference is on the solution of the sub-problem (3.3). Now it becomes:

$$\begin{aligned} \min_{\alpha_i, \alpha_j} \quad & \frac{1}{2} [\alpha_i \quad \alpha_j] \begin{bmatrix} Q_{ii} & Q_{ij} \\ Q_{ji} & Q_{jj} \end{bmatrix} \begin{bmatrix} \alpha_i \\ \alpha_j \end{bmatrix} + (Q_{i,N} \boldsymbol{\alpha}_N - 1) \alpha_i + (Q_{j,N} \boldsymbol{\alpha}_N - 1) \alpha_j \\ \text{subject to} \quad & y_i \alpha_i + y_j \alpha_j = \Delta - \mathbf{y}_N^T \boldsymbol{\alpha}_N^k, \\ & 0 \leq \alpha_i \leq C_i, 0 \leq \alpha_j \leq C_j, \end{aligned} \tag{5.3}$$

where C_i and C_j can be C_+ or C_- depending on y_i and y_j .

Let $\alpha_i = \alpha_i^k + d_i, \alpha_j = \alpha_j^k + d_j$ and $\hat{d}_i \equiv y_i d_i, \hat{d}_j \equiv y_j d_j$. Then (5.3) can be written as

$$\begin{aligned} \min_{d_i, d_j} \quad & \frac{1}{2} [d_i \quad d_j] \begin{bmatrix} Q_{ii} & Q_{ij} \\ Q_{ij} & Q_{jj} \end{bmatrix} \begin{bmatrix} d_i \\ d_j \end{bmatrix} + [\nabla f(\boldsymbol{\alpha}^k)_i \quad \nabla f(\boldsymbol{\alpha}^k)_j] \begin{bmatrix} d_i \\ d_j \end{bmatrix} \\ \text{subject to} \quad & y_i d_i + y_j d_j = 0, \\ & -\alpha_i^k \leq d_i \leq C - \alpha_i^k, -\alpha_j^k \leq d_j \leq C - \alpha_j^k. \end{aligned} \tag{5.4}$$

Define a_{ij} and b_{ij} as in (3.10). Note that if $a_{ij} \leq 0$, then a modification similar to (3.4). Using $\hat{d}_i = -\hat{d}_j$, the objective function can be written as

$$\frac{1}{2}\bar{a}_{ij}\hat{d}_j^2 + b_{ij}\hat{d}_j.$$

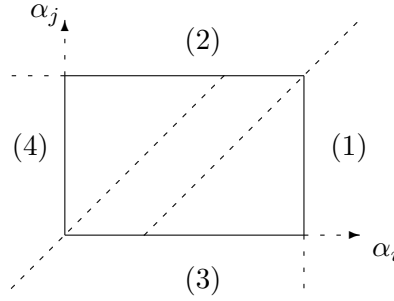
Thus,

$$\begin{aligned}\alpha_i^{new} &= \alpha_i^k + y_i b_{ij} / \bar{a}_{ij} \\ \alpha_j^{new} &= \alpha_i^k - y_j b_{ij} / \bar{a}_{ij}\end{aligned}\tag{5.5}$$

To modify them back to the feasible region, we first consider the case $y_i \neq y_j$ and write (5.5) as

$$\begin{aligned}\alpha_i^{new} &= \alpha_i^k + (-\nabla f(\boldsymbol{\alpha}^k)_i - \nabla f(\boldsymbol{\alpha}^k)_j) / \bar{a}_{ij} \\ \alpha_j^{new} &= \alpha_i^k + (-\nabla f(\boldsymbol{\alpha}^k)_i - \nabla f(\boldsymbol{\alpha}^k)_j) / \bar{a}_{ij}\end{aligned}$$

If $\boldsymbol{\alpha}^{new}$ is not feasible, $(\alpha_i^{new}, \alpha_j^{new})$ is in one of the following four regions:



If it is in region 1, α_i^{k+1} is set to be C_i first and then

$$\alpha_j^{k+1} = C_i - (\alpha_i^k - \alpha_j^k).$$

Of course we must check if it is in region 1 first. If so, we have

$$\alpha_i^k - \alpha_j^k > C_i - C_j \text{ and } \alpha_i^{new} \geq C_i.$$

Other cases are similar. Therefore, we have the following procedure to identify $(\alpha_i^{new}, \alpha_j^{new})$ in different regions and change it back to the feasible set.

```
if (y[i] != y[j])
{
    double quad_coef = Q_i[i] + Q_j[j] + 2 * Q_i[j];
    if (quad_coef <= 0)
        quad_coef = TAU;
    double delta = (-G[i] - G[j]) / quad_coef;
    double diff = alpha[i] - alpha[j];
```

```

alpha[i] += delta;
alpha[j] += delta;

if(diff > 0)
{
    if(alpha[j] < 0) // in region 3
    {
        alpha[j] = 0;
        alpha[i] = diff;
    }
}
else
{
    if(alpha[i] < 0) // in region 4
    {
        alpha[i] = 0;
        alpha[j] = -diff;
    }
}
if(diff > C_i - C_j)
{
    if(alpha[i] > C_i) // in region 1
    {
        alpha[i] = C_i;
        alpha[j] = C_i - diff;
    }
}
else
{
    if(alpha[j] > C_j) // in region 2
    {
        alpha[j] = C_j;
        alpha[i] = C_j + diff;
    }
}
}

```

6 Multi-class classification

We use the “one-against-one” approach (Knerr et al., 1990) in which $k(k-1)/2$ classifiers are constructed and each one trains data from two different classes. The first use of this strategy on SVM was in (Friedman, 1996; Kreßel, 1999). For training data from the i th

and the j th classes, we solve the following binary classification problem:

$$\begin{aligned}
& \min_{\mathbf{w}^{ij}, b^{ij}, \xi^{ij}} && \frac{1}{2}(\mathbf{w}^{ij})^T \mathbf{w}^{ij} + C(\sum_t (\xi^{ij})_t) \\
& \text{subject to} && ((\mathbf{w}^{ij})^T \phi(\mathbf{x}_t)) + b^{ij} \geq 1 - \xi_t^{ij}, \text{ if } \mathbf{x}_t \text{ in the } i\text{th class,} \\
& && ((\mathbf{w}^{ij})^T \phi(\mathbf{x}_t)) + b^{ij} \leq -1 + \xi_t^{ij}, \text{ if } \mathbf{x}_t \text{ in the } j\text{th class,} \\
& && \xi_t^{ij} \geq 0.
\end{aligned}$$

In classification we use a voting strategy: each binary classification is considered to be a voting where votes can be cast for all data points \mathbf{x} - in the end point is designated to be in a class with maximum number of votes.

In case that two classes have identical votes, though it may not be a good strategy, now we simply select the one with the smallest index.

There are other methods for multi-class classification. Some reasons why we choose this “1-against-1” approach and detailed comparisons are in (Hsu and Lin, 2002).

7 Model Selection

LIBSVM provides a model selection tool using the RBF kernel: cross validation via parallel grid search. Currently, we support only C -SVC where two parameters are considered: C and γ . They can be easily modified for other kernels such as linear and polynomial.

For median-sized problems, cross validation might be the most reliable way for model selection. First, the training data is separated to several folds. Sequentially a fold is considered as the validation set and the rest are for training. The average of accuracy on predicting the validation sets is the cross validation accuracy.

Our implementation is as follows. Users provide a possible interval of C (or γ) with the grid space. Then, all grid points of (C, γ) are tried to see which one gives the highest cross validation accuracy. Users then use the best parameter to train the whole training set and generate the final model.

For easy implementation, we consider each SVM with parameters (C, γ) as an independent problem. As they are different jobs, we can easily solve them in parallel. Currently, LIBSVM provides a very simple tool so that jobs are dispatched to a cluster of computers which share the same file system.

Note that now under the same (C, γ) , the one-against-one method is used for training multi-class data. Hence, in the final model, all $k(k-1)/2$ decision functions share the same (C, γ) .

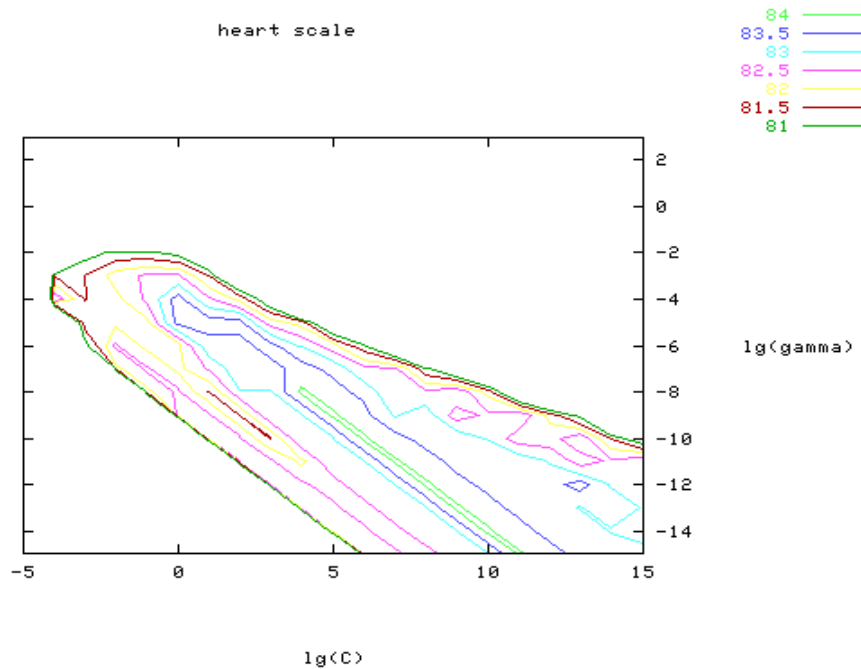


Figure 1: Contour plot of heart_scale included in the LIBSVM package

LIBSVM also outputs the contour plot of cross validation accuracy. An example is in Figure 1.

8 Probability Estimates

Originally support vector classification (regression) predicts only class label (approximate target value) but not probability information. In the following we briefly describe how we extend SVM for probability estimates. More details are in (Wu et al., 2004) for classification and in (Lin and Weng, 2004) for regression.

Given k classes of data, for any \mathbf{x} , the goal is to estimate

$$p_i = p(y = i \mid \mathbf{x}), i = 1, \dots, k.$$

Following the setting of the one-against-one (i.e., pairwise) approach for multi-class classification, we first estimated pairwise class probabilities

$$r_{ij} \approx p(y = i \mid y = i \text{ or } j, \mathbf{x})$$

using an improved implementation (Lin et al., 2003) of (Platt, 2000):

$$r_{ij} \approx \frac{1}{1 + e^{A\hat{f} + B}}, \quad (8.1)$$

where A and B are estimated by minimizing the negative log-likelihood function using known training data and their decision values \hat{f} . Labels and decision values are required to be independent so here we conduct *five-fold cross-validation* to obtain decision values.

Then the second approach in (Wu et al., 2004) is used to obtain p_i from all these r_{ij} 's. It solves the following optimization problem:

$$\min_{\mathbf{p}} \frac{1}{2} \sum_{i=1}^k \sum_{j:j \neq i} (r_{ji}p_i - r_{ij}p_j)^2 \quad \text{subject to} \quad \sum_{i=1}^k p_i = 1, p_i \geq 0, \forall i. \quad (8.2)$$

The objective function comes from the equality

$$p(y = j \mid y = i \text{ or } j, \mathbf{x}) \cdot p(y = i \mid \mathbf{x}) = p(y = i \mid y = i \text{ or } j, \mathbf{x}) \cdot p(y = j \mid \mathbf{x})$$

and can be reformulated as

$$\min_{\mathbf{p}} \frac{1}{2} \mathbf{p}^T Q \mathbf{p}, \quad (8.3)$$

where

$$Q_{ij} = \begin{cases} \sum_{s:s \neq i} r_{si}^2 & \text{if } i = j, \\ -r_{ji}r_{ij} & \text{if } i \neq j. \end{cases} \quad (8.4)$$

This problem is convex, so the optimality conditions that there is a scalar b such that

$$\begin{bmatrix} Q & \mathbf{e} \\ \mathbf{e}^T & 0 \end{bmatrix} \begin{bmatrix} \mathbf{p} \\ b \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ 1 \end{bmatrix}. \quad (8.5)$$

Here \mathbf{e} is the $k \times 1$ vector of all ones, $\mathbf{0}$ is the $k \times 1$ vector of all zeros, and b is the Lagrangian multiplier of the equality constraint $\sum_{i=1}^k p_i = 1$. Instead of directly solving the linear system (8.5), we derive a simple iterative method in the following.

As

$$-\mathbf{p}^T Q \mathbf{p} = -\mathbf{p}^T Q (-bQ^{-1}\mathbf{e}) = b\mathbf{p}^T \mathbf{e} = b,$$

the solution \mathbf{p} satisfies

$$Q_{tt}p_t + \sum_{j:j \neq t} Q_{tj}p_j - \mathbf{p}^T Q \mathbf{p} = 0, \text{ for any } t. \quad (8.6)$$

Using (8.6), we consider the following algorithm:

Algorithm 2

1. Start with some initial $p_i \geq 0, \forall i$ and $\sum_{i=1}^k p_i = 1$.

2. Repeat ($t = 1, \dots, k, 1, \dots$)

$$p_t \leftarrow \frac{1}{Q_{tt}} [- \sum_{j:j \neq t} Q_{tj} p_j + \mathbf{p}^T Q \mathbf{p}] \quad (8.7)$$

$$\text{normalize } \mathbf{p} \quad (8.8)$$

until (8.5) is satisfied.

This procedure guarantees to find a global optimum of (8.2). Using some tricks, we do not need to recalculate $\mathbf{p}^T Q \mathbf{p}$ in each iteration. Detailed implementation notes are in Appendix C of (Wu et al., 2004). We consider a relative stopping condition for Algorithm 2:

$$\|Q\mathbf{p} - \mathbf{p}^T Q \mathbf{p} \mathbf{e}\|_1 = \max_t |(Q\mathbf{p})_t - \mathbf{p}^T Q \mathbf{p}| < 0.005/k.$$

When k is large, \mathbf{p} will be closer to zero, so we decrease the tolerance by a factor of k .

Next, we discuss SVR probability inference. For a given set of training data $\mathcal{D} = \{(\mathbf{x}_i, y_i) \mid \mathbf{x}_i \in R^n, y_i \in R, i = 1, \dots, l\}$, we suppose that the data are collected from the model:

$$y_i = f(\mathbf{x}_i) + \delta_i, \quad (8.9)$$

where $f(\mathbf{x})$ is the underlying function and δ_i are independent and identically distributed random noises. Given a test data \mathbf{x} , the distribution of y given \mathbf{x} and \mathcal{D} , $P(y \mid \mathbf{x}, \mathcal{D})$, allows one to draw probabilistic inferences about y ; for example, one can construct a predictive interval $\mathcal{I} = \mathcal{I}(\mathbf{x})$ such that $y \in \mathcal{I}$ with a pre-specified probability. Denoting \hat{f} as the estimated function based on \mathcal{D} using SVR, then $\zeta = \zeta(\mathbf{x}) \equiv y - \hat{f}(\mathbf{x})$ is the out-of-sample residual (or prediction error), and $y \in \mathcal{I}$ is equivalent to $\zeta \in \mathcal{I} - \hat{f}(\mathbf{x})$. We propose to model the distribution of ζ based on a set of out-of-sample residuals $\{\zeta_i\}_{i=1}^l$ using training data \mathcal{D} . The ζ_i 's are generated by first conducting a k -fold cross validation to get \hat{f}_j , $j = 1, \dots, k$, and then setting $\zeta_i \equiv y_i - \hat{f}_j(\mathbf{x}_i)$ for (\mathbf{x}_i, y_i) in the j th fold. It is conceptually clear that the distribution of ζ_i 's may resemble that of the prediction error ζ .

Figure 2 illustrates ζ_i 's from a real data. Basically, a discretized distribution like histogram can be used to model the data; however, it is complex because all ζ_i 's must be retained. On the contrary, distributions like Gaussian and Laplace, commonly used as noise models, require only location and scale parameters. In Figure 2 we plot the fitted curves using these two families and the histogram of ζ_i 's. The figure shows that the distribution of ζ_i 's seems symmetric about zero and that both Gaussian and Laplace reasonably capture the shape of ζ_i 's. Thus, we propose to model ζ_i by zero-mean Gaussian and Laplace, or equivalently, model the conditional distribution of y given $\hat{f}(\mathbf{x})$ by Gaussian and Laplace with mean $\hat{f}(\mathbf{x})$.

(Lin and Weng, 2004) discussed a method to judge whether a Laplace and Gaussian distribution should be used. Moreover, they experimentally show that in all cases they have tried, Laplace is better. Thus, here we consider the zero-mean Laplace with a density function:

$$p(z) = \frac{1}{2\sigma} e^{-\frac{|z|}{\sigma}}. \quad (8.10)$$

Assuming that ζ_i are independent, we can estimate the scale parameter by maximizing the likelihood. For Laplace, the maximum likelihood estimate is

$$\sigma = \frac{\sum_{i=1}^l |\zeta_i|}{l}. \quad (8.11)$$

(Lin and Weng, 2004) pointed out that some “very extreme” ζ_i may cause inaccurate estimation of σ . Thus, they propose to estimate the scale parameter by discarding ζ_i ’s which exceed $\pm 5 \times$ (standard deviation of ζ_i). Thus, for any new data \mathbf{x} , we consider that

$$y = \hat{f}(\mathbf{x}) + z,$$

where z is a random variable following the Laplace distribution with parameter σ .

In theory, the distribution of ζ may depend on the input \mathbf{x} , but here we assume that it is free of \mathbf{x} . This is similar to the model (8.1) for classification. Such an assumption works well in practice and leads to a simple model.

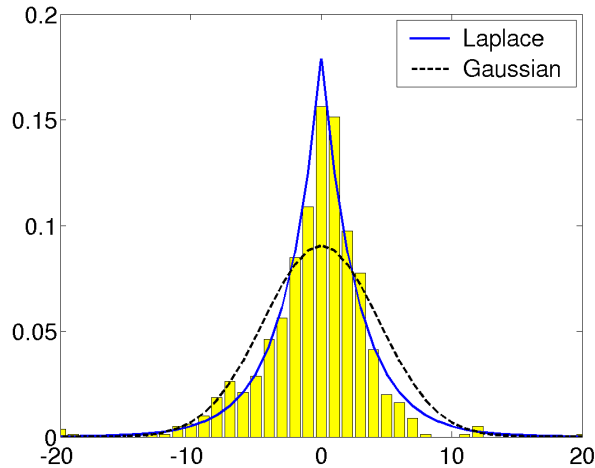


Figure 2: Histogram of ζ_i ’s from a data set and the modeling via Laplace and Gaussian distributions. The x-axis is ζ_i using five-fold CV and the y-axis is the normalized number of data in each bin of width 1.

Acknowledgments

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