

Support Vector Regression using Deflected Subgradient Methods

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Abstract

Project aim is developing the implementation of a model which follows an SVR-type approach including various different kernels. The implementation uses as optimization algorithm a dual approach with appropriate choices of the constraints to be dualized, where the Lagrangian Dual is solved by an algorithm of the class of deflected sub-gradient methods.

1 Introduction

SVR objective is predicting a uni-dimensional real-valued output y through the use of an *objective function* built by optimization using an ε -insensitive loss function. Another fundamental aspect about SVR is keeping the function *as flat as possible* through the tuning of a C parameter in order to avoid overfitting and generating a correct trade-off between accuracy and generalization.

The resulting function can be generically described as:

$$f(x) = wx + b \quad (1)$$

Keeping the above function *as flat as possible* is equivalent to an optimization problem formulated as having minimum $\|w\|$, or, for a more convenient mathematical derivation, minimum $\|w\|^2$, not changing the semantics of the problem.

This brings us to a convex minimization problem, which will be called *primal problem*:

$$\min_{w, \xi_i, \xi_i^*} \frac{1}{2} \|w\|^2 + C \sum_i (\xi_i + \xi_i^*) \quad (2)$$

Where ξ and ξ^* are called *slack variables*, used in conjunction with C to create a *regularization factor* and consequently a *penalty measure* to elements which are not part of the ε -tube. Slack variables allow the definition of constraints applicable to (2):

$$y_i - w^T \phi(x_i) - b \leq \varepsilon + \xi_i, \quad (3a)$$

$$b + w^T \phi(x_i) - y_i \leq \varepsilon + \xi_i, \quad (3b)$$

$$\xi_i, \xi_i^* \geq 0 \quad (3c)$$

x_i input, y_i output

2 Dual Representation

As expressed in the abstract, the implementation will follow a dual approach, which in SVR models is preferred due to the applicability and efficiency of the use of *kernels*. *Dual problem* formulation can be achieved defining the *Lagrangian* function:

$$\begin{aligned}
\mathcal{L}(\alpha, \alpha^*, \mu, \mu^*) = & \frac{1}{2} \|w\|^2 \\
& + C \sum_{i=1}^m (\xi_i + \xi_i^*) \\
& + \sum_{i=1}^m (\alpha_i (y_i - w^T \phi(x_i) - b - \varepsilon - \xi_i)) \\
& + \sum_{i=1}^m (\alpha_i^* (w^T \phi(x_i) + b - y_i - \varepsilon - \xi_i^*)) \\
& - \sum_{i=1}^m (\mu_i \xi_i + \mu_i^* \xi_i^*)
\end{aligned} \tag{4}$$

From which the following optimization problem can be obtained (full derivation shown in 3):

$$\begin{aligned}
\max_{\alpha_i, \alpha_i^*} - & \frac{1}{2} \sum_i \sum_j (\alpha_i - \alpha_i^*) (\alpha_j - \alpha_j^*) K(x_i, x_j) \\
& - \epsilon \sum_i (\alpha_i + \alpha_i^*) \\
& + \sum_i y_i (\alpha_i - \alpha_i^*)
\end{aligned} \tag{5}$$

With constraints:

$$\forall i \alpha_i, \alpha_i^* \geq 0 \quad (KKT \text{ condition}) \tag{6a}$$

$$\forall i \alpha_i, \alpha_i^* \in [0, C] \quad (from \text{ derivation}) \tag{6b}$$

$$\forall i \sum (\alpha_i - \alpha_i^*) = 0 \quad (from \text{ derivation}) \tag{6c}$$

$$\forall i \alpha_i \alpha_i^* = 0 \quad (from \text{ model construction}) \tag{6d}$$

At this point a reformulation of (5) is necessary to follow the task objective, which is solving the *Lagrangian Dual* maximization with a subgradient method, therefore requiring a *non-differentiable function*. Such function is achievable with a simple variable substitution:

$$\begin{aligned}\beta_i &\longleftarrow (\alpha_i - \alpha_i^*) \\ |\beta_i| &\longleftarrow (\alpha_i + \alpha_i^*)\end{aligned}$$

Bringing the definitive dual problem definition:

$$\begin{aligned}\max_{\beta_i} & -\frac{1}{2} \sum_i \sum_j \beta_i \beta_j K(x_i, x_j) \\ & - \epsilon \sum_i |\beta_i| \\ & + \sum_i y_i \beta_i\end{aligned}\tag{7}$$

$$\text{With the constraints} \quad \begin{cases} \sum_i \beta_i = 0 \\ \beta_i \in [-C, C] \\ |\beta_i| \in [0, C] \end{cases}$$

It is important to notice how the above formulation defines a convex non-differentiable problem which still maintains the *strong duality* property of SVR since it is possible to reshape (5) to a quadratic problem, as shown in APPENDIX B (qui la nostra prossima idea per l'appendice B era ripartire da (5) e mostrare come si può arrivare a formulare il problema quadratico tramite l'uso della matrice $Q = [K \quad -K; -K \quad K]$, sarebbe sufficiente come dimostrazione?).

Having the *strong duality* property assures that the optimal solution of the dual problem coincides with the one of the primal problem.

3 APPENDIX A

Define the Lagrangian function

$$\begin{aligned}
\mathcal{L} = \frac{1}{2} \|w\|^2 + C \sum_i (\xi_i + \xi_i^*) &+ \sum_i \alpha_i (y_i - w\phi_i - b - \varepsilon - \xi_i) \\
&+ \sum_i \alpha_i (-y_i + w\phi_i - b - \varepsilon - \xi_i^*) \\
&- \sum_i \mu_i \xi_i \\
&- \sum_i \mu_i^* \xi_i^*
\end{aligned} \tag{8}$$

where $\forall_i \xi_i \xi_i^* \geq 0$

Variables of the two definition of the problem:

$$\begin{array}{ll}
\textit{Primal problem} & w, b, \xi_i, \xi_i^* \\
\textit{Dual Problem} & \alpha_i, \alpha_i^*, \mu_i, \mu_i^*
\end{array}$$

Next step is try to simplify the definition of the Lagrangian wrt the problem that needs to be solved. Since the objective is to find the *minimum* the developments proceeds imposing this condition.

$$\frac{\partial \mathcal{L}}{\partial w} = 0 \quad \longrightarrow \quad w + \sum_i \alpha_i (-\phi_i) + \sum_i \alpha_i^* \phi_i = 0 \tag{9a}$$

$$\frac{\partial \mathcal{L}}{\partial b} = 0 \quad \longrightarrow \quad \sum_i -\alpha_i + \sum_i \alpha_i^* = 0 \tag{9b}$$

$$\frac{\partial \mathcal{L}}{\partial \xi_i} = 0 \quad \longrightarrow \quad C - \alpha_i - \mu_i = 0 \tag{9c}$$

$$\frac{\partial \mathcal{L}}{\partial \xi_i^*} = 0 \quad \longrightarrow \quad C - \alpha_i^* - \mu_i^* = 0 \tag{9d}$$

From (9a) the definition of w can be derived

$$w = \sum_i (\alpha_i - \alpha_i^*) \phi_i \tag{10}$$

From (9b) the first constraint on the Lagrangian variables is obtained

$$\sum_i (\alpha_i^* - \alpha_i) = 0 \tag{11}$$

While from (9c)/(9d) with some further development the second constraint on the Lagrangian variables can be defined

$$\begin{aligned}
& \alpha_i, \alpha_i^*, \mu_i, \mu_i^* \geq 0 \quad \forall_i \\
& C = \alpha_i + \mu_i \quad \longrightarrow \quad \alpha_i = C - \mu_i \\
& \implies \alpha_i \in [0, C] \\
& \text{and equivalently } \alpha_i^* \in [0, C]
\end{aligned}$$

Simplify (8) using the substitution (10)

$$\begin{aligned}
\mathcal{L} = & \frac{1}{2} \sum_i \sum_j (\alpha_i - \alpha_i^*)(\alpha_j - \alpha_j^*) \phi_i \phi_j \\
& - \sum_i \sum_j (\alpha_i - \alpha_i^*)(\alpha_j - \alpha_j^*) \phi_i \phi_j \\
& + \sum_i (\alpha_i - \alpha_i^*) y_i + \sum_i (\alpha_i - \alpha_i^*) b - \sum_i (\alpha_i + \alpha_i^*) \varepsilon \\
& + \sum_i \alpha_i (-\xi_i) + \sum_i \alpha_i^* (-\xi_i^*) \\
& - \sum_i \mu_i \xi_i - \sum_i \mu_i^* \xi_i^* \\
& + C \sum_i \xi_i + \xi_i^*
\end{aligned}$$

Apply condition (11) and (9c) to simplify some terms and obtain the final formulation

$$\begin{aligned}
\mathcal{L}(\alpha, \alpha^*) = & -\frac{1}{2} \sum_i \sum_j (\alpha_i - \alpha_i^*)(\alpha_j - \alpha_j^*) \phi_i \phi_j \\
& + \sum_i (\alpha_i - \alpha_i^*) y_i \\
& - \sum_i (\alpha_i + \alpha_i^*) \varepsilon
\end{aligned}$$

With the constraints

$$\begin{cases} \sum_i (\alpha_i^* - \alpha_i) = 0 \\ \alpha_i \in [0, C] \\ \alpha_i^* \in [0, C] \end{cases}$$