Support Vector Regression using Deflected Subgradient Methods

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Contents

1	Introduction	2
2	Dual Representation	3
3	APPENDIX A	5

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 subgradient 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:

$$f(x) = wx + b \tag{1}$$

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:

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

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

$$b + w^{T} \phi(x_i) - y_i \le \varepsilon + \xi_i, \tag{3b}$$

$$\xi_i, \xi_i^* \ge 0 \tag{3c}$$

 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:

$$\mathcal{L}(\alpha, \alpha^*, \mu, \mu^*) = \frac{1}{2} \|w\|^2$$

$$+ C \sum_{i=1}^{m} (\xi_i + \xi_i^*)$$

$$+ \sum_{i=1}^{m} (\alpha_i (y_i - w^T \phi(x_i) - b - \varepsilon - \xi_i))$$

$$+ \sum_{i=1}^{m} (\alpha_i^* (w^T \phi(x_i) + b - y_i - \varepsilon - \xi_i^*))$$

$$- \sum_{i=1}^{m} (\mu_i \xi_i + \mu_i^* \xi_i^*)$$

$$(4)$$

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

$$\max_{\alpha_i, \alpha_i^*} -\frac{1}{2} \sum_i \sum_j (\alpha_i - \alpha_i^*)(\alpha_j - \alpha_j^*) K(x_i, x_j)$$

$$-\epsilon \sum_i (\alpha_i + \alpha_i^*)$$

$$+ \sum_i y_i (\alpha_i - \alpha_i^*)$$
(5)

With constraints:

$$\forall i \ \alpha_i, \alpha_i^* \ge 0$$
 (KKT condition) (6a)

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

$$\forall i \ \sum (\alpha_i - \alpha_i^*) = 0 \qquad (from \ derivation)$$
 (6c)

$$\forall i \ \alpha_i \alpha_i^* = 0 \qquad (from \ model \ construction) \qquad (6d)$$

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:

$$\beta_i \longleftarrow (\alpha_i - \alpha_i^*)$$

 $|\beta_i| \longleftarrow (\alpha_i + \alpha_i^*)$

Bringing the definitive dual problem definition:

$$\max_{\beta_{i}} - \frac{1}{2} \sum_{i} \sum_{j} \beta_{i} \beta_{j} K(x_{i}, x_{j})$$

$$- \epsilon \sum_{i} |\beta_{i}|$$

$$+ \sum_{i} y_{i} \beta_{i}$$

$$With the constraints$$

$$\begin{cases} \sum_{i} \beta_{i} = 0 \\ \beta_{i} \in [-C, C] \end{cases}$$
(7)

It is important to notice how the above formulation defines a convex nondifferentiable problem which still maintains the *strong duality* propriety, assuring that the optimal solution of the dual problem (*computationally less intensive*) coincides with the one of the primal problem.

3 APPENDIX A

Define the Lagrangian function

$$\mathcal{L} = \frac{1}{2} \|w\|^2 + C \sum_{i} (\xi_i + \xi_i^*) + \sum_{i} \alpha_i (y_i - w\phi_i - b - \varepsilon - \xi_i) + \sum_{i} \alpha_i (-y_i + w\phi_i - b - \varepsilon - \xi_i^*) - \sum_{i} \mu_i \xi_i - \sum_{i} \mu_i^* \xi_i^*$$
(8)

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

Variables of the two definition of the problem:

Primal problem
$$w, b, \xi_i, \xi_i^*$$

Dual Problem $\alpha_i, \alpha_i^*, \mu_i, \mu_i^*$

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.

$$\frac{\partial \mathcal{L}}{\partial w} = 0 \qquad \qquad w + \sum_{i} \alpha_{i}(-\phi_{i}) + \sum_{i} \alpha_{i}^{*}\phi_{i} = 0 \qquad (9a)$$

$$\frac{\partial \mathcal{L}}{\partial b} = 0 \qquad \longrightarrow \qquad \sum_{i} -\alpha_{i} + \sum_{i} \alpha_{i}^{*} = 0 \qquad (9b)$$

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

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

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

$$\alpha_i, \ \alpha_i^*, \ \mu_i, \ \mu_i^* \ge 0 \quad \forall_i$$

$$C = \alpha_i + \mu_i \quad \longrightarrow \quad \alpha_i = C - \mu_i$$

$$\Longrightarrow \quad \alpha_i \in [0, \ C]$$
and equivalently $\alpha_i^* \in [0, \ C]$

Simplify (8) using the substitution (10)

$$\mathcal{L} = \frac{1}{2} \sum_{i} \sum_{j} (\alpha_{i} - \alpha_{i}^{*})(\alpha_{j} - \alpha_{j}^{*}) \phi_{i} \phi_{j}$$

$$- \sum_{i} \sum_{j} (\alpha_{i} - \alpha_{i}^{*})(\alpha_{j} - \alpha_{j}^{*}) \phi_{i} \phi_{j}$$

$$+ \sum_{i} (\alpha_{i} - \alpha_{i}^{*}) y_{i} + \sum_{i} (\alpha_{i} - \alpha_{i}^{*}) b - \sum_{i} (\alpha_{i} + \alpha_{i}^{*}) \varepsilon$$

$$+ \sum_{i} \alpha_{i} (-\xi_{i}) + \sum_{i} \alpha_{i}^{*} (-\xi_{i}^{*})$$

$$- \sum_{i} \mu_{i} \xi_{i} - \sum_{i} \mu_{i}^{*} \xi_{i}^{*}$$

$$+ C \sum_{i} \xi_{i} + \xi_{i}^{*}$$

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

$$\mathcal{L}(\alpha, \alpha^*) = -\frac{1}{2} \sum_{i} \sum_{j} (\alpha_i - \alpha_i^*)(\alpha_j - \alpha_j^*) \phi_i \phi_j$$

$$+ \sum_{i} (\alpha_i - \alpha_i^*) y_i$$

$$- \sum_{i} (\alpha_i + \alpha_i^*) \varepsilon$$

$$With the constraints \begin{cases} \sum_{i} (\alpha_i^* - \alpha_i) = 0 \\ \alpha_i \in [0, C] \\ \alpha_i^* \in [0, C] \end{cases}$$