Support Vector Machines

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Ch. 14 of I2ML (Secs. 14.4, 14.7 – 14.9, and 14.11 – 14.14 excluded)

Relaxing the Constraints

- ▶ In practice, a separating hyperplane may not exist, possibly due to the fact that the data is not linearly separable or a high noise level which causes a large overlap of the classes.
- Even if a separating hyperplane exists, it is not always the best solution to the classification problem when there exist outliers in the data.
 - A mislabeled example can become an outlier which affects the location of the separating hyperplane.

Slack Variables

► A soft-margin SVM allows for the possibility of violating the inequality constraints

$$r^t(\mathbf{w}^T\mathbf{x}^t + w_0) \geq 1$$

by introducing slack variables

$$\xi_t \geq 0, \quad t = 1, \dots, N$$

which store the deviation from the margin.

Relaxed separation constraints:

$$r^t(\mathbf{w}^T\mathbf{x}^t + w_0) \geq 1 - \xi_t$$

Penalty

- **b** By making ξ_t large enough, the constraint on (\mathbf{x}^t, r^t) can always be met.
- In order not to obtain the trivial solution where all ξ_t take on large values, we should penalize them in the objective function.
- ▶ Three cases for ξ_t :
 - $-\xi_t = 0$: no problem with \mathbf{x}^t (no penalty)
 - 0 < ξ_t < 1: \mathbf{x}^t lies on the right side of the hyperplane but in the margin (small penalty)
 - $-\xi_t > 1$: \mathbf{x}^t lies on the wrong side of the hyperplane (large penalty)
- ▶ Number of misclassifications: $\#\{\xi_t > 1\}$
- Number of nonseparable instances: $\#\{\xi_t > 0\}$
- ► Soft error as additional penalty term:

$$\sum_{t=1}^{N} \xi_t$$

Primal Optimization Problem

Primal optimization problem:

$$\begin{aligned} & \underset{\mathbf{w}, \ w_0, \ \{\xi_t\}}{\text{minimize}} & & \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{t=1}^{N} \xi_t \\ & \text{subject to} & & r^t (\mathbf{w}^T \mathbf{x}^t + w_0) \geq 1 - \xi_t, \quad \forall t \\ & & \quad \xi_t \geq 0, \quad \forall t \end{aligned}$$

where $C \ge 0$ is a regularization parameter (which trades off model complexity in terms of the number of support vectors and data misfit in terms of the number of nonseparable points).

- ▶ Both the misclassified instances and the ones in the margin are penalized for better generalization, though the latter ones would be correctly classified during testing.
- For the same reason as before, we will resort to the dual problem.

Lagrangian

Lagrangian:

$$\mathcal{L}(\mathbf{w}, w_0, \{\xi_t\}, \{\alpha_t\}, \{\mu_t\})$$

$$= \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{t=1}^{N} \xi_t - \sum_{t=1}^{N} \alpha_t \left[r^t (\mathbf{w}^T \mathbf{x}^t + w_0) - 1 + \xi_t \right] - \sum_{t=1}^{N} \mu_t \xi_t$$

where the new Lagrange multipliers $\mu_t \geq 0$.

Eliminating Primal Variables

▶ Setting the gradients of \mathcal{L} w.r.t. **w**, w_0 , and $\{\xi_t\}$ to 0:

$$\frac{\partial \mathcal{L}}{\partial \mathbf{w}} = \mathbf{0} \quad \Rightarrow \quad \mathbf{w} = \sum_{t} \alpha_{t} r^{t} \mathbf{x}^{t} \tag{4}$$

$$\frac{\partial \mathcal{L}}{\partial w_0} = 0 \quad \Rightarrow \quad \sum_t \alpha_t r^t = 0 \tag{5}$$

$$\frac{\partial \mathcal{L}}{\partial \xi_t} = 0 \quad \Rightarrow \quad \mu_t = C - \alpha_t, \quad \forall t$$
 (6)

Plugging (4), (5), and (6) into \mathcal{L} gives the objective function G to maximize for the dual problem:

$$G(\{\alpha_t\}) = -\frac{1}{2} \sum_{t} \sum_{t'} \alpha_t \alpha_{t'} r^t r^{(t')} (\mathbf{x}^t)^T \mathbf{x}^{(t')} + \sum_{t} \alpha_t$$

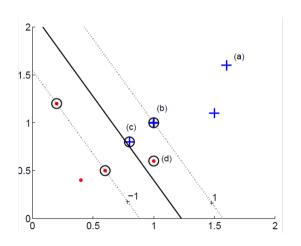
▶ Since $\mu_t \ge 0$, $\forall t$, (6) implies that $0 \le \alpha_t \le C$, $\forall t$.

Dual Optimization Problem

Dual optimization problem:

- Similar to the hard-margin case (i.e., the separable case), instances that are not support vectors (lie on the correct side of the boundary with sufficient margin) vanish with $\alpha_t = 0$.
- ▶ The primal variables \mathbf{w} and w_0 can be computed similarly based on the SVs.
 - The SVs have their $\alpha_t > 0$ and they define **w**.
 - Of SVs, those whose $\alpha_t < C$ are the ones that are on the margin which can be used to calculate w_0 (they have $\xi_t = 0$ and satisfy $r^t(\mathbf{w}^T\mathbf{x}^t + w_0) = 1$).
 - Those instances that are in the margin or misclassified have their $\alpha_t = C$.

Soft-Margin Support Vector Machine



Support Vectors

- ▶ The nonseparable instances that we store as support vectors are the instances that we would have trouble correctly classifying if they were not in the training set; they would either be misclassified or classified correctly but not with enough confidence.
- ► An important result from Vapnik's statistical learning theory is that the expected test error rate has an upper bound which depends on the number of support vectors:

$$E_N[P(\text{error})] \leq \frac{E_N[\# \text{ of SVs}]}{N}$$

- where $E_N[\cdot]$ denotes the expectation over training sets of size N.
- ▶ It shows that the error rate depends on the number of support vectors and not on the input dimensionality.

Hinge Loss

▶ In the soft-margin SVM, we define an error ξ_t if the instance (\mathbf{x}^t, r^t) is nonseparable, which can be described as a hinge loss as

$$L_{\mathsf{hinge}}(y^t, r^t) = (1 - r^t y^t)_+ = egin{cases} 0 & \mathsf{if} \ r^t y^t \geq 1 \ 1 - y^t r^t & \mathsf{otherwise} \end{cases}$$

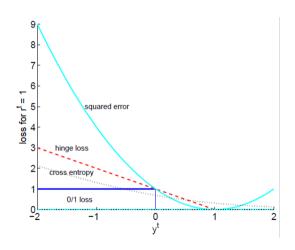
where $y^t = \mathbf{w}^T \mathbf{x}^t + w_0$.

► The soft-margin SVM problem can be equivalently formulated as

minimize
$$\frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{t=1}^{N} (1 - r^t y^t)_+$$
 subject to
$$y^t = \mathbf{w}^T \mathbf{x}^t + w_0, \quad \forall t$$

► The hinge loss, again, reveals the nature of solution sparsity in SVM, i.e., predictions only depend on a subset of the training data.

More Loss Functions



Remark on SVMs

- ► The SVM problem can be case as convex programming problem (every local solution to a convex programming problem is a globally optimal solution), which is contrast to neural networks, where many local minima usually exist.
- ▶ In both training and testing, training data only appear in the form of dot products between vectors, which will become important later on.

Outline

Introduction

Hard-Margin Support Vector Machine

Soft-Margin Support Vector Machine

Kernel Extension

Support Vector Regression

Key Ideas of Kernel Methods

- Instead of defining a nonlinear model in the original (input) space, the problem is mapped to a new (feature) space by performing a nonlinear transformation using suitably chosen basis functions.
- A linear model is then applied in the new space.
- ► This approach can be used in both classification and regression problems.
- ▶ In the particular case of support vector machines, it leads to certain simplifications, where the basis functions are often defined implicitly via defining kernel functions directly.

Basis Functions

Basis Functions:

$$\mathbf{z} = \phi(\mathbf{x})$$
 where $z_j = \phi_j(\mathbf{x}), j = 1, \dots, k$

mapping from the d-dimensional **x**-space to the k-dimensional **z**-space.

Discriminant function:

$$g(\mathbf{z}) = \mathbf{w}^T \mathbf{z} + w_0$$

 $g(\mathbf{x}) = \mathbf{w}^T \phi(\mathbf{x}) + w_0 = \sum_{j=1}^k w_j \phi_j(\mathbf{x}) + w_0$

▶ Usually, $k \gg d$, N (in fact k can even be infinite). The dual form is preferred because its complexity depends on N but that of the primal form depends on k.

Primal Optimization Problem

- ► We use the general case of soft-margin nonlinear SVM because we have no guarantee that the problem is linearly separable in this new space.
- Primal optimization problem:

$$\begin{aligned} & \underset{\mathbf{w}, \ w_0, \ \{\xi_t\}}{\text{minimize}} & & \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{t=1}^{N} \xi_t \\ & \text{subject to} & & r^t(\mathbf{w}^T \phi(\mathbf{x}^t) + w_0) \geq 1 - \xi_t, \quad \forall t \\ & & \xi_t \geq 0, \quad \forall t \end{aligned}$$

where C > 0.

We will resort to the dual problem.

Lagrangian

► Lagrangian:

$$\mathcal{L}(\mathbf{w}, \{\xi_t\}, \{\alpha_t\}, \{\mu_t\})$$

$$= \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{t=1}^{N} \xi_t - \sum_{t=1}^{N} \alpha_t \Big[r^t (\mathbf{w}^T \phi(\mathbf{x}^t) + w_0) - 1 + \xi_t \Big] - \sum_{t=1}^{N} \mu_t \xi_t$$

where the Lagrange multipliers α_t , $\mu_t \geq 0$.

Dual Optimization Problem - I

▶ Setting the gradients of \mathcal{L} w.r.t. **w**, w_0 , and $\{\xi_t\}$ to 0:

$$\frac{\partial \mathcal{L}}{\partial \mathbf{w}} = \mathbf{0} \quad \Rightarrow \quad \mathbf{w} = \sum_{t} \alpha_{t} r^{t} \phi(\mathbf{x}^{t}) \tag{7}$$

$$\frac{\partial \mathcal{L}}{\partial w_0} = 0 \quad \Rightarrow \quad \sum_t \alpha_t r^t = 0 \tag{8}$$

$$\frac{\partial \mathcal{L}}{\partial \xi_t} = 0 \quad \Rightarrow \quad \mu_t = C - \alpha_t, \quad \forall t$$
 (9)

▶ Plugging (7) and (8) into \mathcal{L} gives the objective function G for the dual problem:

$$G(\{\alpha_t\}) = -\frac{1}{2} \sum_{t} \sum_{t'} \alpha_t \alpha_{t'} r^t r^{(t')} \phi(\mathbf{x}^t)^T \phi(\mathbf{x}^{(t')}) + \sum_{t} \alpha_t$$

Dual Optimization Problem - II

► Dual optimization problem:

$$\begin{aligned} & \underset{\{\alpha_t\}}{\text{maximize}} & & \sum_t \alpha_t - \frac{1}{2} \sum_t \sum_{t'} \alpha_t \alpha_{t'} r^t r^{(t')} \phi(\mathbf{x}^t)^T \phi(\mathbf{x}^{(t')}) \\ & \text{subject to} & & \sum_t \alpha_t r^t = 0 \\ & & & 0 \leq \alpha_t \leq C, \ \forall t \end{aligned}$$

Kernel Functions – I

▶ In kernel SVM, we have $K(\mathbf{x}^t, \mathbf{x}^{(t')}) \equiv \phi(\mathbf{x}^t)^T \phi(\mathbf{x}^{(t')})$ which is a kernel function (a.k.a. positive definite kernel, Mercer kernel, or reproducing kernel).

- ▶ Instead of mapping two instances \mathbf{x}^t and $\mathbf{x}^{(t')}$ to the **z**-space and doing a dot product there, we directly apply the kernel function in the original **x**-space.
- ► Kernel matrix (a.k.a. Gram matrix):

$$\mathbf{K} = \left[\mathcal{K}(\mathbf{x}^t, \mathbf{x}^{(t')})
ight]_{t,t'=1}^N$$

which, like a covariance matrix, is symmetric and positive semidefinite.

Kernel Functions – II

► Solution:

$$\mathbf{w} = \sum_{t} \alpha_{t} r^{t} \mathbf{z}^{t} = \sum_{\mathbf{x}^{t} \in \mathcal{SV}} \alpha_{t} r^{t} \phi(\mathbf{x}^{t})$$

Discriminant function:

$$g(\mathbf{x}) = \mathbf{w}^T \phi(\mathbf{x}) + w_0 = \sum_{\mathbf{x}^t \in \mathcal{SV}} \alpha_t r^t \phi(\mathbf{x}^t)^T \phi(\mathbf{x}) + w_0 = \sum_{\mathbf{x}^t \in \mathcal{SV}} \alpha_t r^t K(\mathbf{x}^t, \mathbf{x}) + w_0$$

where the kernel function also shows up in the discriminant.

Some Common Kernel Functions – I

► Polynomial kernel:

$$K(\mathbf{x}, \mathbf{x}') = (\mathbf{x}^T \mathbf{x}' + 1)^q$$

where q is the degree.

E.g., when q = 2 and d = 2,

$$K(\mathbf{x}, \mathbf{x}') = (\mathbf{x}^T \mathbf{x}' + 1)^2$$

$$= (x_1 x_1' + x_2 x_2' + 1)^2$$

$$= 1 + 2x_1 x_1' + 2x_2 x_2' + 2x_1 x_1' x_2 x_2' + (x_1)^2 (x_1')^2 + (x_2)^2 (x_2')^2$$

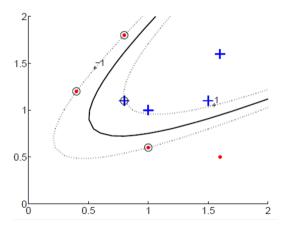
which corresponds to the inner product of the basis function

$$\phi(\mathbf{x}) = \left(1, \sqrt{2}x_1, \sqrt{2}x_2, \sqrt{2}x_1x_2, (x_1)^2, (x_2)^2\right)^T$$

When q = 1, we have the linear kernel corresponding to the original formulation.

Some Common Kernel Functions - II

▶ Polynomial kernel of degree 2:



Some Common Kernel Functions - III

▶ Radial basis function (RBF) kernel (or Gaussian radial kernel):

$$K(\mathbf{x}, \mathbf{x}') = \exp\left[-\frac{\|\mathbf{x} - \mathbf{x}'\|^2}{2s^2}\right]$$

which is a spherical kernel where \mathbf{x}' is the center and s, supplied by the user, defines the radius.

- ▶ The feature space of the RBF kernel has an infinite number of dimensions.
- ▶ It can be generalized to

$$K(\mathbf{x}, \mathbf{x}') = \exp\left[-rac{\mathcal{D}(\mathbf{x}, \mathbf{x}')}{2s^2}
ight]$$

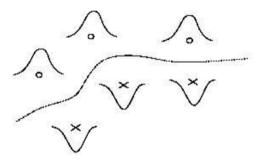
where $\mathcal{D}(\cdot, \cdot)$ is some distance function.

▶ When taking the Mahalanobis distance, we have the Mahalanobis kernel

$$K(\mathbf{x}, \mathbf{x}') = \exp \left[-\frac{(\mathbf{x} - \mathbf{x}')^T \mathbf{S}^{-1} (\mathbf{x} - \mathbf{x}')}{2s^2} \right]$$

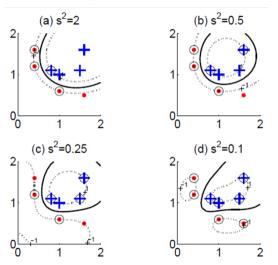
Some Common Kernel Functions – IV

▶ Discriminant function with RBF kernel: amounts to putting bumps of various sizes on the training set



Some Common Kernel Functions - V

▶ Gaussian kernel with different spread values, s^2 :



Some Common Kernel Functions - VI

► Sigmoidal kernel (or hyperbolic tangent kernel):

$$K(\mathbf{x}, \mathbf{x}') = \tanh(\kappa \mathbf{x}^T \mathbf{x}' + \theta)$$

which, strictly speaking, is not positive semidefinite for certain parameter values κ and θ .

▶ This is similar to multilayer perceptrons that we discussed in last lecture.

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t₂ Loss Function

We start with a linear model for regression as

$$f(\mathbf{x}) = \mathbf{w}^T \mathbf{x} + w_0$$

and we have used the squared loss in ordinary linear regression

$$E_2^t(r^t, f(\mathbf{x}^t)) = |r^t - f(\mathbf{x}^t)|^2$$

► Total loss:

$$E_2 = \sum_t E_2^t(r^t, f(\mathbf{x}^t)) = \sum_t |r^t - f(\mathbf{x}^t)|^2$$

► Squared regression (or least squares regression):

$$\underset{\mathbf{w}, w_0}{\text{minimize}} \quad \frac{1}{N} \sum_{t=1}^{N} |r^t - f(\mathbf{x}^t)|^2$$

ϵ -Insensitive Loss Function – I

▶ In order for the sparseness property of support vectors in SVM for classification to carry over to regression, we do not use the squared loss but the ϵ -insensitive loss function:

$$E_{\epsilon}^t(r^t, f(\mathbf{x}^t)) = (|r^t - f(\mathbf{x}^t)| - \epsilon)_+ = \begin{cases} 0 & \text{if } |r^t - f(\mathbf{x}^t)| \le \epsilon \\ |r^t - f(\mathbf{x}^t)| - \epsilon & \text{otherwise} \end{cases}$$

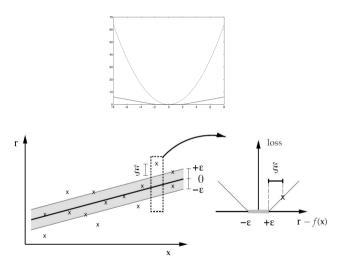
- Two characteristics:
 - Errors are tolerated up to a threshold of ϵ , i.e., no loss for point lying inside an ϵ -tube around the prediction.
 - Errors beyond ϵ have a linear (rather than quadratic) effect so that the model is more more tolerant to noise and robust against noise.
- ► Total loss:

$$E_{\epsilon} = \sum_{t} E_{\epsilon}^{t}(r^{t}, f(\mathbf{x}^{t})) = \sum_{t} (|r^{t} - f(\mathbf{x}^{t})| - \epsilon)_{+}$$

► Tube regression:

$$\underset{\mathbf{w}, w_0}{\text{minimize}} \quad \frac{1}{N} \sum_{t=1}^{N} (|r^t - f(\mathbf{x}^t)| - \epsilon)_+$$

ϵ -Insensitive Loss Function — II



Support Vector Regression

► Support vector (machine) regression (SVR) is given as

$$\underset{\mathbf{w}, w_0}{\text{minimize}} \quad \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{t} (|r^t - f(\mathbf{x}^t)| - \epsilon)_+$$

where C trades off the model complexity (i.e., the flatness of the model) and data misfit.

- The value of ϵ determines the width of the tube (a smaller value indicates a lower tolerance for error) and also affects the number of support vectors and, consequently, the solution sparsity.
 - If ϵ is decreased, the boundary of the tube is shifted inward. Therefore, more datapoints are around the boundary indicating more support vectors.
 - Similarly, increasing ϵ will result in fewer points around the boundary.
- A convex problem, but not a standard QP.
- ▶ We will rewrite it to a form similar to SVM which can be QP-solvable.

Primal Optimization Problem

- We introduce slack variables ξ_t^+ and ξ_t^- to account for deviations out of the ϵ -zone.
- Primal optimization problem:

$$\begin{aligned} & \underset{\mathbf{w}, \ w_0, \ \{\xi_t^+\}, \ \{\xi_t^-\}}{\text{minimize}} & \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_t (\xi_t^+ + \xi_t^-) \\ & \text{subject to} & r^t - (\mathbf{w}^T \mathbf{x}^t + w_0) \leq \epsilon + \xi_t^+, \quad \forall t \\ & (\mathbf{w}^T \mathbf{x}^t + w_0) - r^t \leq \epsilon + \xi_t^-, \quad \forall t \\ & \xi_t^+, \xi_t^- \geq 0, \quad \forall t \end{aligned}$$

which is a standard QP.

- ► Two types of slack variables:
 - $-\xi_t^+$: for positive deviation such that $r^t (\mathbf{w}^T \mathbf{x}^t + w_0) > \epsilon$.
 - $-\xi_t^-$: for negative deviation such that $(\mathbf{w}^T\mathbf{x}^t + w_0) r^t > \epsilon$.
- ▶ If $r^t (\mathbf{w}^T \mathbf{x}^t + w_0) \le \epsilon$ and $(\mathbf{w}^T \mathbf{x}^t + w_0) r^t \le \epsilon$, then $\xi_t^+ = \xi_t^- = 0$, contributing no cost to the objective function.

Lagrangian

- Similar to SVM for classification, the optimization problem for SVR can also be rewritten in the dual form.
- ► Lagrangian:

$$\mathcal{L}(\mathbf{w}, w_0, \{\xi_t^+\}, \{\xi_t^-\}, \{\alpha_t^+\}, \{\alpha_t^-\}, \{\mu_t^+\}, \{\mu_t^-\})$$

$$= \frac{1}{2} ||\mathbf{w}||^2 + C \sum_t (\xi_t^+ + \xi_t^-)$$

$$- \sum_t \alpha_t^+ \left[\epsilon + \xi_t^+ - r^t + (\mathbf{w}^T \mathbf{x}^t + w_0) \right] - \sum_t \alpha_t^- \left[\epsilon + \xi_t^- + r^t - (\mathbf{w}^T \mathbf{x}^t + w_0) \right]$$

$$- \sum_t (\mu_t^+ \xi_t^+ + \mu_t^- \xi_t^-)$$

where
$$\alpha_t^+$$
, α_t^- , μ_t^+ , $\mu_t^- > 0$.

Eliminating Primal Variables

▶ Setting the gradients of \mathcal{L} w.r.t. **w**, w_0 , $\{\xi_t^+\}$, and $\{\xi_t^-\}$ to 0:

$$\frac{\partial \mathcal{L}}{\partial \mathbf{w}} = \mathbf{0} \quad \Rightarrow \quad \mathbf{w} = \sum_{t} (\alpha_{t}^{+} - \alpha_{t}^{-}) \mathbf{x}^{t}$$
 (10)

$$\frac{\partial \mathcal{L}}{\partial w_0} = 0 \quad \Rightarrow \quad \sum_t (\alpha_t^+ - \alpha_t^-) = 0 \tag{11}$$

$$\frac{\partial \mathcal{L}}{\partial \varepsilon_{t}^{+}} = 0 \quad \Rightarrow \quad \mu_{t}^{+} = C - \alpha_{t}^{+}, \quad \forall t$$
 (12)

$$\frac{\partial \mathcal{L}}{\partial \xi_t^-} = 0 \quad \Rightarrow \quad \mu_t^- = C - \alpha_t^-, \quad \forall t \tag{13}$$

▶ Plugging (9), (10), (11), and (12) into \mathcal{L} gives the objective function G for the dual problem:

$$G(\{\alpha_t^+\}, \{\alpha_t^-\}) = -\frac{1}{2} \sum_t \sum_{t'} (\alpha_t^+ - \alpha_t^-) (\alpha_{t'}^+ - \alpha_{t'}^-) (\mathbf{x}^t)^T \mathbf{x}^{(t')}$$

$$-\epsilon \sum_t (\alpha_t^+ + \alpha_t^-) + \sum_t r^t (\alpha_t^+ - \alpha_t^-)$$
gression

Dual Optimization Problem – I

► Dual optimization problem:

$$\begin{aligned} & \underset{\{\alpha_t^+\}, \, \{\alpha_t^-\}}{\text{maximize}} && -\frac{1}{2} \sum_t \sum_{t'} (\alpha_t^+ - \alpha_t^-) (\alpha_{t'}^+ - \alpha_{t'}^-) (\mathbf{x}^t)^T \mathbf{x}^{(t')} \\ && -\epsilon \sum_t (\alpha_t^+ + \alpha_t^-) + \sum_t r^t (\alpha_t^+ - \alpha_t^-) \end{aligned} \\ & \text{subject to} && \sum_t (\alpha_t^+ - \alpha_t^-) = 0 \\ && 0 \leq \alpha_t^+ \leq C, \; \forall t \\ && 0 \leq \alpha_t^- \leq C, \; \forall t \end{aligned}$$

- Instances in the ϵ -tube ($\alpha_t^+ = \alpha_t^- = 0$) are instances fitted with enough precision.
- ▶ The support vectors satisfy either $\alpha_t^+ > 0$ or $\alpha_t^- > 0$ and are of two types.
 - instances on the boundary of the ϵ -tube (either 0 < α_t^+ < C or 0 < α_t^- < C), and we use these to calculate w_0
 - instances outside the ϵ -tube are instances for which we do not have a good fit (either $\alpha_t^+=C$ or $\alpha_t^-=C$)

Dual Optimization Problem - II

▶ We have the fitted line as a weighted sum of the support vectors:

$$f(\mathbf{x}) = \mathbf{w}^T \mathbf{x} + w_0 = \sum_{\mathbf{x}^t \in \mathcal{SV}} (\alpha_t^+ - \alpha_t^-) (\mathbf{x}^t)^T \mathbf{x} + w_0$$

- Due to the sparseness property of the ϵ -insensitive loss function, only a small fraction of the training instances are support vectors which are used in defining the regression function (like the discriminant function for classification).
- Nonlinear (kernel) extension is possible by introducing appropriate kernel functions.

SVR

